

Supporting Information

Pyridinyl Amide Ion Pairs as Lewis Base Organocatalysts

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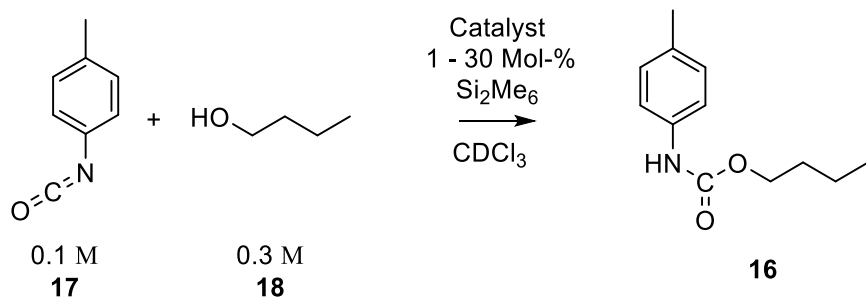
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Experimental Part

Benchmark Reaction 1 – Urethane Synthesis

Due to the significance of catalytic activation of isocyanates for nucleophilic attack and our recent experience on the subject, we chose the synthesis of urethane **16** from *p*-methyl isocyanate **17** and 1-butanol **18** as the primary benchmark reaction (**Scheme S1**).^[1] Moreover, this reaction being a classic addition does not generate acids as it is the case with acetylation or silylation reactions, which also have been employed by our group to benchmark catalyst activity.^[2] Since the CDCl₃ solvent signal is not clearly distinguishable in most of our aromatic moieties containing reactions, we chose to include hexamethyldisilane as inert internal standard. In order to minimize the oligomerization of isocyanate **17** as a potential side reaction, 3 equivalents of alcohol **18** were used.^[1]



Scheme S1. Synthesis of urethane **16** used as benchmark reaction for investigated catalyst systems.

Benchmark reactions were done as described in the main part of this publication.

Figure S1 shows a typical GC-spectrum including the signals for starting materials, the product, solvent and internal standard.

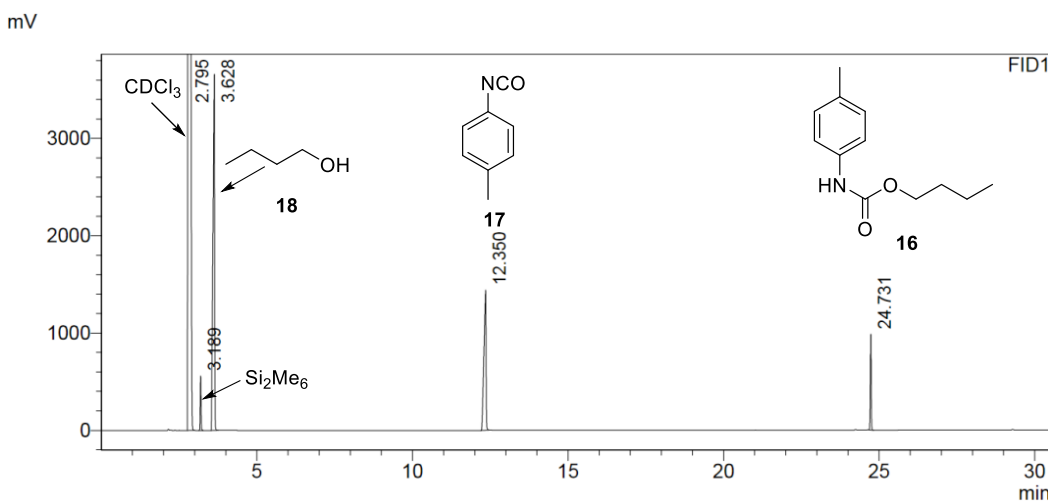


Figure S1. Typical GC-spectrum of the investigated reaction.

Data Processing

NMR:

Measured spectra were imported into MestReNova (Version 12.0.3) and superimposed. The following steps were applied to the superimposed spectra in this order:

- Reference set (Si₂Me₆ set to 0.02 ppm)
- Automatic phase correction
- Automatic baseline correction (Whittaker Smoother)

Three areas containing the signals highlighted in **Figure S2** were integrated:

- **Integral U1:** 4.25 ppm → 4.0 ppm = urethane signal **16B** (CH₂) at 4.15 ppm
- **Integral U2:** 3.75 ppm → 3.5 ppm = butanol signal **18B** at 3.63 ppm (CH₂)
- **Integral U3:** 2.4 ppm → 2.3 ppm = combined methyl signals of isocyanate (**17A**) at 2.30 ppm and urethane (**16A**) at 2.28 ppm

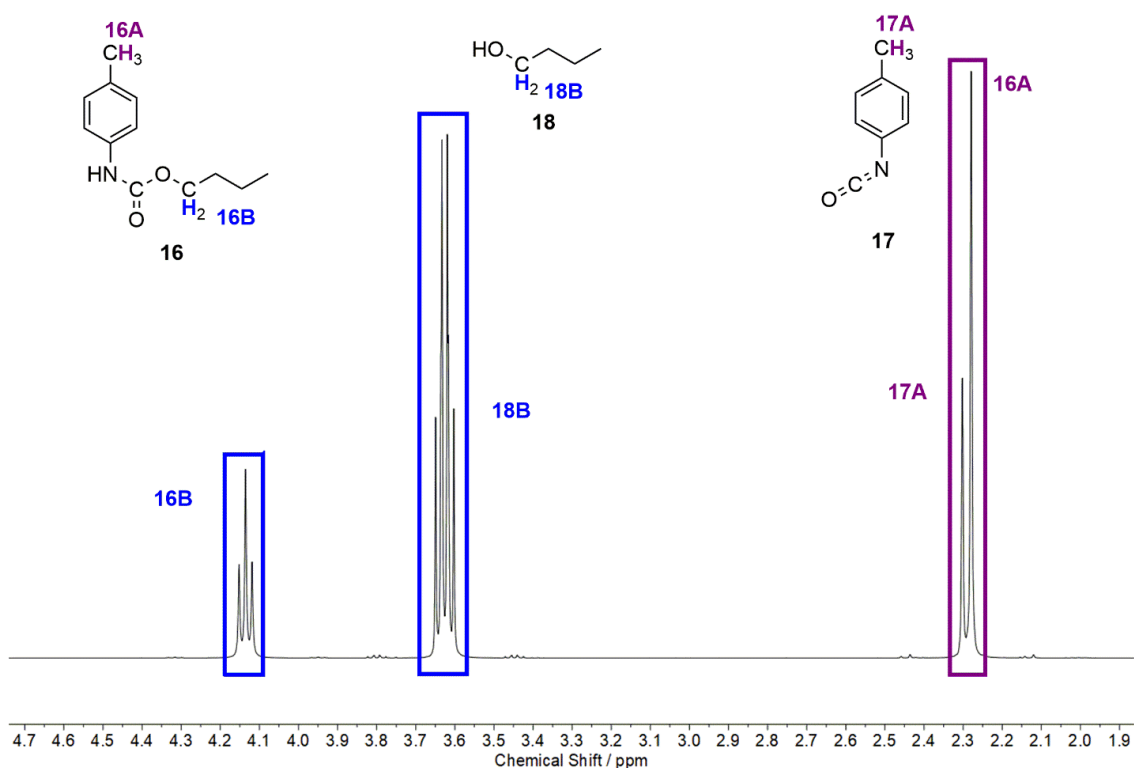


Figure S2. Integrals of interest for the synthesis of urethane **16** from isocyanate **17** and butanol **18**.

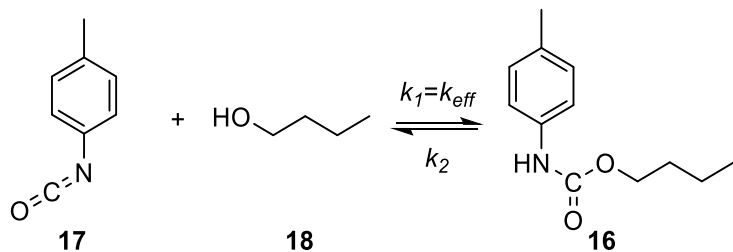
The values of these integrals were used to calculate turnover according to Equation S1:

$$T_{Uret} / \% = \frac{3 \times \mathbf{Integral\ U1}}{2 * \mathbf{Integral\ U3}} \times 100 = \frac{3 \times \mathbf{16B}}{2 * (\mathbf{16A} + \mathbf{17A})} \times 100 \quad \text{Eq. S1}$$

The values obtained for turnover T_{Uret} were used for calculating concentrations of **16** at the time t based on initial concentrations c_0 as shown by Equation S2:

$$c_t [\mathbf{16}] / \text{mol L}^{-1} = \frac{c_0 [\mathbf{16}] \times (100 - T_{Uret}(t))}{100} \quad \text{Eq. S2}$$

Simulation of kinetic parameters was done using COPASI^[3]. The obtained values for t and c_i [**16**] were imported into the program and the *Parameter Estimation* (default settings) option was used for the simplified model shown in Scheme S2.



Scheme S2. Simplified model used for fitting of the experimental data obtained for the Urethane synthesis in COPASI.

The values obtained for k_{eff} were then used to compare the activity of different catalysts to each other as detailed in the next section.

GC:

We noticed, that under the chosen conditions, some decomposition of urethane **16** happened in the GC machine, especially after several injections of reaction mixture as visible from the spectrum of purified (as specified in the synthetic section) urethane in $CDCl_3$ shown in **Figure S3**.

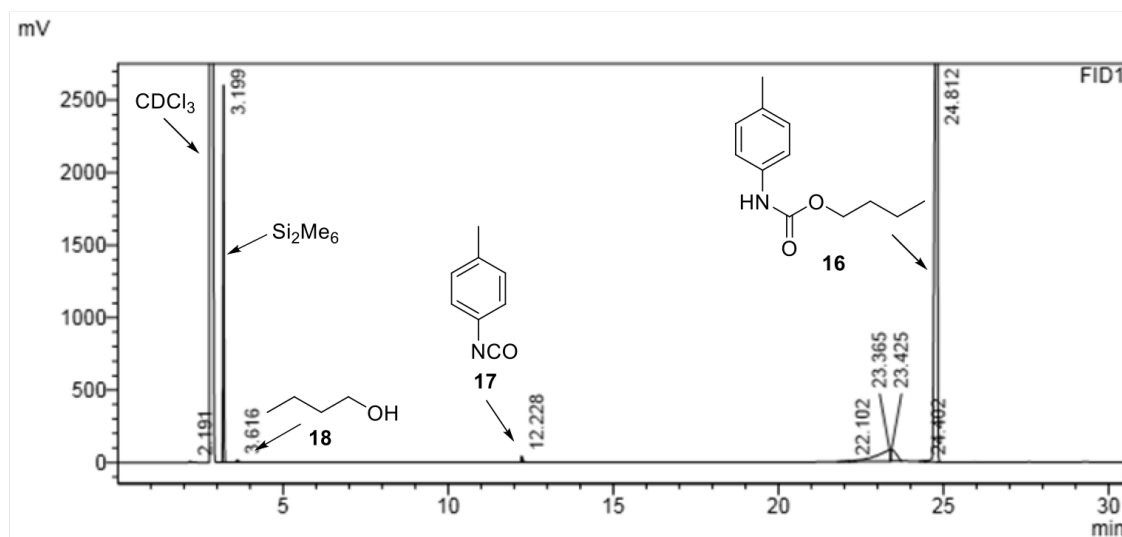


Figure S3. GC-spectrum of urethane **16** showing decomposition in the injector leading to distinct peaks for butanol **18** and isocyanate **17**. The broad signal at ca. 22 – 24 min is attributed to gradual decomposition on the column at higher temperatures.

Unfortunately, the short cleaning runs performed in between the measurements did not help solving the issue. We assume that the very small amounts of butanol **18** and isocyanate **17** indicate initial decomposition in the injector at 200 °C. In the reaction mixture, there would be no way of quantifying this, but we decided the amount was negligible. However, The broad signal at ca. 22 – 24 min accounts for up to 5 % of the integral of the peak of urethane **16** and we attributed it to gradual decomposition on the column at higher temperatures. This is in agreement with the known pyrolysis of urethanes at elevated temperatures, and so we decided to add the integral of this signal to the integral of the distinct urethane peak.

To be able to transform the integrals obtained for the product, urethane **16**, we measured different ratios of compound **16** and the internal standard Si_2Me_6 in CDCl_3 . We then plotted the ratio of the concentrations of urethane and internal standard to the ratio of the Integrals of the same compounds generating the straight calibration lines shown in **Figure S4**.

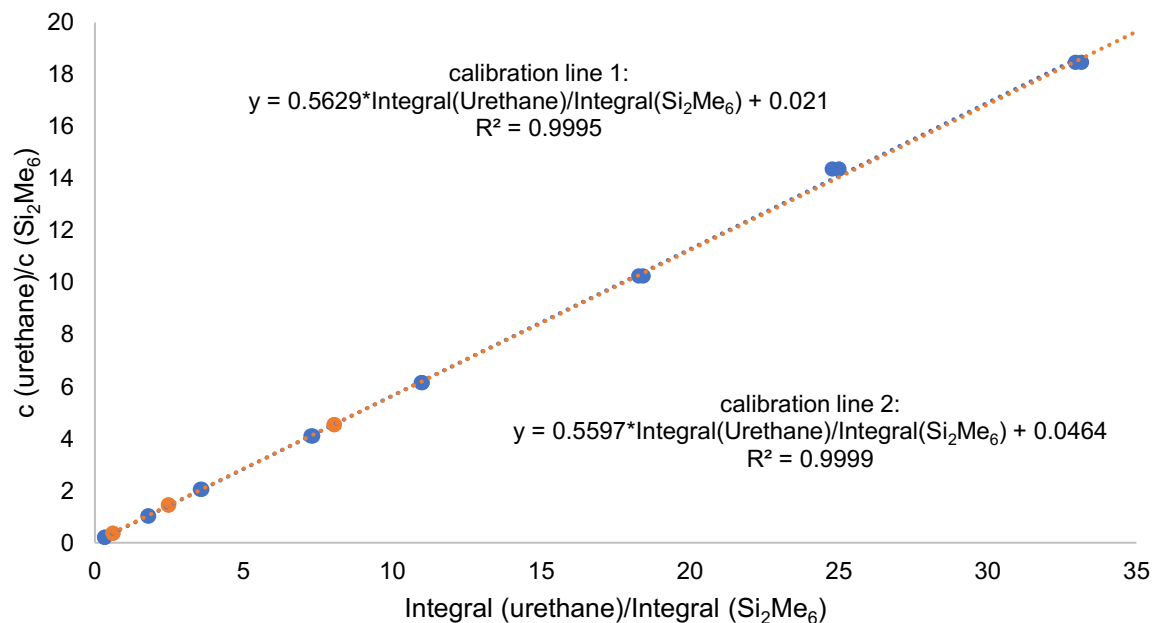


Figure S4. Straight calibration lines for $c(\text{urethane})/c(\text{Si}_2\text{Me}_6)$ to $\text{Integral}(\text{urethane})/\text{Integral}(\text{Si}_2\text{Me}_6)$.

From the fits of the straight calibration lines, equations Eq. S3 and Eq. S4 were derived, that give the concentration of urethane **16** at the time t : $c_t[\mathbf{16}]$.

$$c_{t1}[\mathbf{16}] / \text{mol L}^{-1} = (0.5629 \times \frac{\text{Int}(\mathbf{16})}{\text{Int}(\text{Si}_2\text{Me}_6)} + 0.021) \times c(\text{Si}_2\text{Me}_6) \quad \text{Eq. S3}$$

$$c_{t2}[\mathbf{16}] / \text{mol L}^{-1} = (0.5597 \times \frac{\text{Int}(\mathbf{16})}{\text{Int}(\text{Si}_2\text{Me}_6)} + 0.0464) \times c(\text{Si}_2\text{Me}_6) \quad \text{Eq. S4}$$

The obtained values for $c_{t1}[\mathbf{16}]$ and $c_{t2}[\mathbf{16}]$ were averaged obtaining $c_t[\mathbf{16}]$ and Simulation of kinetic parameters was done using COPASI^[3]. The values for t and $c_t[\mathbf{16}]$ were imported into the program and the *Parameter Estimation* (default settings) option was used for the simplified model shown in Scheme S2.

The values obtained for k_{eff} were then used to compare the activity of different catalysts to each other as detailed in the next section.

Kinetic Data for the Urethane Synthesis Benchmark Reaction

Table S1 gives details for the urethane synthesis benchmark reactions that were done in the course of this study while **Figure S5 – Figure S81** shows the fitted turnover curves that are obtained as graphical output by COPASI:

Table S1. Details for the urethane synthesis benchmark reactions.

Experiment	Method	Catalyst	mol-% catalyst (compared to isocyanate 17)	c(Catalyst) / mol L ⁻¹	keff / L mol ⁻¹ s ⁻¹
urethane_01	NMR	none	0.0	0.00E+00	4.54E-05
urethane_02	NMR	1a	3.0	3.00E-03	2.80E-04
urethane_03	NMR	1a	15.1	1.50E-02	1.27E-03
urethane_04	NMR	1a	30.2	3.00E-02	2.35E-03
urethane_05	NMR	1b	0.1	9.98E-05	6.02E-05
urethane_06	NMR	1b	0.1	1.00E-04	5.91E-05
urethane_07	NMR	1b	1.0	9.98E-04	2.61E-04
urethane_08	NMR	1b	1.0	1.00E-03	2.72E-04
urethane_09	NMR	1b	3.0	2.97E-03	7.69E-04
urethane_10	NMR	1b	3.0	2.97E-03	7.31E-04
urethane_11	NMR	1b	5.0	4.99E-03	1.22E-03
urethane_12	NMR	1b	5.0	5.01E-03	1.19E-03
urethane_13	NMR	1b	29.7	2.97E-02	6.63E-03
urethane_14	NMR	1c	0.1	1.00E-04	4.95E-05
urethane_15	NMR	1c	1.0	9.99E-04	1.45E-04
urethane_16	NMR	1c	1.0	9.99E-04	1.42E-04
urethane_17	NMR	1c	2.0	2.00E-03	2.50E-04
urethane_18	NMR	1c	1.0	2.00E-03	1.59E-04
urethane_19	NMR	1c	3.0	3.00E-03	4.49E-04
urethane_20	NMR	1c	3.0	3.00E-03	3.47E-04
urethane_21	NMR	1c	3.0	3.00E-03	3.51E-04
urethane_22	NMR	1c	5.0	5.00E-03	6.45E-04
urethane_23	NMR	1c	10.0	1.00E-02	1.14E-03
urethane_24	NMR	1c	20.0	2.00E-02	2.64E-03
urethane_25	NMR	1d	1.0	9.99E-04	1.72E-04
urethane_26	NMR	1d	3.0	3.00E-03	5.05E-04
urethane_27	NMR	1d	5.0	5.00E-03	8.43E-04
urethane_28	NMR	1d	5.0	5.00E-03	7.44E-04
urethane_29	NMR	1e	1.0	9.95E-04	2.43E-04
urethane_30	NMR	1e	3.0	2.99E-03	6.57E-04
urethane_31	NMR	1e	5.0	4.98E-03	1.09E-03
urethane_32	NMR	1f	1.0	9.99E-04	2.38E-04
urethane_33	NMR	1f	3.0	3.00E-03	6.42E-04
urethane_34	NMR	1f	5.0	5.00E-03	1.04E-03
urethane_35	NMR	6aa	3.0	3.02E-03	3.65E-04
urethane_36	NMR	6aa	5.0	4.98E-03	6.07E-04
urethane_37	NMR	6aa	19.9	1.99E-02	2.02E-03
urethane_38	NMR	6ab	3.0	3.00E-03	3.89E-04

Table S1 (continuation). Details for the urethane synthesis benchmark reactions.

urethane_39	NMR	6ac	3.0	3.00E-03	4.66E-04
urethane_40	NMR	6ac	3.0	3.00E-03	4.76E-04
urethane_41	NMR	6bc	3.0	3.00E-03	1.49E-03
urethane_42	NMR	6bc	3.0	3.00E-03	1.43E-03
urethane_43	NMR	6bc	3.0	3.01E-03	1.41E-03
urethane_44	NMR	6bc	15.0	1.50E-02	6.94E-03
urethane_45	NMR	6bf	3.0	3.00E-03	1.43E-03
urethane_46	NMR	6cg	1.2	1.20E-03	8.04E-04
urethane_47	NMR	6cg	3.0	3.01E-03	1.99E-03
urethane_48	NMR	6cg	6.0	5.98E-03	3.96E-03
urethane_49	NMR	6cg	11.9	1.20E-02	7.78E-03
urethane_50	NMR	15g	3.0	3.00E-03	8.32E-04
urethane_51	NMR	15g	3.0	3.00E-03	8.36E-04
urethane_52	NMR	15g	6.0	6.00E-03	1.61E-03
urethane_53	NMR	15g	12.0	1.20E-02	3.22E-03
urethane_54	NMR	22	3.0	3.04E-03	3.55E-05
urethane_55	NMR	22	30.3	3.04E-02	3.50E-05
urethane_56	NMR	23	15.0	1.50E-02	1.14E-04
urethane_57	NMR	23	30.1	3.01E-02	1.74E-04
urethane_58	NMR	23	30.1	3.01E-02	1.70E-04
urethane_59	NMR	24	3.0	3.00E-03	3.63E-05
urethane_60	GC	1b	0.1	9.98E-05	6.77E-05
urethane_61	GC	1b	0.1	1.00E-04	6.57E-05
urethane_62	GC	1b	1.0	9.98E-04	2.84E-04
urethane_63	GC	1b	1.0	1.00E-03	2.94E-04
urethane_64	GC	1b	5.0	4.99E-03	1.46E-03
urethane_65	GC	1b	5.0	5.01E-03	1.62E-03
urethane_66	GC	1c	0.1	1.00E-04	5.09E-05
urethane_67	GC	1c	1.0	9.99E-04	1.27E-04
urethane_68	GC	1c	1.0	9.99E-04	1.47E-04
urethane_69	GC	1c	5.0	5.00E-03	6.64E-04
urethane_70	GC	1c	10.0	1.00E-02	1.37E-03
urethane_71	GC	1d	5.0	5.00E-03	8.07E-04
urethane_72	GC	1d	5.0	5.00E-03	9.04E-04
urethane_73	GC	1e	3.0	2.99E-03	7.21E-04
urethane_74	GC	1e	5.0	4.98E-03	1.23E-03
urethane_75	GC	1f	1.0	9.99E-04	2.43E-04
urethane_76	GC	1f	3.0	3.00E-03	6.80E-04
urethane_77	GC	1f	5.0	5.00E-03	1.14E-03

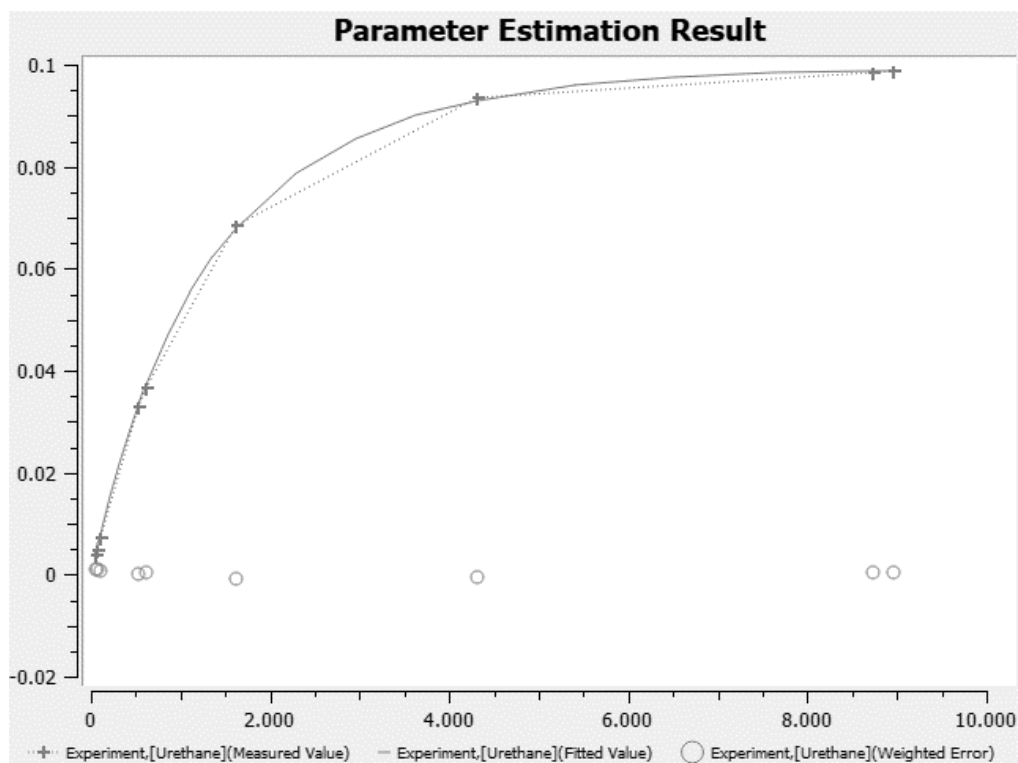


Figure S5. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_01. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 10000 min.

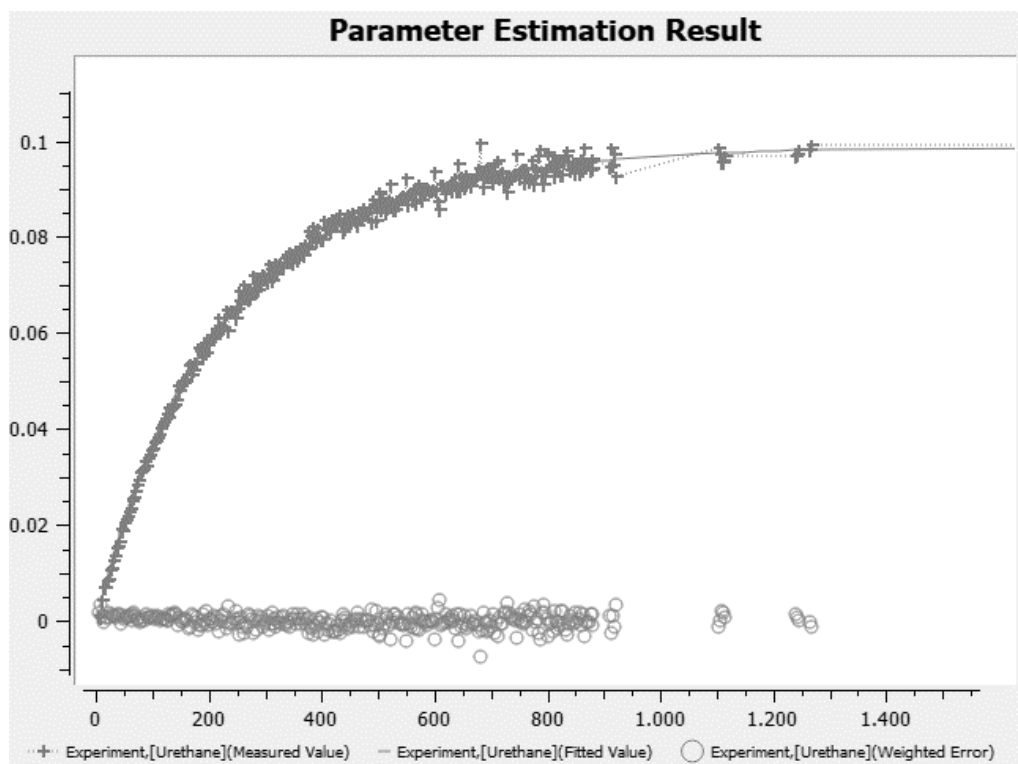


Figure S6. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_02. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 1400 min.

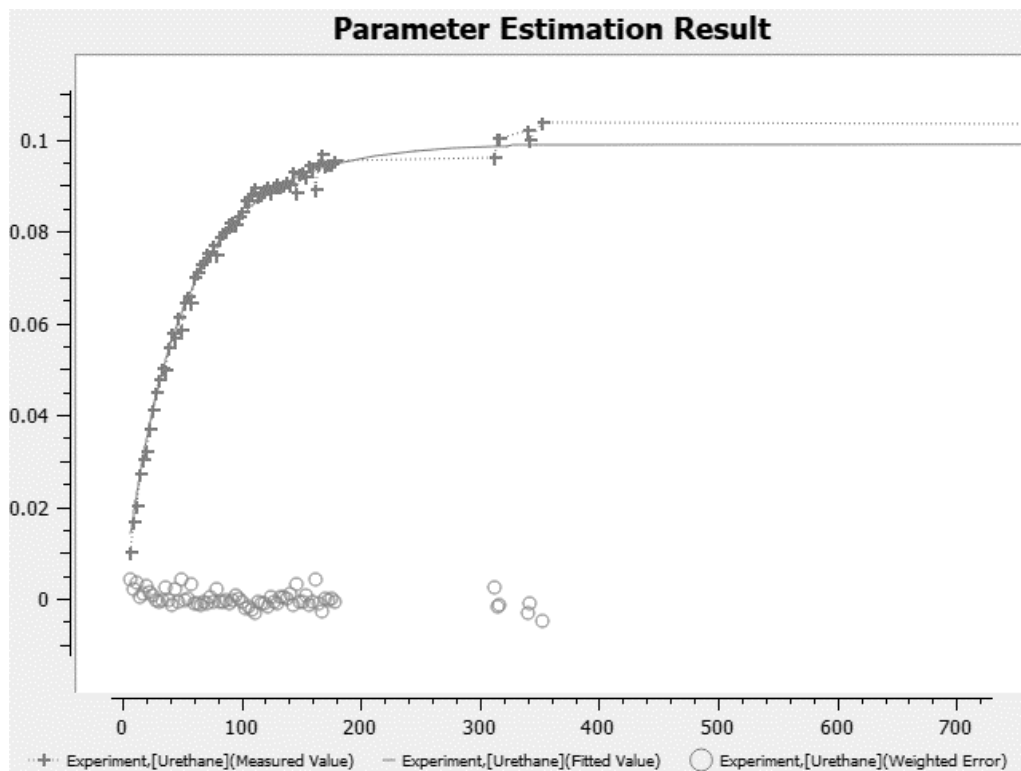


Figure S7. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_03. Vertical axis gives the concentration of urethane **16** in mol L⁻¹, horizontal axis gives the time from 0 min to 700 min.

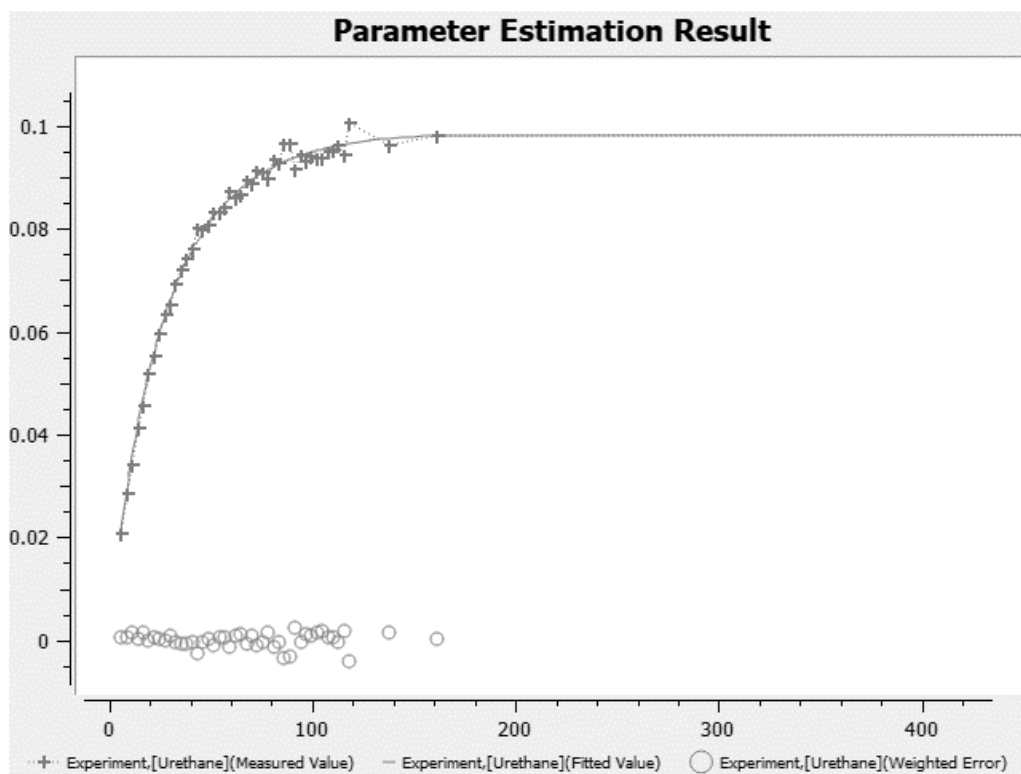


Figure S8. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_04. Vertical axis gives the concentration of urethane **16** in mol L⁻¹, horizontal axis gives the time from 0 min to 400 min.

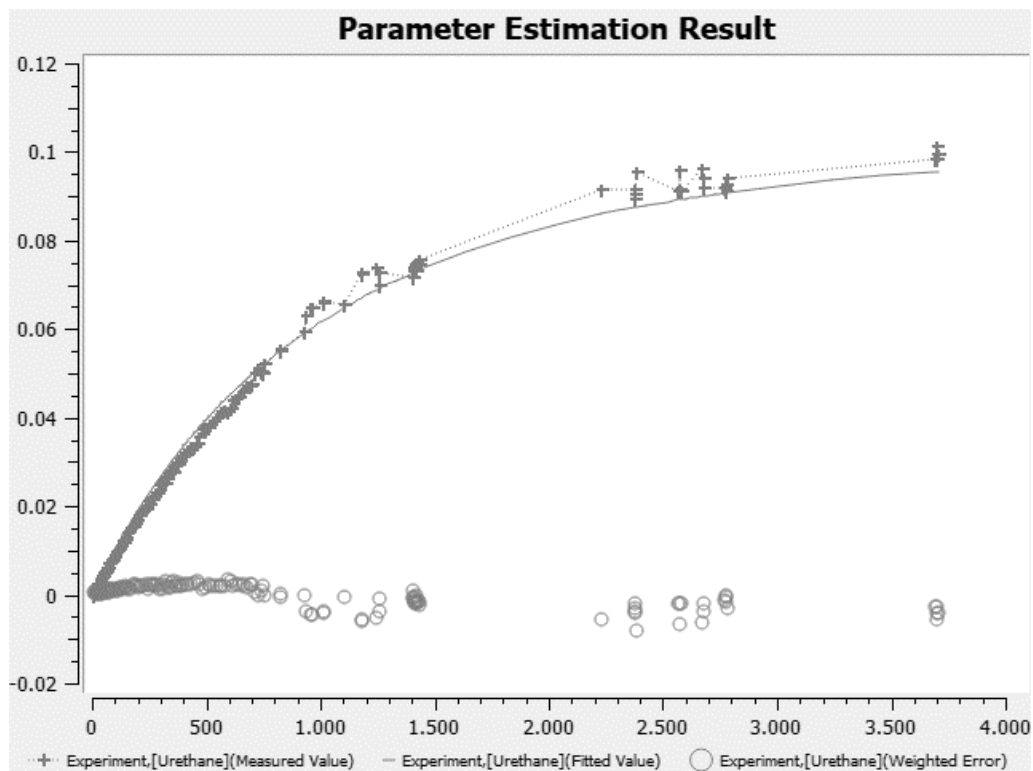


Figure S9. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_05. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 4000 min.

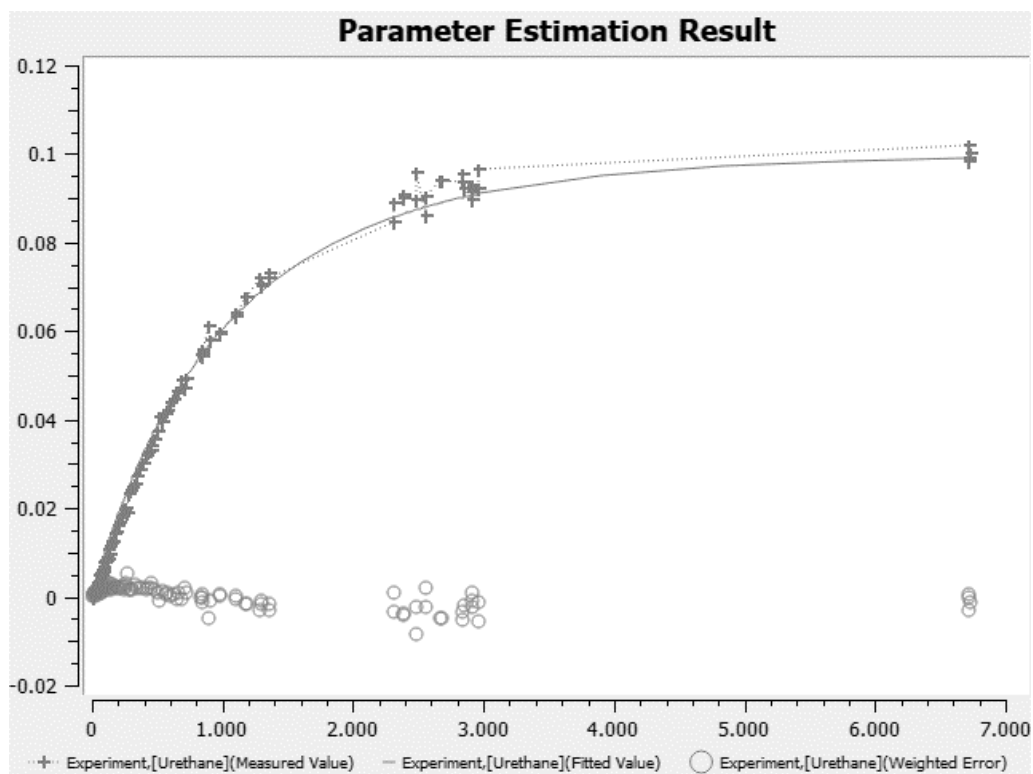


Figure S10. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_06. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 7000 min.

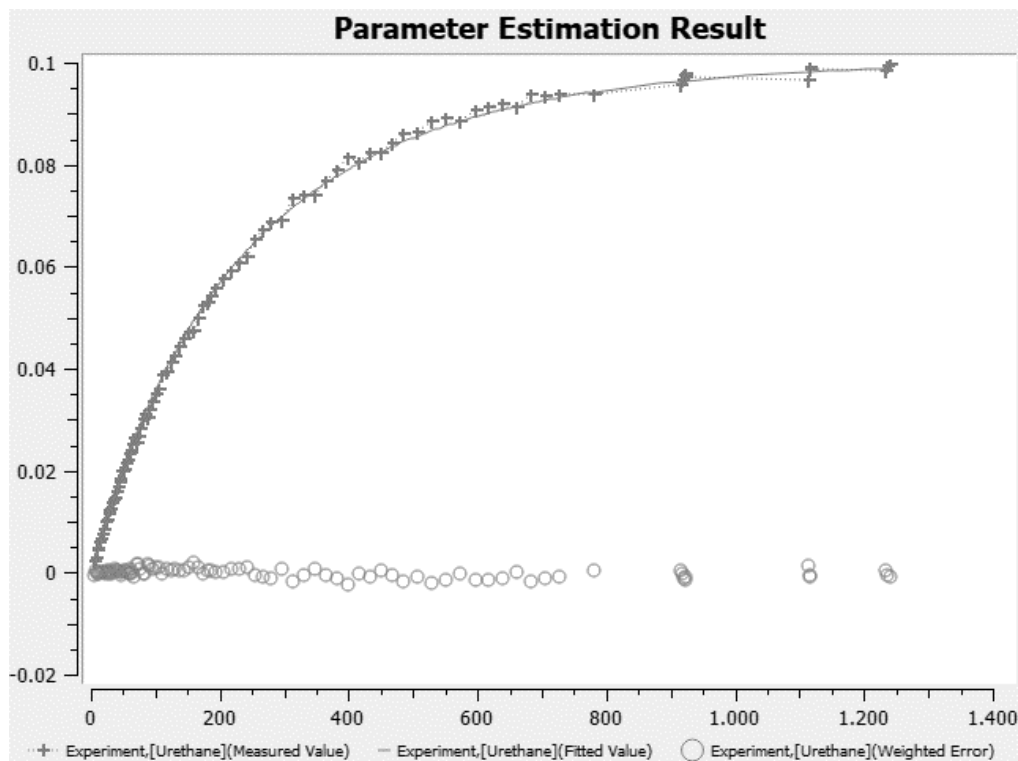


Figure S11. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_07. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 1400 min.

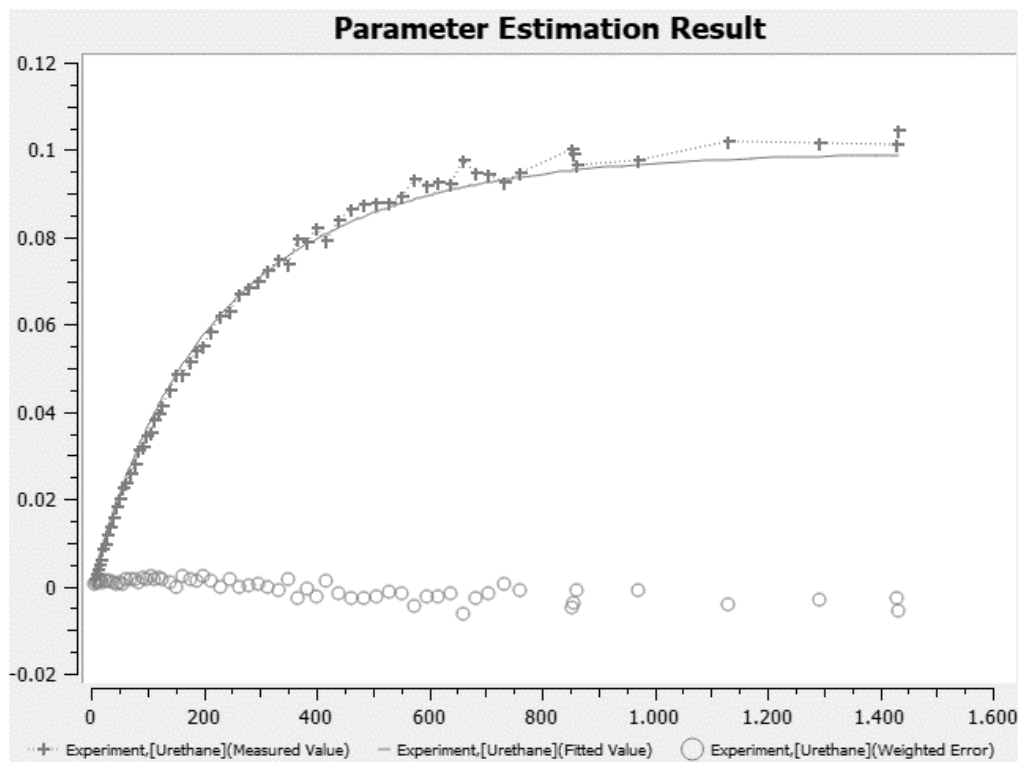


Figure S12. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_08. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 1600 min.

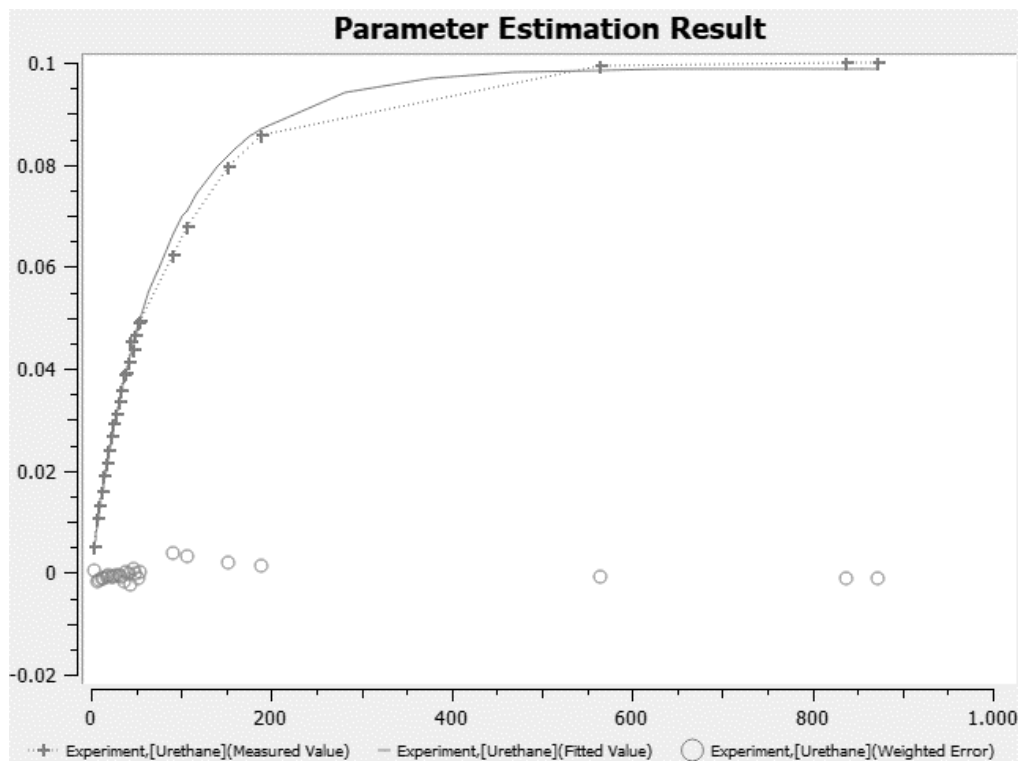


Figure S13. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_09. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 1000 min.

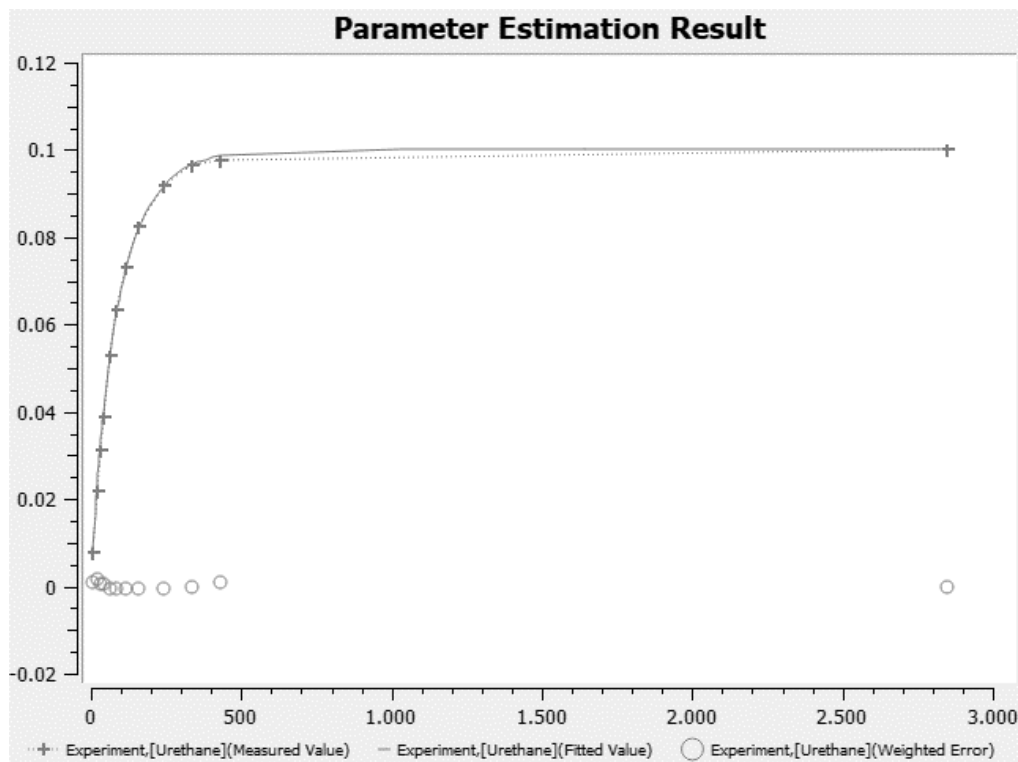


Figure S14. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_10. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 3000 min.

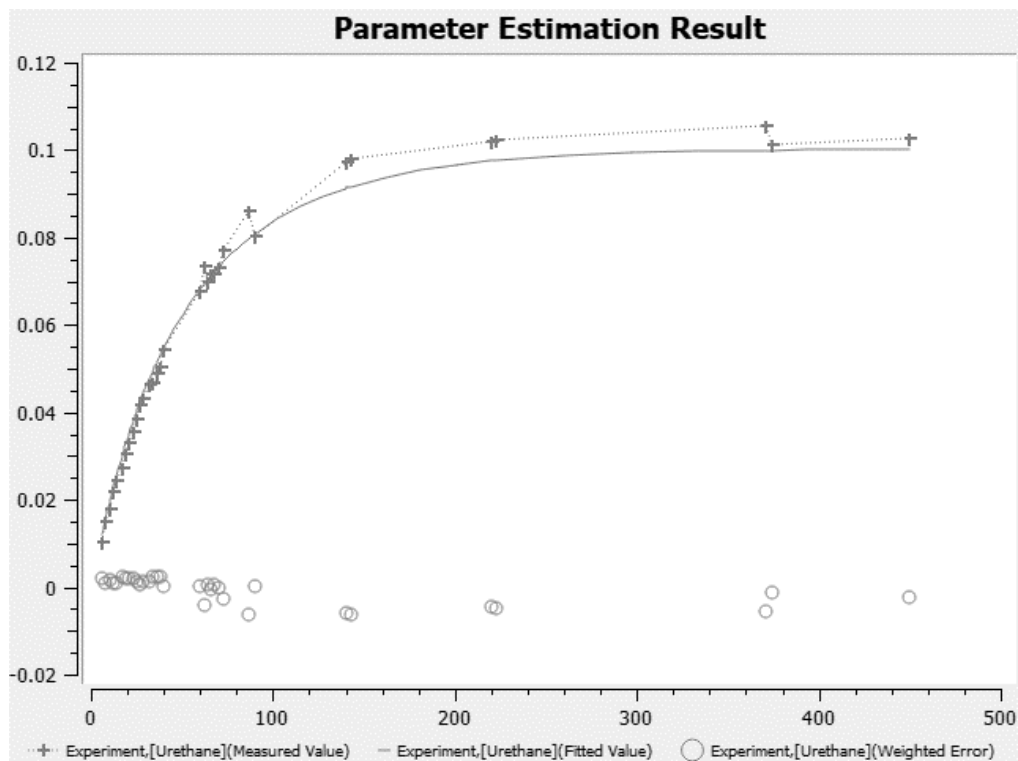


Figure S15. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_11. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 500 min.

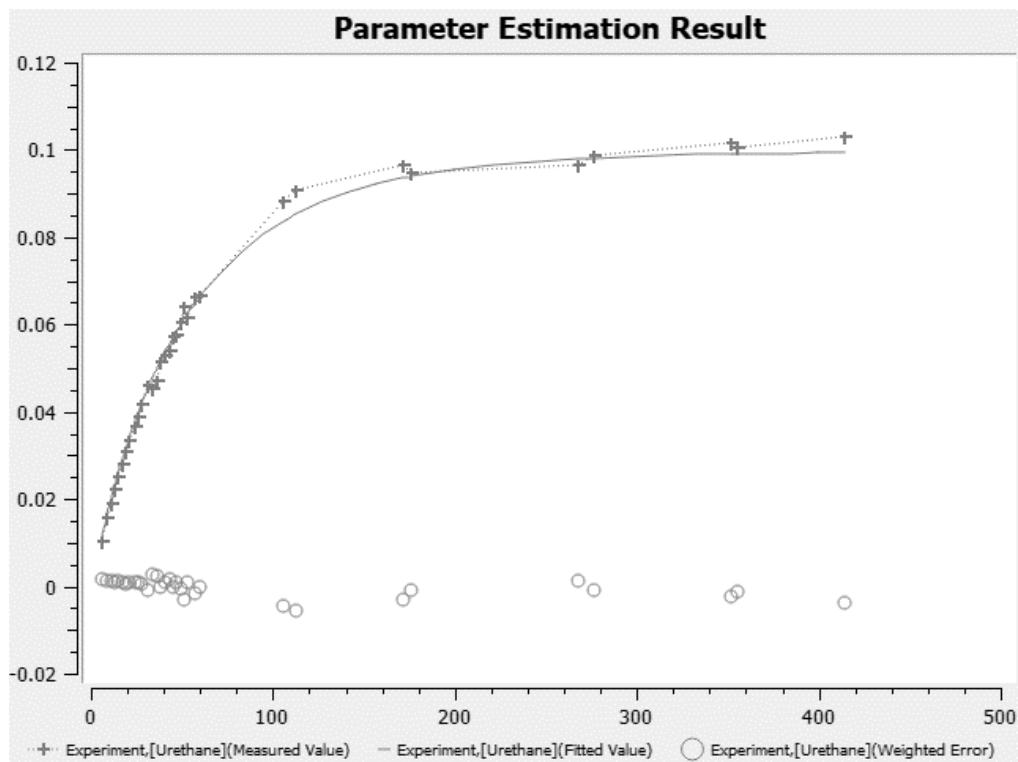


Figure S16. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_12. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 500 min.

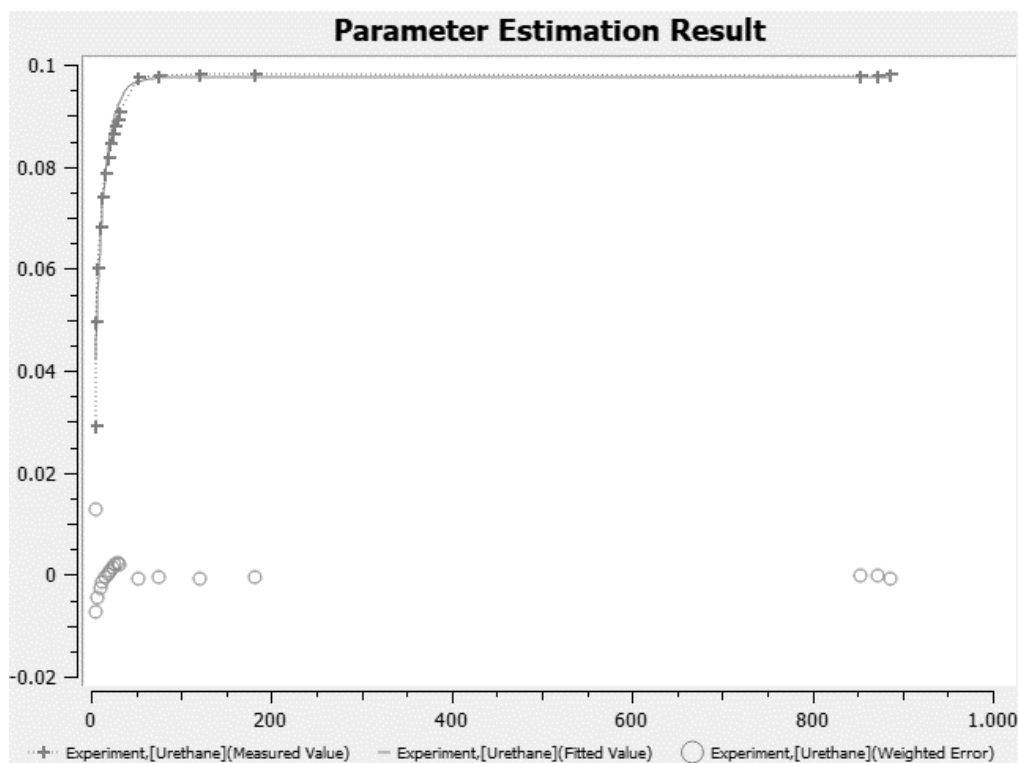


Figure S17. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_13. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 1000 min.

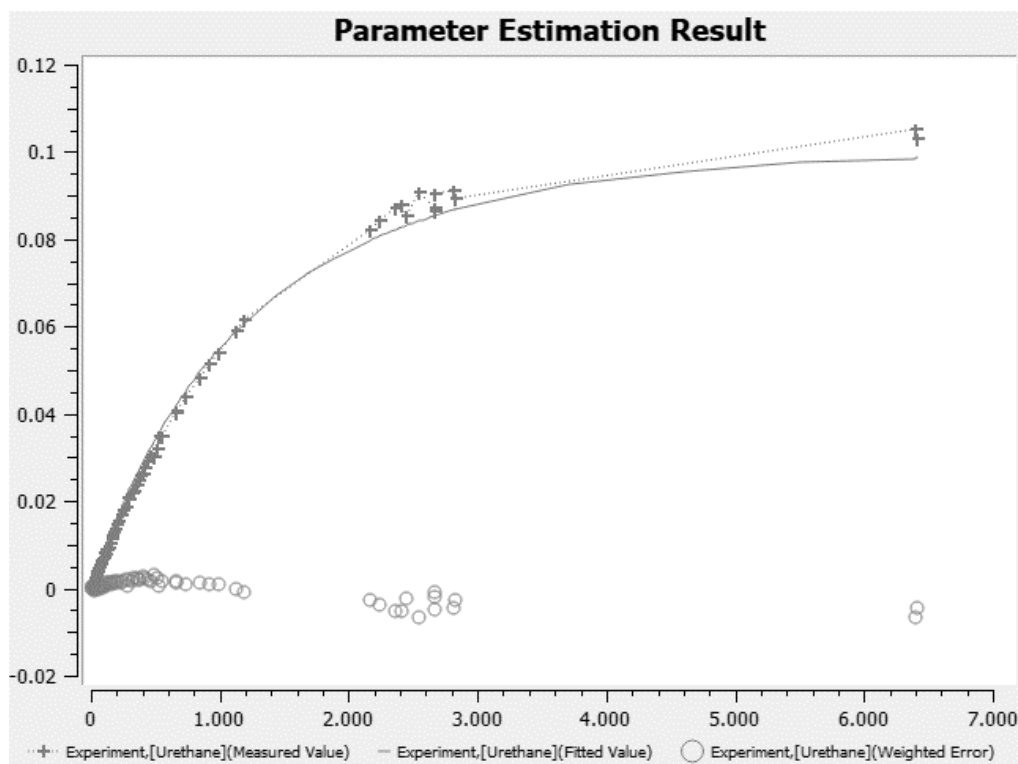


Figure S18. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_14. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 7000 min.

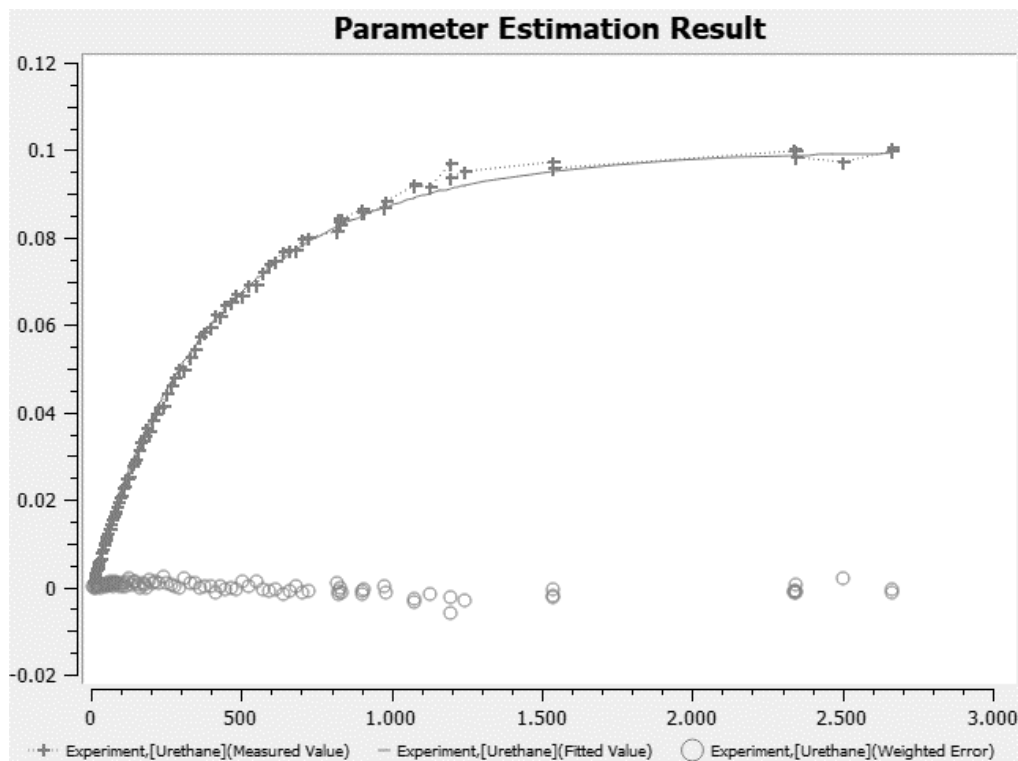


Figure S19. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_15. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 3000 min.

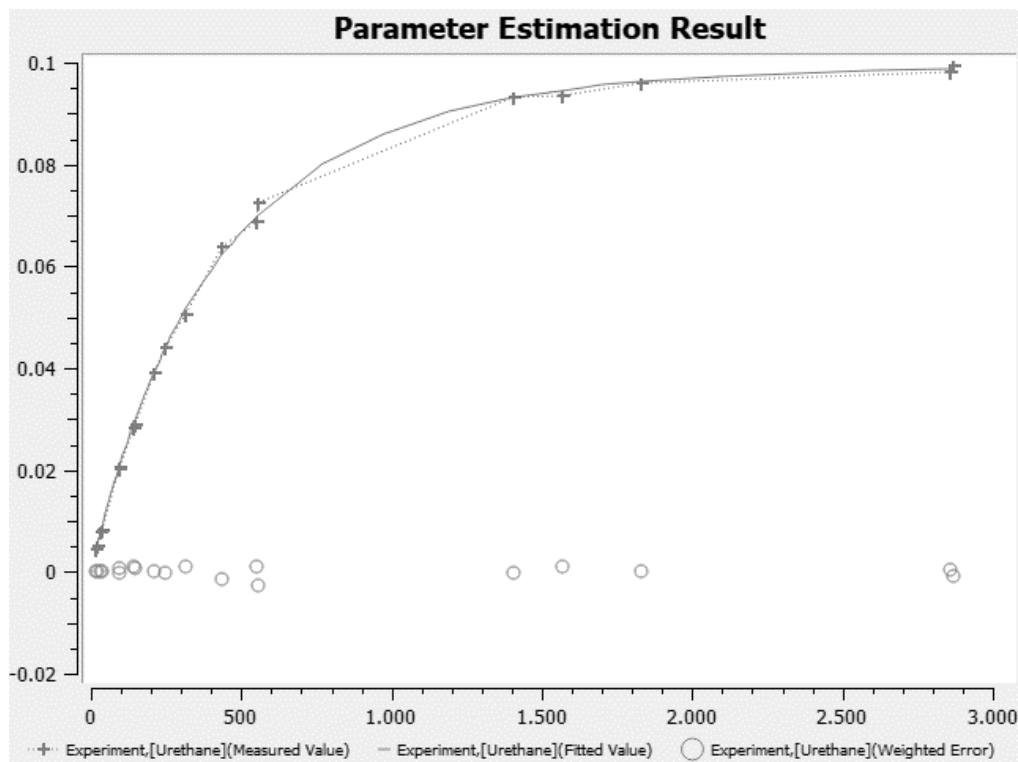


Figure S20. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_16. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 3000 min.

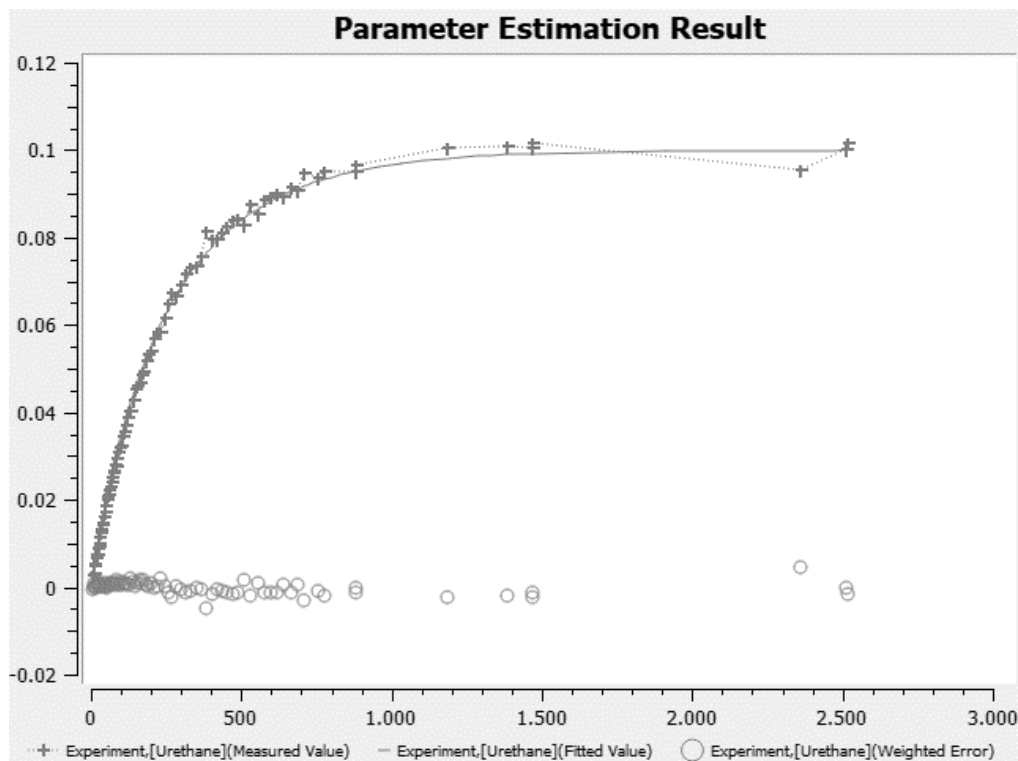


Figure S21. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_17. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 3000 min.

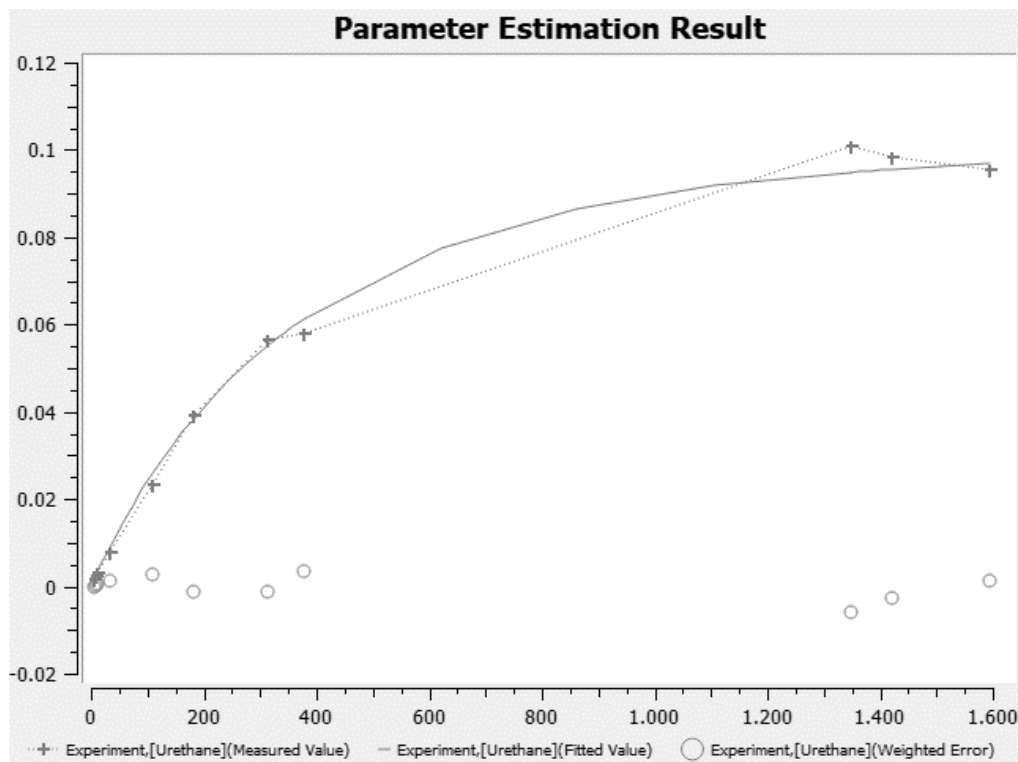


Figure S22. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_18. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 1600 min.

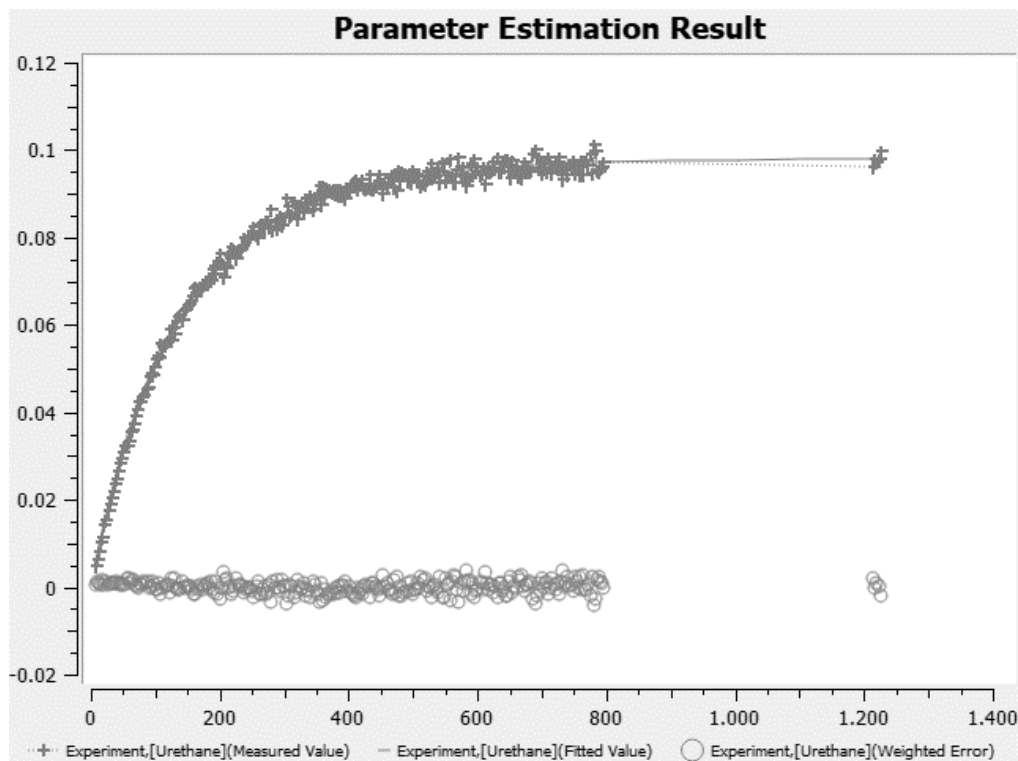


Figure S23. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_19. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 1400 min.

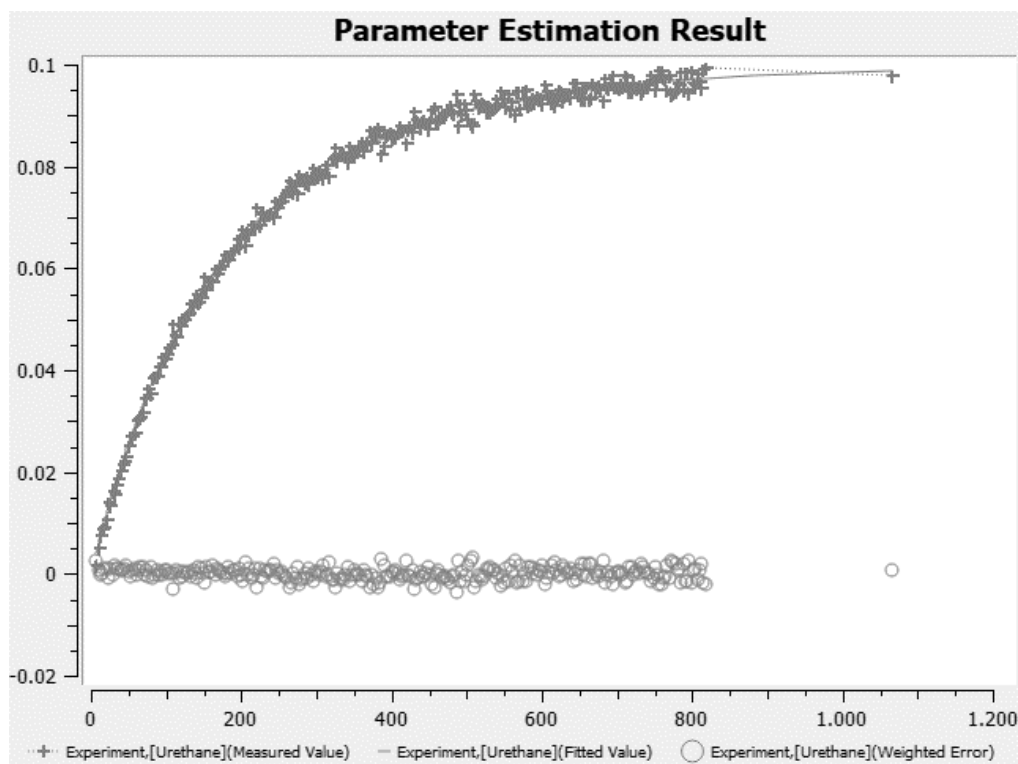


Figure S24. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_20. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 1200 min.

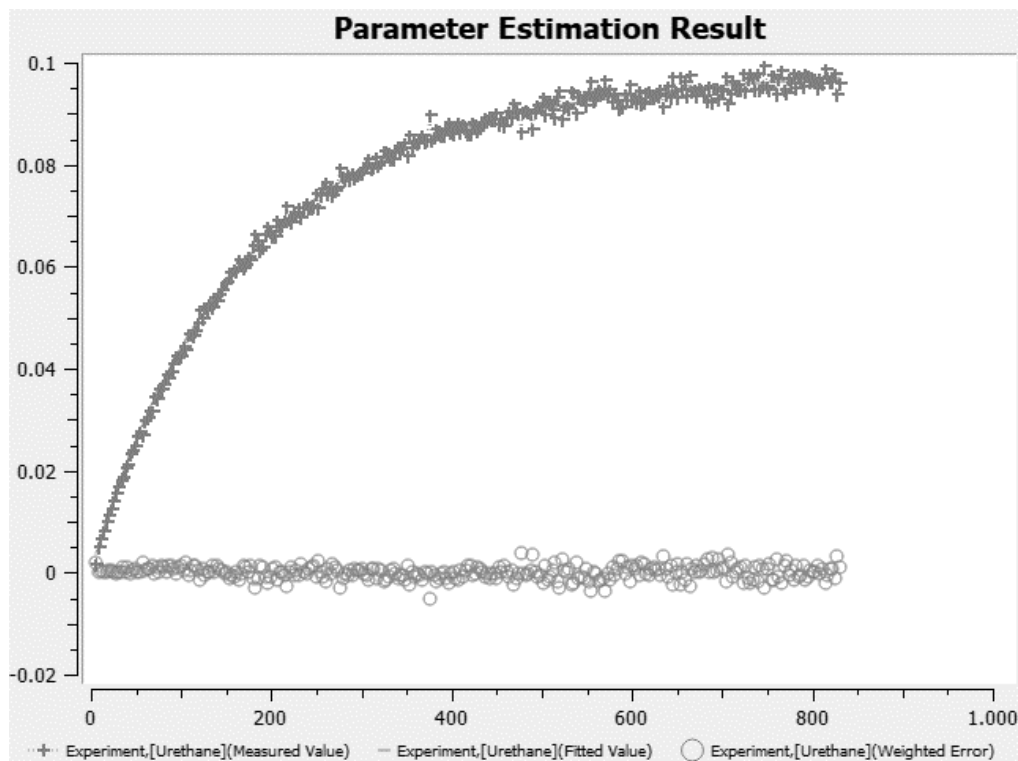


Figure S25. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_21. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 1000 min.

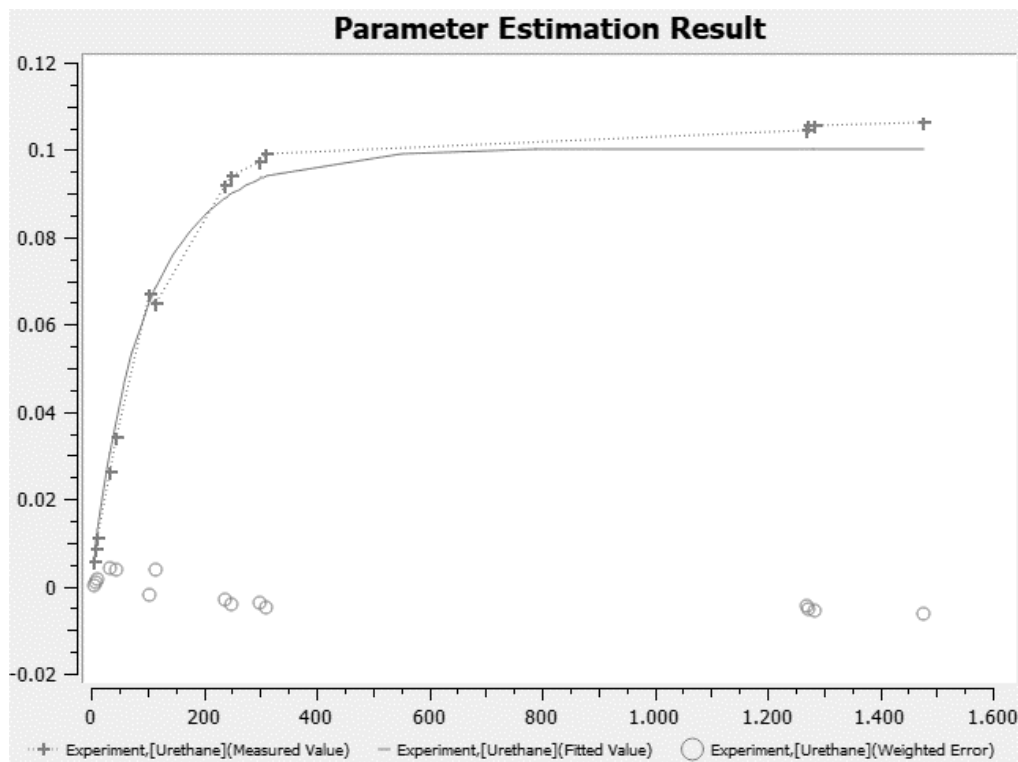


Figure S26. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_22. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 1600 min.

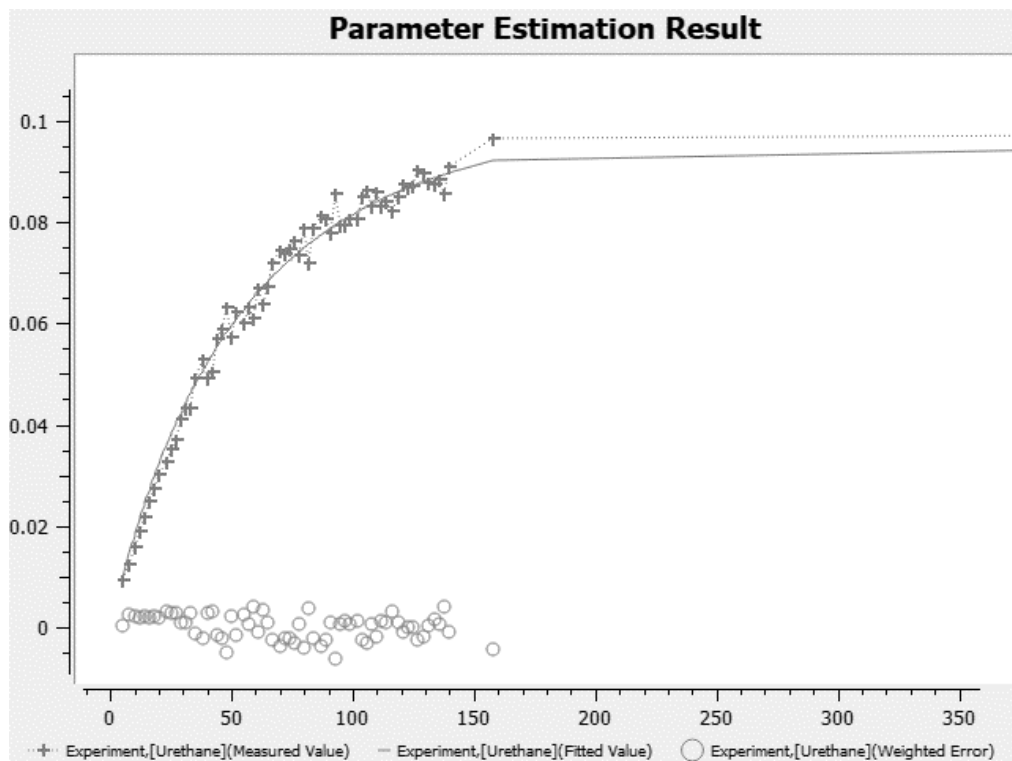


Figure S27. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_23. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 350 min.

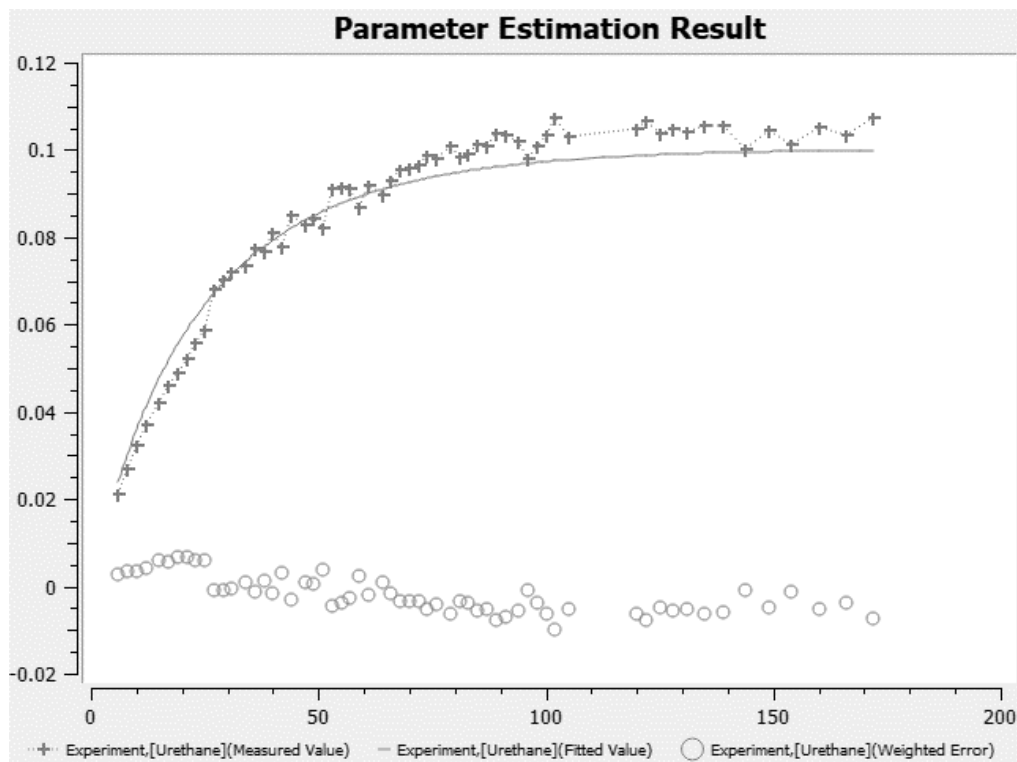


Figure S28. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_24. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 200 min.

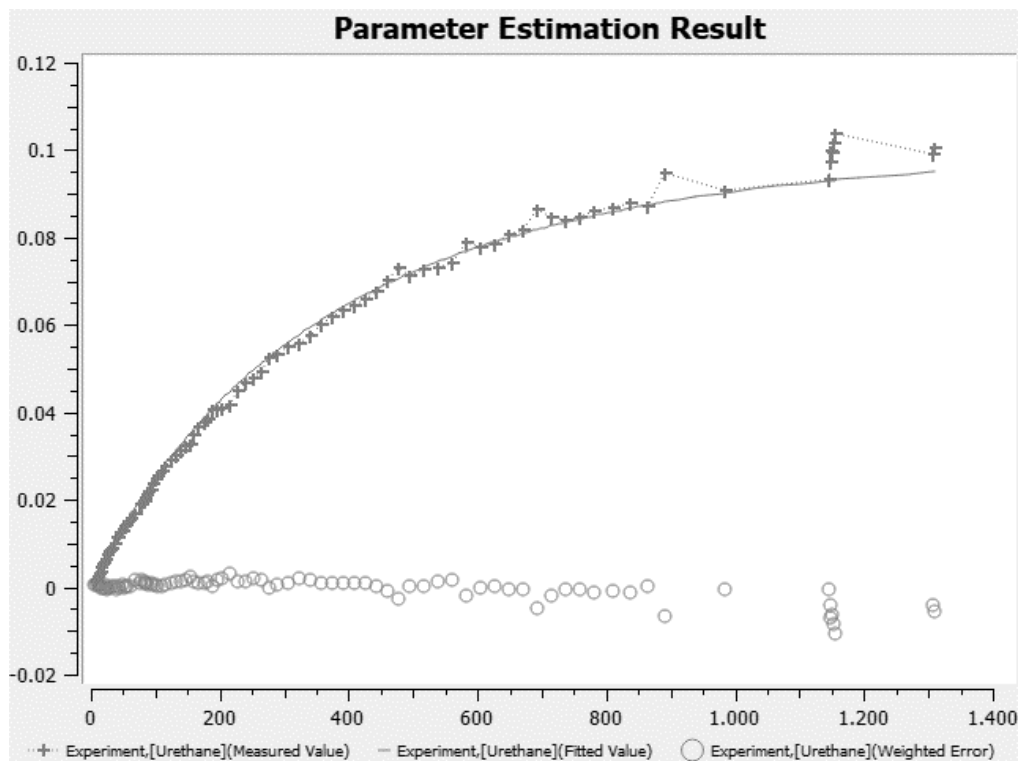


Figure S29. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_25. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 1400 min.

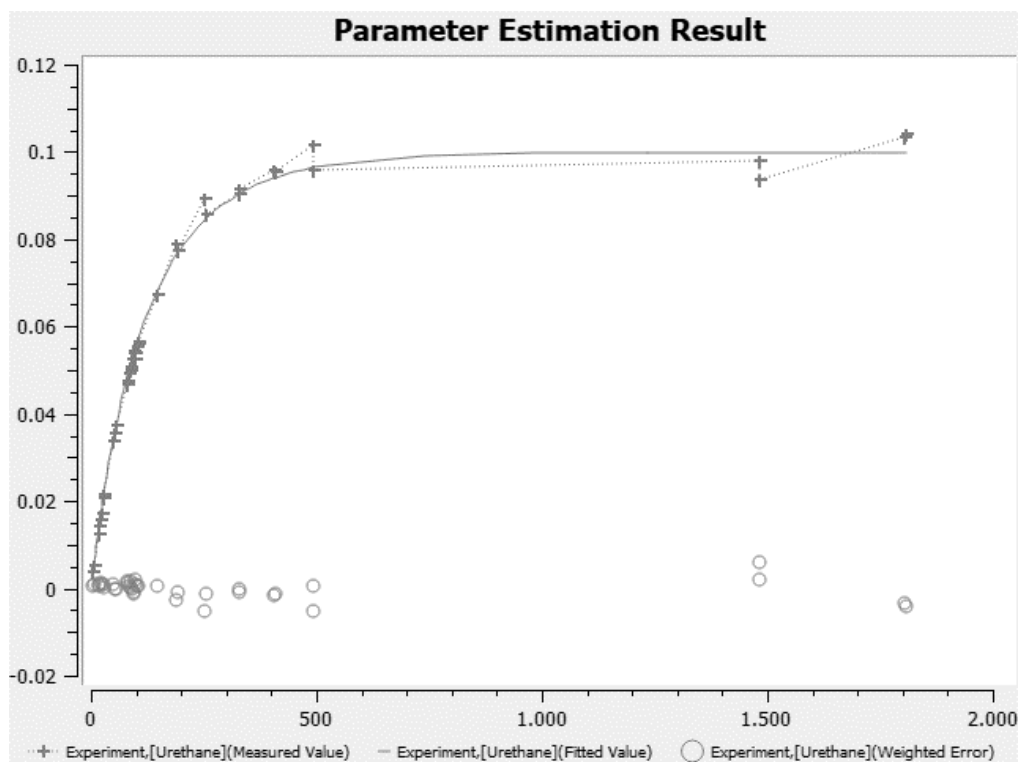


Figure S30. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_26. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 2000 min.

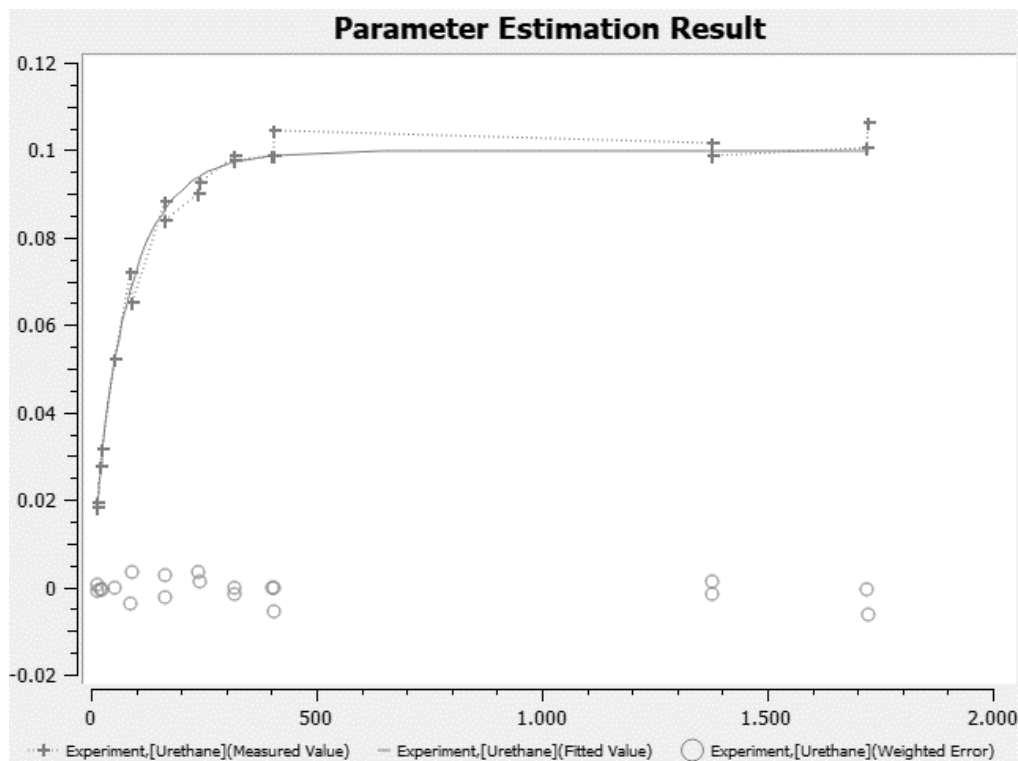


Figure S31. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_27. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 2000 min.

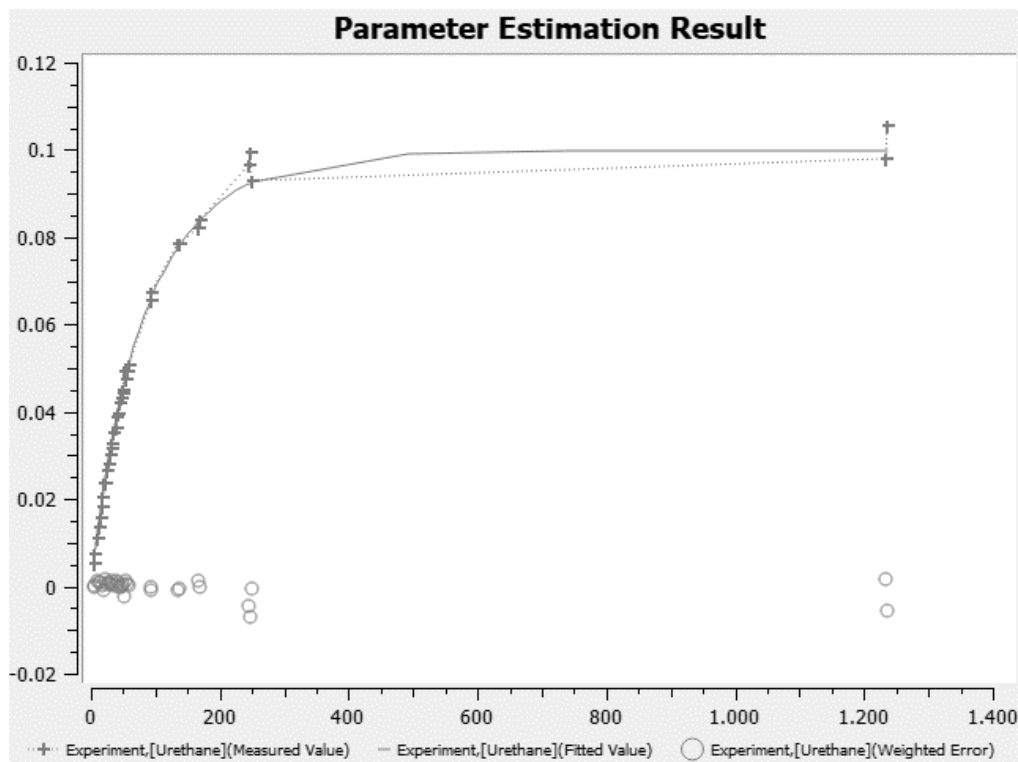


Figure S32. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_28. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 1400 min.

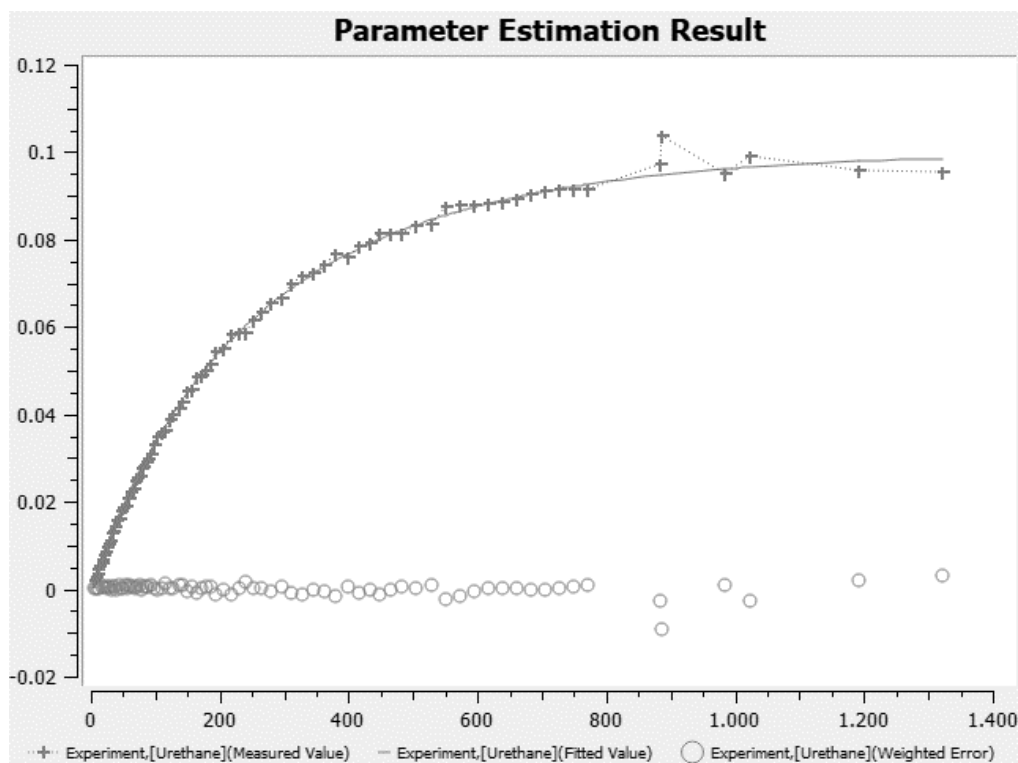


Figure S33. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_29. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 1400 min.

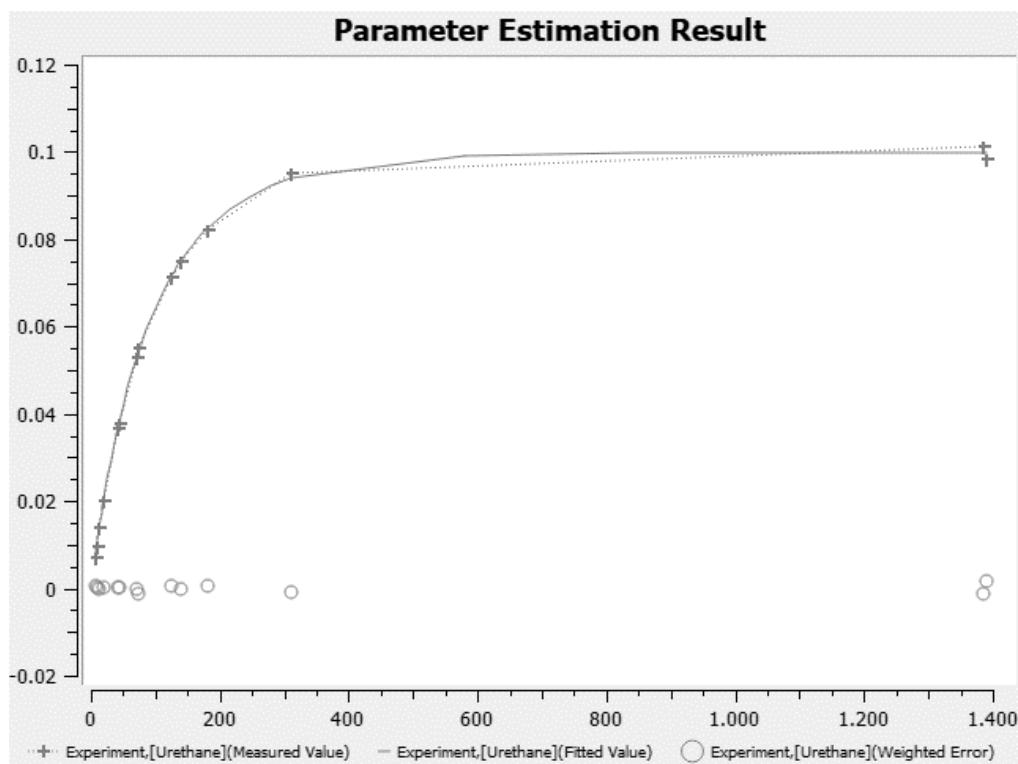


Figure S34. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_30. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 1400 min.

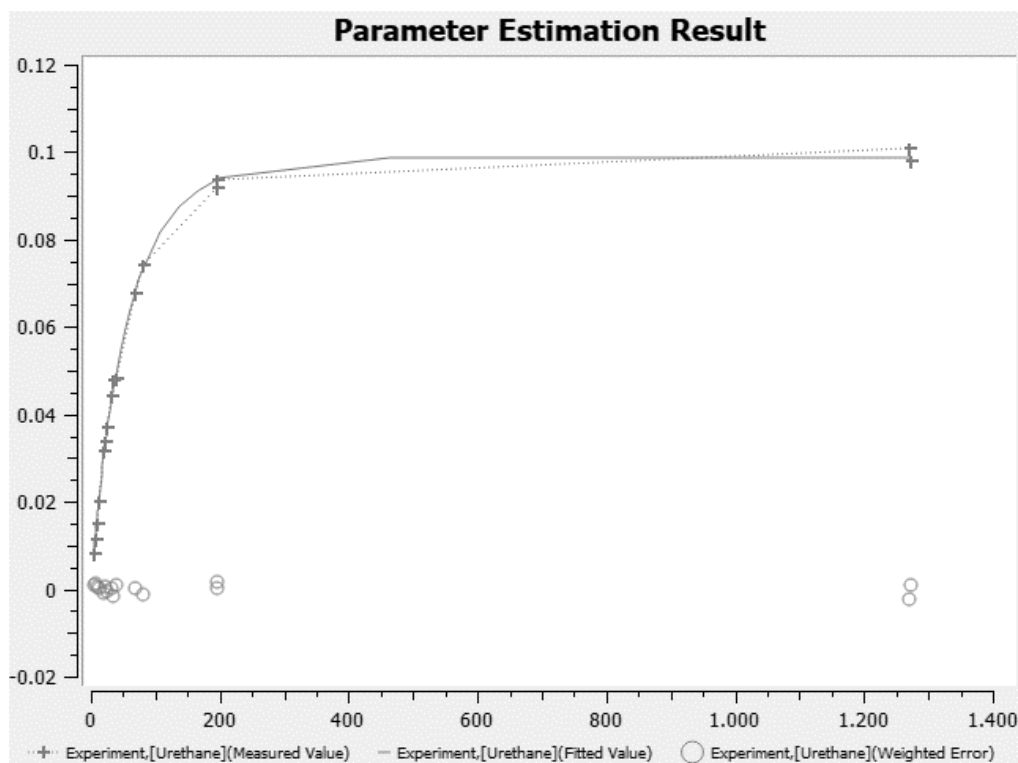


Figure S35. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_31. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 1400 min.

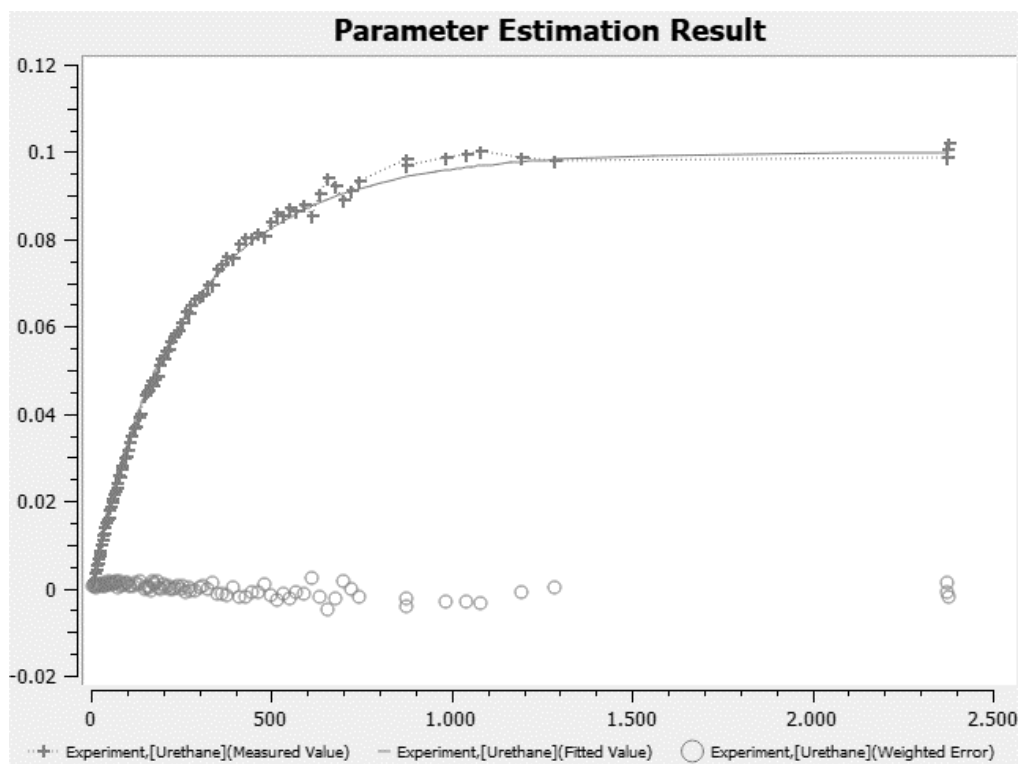


Figure S36. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_32. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 2500 min.

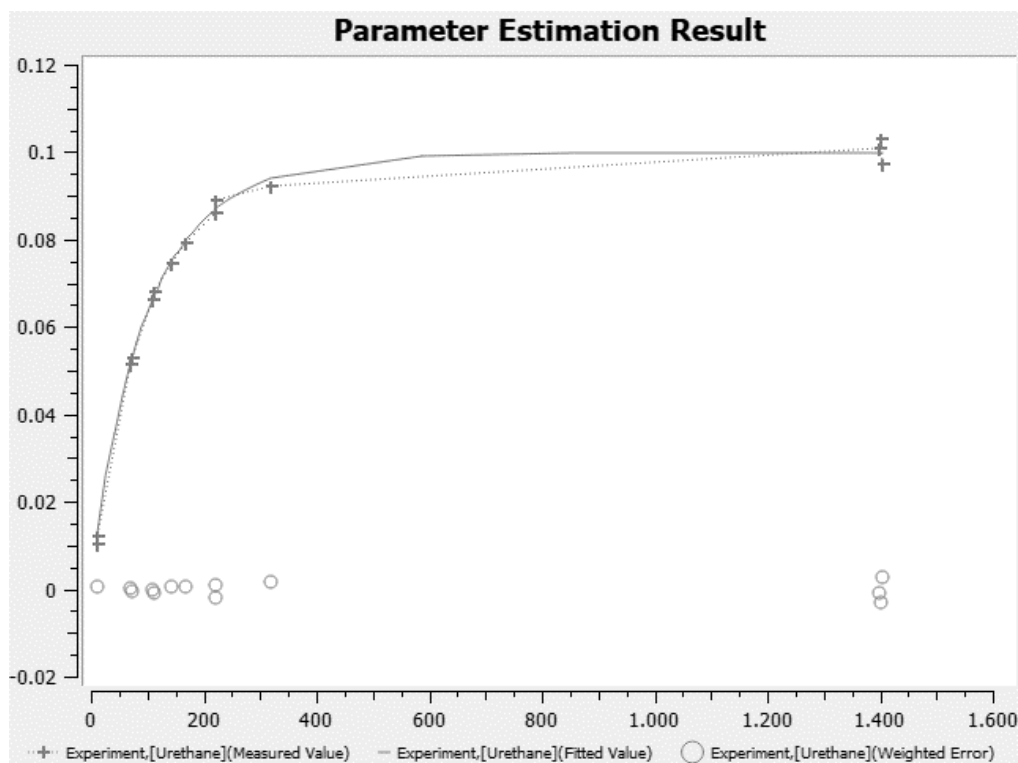


Figure S37. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_33. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 1600 min.

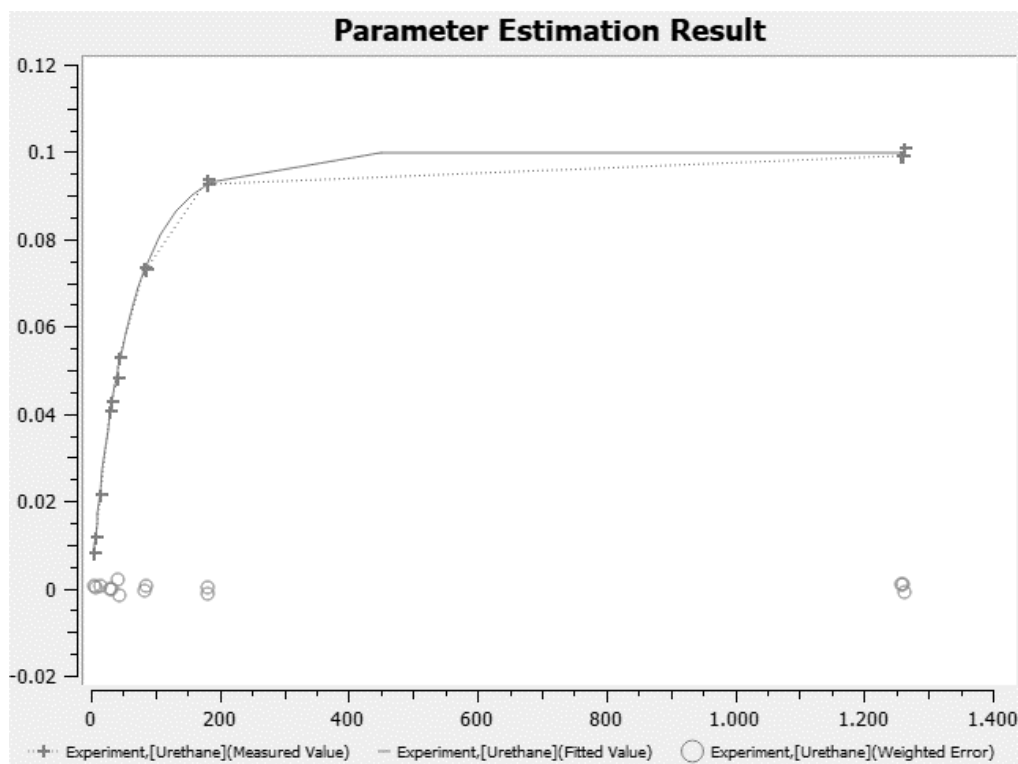


Figure S38. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_34. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 1400 min.

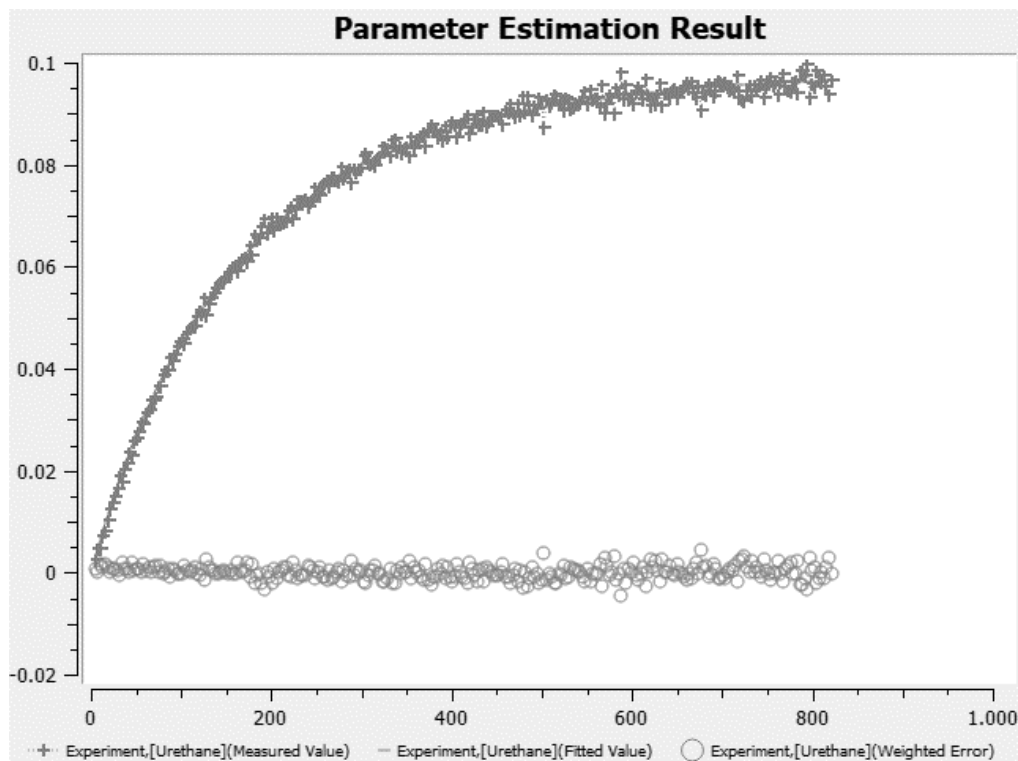


Figure S39. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_35. Vertical axis gives the concentration of urethane **16** in mol L⁻¹, horizontal axis gives the time from 0 min to 1000 min.

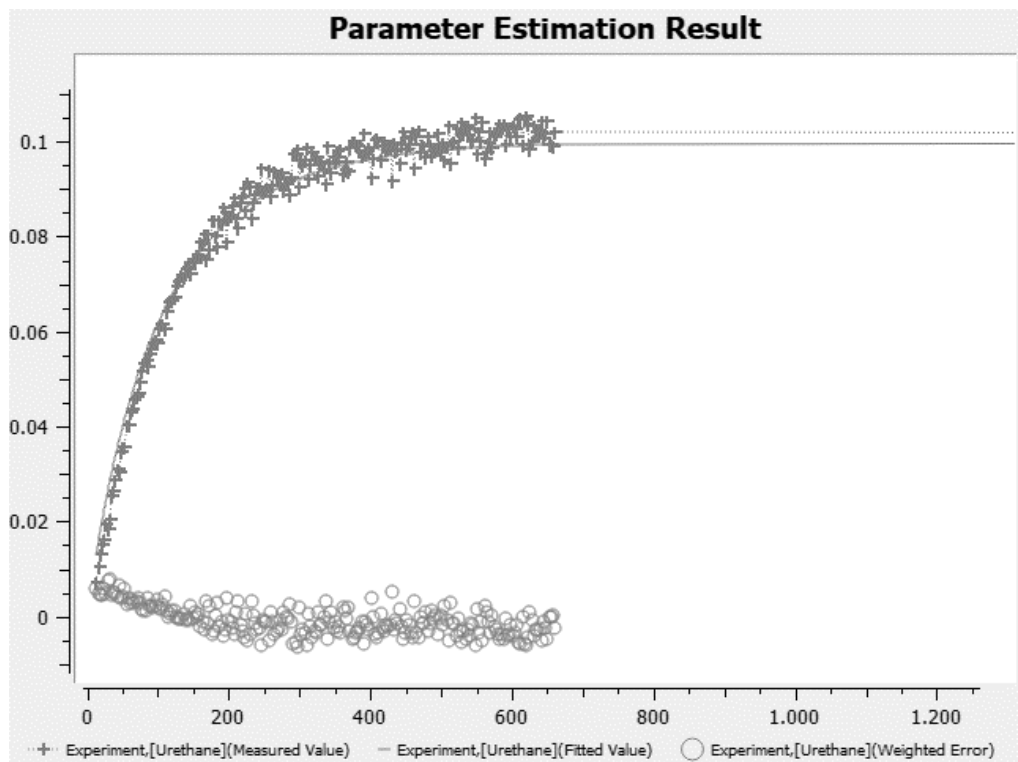


Figure S40. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_36. Vertical axis gives the concentration of urethane **16** in mol L⁻¹, horizontal axis gives the time from 0 min to 1200 min.

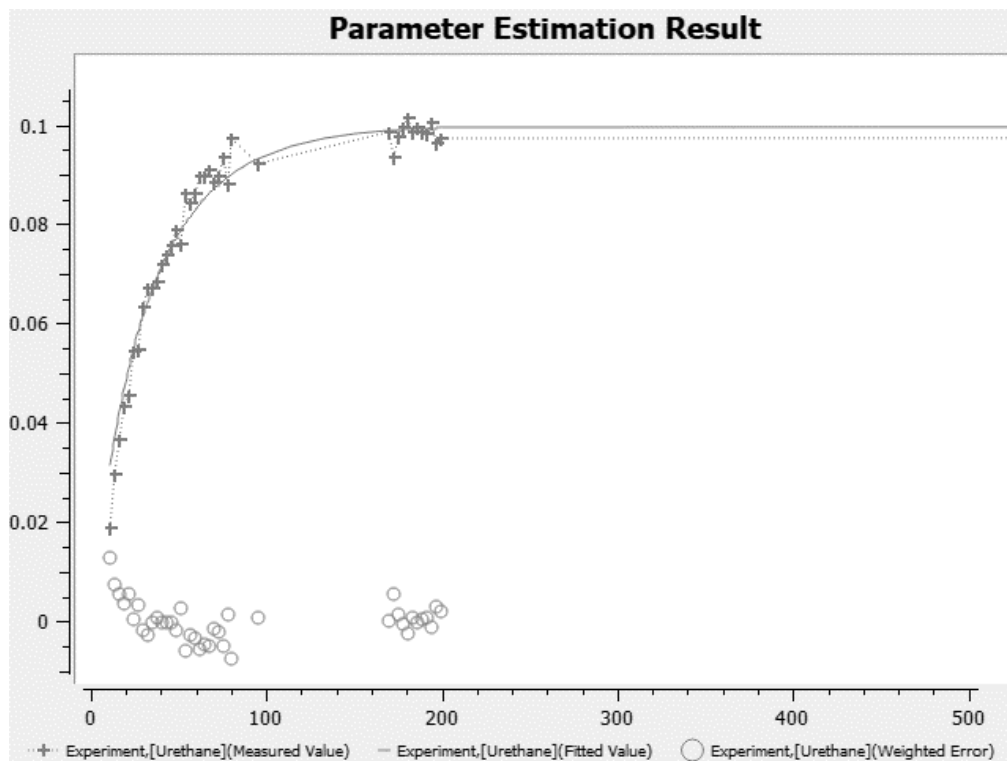


Figure S41. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_37. Vertical axis gives the concentration of urethane **16** in mol L⁻¹, horizontal axis gives the time from 0 min to 500 min.

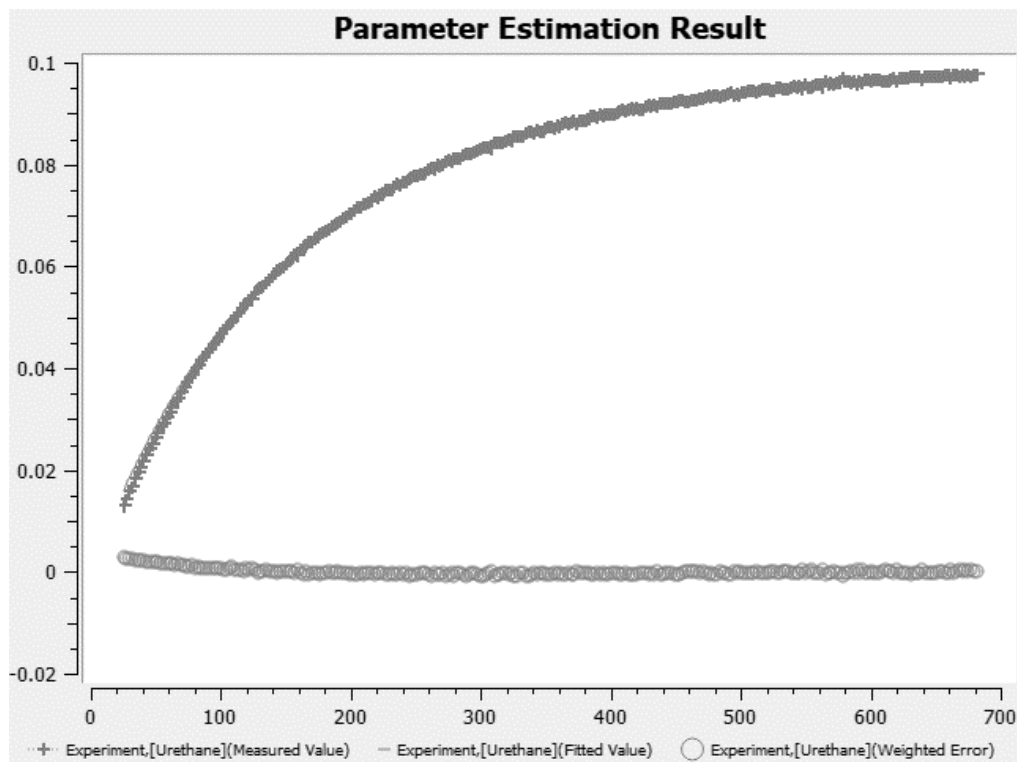


Figure S42. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_38. Vertical axis gives the concentration of urethane **16** in mol L⁻¹, horizontal axis gives the time from 0 min to 700 min.

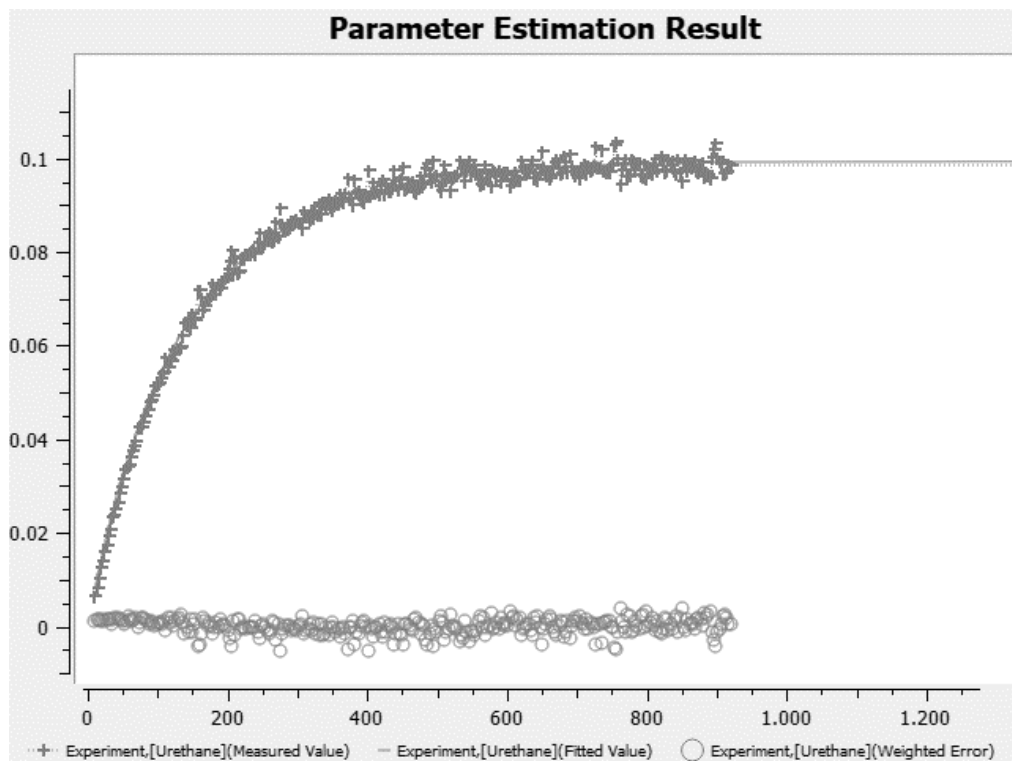


Figure S43. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_39. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 1200 min.

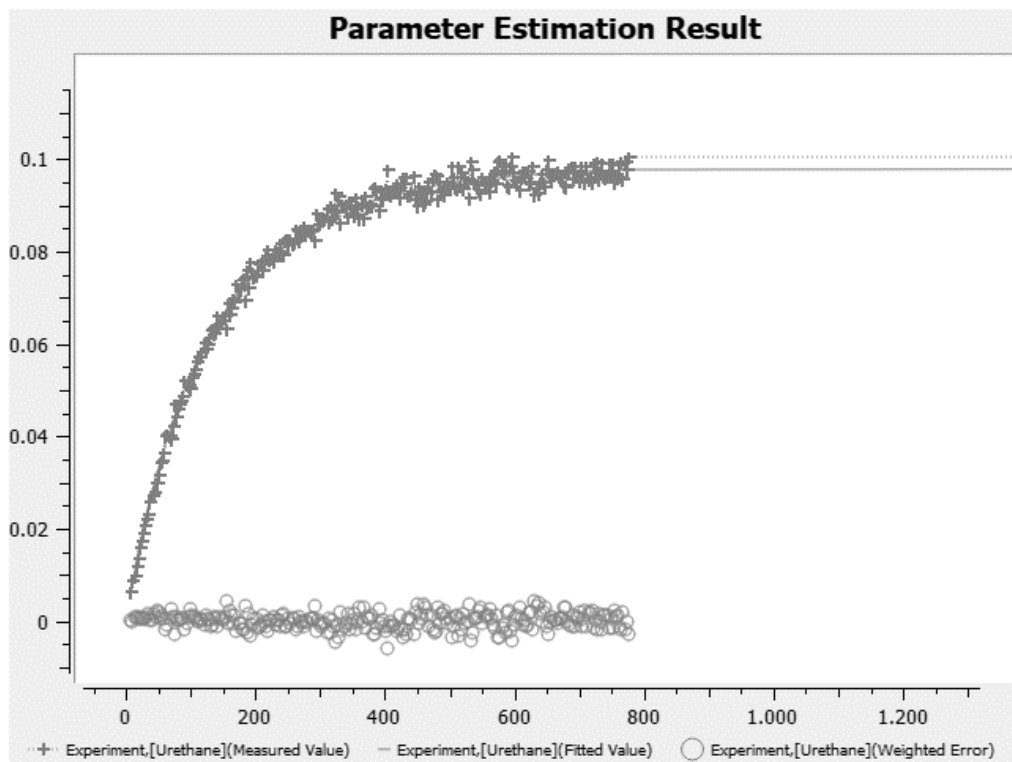


Figure S44. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_40. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 1200 min.

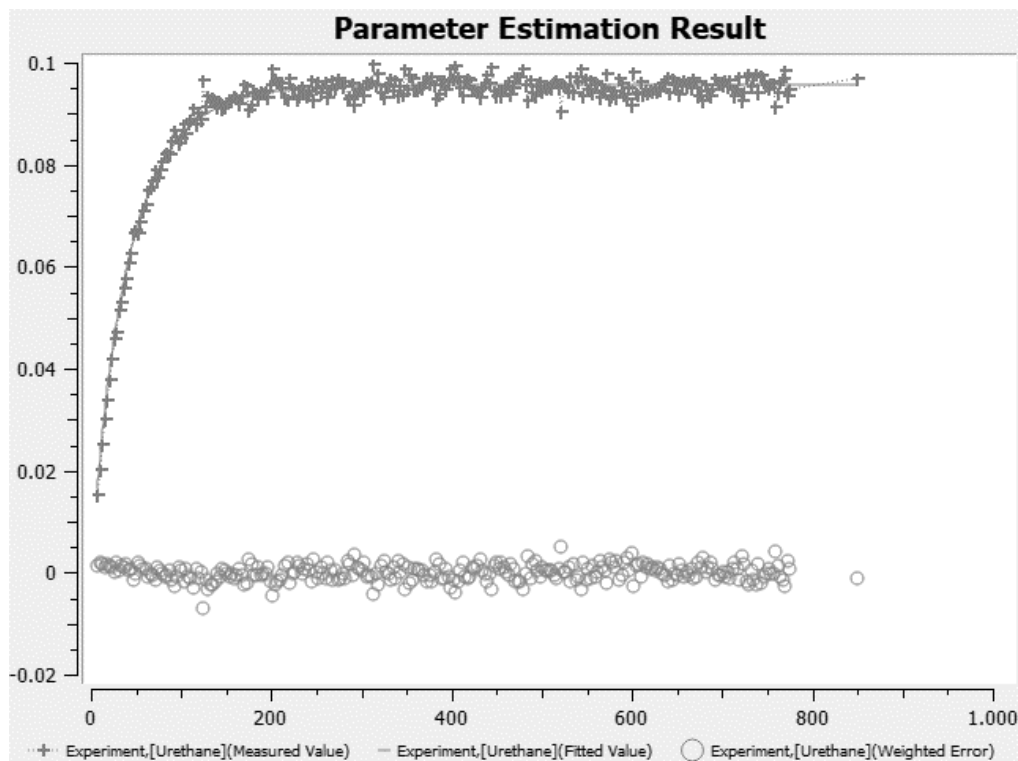


Figure S45. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_41. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 1100 min.

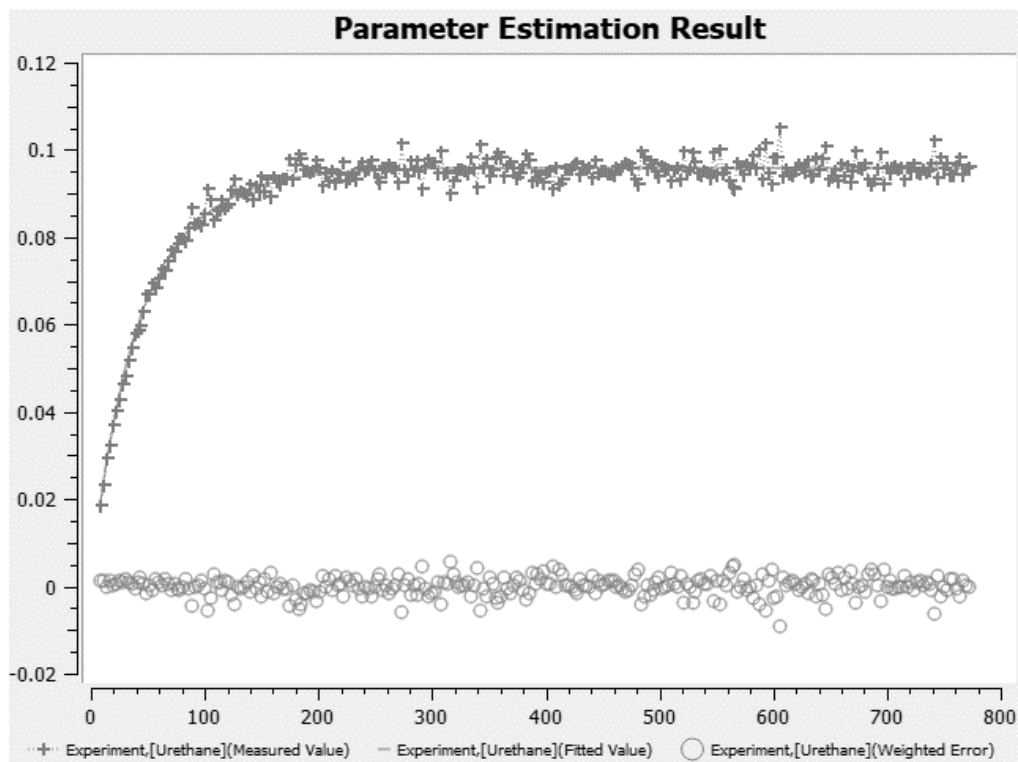


Figure S46. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_42. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 800 min.

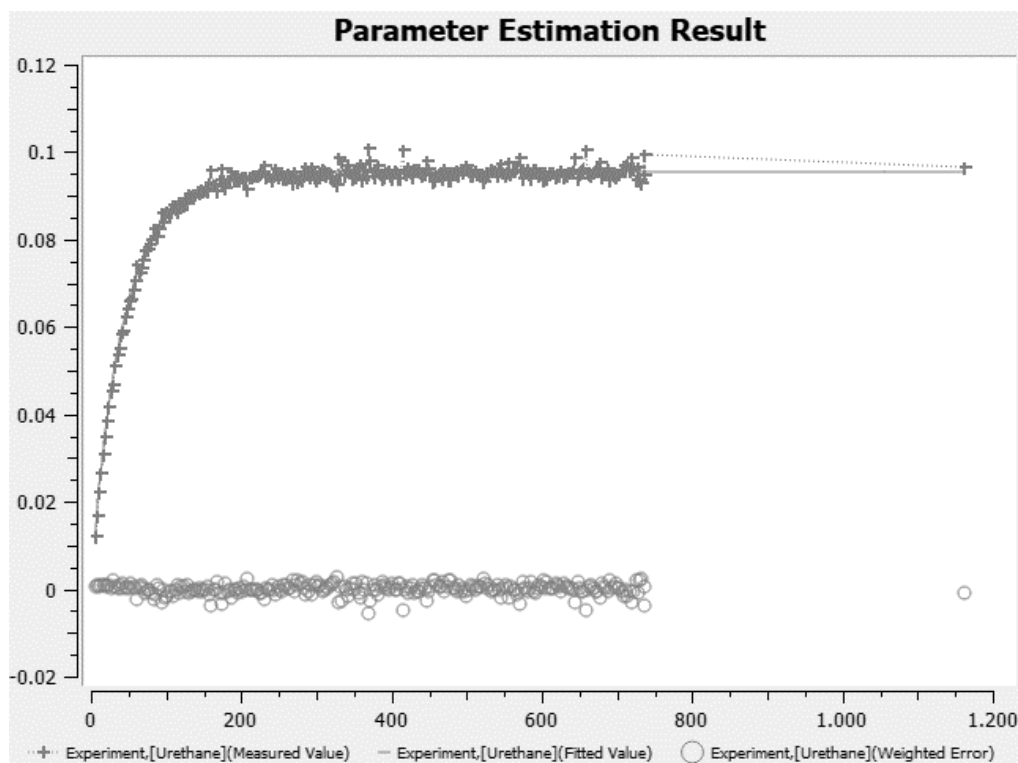


Figure S47. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_43. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 1200 min.

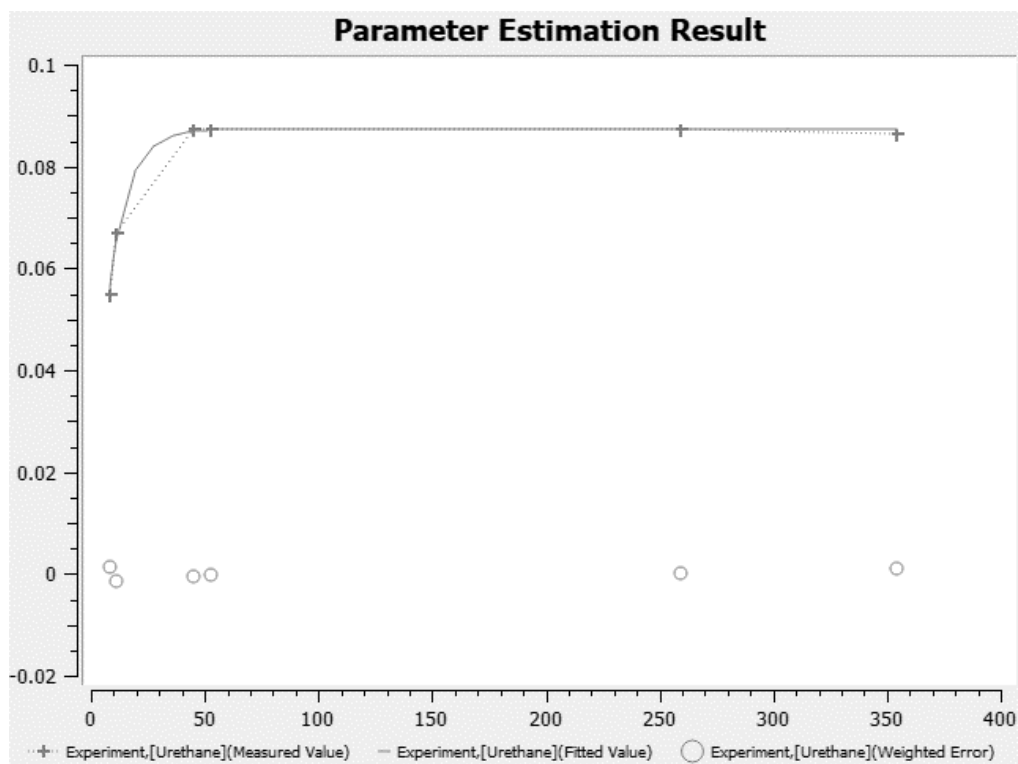


Figure S48. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_44. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 400 min.

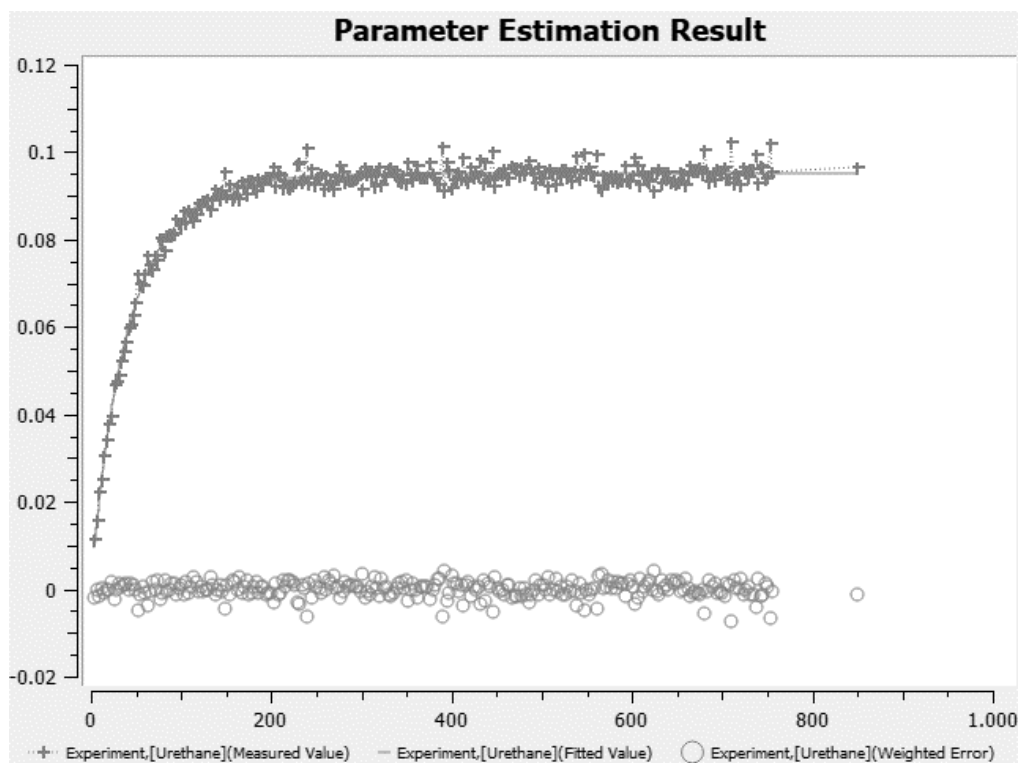


Figure S49. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_45. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 1000 min.

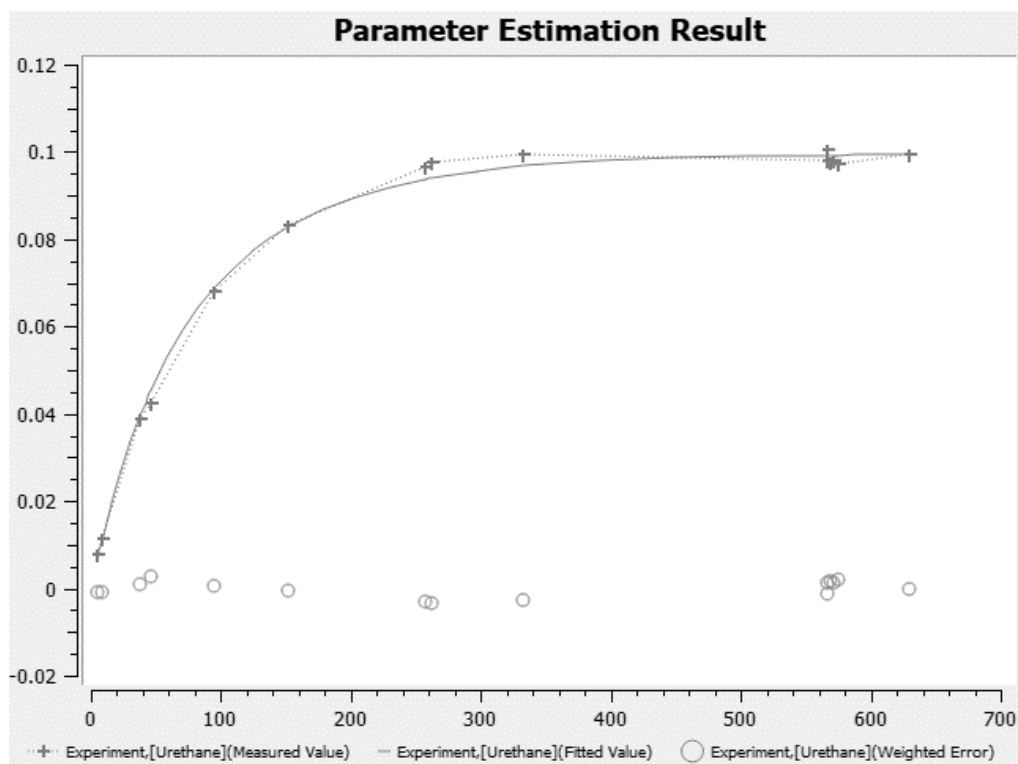


Figure S50. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_46. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 700 min.

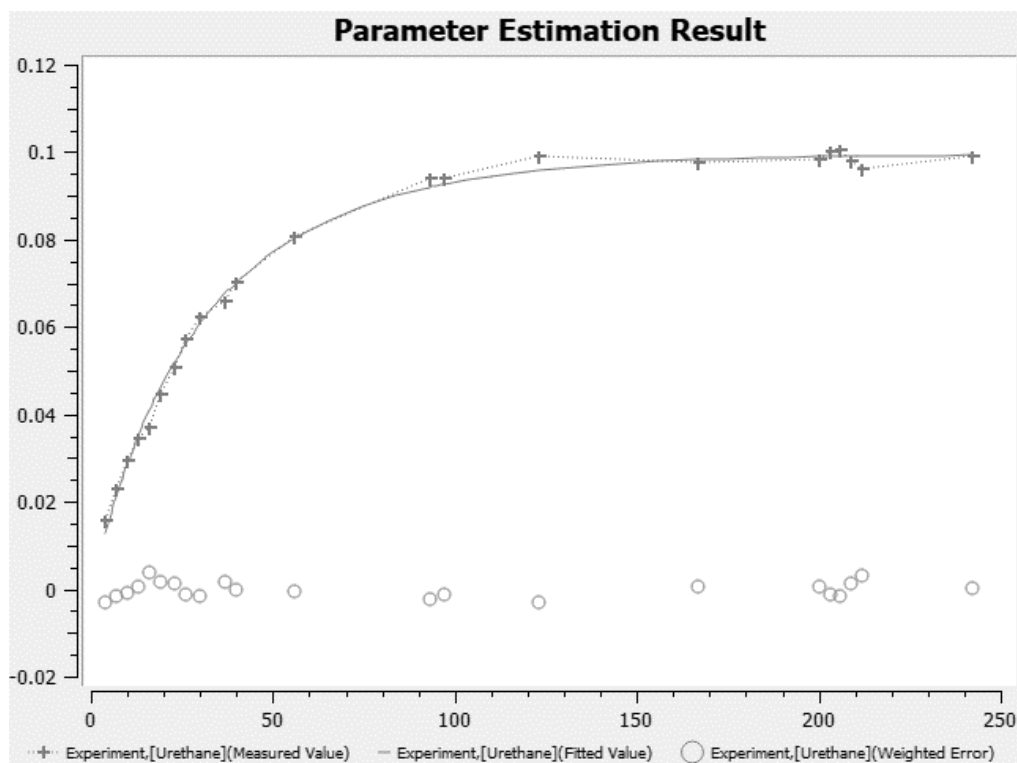


Figure S51. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_47. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 250 min.

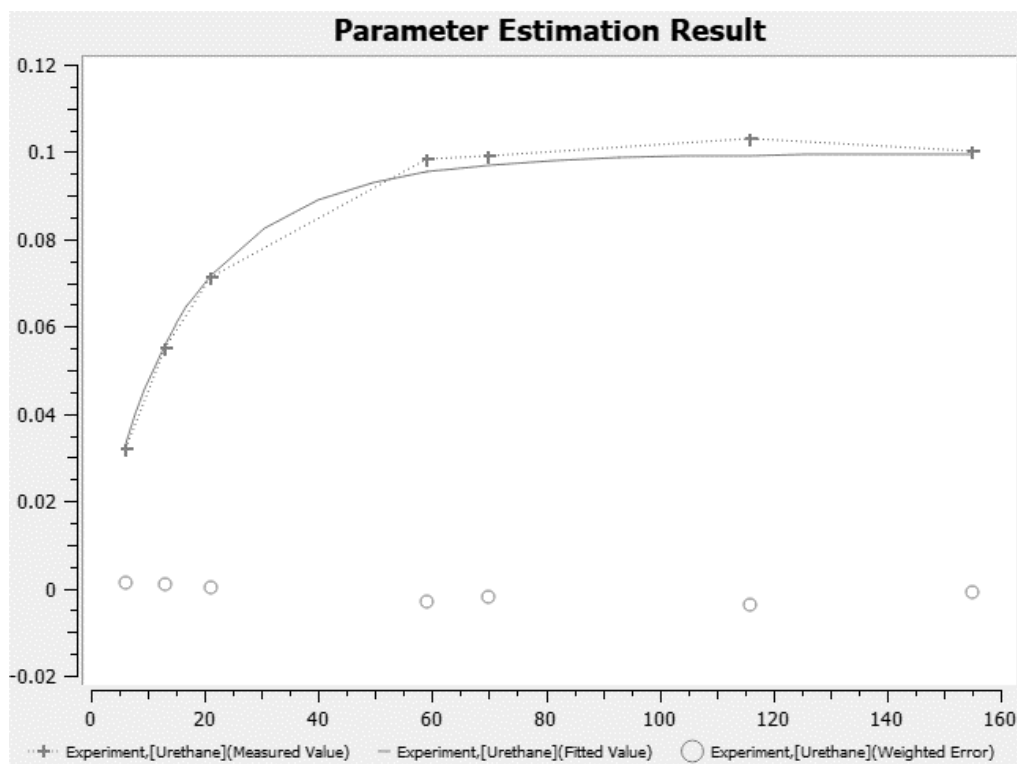


Figure S52. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_48. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 160 min.

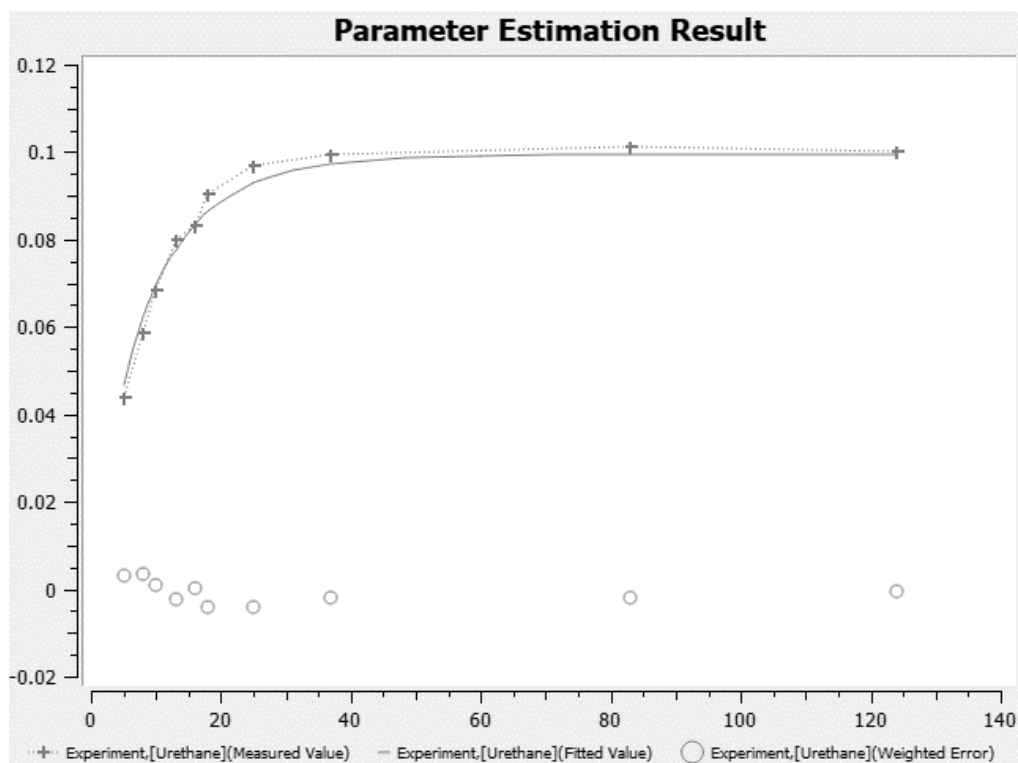


Figure S53. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_49. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 140 min.

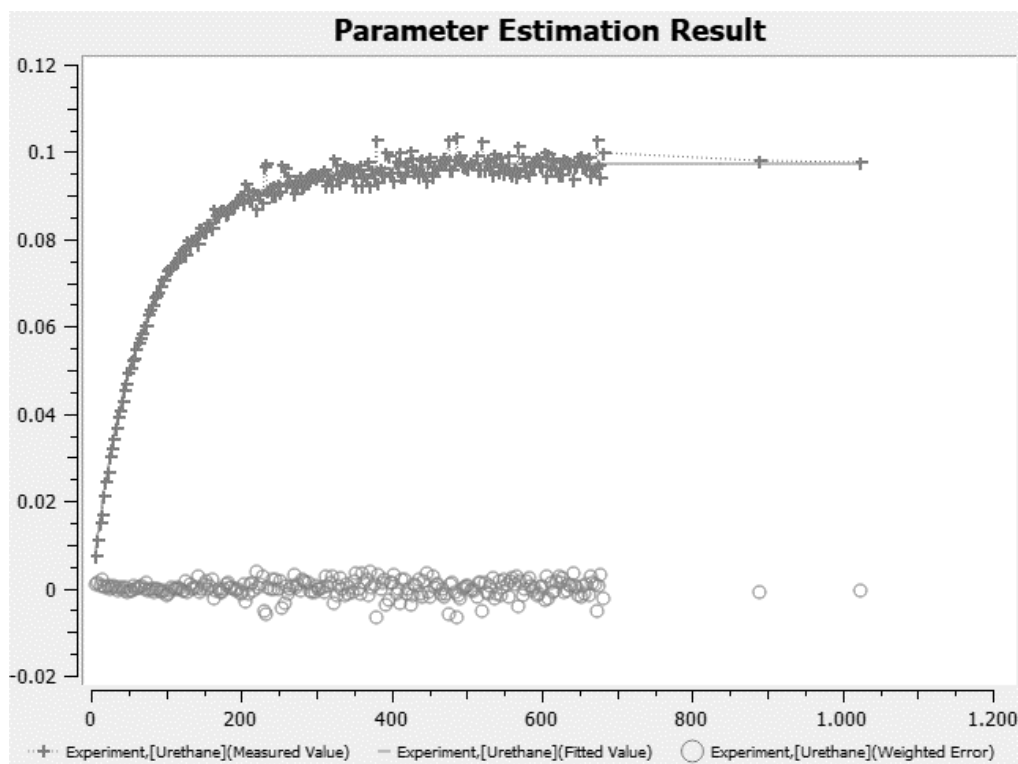


Figure S54. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_50. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 1200 min.

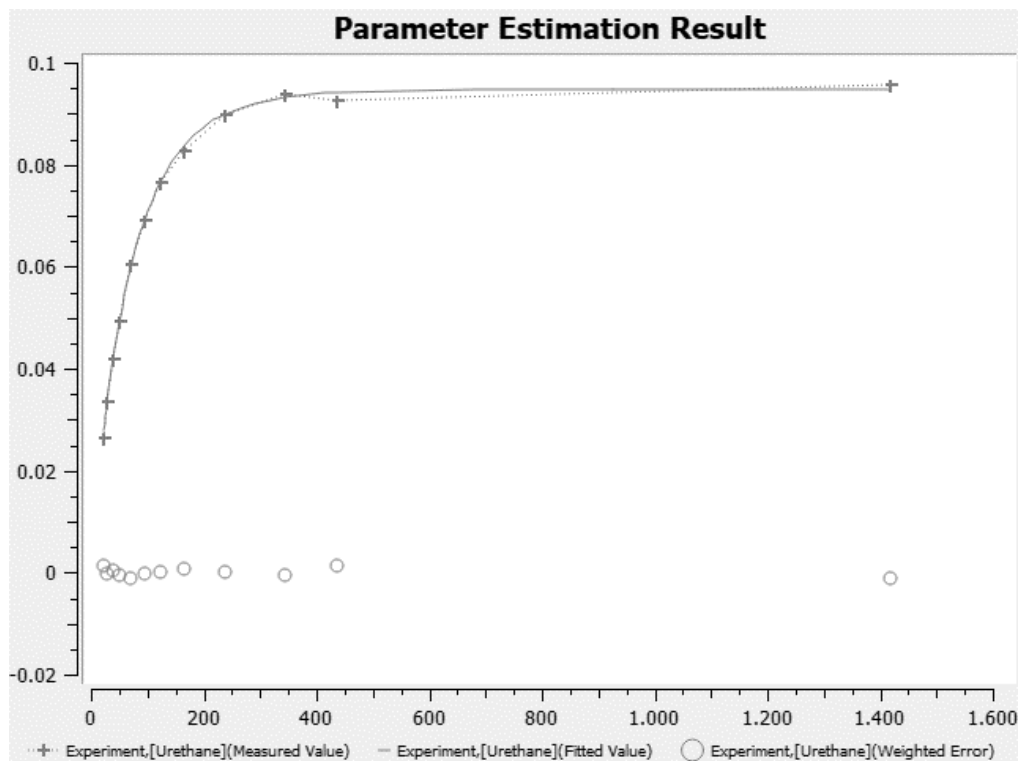


Figure S55. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_51. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 1600 min.

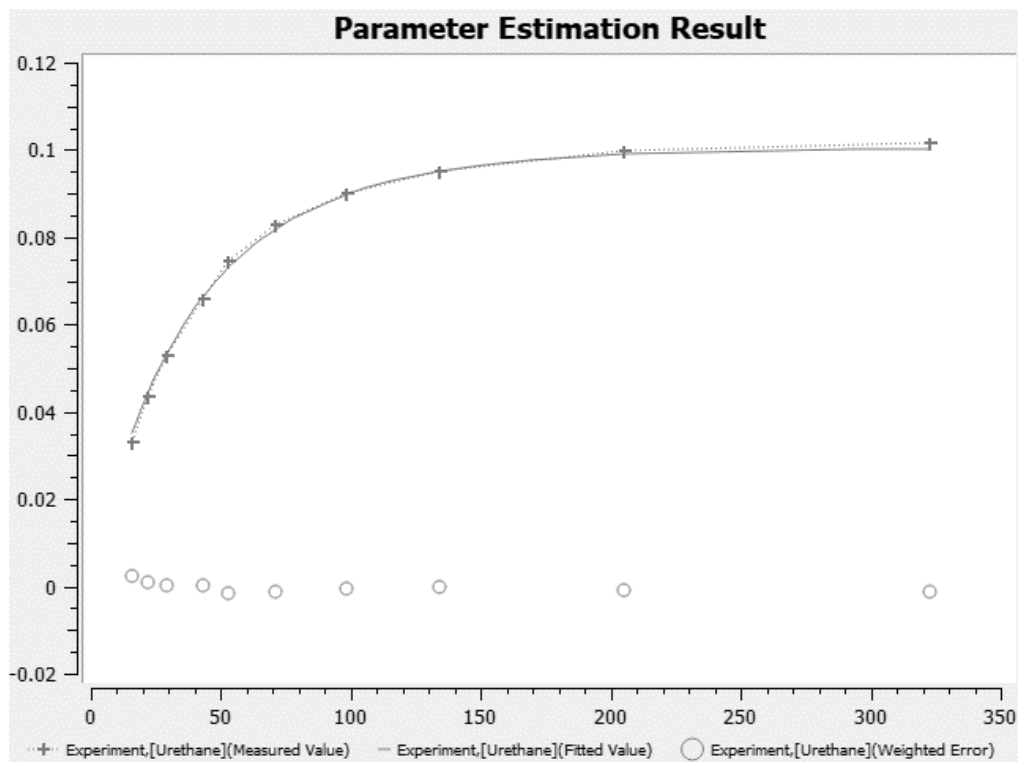


Figure S56. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_52. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 350 min.

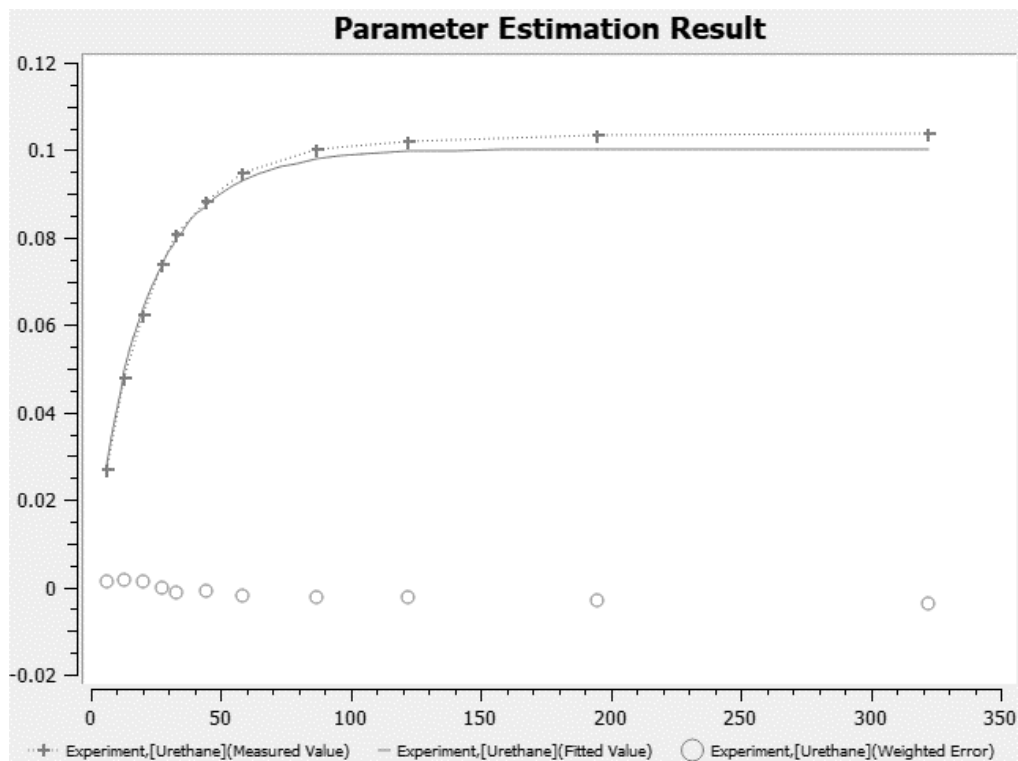


Figure S57. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_53. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 350 min.

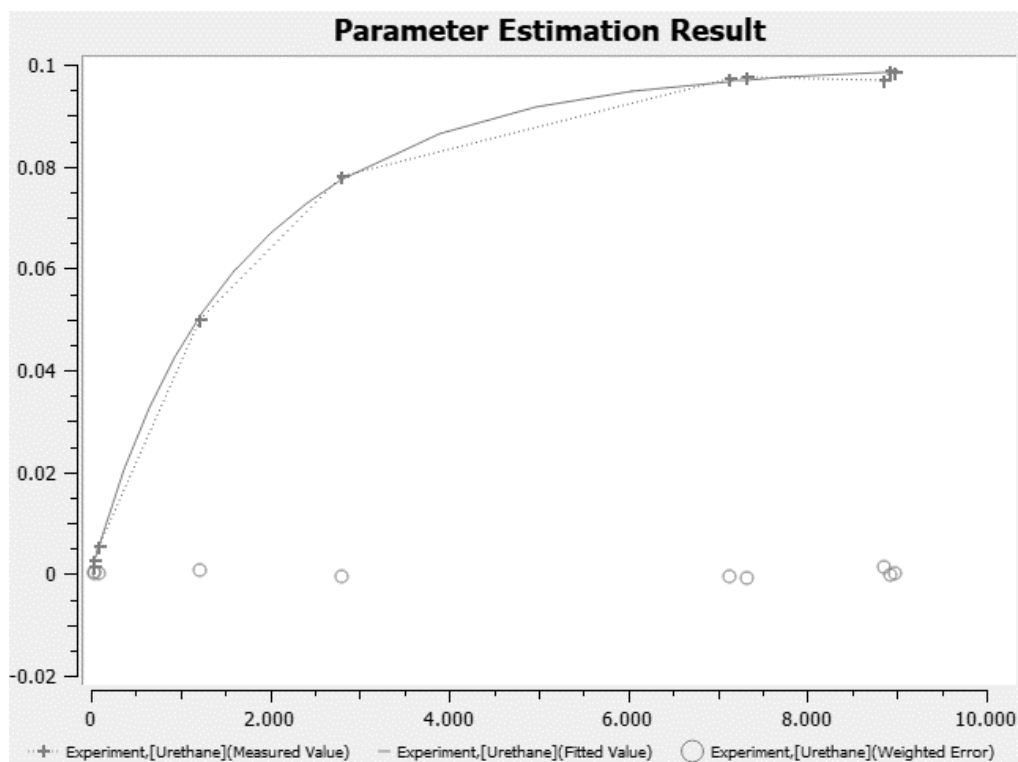


Figure S58. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_54. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 10000 min.

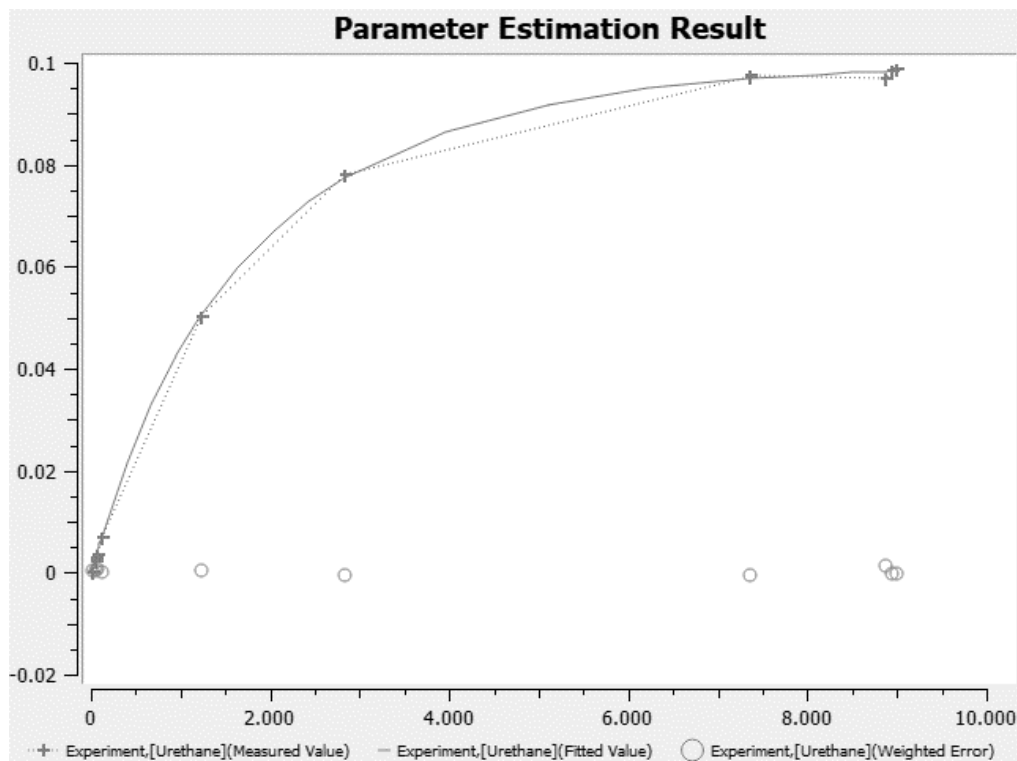


Figure S59. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_55. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 10000 min.

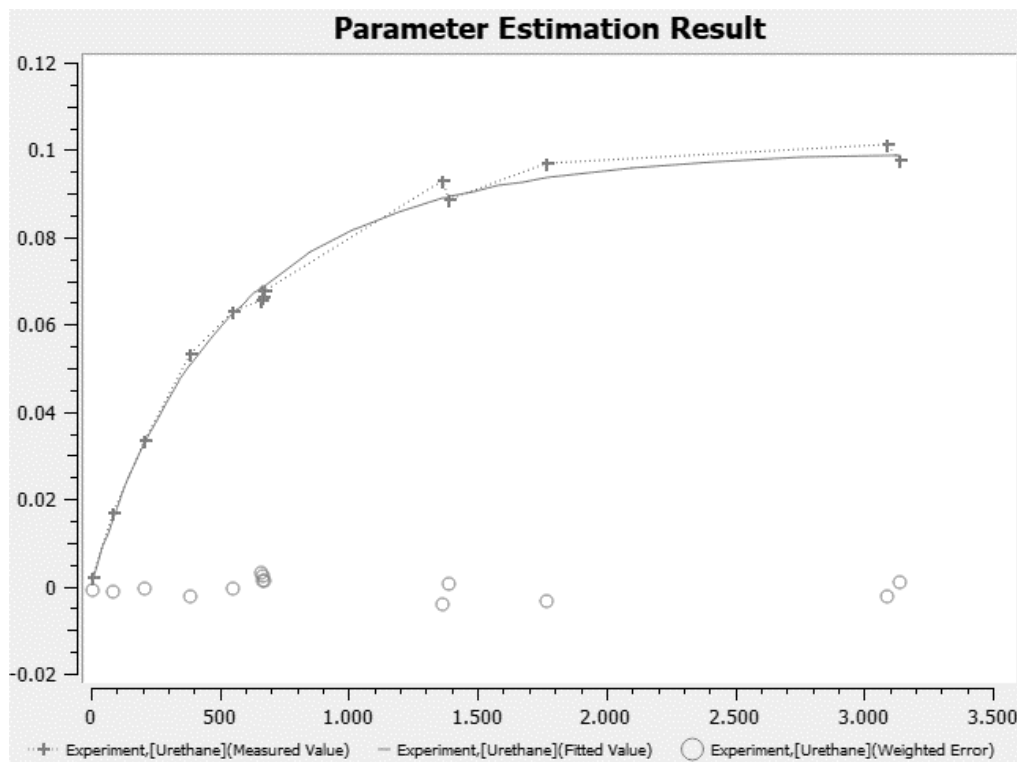


Figure S60. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_56. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 3500 min.

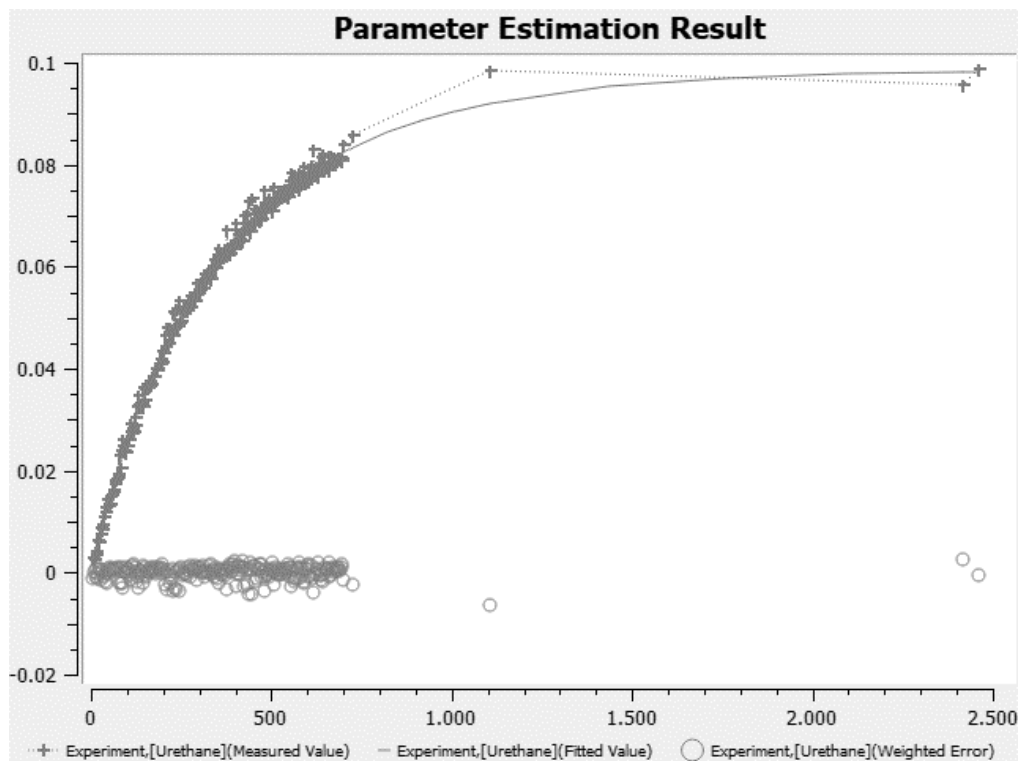


Figure S61. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_57. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 2500 min.

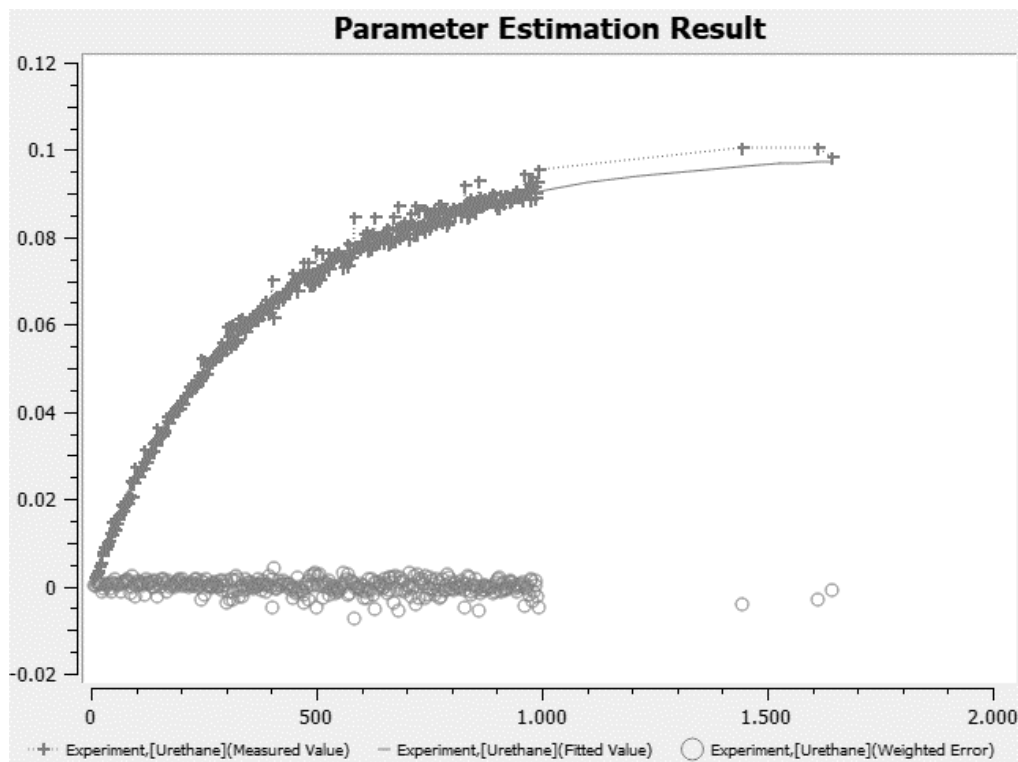


Figure S62. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_58. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 2000 min.

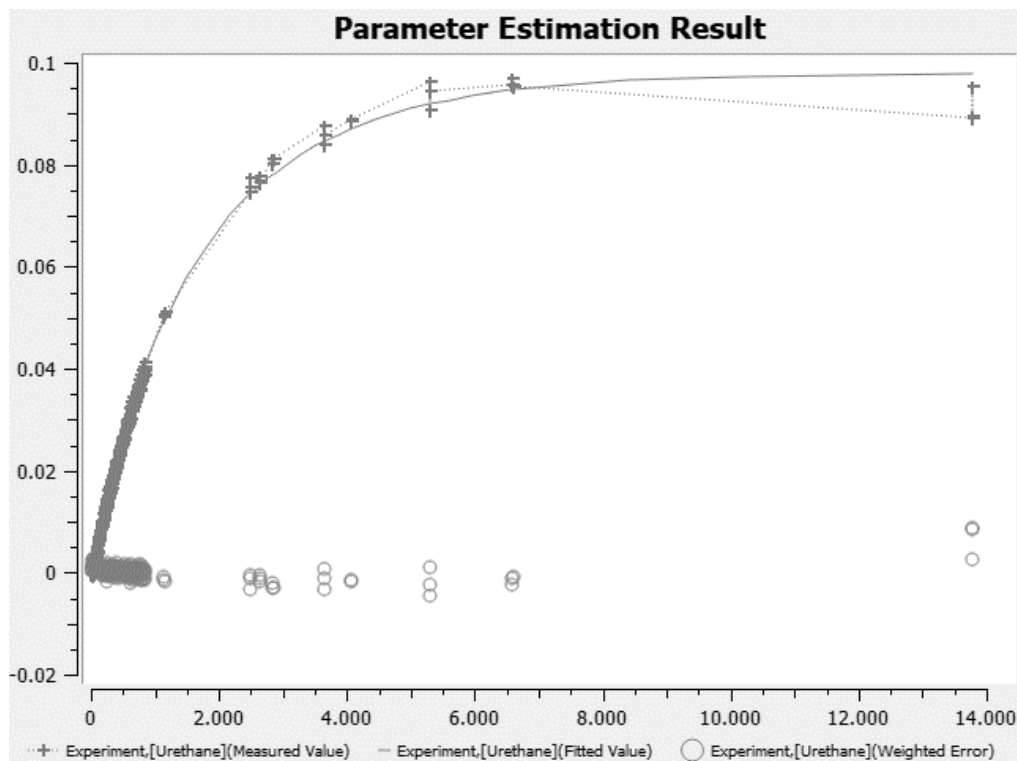


Figure S63. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_59. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 14000 min.

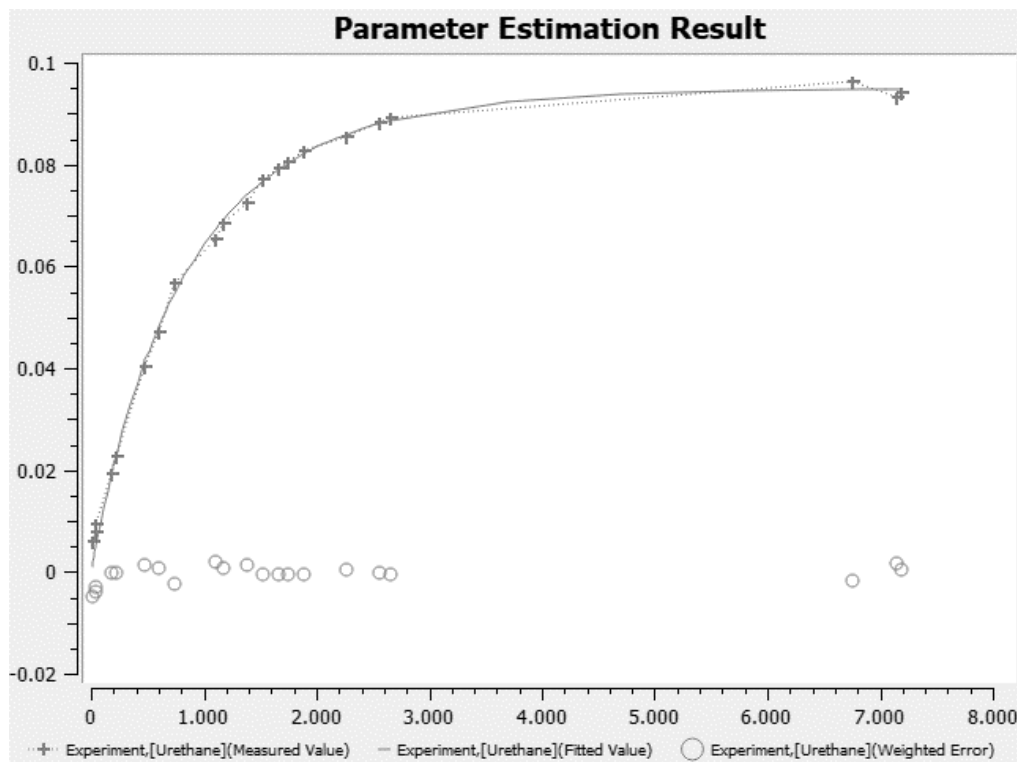


Figure S64. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_60. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 8000 min.

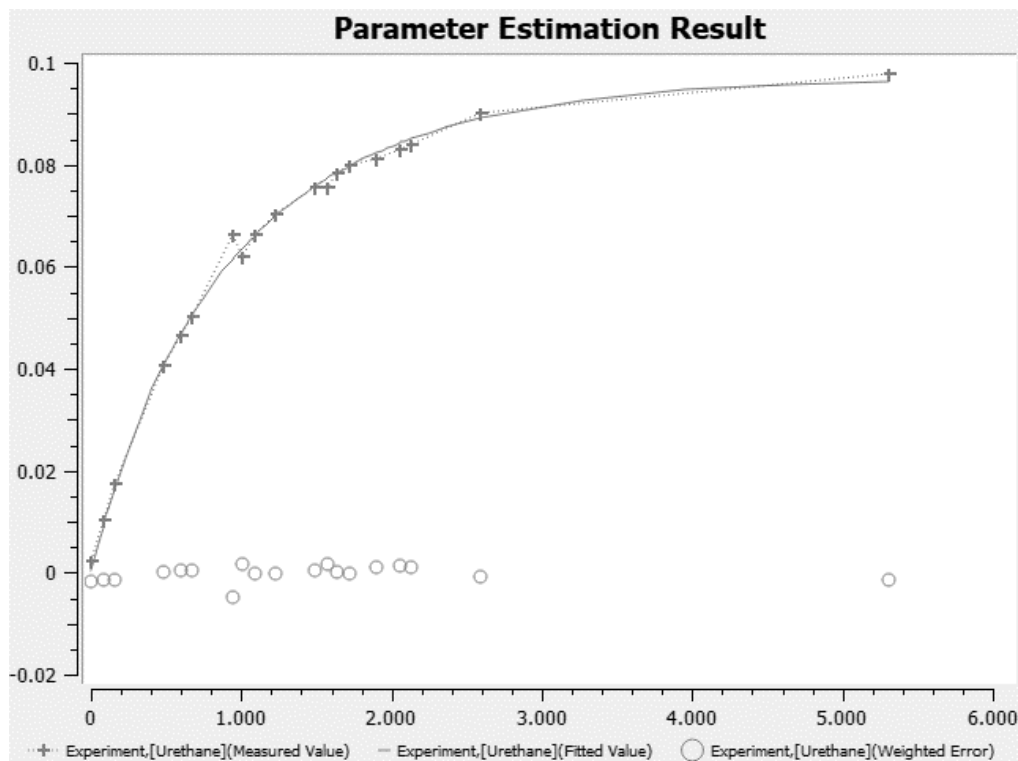


Figure S65. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_61. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 6000 min.

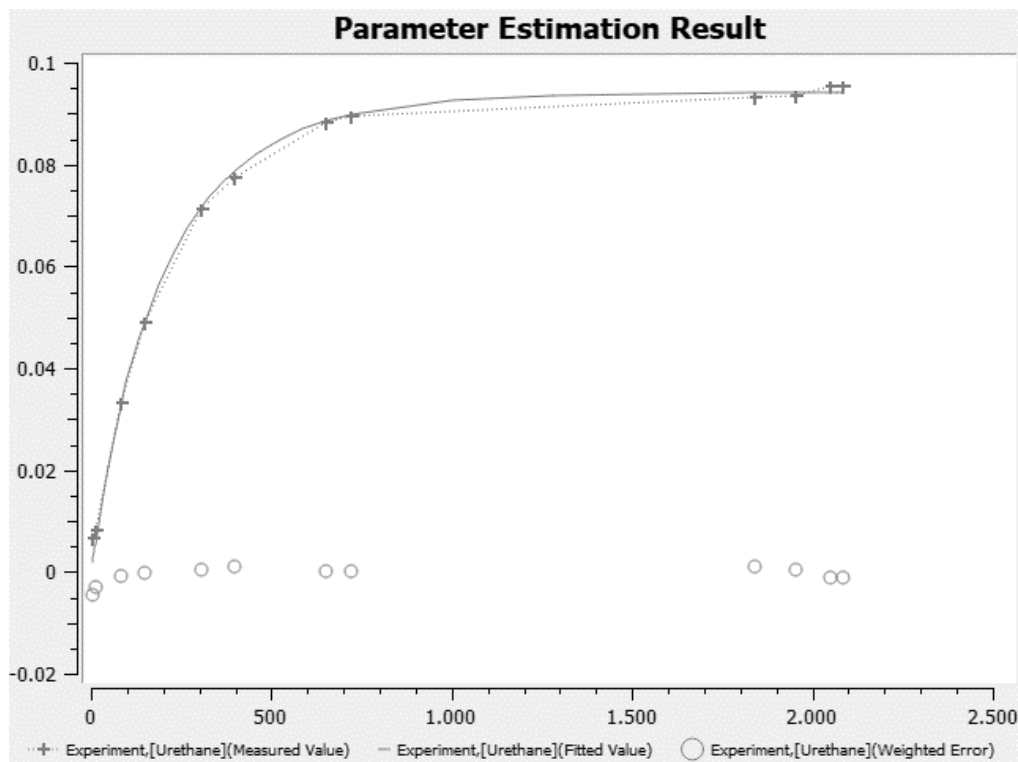


Figure S66. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_62. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 2500 min.

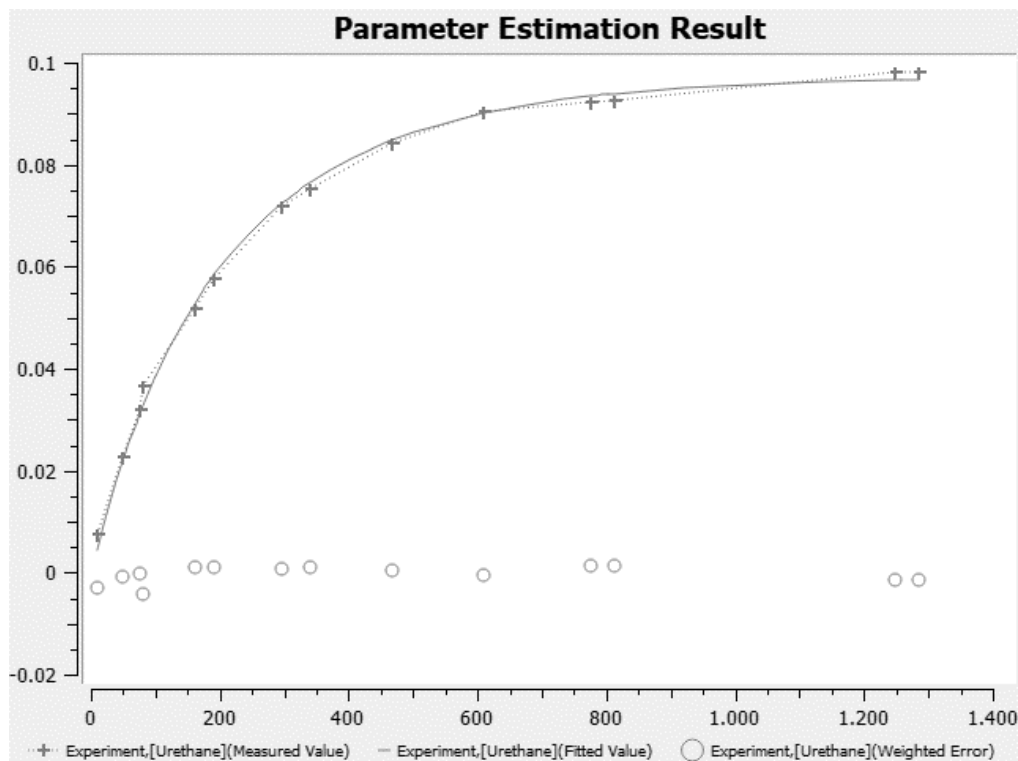


Figure S67. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_63. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 1400 min.

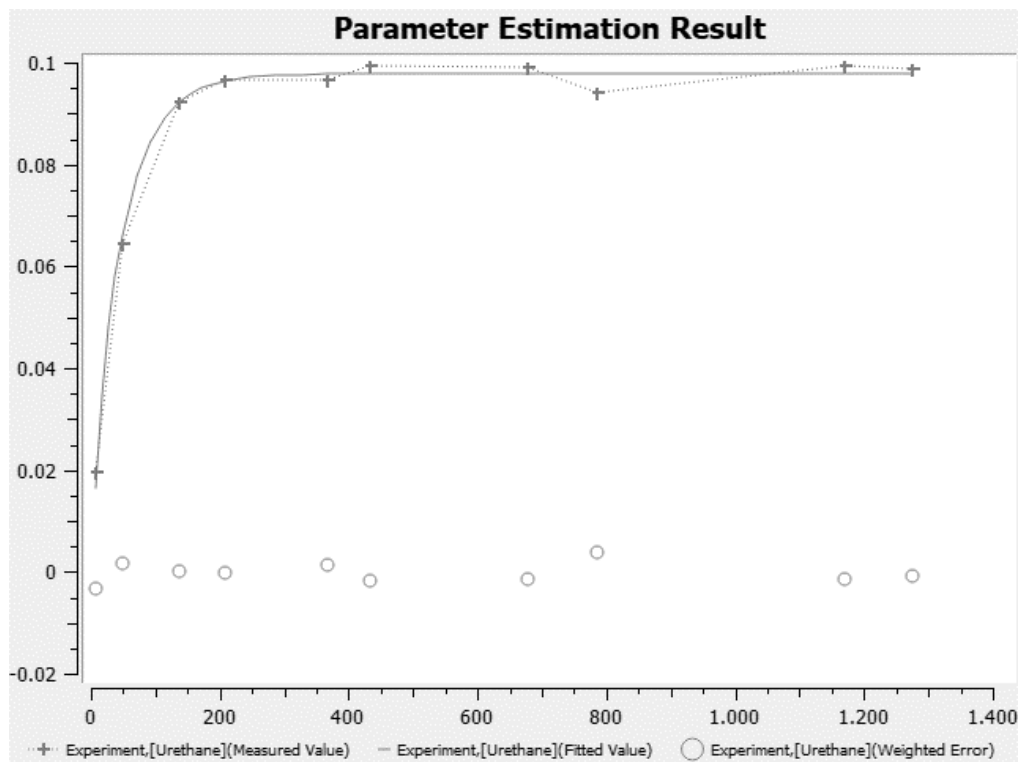


Figure S68. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_64. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 1400 min.

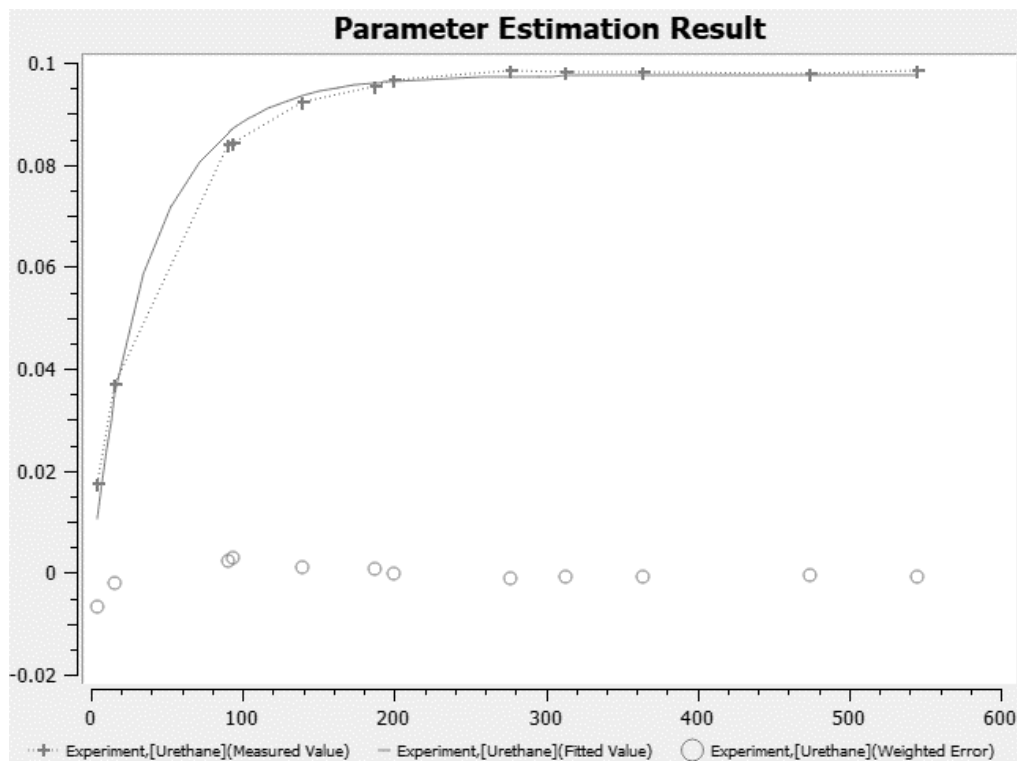


Figure S69. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_65. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 600 min.

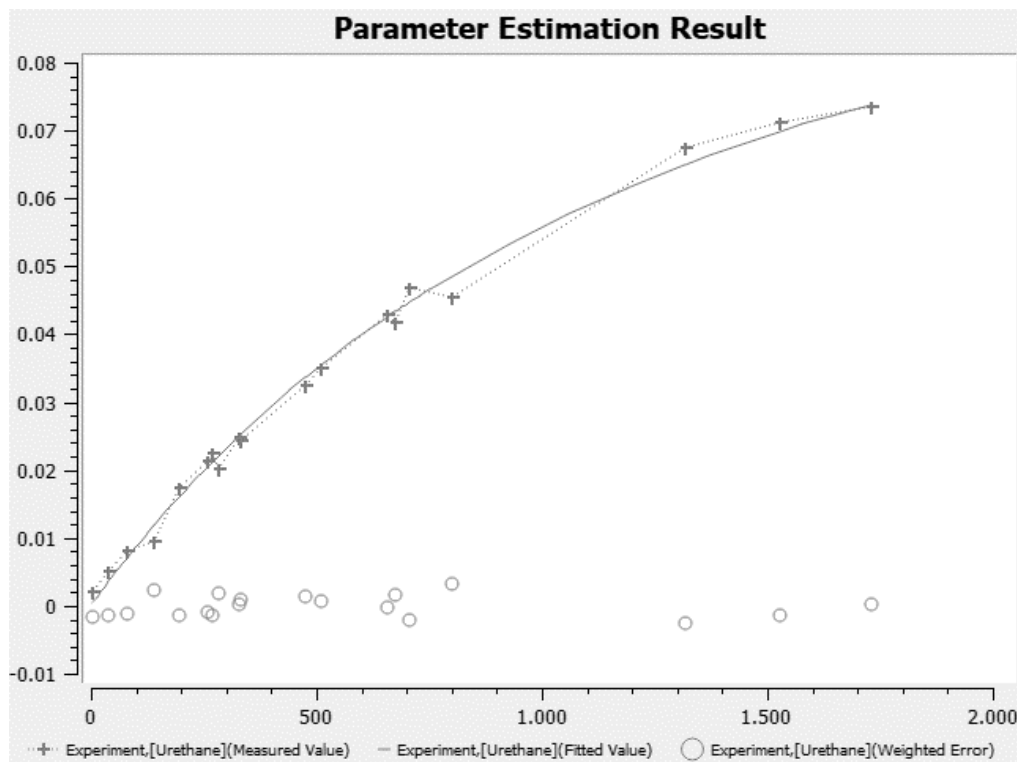


Figure S70. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_66. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 2000 min.

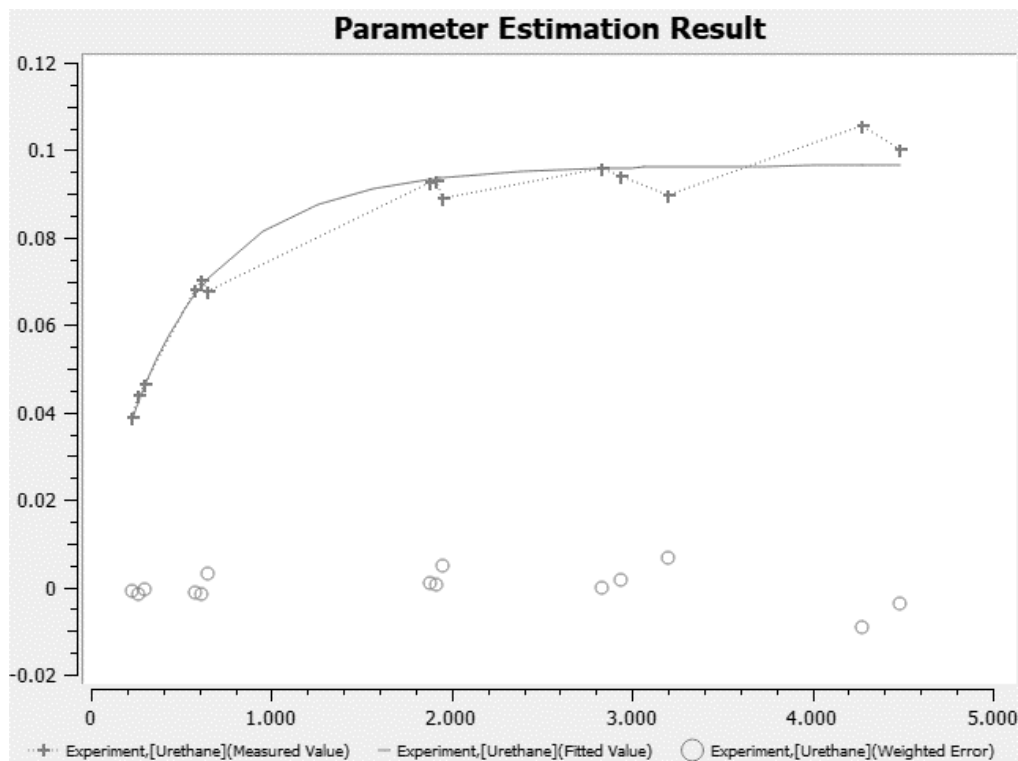


Figure S71. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_67. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 5000 min.

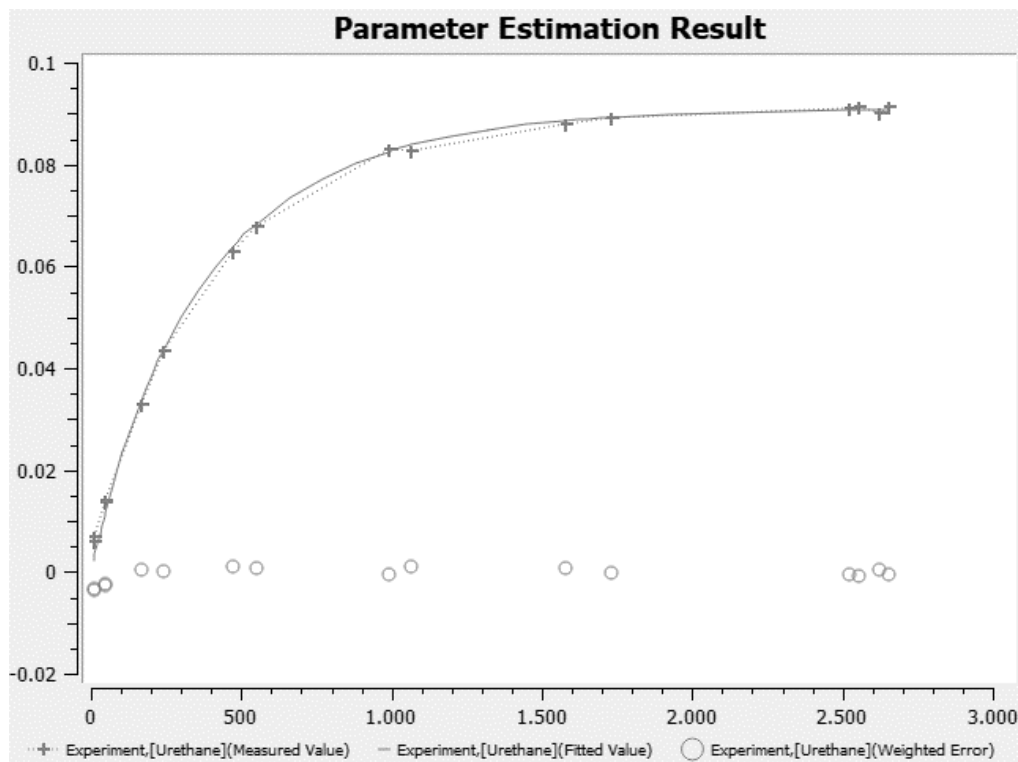


Figure S72. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_68. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 3000 min.

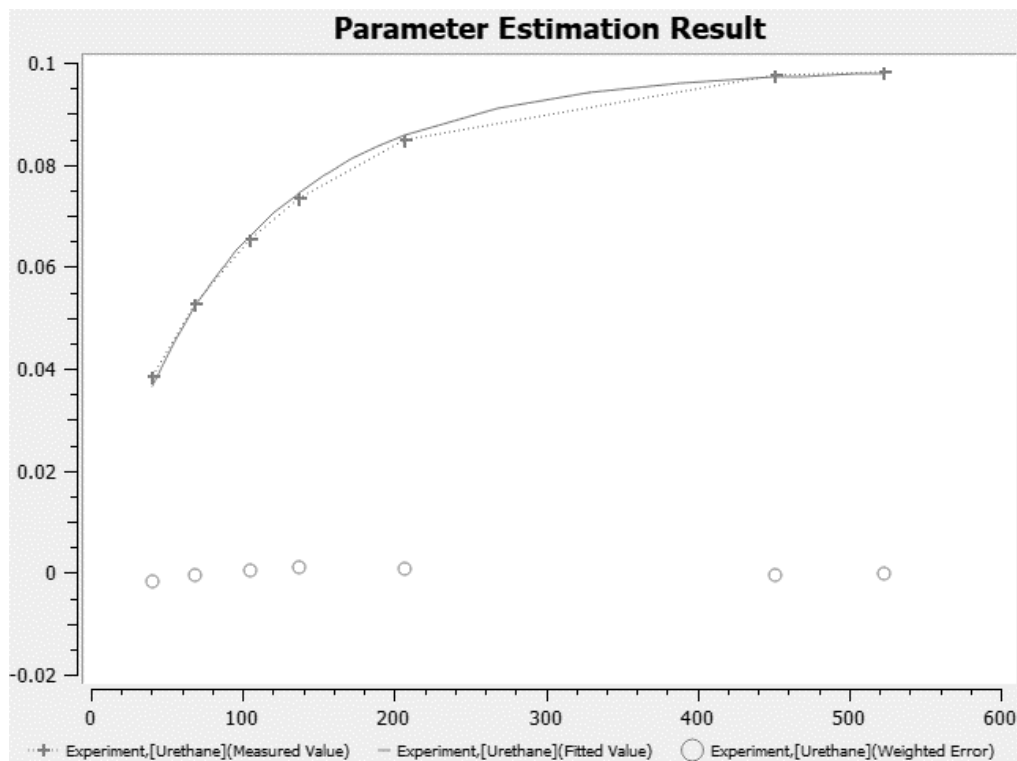


Figure S73. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_69. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 600 min.

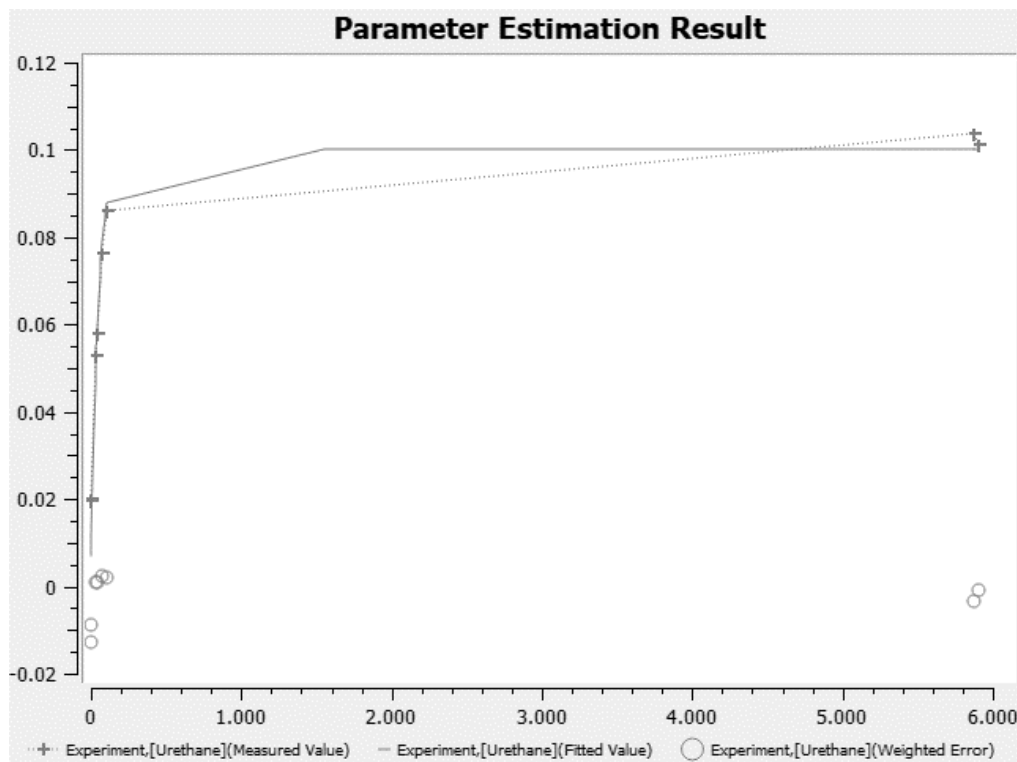


Figure S74. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_70. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 6000 min.

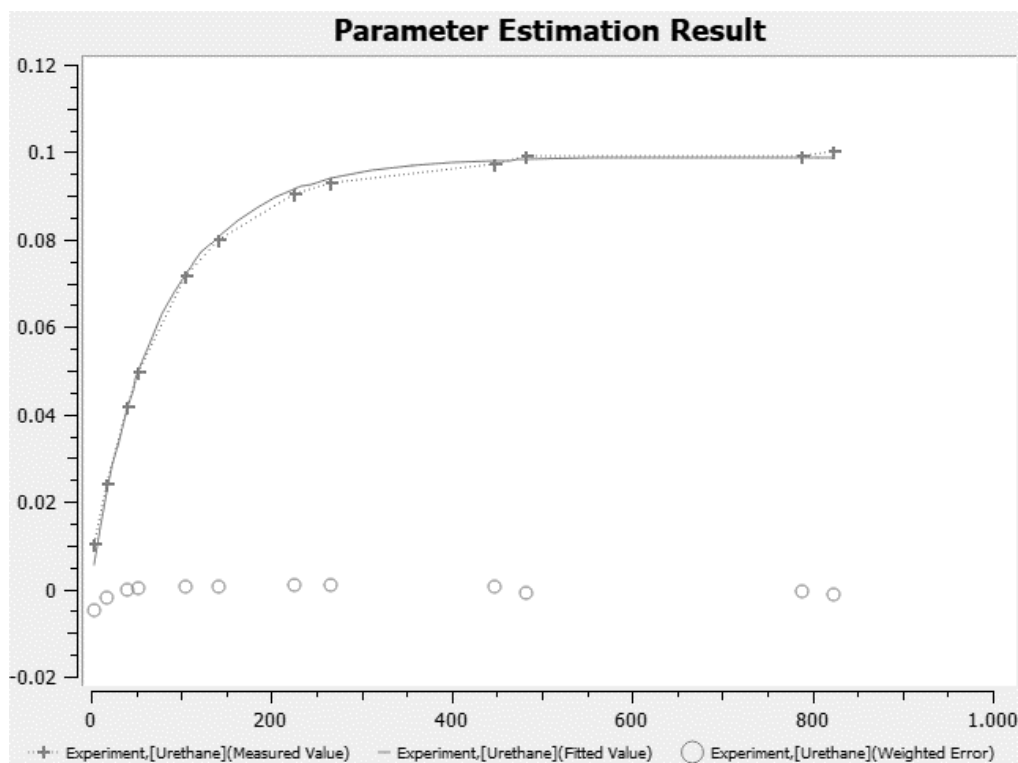


Figure S75. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_71. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 1000 min.

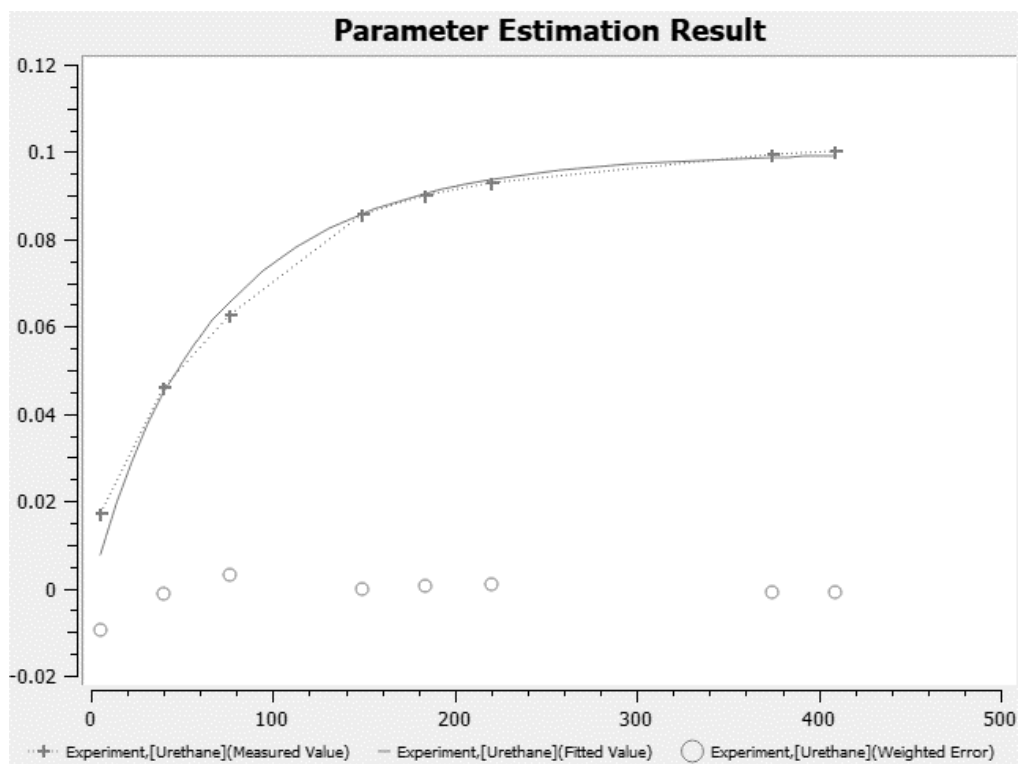


Figure S76. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_72. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 500 min.

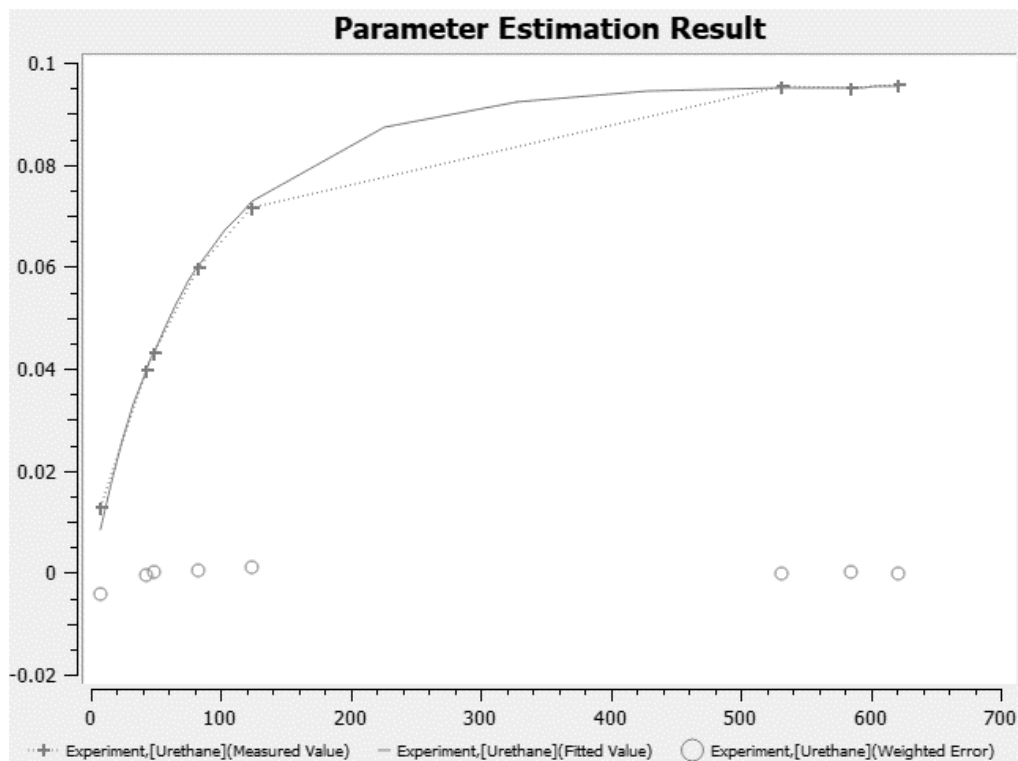


Figure S77. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_73. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 700 min.

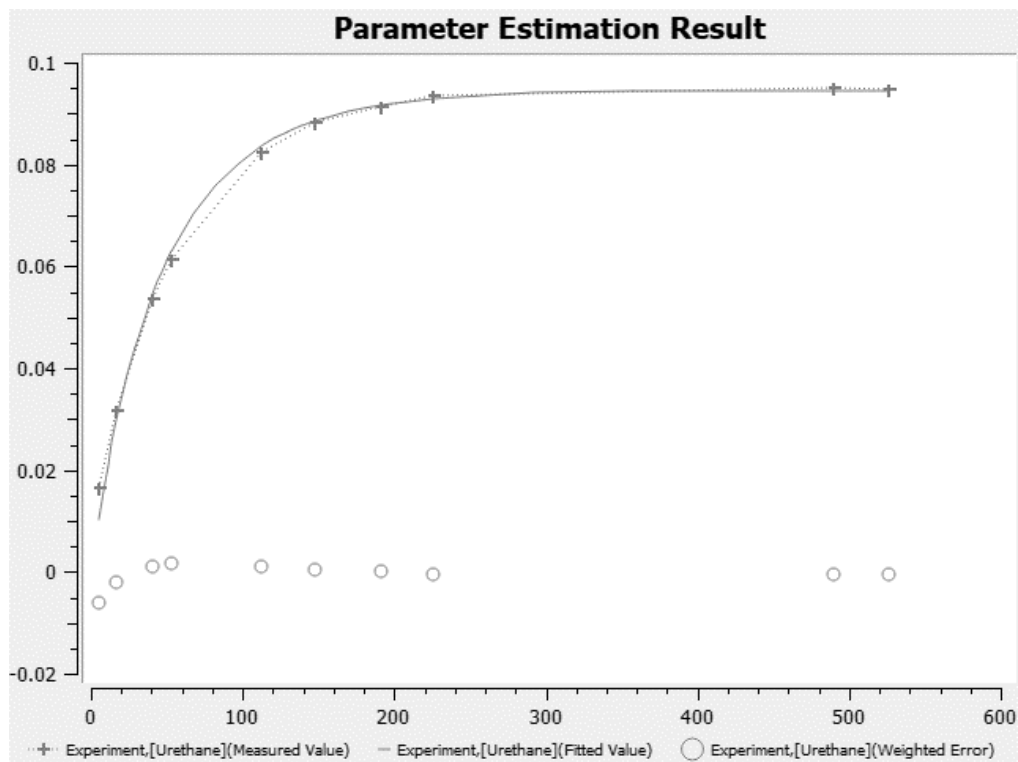


Figure S78. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_74. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 600 min.

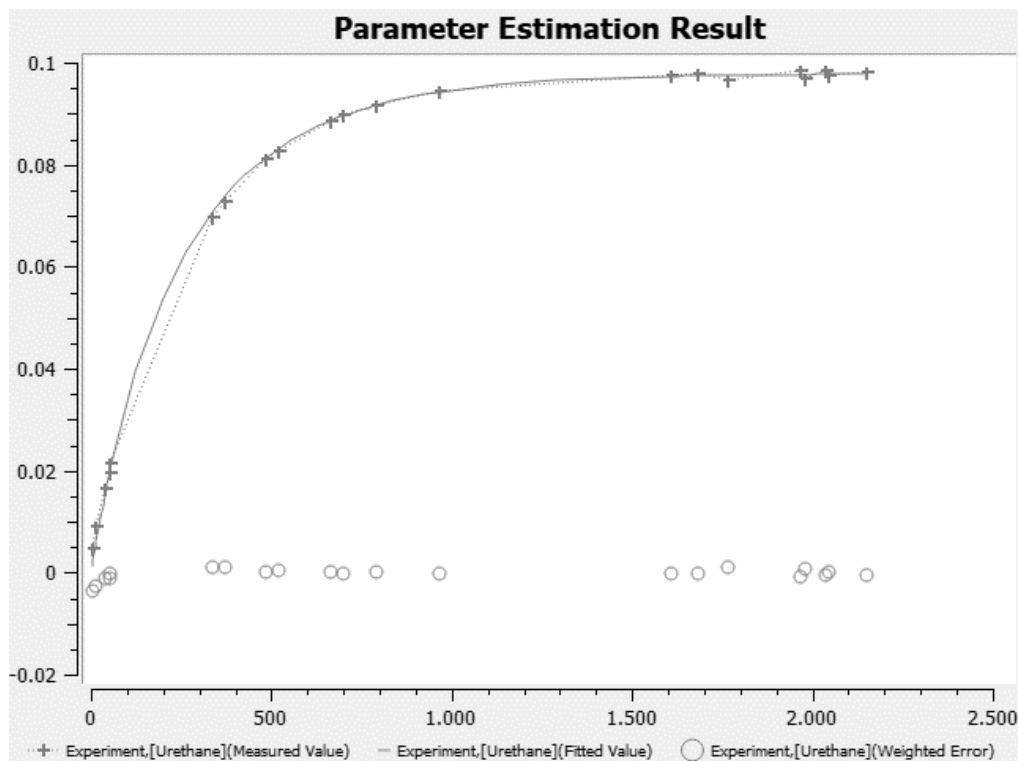


Figure S79. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_75. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 2500 min.

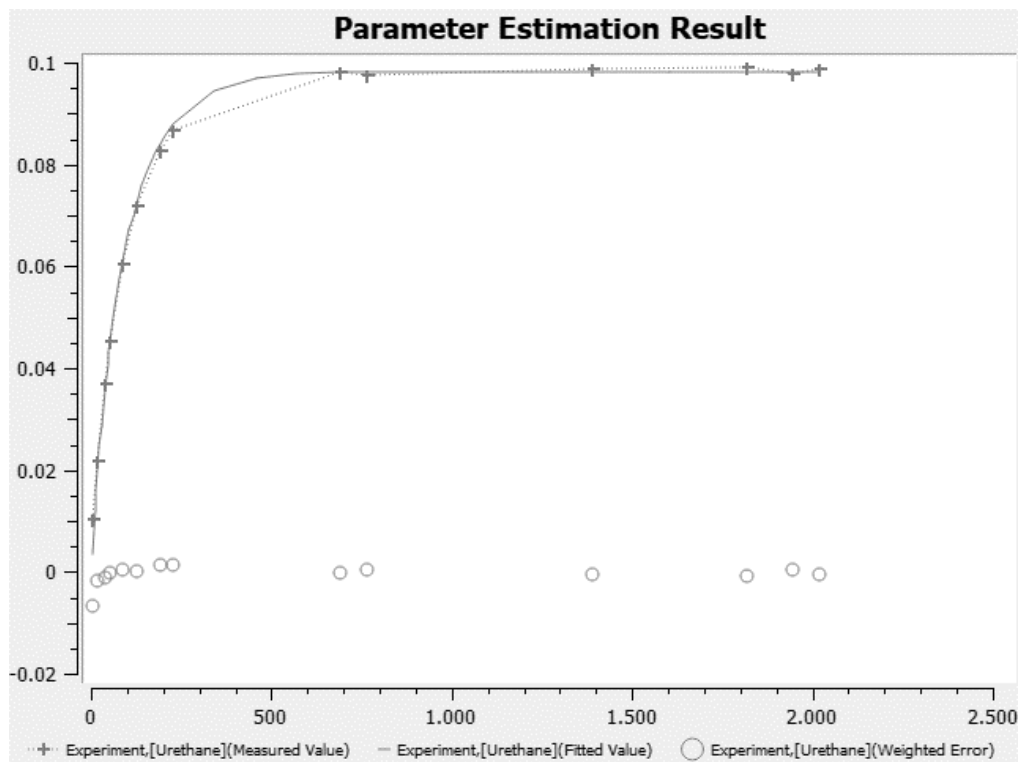


Figure S80. Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_76. Vertical axis gives the concentration of urethane 16 in mol L⁻¹, horizontal axis gives the time from 0 min to 2500 min.

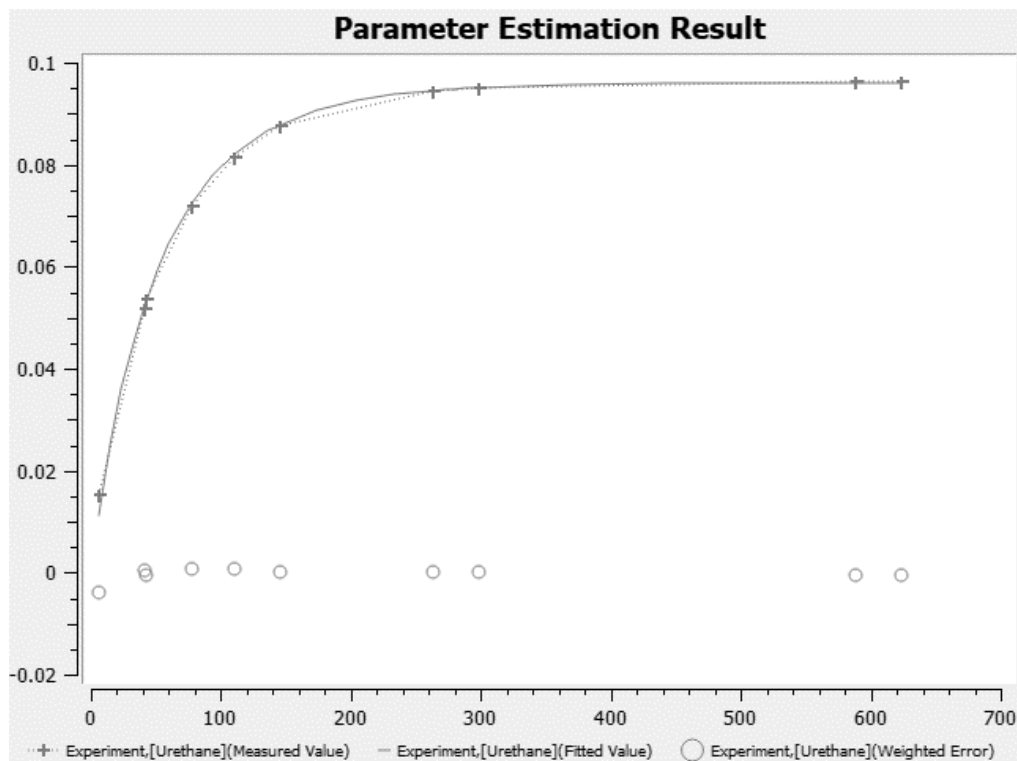
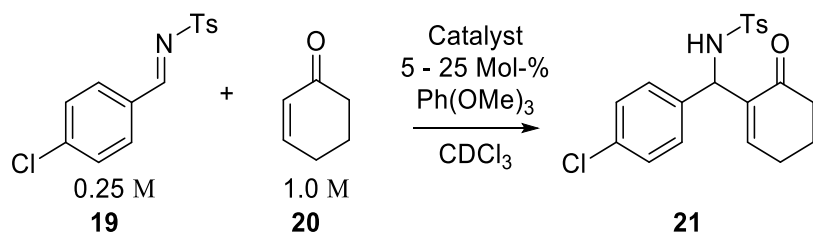


Figure S81 Fitted turnover curve obtained as graphical output by COPASI for experiment urethane_77. Vertical axis gives the concentration of urethane **16** in mol L⁻¹, horizontal axis gives the time from 0 min to 700 min.

Benchmark Reaction 2 - Aza-Morita-Baylis-Hillman Reaction

To show the efficiency of the investigated anionic pyridine catalysts, we decided to further test the ones that had performed best in the urethane synthesis. Therefore, we selected an electrophile that is considered very hard to activate, cyclohex-2-en-1-one **20** and decided to observe the corresponding *aza*-Morita-Baylis-Hillman (MBH) reaction with an activated imine. As reported by Shi (classical N- and P-bases), Ye (N-heterocyclic carbenes) and Zipse (bi- and tricyclic aminopyridines), this reaction is sluggish at best, taking at least 24 h to finish and shows no conversion at all without addition of an appropriate catalyst.^[4] Since the CDCl₃ solvent signal is not clearly distinguishable in most of our reactions that are containing aromatic moieties, we chose to include 1,3,5-trimethoxybenzene as inert internal standard for the benchmark reaction shown in **Scheme S3**. Benchmark reactions were done as described in the main part of this publication.



Scheme S3. *aza*-MBH reaction of tosyl imine **19** and cyclohex-2-en-1-one **20**.

Data Processing

Since no other products than amine **21** were identified, we decided to measure conversion solely by the integrals of starting material **19** and product **21**.

Measured spectra were imported into MestReNova (Version 12.0.3) and superimposed. The following was done for the superimposed spectra in this order:

- Reference set (Ph(OMe)₃ set to 3.70 ppm)
- Automatic phase correction
- Automatic baseline correction (Whittaker Smoother)

Three areas containing the signals highlighted in **Figure S82** were integrated:

- **Integral MBH1:** 9.05 ppm → 8.8 ppm = signal of tosyl imine **19** (CH) at 8.9 ppm
- **Integral MBH2:** 5.2 ppm → 4.95 ppm = signal of tosyl amine **21** at 5.1 ppm (CH)

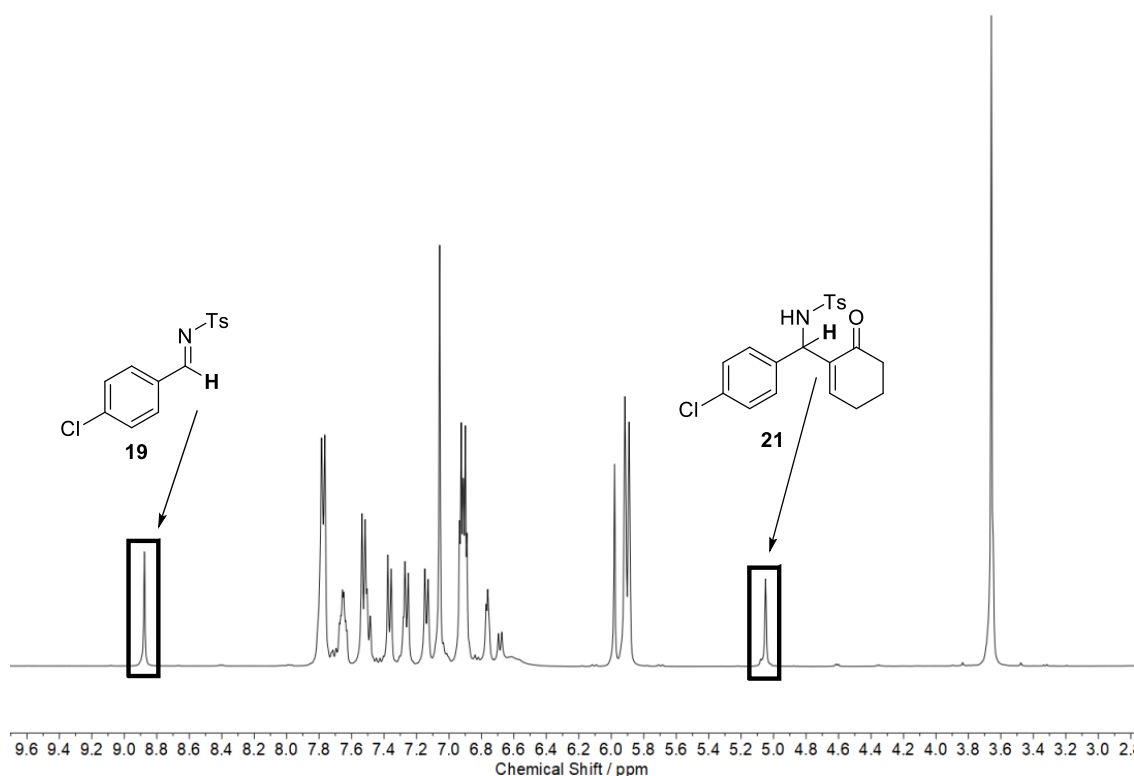


Figure S82. Integrals of interest for the synthesis of tosyl amine **21** from tosyl imine **19** in a typical spectrum of the aza-MBH benchmark reaction.

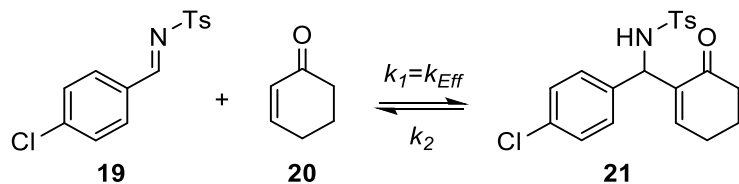
The values of these integrals were used to calculate turnovers according to Equation S5:

$$T_{MBH} / \% = \frac{\text{Integral MBH2}}{(\text{Integral MBH2} + \text{Integral MBH1})} \times 100 = \frac{\mathbf{21}}{(\mathbf{19} + \mathbf{21})} \times 100 \quad \text{Eq. S5}$$

The values obtained for turnover T_{MBH} were used for calculating concentrations of **21** at the time t based on initial concentrations c_0 as shown by Equation S6:

$$c_t [\mathbf{21}] / \text{mol L}^{-1} = \frac{c_0 [\mathbf{19}] \times (100 - T_{MBH(t)})}{100} \quad \text{Eq. S6}$$

Simulation of kinetic parameters was done using COPASI^[3]. The obtained values for t and $c_t[21]$ were imported into the program and the *Parameter Estimation* (default settings) option was used for the simplified model shown in **Scheme S4**.



Scheme S4. Simplified model used for fitting the experimental data obtained for aza-MBH benchmark reactions in COPASI.

The values obtained for k_{eff} were then used to compare the activity of different catalysts to each other as detailed in the next section.

Kinetic Data for the aza-MBH Benchmark Reaction

Table S2 gives details for the aza-MBH benchmark reactions that were done in the course of this study while **Figure S83** – **Figure S99** show the fitted turnover curves that are obtained as graphical output by COPASI:

Table S2. Details for the aza-MBH benchmark reactions.

Experiment	Catalyst	mol-% catalyst (compared to sulfonimine 19)	c(Catalyst) / mol L ⁻¹	k_{eff} / L mol ⁻¹ s ⁻¹
mbh_1	none	0.0	---	---
mbh_2	1a	25.0	6.26E-02	1.51E-06
mbh_3	1a	25.0	6.27E-02	1.41E-06
mbh_4	1c	12.5	3.12E-02	1.51E-05
mbh_5	1c	12.5	3.12E-02	1.95E-05
mbh_6	1c	24.9	6.25E-02	2.97E-05
mbh_7	1c	24.9	6.25E-02	3.51E-05
mbh_8	22	25.0	6.25E-02	---
mbh_9	6bc	5.7	1.44E-02	6.73E-05
mbh_10	6bc	11.5	2.88E-02	1.60E-04
mbh_11	6bc	12.4	3.12E-02	1.62E-04
mbh_12	6bc	12.4	3.12E-02	2.02E-04
mbh_13	6bc	24.9	6.24E-02	3.42E-04
mbh_14	6bc	24.9	6.24E-02	3.69E-04
mbh_15	6cg	5.0	1.25E-02	8.53E-05
mbh_16	6cg	12.5	3.13E-02	2.49E-04
mbh_17	6cg	25.1	6.27E-02	4.81E-04

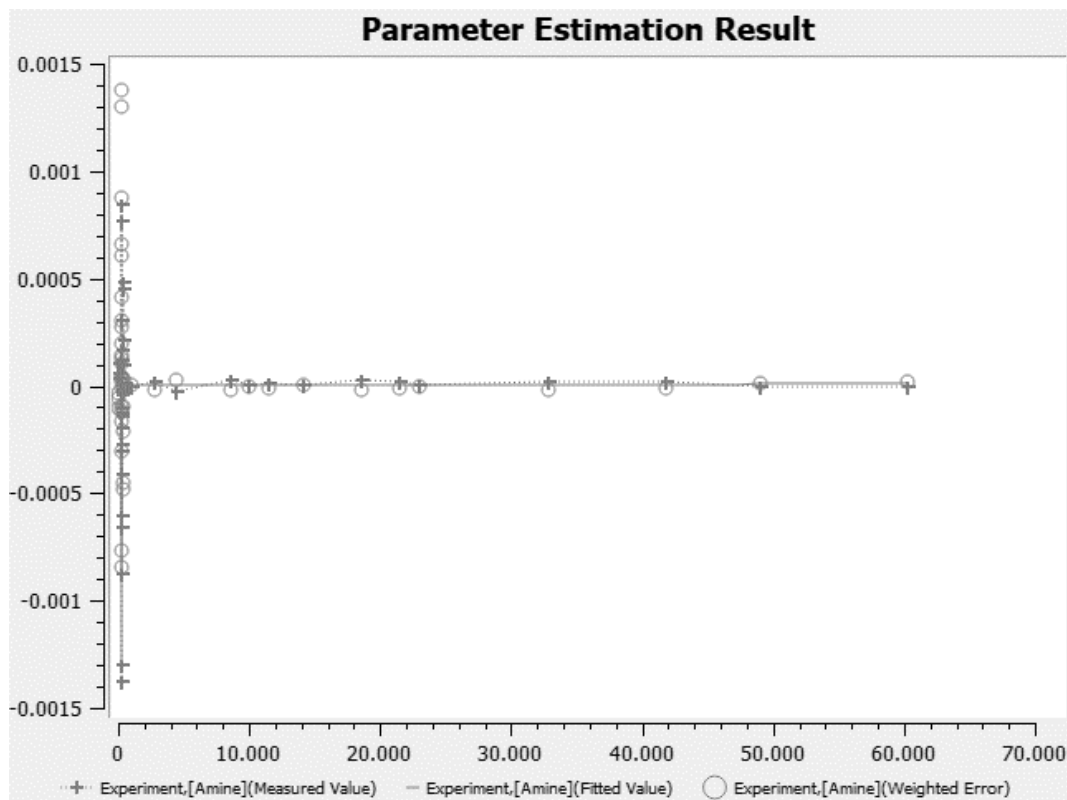


Figure S83. Fitted turnover curve obtained as graphical output by COPASI for experiment mbh_01. Vertical axis gives the concentration of amine **21** in mol L⁻¹, horizontal axis gives the time from 0 min to 70000 min.

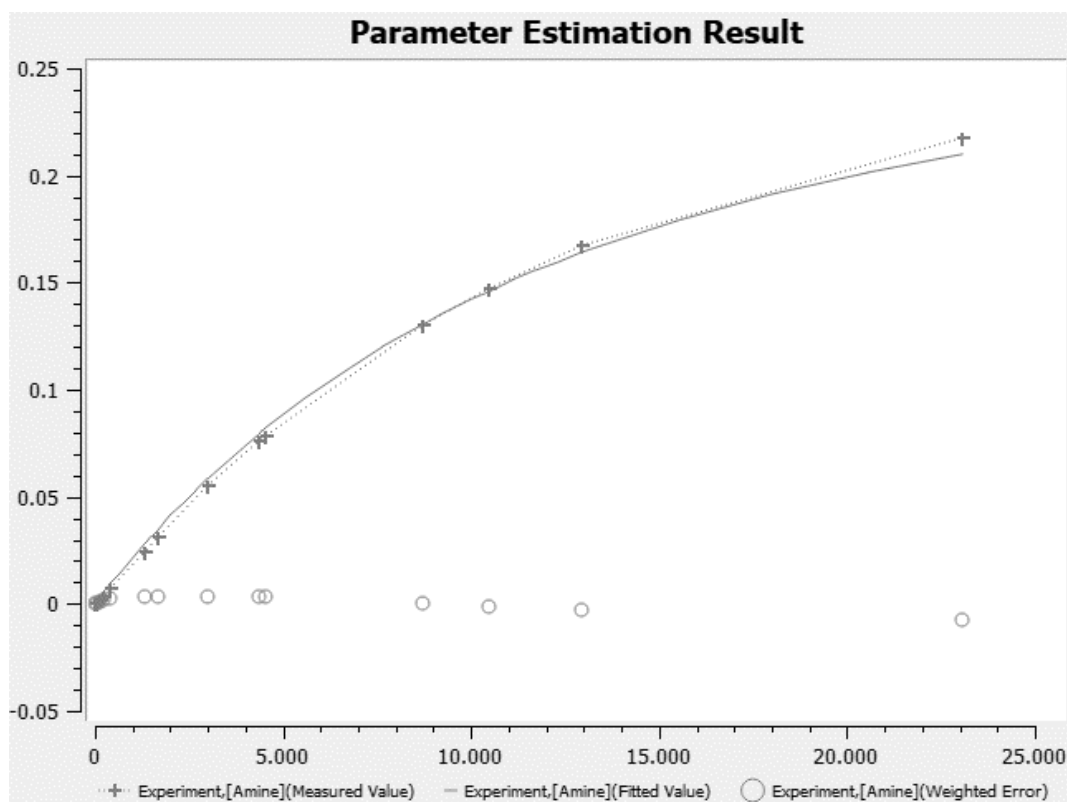


Figure S84. Fitted turnover curve obtained as graphical output by COPASI for experiment mbh_02. Vertical axis gives the concentration of amine **21** in mol L⁻¹, horizontal axis gives the time from 0 min to 25000 min.

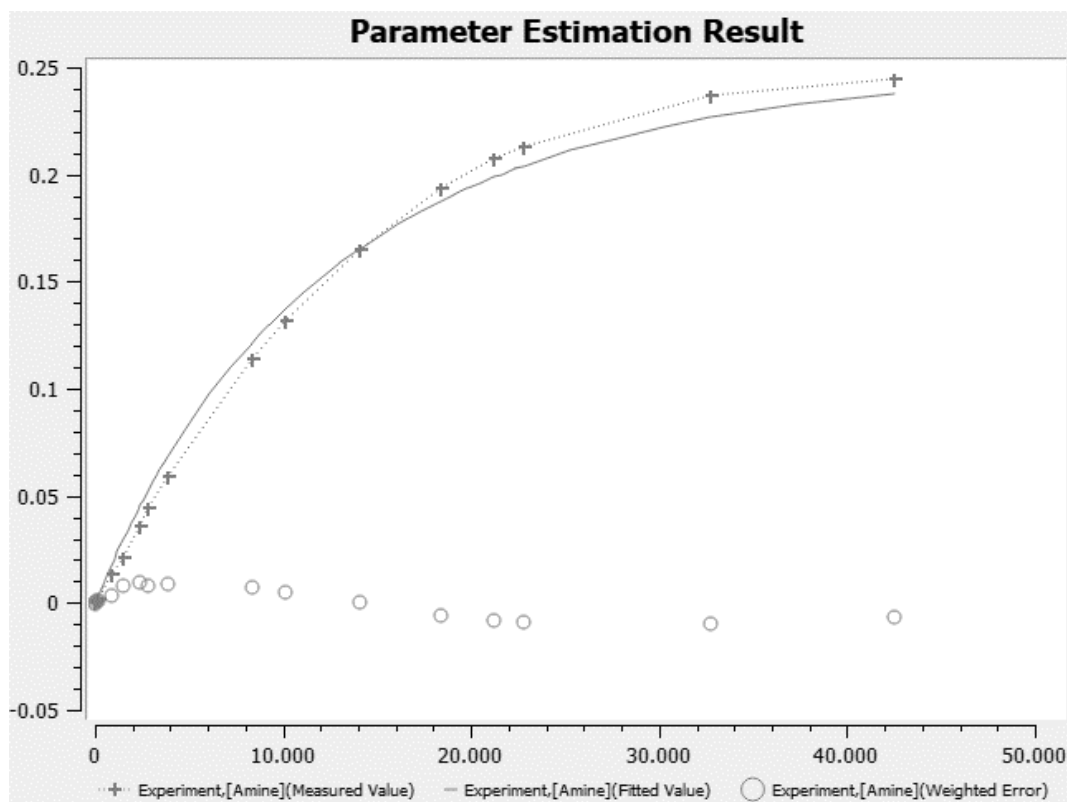


Figure S85. Fitted turnover curve obtained as graphical output by COPASI for experiment mbh_03. Vertical axis gives the concentration of amine **21** in mol L⁻¹, horizontal axis gives the time from 0 min to 50000 min.

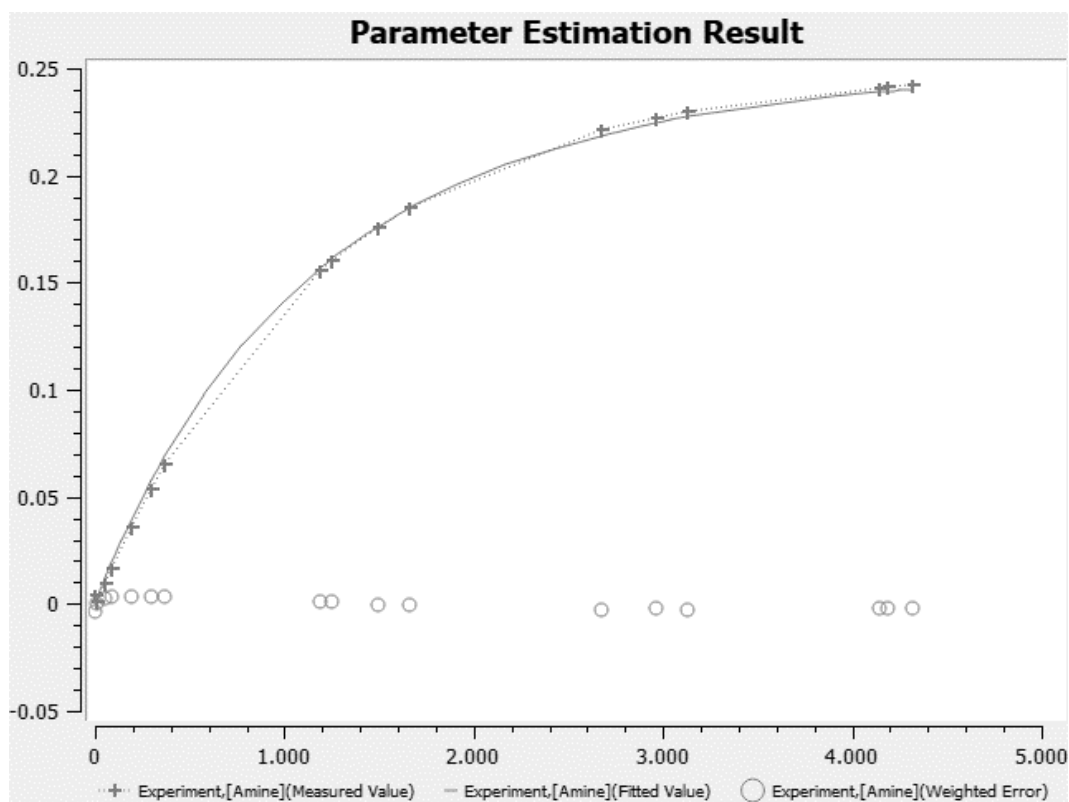


Figure S86. Fitted turnover curve obtained as graphical output by COPASI for experiment mbh_04. Vertical axis gives the concentration of amine **21** in mol L⁻¹, horizontal axis gives the time from 0 min to 5000 min.

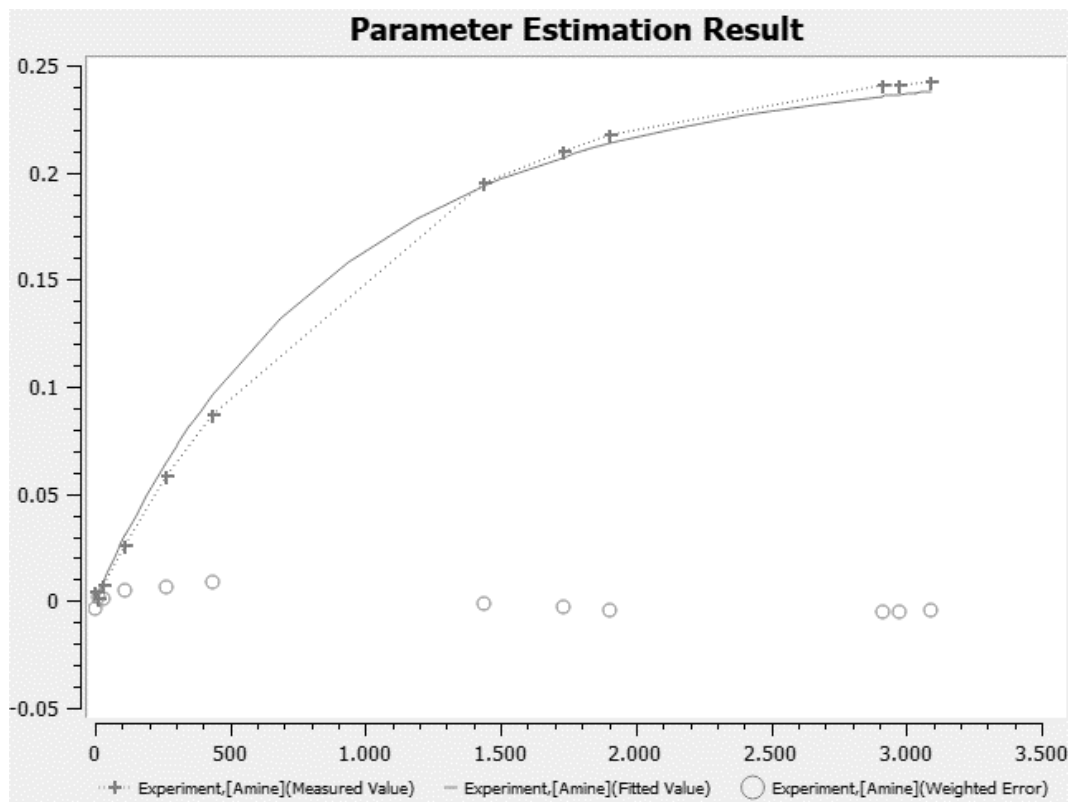


Figure S87. Fitted turnover curve obtained as graphical output by COPASI for experiment mbh_05. Vertical axis gives the concentration of amine **21** in mol L⁻¹, horizontal axis gives the time from 0 min to 3500 min.

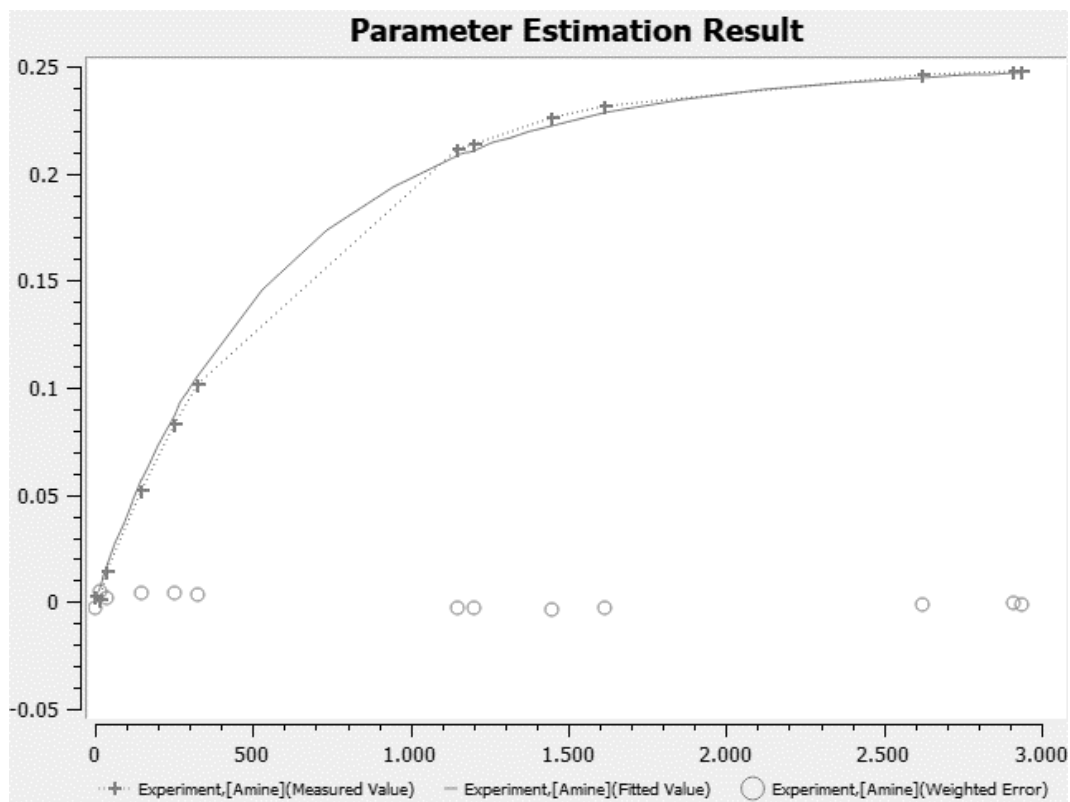


Figure S88. Fitted turnover curve obtained as graphical output by COPASI for experiment mbh_06. Vertical axis gives the concentration of amine **21** in mol L⁻¹, horizontal axis gives the time from 0 min to 3000 min.

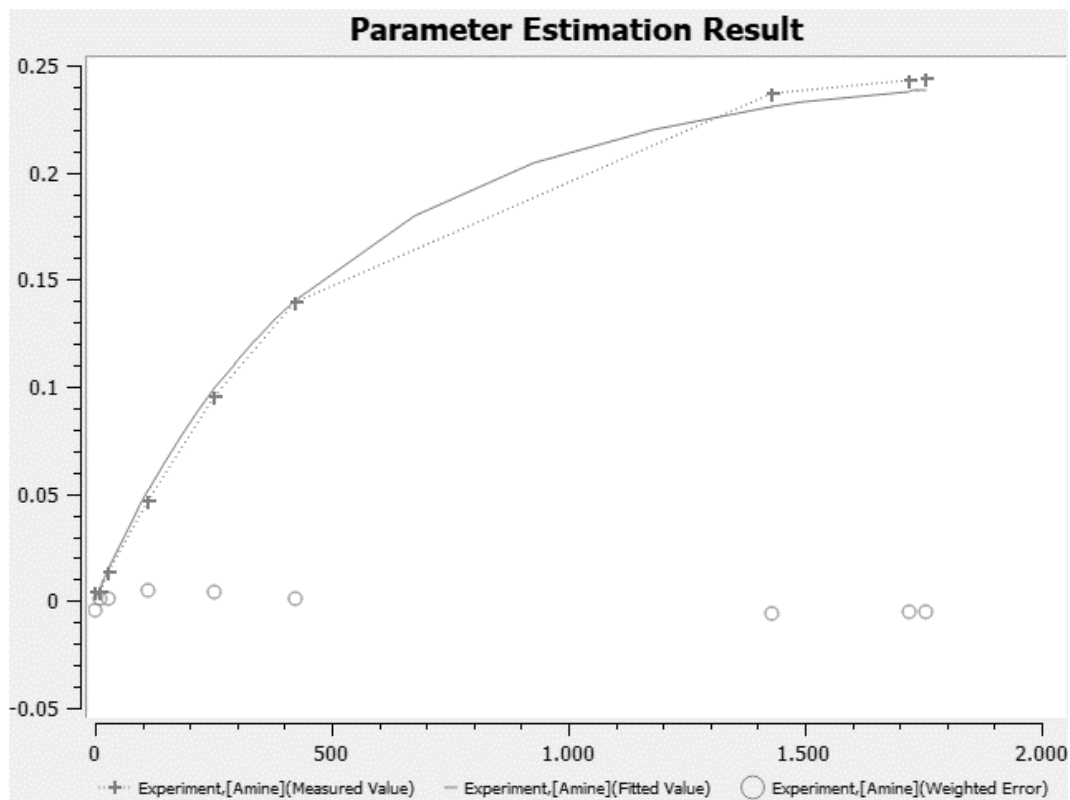


Figure S89. Fitted turnover curve obtained as graphical output by COPASI for experiment mbh_07. Vertical axis gives the concentration of amine **21** in mol L⁻¹, horizontal axis gives the time from 0 min to 2000 min.

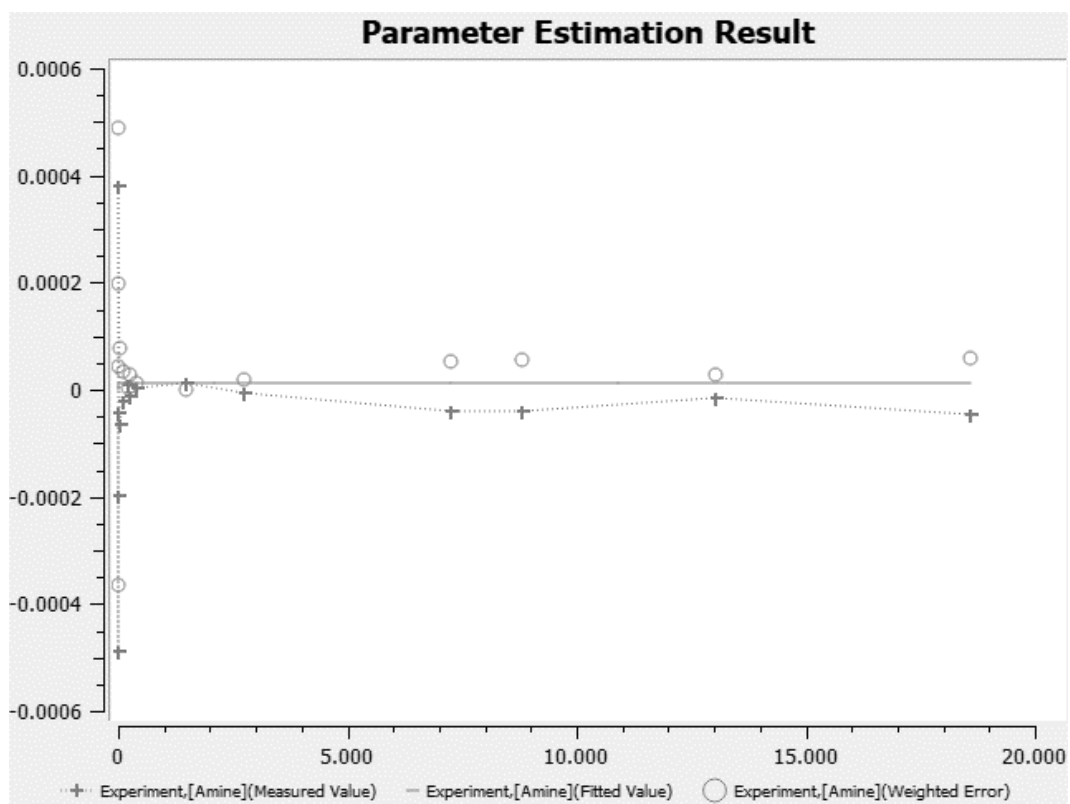


Figure S90. Fitted turnover curve obtained as graphical output by COPASI for experiment mbh_08. Vertical axis gives the concentration of amine **21** in mol L⁻¹, horizontal axis gives the time from 0 min to 20000 min.

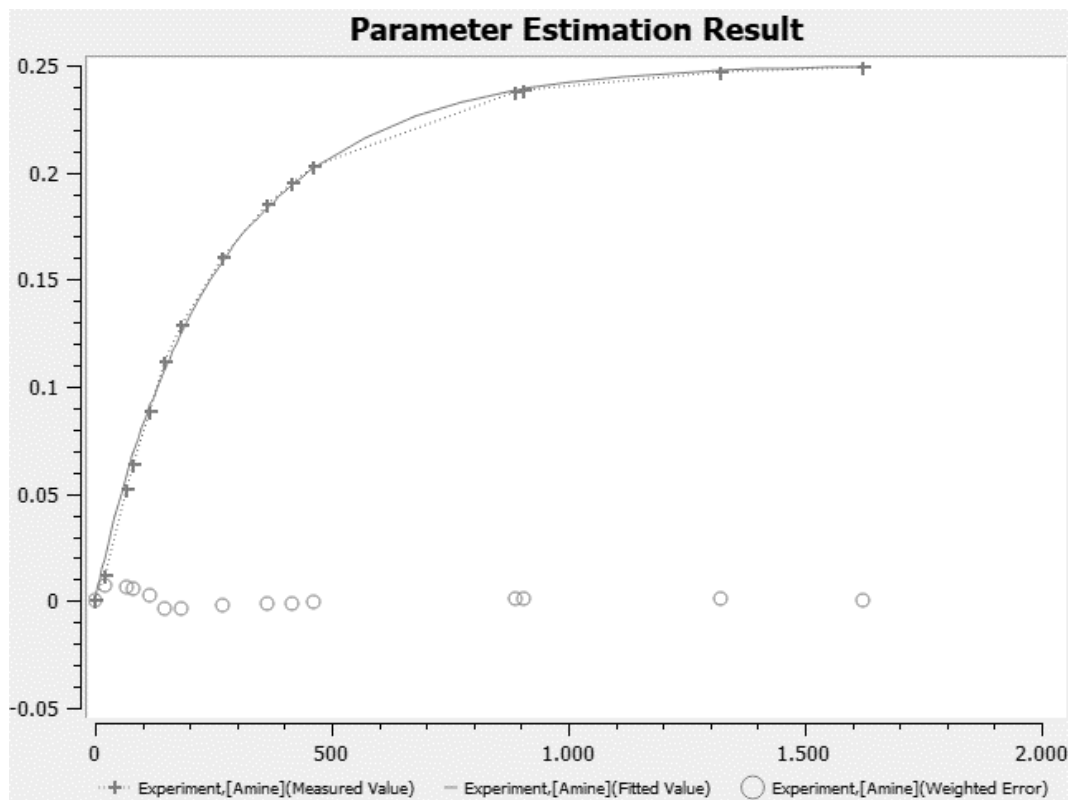


Figure S91. Fitted turnover curve obtained as graphical output by COPASI for experiment mbh_09. Vertical axis gives the concentration of amine **21** in mol L⁻¹, horizontal axis gives the time from 0 min to 2000 min.

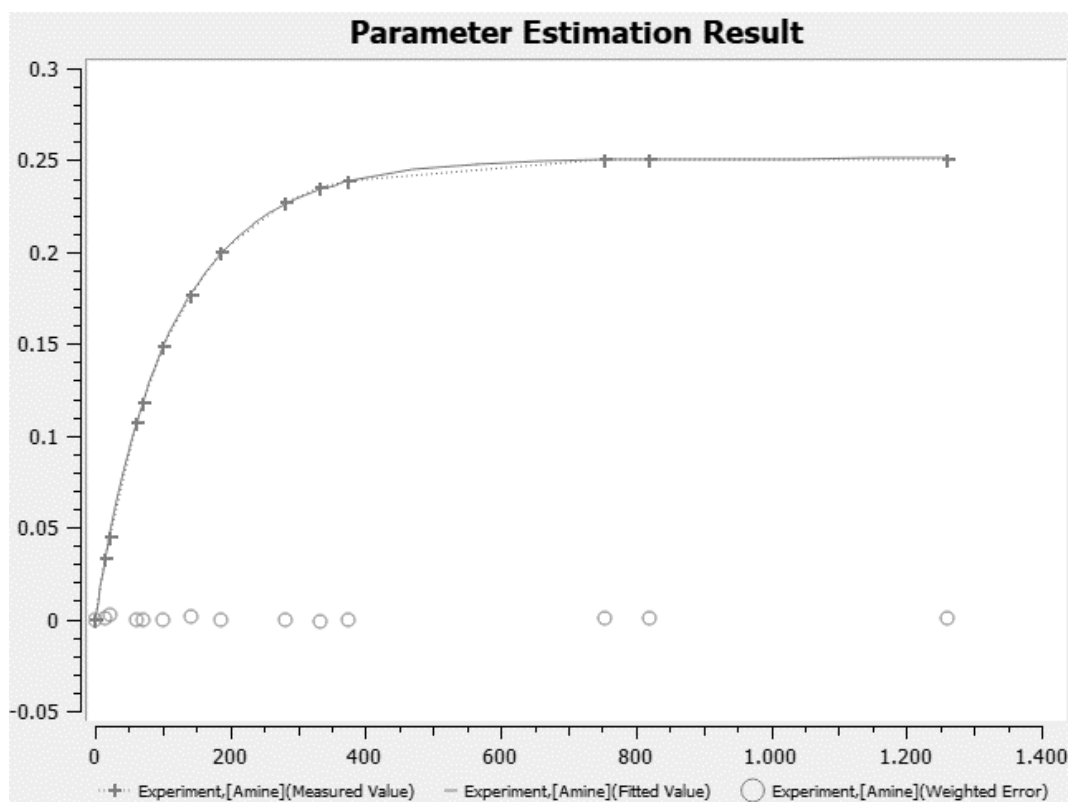


Figure S92. Fitted turnover curve obtained as graphical output by COPASI for experiment mbh_10. Vertical axis gives the concentration of amine **21** in mol L⁻¹, horizontal axis gives the time from 0 min to 1400 min.

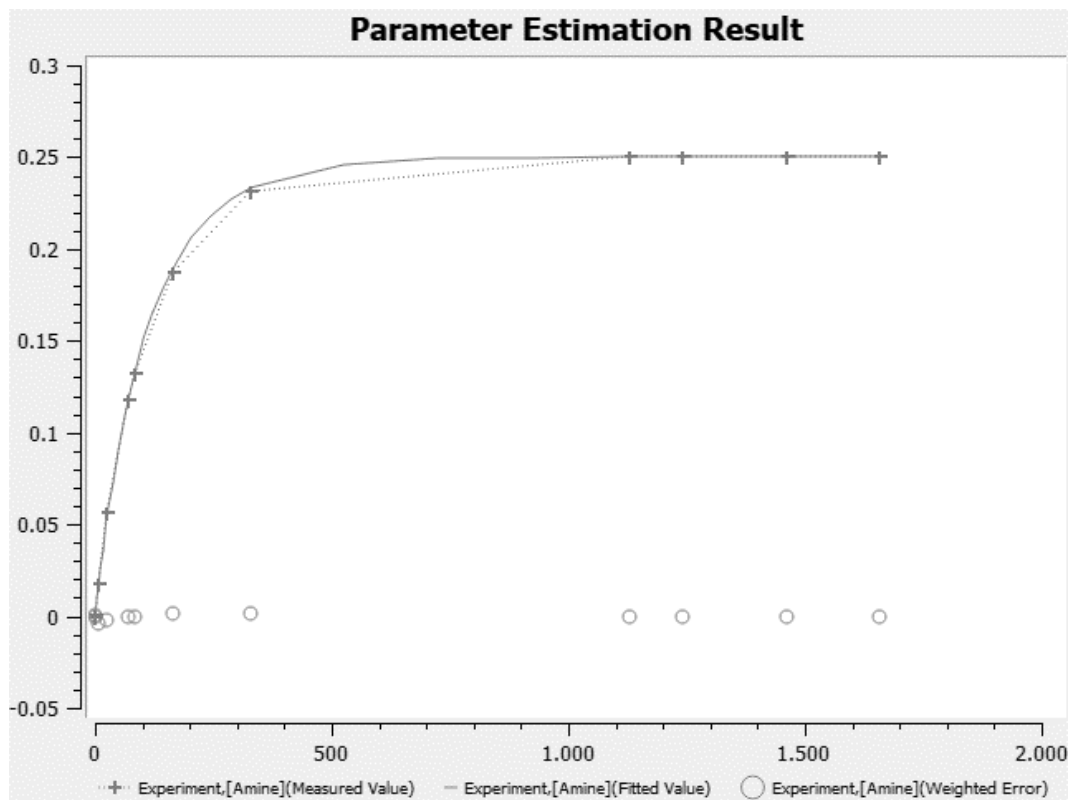


Figure S93. Fitted turnover curve obtained as graphical output by COPASI for experiment mbh_11. Vertical axis gives the concentration of amine **21** in mol L⁻¹, horizontal axis gives the time from 0 min to 2000 min.

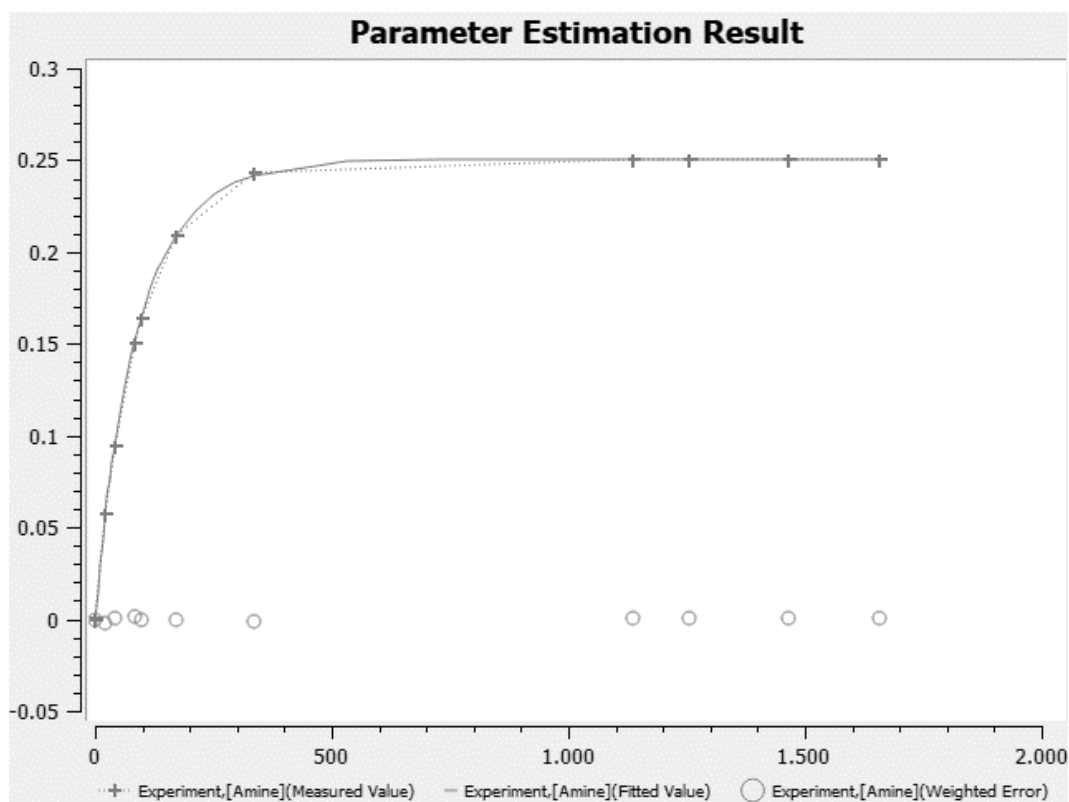


Figure S94. Fitted turnover curve obtained as graphical output by COPASI for experiment mbh_12. Vertical axis gives the concentration of amine **21** in mol L⁻¹, horizontal axis gives the time from 0 min to 2000 min.

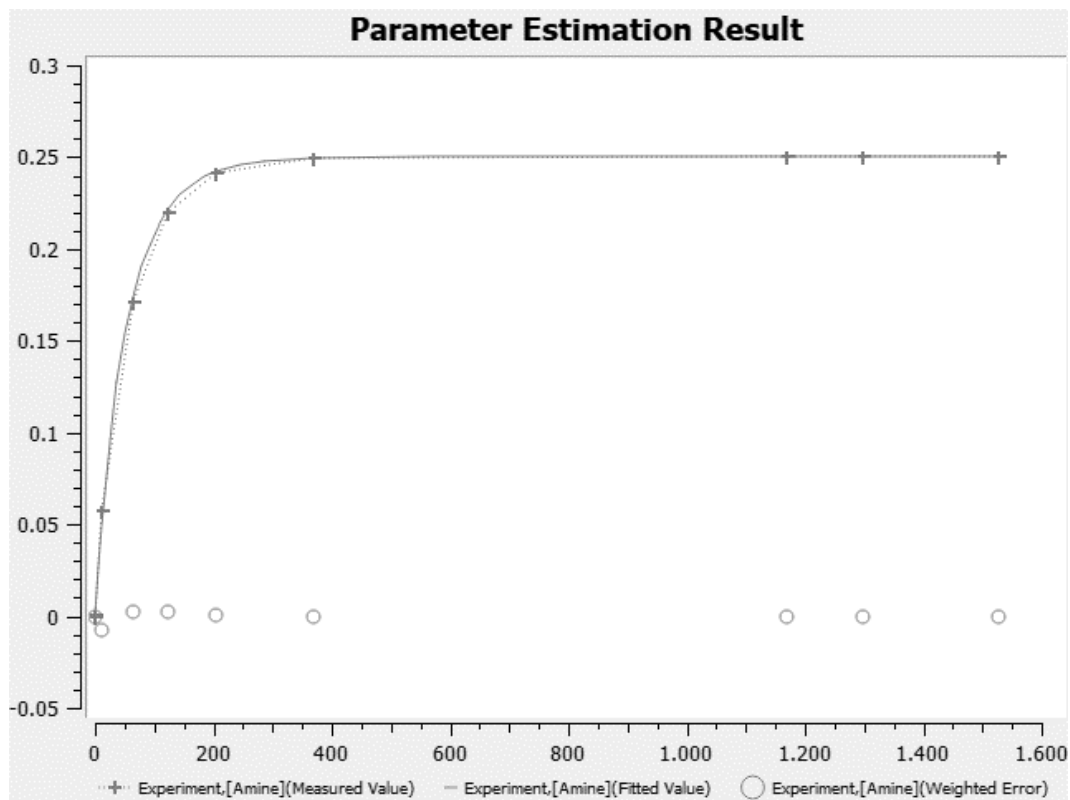


Figure S95. Fitted turnover curve obtained as graphical output by COPASI for experiment mbh_13. Vertical axis gives the concentration of amine **21** in mol L⁻¹, horizontal axis gives the time from 0 min to 1600 min.

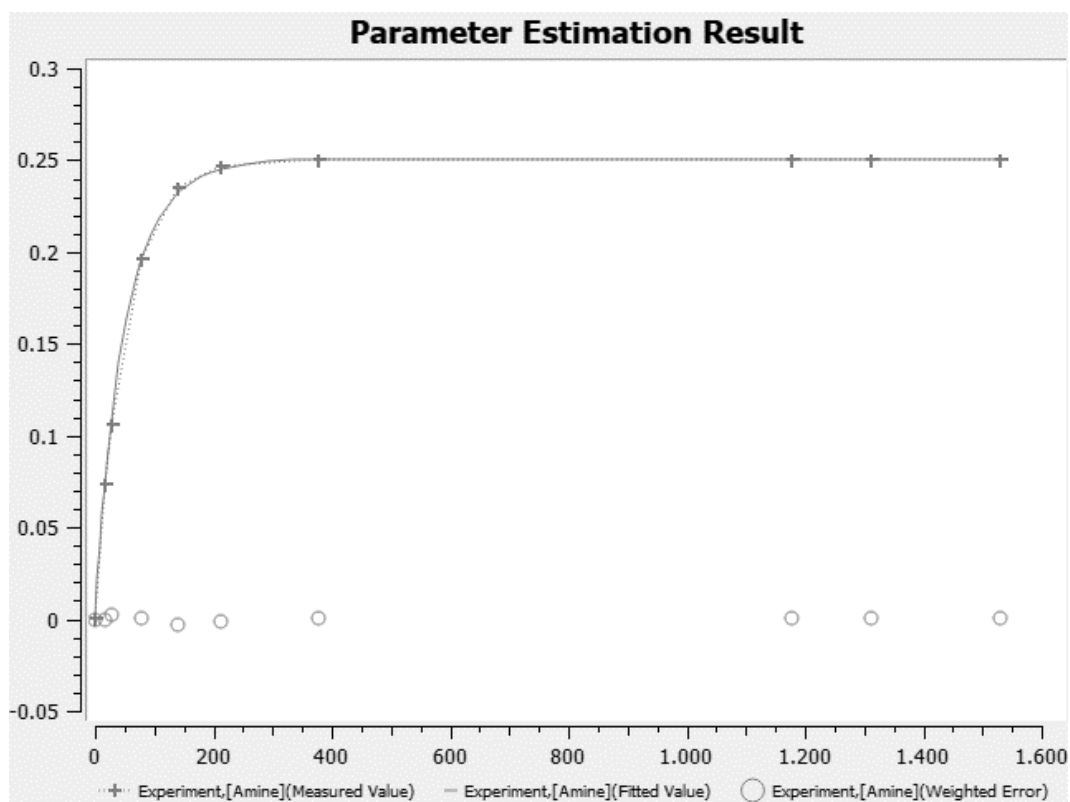


Figure S96. Fitted turnover curve obtained as graphical output by COPASI for experiment mbh_14. Vertical axis gives the concentration of amine **21** in mol L⁻¹, horizontal axis gives the time from 0 min to 1600 min.

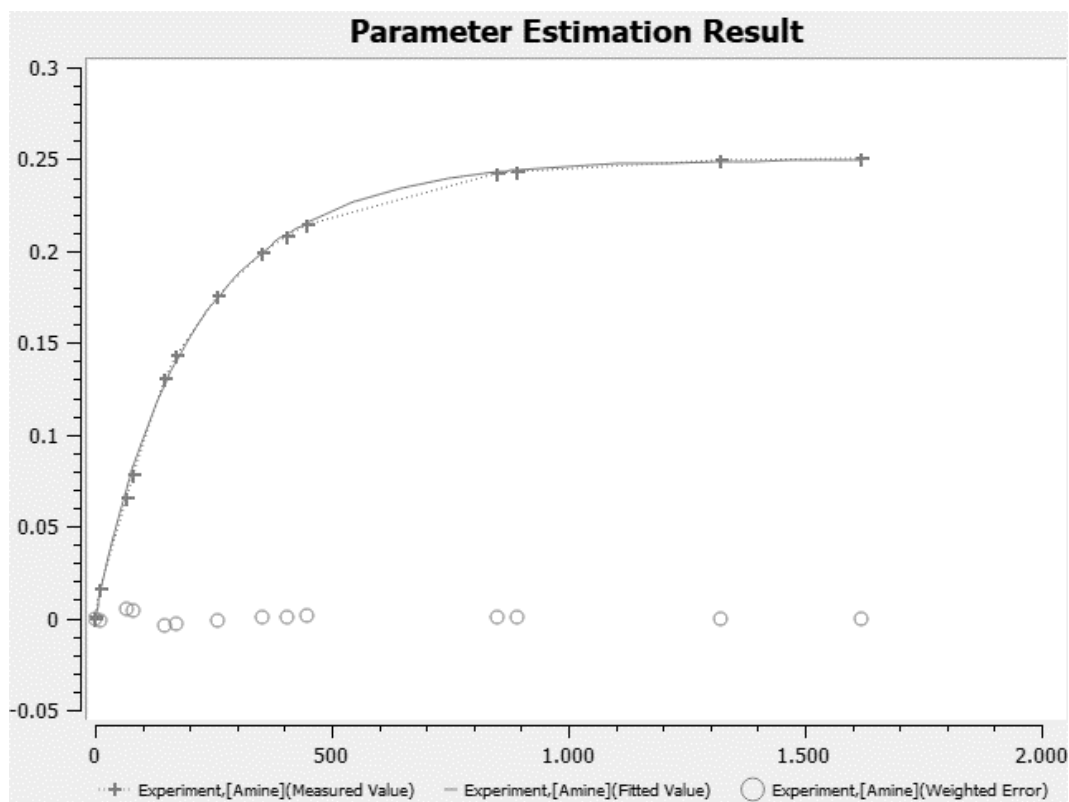


Figure S97. Fitted turnover curve obtained as graphical output by COPASI for experiment mbh_15. Vertical axis gives the concentration of amine **21** in mol L⁻¹, horizontal axis gives the time from 0 min to 2000 min.

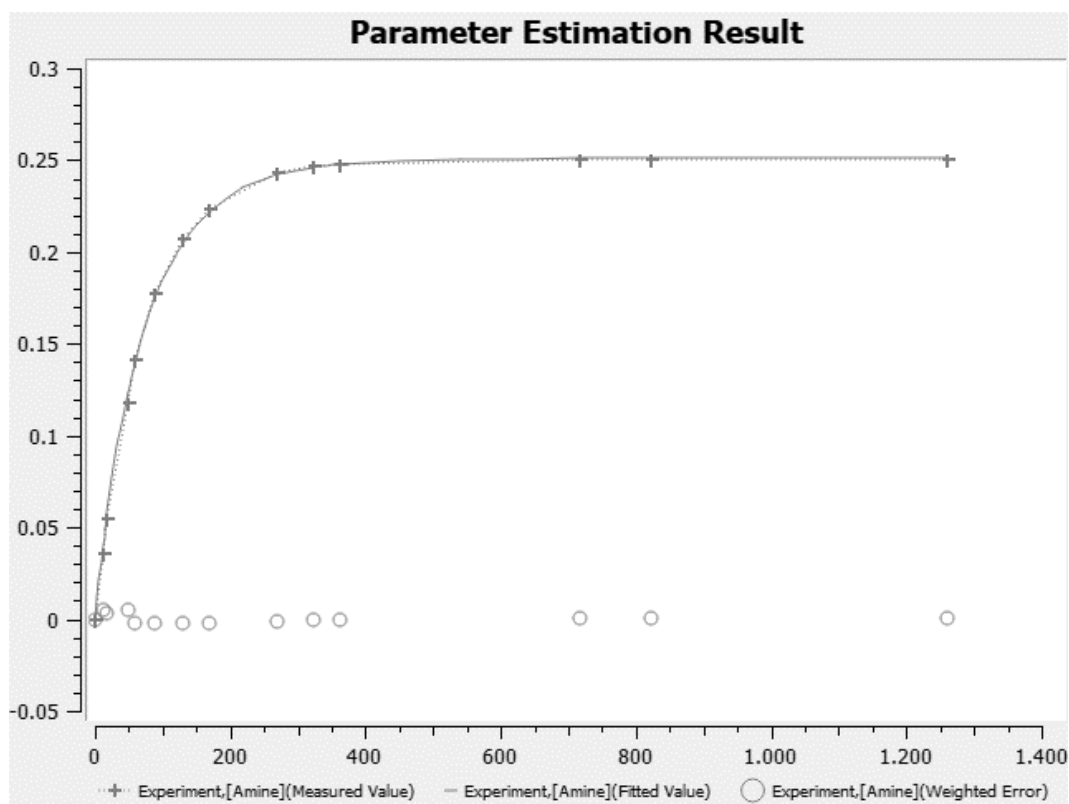


Figure S98. Fitted turnover curve obtained as graphical output by COPASI for experiment mbh_16. Vertical axis gives the concentration of amine **21** in mol L⁻¹, horizontal axis gives the time from 0 min to 1400 min.

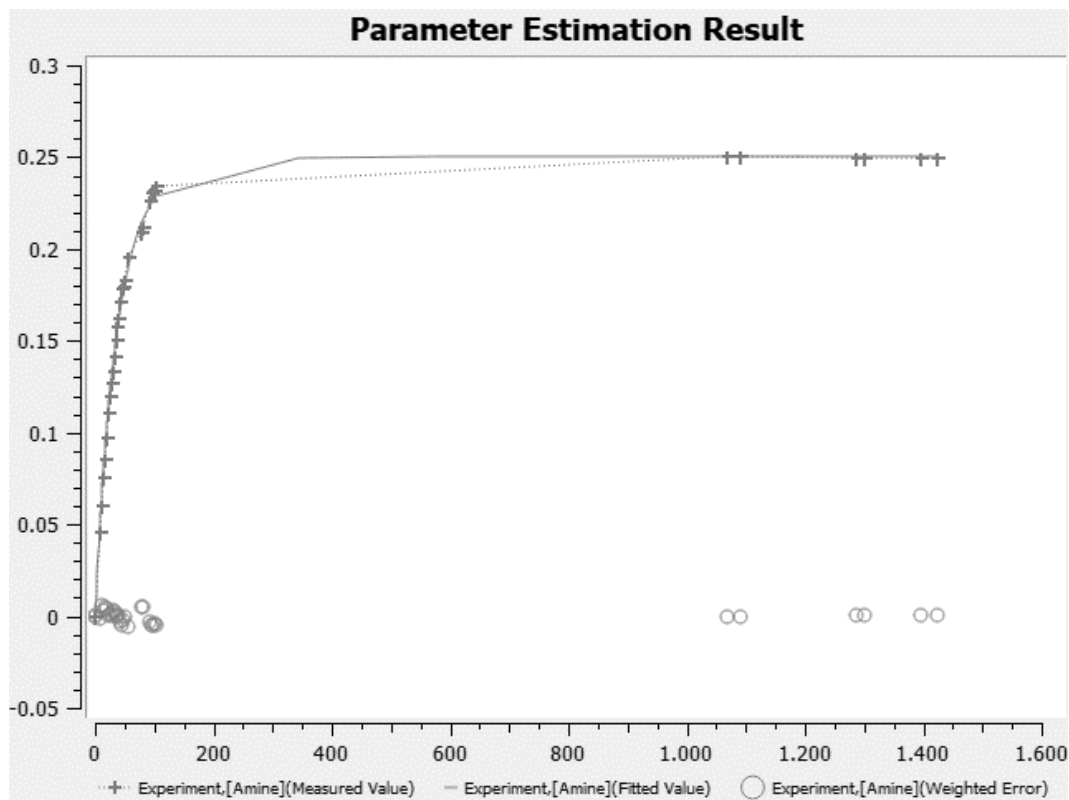


Figure S99. Fitted turnover curve obtained as graphical output by COPASI for experiment mbh_17. Vertical axis gives the concentration of amine **21** in mol L⁻¹, horizontal axis gives the time from 0 min to 1600 min.

Esterification Reactions Mediated by Ion Pair Catalysts

We were interested whether the ion pair catalyst employed in this study would be able to withstand the conditions present in esterification reactions. In classic, Lewis-base catalyzed esterification reactions, HCl or organic acids are generated as byproducts and need to be removed by auxiliary base (such as NEt₃) to prevent protonation and therefore deactivation of the catalyst. The investigated catalyst systems are anionic bases, and able to act as Bronsted bases which would cause them to get deactivated. To test this, we performed a single set of experiments as shown in **Figure S100**, mimicking the conditions of a previous study investigating acylation reactions catalyzed by DMAP (**1a**).^[5]

Turnover was determined by comparison of the integrals of the ¹H-NMR signals of the CH₂-groups of both the ester and the benzyl alcohol as described in the next section and in the same manner as in our previous study of esterification reactions.^[2]

We decided to use only 1 mol-% (with respect to benzyl alcohol) of catalyst **6aa** to be able to easily detect catalyst deactivation. However, judging from the turnover-curves in **Figure S100**, there seems to be no deactivation of the ion pair catalyst. On the contrary, the reaction is sped up by a factor of more than 25 by the addition of 1 mol-% **6aa** compared to the uncatalyzed acylation.

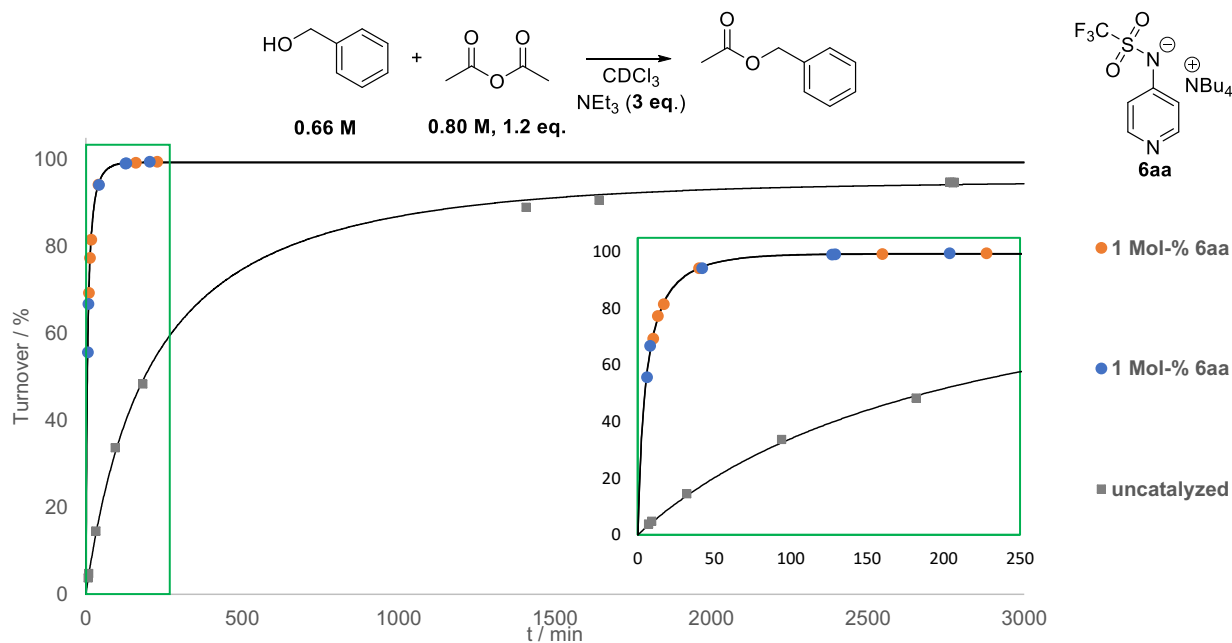


Figure S100. Acylation of benzyl alcohol with acetic anhydride catalyzed by 1 mol-% ion pair catalyst **6aa** and uncatalyzed reaction at 23 °C.

These results encouraged us to try a more challenging combination of alcohols and anhydrides and to compare our most active ion pair catalyst, **6cg** with common, neutral Lewis basic pyridine derivatives. As shown in **Figure S101**, the reaction a 1:1 mixture of 1-phenylethanol and pivalic anhydride was chosen because of a minimization of (uncatalyzed) background reaction and the general challenge of activating pivalic anhydride.

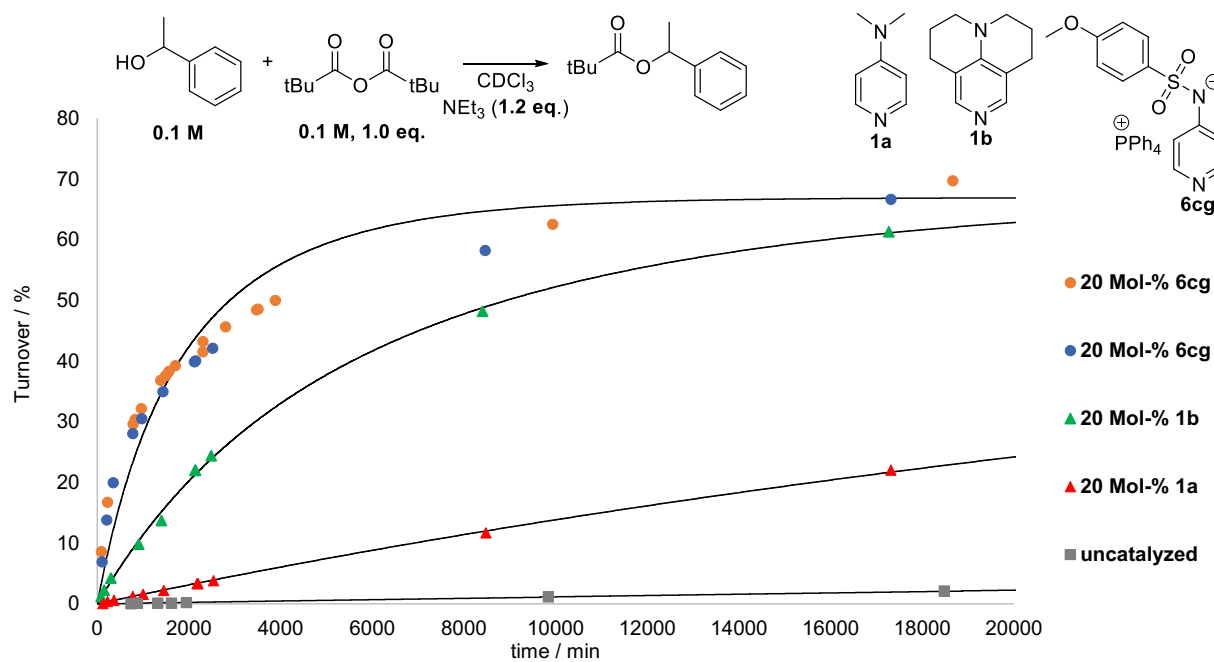


Figure S101. Esterification of 1-phenylethanol, catalyzed by **6cg**, **1b**, **1a** (20 mol-% each compared to 1-phenylethanol), and uncatalyzed reaction at 23 °C.

Again, turnover was determined by comparison of the integrals of the $^1\text{H-NMR}$ signals of the proton attached to the chiral carbon of both the ester and the benzyl alcohol in the same manner as described in the next section and in our previous study of esterification reactions.^[2]

Due to the sluggishness of the reaction, it was not measured until completed in all cases and only observed for about two weeks. Still, a remarkable initial increase of reactivity is observed in the reactions catalyzed by **6cg** compared to DMAP **1a** and even TCAP **1b**. Unlike the neutral catalysts **1a** and **1b**, ion pair **6cg** is however unable to retain this performance under the investigated conditions. The turnover curve shows a distinct bend from about 20 % turnover on. We expect this to be caused by partial protonation of the catalyst's anion. This would also explain, why the shape of the simulated curve (done by COPASI, see below) gives a bad fit. However, the uncatalyzed reaction shows that the reaction would be expected to "flatline" if all catalyst was deactivated. Therefore, we think there is still some active catalyst in the mixtures even after one equivalent of acid was formed at 20 % turnover, which means that there is an equilibrium with the triethyl ammonium chloride that is not fully on the side of the protonated ion pair catalyst.

Due to the discussed issues with esterification reactions, we did not pursue this kind of chemistry any further and concentrated on addition reactions that do not increase the systems acidity with reaction progress, thus enabling us to benchmark the reactivity of the investigated ion pair catalysts more reliably.

Nevertheless, applications for using such ion pair catalysts for esterification reactions should not be completely ruled out in our opinion. First, the less basic trifluoromethane sulfonic amides appear to do well under classic esterification conditions. Secondly, if used to induce selectivity, usually there is no desire to convert all of the initially present alcohol, but ideally only the targeted isomer/functional group, etc. As we showed in **Figure S101**, the investigated ion pair catalysts have the potential to give superior reactivity in the important first half life and remain highly modular which could potentially be used to impart selectivity.

Sample Preparation and Data Acquisition and Processing for the Esterification Reactions

Three different stock solutions were prepared under N_2 atmosphere:

- **SSF**: 3* the final concentration of the alcohol used and 3* the final concentration of NEt_3 (as given in **Table S3**) and a recorded amount of internal standard Si_2Me_6 in CDCl_3
- **SSG**: 3* the final concentration of the appropriate anhydride in CDCl_3 (as given in **Table S3**)
- **SSH**: 3* the final concentration of the corresponding catalyst in CDCl_3 (as given in **Table S3**)

Samples were prepared by transferring 0.2 mL of SSF, 0.2 mL of SSH and 0.2 mL of SSG (total of 0.6 mL sample volume) into a dried, N_2 -purged NMR tube. The sample was flame sealed under N_2 atmosphere. It was then stored in the bath of a thermostat set at 23 °C. The samples were only taken out of the thermostat for measuring ^1H NMR spectra.

Measured spectra were imported into MestReNova (Version 12.0.3) and superimposed. The following was done for the superimposed spectra in this order:

- Reference set (Si_2Me_6 set to 0.02 ppm)
- Automatic phase correction
- Automatic baseline correction (Whittaker Smoother)

For each reaction, the two signals highlighted in **Figure S102** and **Figure S103** were integrated. These signals represent the H-atoms attached to the α -carbons of the alcohol and the ester respectively:

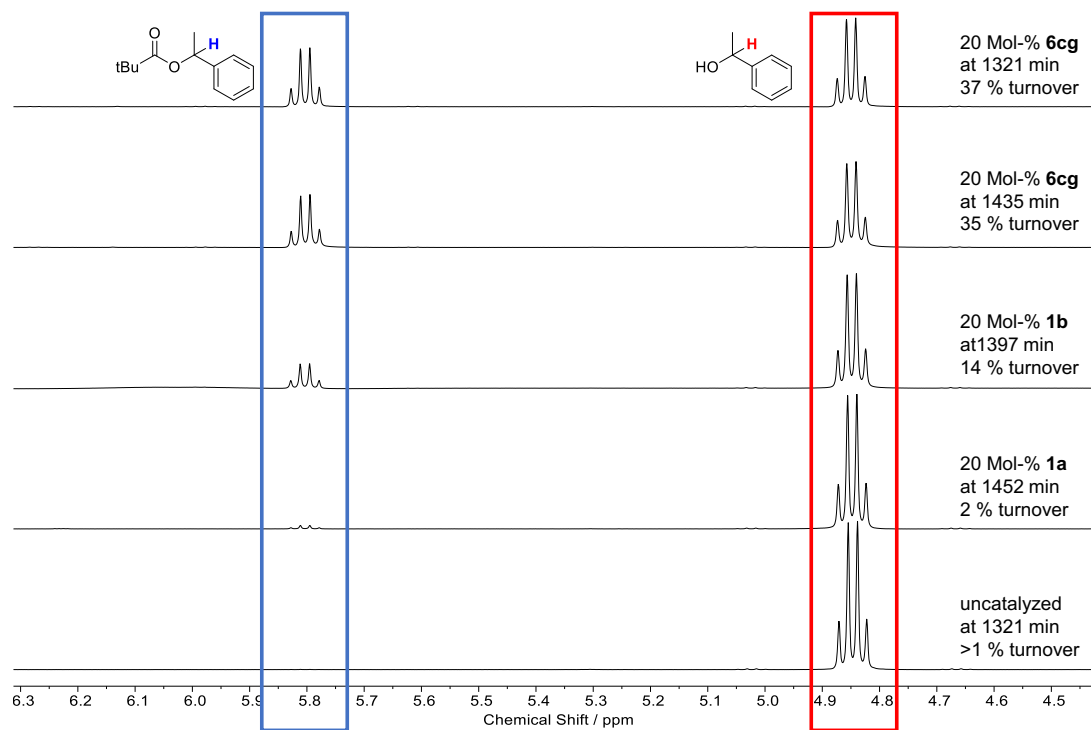


Figure S102. Spectra of the esterification of 1-phenylethanol, catalyzed by different catalysts and uncatalyzed reaction, measured at similar reaction time.

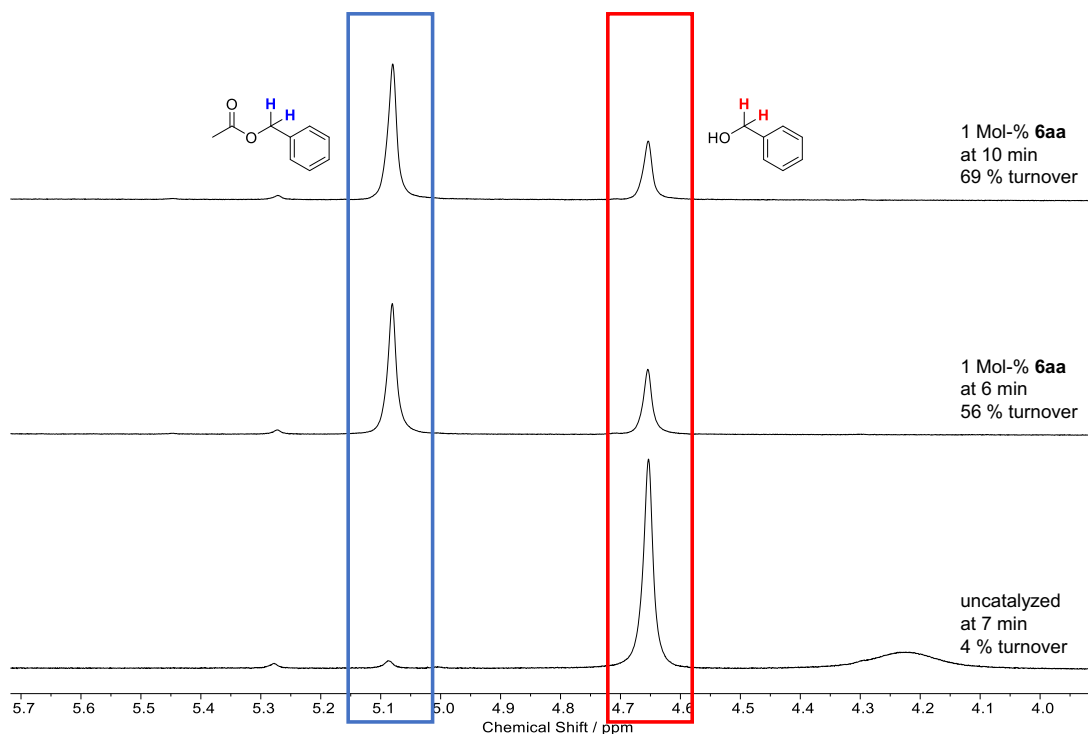


Figure S103. Spectra of the esterification of benzyl alcohol, catalyzed by **6aa** and uncatalyzed reaction.

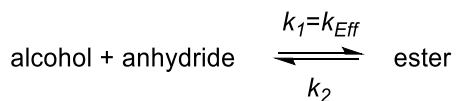
The values of these integrals were used to calculate turnover according to Equation S7:

$$T_{\text{ester}} / \% = \frac{\text{Integral ester}}{\text{Integral ester} + \text{Integral alcohol}} \times 100 \quad \text{Eq. S7}$$

The values obtained for turnover T_{ester} were used for calculating concentrations of the corresponding ester at the time t based on initial concentrations c_0 as shown by Equation S8:

$$c_t [\text{ester}] / \text{mol L}^{-1} = \frac{c_0 \text{alcohol} \times (100 - T_{\text{ester}}(t))}{100} \quad \text{Eq. S8}$$

Simulation of kinetic parameters was done using COPASI^[3]. The obtained values for t and $c_t[\text{ester}]$ were imported into the program and the *Parameter Estimation* (default settings) option was used for the simplified model shown in **Scheme S5**.



Scheme S5. Simplified model used for fitting of the experimental data obtained for the esterification reactions in COPASI.

The fitting curves obtained from COPASI were used to emphasize catalytic performance in **Figure S100** and **Figure S101**.

Kinetic Data for the Esterification Reactions

Table S3 gives the details for the performed esterification reactions while the curves Fitted by COPASI are shown in **Figure S104 – Figure S111**.

Table S3. Details for the esterification benchmark reactions.

experiment	alcohol	anhydride	catalyst
esterification_01	0.66 mol L ⁻¹ benzyl alcohol	0.80 mol L ⁻¹ acetic anhydride	1 mol-% 6aa
esterification_02	0.66 mol L ⁻¹ benzyl alcohol	0.80 mol L ⁻¹ acetic anhydride	1 mol-% 6aa
esterification_03	0.66 mol L ⁻¹ benzyl alcohol	0.80 mol L ⁻¹ acetic anhydride	none
esterification_04	0.1 mol L ⁻¹ 1-phenyl ethanol	0.1 mol L ⁻¹ pivolic anhydride	20 mol-% 6cg
esterification_05	0.1 mol L ⁻¹ 1-phenyl ethanol	0.1 mol L ⁻¹ pivolic anhydride	20 mol-% 6cg
esterification_06	0.1 mol L ⁻¹ 1-phenyl ethanol	0.1 mol L ⁻¹ pivolic anhydride	20 mol-% 1b
esterification_07	0.1 mol L ⁻¹ 1-phenyl ethanol	0.1 mol L ⁻¹ pivolic anhydride	20 mol-% 1a
esterification_08	0.1 mol L ⁻¹ 1-phenyl ethanol	0.1 mol L ⁻¹ pivolic anhydride	none

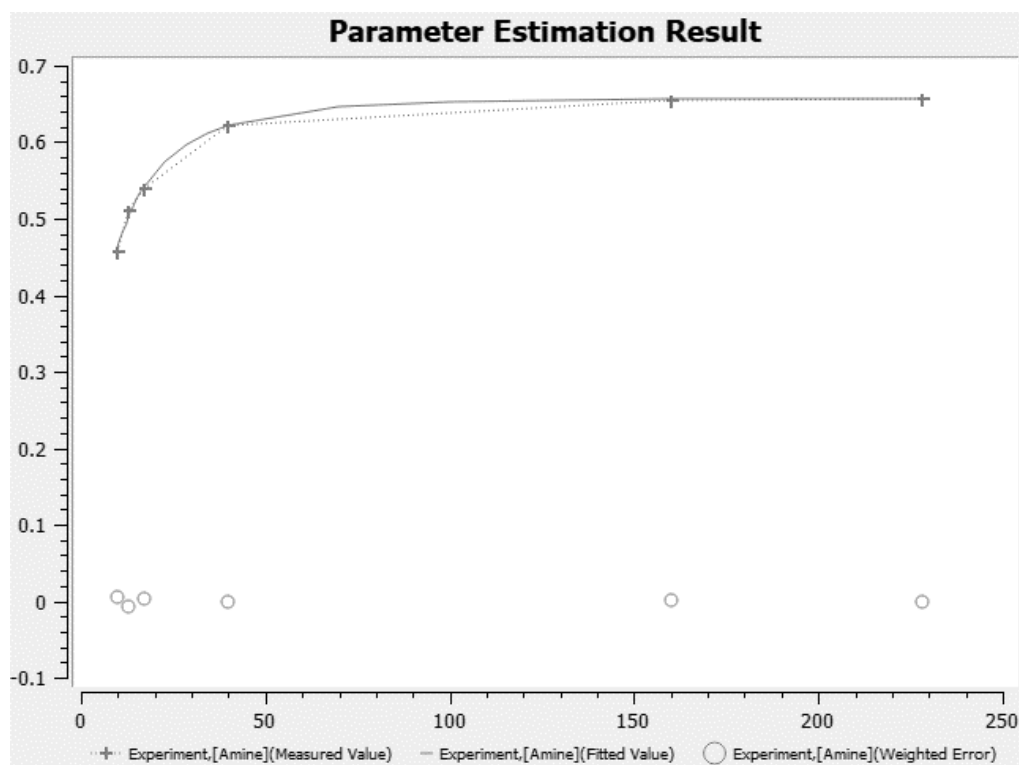


Figure S104. Fitted turnover curve obtained as graphical output by COPASI for experiment esterification_01. Vertical axis gives the concentration of the product ester in mol L⁻¹, horizontal axis gives the time from 0 min to 250 min.

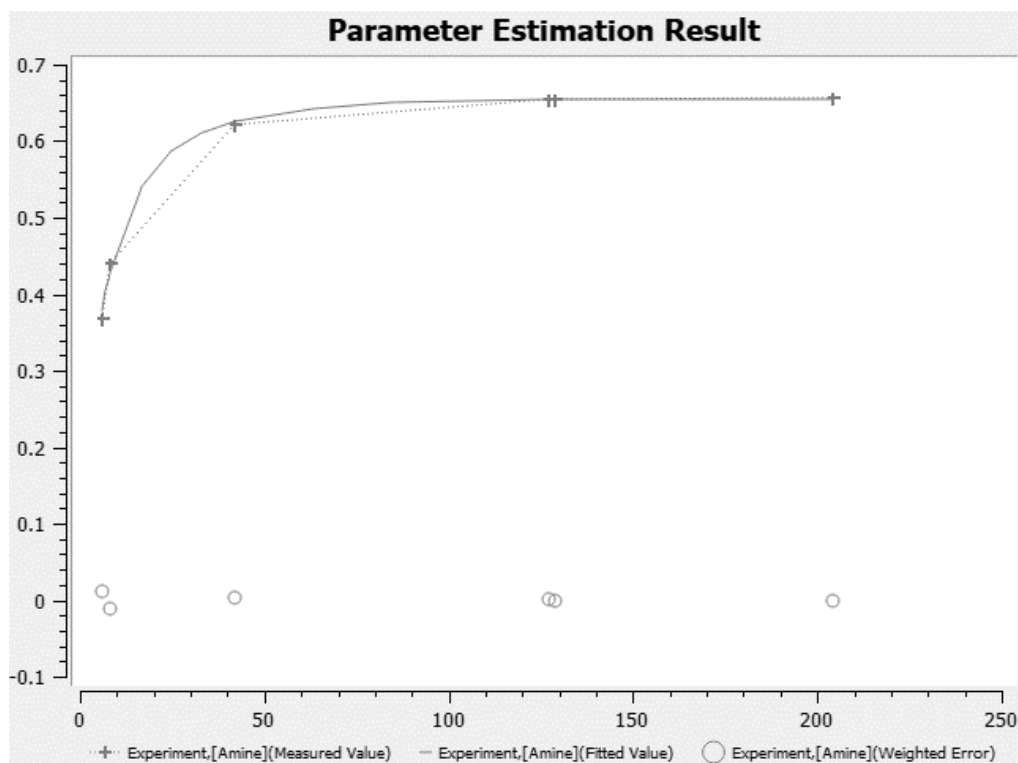


Figure S105. Fitted turnover curve obtained as graphical output by COPASI for experiment esterification_02. Vertical axis gives the concentration of the product ester in mol L⁻¹, horizontal axis gives the time from 0 min to 250 min.

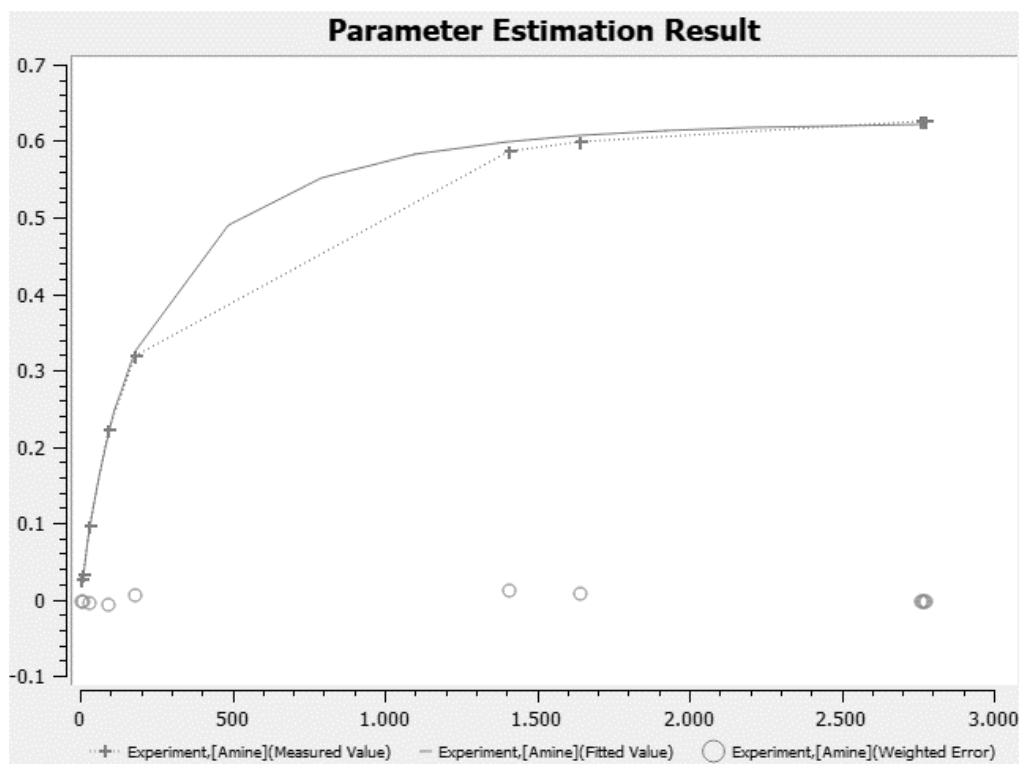


Figure S106. Fitted turnover curve obtained as graphical output by COPASI for experiment esterification_03. Vertical axis gives the concentration of the product ester in mol L⁻¹, horizontal axis gives the time from 0 min to 3000 min.

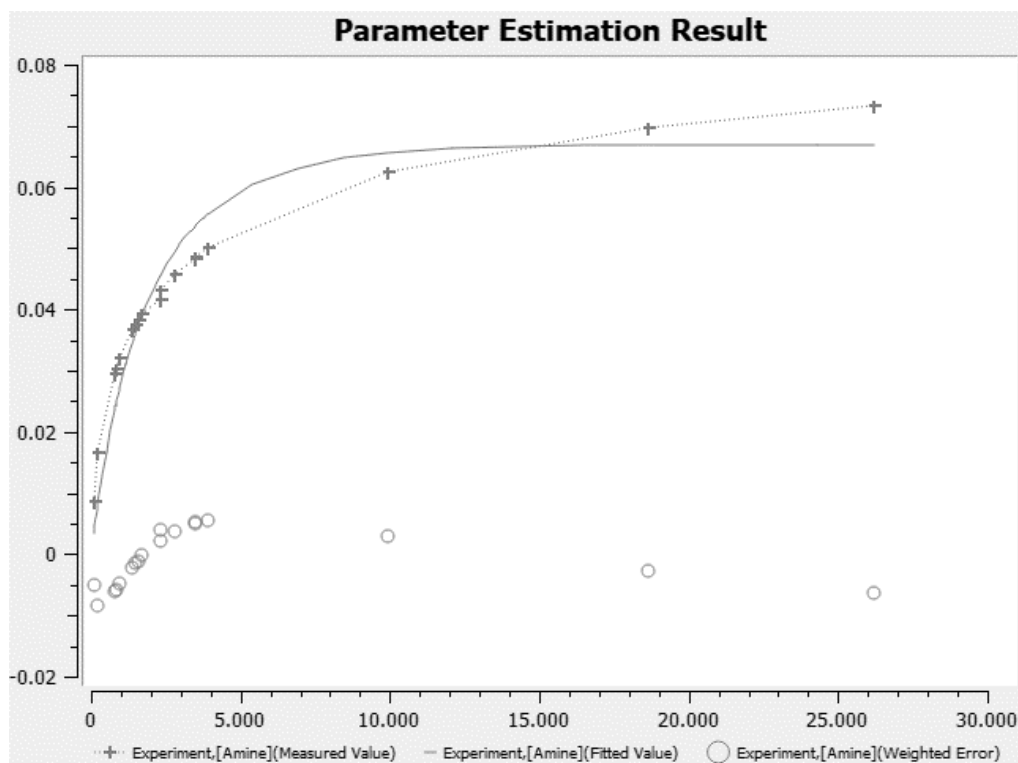


Figure S107. Fitted turnover curve obtained as graphical output by COPASI for experiment esterification_04. Vertical axis gives the concentration of the product ester in mol L^{-1} , horizontal axis gives the time from 0 min to 30000 min.

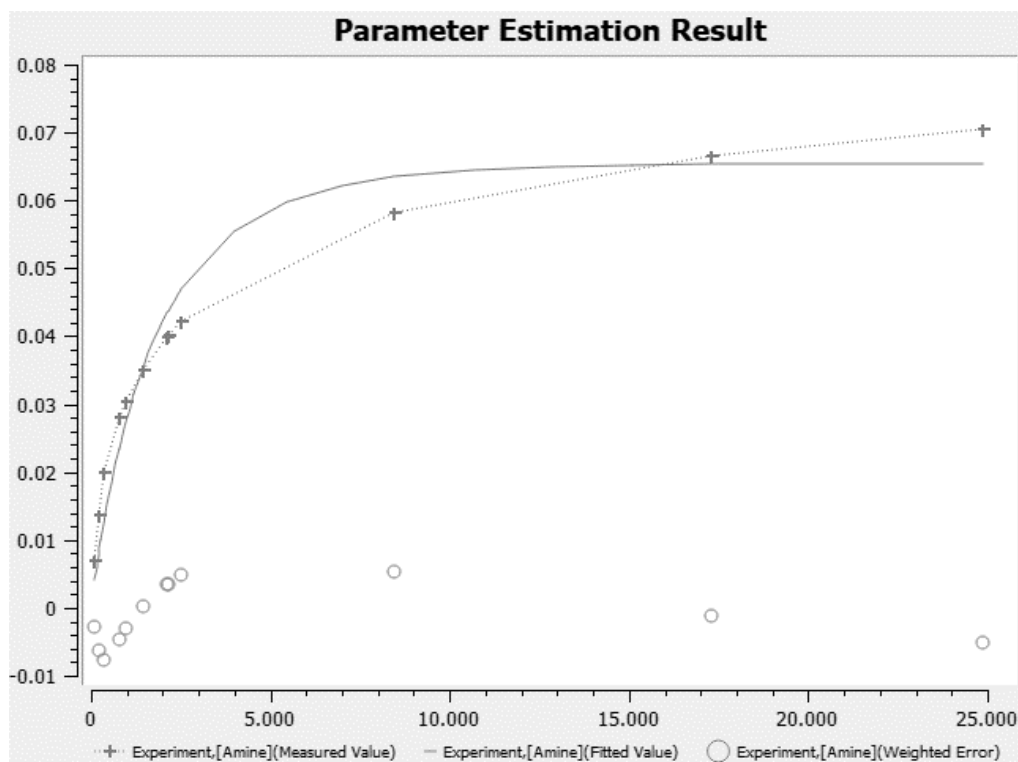


Figure S108. Fitted turnover curve obtained as graphical output by COPASI for experiment esterification_05. Vertical axis gives the concentration of the product ester in mol L^{-1} , horizontal axis gives the time from 0 min to 25000 min.

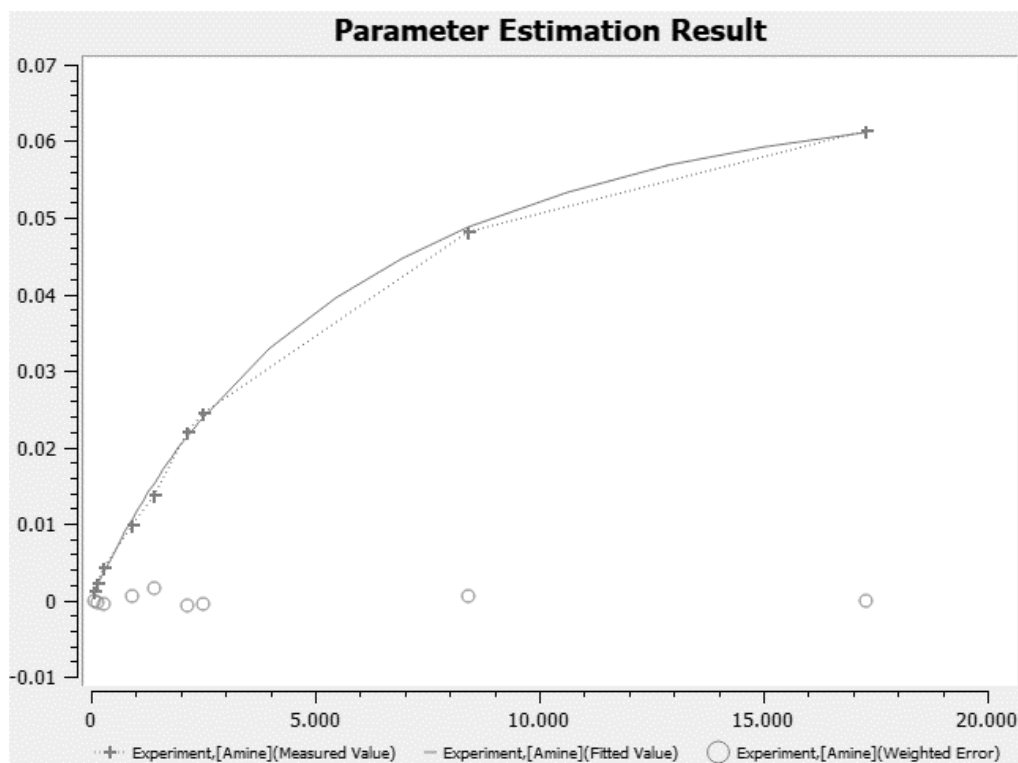


Figure S109. Fitted turnover curve obtained as graphical output by COPASI for experiment esterification_06. Vertical axis gives the concentration of the product ester in mol L^{-1} , horizontal axis gives the time from 0 min to 20000 min.

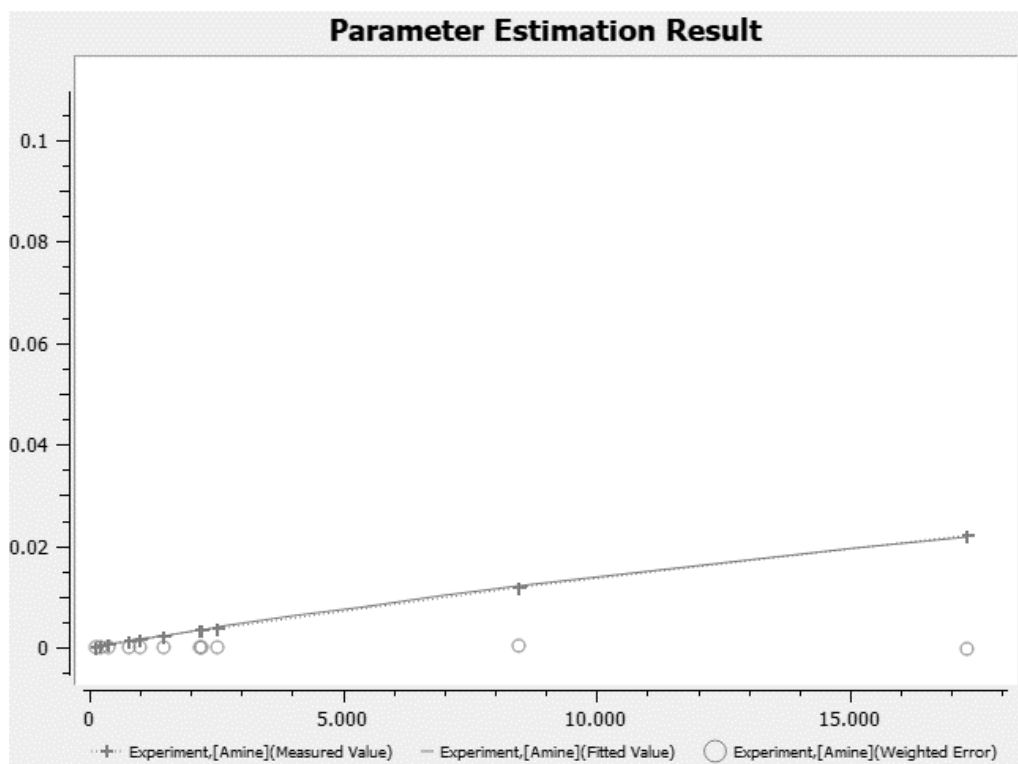


Figure S110. Fitted turnover curve obtained as graphical output by COPASI for experiment esterification_07. Vertical axis gives the concentration of the product ester in mol L^{-1} , horizontal axis gives the time from 0 min to 20000 min.

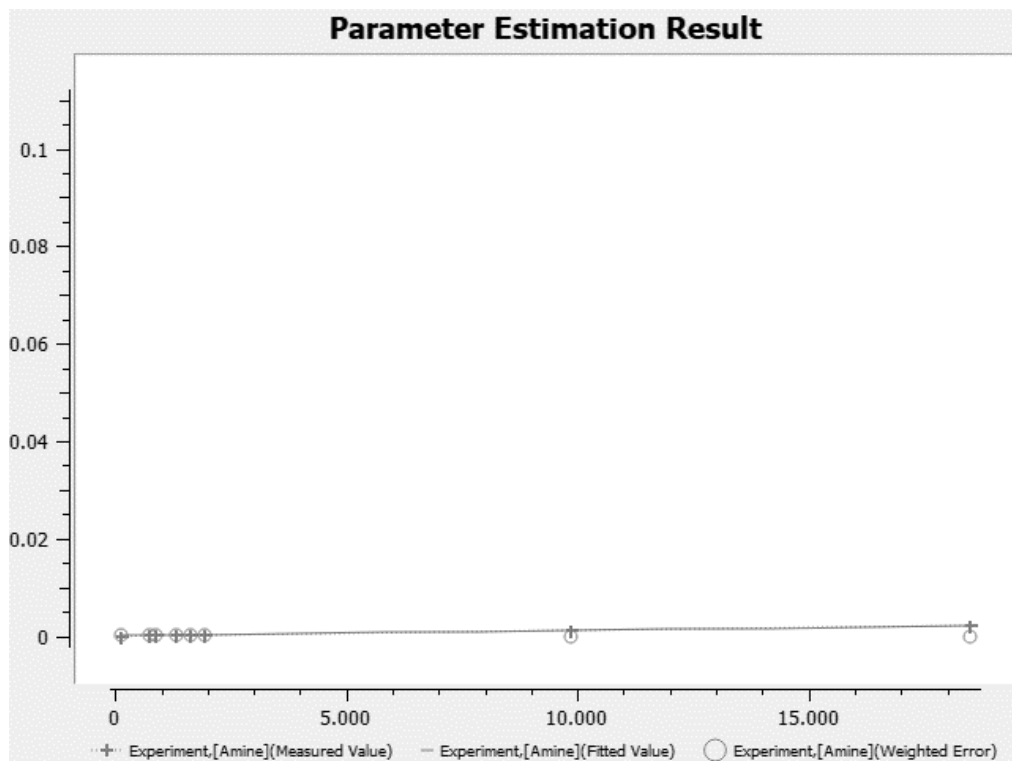


Figure S111. Fitted turnover curve obtained as graphical output by COPASI for experiment esterification_08. Vertical axis gives the concentration of the product ester in mol L⁻¹, horizontal axis gives the time from 0 min to 19000 min.

Deprotonation of More Acidic Cations in Ion Pair Catalysis

When performing the urethane benchmark reactions with catalysts containing the diethyl benzimidazolium cation (**6be**, **6ce**, **7e**) we observed some new, unexpected signals and decided to investigate 1:1 mixtures of the catalyst and isocyanate **17** in CDCl₃. **Figure S112** and **Figure S113** show spectra of these mixtures and spectra of the pure catalyst and isocyanate solutions.

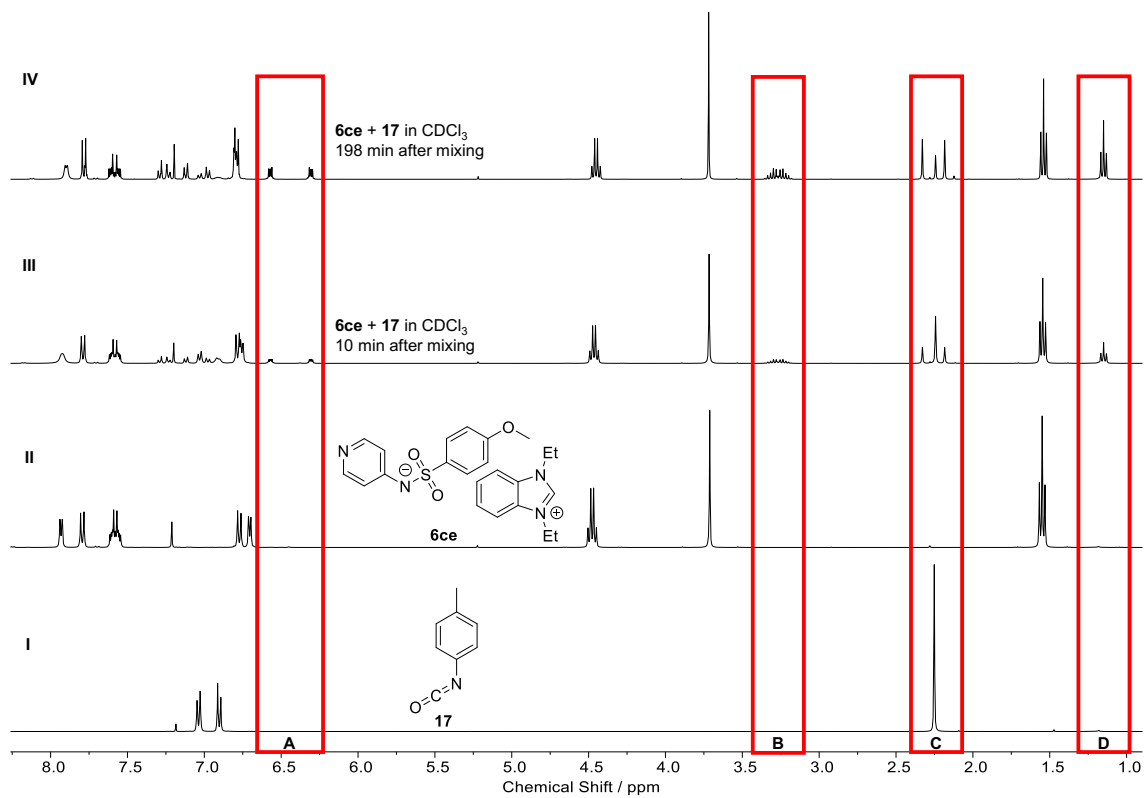


Figure S112. Stacked ^1H NMR spectra of stock solution of isocyanate **17** (I), stock solution of catalyst **6ce** (II), and a 1:1 mixture (molar) of both stock solutions after different times of reaction (III, IV). All spectra are recorded in CDCl_3 at 400 MHz.

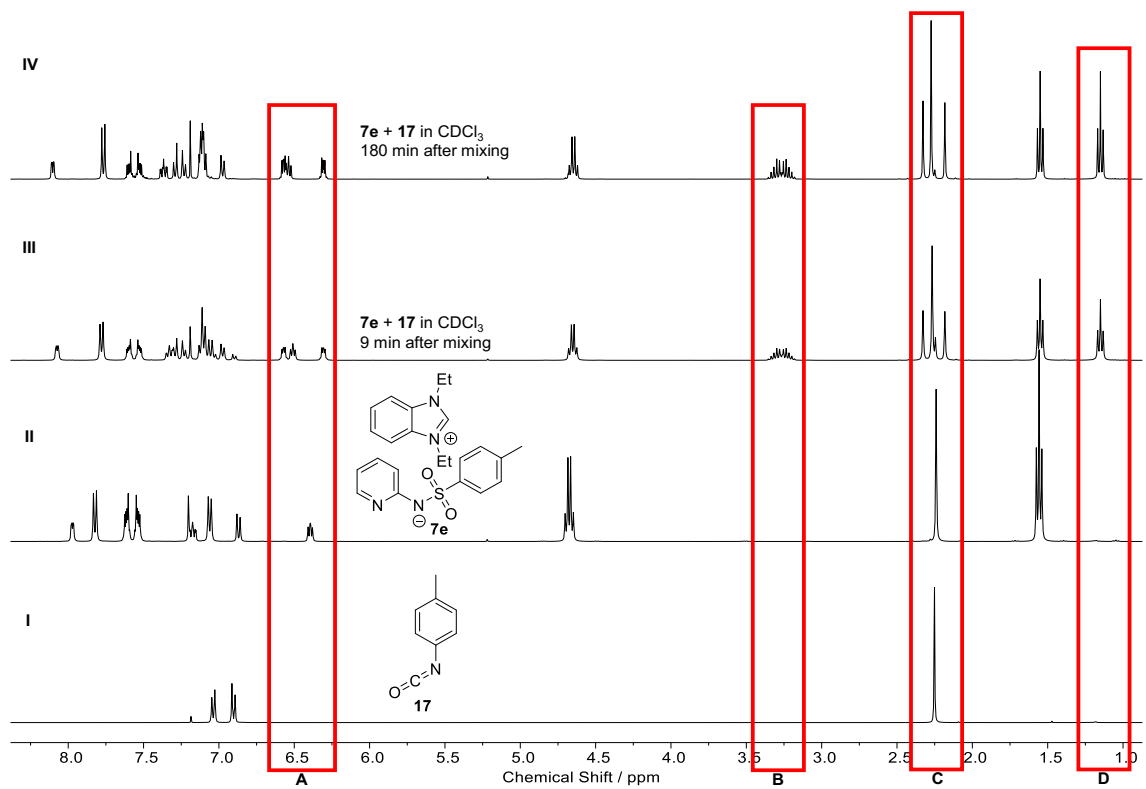


Figure S113. Stacked ^1H NMR spectra of stock solution of isocyanate **17** (I), stock solution of catalyst **7e** (II), and a 1:1 mixture (molar) of both stock solutions after different times of reaction (III, IV). All spectra are recorded in CDCl_3 at 400 MHz.

Both Figures show the same signals -although more pronounced- that we observed in the urethane benchmark reactions employing catalysts containing the benzimidazolium cation. More specifically, we observed a new set of multiplets (signals **A**), that by its distinct shape can be attributed to one of the aromatic protons of the benzimidazolium cation as shown in **Figure S114**, although shifted by more than one ppm high-field. A very similar shift was reported by Lemal *et al.* for a comparable system: They found signals at 6.63 and 6.53 ppm for the corresponding *N*-heterocyclic carbene (NHC)-dimer of compound **26** in diglyme-*d*₁₄ at room temperature. Upon heating to 110 °C, the signals shifted to 7.29 and 7.10 ppm and were attributed to the corresponding NHC.^[6]

We decided to get an ESI-HR-MS of the reaction mixture and found the dominant signal in the positive spectrum to be of mass 308.17571 (**7e** + **17**) and 308.17572 (**6ce** + **17**) respectively.

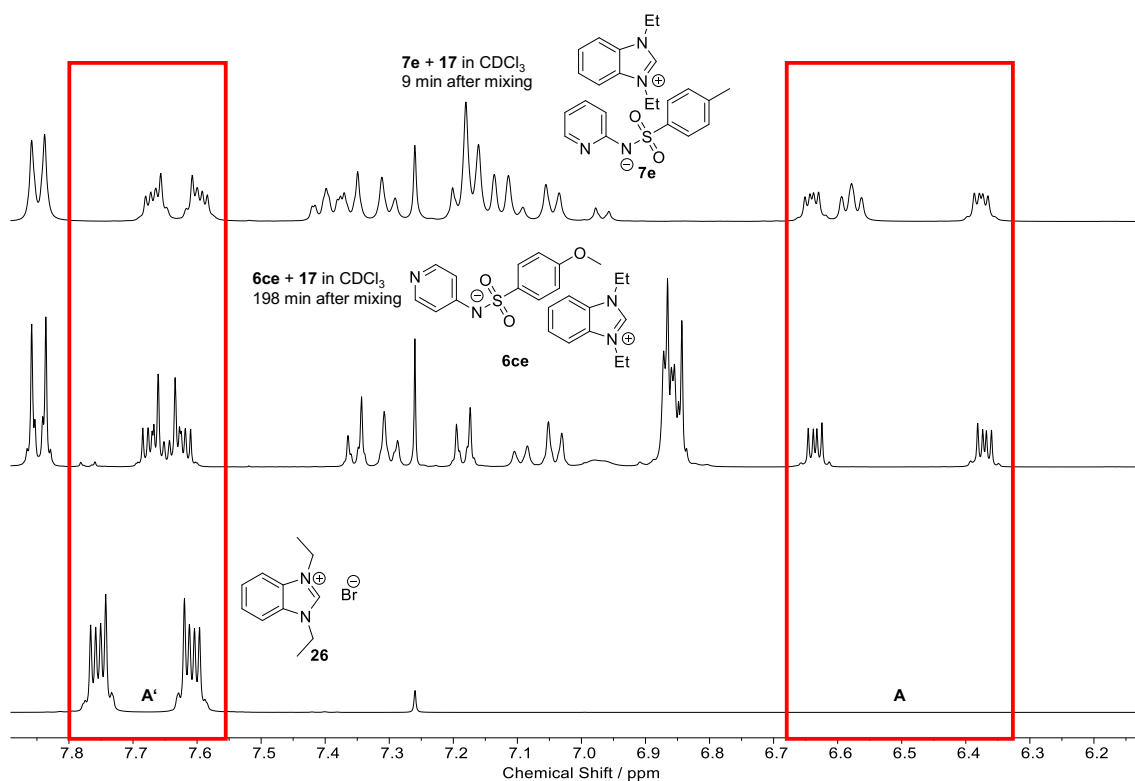
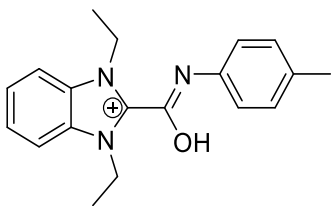


Figure S114. Detailed view of the signals in area **A** and the area **A'**, where the original signals of the corresponding aryl protons are found.

These findings, together with the reported shifts for the NHC dimer referenced above allowed us to propose the structure given in **Scheme S6** or an isomer of this structure. This is further supported by 2D NMR spectra directly linking one of the isocyanate *p*-methyl-signals in area **C** to the rest of the new signals via a single, well-separated ¹³C signal (**Figure S115**) and the integrals being in very good agreement as shown in **Figure S116**.



Exact Mass: 308.17574

Scheme S6. Structure proposed for the result of the positive ESI-HR-MS.

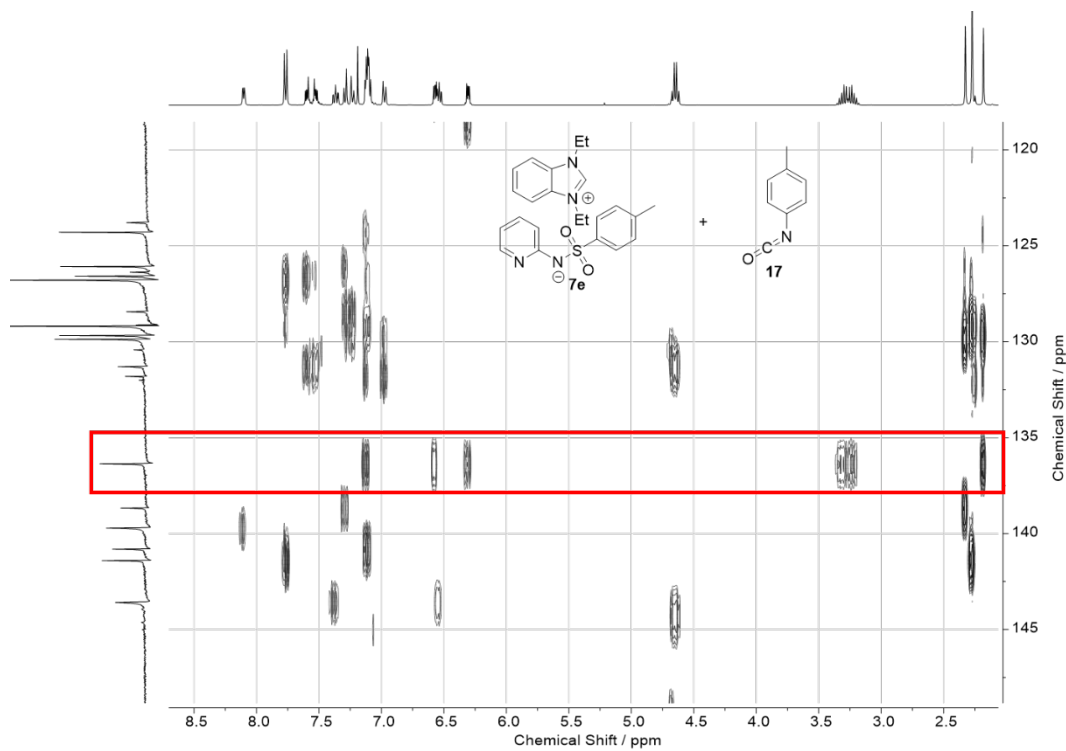


Figure S115. ^1H - ^{13}C HMBC NMR spectrum of a 1:1 mixture of **7e** and **17**. The ^{13}C signal interacting with both protons of the benzimidazole-unit and the isocyanate **17** is highlighted.

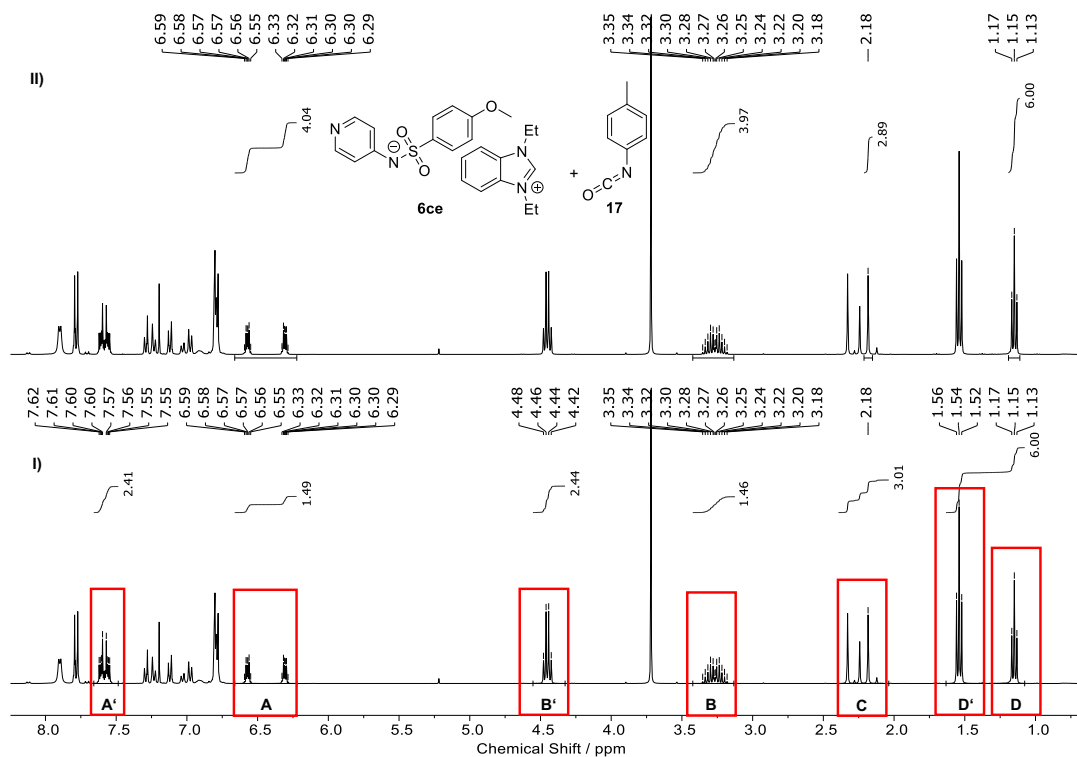


Figure S116. Identical ^1H NMR spectrum of a 1:1 mixture of **6ce** and **17**. Original signals and the new ones (**capital letter'** and **capital letter**) respectively are indicated in spectrum I).

Spectra I) and II) are identical and differ only with respect to the integrated areas.

Spectrum I) gives separate integrals for **A'** and **A** adding up to four protons (aryl signals of benzimidazole-compounds) and **B'** and **B** adding up to four protons (CH_2 -signals of benzimidazole-compounds). The integral area containing all different signals produced by the *p*-methyl signal of the isocyanate **C** adds up to three protons and **D'** and **D** are adding up to six protons representing the CH_3 -groups of the benzimidazole-compounds.

Spectrum II), on the other hand gives only the well-separated integrals of the proposed NHC-isocyanate adduct species in the expected ratio of 4/4/3/6, confirming our assignment of the majorly formed compound.

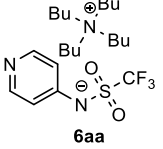
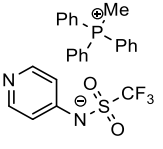
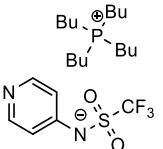
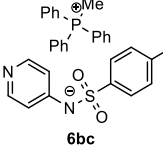
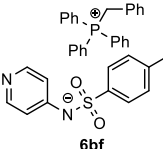
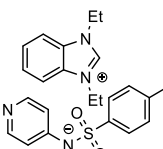
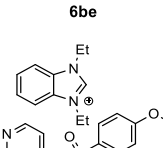
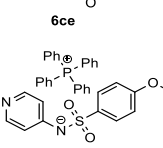
In conclusion, these experiments showed why the attempted benchmark-reactions with ion pair catalysts containing benzimidazolium counter ions gave "wild" mixtures with low estimated turnovers, because the ion pairs acted as *in-situ* generators of the corresponding NHCs that reacted with the abundantly present isocyanate **17** to form adducts as detected by NMR and HR-MS. Furthermore, not identified products were generated as well. In case of the triphenylmethyl phosphonium and the benzyltriphenyl phosphonium cation, similar, although less pronounced effects are observed, although for low catalyst concentrations (3 mol-%), there is no effect detectable beyond the experimental error of the measurements itself.

Crystallographic Data

Table of selected anion-cation interactions observed by single-crystal X-ray diffraction

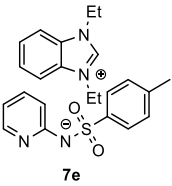
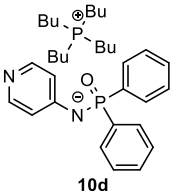
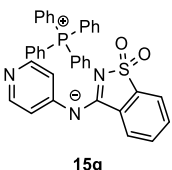
Values were obtained using the inbuilt "Contacts"-function of Mercury 3.8 (Short Contacts, intermolecular, < sum of vdW radii (150 pm)) on unit cells.

Table S4. Selected anion-cation interactions observed by single-crystal X-ray diffraction.

Entry	Catalyst	heteroatom(anion)→P/N(cation) ^a	pyridine-N →cation ^a	amide-N →cation ^a	heteroatom(anion)→cation ^a
1	 6aa	395.0 (O→N)	257.3 (α-H)	246.3 (α-H)	244.9 (O→β-H)
2	 6ac	394.5 (pyridine-N→P)	248.6 (β-H)	249.4 (α-H)	245.0 (O→β-H)
3	 6ad	394.4 (O→P)	253.4 (α-H)	264.2 (α-H)	238.1 (O→α-H)
4	 6bc	399.5 (O→P)	254.2 (α-H)	254.2 (α-H)	234.1 (O→α-H)
5	 6bf	420.1 (O→P)	278.9 (δ-H)	291.0 (β-H)	230.8 (O→α-H)
6	 6be	366.8 (O→N)	270.2 (β-H)	268.0 (α-H)	213.3 (O→α-H)
7	 6ce	391.0 (SO ₂ -O→N)	244.7 (α-H)	255.9 (α-H)	222.0 (SO ₂ -O→ α-H)
8	 6cg	467.9 (Me-O→P)	285.7 (α-H)	267.6 (β-H)	241.4 (Me-O→α-H)

^a in pm.

Table S4 (continuation). Selected anion-cation interactions observed by single-crystal X-ray diffraction.

9	 7e	388.4 (O→N)	243.6 (α-H)	217.6 (α-H)	217.6 (amide-N→α-H)
10	 10d	368.9 (O→P)	247.9 (α-H)	286.2 (δ-H)	219.5 (O→α-H)
11	 15g	506.6 (O→P)	251.8 (γ-H)	280.1 (β-H)	238.3 (O→γ-H)

^a in pm.

As discussed in the main part of this publication, we found that in the solid state the cation is usually rather closer to the amide moiety as indicated by columns 3 and 7. The only true exception is the structurally different ion pair **7e**. In the case of our most active example **6cg**, the closest interactions originate from the methoxy group's oxygen still indicating that the cation is not coordinated by the pyridine part.

Tetrabutylammonium pyridin-4-yl((trifluoromethyl)sulfonyl)amide **6aa**

Figure S117 shows a single ion pair, **Figure S118** gives the unit cell and crystallographic data for catalyst system **6aa** is given in **Table S5**:

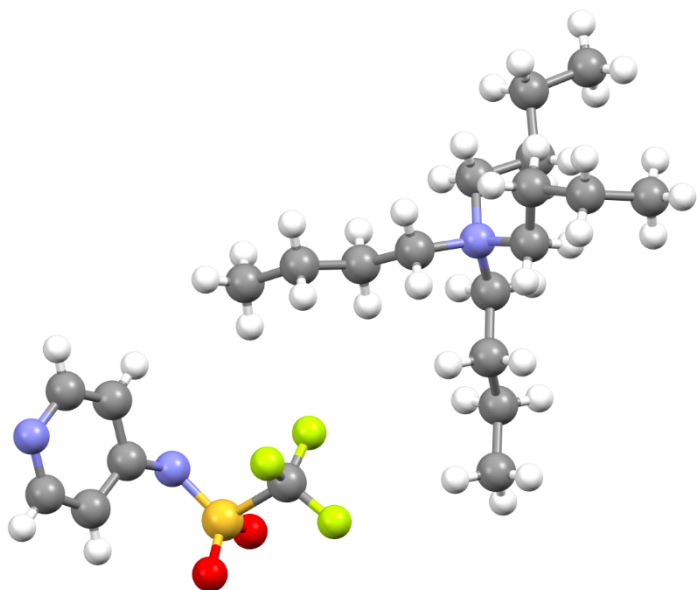


Figure S117. Ion pair of catalyst **6aa**.

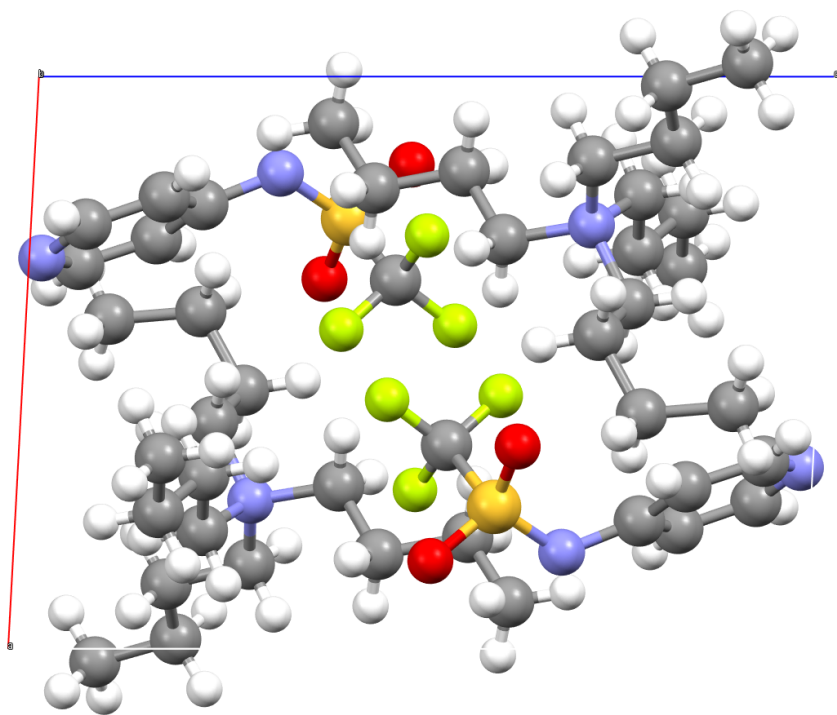


Figure S118. Unit cell of catalyst **6aa** viewed along the *b*-axis.

Table S5. Crystallographic details for ion pair catalyst **6aa**.

net formula	C ₂₂ H ₄₀ F ₃ N ₃ O ₂ S
<i>M_r</i> /g mol ⁻¹	467.63
crystal size/mm	0.100 × 0.080 × 0.050
<i>T</i> /K	100.(2)
radiation	MoKα
diffractometer	'Bruker D8 Venture TXS'
crystal system	triclinic
space group	'P -1'
<i>a</i> /Å	9.7164(18)
<i>b</i> /Å	10.1395(15)
<i>c</i> /Å	13.851(3)
<i>α</i> /°	71.337(5)
<i>β</i> /°	88.764(6)
<i>γ</i> /°	77.117(10)
<i>V</i> /Å ³	1258.5(4)
<i>Z</i>	2
calc. density/g cm ⁻³	1.234
<i>μ</i> /mm ⁻¹	0.173
absorption correction	Multi-Scan
transmission factor range	0.9346–0.9705
refls. measured	24387
<i>R</i> _{int}	0.0406
mean <i>σ</i> (<i>I</i>)/ <i>I</i>	0.0301
<i>θ</i> range	2.723–26.450
observed refls.	4504
<i>x</i> , <i>y</i> (weighting scheme)	0.0343, 0.6485
hydrogen refinement	constr
refls in refinement	5178
parameters	284
restraints	0
<i>R</i> (<i>F</i> _{obs})	0.0346
<i>R</i> _w (<i>F</i> ²)	0.0903
<i>S</i>	1.053
shift/error _{max}	0.001
max electron density/e Å ⁻³	0.361
min electron density/e Å ⁻³	-0.436

Methyltriphenylphosphonium pyridin-4-yl((trifluoromethyl)sulfonyl)amide **6ac**

Figure S119 shows a single ion pair, **Figure S120** gives the unit cell and crystallographic data for catalyst system **6ac** is given in **Table S6**:

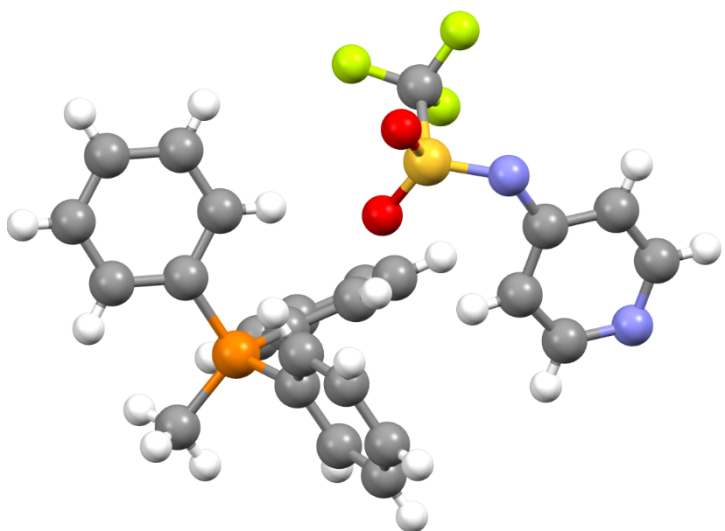


Figure S119. Ion pair of catalyst **6ac**.

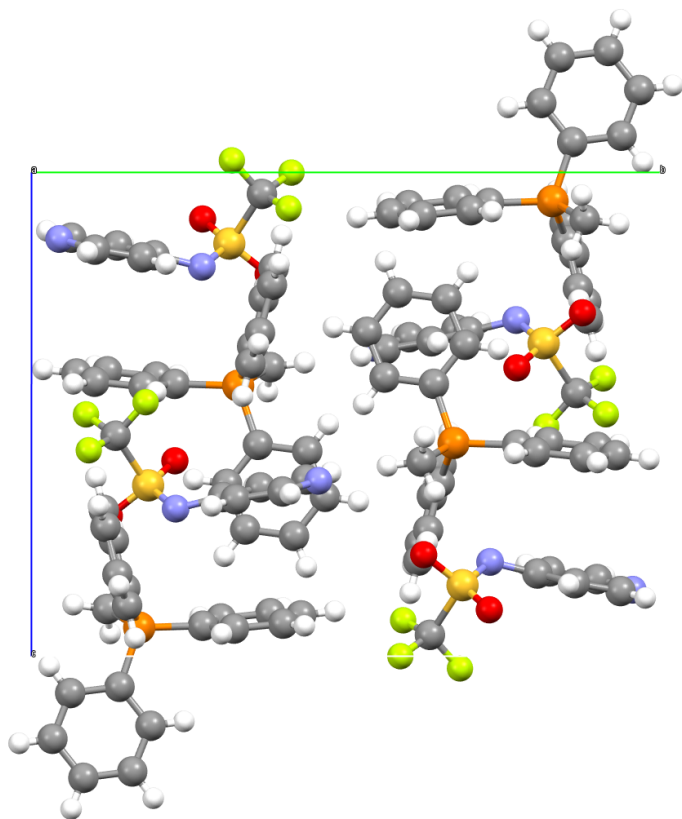


Figure S120. Unit cell of catalyst **6ac** viewed along the *a*-axis.

Table S6. [Table S6]. Crystallographic details for ion pair catalyst **6ac**.

net formula	C ₂₅ H ₂₂ F ₃ N ₂ O ₂ PS
<i>M_r</i> /g mol ⁻¹	502.47
crystal size/mm	0.100 × 0.090 × 0.060
<i>T</i> /K	100.(2)
radiation	MoKα
diffractometer	'Bruker D8 Venture TXS'
crystal system	monoclinic
space group	'P 1 21/n 1'
<i>a</i> /Å	10.2414(4)
<i>b</i> /Å	17.5228(6)
<i>c</i> /Å	14.1388(5)
α /°	90
β /°	107.3215(12)
γ /°	90
<i>V</i> /Å ³	2422.25(15)
<i>Z</i>	4
calc. density/g cm ⁻³	1.378
μ /mm ⁻¹	0.248
absorption correction	Multi-Scan
transmission factor range	0.9303–0.9705
refls. measured	30328
<i>R</i> _{int}	0.0463
mean $\sigma(I)/I$	0.0395
θ range	3.137–30.508
observed refls.	6189
<i>x</i> , <i>y</i> (weighting scheme)	0.0365, 1.4492
hydrogen refinement	constr
refls in refinement	7370
parameters	308
restraints	0
<i>R</i> (<i>F</i> _{obs})	0.0371
<i>R</i> _w (<i>F</i> ²)	0.0993
<i>S</i>	1.048
shift/error _{max}	0.001
max electron density/e Å ⁻³	0.423
min electron density/e Å ⁻³	-0.468

Tetrabutylphosphonium pyridin-4-yl((trifluoromethyl)sulfonyl)amide **6ad**

One of the butyl-chains of the phosphonium-cation is disordered. A split model was applied, the site occupation factor is ca. 1:1.

Figure S121 shows a single ion pair, **Figure S122** gives the unit cell and crystallographic data for catalyst system **6ad** is given in **Table S7**:

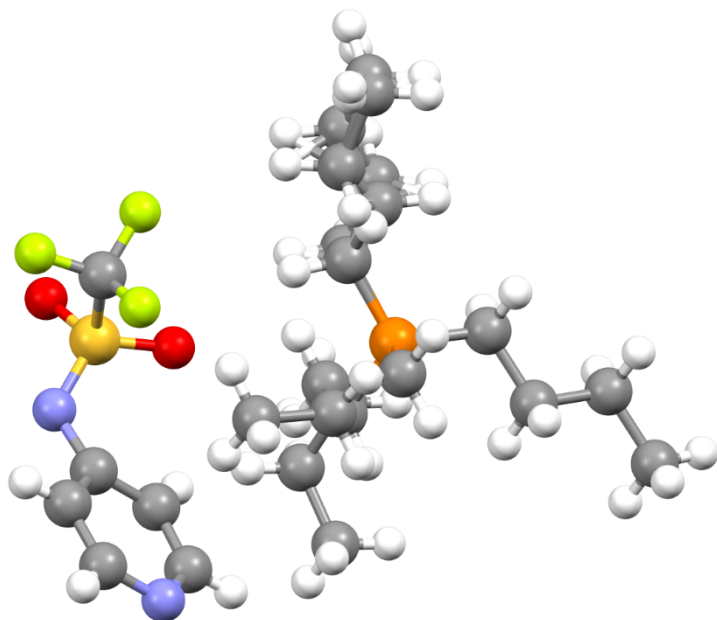


Figure S121. Ion pair of catalyst **6ad**.

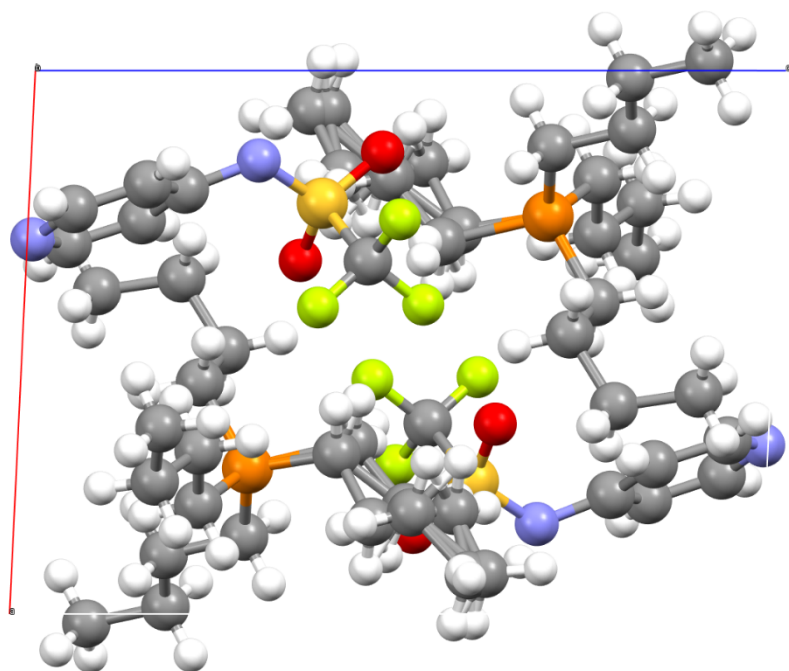


Figure S122. Unit cell of catalyst **6ad** viewed along the *b*-axis.

Table S7. Crystallographic details for ion pair catalyst **6ad**.

net formula	C ₂₂ H ₄₀ F ₃ N ₂ O ₂ PS
<i>M_r</i> /g mol ⁻¹	484.59
crystal size/mm	0.100 × 0.090 × 0.040
<i>T</i> /K	100.(2)
radiation	MoKα
diffractometer	'Bruker D8 Venture TXS'
crystal system	triclinic
space group	'P -1'
<i>a</i> /Å	9.8521(3)
<i>b</i> /Å	10.4233(4)
<i>c</i> /Å	13.8342(5)
<i>α</i> °	72.0296(13)
<i>β</i> °	88.1523(12)
<i>γ</i> °	75.7263(12)
<i>V</i> /Å ³	1308.15(8)
<i>Z</i>	2
calc. density/g cm ⁻³	1.230
<i>μ</i> /mm ⁻¹	0.226
absorption correction	Multi-Scan
transmission factor range	0.8946–0.9705
refls. measured	15218
<i>R</i> _{int}	0.0394
mean <i>σ</i> (<i>I</i>)/ <i>I</i>	0.0573
<i>θ</i> range	3.167–28.279
observed refls.	4801
<i>x</i> , <i>y</i> (weighting scheme)	0.0395, 0.7033
hydrogen refinement	constr
refls in refinement	6472
parameters	322
restraints	0
<i>R</i> (<i>F</i> _{obs})	0.0473
<i>R</i> _w (<i>F</i> ²)	0.1164
<i>S</i>	1.032
shift/error _{max}	0.001
max electron density/e Å ⁻³	0.398
min electron density/e Å ⁻³	-0.368

One side chain disordered, split model applied, sof ratio ca. 1:1.

Methyltriphenylphosphonium pyridin-4-yl(tosyl)amide **6bc**

Figure S123 shows a single ion pair, **Figure S124** gives the unit cell and crystallographic data for catalyst system **6bc** is given in **Table S8**:

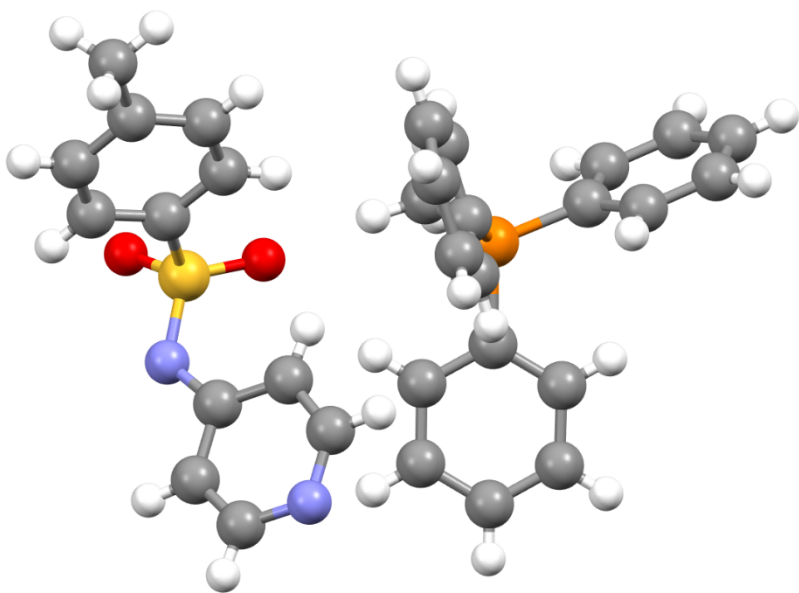


Figure S123. Ion pair of catalyst **6bc**.

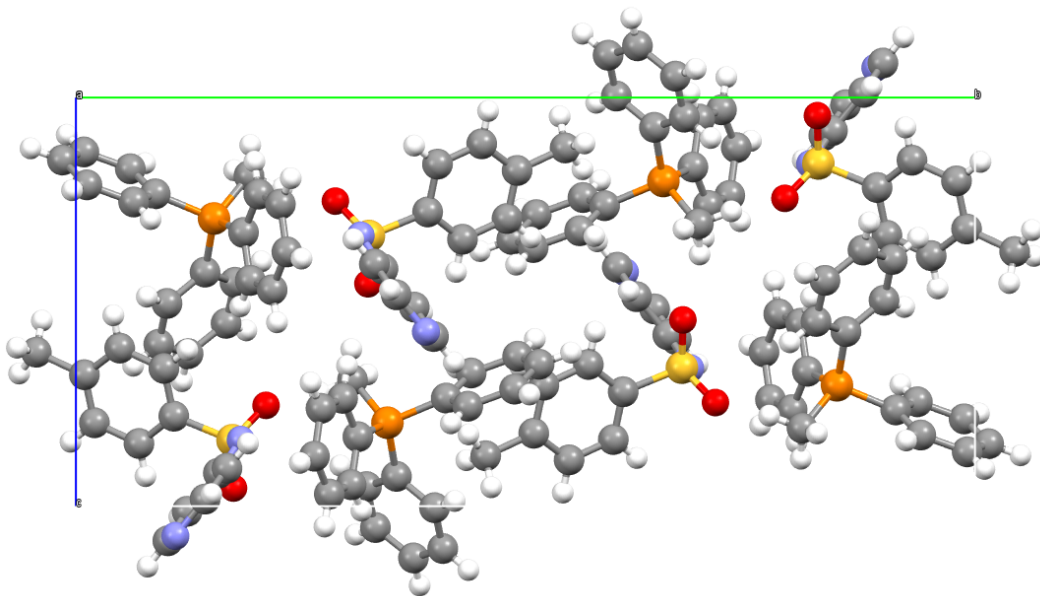


Figure S124. Unit cell of catalyst **6bc** viewed along the *a*-axis.

Table S8. Crystallographic details for ion pair catalyst **6bc**.

net formula	C ₃₁ H ₂₉ N ₂ O ₂ PS
<i>M</i> _r /g mol ⁻¹	524.59
crystal size/mm	0.100 × 0.090 × 0.050
<i>T</i> /K	100.(2)
radiation	MoKα
diffractometer	'Bruker D8 Venture TXS'
crystal system	monoclinic
space group	'P 1 21/n 1'
<i>a</i> /Å	9.6174(6)
<i>b</i> /Å	24.8400(18)
<i>c</i> /Å	11.3600(7)
<i>α</i> /°	90
<i>β</i> /°	97.197(3)
<i>γ</i> /°	90
<i>V</i> /Å ³	2692.5(3)
<i>Z</i>	4
calc. density/g cm ⁻³	1.294
<i>μ</i> /mm ⁻¹	0.211
absorption correction	Multi-Scan
transmission factor range	0.9338–0.9705
refls. measured	43294
<i>R</i> _{int}	0.0378
mean <i>σ</i> (<i>I</i>)/ <i>I</i>	0.0286
<i>θ</i> range	3.258–30.507
observed refls.	7198
<i>x</i> , <i>y</i> (weighting scheme)	0.0355, 1.8155
hydrogen refinement	constr
refls in refinement	8205
parameters	336
restraints	0
<i>R</i> (<i>F</i> _{obs})	0.0360
<i>R</i> _w (<i>F</i> ²)	0.0963
<i>S</i>	1.073
shift/error _{max}	0.001
max electron density/e Å ⁻³	0.447
min electron density/e Å ⁻³	-0.450

Benzyltriphenylphosphonium pyridin-4-yl(tosyl)amide **6bf**

Figure S125 shows a single ion pair, **Figure S126** gives the unit cell and crystallographic data for catalyst system **6bf** is given in **Table S9**:

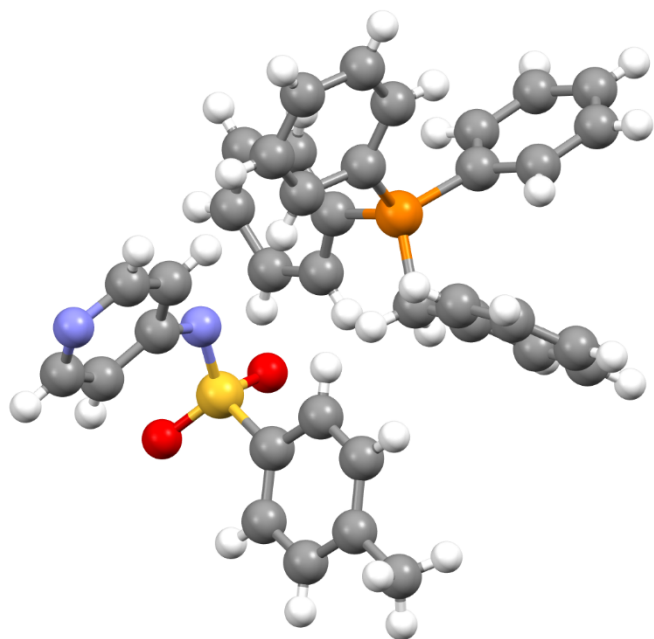


Figure S125. Ion pair of catalyst **6bf**.

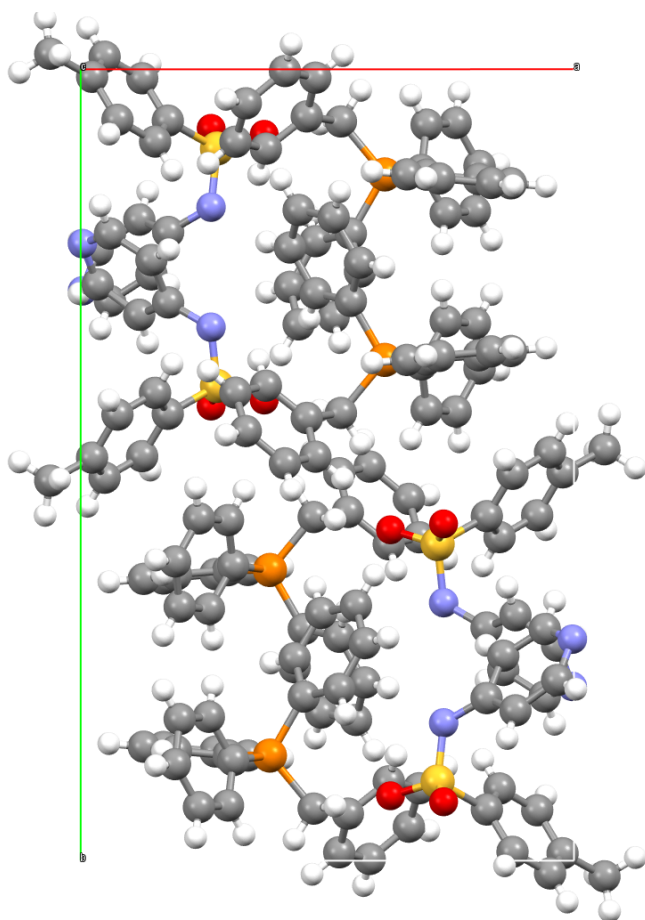


Figure S126. Unit cell of catalyst **6bf** viewed along the *c*-axis.

Table S9. Crystallographic details for ion pair catalyst **6bf**.

net formula	C ₃₇ H ₃₃ N ₂ O ₂ PS
<i>M_r</i> /g mol ⁻¹	600.68
crystal size/mm	0.060 × 0.050 × 0.040
<i>T</i> /K	296.(2)
radiation	MoKα
diffractometer	'Bruker D8Quest'
crystal system	monoclinic
space group	'P 1 21/c 1'
<i>a</i> /Å	13.7440(17)
<i>b</i> /Å	20.825(3)
<i>c</i> /Å	11.4009(18)
<i>α</i> /°	90
<i>β</i> /°	109.349(4)
<i>γ</i> /°	90
<i>V</i> /Å ³	3078.8(8)
<i>Z</i>	4
calc. density/g cm ⁻³	1.296
<i>μ</i> /mm ⁻¹	0.194
absorption correction	Multi-Scan
transmission factor range	0.94–0.99
refls. measured	58691
<i>R</i> _{int}	0.0812
mean <i>σ</i> (<i>I</i>)/ <i>I</i>	0.0397
<i>θ</i> range	3.142–26.372
observed refls.	5029
<i>x</i> , <i>y</i> (weighting scheme)	0.0525, 2.6093
hydrogen refinement	constr
refls in refinement	6275
parameters	389
restraints	3
<i>R</i> (<i>F</i> _{obs})	0.0628
<i>R</i> _w (<i>F</i> ²)	0.1453
<i>S</i>	1.080
shift/error _{max}	0.001
max electron density/e Å ⁻³	0.314
min electron density/e Å ⁻³	-0.316

DELU applied for C17-C18 and C18-C19.

1,3-diethyl-benzimidazolium pyridin-4-yl(tosyl)amide **6be**

Figure S127 shows a single ion pair, **Figure S128** gives the unit cell and crystallographic data for catalyst system **6be** is given in **Table S10**:

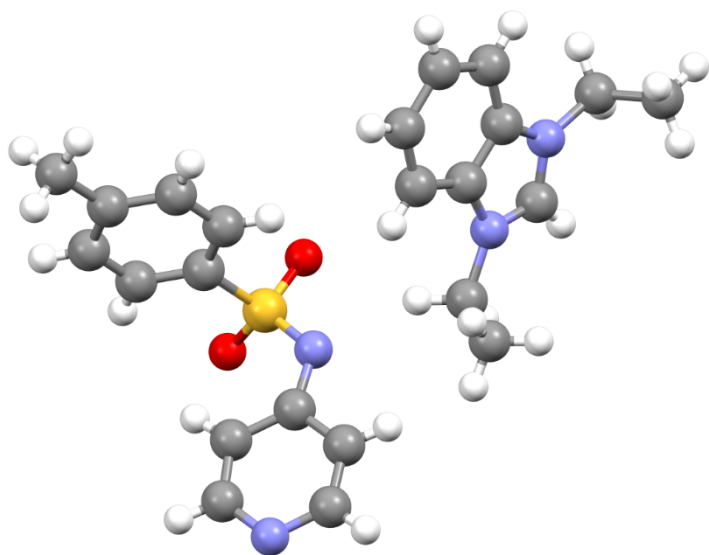


Figure S127. Ion pair of catalyst **6be**.

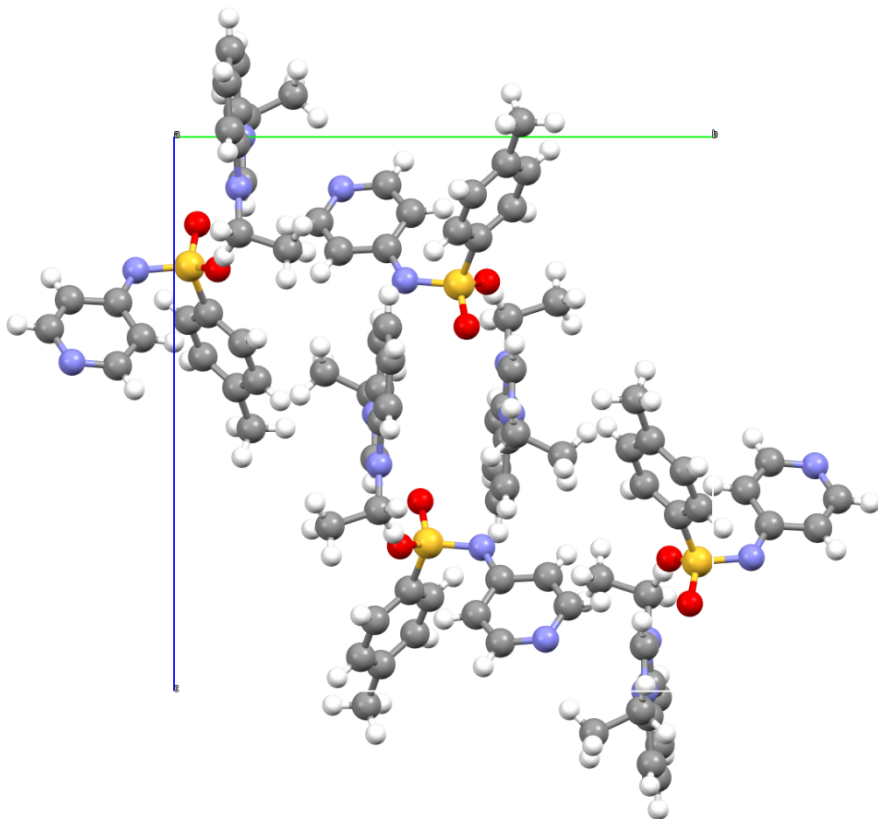


Figure S128. Unit cell of catalyst **6be** viewed along the *a*-axis.

Table S10. Crystallographic details for ion pair catalyst **6be**.

net formula	C ₂₃ H ₂₆ N ₄ O ₂ S
<i>M_r</i> /g mol ⁻¹	422.54
crystal size/mm	0.080 × 0.050 × 0.030
<i>T</i> /K	112.(2)
radiation	MoKα
diffractometer	'Bruker D8 Venture TXS'
crystal system	monoclinic
space group	'P 1 21/c 1'
<i>a</i> /Å	8.6461(8)
<i>b</i> /Å	15.4957(14)
<i>c</i> /Å	16.3096(13)
<i>α</i> /°	90
<i>β</i> /°	102.024(3)
<i>γ</i> /°	90
<i>V</i> /Å ³	2137.2(3)
<i>Z</i>	4
calc. density/g cm ⁻³	1.313
<i>μ</i> /mm ⁻¹	0.179
absorption correction	Multi-Scan
transmission factor range	0.97–0.99
refls. measured	37309
<i>R</i> _{int}	0.0531
mean <i>σ</i> (<i>I</i>)/ <i>I</i>	0.0314
<i>θ</i> range	2.872–27.097
observed refls.	3986
<i>x</i> , <i>y</i> (weighting scheme)	0.0381, 1.4408
hydrogen refinement	constr
refls in refinement	4709
parameters	274
restraints	0
<i>R</i> (<i>F</i> _{obs})	0.0376
<i>R</i> _w (<i>F</i> ²)	0.0993
<i>S</i>	1.034
shift/error _{max}	0.001
max electron density/e Å ⁻³	0.251
min electron density/e Å ⁻³	-0.440

Tetraphenylphosphonium ((4-methoxyphenyl)sulfonyl)(pyridin-4-yl)amide **6cg**

Figure S129 shows a single ion pair, **Figure S130** gives the unit cell and crystallographic data for catalyst system **6cg** is given in **Table S11**:

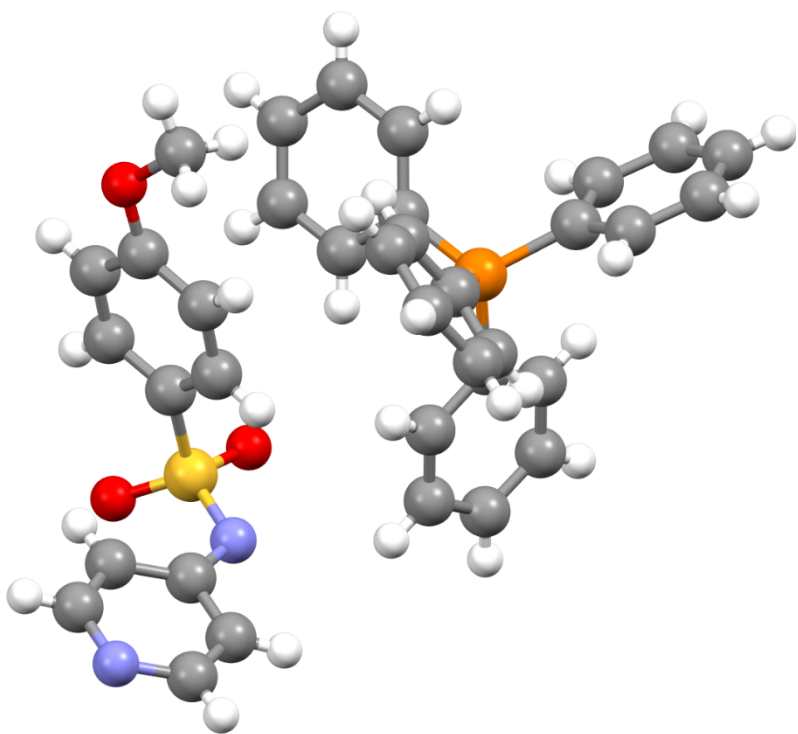


Figure S129. Ion pair of catalyst **6cg**.

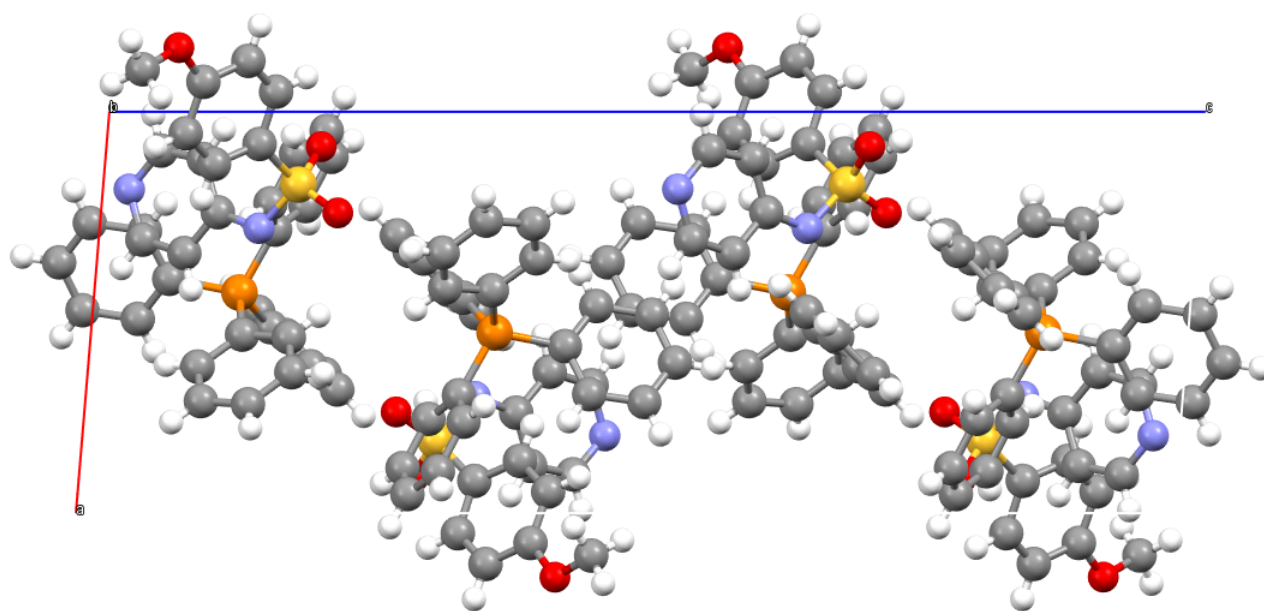


Figure S130. Unit cell of catalyst **6cg** viewed along the *b*-axis.

Table S11. Crystallographic details for ion pair catalyst **6cg**.

net formula	C ₃₆ H ₃₁ N ₂ O ₃ PS
<i>M_r</i> /g mol ⁻¹	602.66
crystal size/mm	0.090 × 0.070 × 0.050
<i>T</i> /K	298.(2)
radiation	MoKα
diffractometer	'Bruker D8 Venture TXS'
crystal system	monoclinic
space group	'P 1 21/c 1'
<i>a</i> /Å	9.8948(3)
<i>b</i> /Å	11.5408(3)
<i>c</i> /Å	26.9578(7)
<i>α</i> /°	90
<i>β</i> /°	94.7690(10)
<i>γ</i> /°	90
<i>V</i> /Å ³	3067.76(15)
<i>Z</i>	4
calc. density/g cm ⁻³	1.305
<i>μ</i> /mm ⁻¹	0.197
absorption correction	Multi-Scan
transmission factor range	0.95–0.99
refls. measured	32004
<i>R</i> _{int}	0.0384
mean <i>σ</i> (<i>I</i>)/ <i>I</i>	0.0319
<i>θ</i> range	2.867–27.103
observed refls.	5056
<i>x</i> , <i>y</i> (weighting scheme)	0.0440, 1.4908
hydrogen refinement	constr
refls in refinement	6770
parameters	389
restraints	0
<i>R</i> (<i>F</i> _{obs})	0.0436
<i>R</i> _w (<i>F</i> ²)	0.1165
<i>S</i>	1.030
shift/error _{max}	0.001
max electron density/e Å ⁻³	0.262
min electron density/e Å ⁻³	-0.309

1,3-diethyl-benzimidazolium ((4-methoxyphenyl)sulfonyl)(pyridin-4-yl)amide **6ce**

Figure S131 shows a single ion pair, **Figure S132** gives the unit cell and crystallographic data for catalyst system **6ce** is given in **Table S12**:

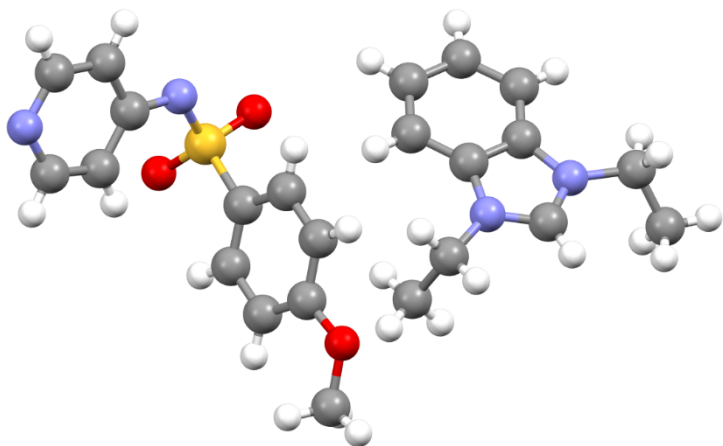


Figure S131. Ion pair of catalyst **6ce**.

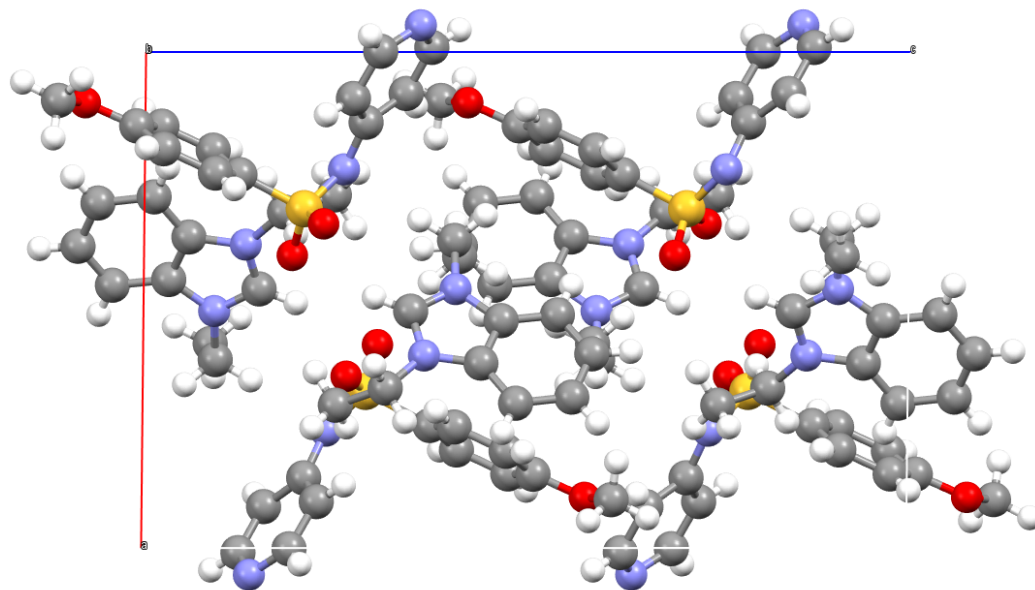


Figure S132. Unit cell of catalyst **6ce** viewed along the *b*-axis.

Table S12. Crystallographic details for ion pair catalyst **6ce**.

net formula	C ₂₃ H ₂₆ N ₄ O ₃ S
<i>M_r</i> /g mol ⁻¹	438.54
crystal size/mm	0.090 × 0.040 × 0.030
<i>T</i> /K	107.(2)
radiation	MoKα
diffractometer	'Bruker D8 Venture TXS'
crystal system	monoclinic
space group	'P 1 21/c 1'
<i>a</i> /Å	11.9827(9)
<i>b</i> /Å	9.6390(7)
<i>c</i> /Å	18.4664(15)
<i>α</i> /°	90
<i>β</i> /°	90.582(3)
<i>γ</i> /°	90
<i>V</i> /Å ³	2132.8(3)
<i>Z</i>	4
calc. density/g cm ⁻³	1.366
<i>μ</i> /mm ⁻¹	0.185
absorption correction	Multi-Scan
transmission factor range	0.95–0.99
refls. measured	28433
<i>R</i> _{int}	0.0481
mean <i>σ</i> (<i>I</i>)/ <i>I</i>	0.0322
<i>θ</i> range	2.934–26.372
observed refls.	3618
<i>x</i> , <i>y</i> (weighting scheme)	0.0382, 1.6219
hydrogen refinement	constr
refls in refinement	4342
parameters	283
restraints	1
<i>R</i> (<i>F</i> _{obs})	0.0402
<i>R</i> _w (<i>F</i> ²)	0.1050
<i>S</i>	1.050
shift/error _{max}	0.001
max electron density/e Å ⁻³	0.378
min electron density/e Å ⁻³	-0.408

1,3-diethyl-benzimidazolium pyridin-2-yl(tosyl)amide **7e**

Figure S133 shows a single ion pair, **Figure S134** gives the unit cell and crystallographic data for catalyst system **7e** is given in **Table S13**:

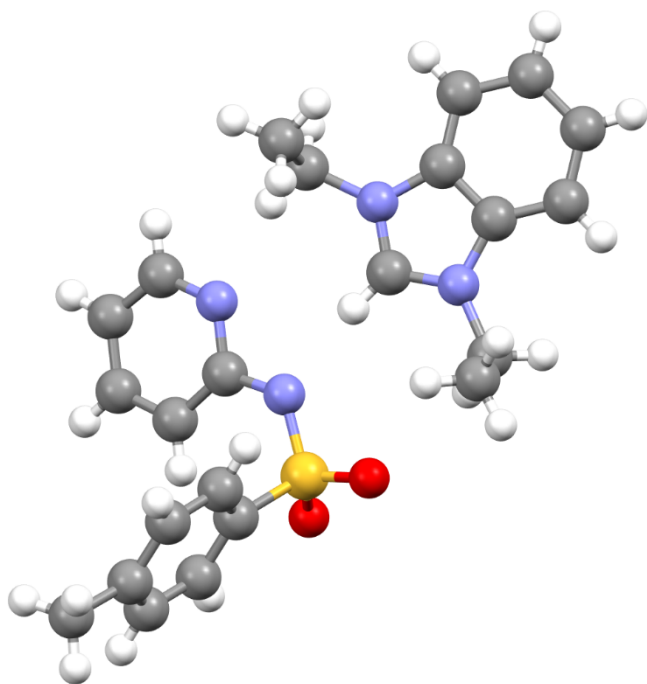


Figure S133. Ion pair of catalyst **7e**.

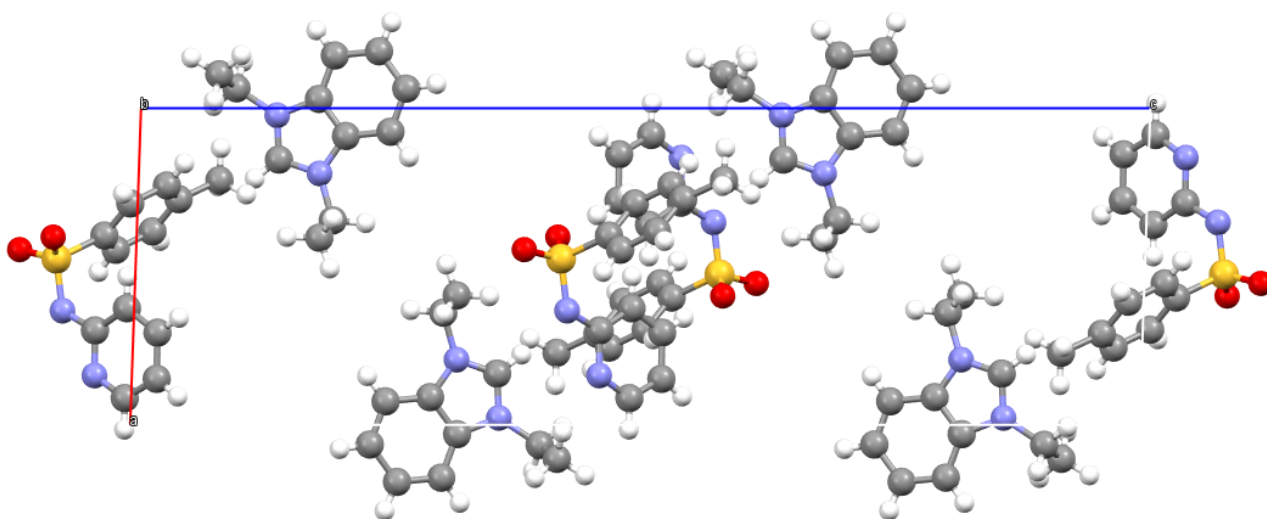


Figure S134. Unit cell of catalyst **7e** viewed along the *b*-axis.

Table S13. Crystallographic details for ion pair catalyst **7e**.

net formula	C ₂₃ H ₂₆ N ₄ O ₂ S
<i>M_r</i> /g mol ⁻¹	422.54
crystal size/mm	0.080 × 0.040 × 0.030
<i>T</i> /K	106.(2)
radiation	MoK α
diffractometer	'Bruker D8 Venture TXS'
crystal system	monoclinic
space group	'P 1 21/c 1'
<i>a</i> /Å	9.5001(3)
<i>b</i> /Å	14.8911(4)
<i>c</i> /Å	30.2630(9)
α /°	90
β /°	91.9590(10)
γ /°	90
<i>V</i> /Å ³	4278.7(2)
<i>Z</i>	8
calc. density/g cm ⁻³	1.312
μ /mm ⁻¹	0.179
absorption correction	Multi-Scan
transmission factor range	0.94–0.99
refls. measured	63746
<i>R</i> _{int}	0.0532
mean $\sigma(I)/I$	0.0294
θ range	2.544–25.350
observed refls.	6407
<i>x</i> , <i>y</i> (weighting scheme)	0.0379, 2.4800
hydrogen refinement	constr
refls in refinement	7815
parameters	547
restraints	0
<i>R</i> (<i>F</i> _{obs})	0.0385
<i>R</i> _w (<i>F</i> ²)	0.0949
<i>S</i>	1.062
shift/error _{max}	0.001
max electron density/e Å ⁻³	0.285
min electron density/e Å ⁻³	-0.433

1,1,1-trifluoro-N-(pyridin-4(1H)-ylidene)methanesulfonamide **8a**

Recrystallization was done from H₂O.

Figure S135 shows a single molecule, **Figure S136** gives the unit cell and crystallographic data for sulfonamide **8a** is given in **Table S14**:

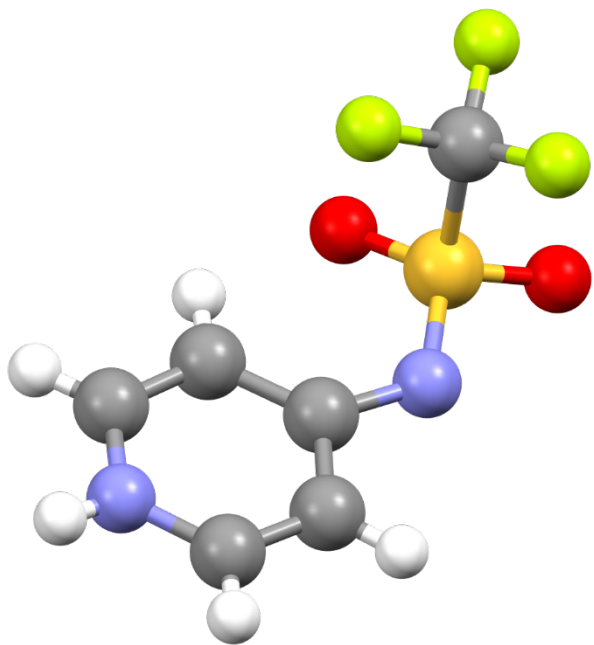


Figure S135. Molecule of sulfonamide **8a**.

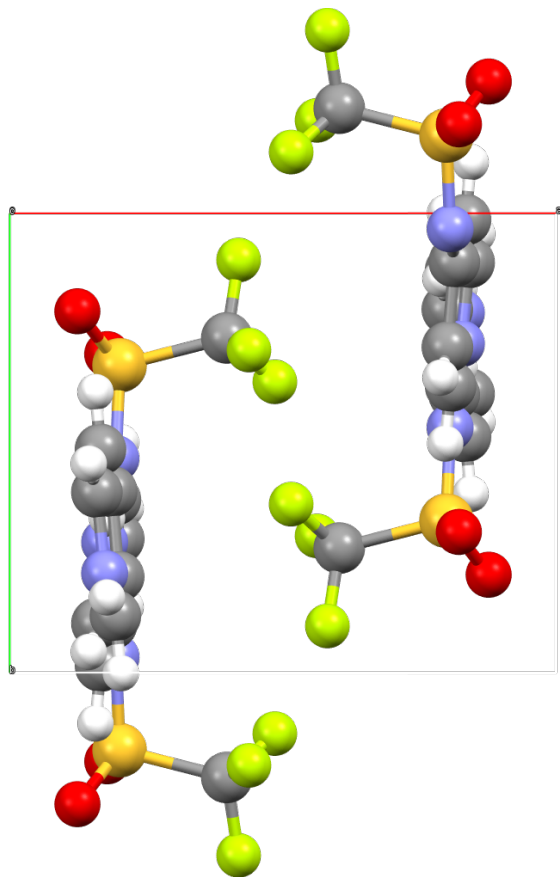


Figure S136. Unit cell of sulfonamide **8a** viewed along the c-axis.

Table S14. [Table S14]. Crystallographic details for sulfonamide **8a**.

net formula	C ₆ H ₅ F ₃ N ₂ O ₂ S
<i>M</i> _r /g mol ⁻¹	226.18
crystal size/mm	0.090 × 0.050 × 0.040
<i>T</i> /K	105.(2)
radiation	MoKα
diffractometer	'Bruker D8 Venture TXS'
crystal system	monoclinic
space group	'P 1 21/c 1'
<i>a</i> /Å	9.3732(7)
<i>b</i> /Å	7.5696(5)
<i>c</i> /Å	12.4533(8)
<i>α</i> /°	90
<i>β</i> /°	106.212(2)
<i>γ</i> /°	90
<i>V</i> /Å ³	848.44(10)
<i>Z</i>	4
calc. density/g cm ⁻³	1.771
<i>μ</i> /mm ⁻¹	0.407
absorption correction	Multi-Scan
transmission factor range	0.94–0.98
refls. measured	17191
<i>R</i> _{int}	0.0431
mean <i>σ</i> (<i>I</i>)/ <i>I</i>	0.0273
<i>θ</i> range	3.185–30.505
observed refls.	2260
<i>x</i> , <i>y</i> (weighting scheme)	0.0370, 0.5851
hydrogen refinement	H(C) constr, H(N) refall
refls in refinement	2573
parameters	131
restraints	0
<i>R</i> (<i>F</i> _{obs})	0.0326
<i>R</i> _w (<i>F</i> ²)	0.0892
<i>S</i>	1.070
shift/error _{max}	0.001
max electron density/e Å ⁻³	0.458
min electron density/e Å ⁻³	-0.383

4-methyl-N-(pyridin-4(1H)-ylidene)benzenesulfonamide **8b**

Recrystallization was done from DMSO.

Figure S137 shows a single molecule, **Figure S138** gives the unit cell and crystallographic data for sulfonamide **8b** is given in **Table S15**:

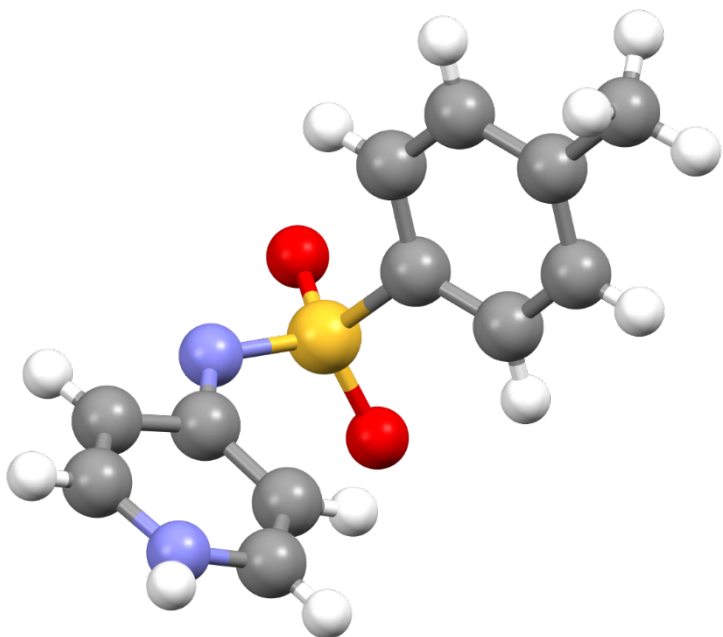


Figure S137. Molecule of sulfonamide **8b**.

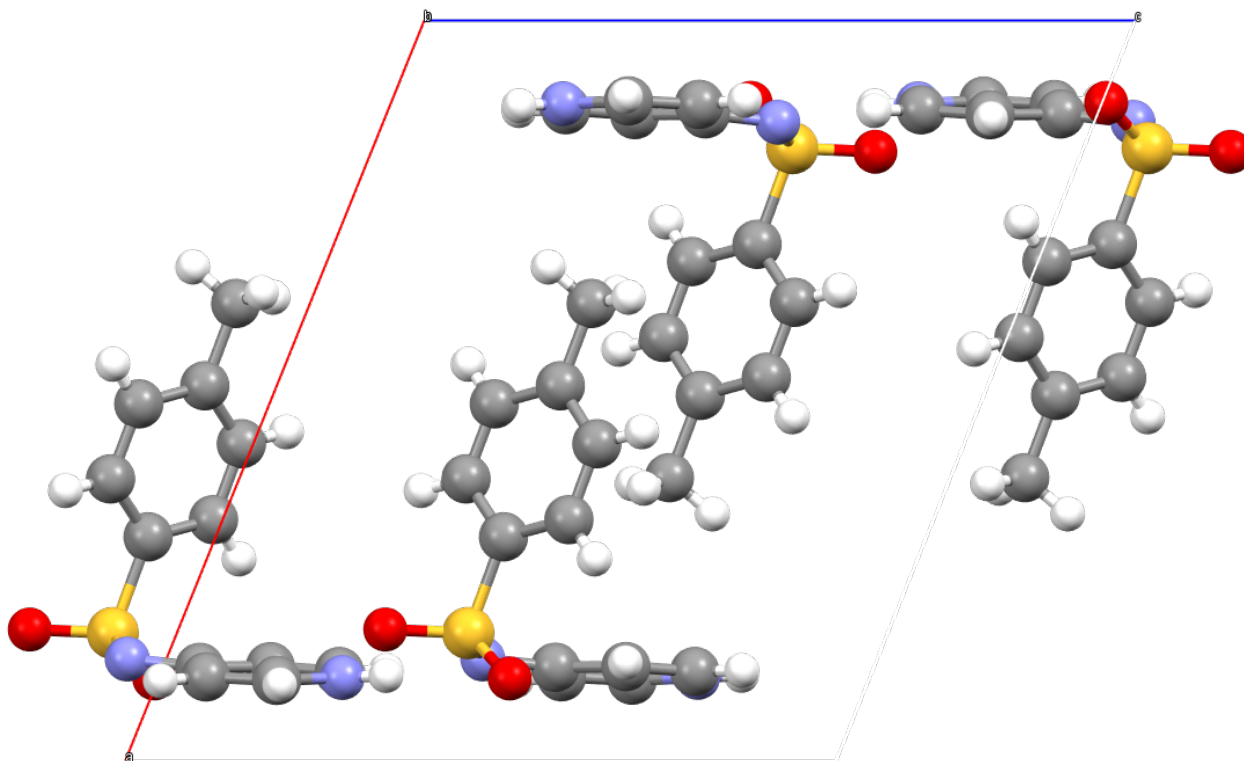


Figure S138. Unit cell of sulfonamide **8b** viewed along the *b*-axis.

Table S15. Crystallographic details for sulfonamide **8b**.

net formula	C ₁₂ H ₁₂ N ₂ O ₂ S
<i>M_r</i> /g mol ⁻¹	248.30
crystal size/mm	0.100 × 0.100 × 0.050
<i>T</i> /K	105.(2)
radiation	MoKα
diffractometer	'Bruker D8 Venture TXS'
crystal system	monoclinic
space group	'P 1 21/c 1'
<i>a</i> /Å	13.7763(6)
<i>b</i> /Å	7.4726(3)
<i>c</i> /Å	12.2799(6)
<i>α</i> /°	90
<i>β</i> /°	112.0110(10)
<i>γ</i> /°	90
<i>V</i> /Å ³	1172.01(9)
<i>Z</i>	4
calc. density/g cm ⁻³	1.407
<i>μ</i> /mm ⁻¹	0.267
absorption correction	Multi-Scan
transmission factor range	0.86–0.99
refls. measured	17184
<i>R</i> _{int}	0.0440
mean <i>σ</i> (<i>I</i>)/ <i>I</i>	0.0302
<i>θ</i> range	3.158–27.481
observed refls.	2170
<i>x</i> , <i>y</i> (weighting scheme)	0.0313, 1.7564
hydrogen refinement	H(C) constr, H(N) refall
refls in refinement	2675
parameters	159
restraints	0
<i>R</i> (<i>F</i> _{obs})	0.0455
<i>R</i> _w (<i>F</i> ²)	0.1168
<i>S</i>	1.102
shift/error _{max}	0.001
max electron density/e Å ⁻³	0.399
min electron density/e Å ⁻³	-0.520

4N-(1,4-dihydropyridin-4-yl)-4-methoxybenzenesulfonamide **8c**

Recrystallization was done from a 1/2 mixture of pyridine/H₂O.

8c crystallized with one molecule of H₂O per sulfonamide, which coordinates at the amide-N.

Figure S139 shows a single molecule, **Figure S140** gives the unit cell and crystallographic data for sulfonamide **8c** is given in **Table S16**:

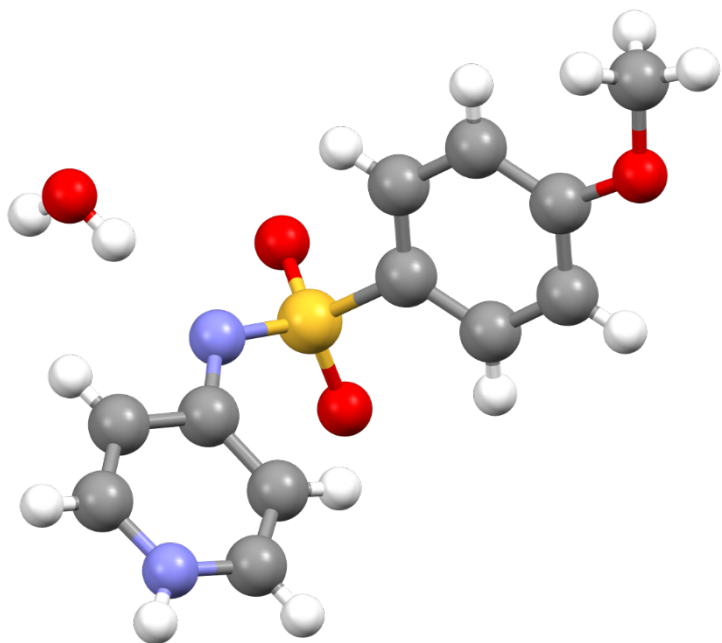


Figure S139. Molecule of sulfonamide **8c**.

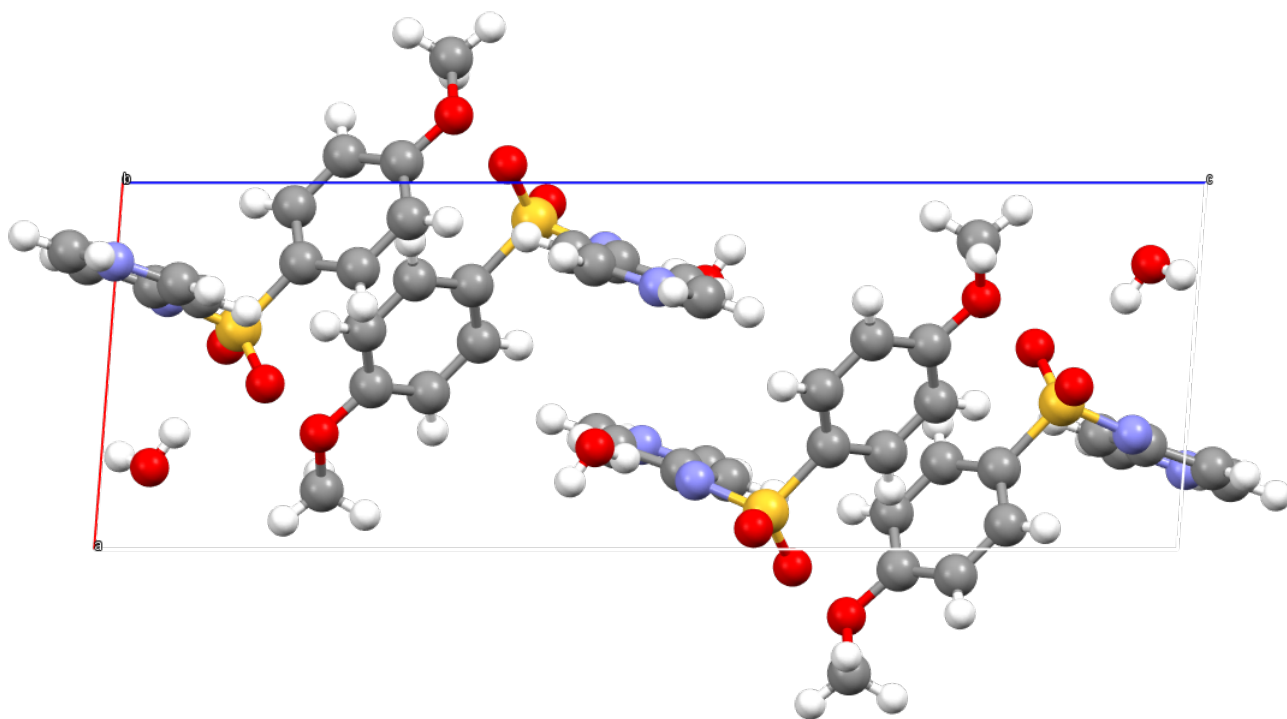


Figure S140. Unit cell of sulfonamide **8c** viewed along the *b*-axis.

Table S16. Crystallographic details for sulfonamide **8c**.

net formula	C ₁₂ H ₁₄ N ₂ O ₄ S
<i>M_r</i> /g mol ⁻¹	282.31
crystal size/mm	0.100 × 0.050 × 0.030
<i>T</i> /K	105.(2)
radiation	MoK α
diffractometer	'Bruker D8 Venture TXS'
crystal system	monoclinic
space group	'P 1 21/n 1'
<i>a</i> /Å	7.1584(4)
<i>b</i> /Å	8.4697(4)
<i>c</i> /Å	21.0760(11)
α /°	90
β /°	94.450(2)
γ /°	90
<i>V</i> /Å ³	1273.98(11)
<i>Z</i>	4
calc. density/g cm ⁻³	1.472
μ /mm ⁻¹	0.266
absorption correction	Multi-Scan
transmission factor range	0.92–0.99
refls. measured	23725
<i>R</i> _{int}	0.0440
mean $\sigma(I)/I$	0.0319
θ range	2.942–30.497
observed refls.	3297
<i>x</i> , <i>y</i> (weighting scheme)	0.0388, 0.8028
hydrogen refinement	H(C) constr, H(N,O) refall
refls in refinement	3887
parameters	185
restraints	0
<i>R</i> (<i>F</i> _{obs})	0.0353
<i>R</i> _w (<i>F</i> ²)	0.0975
<i>S</i>	1.052
shift/error _{max}	0.001
max electron density/e Å ⁻³	0.402
min electron density/e Å ⁻³	-0.422

8c crystallized with one molecule of H₂O per sulfonamide, which coordinates at the amide-N.

Tetrabutylphosphonium (diphenylphosphoryl)(pyridin-4-yl)amide **10d**

Disorder is addressed by a split-model. The unit cell contains two asymmetric units which in turn consist of three ion pairs.

Figure S141 shows single ion pair, **Figure S142** gives the unit cell and crystallographic data for catalyst system **10d** is given in **Table S17**:

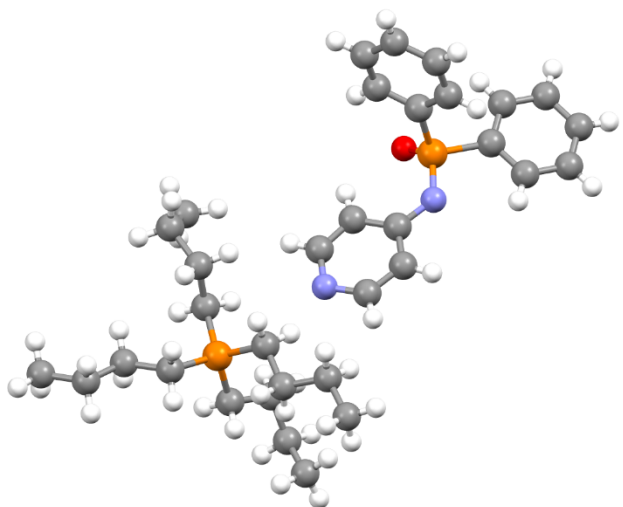


Figure S141. Ion pair of catalyst **10d**.

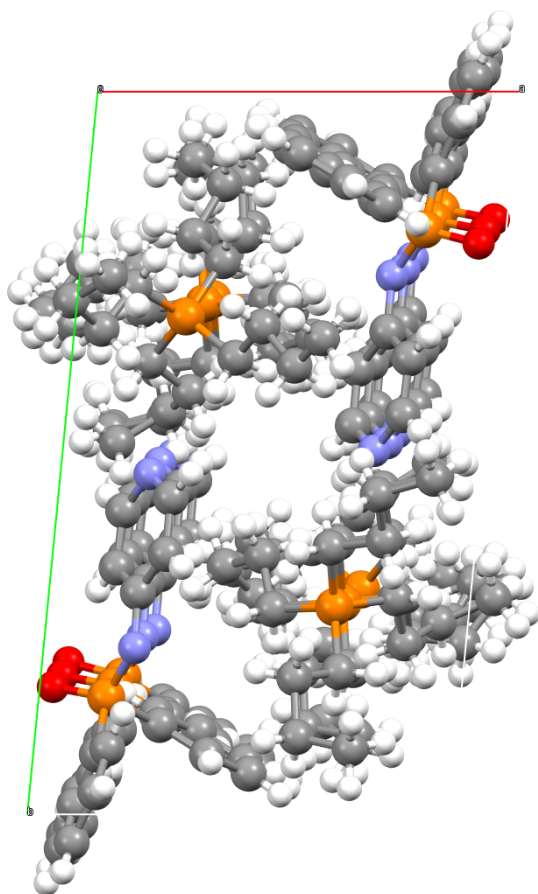


Figure S142. Unit cell of catalyst **10d** viewed along the *c*-axis.

Table S17. Crystallographic details for ion pair catalyst 10d.

net formula	C ₃₃ H ₅₀ N ₂ OP ₂
<i>M_r</i> /g mol ⁻¹	552.69
crystal size/mm	0.436 × 0.191 × 0.138
<i>T</i> /K	143(2)
radiation	MoKα
diffractometer	'Oxford XCalibur'
crystal system	triclinic
space group	'P -1'
<i>a</i> /Å	10.0606(4)
<i>b</i> /Å	17.2822(5)
<i>c</i> /Å	28.0572(12)
<i>α</i> /°	97.836(3)
<i>β</i> /°	99.154(4)
<i>γ</i> /°	94.177(3)
<i>V</i> /Å ³	4748.9(3)
<i>Z</i>	6
calc. density/g cm ⁻³	1.160
<i>μ</i> /mm ⁻¹	0.165
absorption correction	multi-scan
transmission factor range	0.98885–1.00000
refls. measured	25735
<i>R</i> _{int}	0.0466
mean <i>σ</i> (<i>I</i>)/ <i>I</i>	0.1289
<i>θ</i> range	4.214–25.025
observed refls.	8233
<i>x</i> , <i>y</i> (weighting scheme)	0.0593, 0
hydrogen refinement	constr
refls in refinement	16587
parameters	1038
restraints	6
<i>R</i> (<i>F</i> _{obs})	0.0733
<i>R</i> _w (<i>F</i> ²)	0.1907
<i>S</i>	1.009
shift/error _{max}	0.001
max electron density/e Å ⁻³	0.596
min electron density/e Å ⁻³	-0.403

Disorder is addressed by a split-model. The unit cell contains two asymmetric units which in turn consist of three ion pairs.

P,P-diphenyl-*N*-(pyridin-4-yl)phosphinic amide **11**

Recrystallization was done from H₂O/EtOH.

11 crystallized with ½ molecule of H₂O per phosphonic amide molecule, which coordinates the amide-O of two molecules of **11** each.

Figure S143 shows a single molecule, **Figure S144** gives the unit cell and crystallographic data for phosphonic amide **11** is given in **Table S18**:

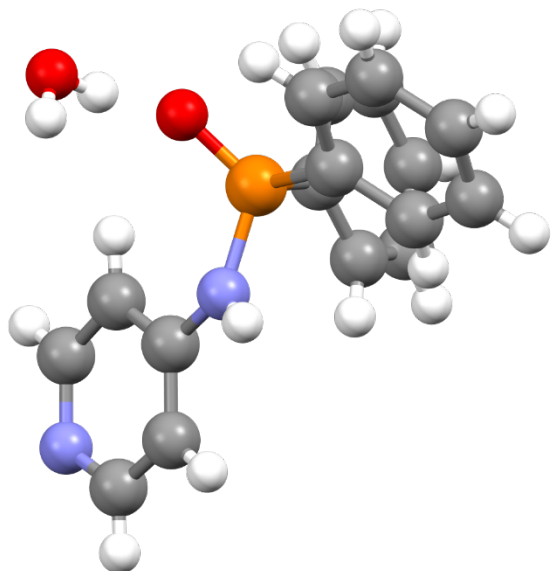


Figure S143. Molecule of phosphonic amide **11**.

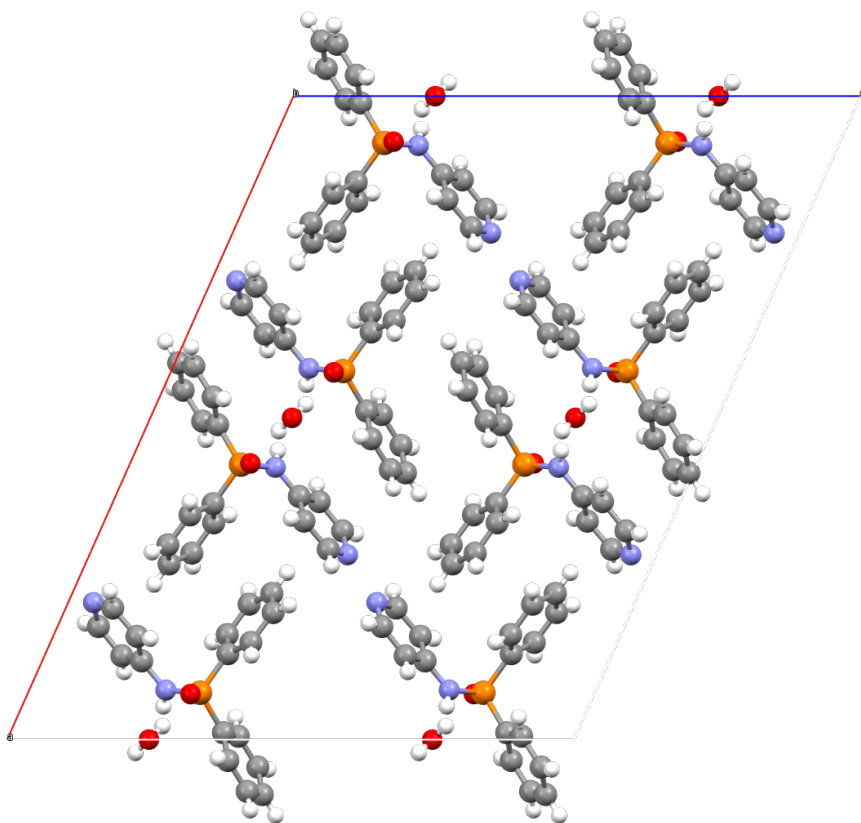


Figure S144. Unit cell of phosphonic amide **11** viewed along the *b*-axis.

Table S18. Crystallographic details for phosphonic amide **11**.

net formula	C ₃₄ H ₃₂ N ₄ O ₃ P ₂
<i>M_r</i> /g mol ⁻¹	606.57
crystal size/mm	0.080 × 0.060 × 0.030
<i>T</i> /K	103.(2)
radiation	MoKα
diffractometer	'Bruker D8 Venture TXS'
crystal system	monoclinic
space group	'C 1 2/c 1'
<i>a</i> /Å	26.0481(8)
<i>b</i> /Å	6.0009(2)
<i>c</i> /Å	20.9637(7)
<i>α</i> /°	90
<i>β</i> /°	113.9890(10)
<i>γ</i> /°	90
<i>V</i> /Å ³	2993.83(17)
<i>Z</i>	4
calc. density/g cm ⁻³	1.346
<i>μ</i> /mm ⁻¹	0.188
absorption correction	Multi-Scan
transmission factor range	0.97–0.99
refls. measured	25369
<i>R</i> _{int}	0.0426
mean <i>σ</i> (<i>I</i>)/ <i>I</i>	0.0272
<i>θ</i> range	3.214–27.485
observed refls.	3097
<i>x</i> , <i>y</i> (weighting scheme)	0.0319, 3.9710
hydrogen refinement	H(C) constr, H(N,O) refall
refls in refinement	3426
parameters	203
restraints	0
<i>R</i> (<i>F</i> _{obs})	0.0321
<i>R</i> _w (<i>F</i> ²)	0.0850
<i>S</i>	1.057
shift/error _{max}	0.001
max electron density/e Å ⁻³	0.399
min electron density/e Å ⁻³	-0.369

11 crystallized with ½ molecule of H₂O per phosphonic amide molecule, which coordinates the amide-O of two molecules of **11** each.

3-(pyridin-4-ylamino)benzo[d]isothiazole 1,1-dioxide **14**

Recrystallization was done from DMSO.

Compound **14** crystallized with one molecule of DMSO per sulfonamide molecule, which coordinates at the H-atom of the secondary amine.

Figure S145 shows a single molecule, **Figure S146** gives the unit cell and crystallographic data for “extended” sulfonamide **14** is given in **Table S19**:

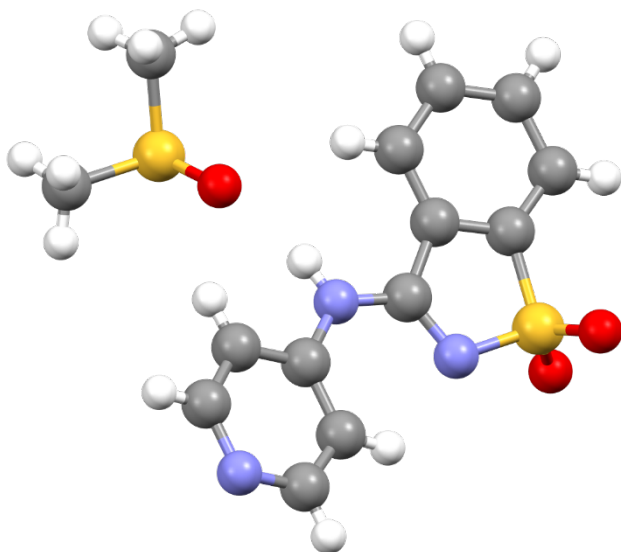


Figure S145. Molecule of sulfonamide **14**.

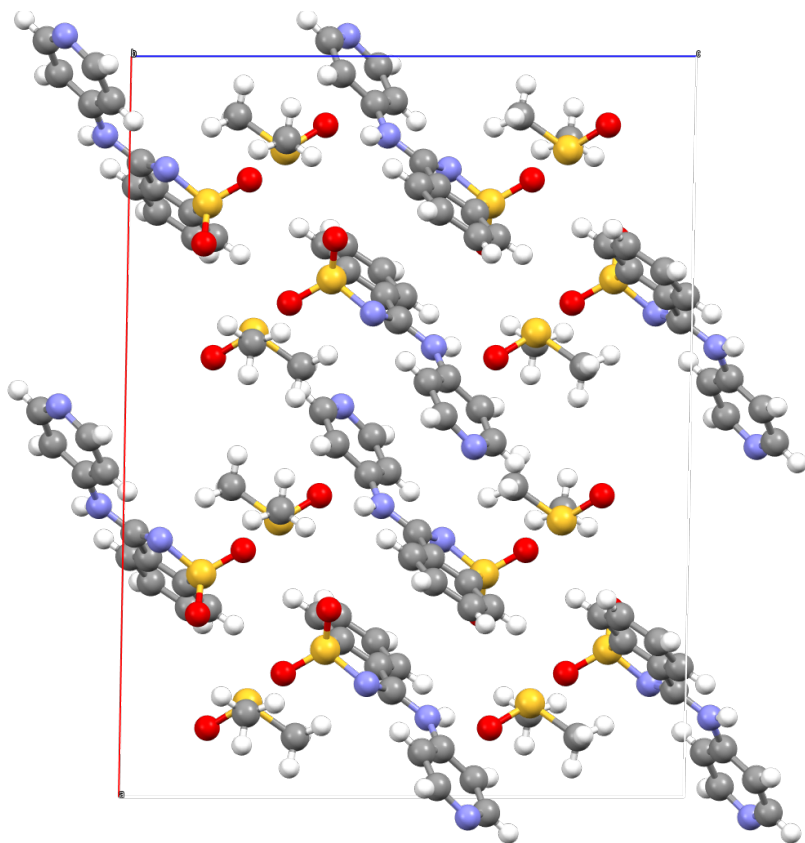


Figure S146. Unit cell of sulfonamide **14** viewed along the *b*-axis.

Table S19. Crystallographic details for sulfonamide **14**.

net formula	C ₁₄ H ₁₅ N ₃ O ₃ S ₂
<i>M_r</i> /g mol ⁻¹	337.41
crystal size/mm	0.100 × 0.090 × 0.070
<i>T</i> /K	105.(2)
radiation	MoKα
diffractometer	'Bruker D8 Venture TXS'
crystal system	monoclinic
space group	'C 1 2/c 1'
<i>a</i> /Å	22.0954(14)
<i>b</i> /Å	8.0559(6)
<i>c</i> /Å	16.8525(11)
<i>α</i> /°	90
<i>β</i> /°	90.975(2)
<i>γ</i> /°	90
<i>V</i> /Å ³	2999.3(4)
<i>Z</i>	8
calc. density/g cm ⁻³	1.494
<i>μ</i> /mm ⁻¹	0.371
absorption correction	Multi-Scan
transmission factor range	0.94–0.97
refls. measured	28539
<i>R</i> _{int}	0.0263
mean <i>σ</i> (<i>I</i>)/ <i>I</i>	0.0191
<i>θ</i> range	3.016–30.503
observed refls.	4234
<i>x</i> , <i>y</i> (weighting scheme)	0.0346, 3.5011
hydrogen refinement	H(C) constr, H(N) refall
refls in refinement	4576
parameters	205
restraints	0
<i>R</i> (<i>F</i> _{obs})	0.0290
<i>R</i> _w (<i>F</i> ²)	0.0812
<i>S</i>	1.080
shift/error _{max}	0.001
max electron density/e Å ⁻³	0.406
min electron density/e Å ⁻³	-0.450

14 crystallized with one molecule of DMSO per sulfonamide molecule, which coordinates at the H-atom of the secondary amine.

Tetraphenylphosphonium (1,1-dioxidobenzo[d]isothiazol-3-yl)(pyridin-4-yl)amide **15g**

Figure S147 shows single ion pair, **Figure S148** gives the unit cell and crystallographic data for catalyst system **15g** is given in **Table S20**:

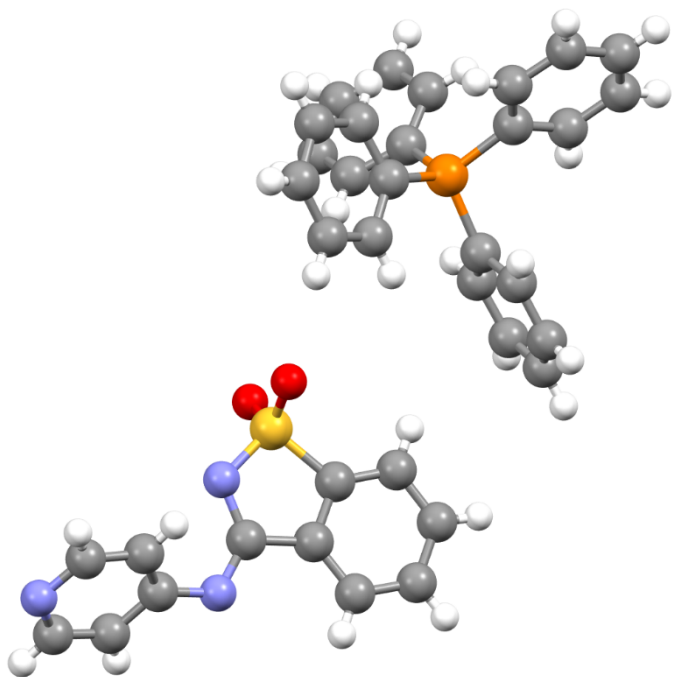


Figure S147. Ion pair of catalyst **15g**.

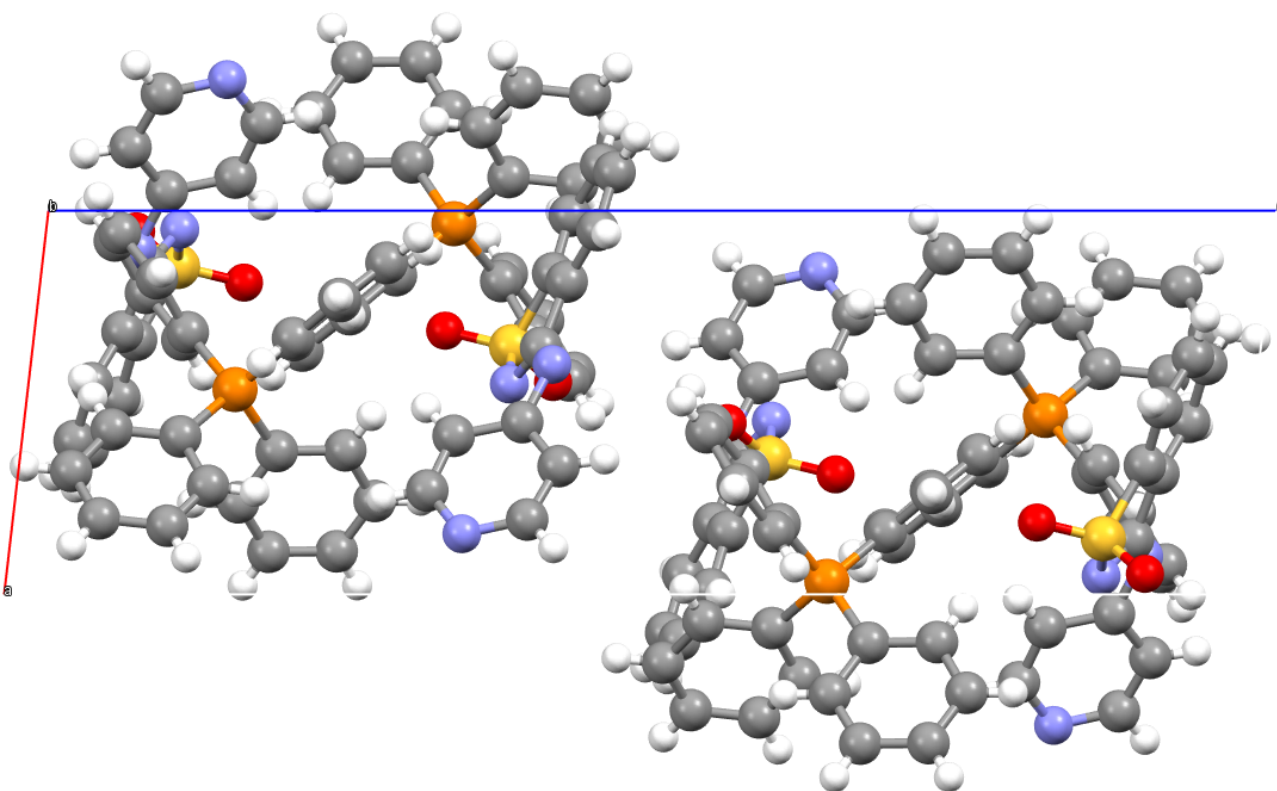


Figure S148. Unit cell of catalyst **15g** viewed along the *b*-axis.

Table S20. Crystallographic details for ion pair catalyst **15g**.

net formula	C ₃₃ H ₅₀ N ₂ OP ₂
<i>M_r</i> /g mol ⁻¹	552.69
crystal size/mm	0.436 × 0.191 × 0.138
<i>T</i> /K	143(2)
radiation	MoKα
diffractometer	'Oxford XCalibur'
crystal system	triclinic
space group	'P -1'
<i>a</i> /Å	10.0606(4)
<i>b</i> /Å	17.2822(5)
<i>c</i> /Å	28.0572(12)
<i>α</i> /°	97.836(3)
<i>β</i> /°	99.154(4)
<i>γ</i> /°	94.177(3)
<i>V</i> /Å ³	4748.9(3)
<i>Z</i>	6
calc. density/g cm ⁻³	1.160
<i>μ</i> /mm ⁻¹	0.165
absorption correction	multi-scan
transmission factor range	0.98885–1.00000
refls. measured	25735
<i>R</i> _{int}	0.0466
mean <i>σ</i> (<i>I</i>)/ <i>I</i>	0.1289
<i>θ</i> range	4.214–25.025
observed refls.	8233
<i>x</i> , <i>y</i> (weighting scheme)	0.0593, 0
hydrogen refinement	constr
refls in refinement	16587
parameters	1038
restraints	6
<i>R</i> (<i>F</i> _{obs})	0.0733
<i>R</i> _w (<i>F</i> ²)	0.1907
<i>S</i>	1.009
shift/error _{max}	0.001
max electron density/e Å ⁻³	0.596
min electron density/e Å ⁻³	-0.403

Butyl *p*-tolylcarbamate **16**

The unit cell contains four asymmetric units which in turn consist of four molecules each.

Figure S149 shows a single molecule, **Figure S150** gives the unit cell and crystallographic data for urethane **16** is given in **Table S21**:

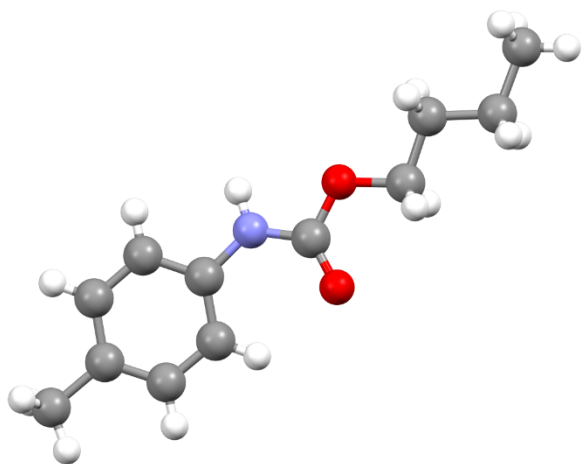


Figure S149. Urethane **16**.

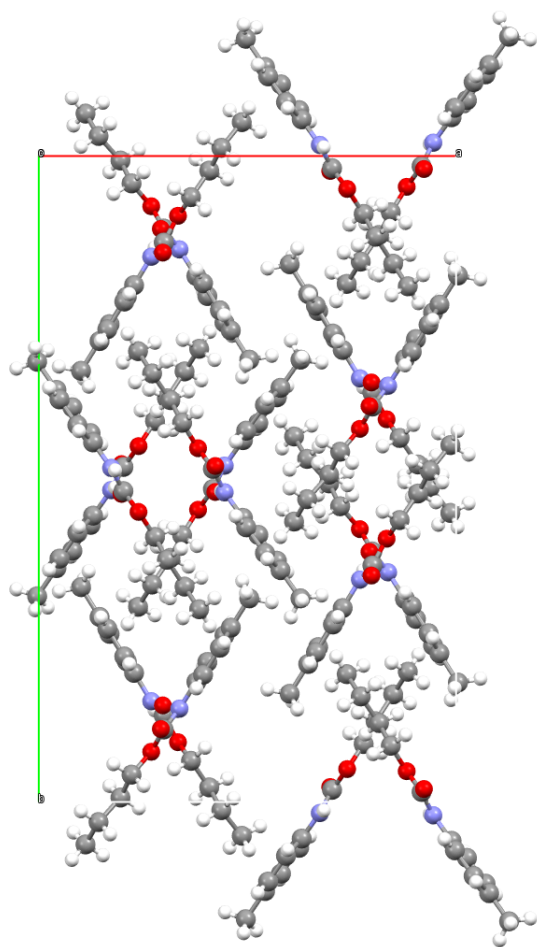


Figure S150. Unit cell of urethane **16** viewed along the *c*-axis.

Table S21. Crystallographic details for urethane **16**.

net formula	C ₁₂ H ₁₇ NO ₂
<i>M_r</i> /g mol ⁻¹	207.26
crystal size/mm	0.100 × 0.030 × 0.030
<i>T</i> /K	153.(2)
radiation	MoKα
diffractometer	'Bruker D8 Venture TXS'
crystal system	monoclinic
space group	'C 1 c 1'
<i>a</i> /Å	18.1807(6)
<i>b</i> /Å	27.4981(7)
<i>c</i> /Å	9.6395(2)
<i>α</i> /°	90
<i>β</i> /°	102.0210(10)
<i>γ</i> /°	90
<i>V</i> /Å ³	4713.4(2)
<i>Z</i>	16
calc. density/g cm ⁻³	1.168
<i>μ</i> /mm ⁻¹	0.079
absorption correction	Multi-Scan
transmission factor range	0.8905–0.9604
refls. measured	29658
<i>R</i> _{int}	0.0493
mean <i>σ</i> (<i>I</i>)/ <i>I</i>	0.0728
<i>θ</i> range	3.145–30.508
observed refls.	10647
<i>x</i> , <i>y</i> (weighting scheme)	0.0640, 0.7848
hydrogen refinement	C-H: constr, N-H: refall
Flack parameter	0.5
refls in refinement	14193
parameters	565
restraints	2
<i>R</i> (<i>F</i> _{obs})	0.0572
<i>R</i> _w (<i>F</i> ²)	0.1410
<i>S</i>	1.019
shift/error _{max}	0.001
max electron density/e Å ⁻³	0.240
min electron density/e Å ⁻³	-0.198

4-methyl-N-(pyridin-2-yl)benzenesulfonamide **25**

Recrystallization was done from H₂O/EtOH.

Figure S151 shows the dimer, **Figure S152** gives the unit cell and crystallographic data for sulfonamide **25** is given in **Table S22**:

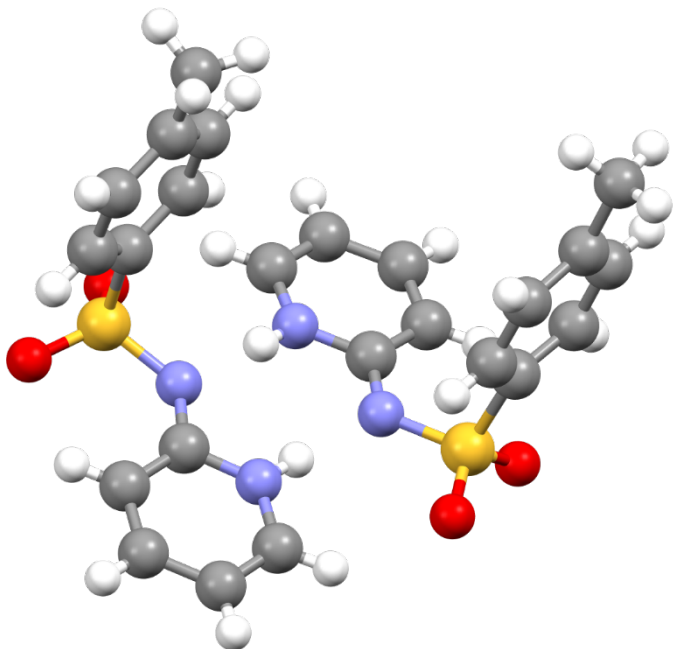


Figure S151. Dimer of sulfonamide **25**.

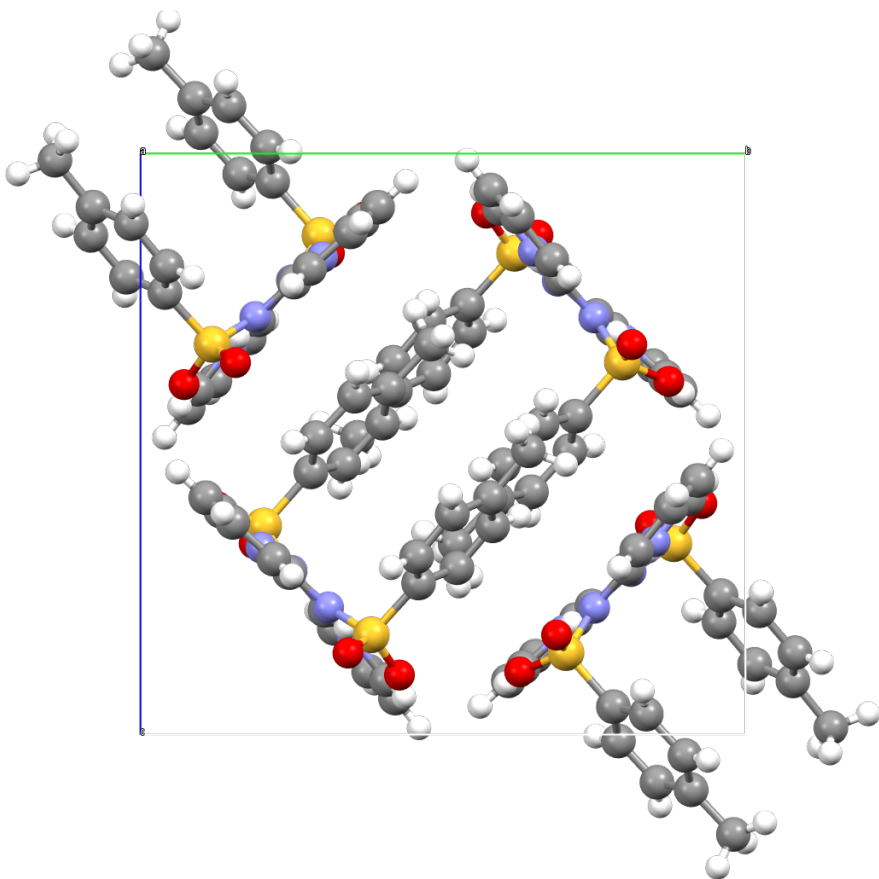


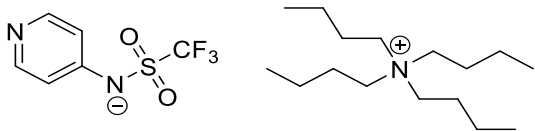
Figure S152. Unit cell of sulfonamide **25** viewed along the *a*-axis.

Table S22. Crystallographic details for sulfonamide **25**.

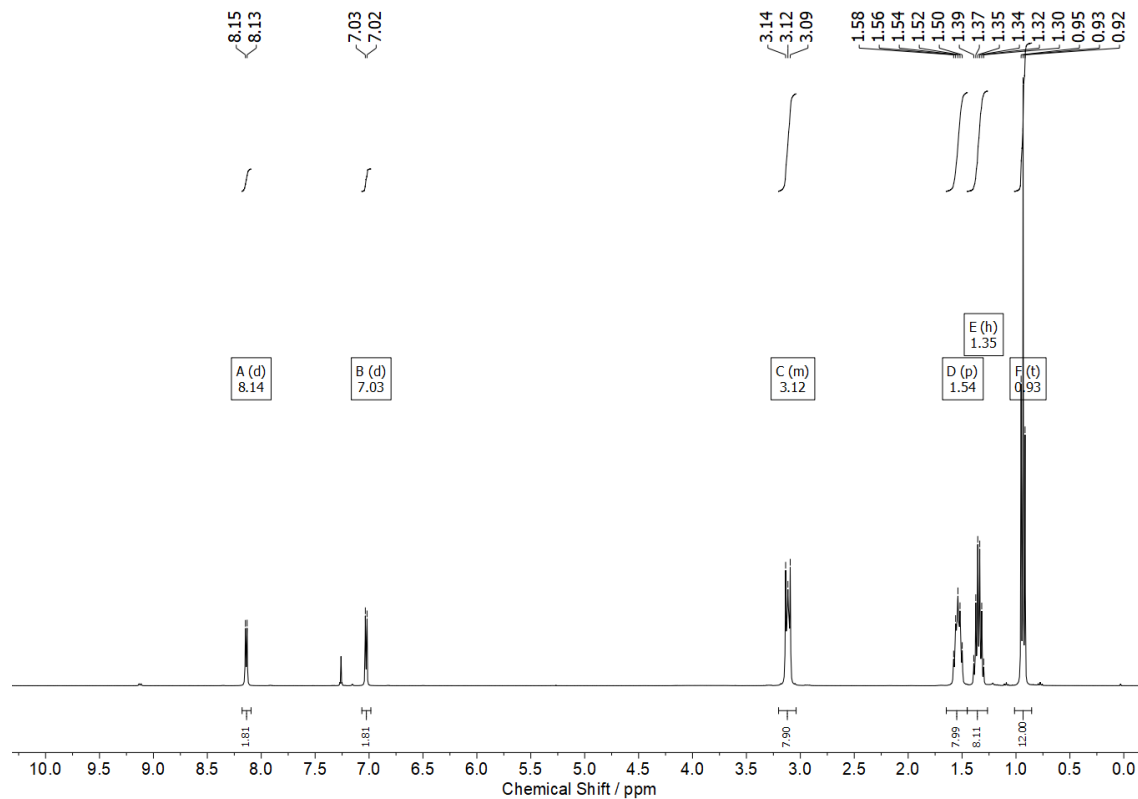
net formula	C ₁₂ H ₁₂ N ₂ O ₂ S
<i>M_r</i> /g mol ⁻¹	248.30
crystal size/mm	0.080 × 0.050 × 0.040
<i>T</i> /K	104.(2)
radiation	MoKα
diffractometer	'Bruker D8 Venture TXS'
crystal system	monoclinic
space group	'P 1 21/c 1'
<i>a</i> /Å	10.7237(4)
<i>b</i> /Å	14.8564(5)
<i>c</i> /Å	14.6583(5)
<i>α</i> /°	90
<i>β</i> /°	103.0200(10)
<i>γ</i> /°	90
<i>V</i> /Å ³	2275.26(14)
<i>Z</i>	8
calc. density/g cm ⁻³	1.450
<i>μ</i> /mm ⁻¹	0.275
absorption correction	Multi-Scan
transmission factor range	0.95–0.99
refls. measured	35558
<i>R</i> _{int}	0.0533
mean <i>σ</i> (<i>I</i>)/ <i>I</i>	0.0341
<i>θ</i> range	2.995–27.484
observed refls.	4271
<i>x</i> , <i>y</i> (weighting scheme)	0.0353, 1.6662
hydrogen refinement	H(C) constr, H(N) refall
refls in refinement	5190
parameters	317
restraints	0
<i>R</i> (<i>F</i> _{obs})	0.0361
<i>R</i> _w (<i>F</i> ²)	0.0967
<i>S</i>	1.073
shift/error _{max}	0.001
max electron density/e Å ⁻³	0.309
min electron density/e Å ⁻³	-0.461

NMR Spectra of Synthesized Compounds

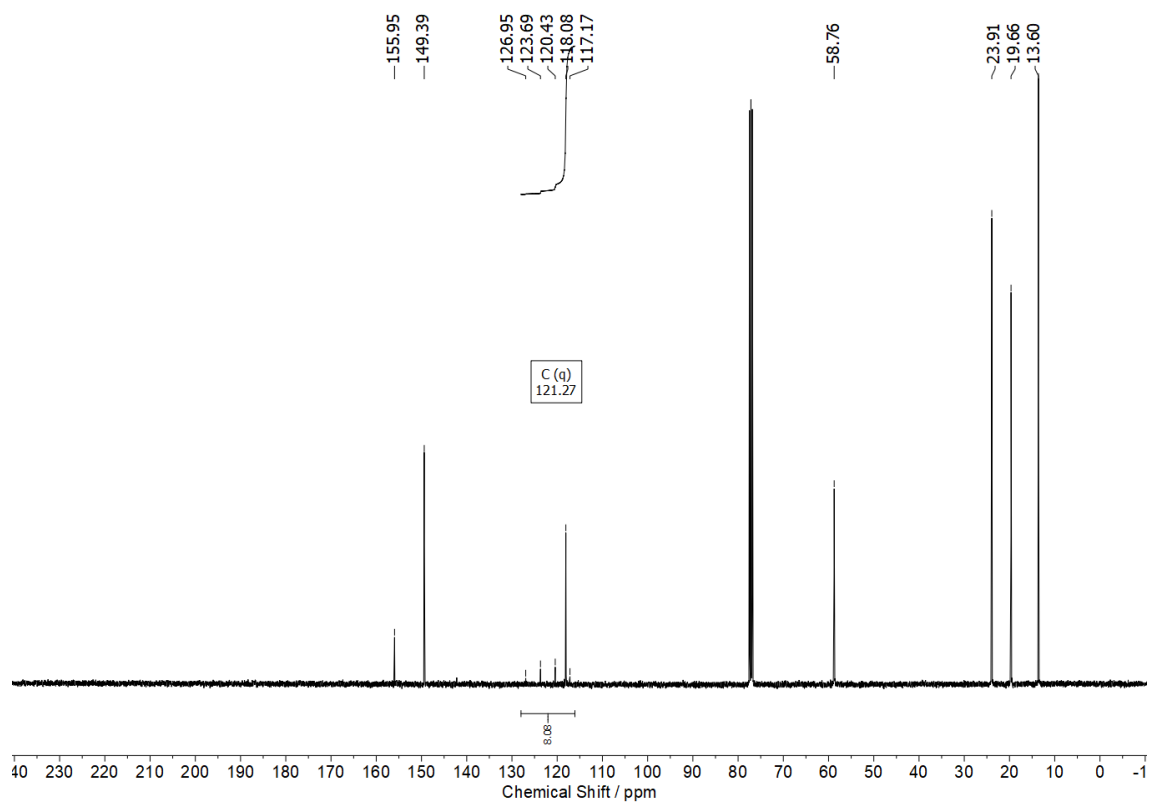
Tetrabutylammonium pyridin-4-yl((trifluoromethyl)sulfonyl)amide **6aa**



a)



b)



c)

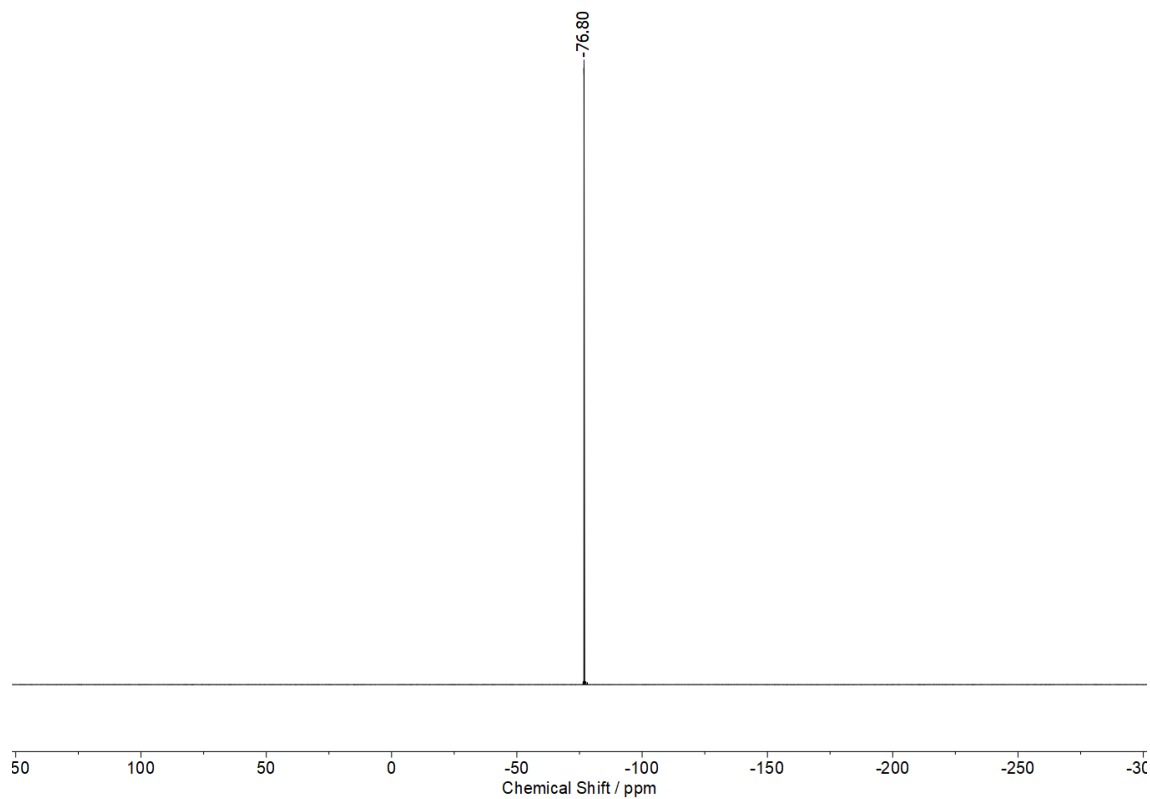
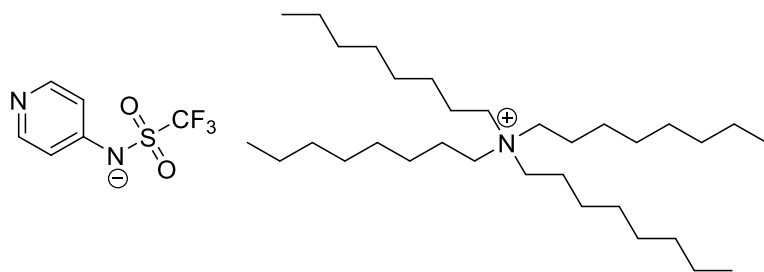
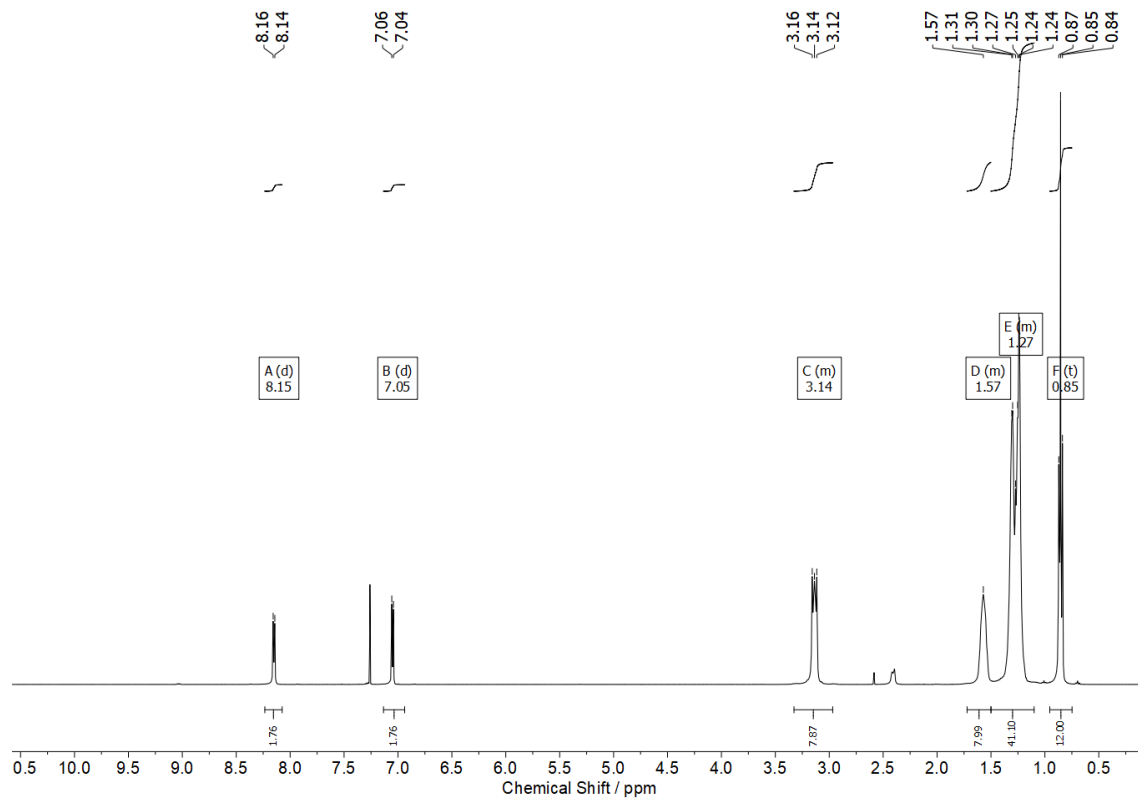


Figure S153. NMR spectra of catalyst **6aa** (CDCl_3 , 400 MHz): a) ^1H NMR spectrum, b) ^{13}C NMR spectrum, c) ^{19}F NMR spectrum.

Tetraoctylammonium pyridin-4-yl((trifluoromethyl)sulfonyl)amide **6ab**



a)



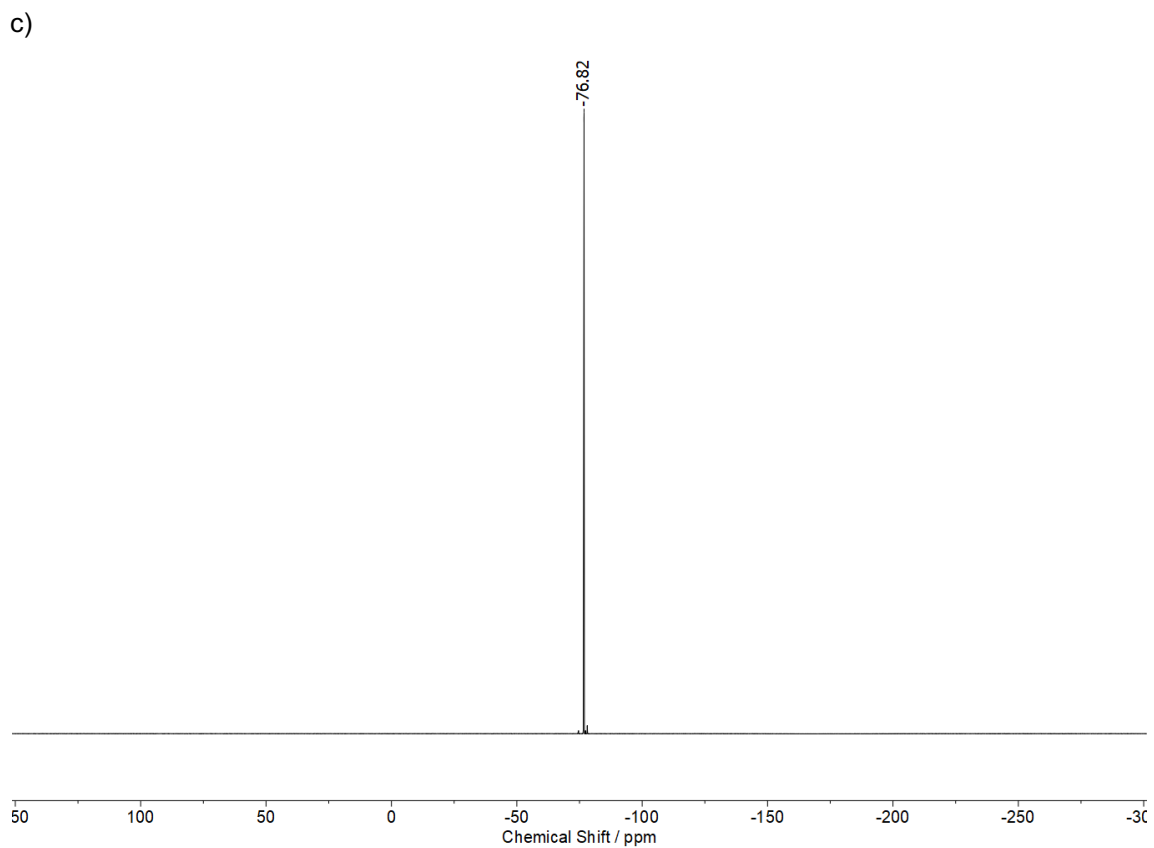
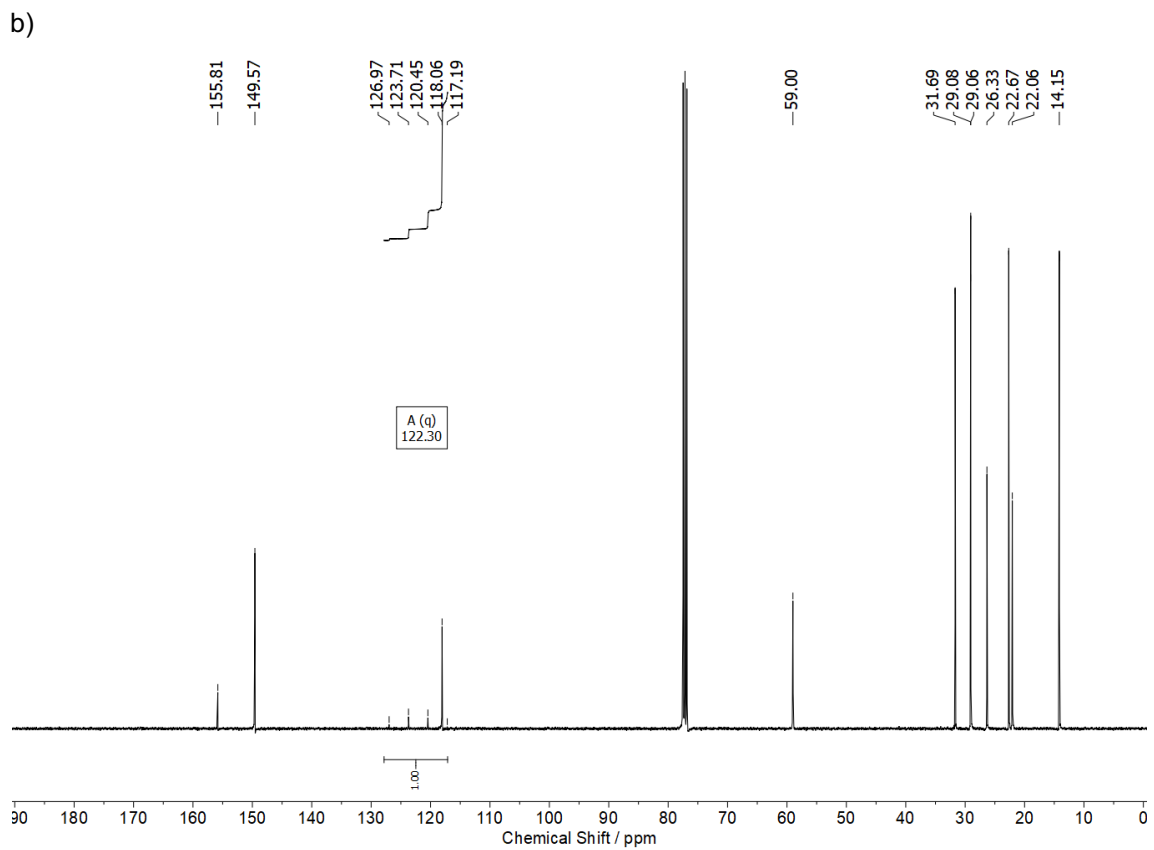
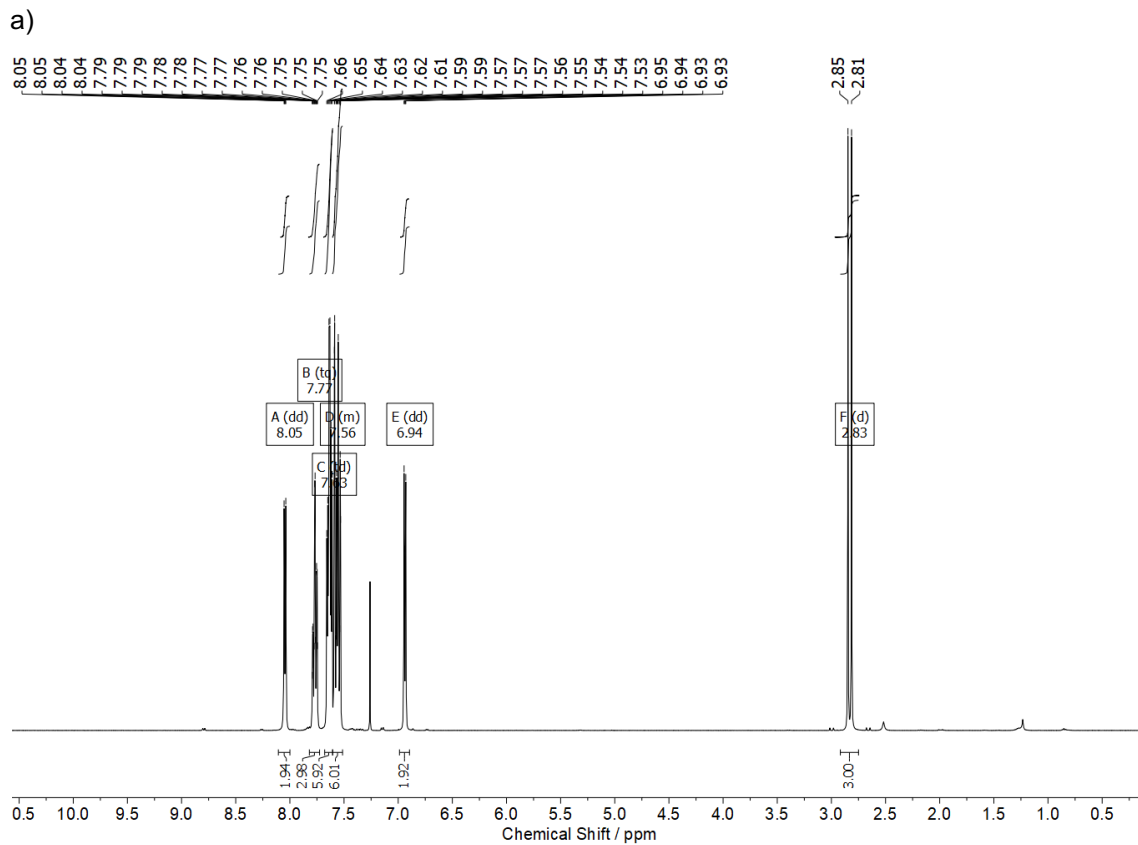
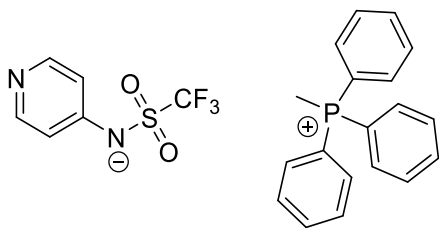
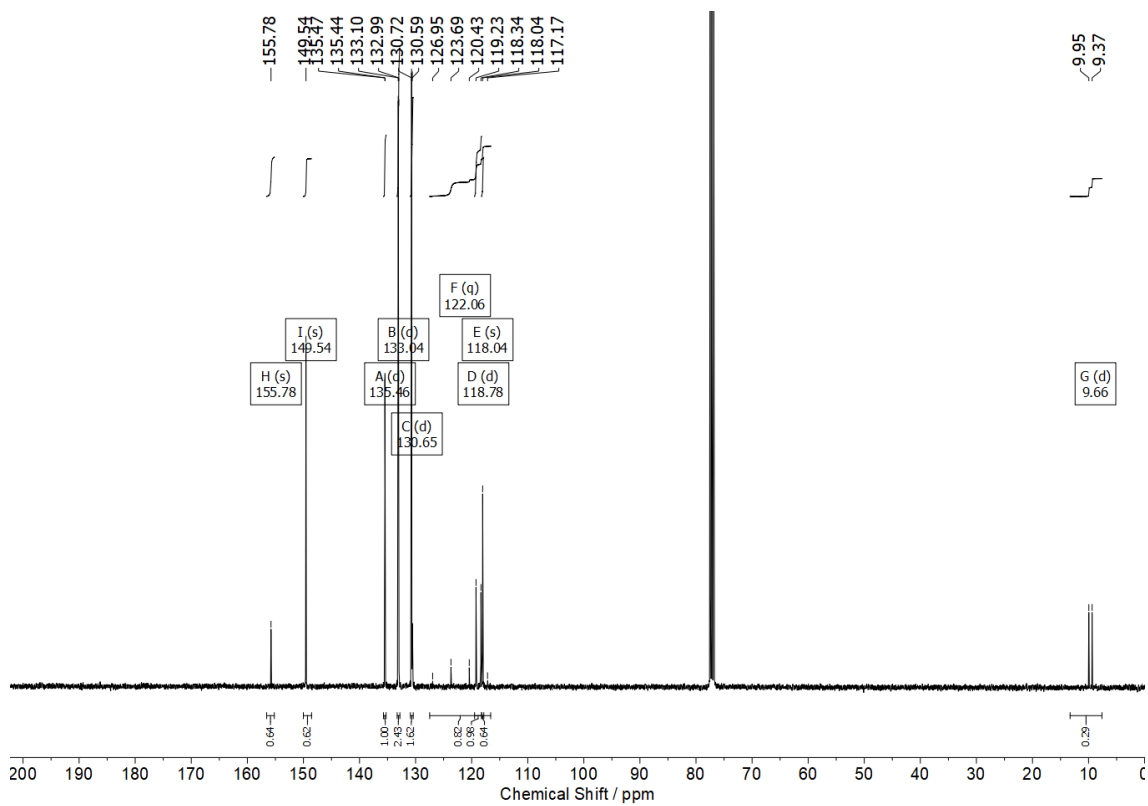


Figure S154. NMR spectra of catalyst **6ab** (CDCl_3 , 400 MHz): a) ^1H NMR spectrum, b) ^{13}C NMR spectrum, c) ^{19}F NMR spectrum.

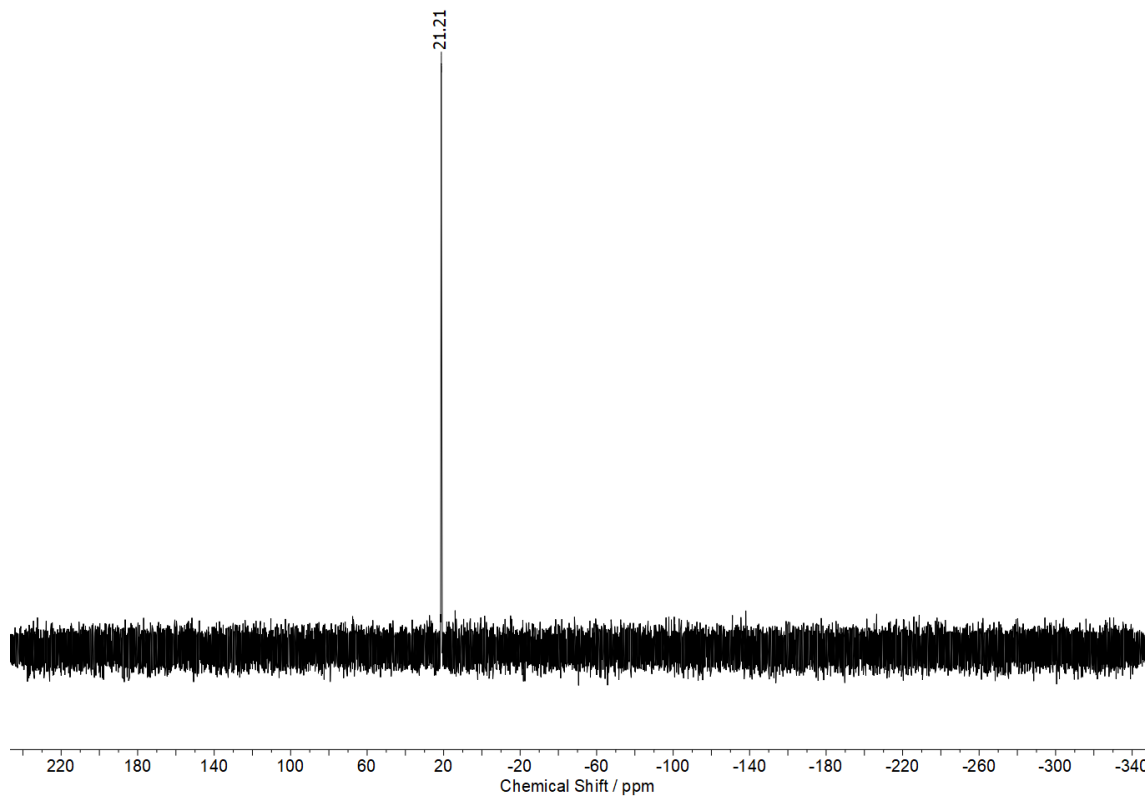
Methyltriphenylphosphonium pyridin-4-yl((trifluoromethyl)sulfonyl)amide **6ac**



b)



c)



d)

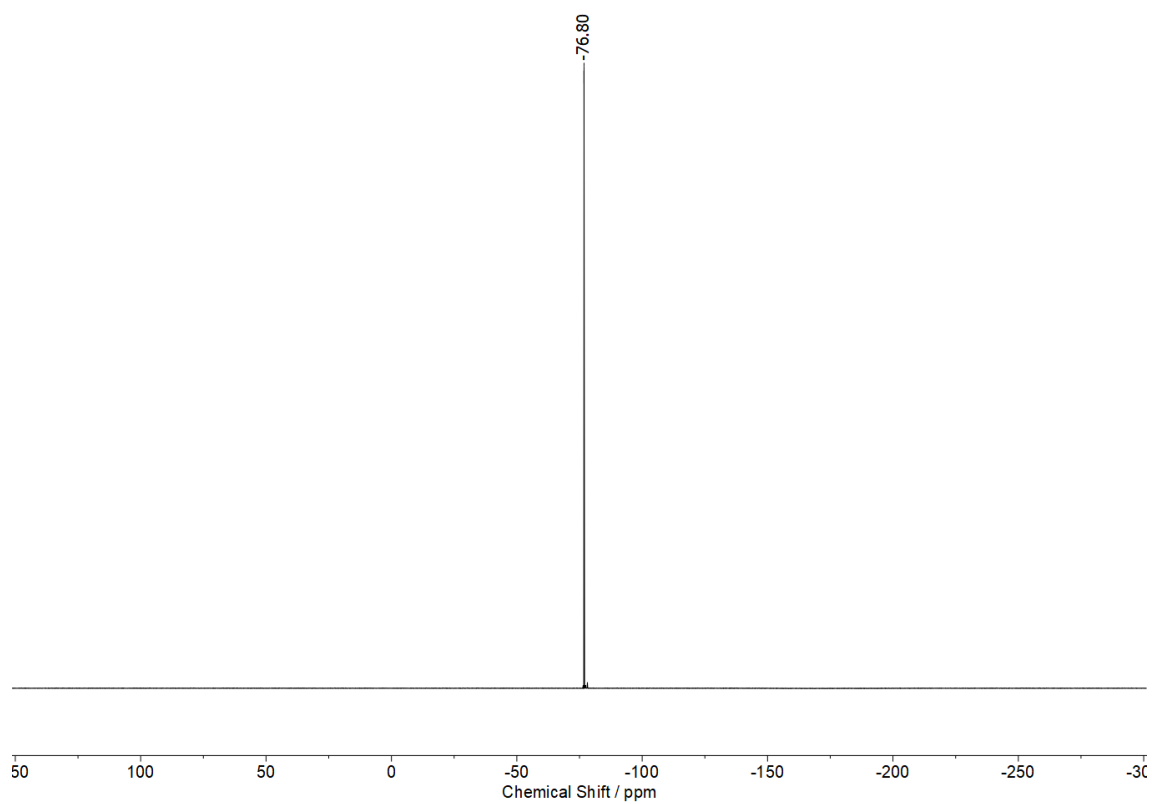
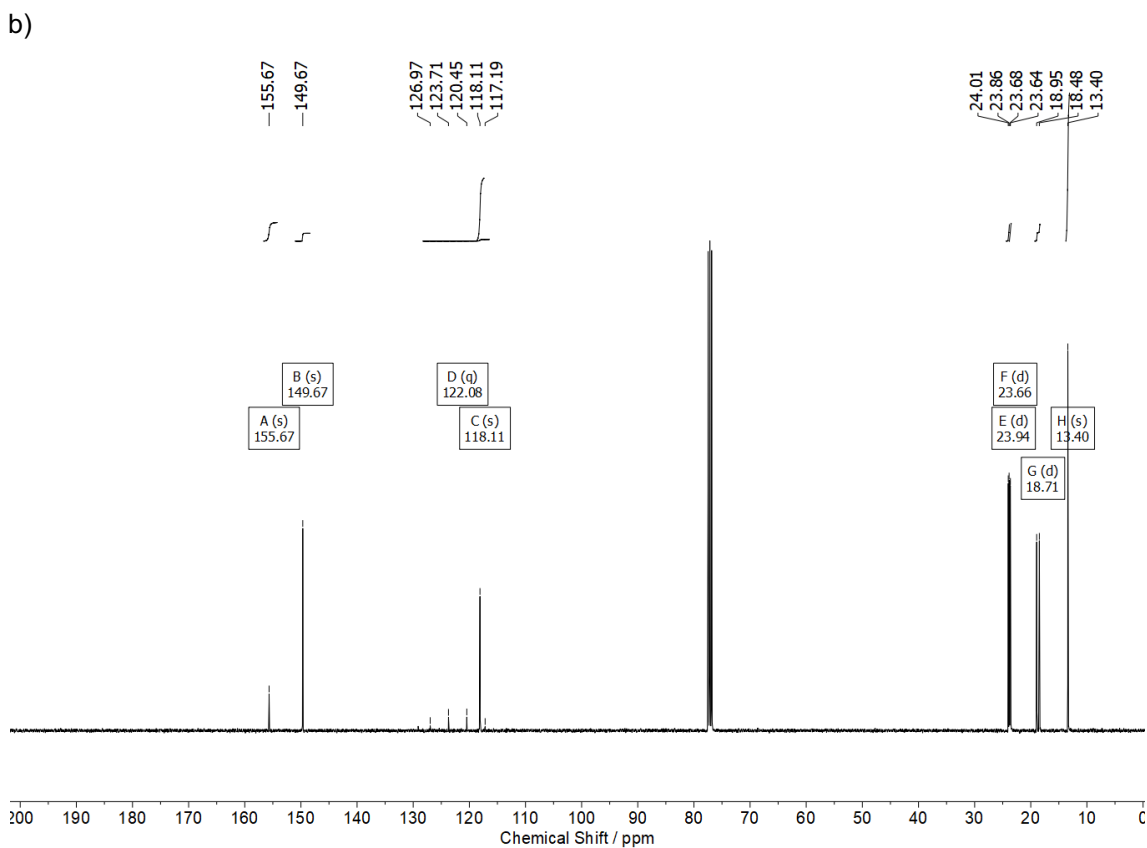
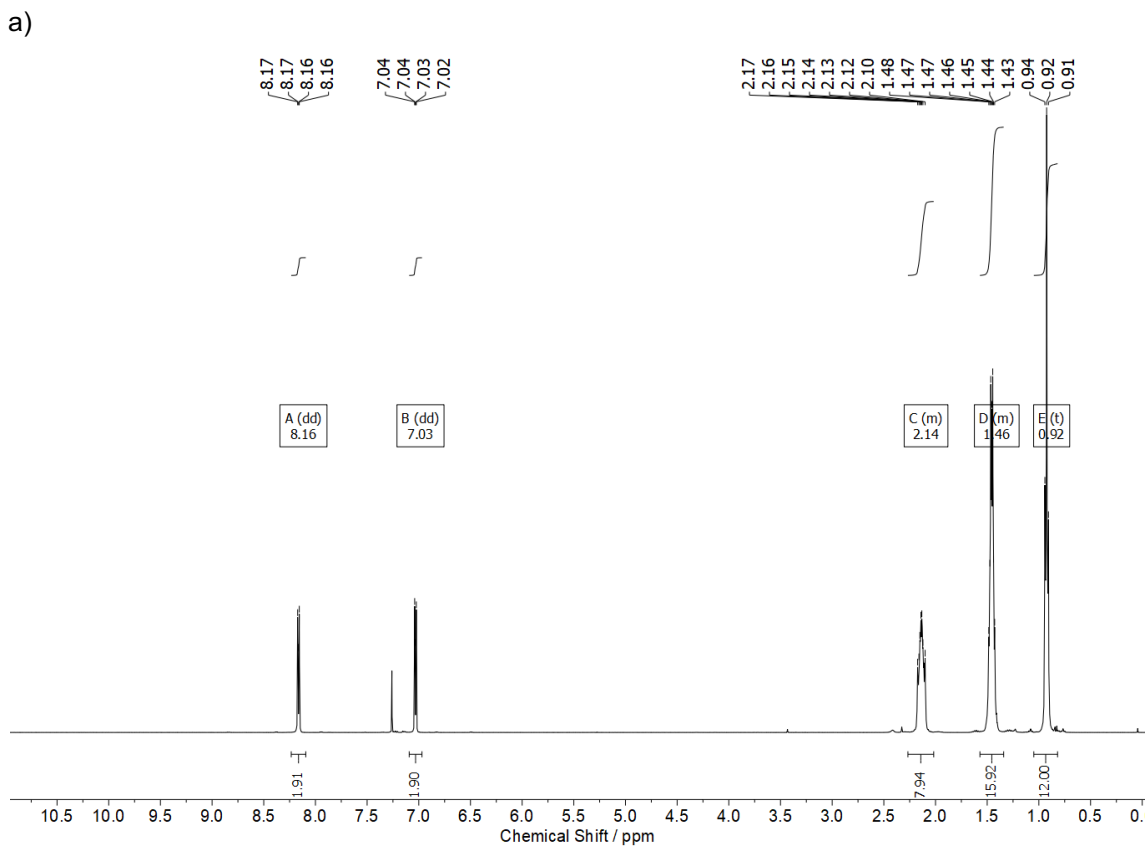
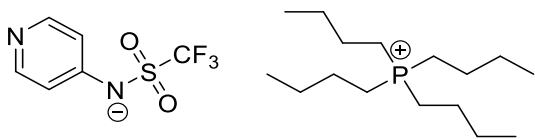
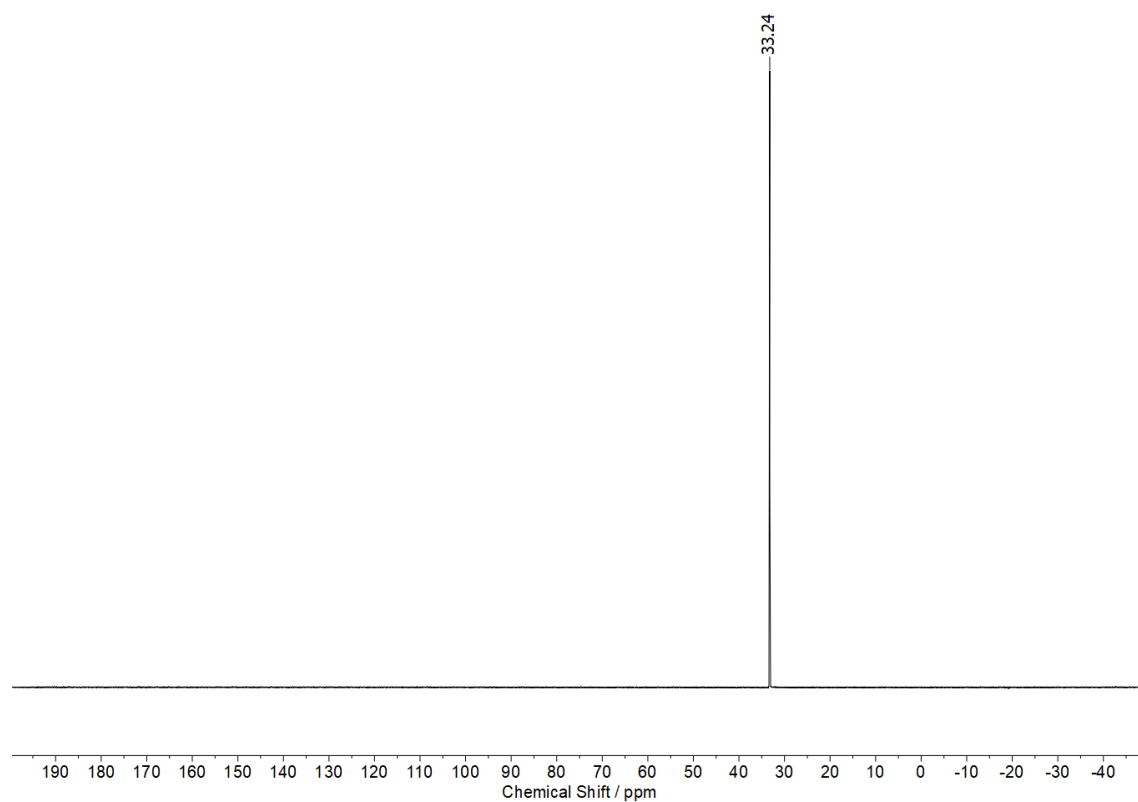


Figure S155. NMR spectra of catalyst **6ac** (CDCl_3 , 400 MHz): a) ^1H NMR spectrum, b) ^{13}C NMR spectrum, c) ^{31}P NMR spectrum, d) ^{19}F NMR spectrum.

Tetrabutylphosphonium pyridin-4-yl((trifluoromethyl)sulfonyl)amide **6ad**



c)



d)

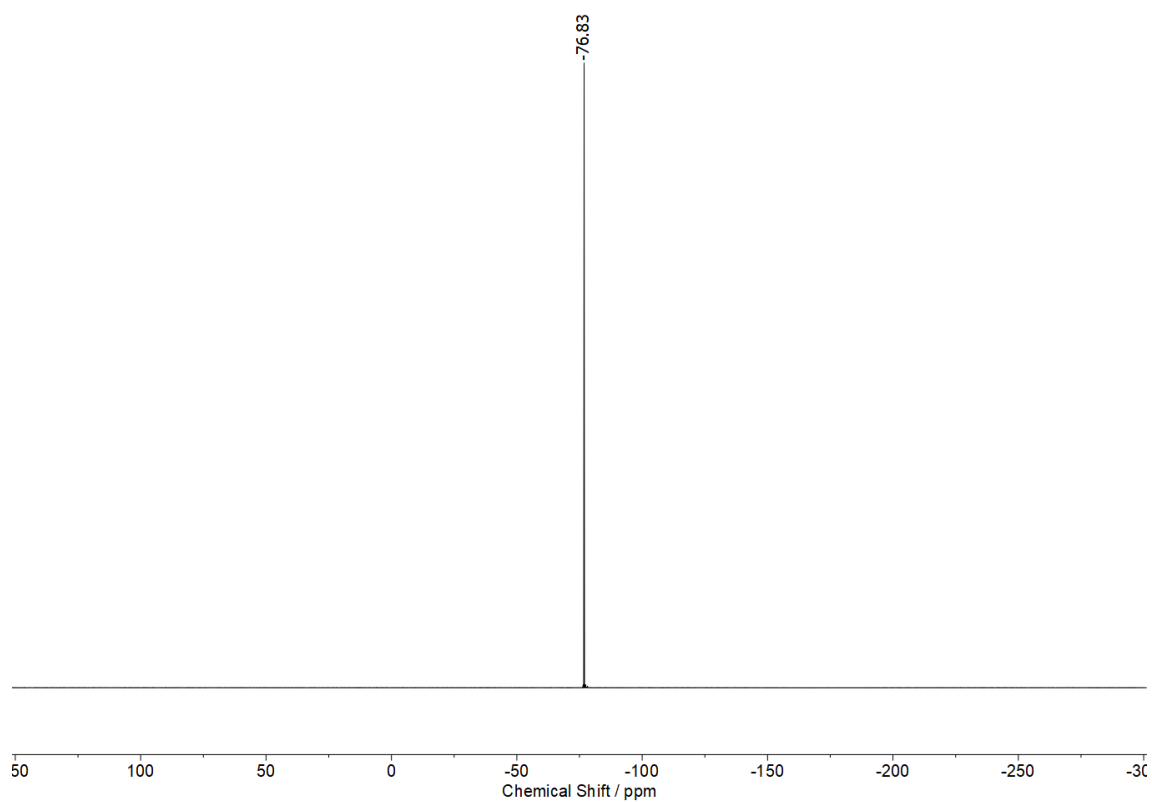
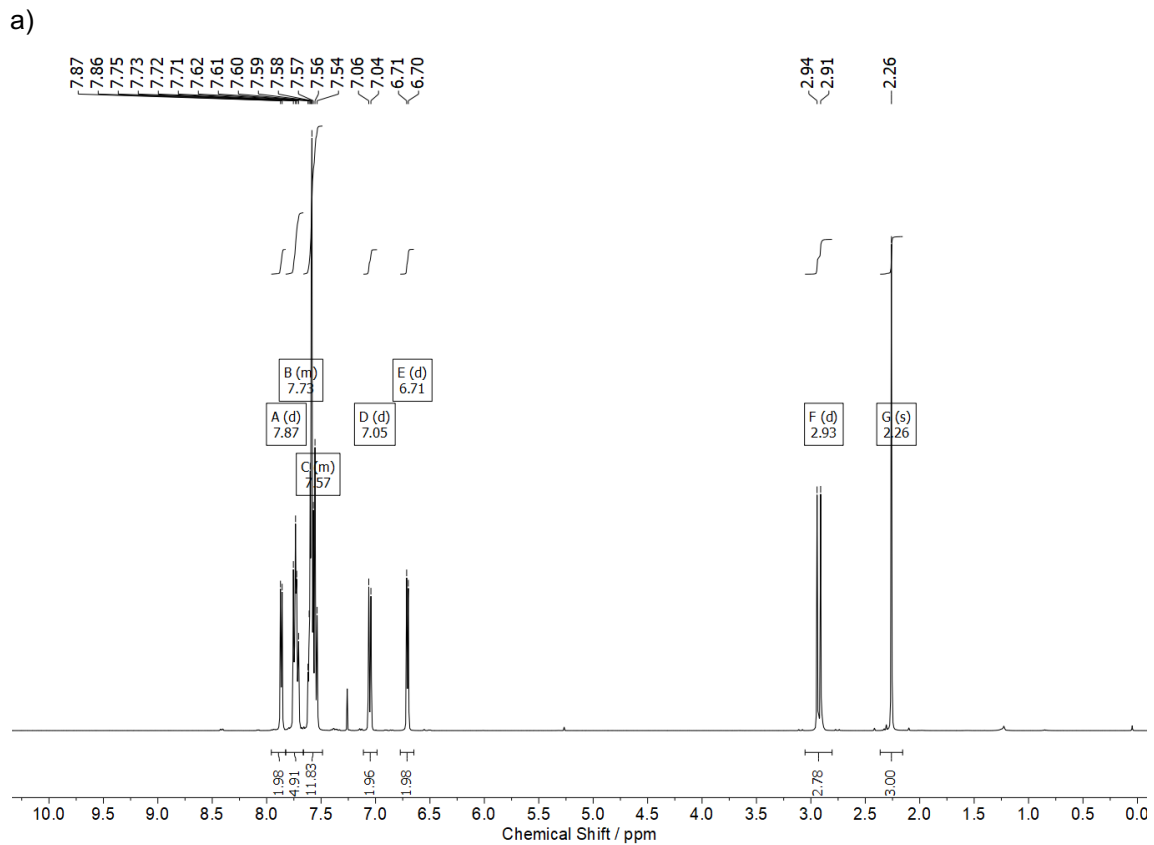
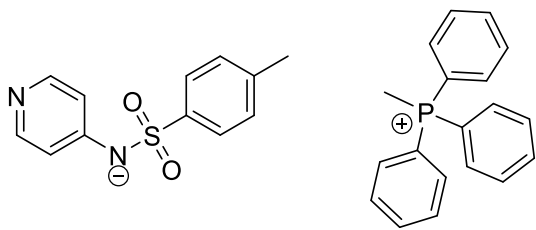


Figure S156. NMR spectra of catalyst **6ad** (CDCl_3 , 400 MHz): a) ^1H NMR spectrum, b) ^{13}C NMR spectrum, c) $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum, d) ^{19}F NMR spectrum.

Methyltriphenylphosphonium pyridin-4-yl(tosyl)amide **6bc**



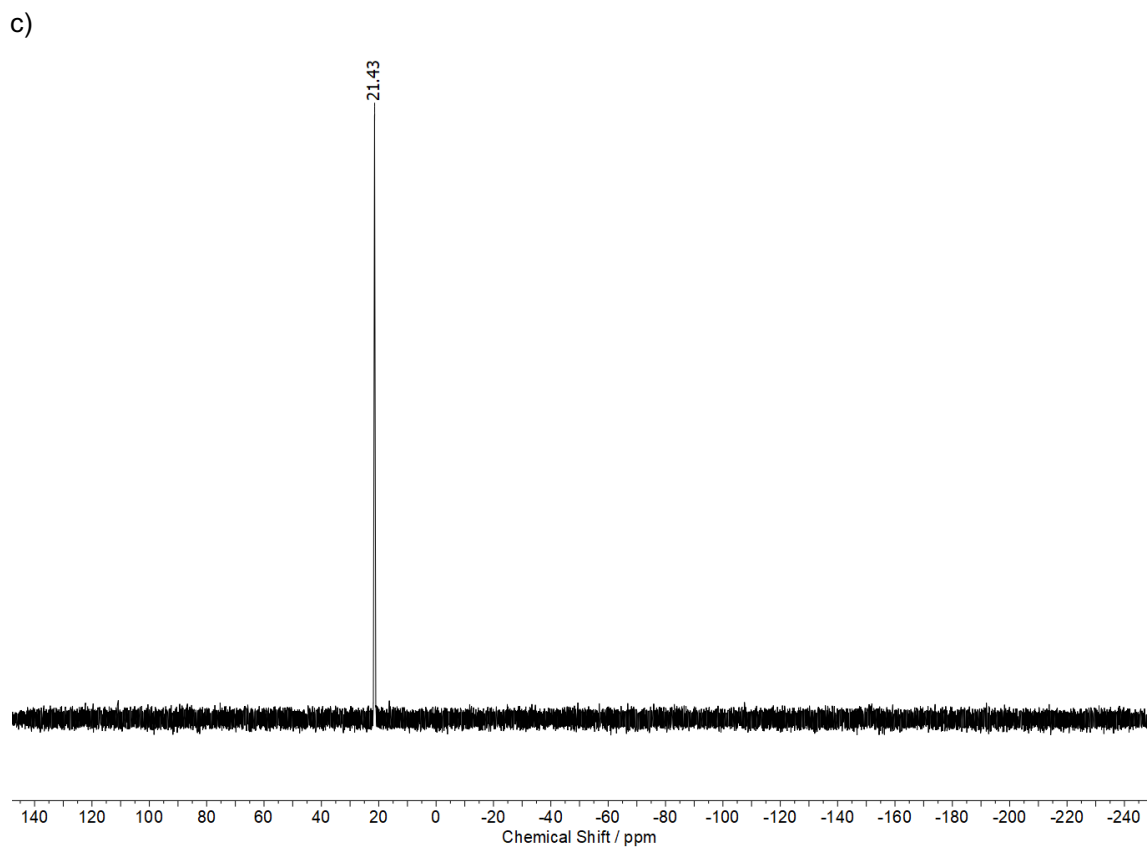
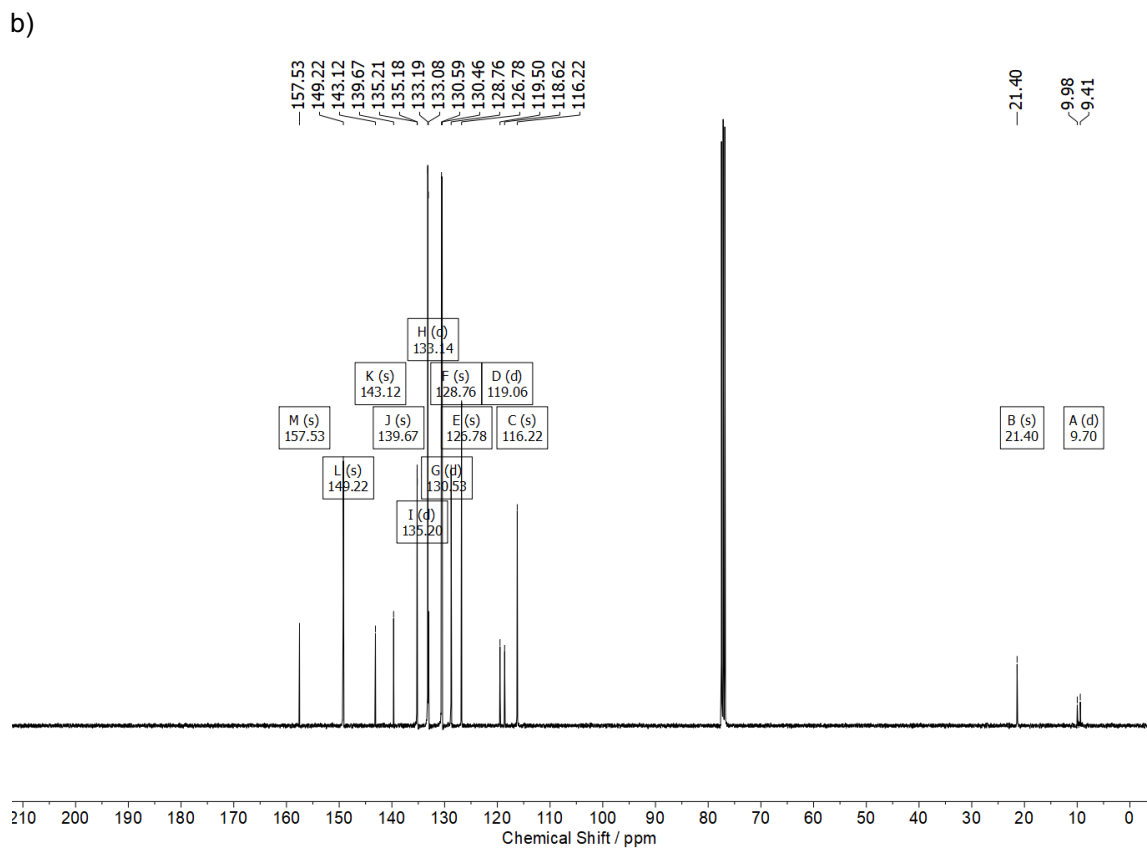
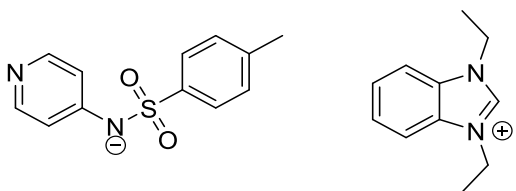
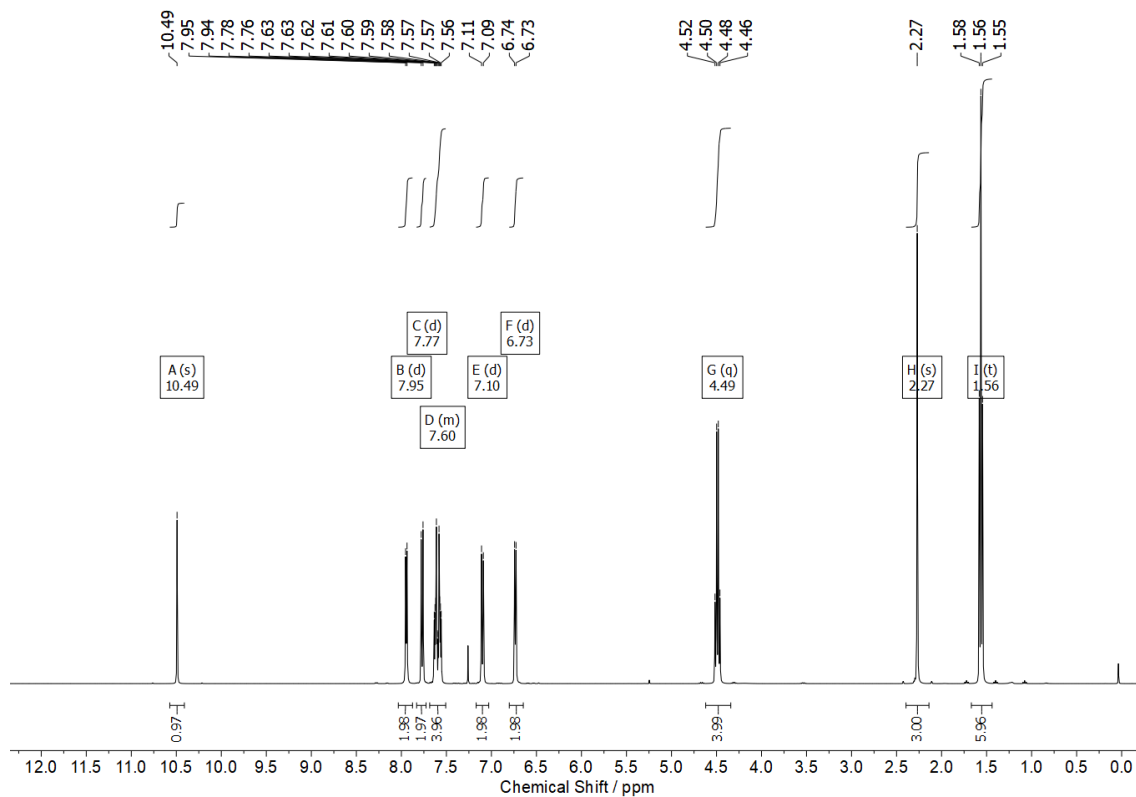


Figure S157. NMR spectra of catalyst **6bc** (CDCl_3 , 400 MHz): a) ^1H NMR spectrum, b) ^{13}C NMR spectrum, c) $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum.

1,3-diethyl-benzimidazolium pyridin-4-yl(tosyl)amide **6be**



a)



b)

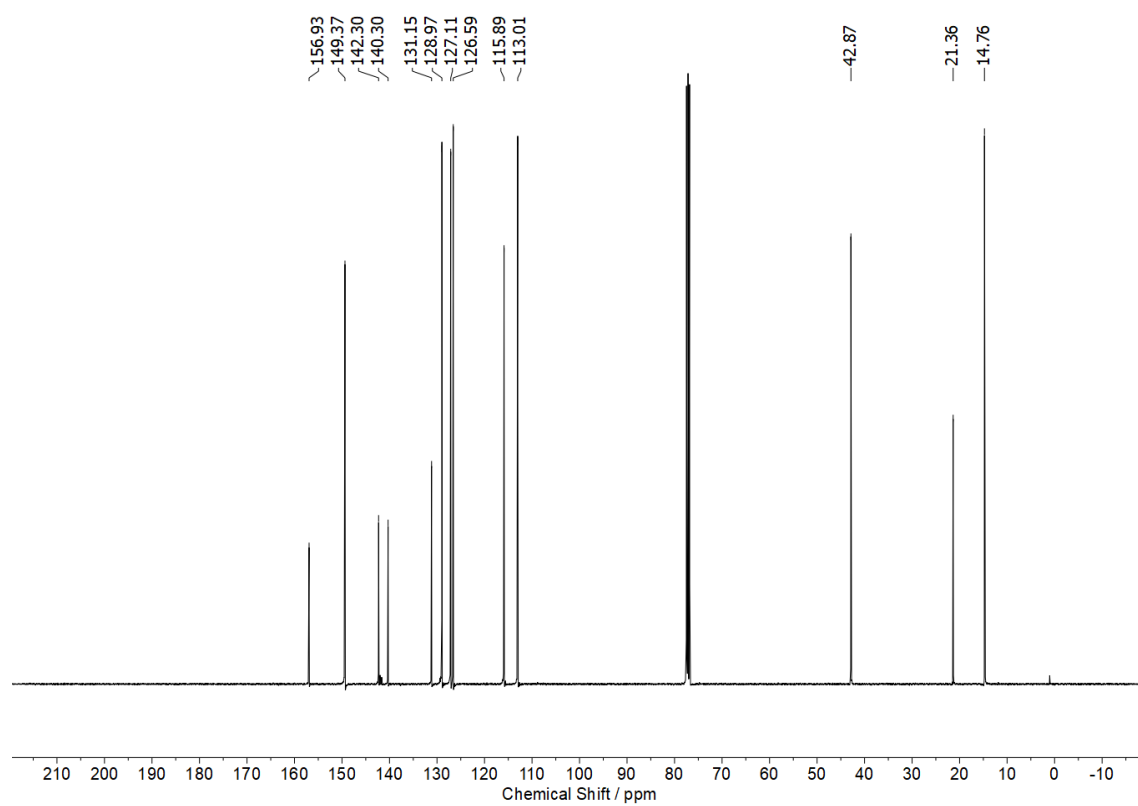
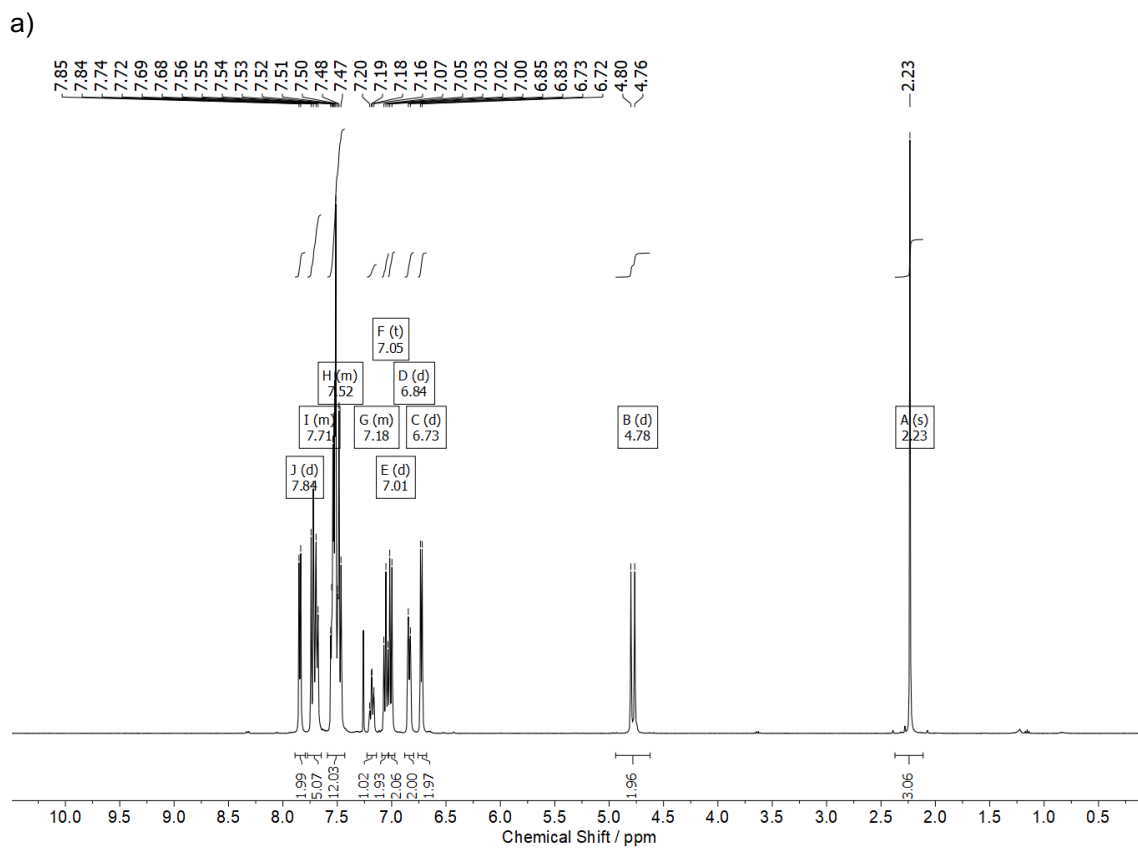
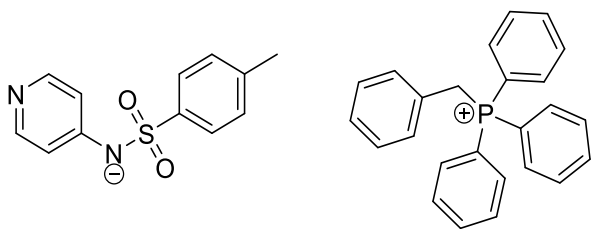


Figure S158. NMR spectra of catalyst **6be** (CDCl_3 , 400 MHz): a) ^1H NMR spectrum, b) ^{13}C NMR spectrum.

Benzyltriphenylphosphonium pyridin-4-yl(tosyl)amide **6bf**



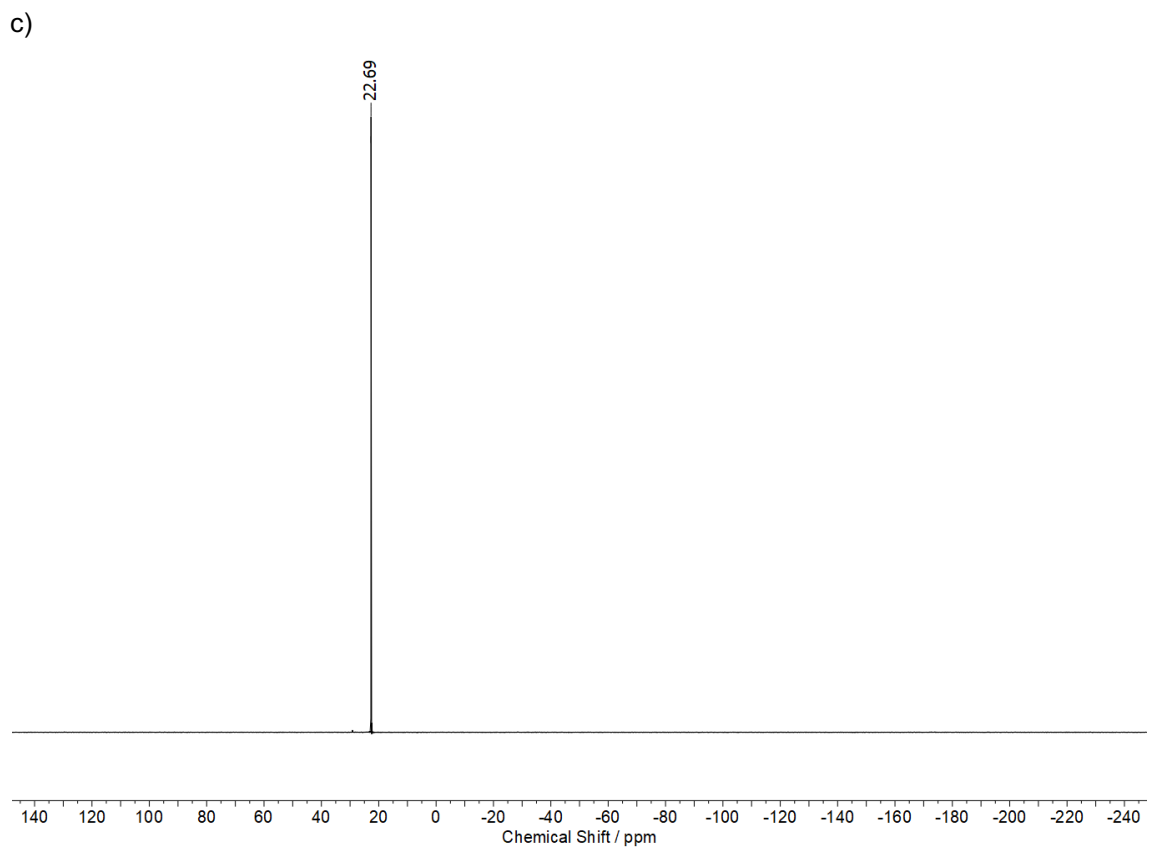
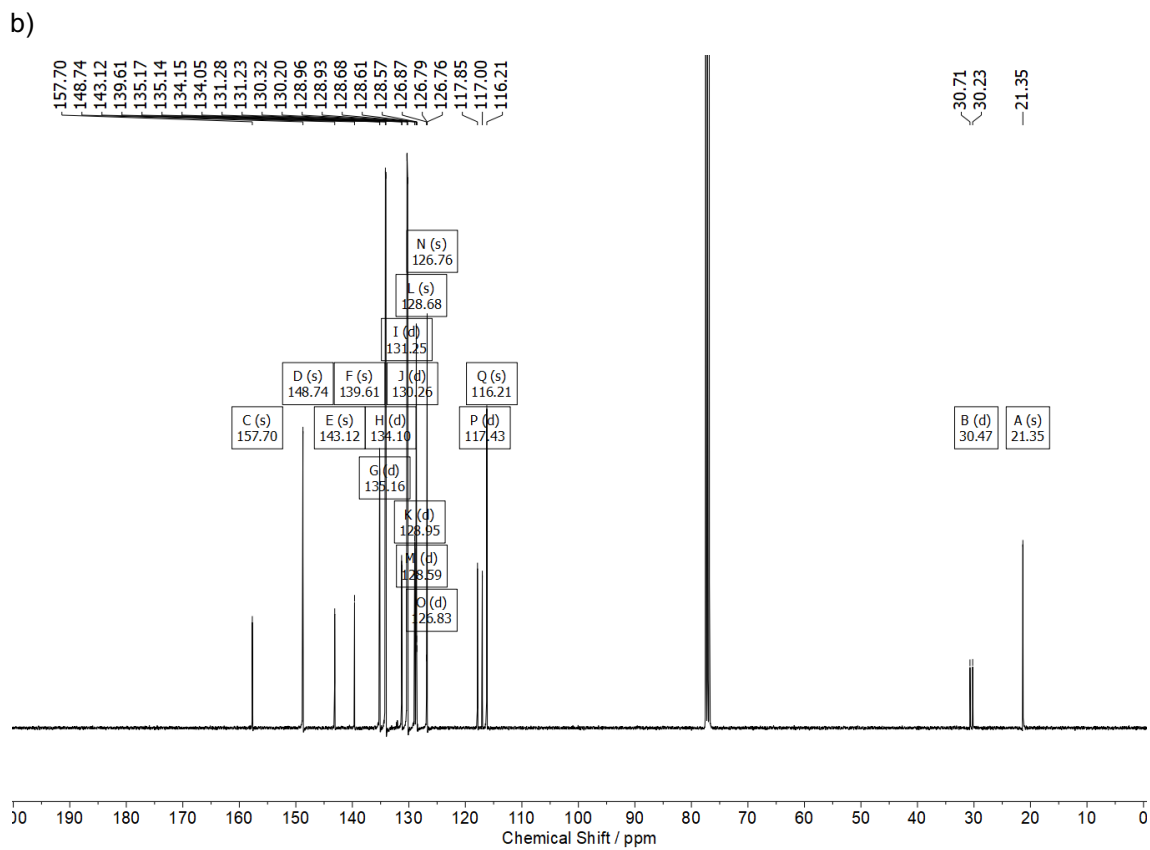
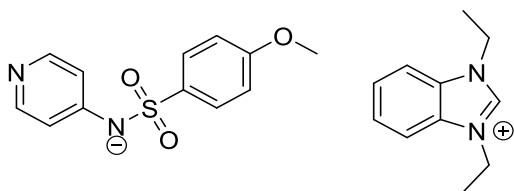
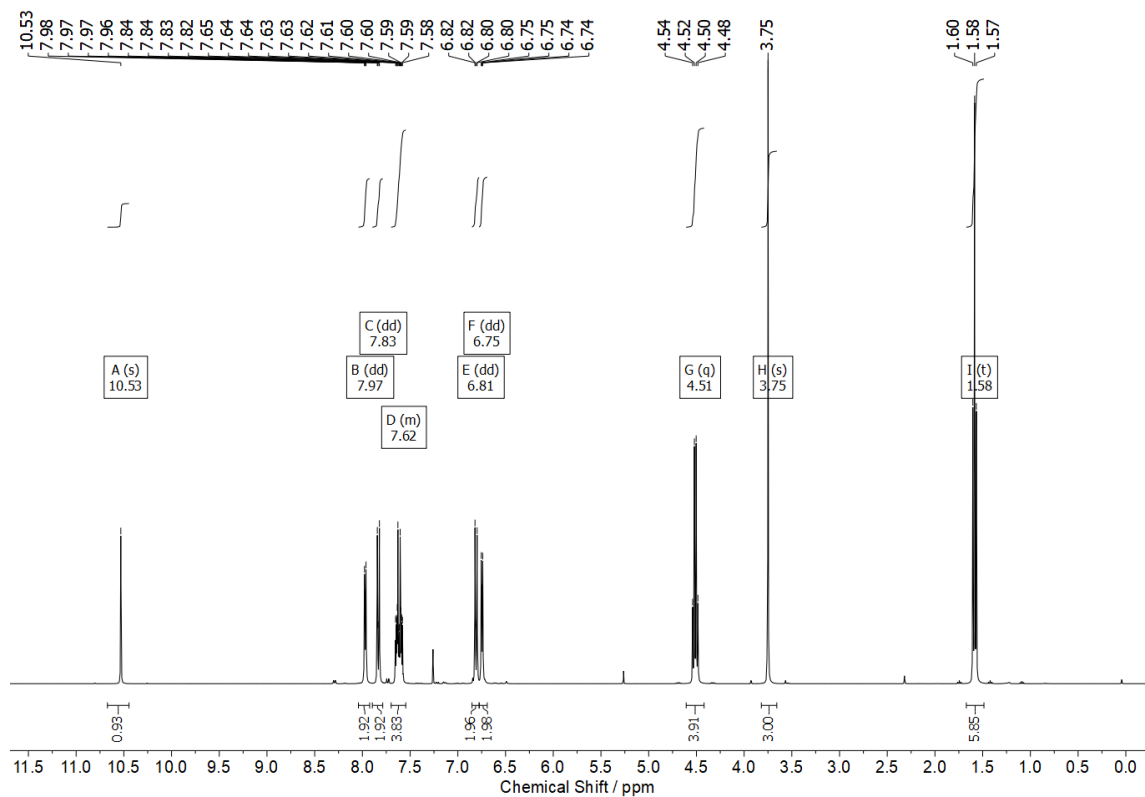


Figure S159. NMR spectra of catalyst **6bf** (CDCl_3 , 400 MHz): a) ^1H NMR spectrum, b) ^{13}C NMR spectrum, c) $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum.

1,3-diethyl-benzimidazolium ((4-methoxyphenyl)sulfonyl)(pyridin-4-yl)amide **6ce**



a)



b)

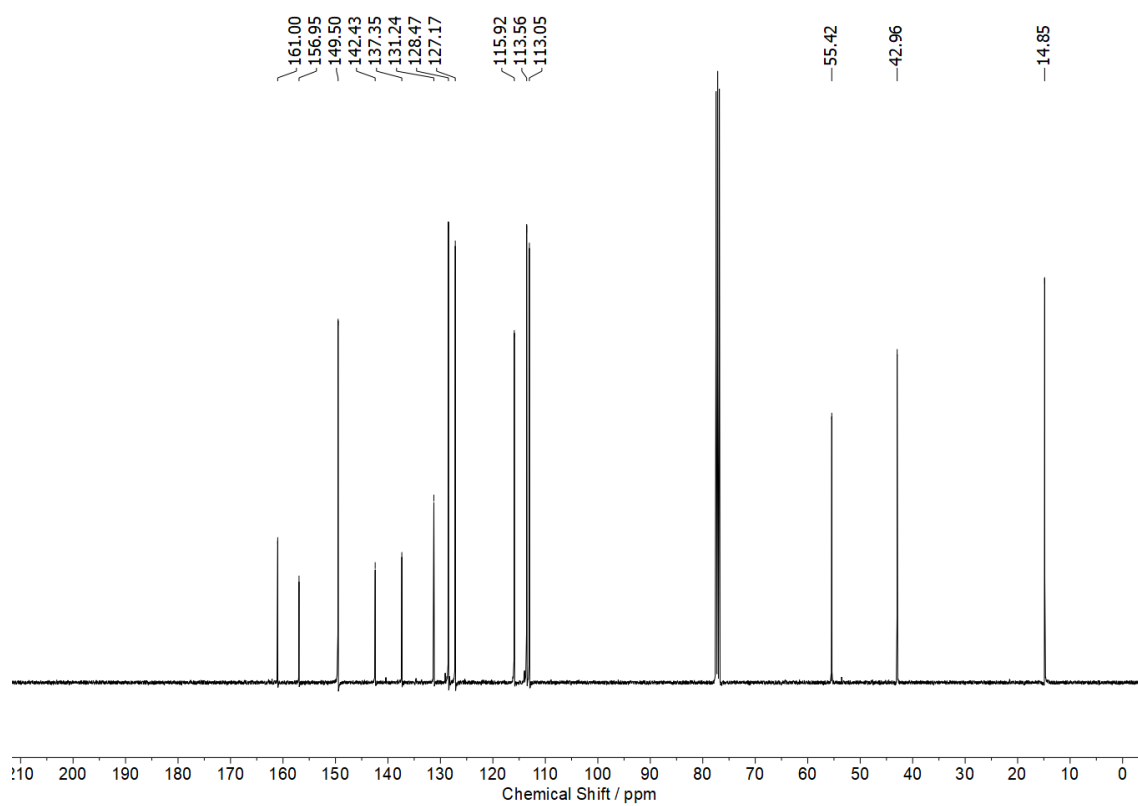
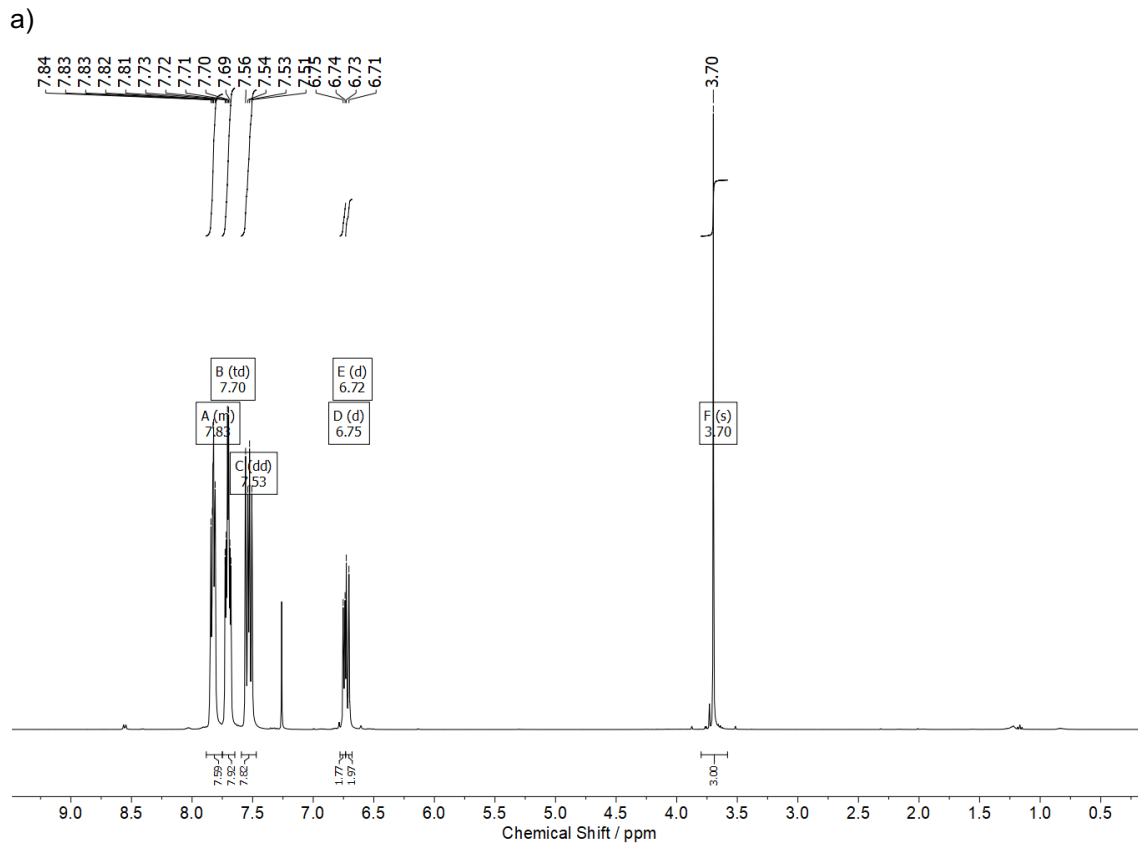
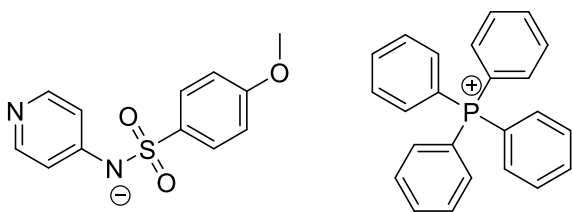


Figure S160. NMR spectra of catalyst **6ce** (CDCl_3 , 400 MHz): a) ^1H NMR spectrum, b) ^{13}C NMR spectrum.

Tetraphenylphosphonium ((4-methoxyphenyl)sulfonyl)(pyridin-4-yl)amide **6cg**



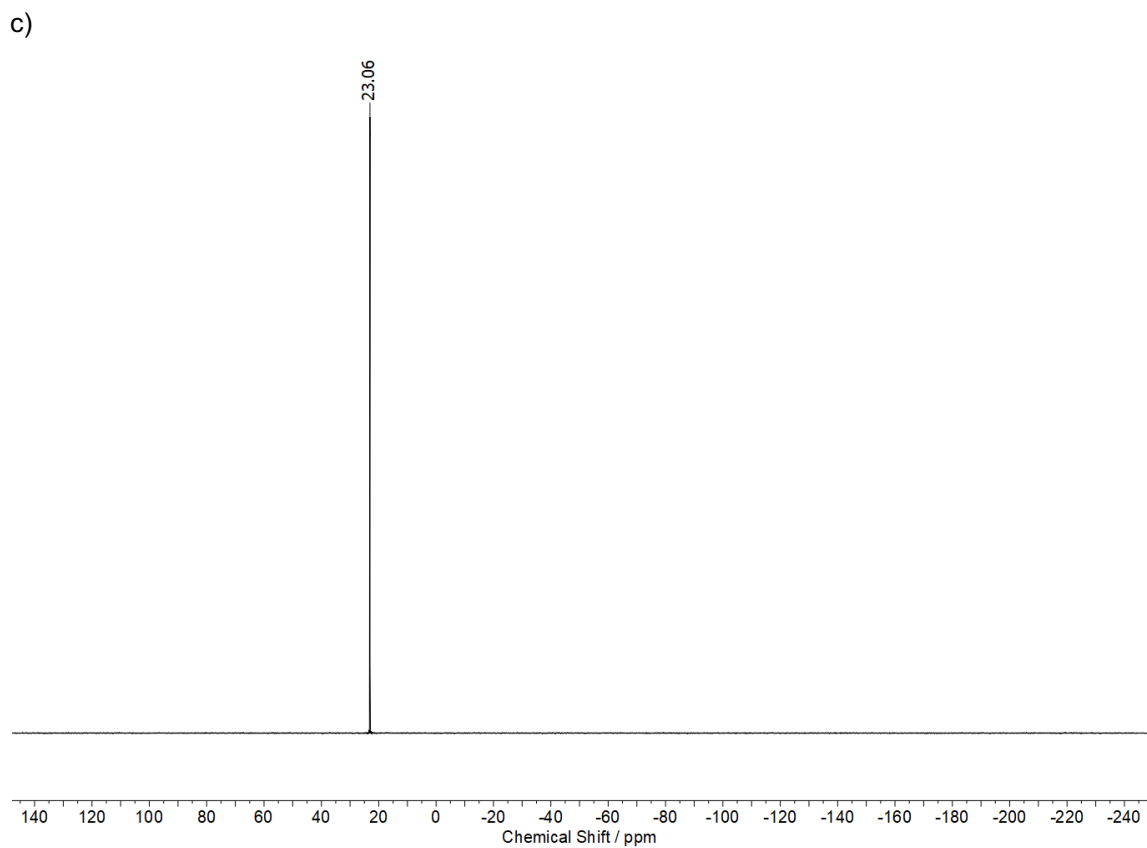
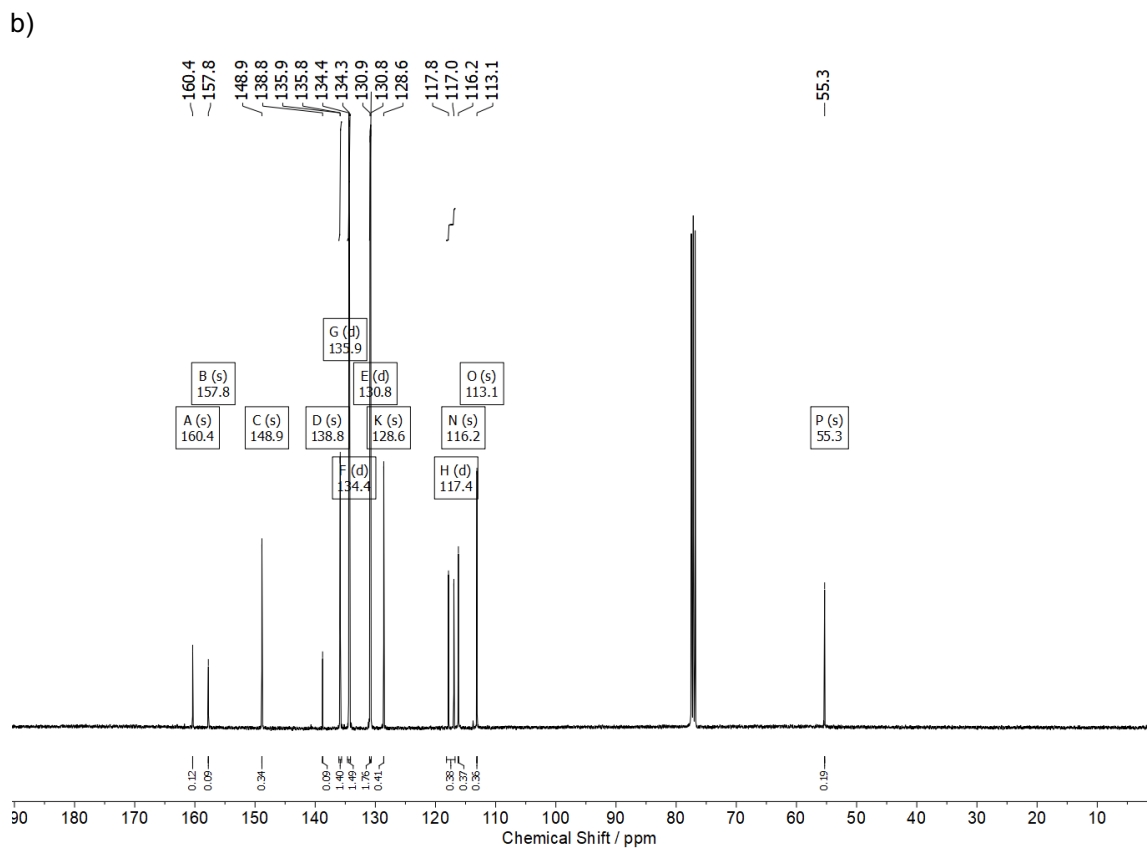
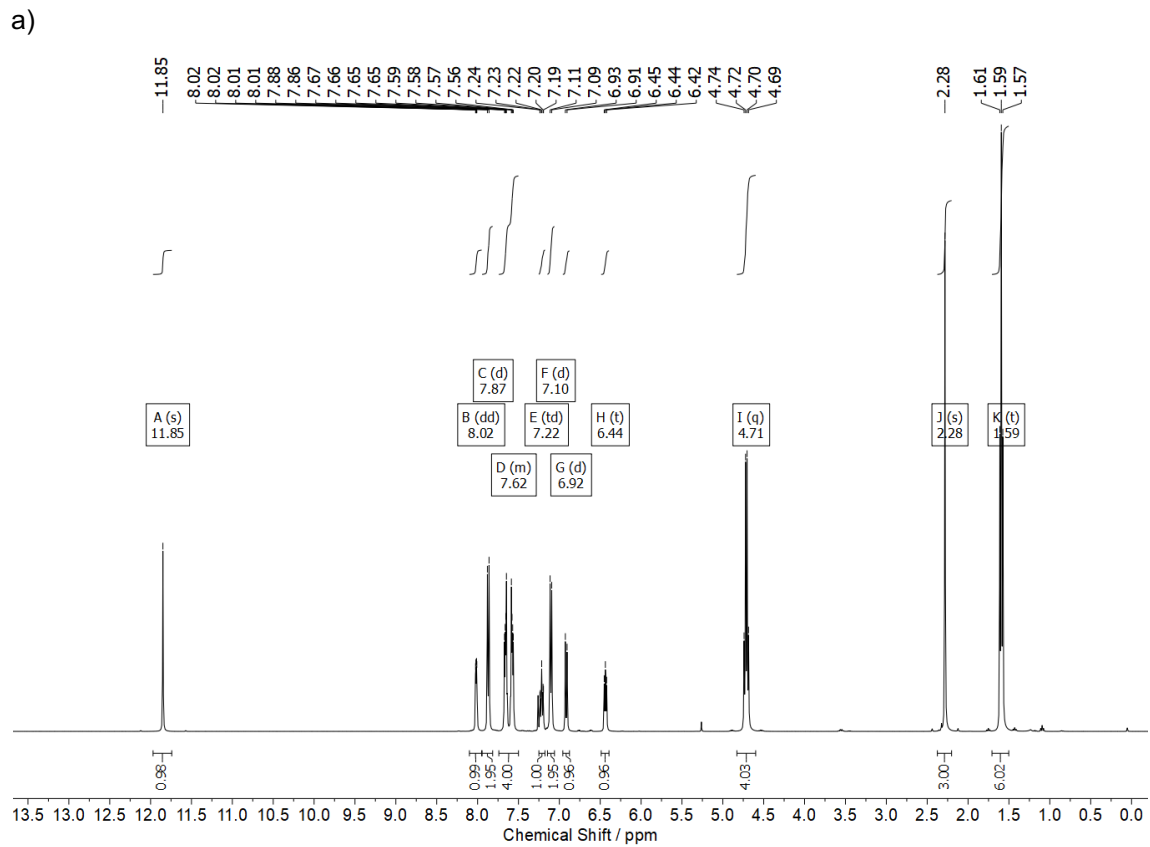
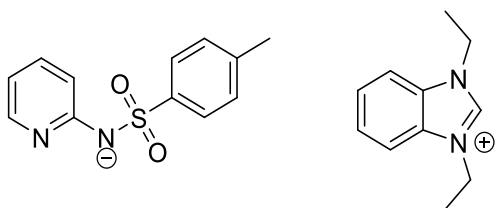


Figure S161. NMR spectra of catalyst **6cg** (CDCl_3 , 400 MHz): a) ^1H NMR spectrum, b) ^{13}C NMR spectrum, c) $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum.

1,3-diethyl-benzimidazolium pyridin-2-yl(tosyl)amide **7e**



b)

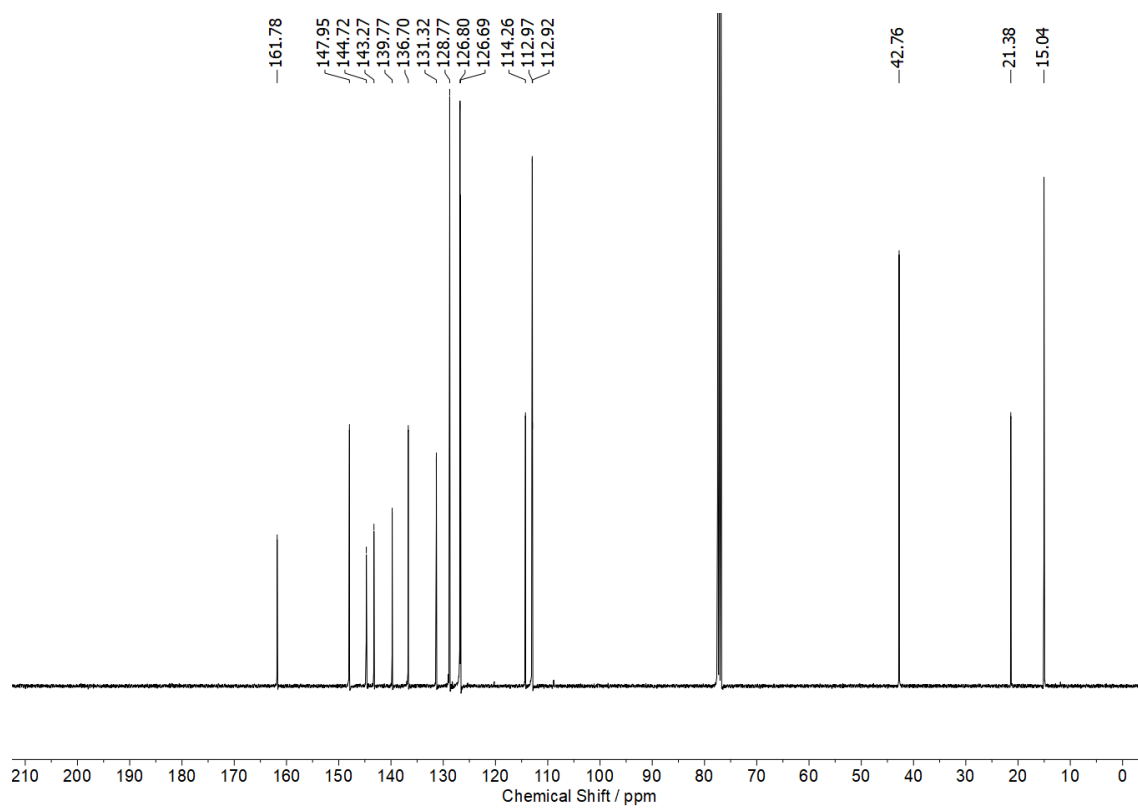
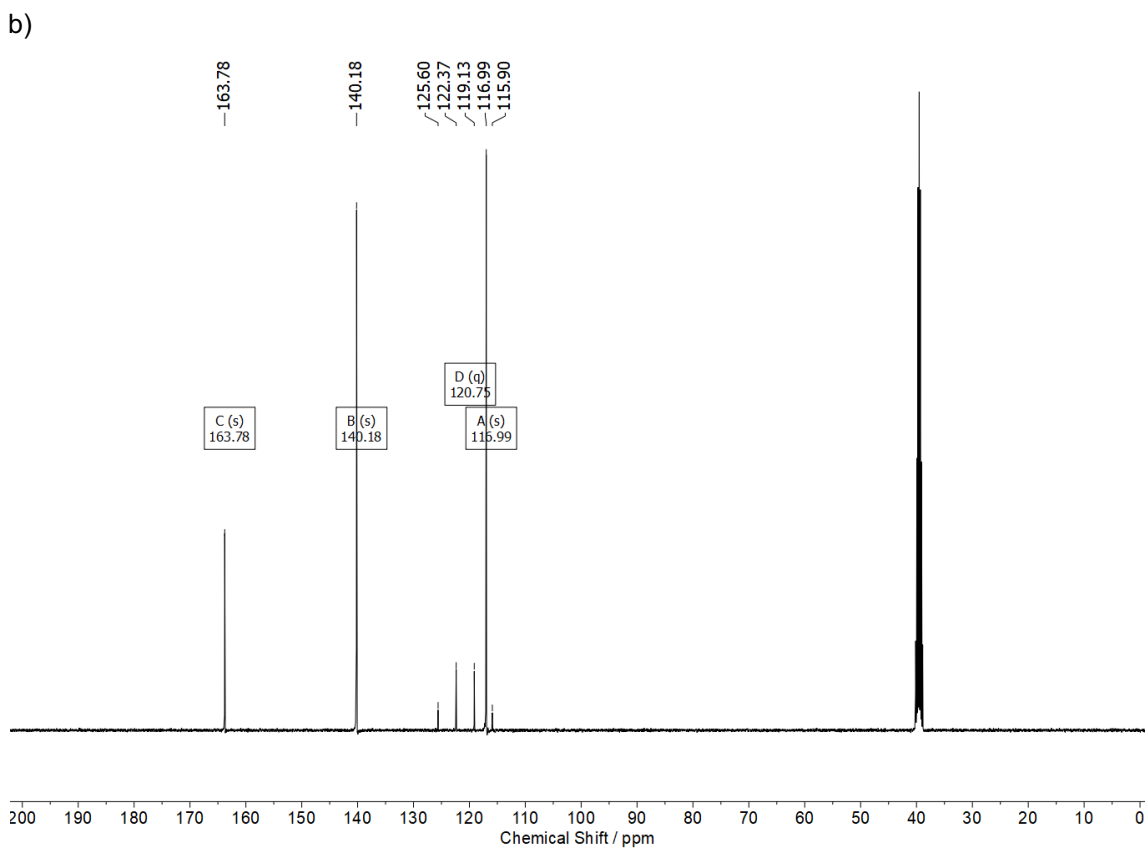
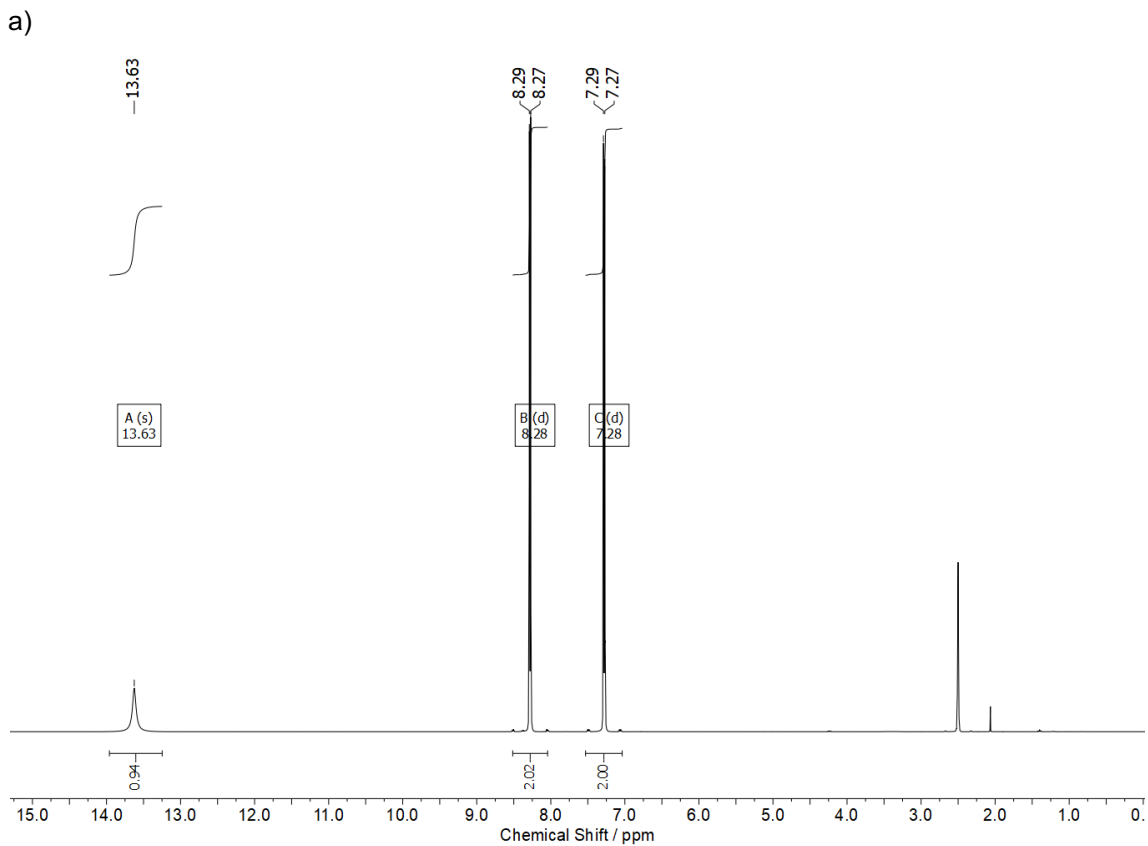
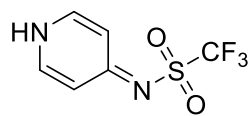


Figure S162. NMR spectra of catalyst **7e** (CDCl_3 , 400 MHz): a) ^1H NMR spectrum, b) ^{13}C NMR spectrum.

1,1,1-trifluoro-N-(pyridin-4(1H)-ylidene)methanesulfonamide **8a**



c)

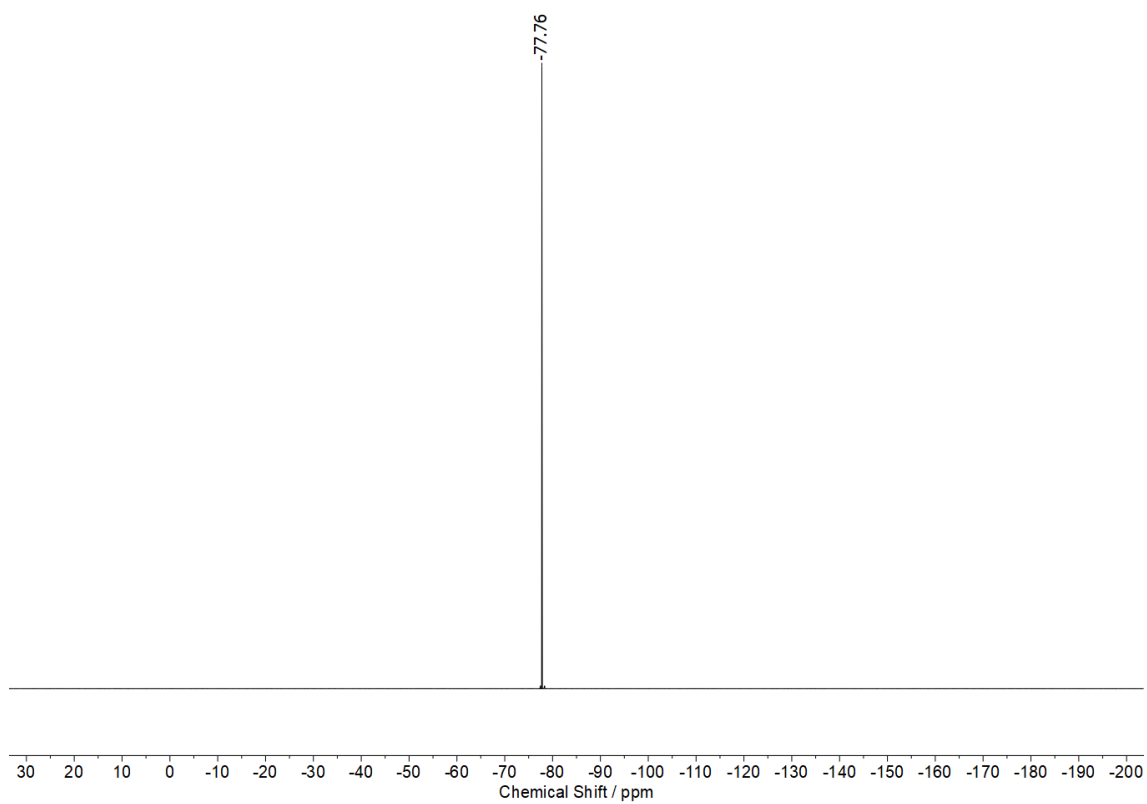
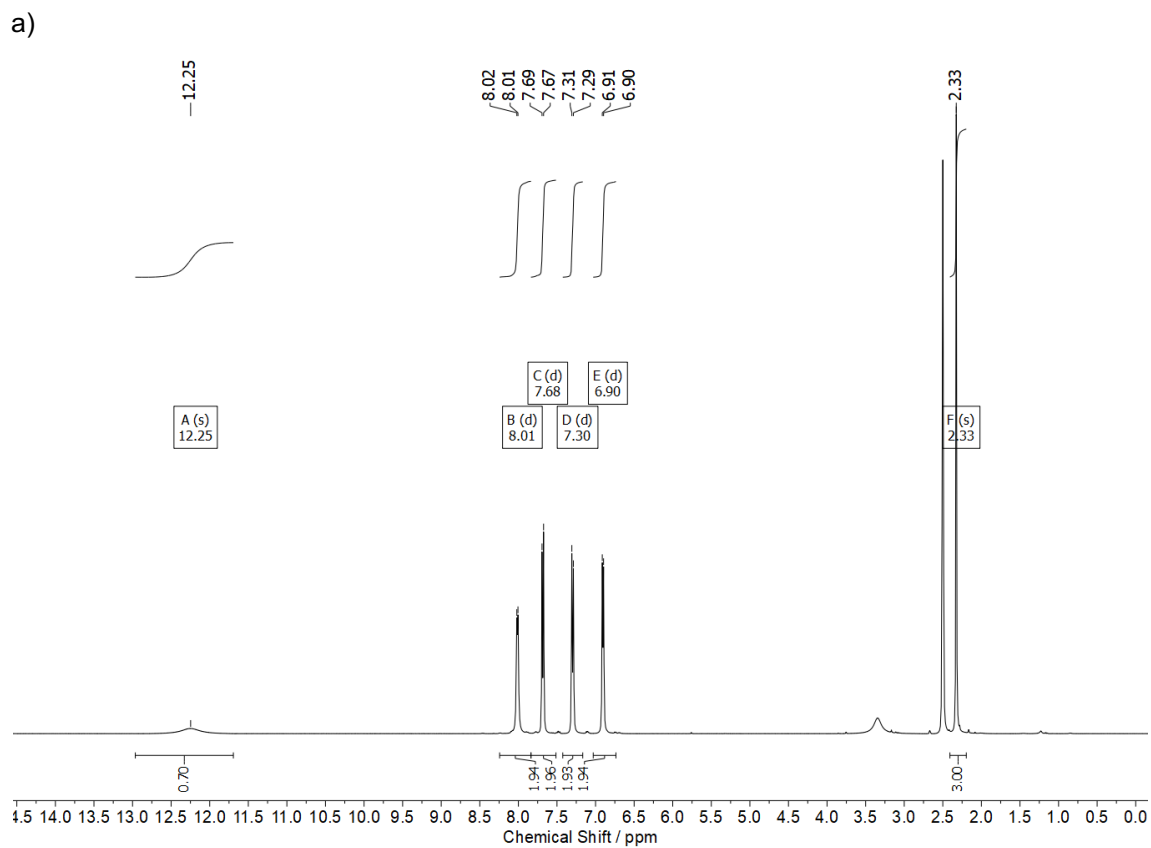
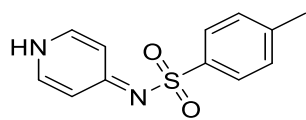


Figure S163. NMR spectra of sulfonamide **8a** (DMSO- d_6), 400 MHz): a) ^1H NMR spectrum, b) ^{13}C NMR spectrum, c) ^{19}F NMR spectrum.

4-methyl-N-(pyridin-4(1H)-ylidene)benzenesulfonamide **8b**



b)

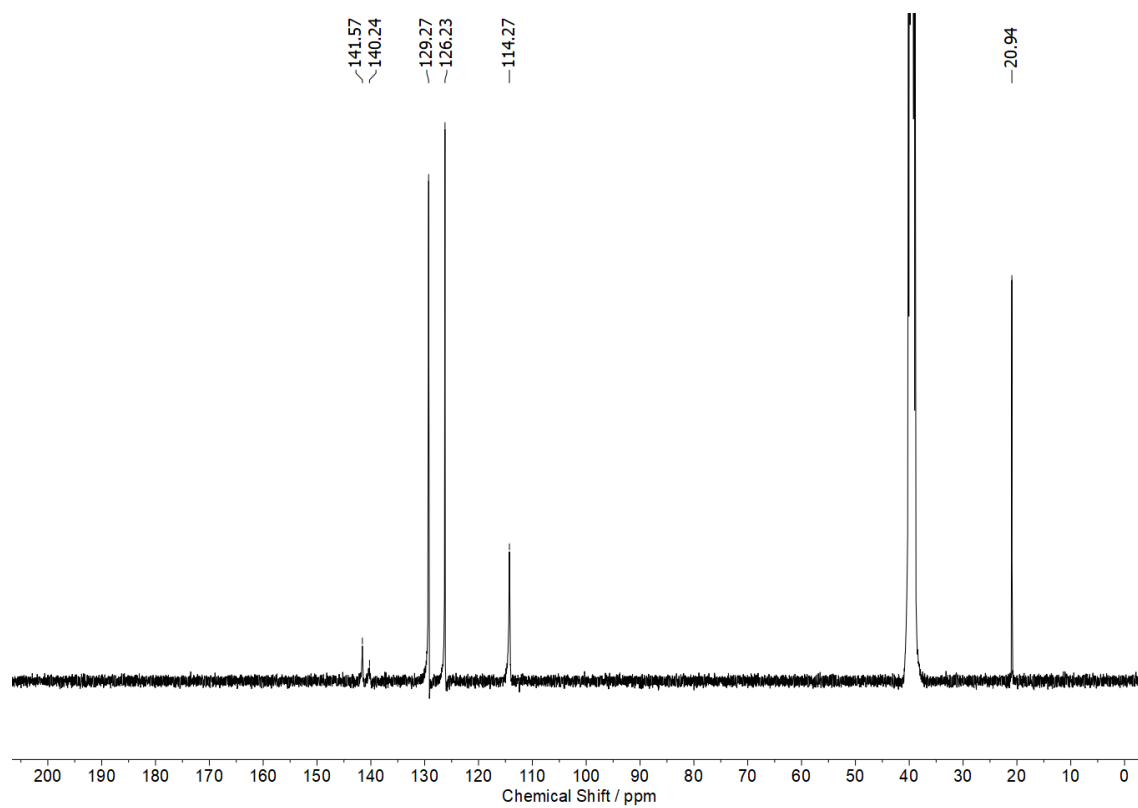
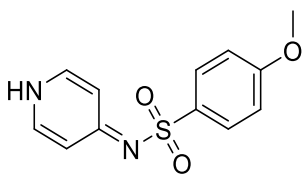
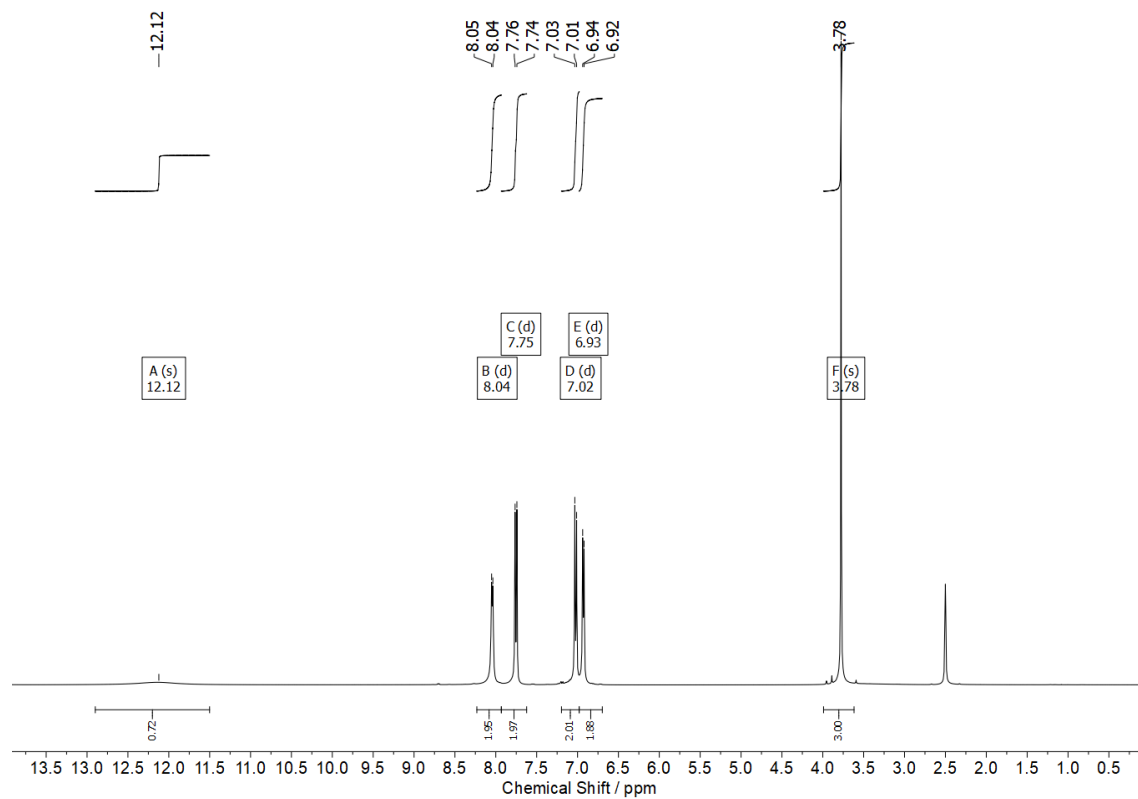


Figure S164. NMR spectra of catalyst **8b** (DMSO-d_6), 400 MHz: a) ^1H NMR spectrum, b) ^{13}C NMR spectrum.

N-(1,4-dihydropyridin-4-yl)-4-methoxybenzenesulfonamide **8c**



a)



b)

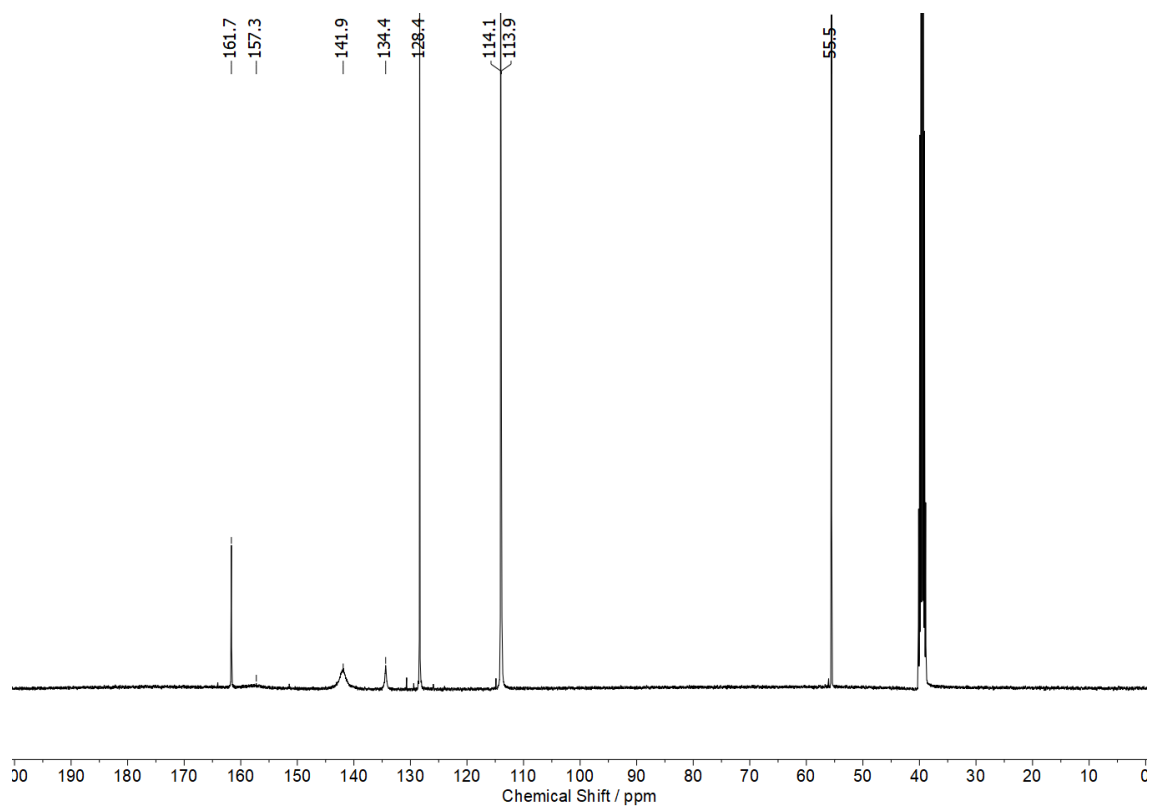
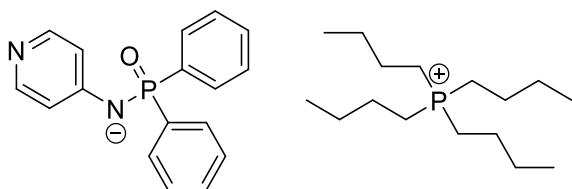
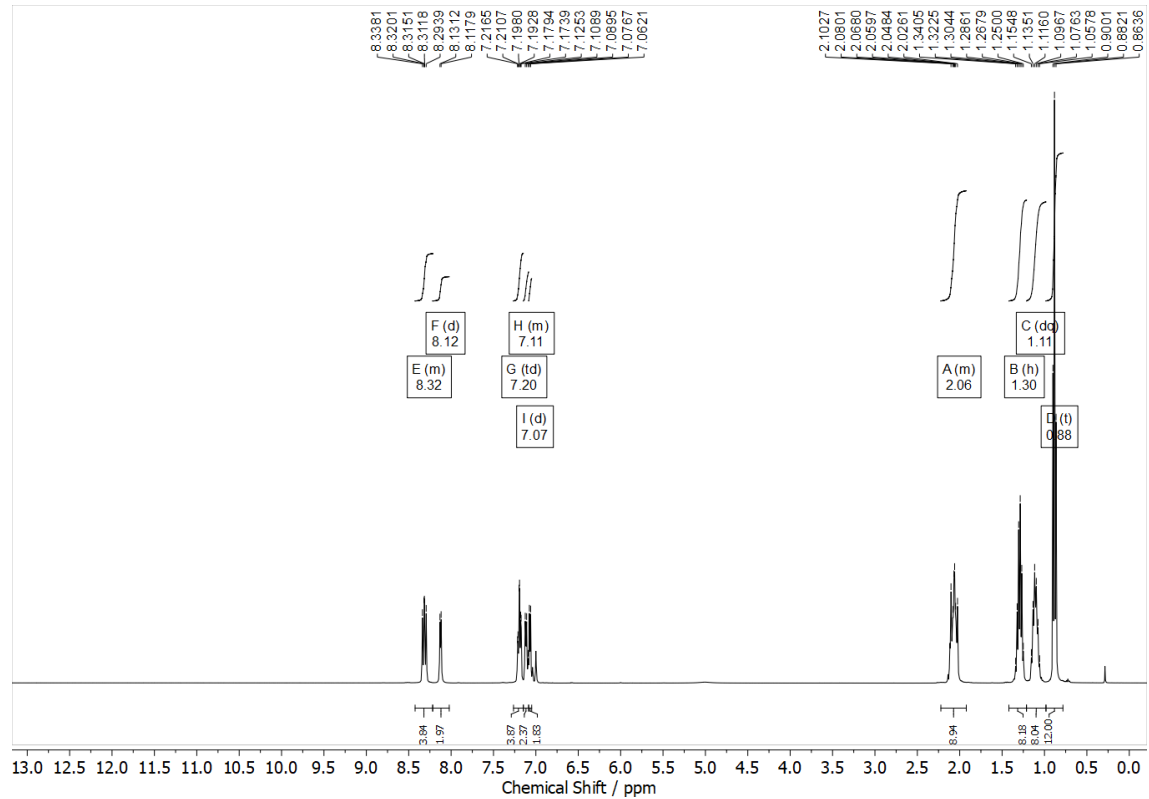


Figure S165. NMR spectra of sulfonamide **8c** (DMSO- d_6 , 400 MHz): a) 1H NMR spectrum, b) ^{13}C NMR spectrum.

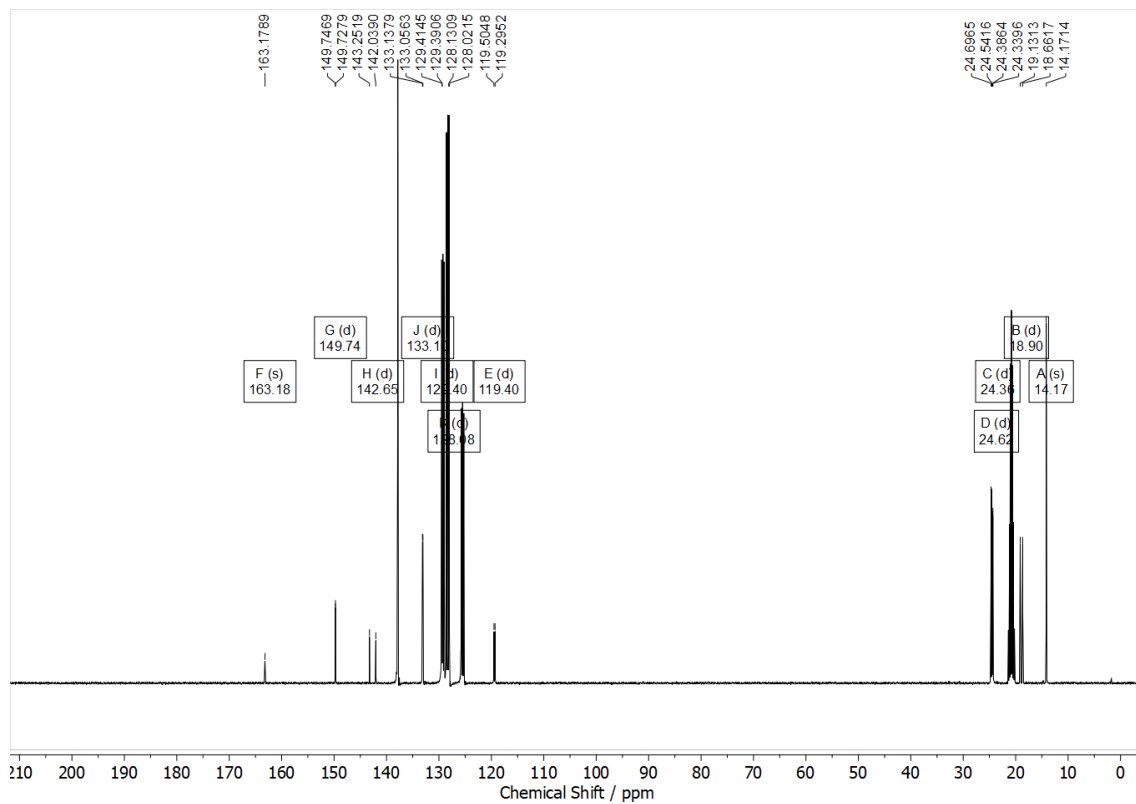
Tetrabutylphosphonium (diphenylphosphoryl)(pyridin-4-yl)amide **10d**



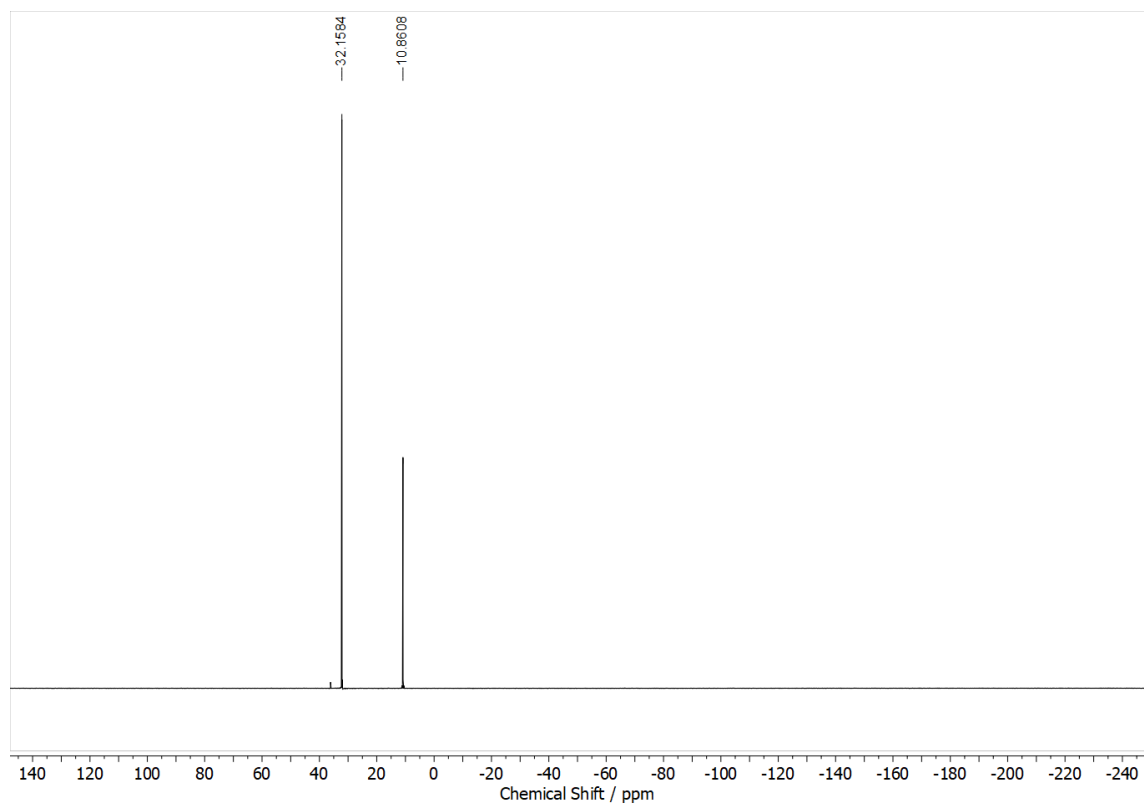
a)



b)



c)



d)

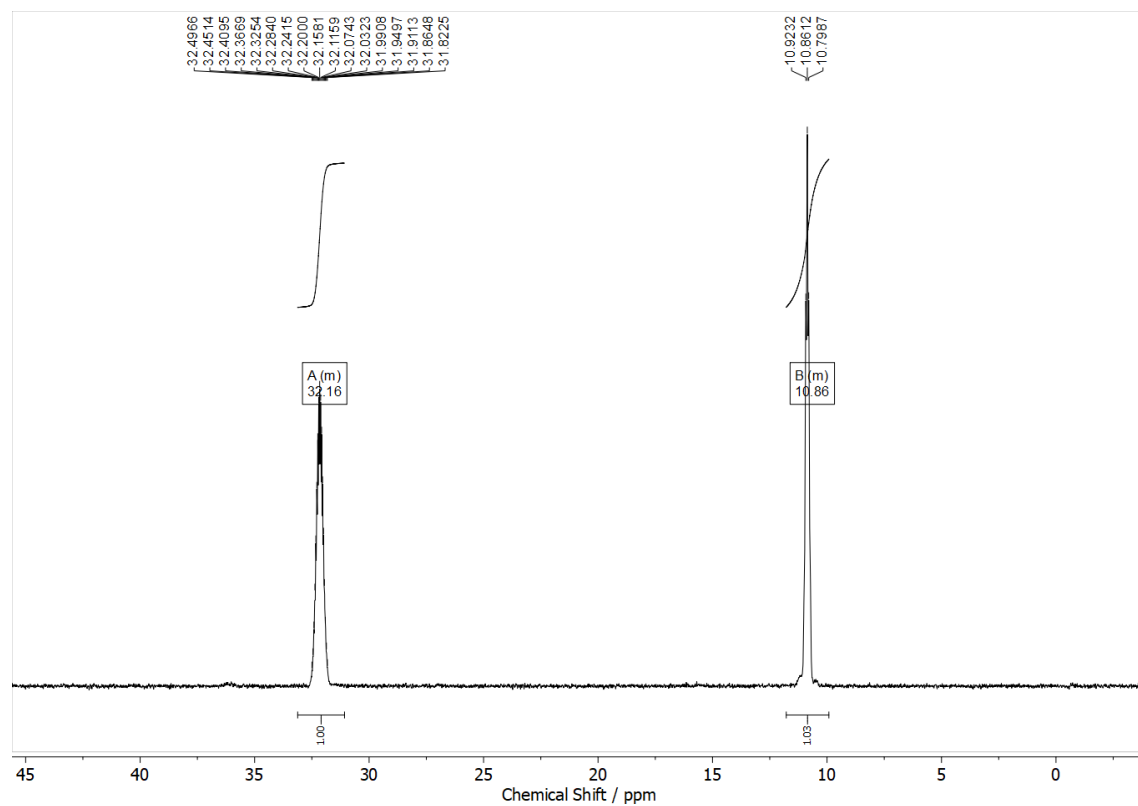
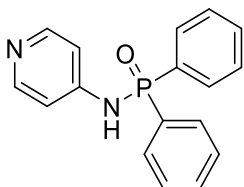
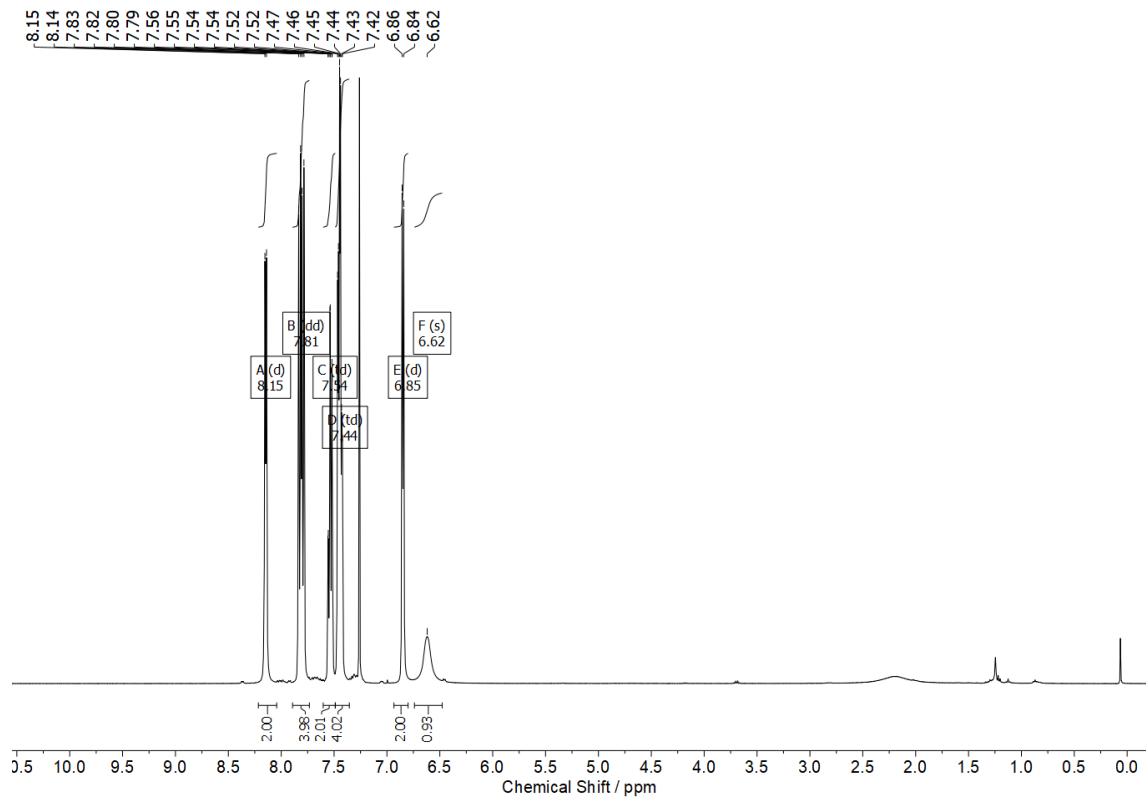


Figure S166. NMR spectra of phosphonic amide catalyst **10d** (CDCl_3 , 400 MHz): a) ^1H NMR spectrum, b) ^{13}C NMR spectrum, c) $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum. d) $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum.

P,P-diphenyl-N-(pyridin-4-yl)phosphinic amide **11**



a)



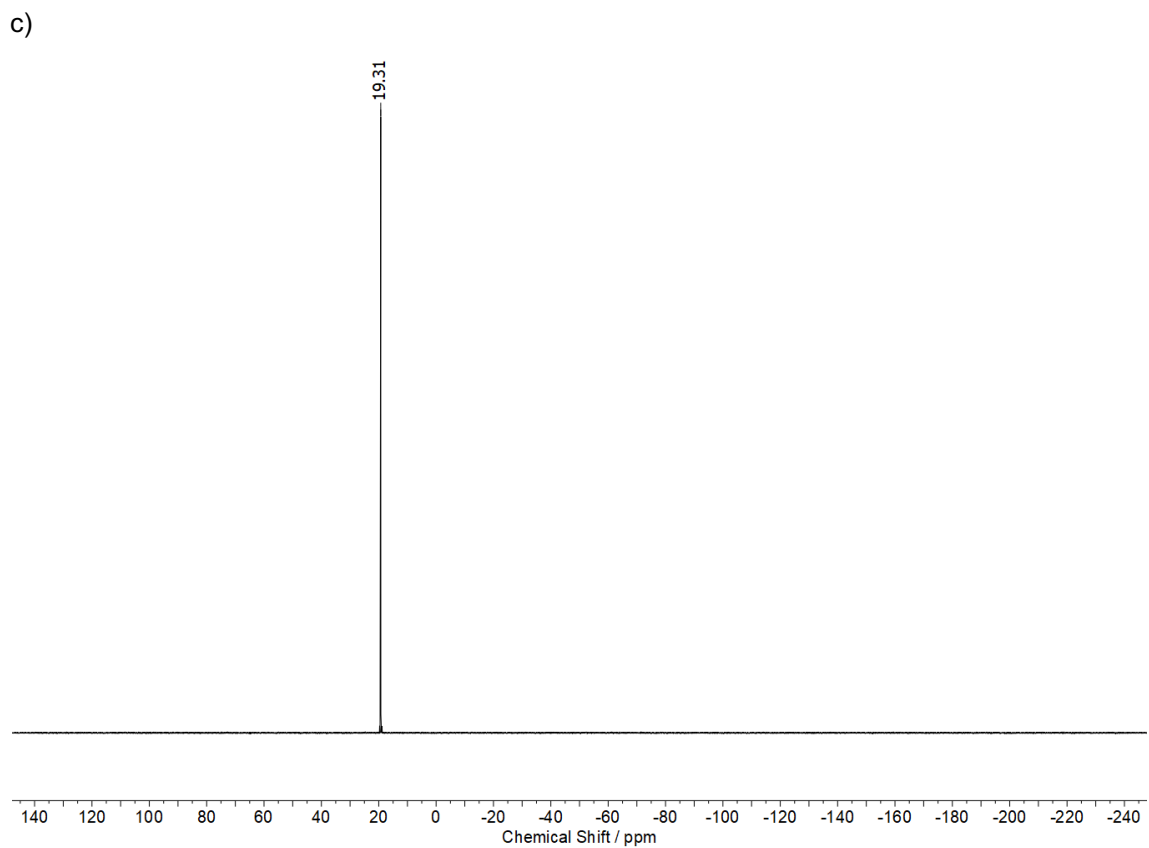
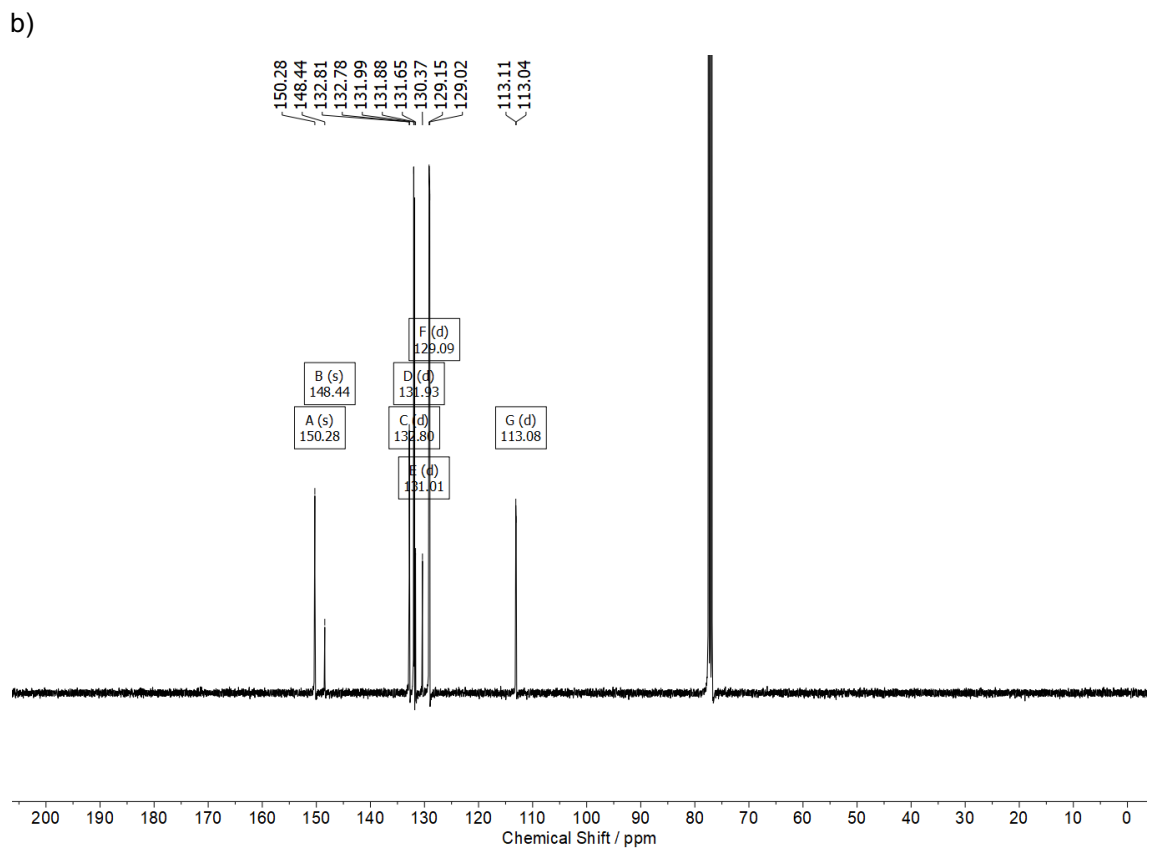
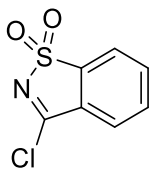
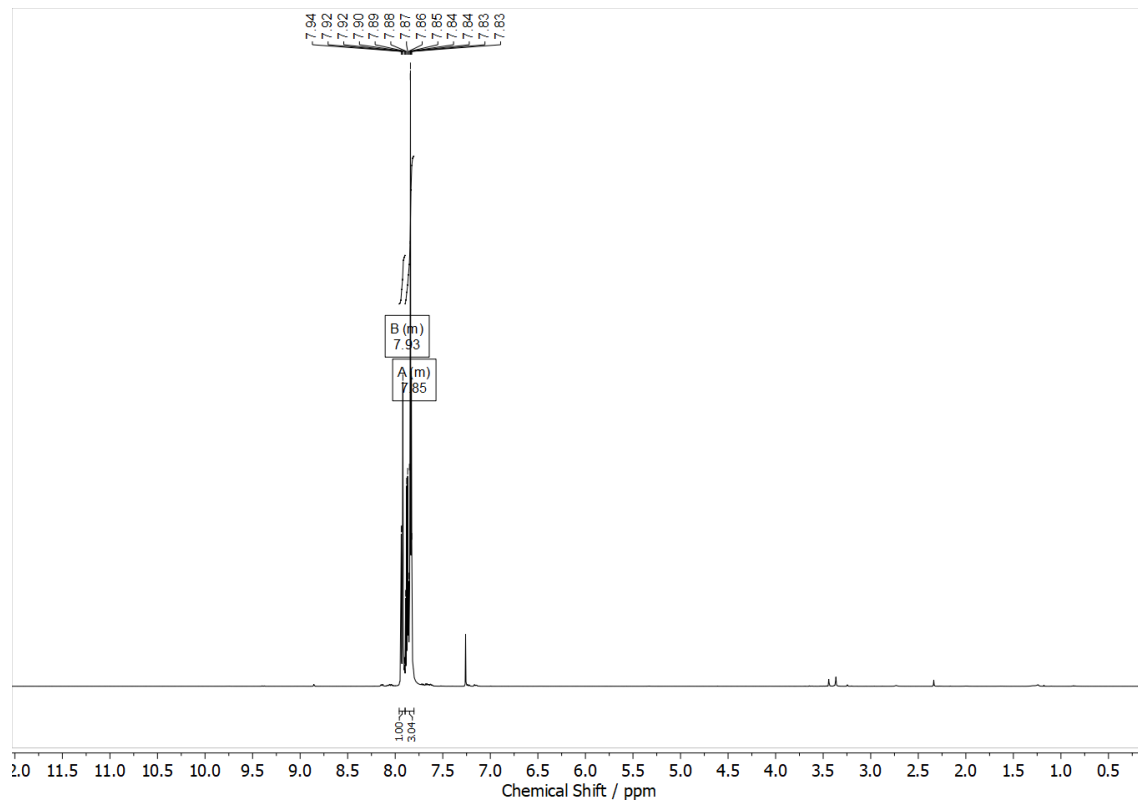


Figure S167. NMR spectra of phosphinic amide **11** CDCl_3 , 400 MHz): a) ^1H NMR spectrum, b) ^{13}C NMR spectrum, c) $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum.

3-chlorobenzo[d]isothiazole 1,1-dioxide **13**



a)



b)

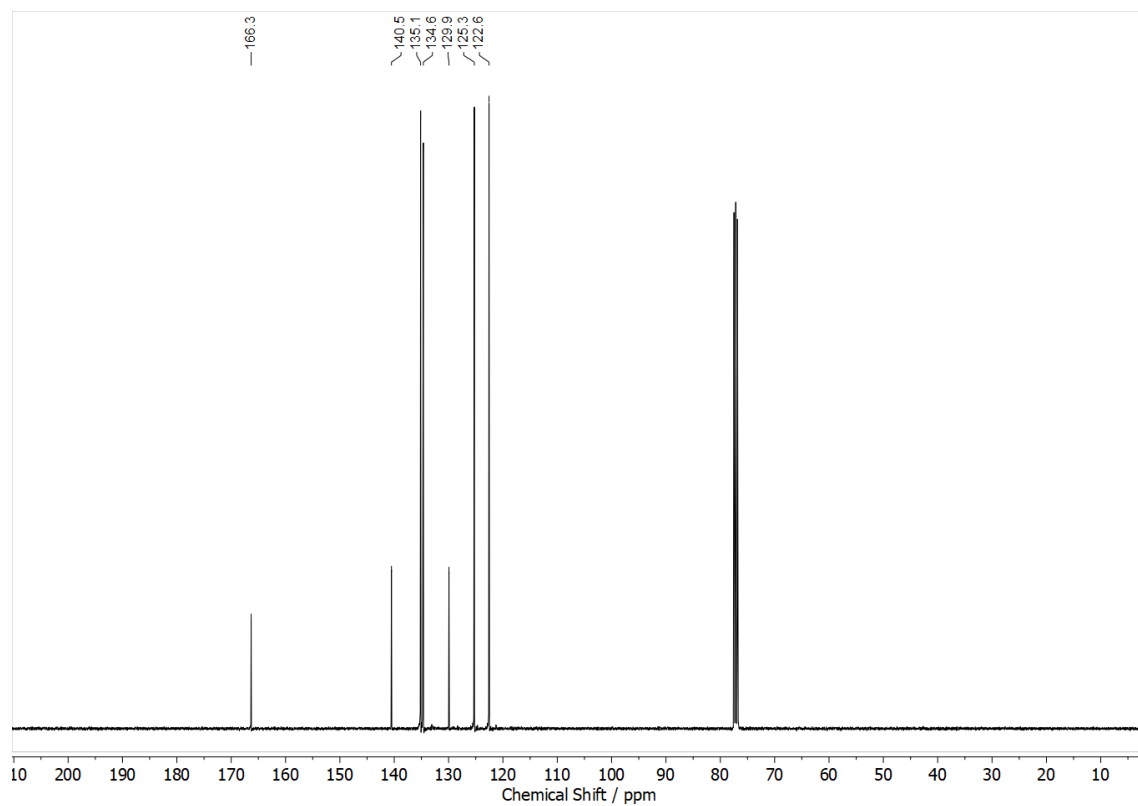
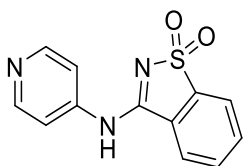
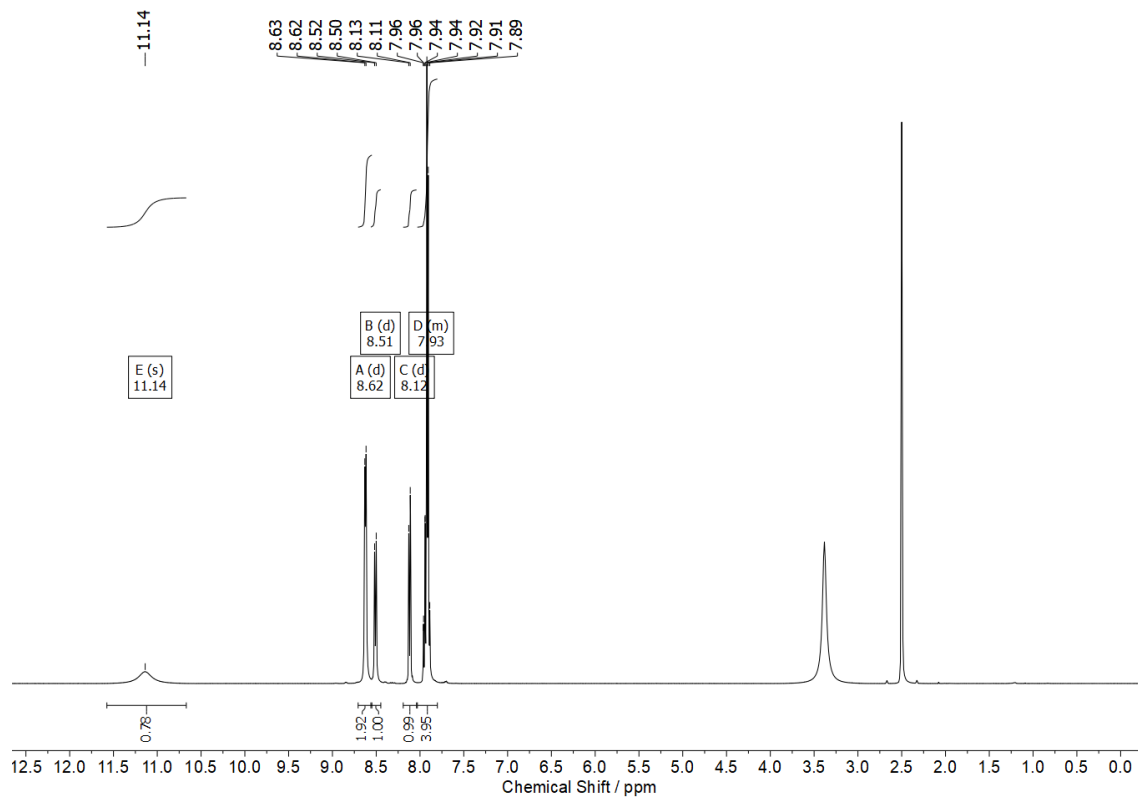


Figure S168. NMR spectra of imidoyl chloride **13** (CDCl_3 , 400 MHz): a) ^1H NMR spectrum, b) ^{13}C NMR spectrum.

3-(pyridin-4-ylamino)benzo[d]isothiazole 1,1-dioxide **14**



a)



b)

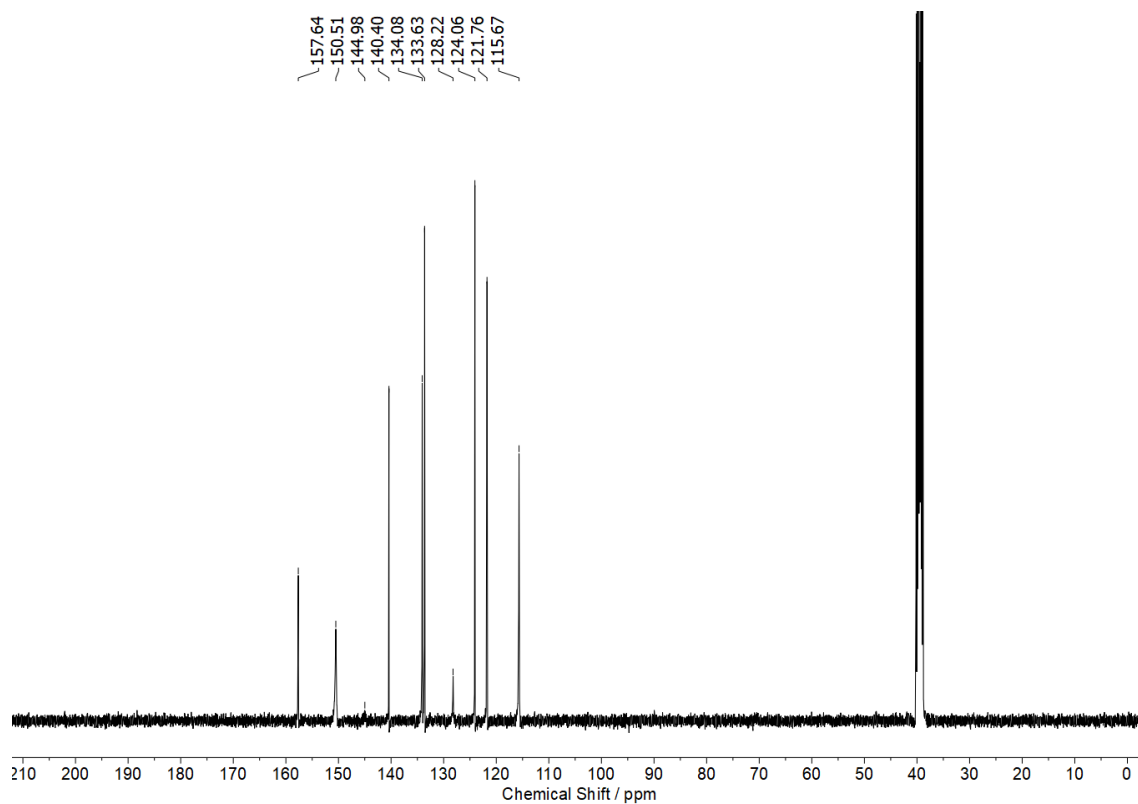
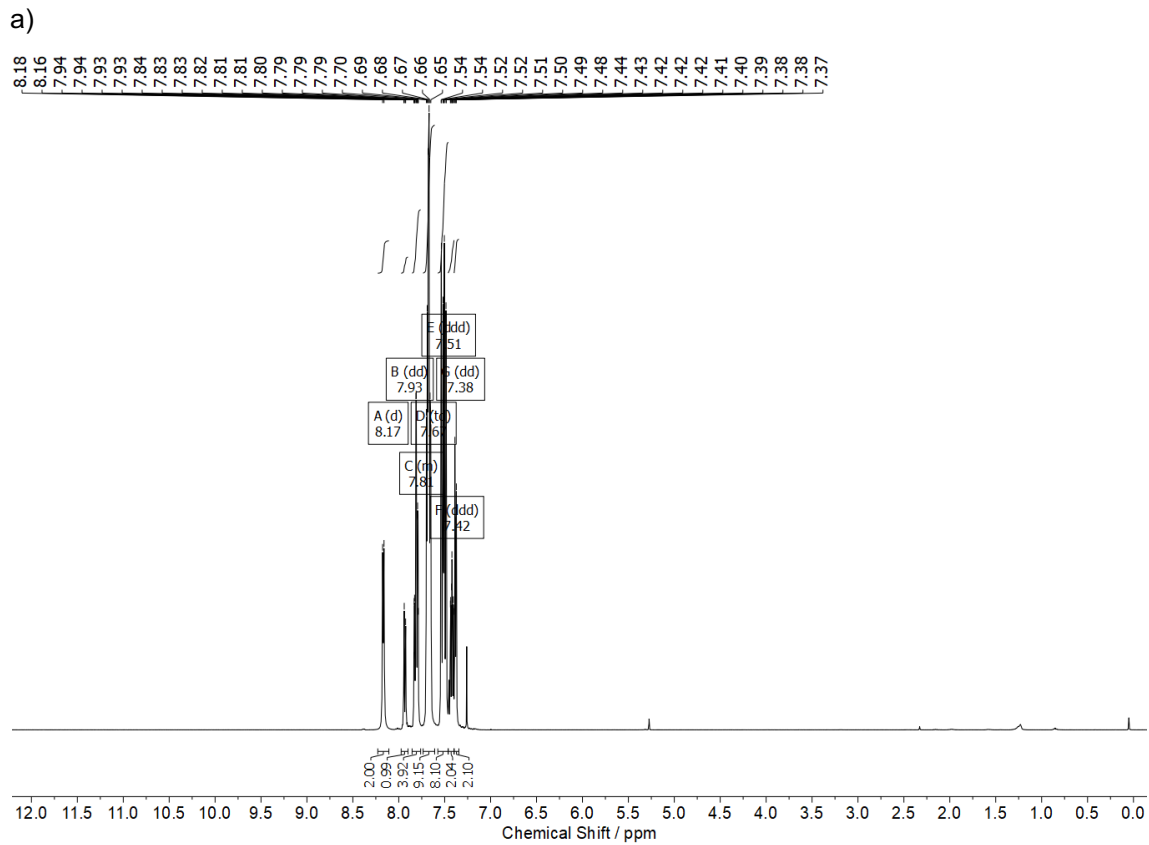
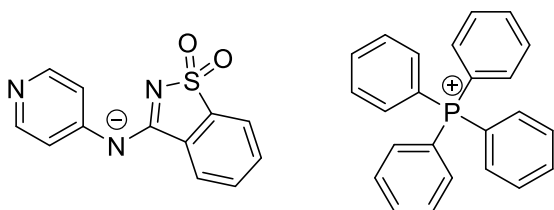


Figure S169. NMR spectra of sulfonamide **14** (DMSO-d₆, 400 MHz): a) ¹H NMR spectrum, b) ¹³C NMR spectrum.

Tetraphenylphosphonium (1,1-dioxidobenzo[d]isothiazol-3-yl)(pyridin-4-yl)amide **15g**



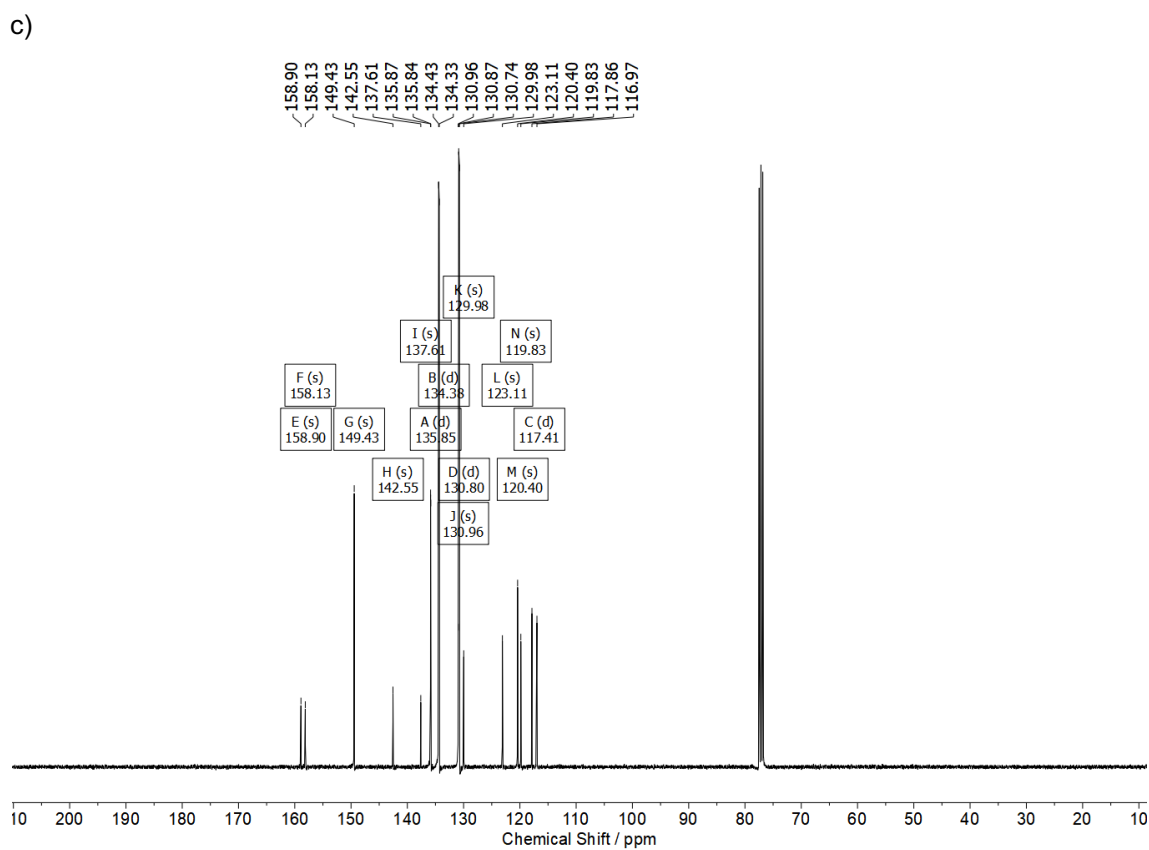
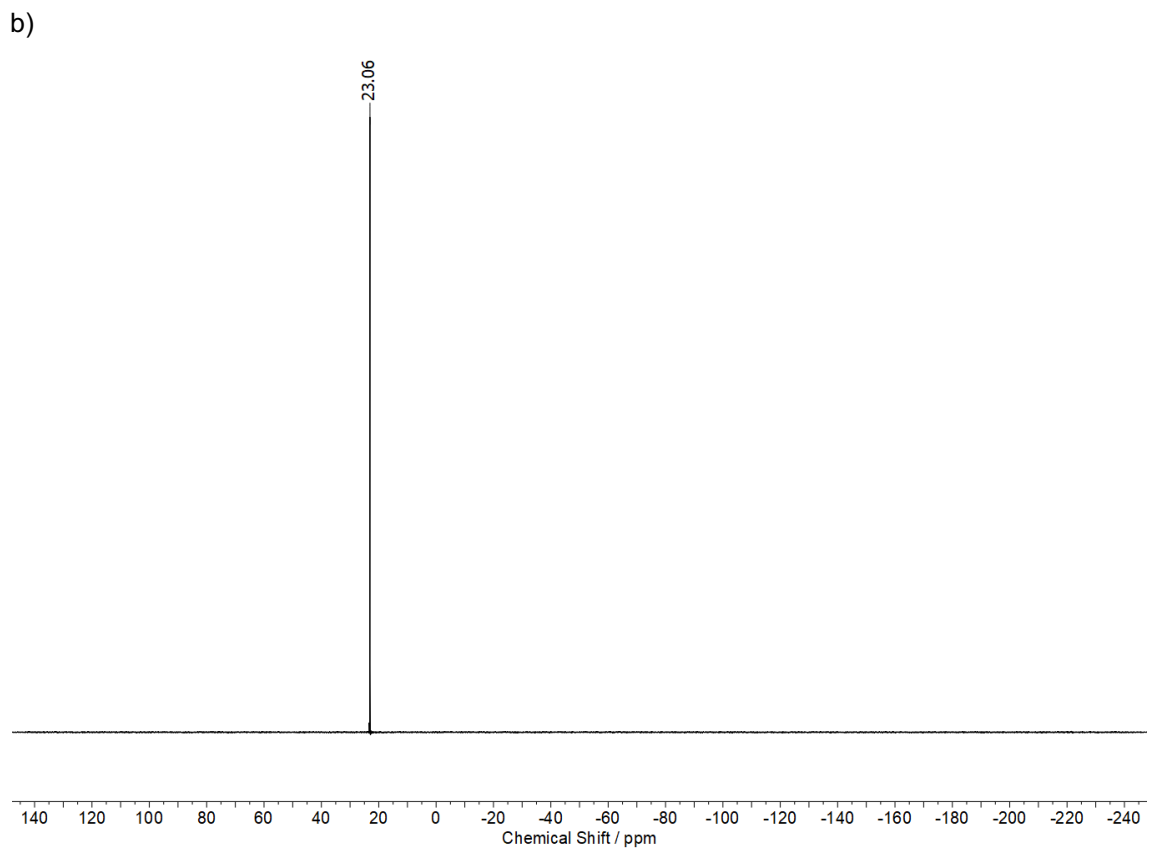
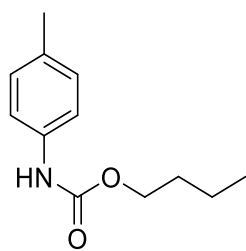
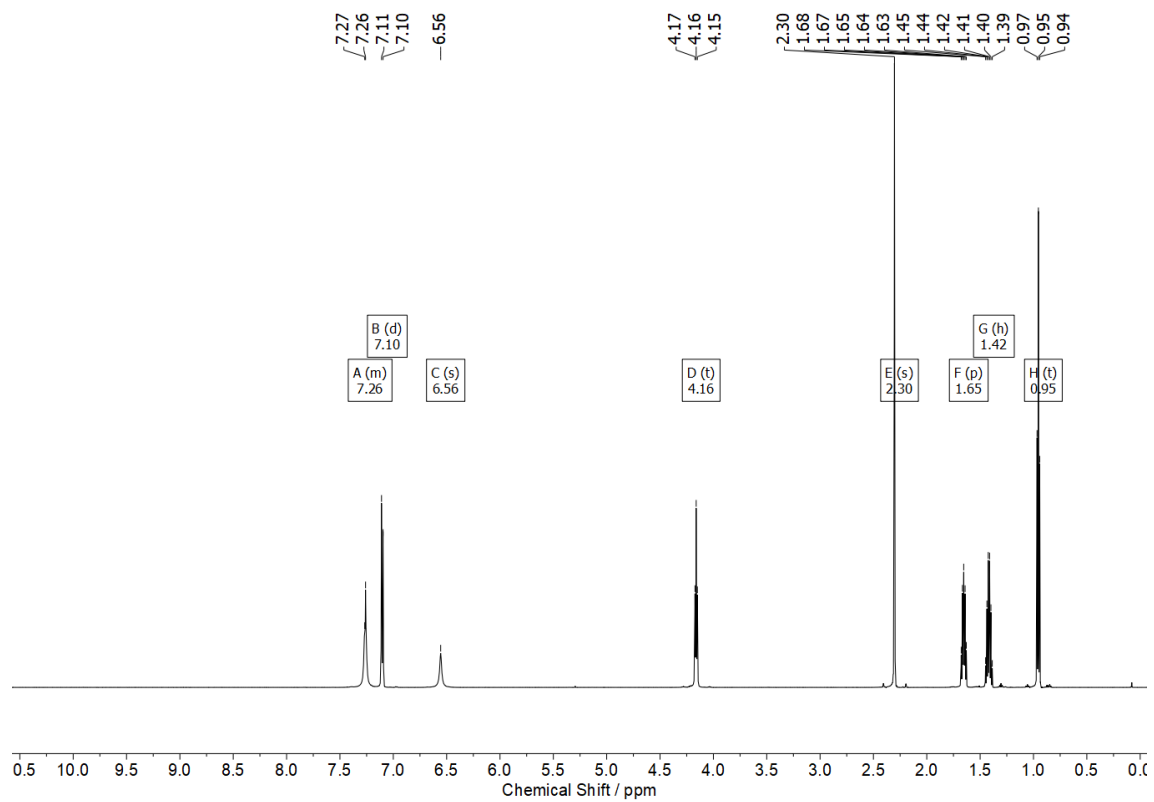


Figure S170. NMR spectra of ion pair catalyst **15g** CDCl_3 , 400 MHz): a) ^1H NMR spectrum, b) ^{13}C NMR spectrum, c) $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum.

Butyl *p*-tolylcarbamate **16**



a)



b)

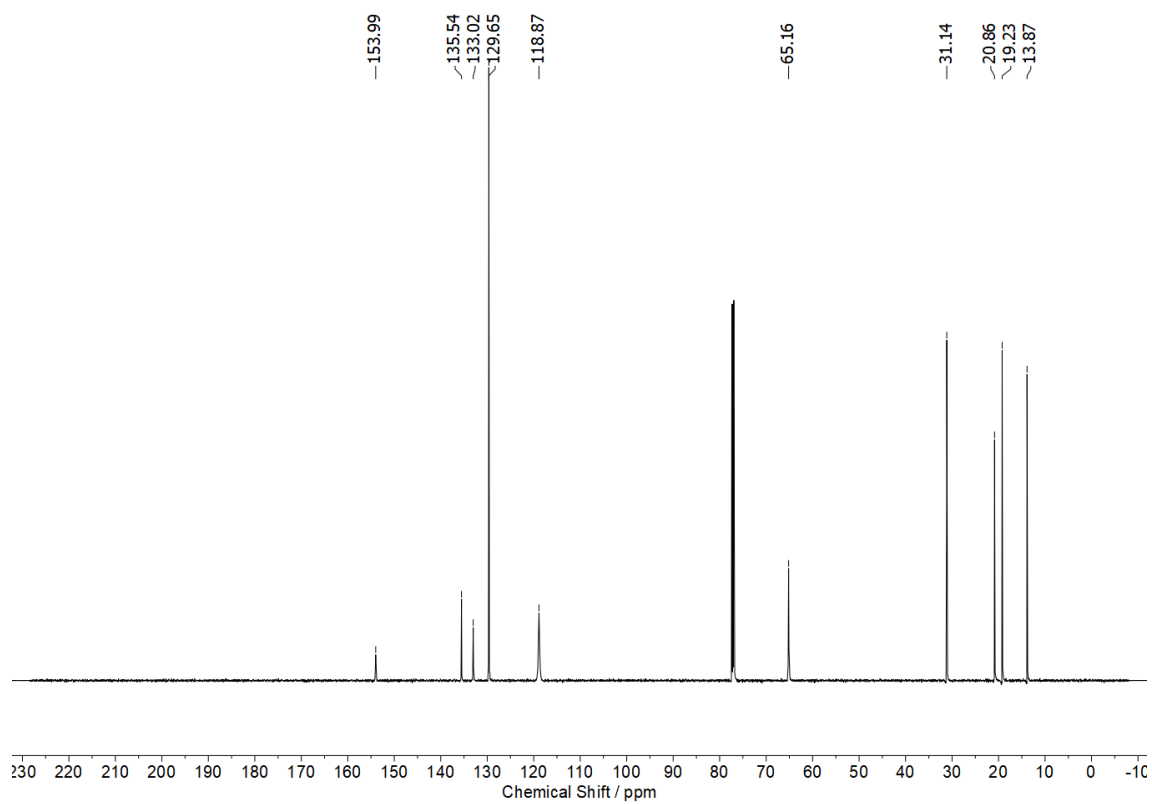
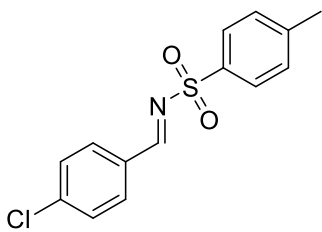
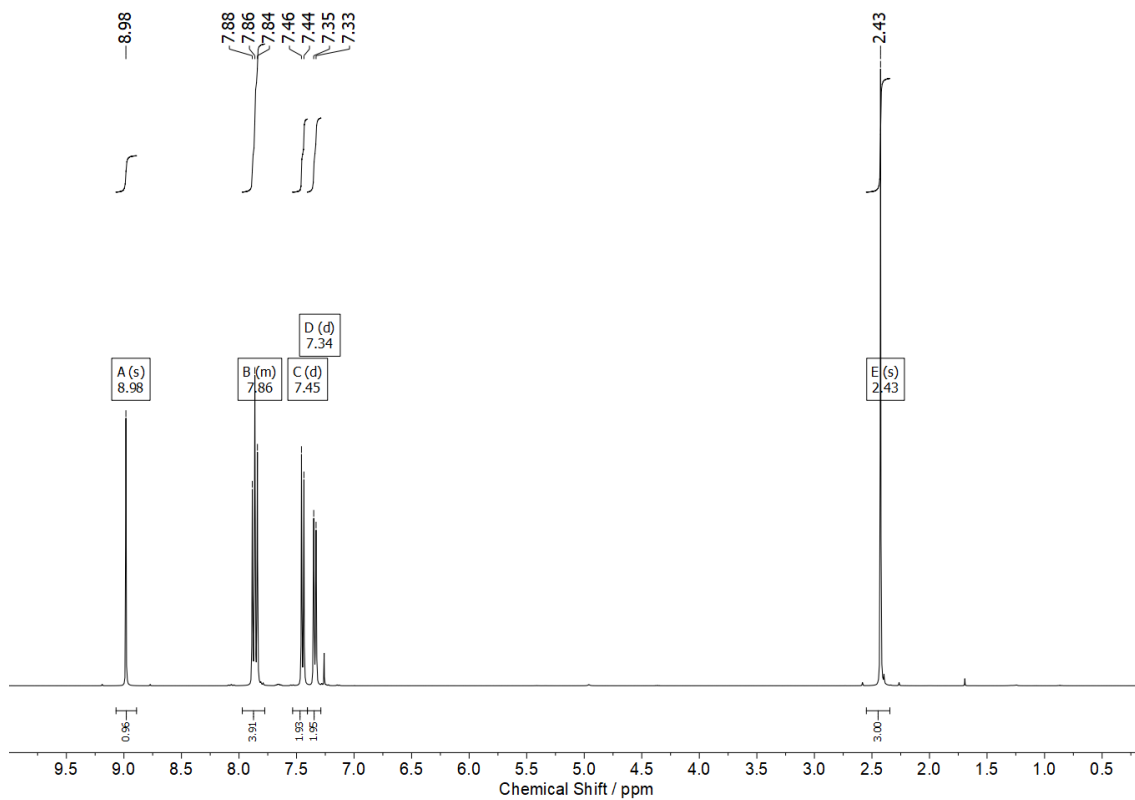


Figure S171. NMR spectra of urethane **16** (CDCl_3 , 600 MHz): a) ^1H NMR spectrum, b) ^{13}C NMR spectrum.

N-(4-chlorobenzylidene)-4-methylbenzenesulfonamide **19**



a)



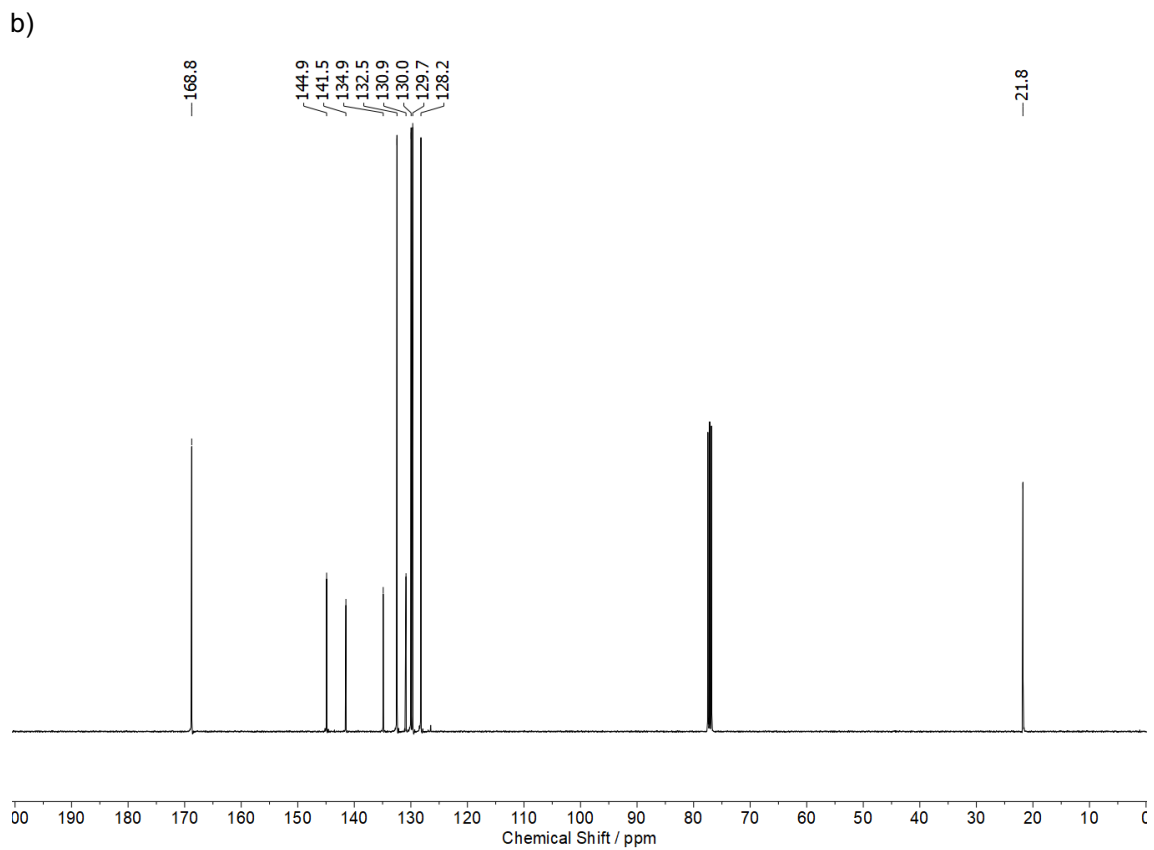
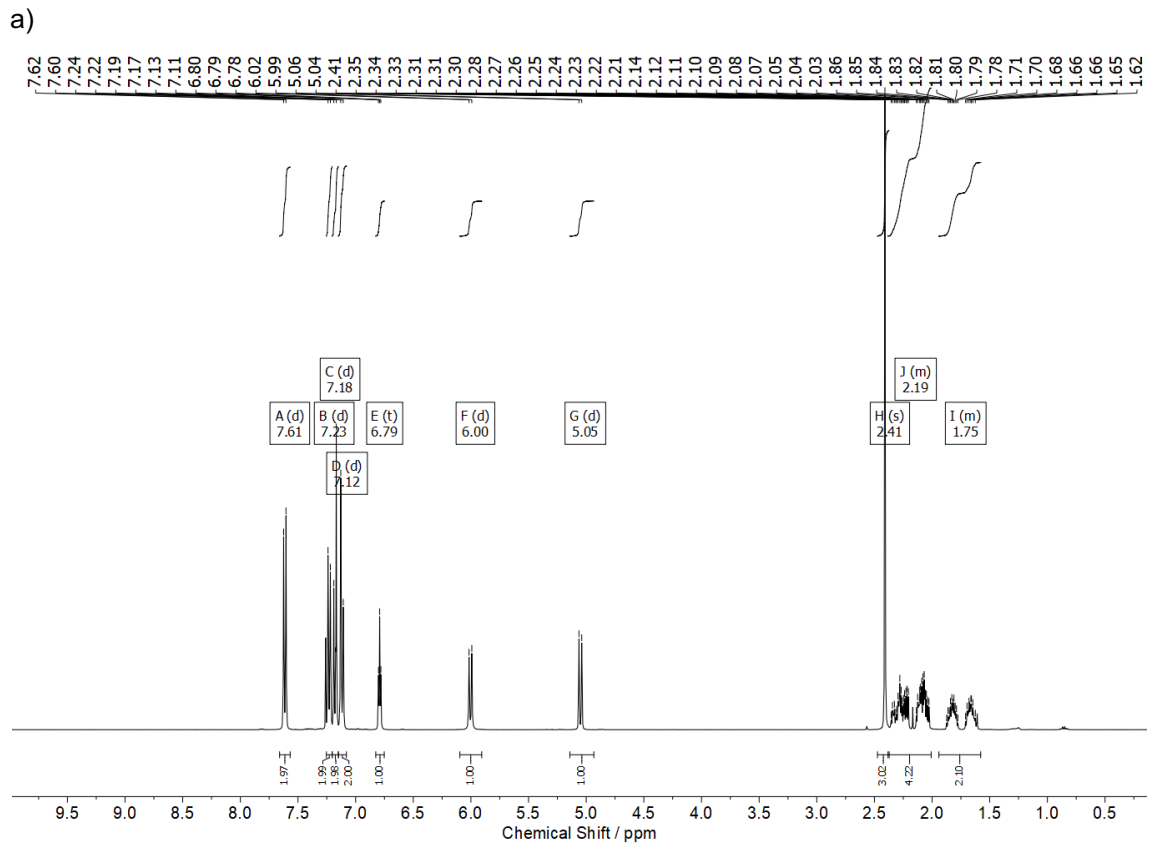
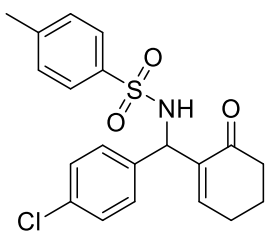


Figure S172. NMR spectra of imine **19** (CDCl_3 , 400 MHz): a) ^1H NMR spectrum, b) ^{13}C NMR spectrum.

N-((4-chlorophenyl)(6-oxocyclohex-1-en-1-yl)methyl)-4-methylbenzenesulfonamide **21**



b)

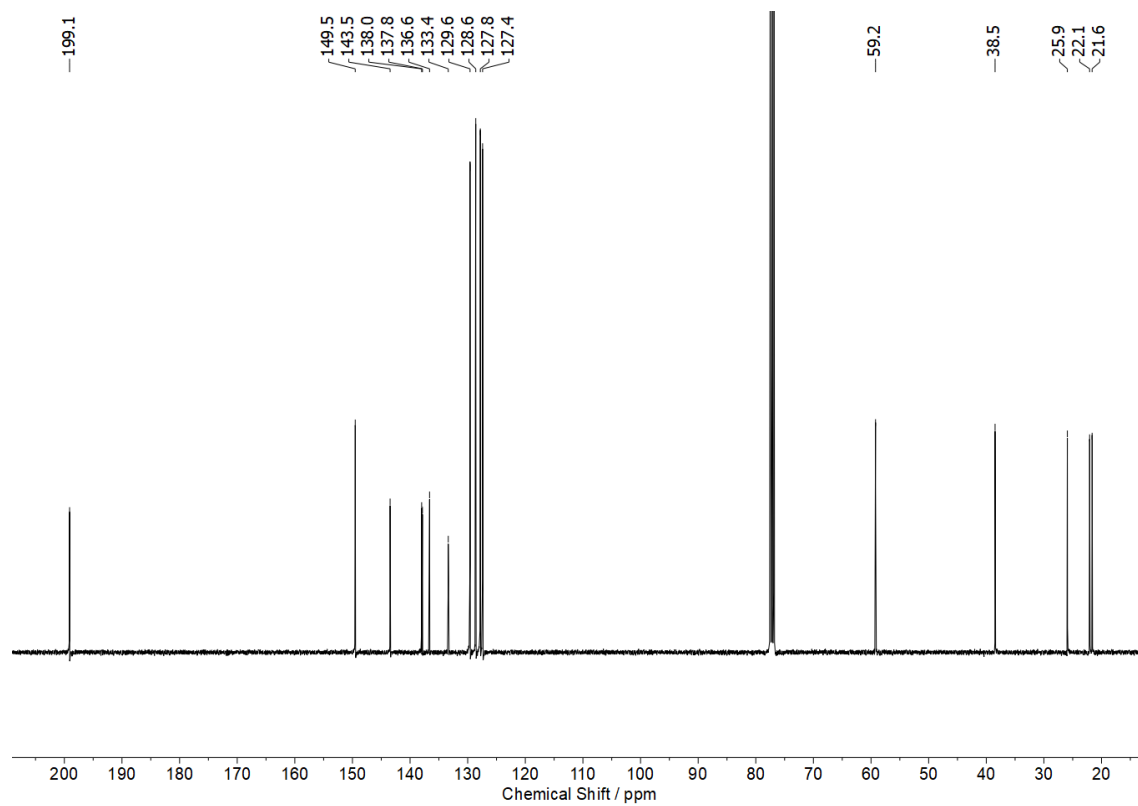
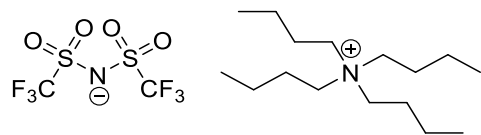
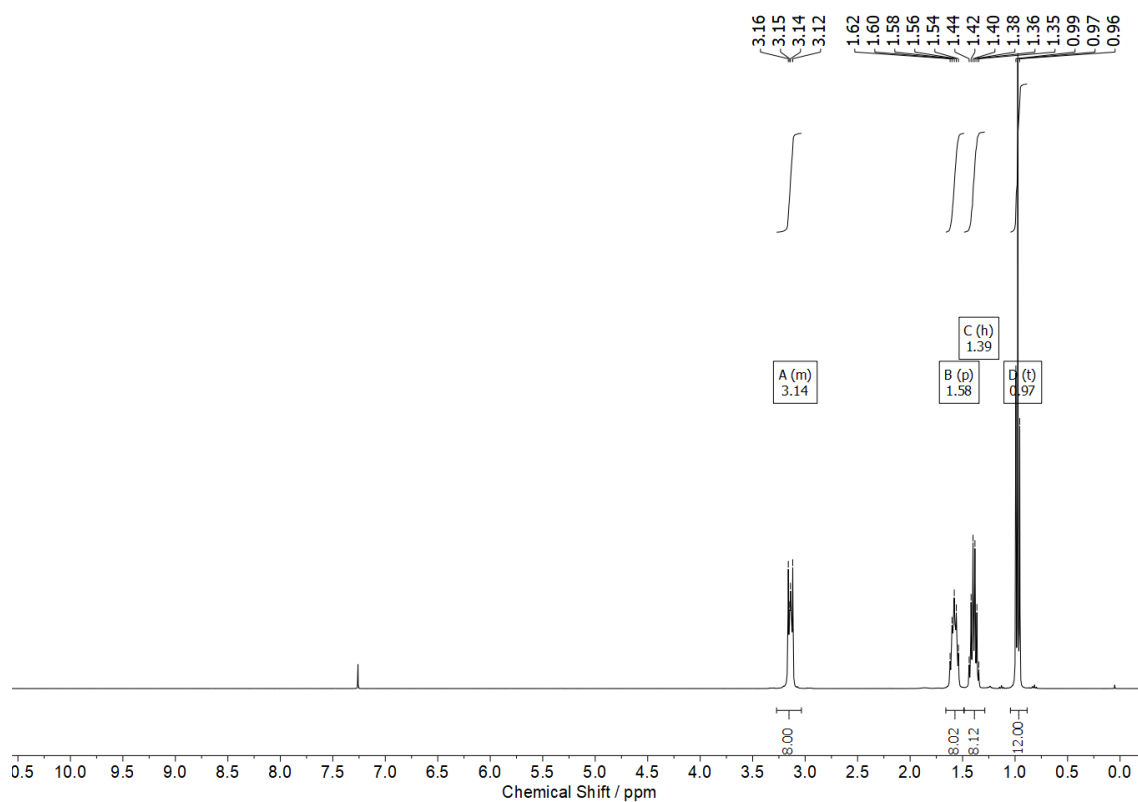


Figure S173. NMR spectra of compound **21** (CDCl_3 , 400 MHz): a) ^1H NMR spectrum, b) ^{13}C NMR spectrum.

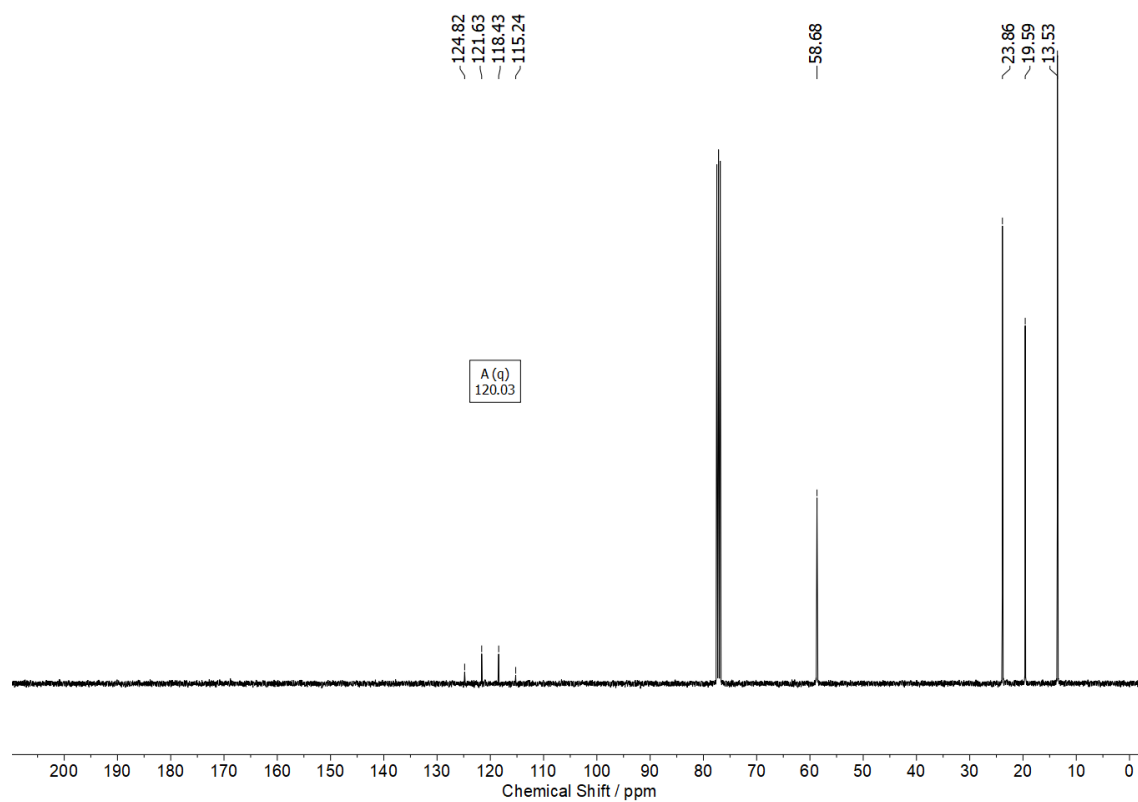
Tetrabutylammonium bis((trifluoromethyl)sulfonyl)amide **24**



a)



b)



c)

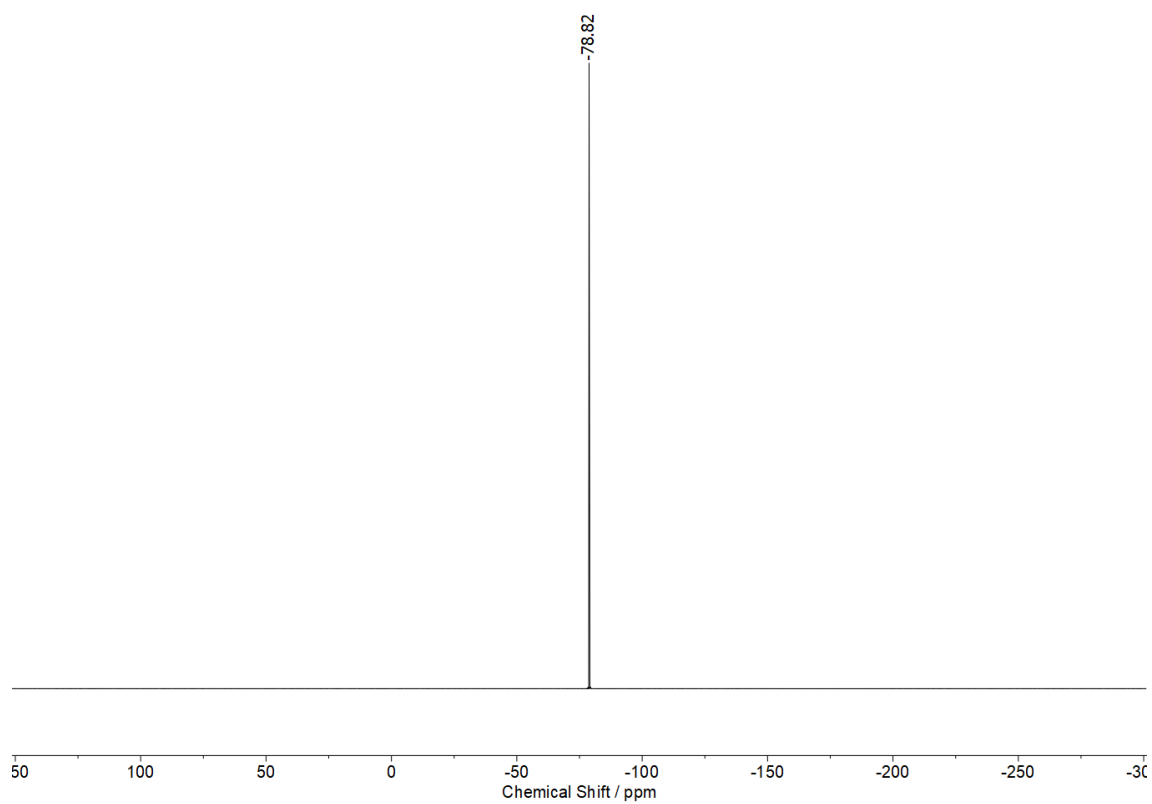
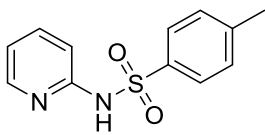
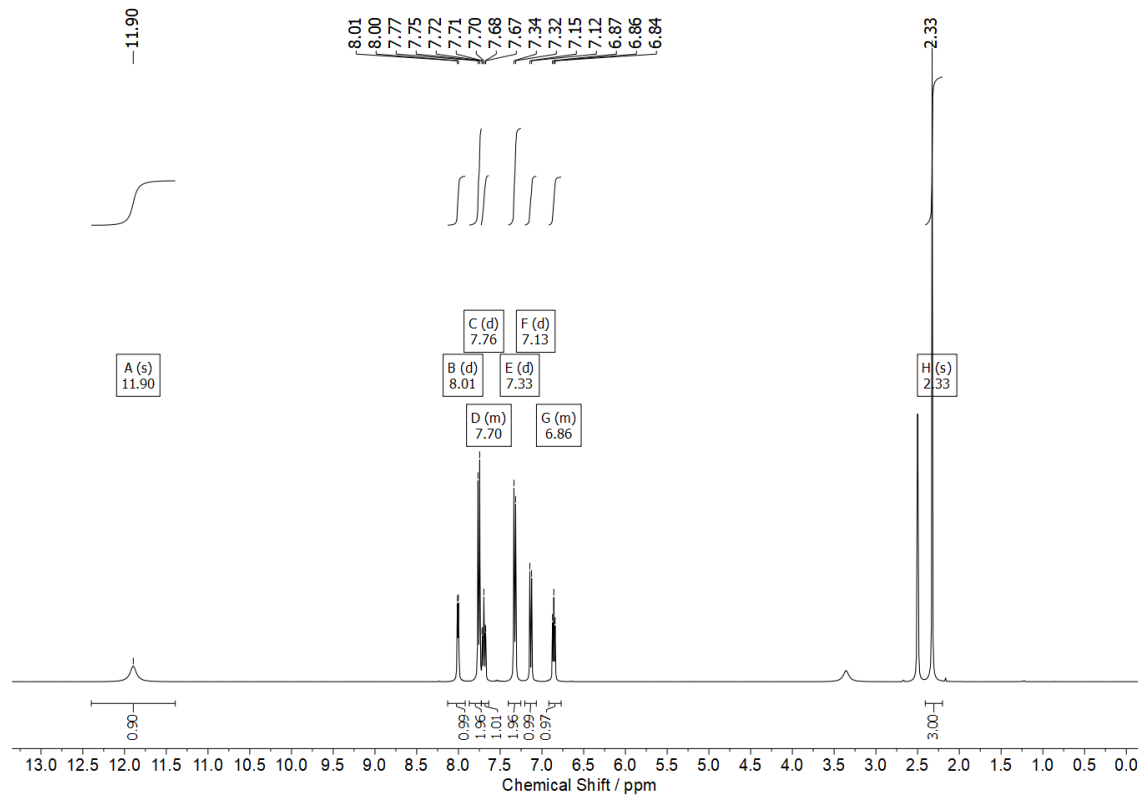


Figure S174. NMR spectra of compound **24** (CDCl_3 , 400 MHz): a) ^1H NMR spectrum, b) ^{13}C NMR spectrum, c) ^{19}F NMR spectrum.

4-methyl-N-(pyridin-2-yl)benzenesulfonamide **25**



a)



b)

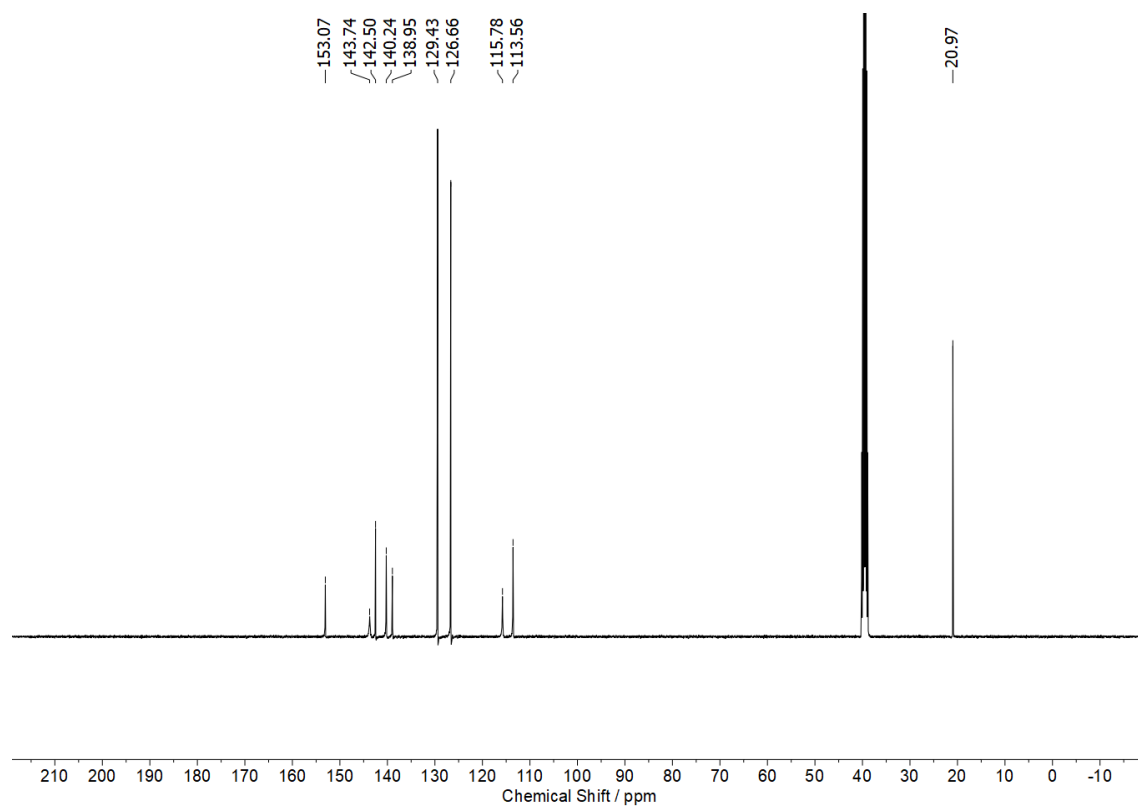
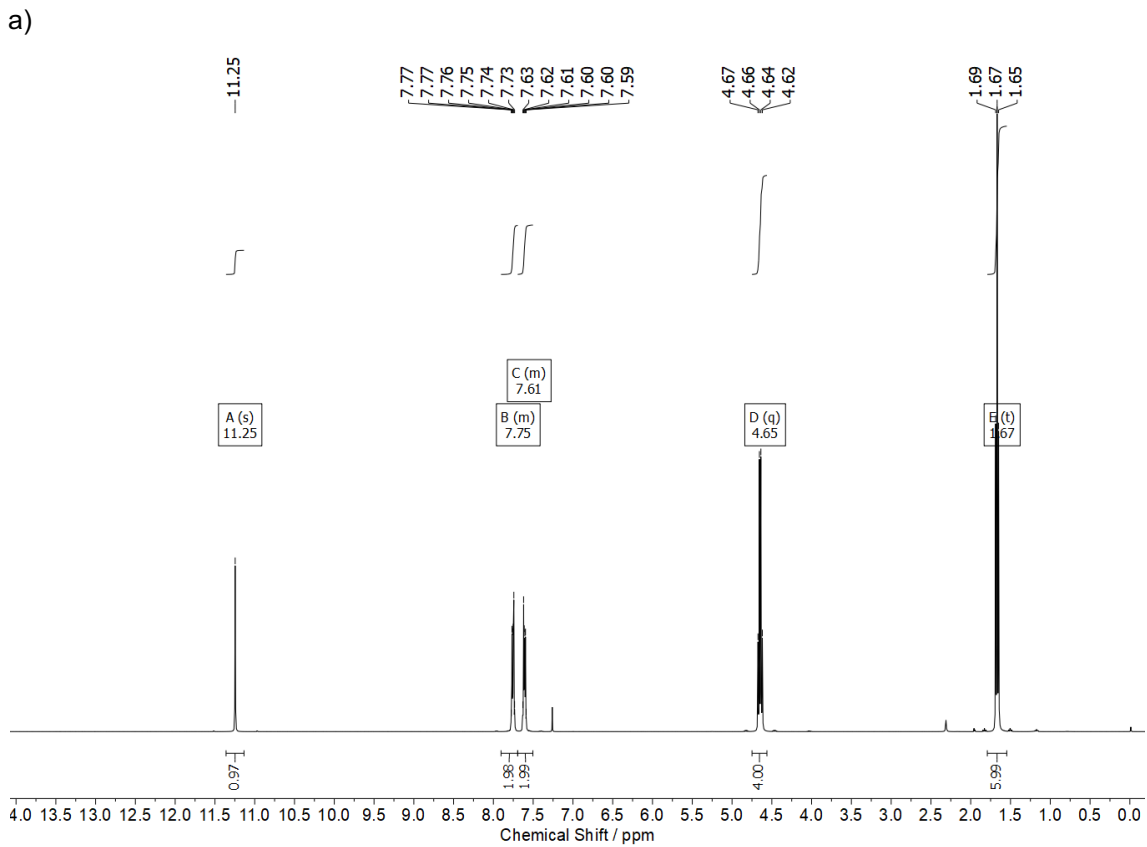
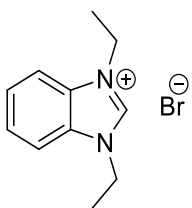


Figure S175. NMR spectra of sulfonamide **25** (DMSO-d₆, 400 MHz): a) ¹H NMR spectrum, b) ¹³C NMR spectrum.

1,3-diethyl-benzimidazolium bromide **26**



b)

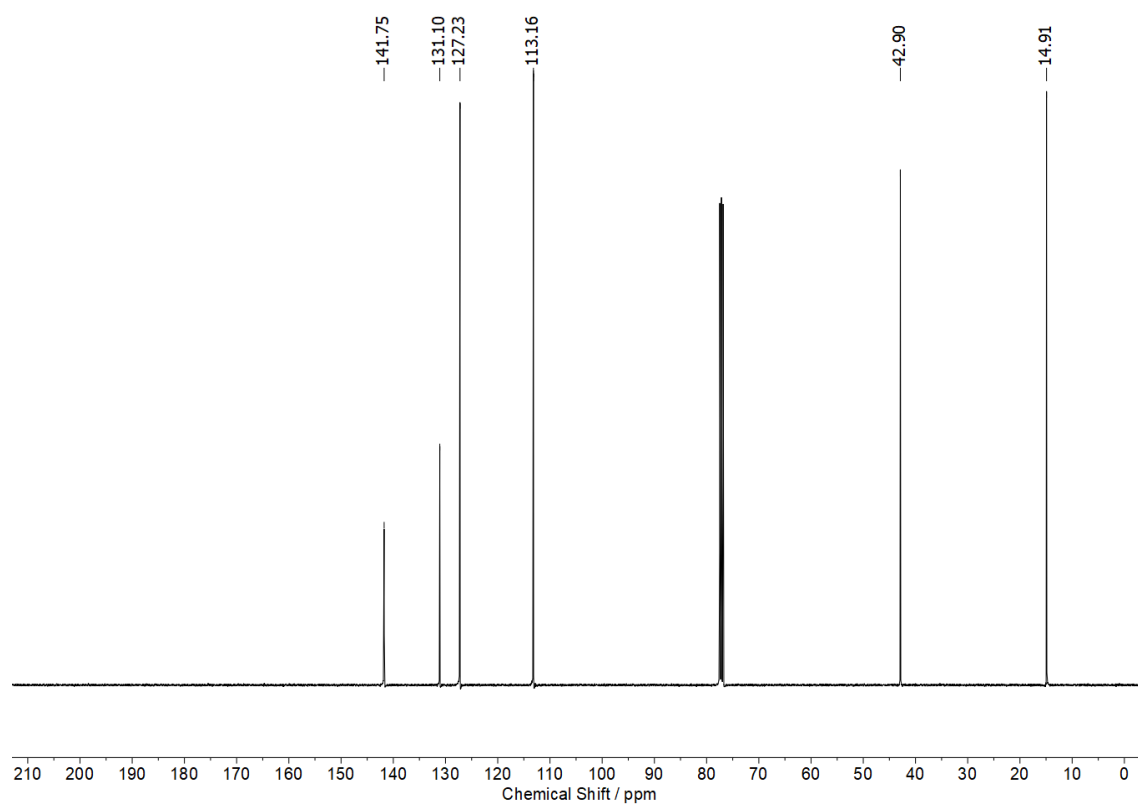


Figure S176. NMR spectra of benzimidazolium bromide **26** (CDCl_3 , 400 MHz): a) ^1H NMR spectrum, b) ^{13}C NMR spectrum.

Computational Part

General Computational Methods

Recent studies by our group showed that reliable results that take dispersive interactions into account are obtained at the DLPNO-CCSD(T)/def2-TZVPP//SMD(CHCl₃)/B3LYP-D3/6-31+G(d) level of theory (abbreviated as CC in the following) and therefore we used it for the calculation of Δ MCA and Δ PIA values in this study.^[7] Initial coordinates for monomolecular systems were generated by applying the OPLS_2005 force field implemented in MacroModel (Schrödinger program package).^[8] Optimizations were done differently for monomolecular systems and ion pairs. In the first case, optimization at the SMD(CHCl₃)/B3LYP-D3/6-31+G(d) level of theory was followed by calculation of thermal corrections at 298.15 K without scaling using the rigid rotor/harmonic oscillator model at the same level.

For ion pair systems, 150 sets of starting coordinates were randomized using the stochastic kick procedure developed by Saunders and further adapted by Sakic.^[9] 50 sets of coordinates were generated starting from the pairing of the best, second best and third best conformers each of cation and anion optimized beforehand. Pre-optimization was done at the SMD(CHCl₃)/B3LYP-D3/6-31+G(d) (abbreviated as DFT in the following) level of theory using the scf=(conver=6) and int=(SG1Grid) options. For this pre-optimization, jobs were submitted (and if not terminated normally) resubmitted in a randomized fashion until at least 100 structures had been terminated normally. Out of these, a minimum of 30 (the energetically most favored ones) conformers were selected and optimized at the SMD(CHCl₃)/B3LYP-D3/6-31+G(d) level of theory followed by calculation of thermal corrections at 298.15 K without scaling using the rigid rotor/harmonic oscillator model at the same level.

All values reported at the SMD(CHCl₃)/B3LYP-D3/6-31+G(d) level of theory were done with Gaussian 09, Revision D.01.^[10]

Single point energies were calculated at the DLPNO-CCSD(T)/def2-TZVPP level of theory with ORCA Version 4.0.0.2 using the fully optimized DFT geometries.^[11] Thermal corrections previously obtained at the SMD(CHCl₃)/B3LYP-D3/6-31+G(d) level were added to generate the final single point values.

All Δ MCA and Δ PIA values given in this study are the best DFT or coupled cluster conformers generated as described above.

To represent tetraalkyl ammonium and tetraalkyl phosphonium cations (as present in catalyst systems (**6aa**, **6ab**, **6ad**, and **10d**), without having to face the huge conformational space that comes with it, we calculated the corresponding tetraethyl phosphonium-containing catalyst systems (**6ah** and **10h**) as shown in **Table S23**.

Table of Calculated Compounds

Table S23 gives the identifier as well as the structure of the compounds calculated for this study.

Table of Calculated Compounds

Table S4: 23 gives the identifier as well as the structure of the compounds calculated for this study.

Table S4: 23. [Table S23] Compounds calculated for this study.

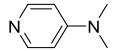
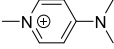
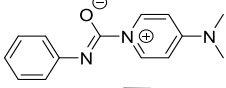
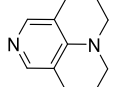
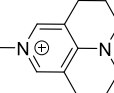
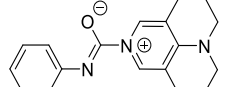
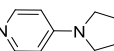
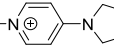
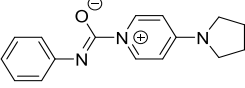
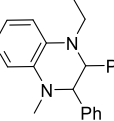
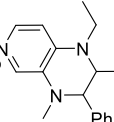
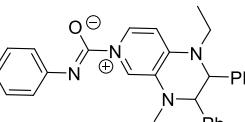
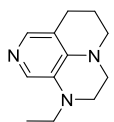
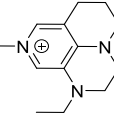
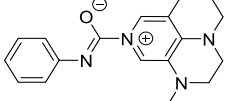
Entry	Identifier	Compound
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2	1a-Me	
3	1a-PhNCO	
4	1b	
5	1b-Me	
6	1b-PhNCO	
7	1c	
8	1c-Me	
9	1c-PhNCO	
10	1d	
11	1d-Me	
12	1d-PhNCO	
13	1e	
14	1e-Me	
15	1e-PhNCO	

Table S23 (continuation). Compounds calculated for this study.

16	1f	
17	1f-Me	
18	1f-PhNCO	
19	1g	
20	1g-Me	
21	1g-PhNCO	
22	6a	
23	6a-Me	
24	6a-Me2	
25	6a-PhNCO	
26	6a-PhNCO2	
27	6ac	
28	6ac-Me	
29	6ac-PhNCO	
30	6ah	

Table S23 (continuation). Compounds calculated for this study.

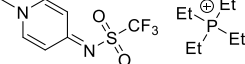
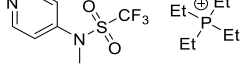
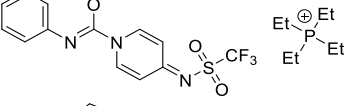
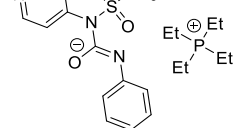
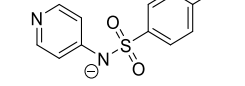
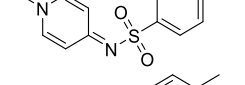
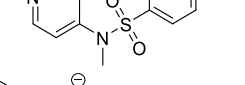
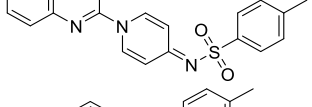
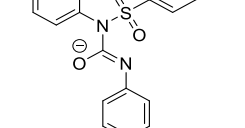
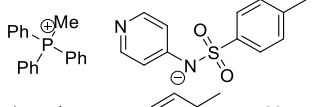
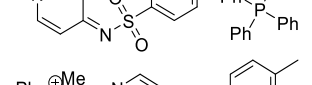
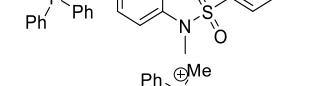
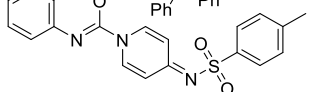
31	6ah-Me	
32	6ah-Me2	
33	6ah-PhNCO	
34	6ah-PhNCO2	
35	6b	
36	6b-Me	
37	6b-Me2	
38	6b-PhNCO	
39	6b-PhNCO2	
40	6bc	
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42	6bc-Me2	
43	6bc-PhNCO	

Table S23 (continuation). Compounds calculated for this study.

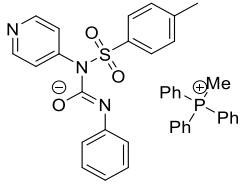
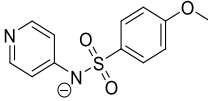
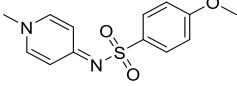
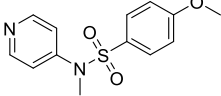
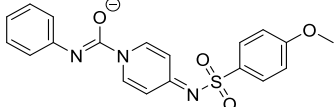
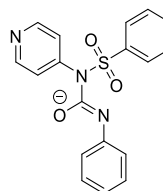
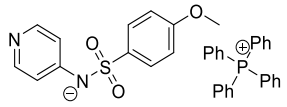
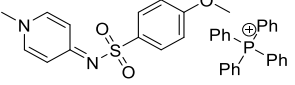
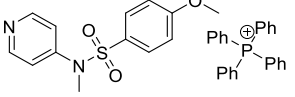
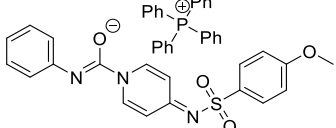
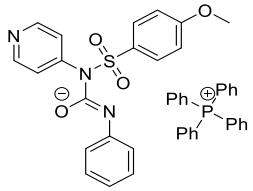
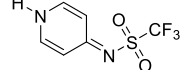
44	6bc-PhNCO2	
45	6c	
46	6c-Me	
47	6c-Me2	
48	6c-PhNCO	
49	6c-PhNCO2	
50	6cg	
51	6cg-Me	
52	6cg-Me2	
53	6cg-PhNCO	
54	6cg-PhNCO2	
55	8a	

Table S23 (continuation). Compounds calculated for this study.

56	10	
57	10-Me	
58	10-Me2	
59	10-PhNCO	
60	10-PhNCO2	
61	10h	
62	10h-Me	
63	10h-PhNCO	
64	11	
65	14	
66	15	
67	15-Me	

Table S23 (continuation). Compounds calculated for this study.

68	15-Me2	
69	15-PhNCO	
70	15-PhNCO2	
72	15g	
73	15g-Me	
74	15g-Me2	
75	15g-PhNCO	
76	15g-PhNCO2	
77	22	
78	22-Me	
79	22-PhNCO	
80	23	

Table S23 (continuation). Compounds calculated for this study.

81	23-Me	
82	23-PhNCO	

Calculated Phenyl Isocyanate Affinities (Δ PIAs) and Methyl Cation Affinities (Δ MCAs)

Table S24 gives the values calculated for Δ PiA and Δ MCA for the neutral catalysts, ion pair catalysts, and anion catalysts.

Table S24. Phenyl Isocyanate Affinities (Δ PIAs) and Methyl Cation Affinities (Δ MCAs).

Entry	Catalyst	Lewis basic atom ^a	ΔH_{298K} SMD(CHCl ₃)/B3LYP-D3/ 6-31+G(d)		ΔH_{298K} DLPNO-CCSD(T)/def2-TZVPP// SMD(CHCl ₃)/B3LYP-D3/6-31+G(d)	
			Δ MCA ^b	Δ PiA ^b	Δ MCA ^b	Δ PiA ^b
1	1a	N1	-37.0	-25.7	-35.2	-24.8
2	1c	N1	-40.9	-27.2	-38.4	-26.3
3	1b	N1	-48.8	-32.5	-43.9	-29.9
4	1d	N1	-45.7	-30.6	-39.0	-27.7
5	1e	N1	-52.2	-34.2	-46.3	-32.2
6	1f	N1	-54.7	-39.3	-47.8	-37.2
7	22	N1	-45.2	+8.2	-53.7	+8.8
8	23	N1	-7.1	-1.7	-2.3	-0.5
9	6ac	N1	-43.2	-38.1	-38.4	-38.3
10	6ah	N1	-40.5	-30.9	-37.9	-31.8
11	6ah	N2	-0.8	+10.7	-12.2	+3.9
12	6bc	N1	-64.8	-56.7	-63.0	-58.1
13	6bc	N2	-57.9	-28.5	-64.0	-34.7
14	6cg	N1	-65.6	-61.2	-62.7	-61.7
15	6cg	N2	-61.2	-24.4	-67.8	-31.4
16	15g	N1	-47.0	-45.7	-43.0	-42.1
17	15g	N2	-32.0	-11.9	-42.8	-27.9
18	10h	N1	-72.2	-53.1	-68.0	-53.3
19	6a	N1	-81.7	-33.9	-84.7	-36.4
20	6a	N2	-48.3	+21.0	-65.2	+14.0
21	6b	N1	-99.9	-46.8	-102.8	-47.6
22	6b	N2	-97.9	-9.5	-109.3	-16.9
23	6c	N1	-100.1	-46.9	-103.5	-47.7
24	6c	N2	-99.8	-10.1	-111.2	-17.5
25	15	N1	-85.5	-34.0	-86.5	-34.3
26	15	N2	-57.7	+3.4	-78.2	-14.5
27	10	N1	-115.3	-56.0	-116.6	-55.4
28	10	N2	-120.5	-42.3	-133.1	-52.6

^a N1 = pyridine-N; N2 = amide-N. ^b in kJ mol⁻¹

Effect of Exclusion of Cations for Computed Affinity Values

Entries 1 - 18 of **Table S24** have already been shown and discussed in the main part of this publication. The results summarized in Entries 19 – 28 of **Table S24** were briefly discussed. They give the affinity values determined from calculations of the anion-isocyanate and anion-methyl cation adducts only. **Figure S177** is a plot of the DFT-derived affinities of the ion pair catalyst adduct to isocyanate and methyl cation (Entries 9, 10, 12, 14, 16, 18 of **Table S24**) vs. those of the corresponding “naked” anion-adduct (Entries 19, 21, 23, 25, 27 of **Table S24**), which shows the effect of including the counter-cation in the calculation. The reference in this case is the symmetrical distribution of the monomolecular systems (unlabeled in the Figure), that do naturally only give one value.

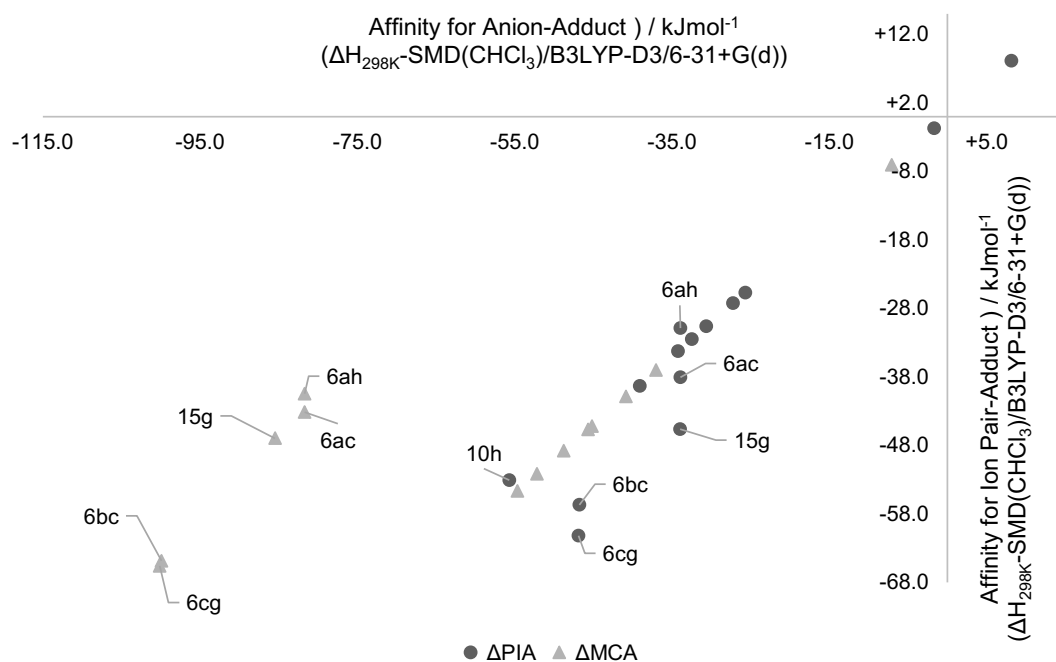


Figure S177. ion pair-adduct affinities vs. anion-adduct affinities for the pyridine-N (in kJ mol^{-1}). Neutral catalysts have been included to show the monomolecular case.

Although the inclusion of the counter-cation is computationally quite expensive (because of the theoretically limitless conformational space, but also the increasing size of the system), there is some obvious benefit. In the case of the Δ PIA values, the ionic catalyst systems noticeably disagree with the symmetrical plot of the neutral organocatalysts. For most of the examples shown here, the exclusion of the cation destabilized the adduct, as was shown in Scheme 3 of the main manuscript of this publication for the case of **6cg**. A similar (although less pronounced) observation is made for catalyst systems **6ac**, **15g**, and **6bc**. Only the systems **6ah**, and **10h** are slightly stabilized by omission of the cation for reasons that we did not manage to discern. The obvious thing to point out though, is that those two are both containing tetraethyl phosphonium counter ions. It seems not impossible, that the added stabilization in the other cases could be attributed to aromatic interactions like π - π stacking.

The effect of the absence of the counter ion in the case of the Δ MCA values is much more pronounced. We propose this to be caused by the quenching of the charged character of the anionic “warhead” under formation of a neutral molecule. Furthermore, the anion-adduct affinities show irregularities with regard to the experimental results: **6bc** and **6cg**, that gave quite different values in our experimental study are similar for both Δ MCA and Δ PIA. Also, the Δ PIA-values calculated for anion-adducts for **6aa**, **6ac** and **15g**, are similar which is not at all observed in the experiment (**Table S24**, Entries 19, 25).

This brings us to **Figure S178**, which shows the effect of inclusion or exclusion of the cation onto the correlation with experimentally determined values. In all cases the pyridine-nitrogen atom is the one considered for calculation of the affinities:

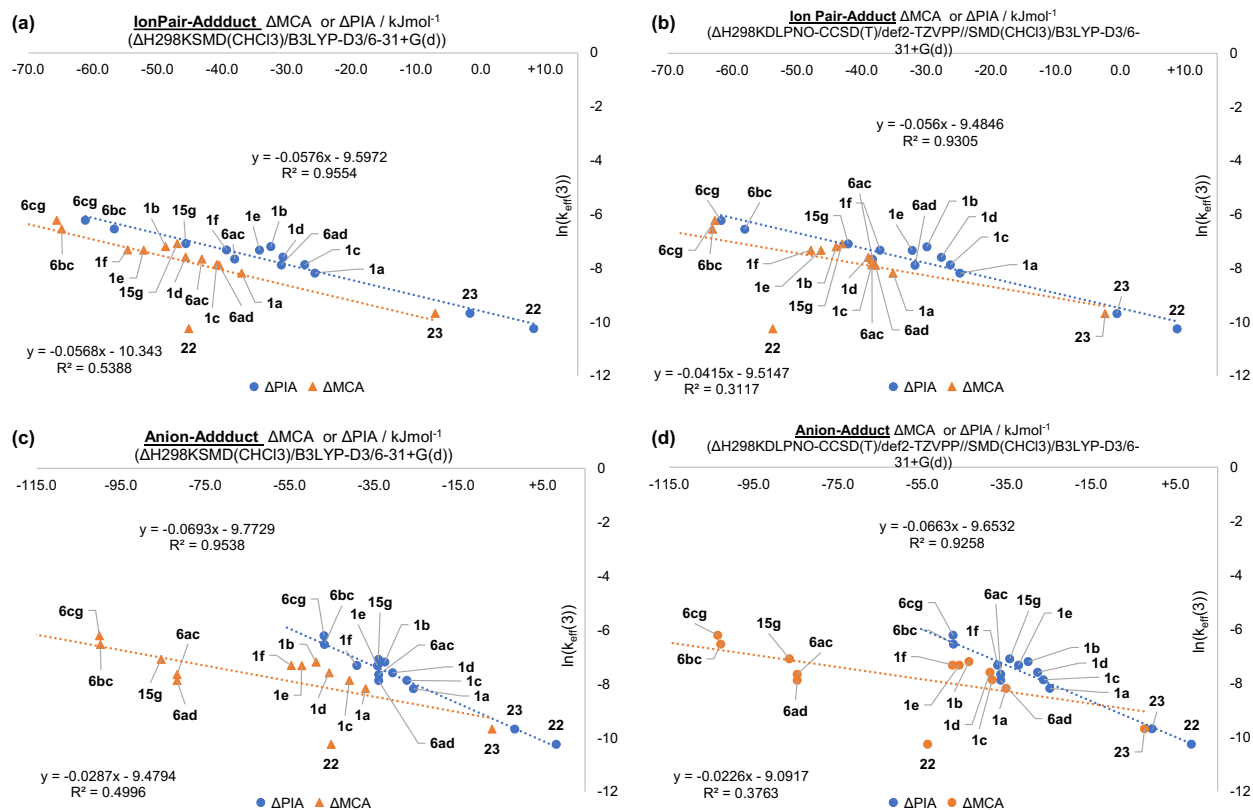


Figure S178. Plots of experimentally determined $\ln(k_{\text{eff}}(3))$ -values of the urethane benchmark reaction vs. calculated Δ MCA and Δ PIA values (all for pyridine-N). (a) vs. DTF-values (already shown in the main body of this publication) and (b) vs. CC-values. (c) is a plot vs. the DFT-derived values when the cation is excluded and (d) gives correlation vs. the affinities obtained at CC level of theory.

We observe that the quality of the correlation does not change when plotting either the ion-pair affinity or the anion affinity values against the experimentally derived values. However, the slope of the fit changes when omitting the cation in the calculations, which indicates some fundamental change to the correlation.

The same trend observed in **Figure S177** is evident again: The Δ PIA values show very good correlation with the experimentally derived values independent of the method. Most noticeable is the shift of **15g**, which in the experiment tested far more reactive than the neutral catalysts and now is amongst them (**Table S24**, Entries 16, 25).

The correlation for the Δ MCA values is quite poor independent of inclusion of the cations due to the values determined for the triphenylphosphine **22** as discussed in the main part of this publication. However, the affinity values for the anion-methyl cation “adduct” are increased massively to overestimate our experimental data much in the same way as triphenylphosphine **22**. For the ionic catalysts, we think this is due to the change of the system from minus one to zero as mentioned above.

In total, the effects discussed above show, that the inclusion of the cation into the calculation of affinities (and likely also mechanistic studies) is a step that should be considered to get a more reliable representation of the catalyst systems.

Since we observe a huge effect of adducts that change their charge, this is probably also of importance for esterification or silylation reactions catalyzed by ion pair pyridinyl systems because of the leaving-group induced change in charge. While Δ PIA values calculated from anion-adducts appear to be usable for ranking of reactivity amongst such ionic systems to some extent, they fail to represent experimental findings when comparison with neutral organocatalysts is desired.

Lewis Basicity of Pyridine-N vs. Amide-N

The results for the Lewis basicity of the competing Nitrogen atoms have already been discussed in the main body of this publication. **Figure S179** shows the effect mentioned there in a graph giving a plot of the affinities obtained for the pyridine-N (N1) vs. those of the amide-N (N2) (all calculated at DFT level of theory). The neutral catalysts values all represent the pyridine-N (or P-atom in the case of **22**) and have been included to show the symmetrical plot for identical values (labeling was omitted for these cases).

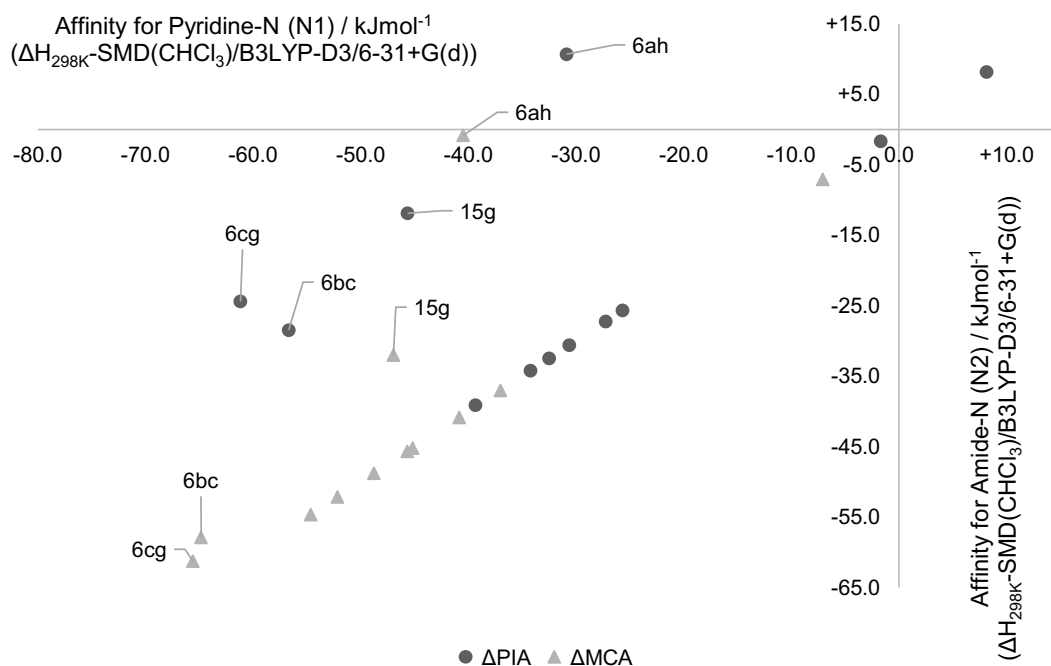


Figure S179. Plot of affinity values for the pyridine-N vs. those for the amide-N obtained at the DFT level of theory.

This graph shows nicely the observed trend of all the pyridine-N affinity values being at generally more favorable than the ones generated for amide-N adducts. The only two cases where this is less pronounced are the Δ MCA values of **6bc** and **6cg**. The Δ PIA values on the other hand show a clear preference for catalytic activation by the pyridine-N for all investigated systems, hinting at the pyridine-N being responsible for the observed catalytic activity.

Figure S180 shows affinity values calculated for pyridine-N and amide-N plotted against experimentally determined $k_{eff}(3)$ values for the urethane benchmark reaction.

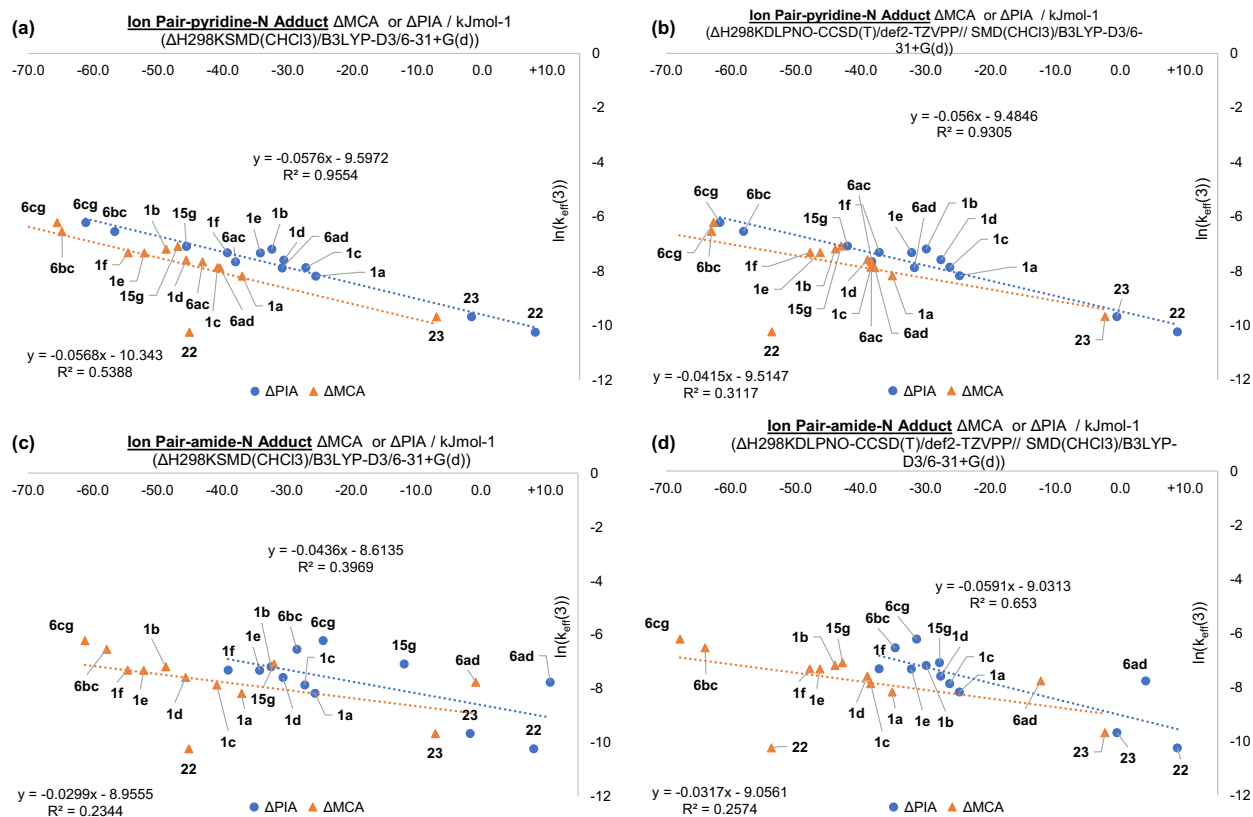


Figure S180. Plots of experimentally determined $\ln(k_{\text{eff}}(3))$ -values of the urethane benchmark reaction vs. calculated Δ MCA and Δ PIA values. (a) and (b) give plots of pyridine-N affinities of DFT and CC methods respectively. (c) and (d) gives plots of amide-N affinities of DFT and CC methods respectively.

Independent of the computational method used, we found that the amide-N derived affinities correlate much poorer with the experimentally determined values. Additionally, the Δ PIA values calculated for the amide-N adducts of all ion pair catalysts are similar or lower than those for the more active organocatalysts, which is contradicted by our experimental observations.

These results combined with the ones discussed above and in the main body of this publication lead us to firmly believe, that the pyridine-N atom is the catalytically active center in the investigated ion pair Lewis base organocatalysts.

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Table of Thermochemical Data (sorted by $\Delta H_{298K}(CC)$)

Nr.	$H_{298K}(DFT)/\text{Hartree}$	$\Delta H_{298K}(DFT)/\text{kJ mol}^{-1}$	$E_{298K}(DFT)/\text{Hartree}$	$H_{298K}(CC)/\text{Hartree}$	$\Delta H_{298K}(CC)/\text{kJ mol}^{-1}$	$E_{298K}(CC)/\text{Hartree}$
1a-001	-382.127410	+0.00	-382.299549	-381.416284	+0.00	-381.573299

Nr.	$H_{298K}(DFT)/\text{Hartree}$	$\Delta H_{298K}(DFT)/\text{kJ mol}^{-1}$	$E_{298K}(DFT)/\text{Hartree}$	$H_{298K}(CC)/\text{Hartree}$	$\Delta H_{298K}(CC)/\text{kJ mol}^{-1}$	$E_{298K}(CC)/\text{Hartree}$
1a-Me-002	-421.853065	+0.39	-422.069489	-421.064066	+0.60	-421.207869
1a-Me-001	-421.853214	+0.00	-422.069542	-421.064295	+0.00	-421.207977

Nr.	$H_{298K}(DFT)/\text{Hartree}$	$\Delta H_{298K}(DFT)/\text{kJ mol}^{-1}$	$E_{298K}(DFT)/\text{Hartree}$	$H_{298K}(CC)/\text{Hartree}$	$\Delta H_{298K}(CC)/\text{kJ mol}^{-1}$	$E_{298K}(CC)/\text{Hartree}$
1a-PhNCO-002	-781.783639	+26.23	-782.070340	-780.357903	+22.39	-780.603868
1a-PhNCO-001	-781.793628	+0.00	-782.080726	-780.366432	+0.00	-780.617834

Nr.	$H_{298K}(DFT)/\text{Hartree}$	$\Delta H_{298K}(DFT)/\text{kJ mol}^{-1}$	$E_{298K}(DFT)/\text{Hartree}$	$H_{298K}(CC)/\text{Hartree}$	$\Delta H_{298K}(CC)/\text{kJ mol}^{-1}$	$E_{298K}(CC)/\text{Hartree}$
1b-Me-002	-576.662400	+0.00	-576.953434	-575.575527	+0.06	-575.794312
1b-Me-001	-576.662368	+0.08	-576.953475	-575.575549	+0.00	-575.794400

Nr.	$H_{298K}(DFT)/\text{Hartree}$	$\Delta H_{298K}(DFT)/\text{kJ mol}^{-1}$	$E_{298K}(DFT)/\text{Hartree}$	$H_{298K}(CC)/\text{Hartree}$	$\Delta H_{298K}(CC)/\text{kJ mol}^{-1}$	$E_{298K}(CC)/\text{Hartree}$
1b-PhNCO-007	-936.591252	+25.41	-936.953034	-934.868003	+21.74	-935.185036
1b-PhNCO-006	-936.591294	+25.30	-936.953227	-934.868007	+21.73	-935.185197
1b-PhNCO-005	-936.591687	+24.27	-936.953564	-934.868396	+20.71	-935.185109
1b-PhNCO-004	-936.591863	+23.81	-936.953737	-934.868463	+20.53	-935.185360
1b-PhNCO-003	-936.600394	+1.41	-936.962542	-934.875935	+0.91	-935.198100
1b-PhNCO-002	-936.600529	+1.05	-936.962650	-934.875959	+0.85	-935.198217
1b-PhNCO-001	-936.600930	+0.00	-936.963097	-934.876283	+0.00	-935.198263

Nr.	$H_{298K}(DFT)/\text{Hartree}$	$\Delta H_{298K}(DFT)/\text{kJ mol}^{-1}$	$E_{298K}(DFT)/\text{Hartree}$	$H_{298K}(CC)/\text{Hartree}$	$\Delta H_{298K}(CC)/\text{kJ mol}^{-1}$	$E_{298K}(CC)/\text{Hartree}$
1b-002	-536.931667	+1.20	-537.178614	-535.923029	+3.05	-536.150546
1b-001	-536.932123	+0.00	-537.179099	-535.924189	+0.00	-536.151986

Nr.	$H_{298K}(DFT)/\text{Hartree}$	$\Delta H_{298K}(DFT)/\text{kJ mol}^{-1}$	$E_{298K}(DFT)/\text{Hartree}$	$H_{298K}(CC)/\text{Hartree}$	$\Delta H_{298K}(CC)/\text{kJ mol}^{-1}$	$E_{298K}(CC)/\text{Hartree}$
1c-Me-002	-499.253370	+0.13	-499.506871	-498.315476	+0.26	-498.495956
1c-Me-001	-499.253421	+0.00	-499.506908	-498.315576	+0.00	-498.496031

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
1c-PhNCO-003	-859.183086	+25.94	-859.507427	-857.608438	+22.55	-857.889460
1c-PhNCO-002	-859.183157	+25.76	-859.507379	-857.608527	+22.32	-857.889434
1c-PhNCO-001	-859.192967	+0.00	-859.517639	-857.617027	+0.00	-857.903369

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
1c-001	-459.526159	+0.00	-459.735742	-458.666309	+0.00	-458.858005

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
1d-005	-1016.125648	+4.51	-1016.554274	-1014.201302	+5.06	-1014.600809
1d-004	-1016.125019	+6.16	-1016.553668	-1014.201511	+4.51	-1014.600943
1d-003	-1016.126551	+2.13	-1016.555089	-1014.202468	+2.00	-1014.601808
1d-002	-1016.126904	+1.21	-1016.555471	-1014.202765	+1.22	-1014.602219
1d-001	-1016.127364	+0.00	-1016.555451	-1014.203229	+0.00	-1014.601766

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
1d-Me-005	-1055.853323	+8.25	-1056.326501	-1053.849974	+7.14	-1054.245677
1d-Me-004	-1055.854370	+5.50	-1056.327149	-1053.850126	+6.74	-1054.245476
1d-Me-003	-1055.855214	+3.29	-1056.327676	-1053.851306	+3.64	-1054.246181
1d-Me-002	-1055.856026	+1.16	-1056.328853	-1053.852273	+1.10	-1054.247612
1d-Me-001	-1055.856466	+0.00	-1056.329413	-1053.852693	+0.00	-1054.247636

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
1d-PhNCO-025	-1415.782913	+32.95	-1416.326219
1d-PhNCO-024	-1415.782976	+32.79	-1416.326526
1d-PhNCO-023	-1415.783231	+32.12	-1416.326692
1d-PhNCO-022	-1415.783940	+30.26	-1416.327312
1d-PhNCO-021	-1415.784050	+29.97	-1416.327704
1d-PhNCO-020	-1415.784232	+29.49	-1416.327386
1d-PhNCO-019	-1415.784564	+28.62	-1416.328386
1d-PhNCO-018	-1415.785624	+25.83	-1416.328782
1d-PhNCO-017	-1415.786134	+24.50	-1416.329634

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
1d-PhNCO-016	-1415.785113	+27.18	-1416.328670	-1413.145389	+23.84	-1413.635484
1d-PhNCO-015	-1415.785144	+27.10	-1416.328509	-1413.145852	+22.62	-1413.635675

1d-PhNCO-014	-1415.785416	+26.38	-1416.328786	-1413.145953	+22.36	-1413.636689
1d-PhNCO-013	-1415.785784	+25.41	-1416.328993	-1413.145959	+22.34	-1413.635057
1d-PhNCO-012	-1415.785659	+25.74	-1416.329060	-1413.146237	+21.61	-1413.636107
1d-PhNCO-011	-1415.786066	+24.67	-1416.329258	-1413.146465	+21.01	-1413.635321
1d-PhNCO-010	-1415.786517	+23.49	-1416.329657	-1413.147077	+19.41	-1413.637972
1d-PhNCO-009	-1415.787146	+21.84	-1416.330065	-1413.147676	+17.83	-1413.637591
1d-PhNCO-008	-1415.787546	+20.79	-1416.330724	-1413.148044	+16.87	-1413.639136
1d-PhNCO-007	-1415.792653	+7.38	-1416.336146	-1413.151298	+8.32	-1413.646588
1d-PhNCO-006	-1415.792519	+7.73	-1416.336124	-1413.152278	+5.75	-1413.647644
1d-PhNCO-005	-1415.793509	+5.13	-1416.336925	-1413.152555	+5.02	-1413.647770
1d-PhNCO-004	-1415.793762	+4.47	-1416.337187	-1413.153220	+3.28	-1413.648411
1d-PhNCO-003	-1415.795038	+1.12	-1416.338624	-1413.154199	+0.71	-1413.648894
1d-PhNCO-002	-1415.795269	+0.51	-1416.338522	-1413.154291	+0.46	-1413.649340
1d-PhNCO-001	-1415.795464	+0.00	-1416.339007	-1413.154468	+0.00	-1413.649226

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
1e-Me-007	-671.272700	+18.29	-671.611402	-670.021437	+13.84	-670.287096
1e-Me-006	-671.273142	+17.13	-671.611849	-670.021931	+12.54	-670.287498
1e-Me-005	-671.277554	+5.55	-671.616679	-670.025080	+4.27	-670.292271
1e-Me-004	-671.277963	+4.47	-671.617100	-670.025122	+4.16	-670.292244
1e-Me-003	-671.278402	+3.32	-671.617172	-670.025359	+3.54	-670.292173
1e-Me-002	-671.279517	+0.39	-671.618500	-670.026524	+0.48	-670.293492
1e-Me-001	-671.279667	+0.00	-671.618370	-670.026708	+0.00	-670.293452

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
1e-PhNCO-032	-1031.202129	+40.56	-1031.611785
1e-PhNCO-031	-1031.203661	+36.54	-1031.613310
1e-PhNCO-030	-1031.205577	+31.51	-1031.614967
1e-PhNCO-029	-1031.206243	+29.76	-1031.616212
1e-PhNCO-028	-1031.206281	+29.66	-1031.615924
1e-PhNCO-027	-1031.206422	+29.29	-1031.616265
1e-PhNCO-026	-1031.206733	+28.47	-1031.616355
1e-PhNCO-025	-1031.206843	+28.18	-1031.616503
1e-PhNCO-024	-1031.206852	+28.16	-1031.616469
1e-PhNCO-023	-1031.206906	+28.02	-1031.616501
1e-PhNCO-022	-1031.206928	+27.96	-1031.616544
1e-PhNCO-021	-1031.207282	+27.03	-1031.616900
1e-PhNCO-020	-1031.207388	+26.75	-1031.617074
1e-PhNCO-019	-1031.207848	+25.54	-1031.617448
1e-PhNCO-018	-1031.207893	+25.43	-1031.617461
1e-PhNCO-017	-1031.208041	+25.04	-1031.617734
1e-PhNCO-016	-1031.208056	+25.00	-1031.617943
1e-PhNCO-015	-1031.208307	+24.34	-1031.617905
1e-PhNCO-014	-1031.208348	+24.23	-1031.618125

1e-PhNCO-013	-1031.208609	+23.55	-1031.618435
1e-PhNCO-012	-1031.208910	+22.76	-1031.618481
1e-PhNCO-011	-1031.209041	+22.41	-1031.618834

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
1e-PhNCO-010	-1031.209124	+22.19	-1031.618990	-1029.320349	+18.58	-1029.685170
1e-PhNCO-009	-1031.215706	+4.91	-1031.625690	-1029.325641	+4.68	-1029.694067
1e-PhNCO-008	-1031.215716	+4.89	-1031.625631	-1029.325856	+4.12	-1029.693945
1e-PhNCO-007	-1031.216193	+3.63	-1031.626016	-1029.326033	+3.65	-1029.694451
1e-PhNCO-006	-1031.216098	+3.88	-1031.625900	-1029.326169	+3.30	-1029.694292
1e-PhNCO-005	-1031.216157	+3.73	-1031.626007	-1029.326206	+3.20	-1029.694405
1e-PhNCO-004	-1031.216996	+1.53	-1031.627058	-1029.326796	+1.65	-1029.695031
1e-PhNCO-003	-1031.217184	+1.03	-1031.627124	-1029.327007	+1.10	-1029.695433
1e-PhNCO-002	-1031.217450	+0.33	-1031.627294	-1029.327221	+0.54	-1029.695309
1e-PhNCO-001	-1031.217577	+0.00	-1031.627363	-1029.327425	+0.00	-1029.695875

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
1e-007	-631.543106	+13.12	-631.837765	-630.371031	+9.01	-630.644395
1e-006	-631.545096	+7.89	-631.839524	-630.371564	+7.61	-630.644775
1e-005	-631.545553	+6.69	-631.840170	-630.371948	+6.60	-630.644833
1e-004	-631.545860	+5.89	-631.840704	-630.372563	+4.98	-630.645560
1e-003	-631.546628	+3.87	-631.841622	-630.372596	+4.90	-630.645670
1e-002	-631.546690	+3.71	-631.841432	-630.372932	+4.01	-630.646164
1e-001	-631.548102	+0.00	-631.842769	-630.374461	+0.00	-630.647647

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
1f-Me-013	-1098.717087	+12.61	-1099.290092
1f-Me-012	-1098.717173	+12.39	-1099.290467
1f-Me-011	-1098.717226	+12.25	-1099.290394

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
1f-Me-010	-1098.717845	+10.62	-1099.290885	-1096.628310	+6.84	-1097.122947
1f-Me-009	-1098.720261	+4.28	-1099.293218	-1096.628516	+6.30	-1097.122812
1f-Me-008	-1098.720281	+4.23	-1099.292731	-1096.629058	+4.88	-1097.122943
1f-Me-007	-1098.721347	+1.43	-1099.294122	-1096.629522	+3.66	-1097.123473
1f-Me-006	-1098.721042	+2.23	-1099.293951	-1096.629741	+3.08	-1097.124282
1f-Me-005	-1098.721162	+1.91	-1099.294524	-1096.629797	+2.94	-1097.124155
1f-Me-004	-1098.721317	+1.51	-1099.294315	-1096.629972	+2.48	-1097.124575
1f-Me-003	-1098.721378	+1.35	-1099.293913	-1096.630126	+2.07	-1097.124339
1f-Me-002	-1098.721771	+0.32	-1099.294162	-1096.630657	+0.68	-1097.124773
1f-Me-001	-1098.721891	+0.00	-1099.294368	-1096.630916	+0.00	-1097.125234

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
1f-PhNCO-019	-1458.651632	+24.04	-1459.295593
1f-PhNCO-018	-1458.651652	+23.99	-1459.295622
1f-PhNCO-017	-1458.651955	+23.20	-1459.295578
1f-PhNCO-016	-1458.652003	+23.07	-1459.295668
1f-PhNCO-015	-1458.652083	+22.86	-1459.295674
1f-PhNCO-014	-1458.652292	+22.31	-1459.295557
1f-PhNCO-013	-1458.657113	+9.65	-1459.301315
1f-PhNCO-012	-1458.657278	+9.22	-1459.301382
1f-PhNCO-011	-1458.657290	+9.19	-1459.301507

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
1f-PhNCO-010	-1458.657423	+8.84	-1459.301352	-1455.928450	+11.75	-1456.523161
1f-PhNCO-009	-1458.657320	+9.11	-1459.301428	-1455.928638	+11.26	-1456.523543
1f-PhNCO-008	-1458.657854	+7.71	-1459.302058	-1455.928994	+10.33	-1456.525546
1f-PhNCO-007	-1458.657535	+8.55	-1459.301659	-1455.929023	+10.25	-1456.523949
1f-PhNCO-006	-1458.657519	+8.59	-1459.301573	-1455.929025	+10.24	-1456.524791
1f-PhNCO-005	-1458.657607	+8.36	-1459.301821	-1455.929247	+9.66	-1456.524327
1f-PhNCO-004	-1458.659430	+3.57	-1459.303131	-1455.931235	+4.44	-1456.526208
1f-PhNCO-003	-1458.660641	+0.39	-1459.304122	-1455.932866	+0.16	-1456.527753
1f-PhNCO-002	-1458.660790	+0.00	-1459.304522	-1455.932890	+0.10	-1456.527707
1f-PhNCO-001	-1458.660587	+0.53	-1459.304329	-1455.932927	+0.00	-1456.527623

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
1f-019	-1058.987541	+4.81	-1059.516398
1f-018	-1058.987603	+4.65	-1059.516400
1f-017	-1058.987604	+4.64	-1059.516379
1f-016	-1058.987771	+4.21	-1059.516347
1f-015	-1058.987783	+4.17	-1059.516477
1f-014	-1058.987982	+3.65	-1059.516729
1f-013	-1058.987994	+3.62	-1059.516601
1f-012	-1058.988106	+3.33	-1059.517058
1f-011	-1058.988256	+2.93	-1059.516767

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
1f-010	-1058.988385	+2.59	-1059.517138	-1056.976337	+4.56	-1057.473995
1f-009	-1058.988394	+2.57	-1059.517118	-1056.976429	+4.31	-1057.473913
1f-008	-1058.988296	+2.83	-1059.516814	-1056.976468	+4.21	-1057.473766
1f-007	-1058.988635	+1.94	-1059.517342	-1056.976718	+3.55	-1057.474317
1f-006	-1058.988654	+1.89	-1059.517156	-1056.976786	+3.38	-1057.474245
1f-005	-1058.988676	+1.83	-1059.517155	-1056.977033	+2.73	-1057.474401
1f-004	-1058.989049	+0.85	-1059.517983	-1056.977203	+2.28	-1057.475176
1f-003	-1058.989270	+0.27	-1059.518161	-1056.977213	+2.26	-1057.475072

1f-002	-1058.989247	+0.33	-1059.518051	-1056.977767	+0.80	-1057.477963
1f-001	-1058.989373	+0.00	-1059.518314	-1056.978072	+0.00	-1057.478355

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
1g-Me-001	-287.928064	+0.00	-288.066040	-287.383966	+0.00	-287.442793

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
1g-PhNCO-002	-647.863222	+25.14	-648.071509	-646.682029	+21.05	-646.856923
1g-PhNCO-001	-647.872796	+0.00	-648.081694	-646.690046	+0.00	-646.870350

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
1g-001	-248.216362	+0.00	-248.310532	-247.749343	+0.00	-247.833295

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
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6ac-038	-2264.548640	+27.25	-2265.003634
6ac-037	-2264.550097	+23.43	-2265.005251
6ac-036	-2264.551062	+20.89	-2265.006159
6ac-035	-2264.552752	+16.46	-2265.007676
6ac-034	-2264.555216	+9.99	-2265.010438
6ac-033	-2264.555685	+8.76	-2265.010686
6ac-032	-2264.555933	+8.10	-2265.011098
6ac-031	-2264.556287	+7.18	-2265.011237
6ac-030	-2264.556628	+6.28	-2265.011770
6ac-029	-2264.556821	+5.77	-2265.012398
6ac-028	-2264.556869	+5.65	-2265.012030
6ac-027	-2264.556956	+5.42	-2265.012278
6ac-026	-2264.556973	+5.37	-2265.011955
6ac-025	-2264.557030	+5.22	-2265.012127
6ac-024	-2264.557064	+5.14	-2265.011983
6ac-023	-2264.557081	+5.09	-2265.012133
6ac-022	-2264.557111	+5.01	-2265.012173
6ac-021	-2264.557182	+4.83	-2265.012236
6ac-020	-2264.557204	+4.77	-2265.012259
6ac-019	-2264.557286	+4.55	-2265.012424
6ac-018	-2264.557304	+4.51	-2265.012629
6ac-017	-2264.557340	+4.41	-2265.012433
6ac-016	-2264.557346	+4.40	-2265.012383
6ac-015	-2264.557453	+4.11	-2265.012560
6ac-014	-2264.557577	+3.79	-2265.012292
6ac-013	-2264.557659	+3.57	-2265.012856

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6ac-012	-2264.557823	+3.14	-2265.012892	-2261.122129	+6.68	-2261.523283
6ac-011	-2264.557881	+2.99	-2265.012872	-2261.122142	+6.64	-2261.527105
6ac-010	-2264.557977	+2.74	-2265.012947	-2261.122278	+6.29	-2261.525030
6ac-009	-2264.557995	+2.69	-2265.012963	-2261.122338	+6.13	-2261.524859
6ac-008	-2264.557683	+3.51	-2265.013038	-2261.122353	+6.09	-2261.527948
6ac-007	-2264.557831	+3.12	-2265.013228	-2261.122377	+6.03	-2261.527961
6ac-006	-2264.558002	+2.67	-2265.012737	-2261.123026	+4.32	-2261.526280
6ac-005	-2264.557779	+3.26	-2265.012816	-2261.123110	+4.10	-2261.527003
6ac-004	-2264.558565	+1.19	-2265.013752	-2261.123201	+3.86	-2261.528809
6ac-003	-2264.559020	+0.00	-2265.013824	-2261.124159	+1.35	-2261.529197
6ac-002	-2264.558915	+0.28	-2265.013895	-2261.124459	+0.56	-2261.531886
6ac-001	-2264.558997	+0.06	-2265.013733	-2261.124672	+0.00	-2261.532301

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6a-002	-1188.707899	+6.91	-1188.827589	-1187.152309	+8.52	-1187.212049
6a-001	-1188.710531	+0.00	-1188.830358	-1187.155553	+0.00	-1187.215384

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
6ac-Me-028	-2304.284084	+8.07	-2304.783332
6ac-Me-027	-2304.284113	+7.99	-2304.783248
6ac-Me-026	-2304.284225	+7.70	-2304.783396
6ac-Me-025	-2304.284483	+7.02	-2304.783590
6ac-Me-024	-2304.284557	+6.83	-2304.783548
6ac-Me-023	-2304.284582	+6.76	-2304.783415
6ac-Me-022	-2304.284645	+6.60	-2304.783619
6ac-Me-021	-2304.284788	+6.22	-2304.784097
6ac-Me-020	-2304.285067	+5.49	-2304.784380
6ac-Me-019	-2304.285084	+5.44	-2304.784112
6ac-Me-018	-2304.285109	+5.38	-2304.784204
6ac-Me-017	-2304.285430	+4.53	-2304.784368
6ac-Me-016	-2304.285468	+4.43	-2304.784096
6ac-Me-015	-2304.285534	+4.26	-2304.784100
6ac-Me-014	-2304.285539	+4.25	-2304.784276
6ac-Me-013	-2304.285608	+4.07	-2304.784219
6ac-Me-012	-2304.285716	+3.78	-2304.784161

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6ac-Me-011	-2304.285729	+3.75	-2304.784921	-2300.772025	+4.99	-2301.183113
6ac-Me-010	-2304.285732	+3.74	-2304.784658	-2300.772483	+3.79	-2301.182997
6ac-Me-009	-2304.285840	+3.46	-2304.784726	-2300.772714	+3.18	-2301.186838

6ac-Me-008	-2304.286729	+1.12	-2304.785737	-2300.773318	+1.59	-2301.183694
6ac-Me-007	-2304.286420	+1.93	-2304.785387	-2300.773326	+1.57	-2301.186969
6ac-Me-006	-2304.286520	+1.67	-2304.785745	-2300.773335	+1.55	-2301.184530
6ac-Me-005	-2304.286665	+1.29	-2304.785774	-2300.773362	+1.48	-2301.185010
6ac-Me-004	-2304.286546	+1.60	-2304.785311	-2300.773427	+1.31	-2301.186806
6ac-Me-003	-2304.286404	+1.98	-2304.785077	-2300.773504	+1.11	-2301.184341
6ac-Me-002	-2304.286430	+1.91	-2304.785074	-2300.773911	+0.04	-2301.188391
6ac-Me-001	-2304.287157	+0.00	-2304.786019	-2300.773925	+0.00	-2301.185721

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
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6ac-PhNCO-027	-2664.224196	+15.13	-2664.794294
6ac-PhNCO-026	-2664.224693	+13.82	-2664.794737
6ac-PhNCO-025	-2664.226645	+8.70	-2664.796657
6ac-PhNCO-024	-2664.227463	+6.55	-2664.797360
6ac-PhNCO-023	-2664.227503	+6.44	-2664.797476
6ac-PhNCO-022	-2664.228037	+5.04	-2664.797850
6ac-PhNCO-021	-2664.228093	+4.89	-2664.798164
6ac-PhNCO-020	-2664.228097	+4.88	-2664.798164
6ac-PhNCO-019	-2664.228154	+4.73	-2664.798215
6ac-PhNCO-018	-2664.228228	+4.54	-2664.798474
6ac-PhNCO-017	-2664.228277	+4.41	-2664.798532
6ac-PhNCO-016	-2664.228291	+4.37	-2664.798393
6ac-PhNCO-015	-2664.228329	+4.27	-2664.798477
6ac-PhNCO-014	-2664.228354	+4.21	-2664.798448
6ac-PhNCO-013	-2664.228365	+4.18	-2664.798686

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
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6ac-PhNCO-012	-2664.228453	+3.95	-2664.798301	-2660.076920	+8.01	-2660.590526
6ac-PhNCO-011	-2664.229445	+1.34	-2664.799432	-2660.078011	+5.15	-2660.590056
6ac-PhNCO-010	-2664.228592	+3.58	-2664.798532	-2660.078291	+4.41	-2660.591607
6ac-PhNCO-009	-2664.228531	+3.74	-2664.798710	-2660.078336	+4.29	-2660.588076
6ac-PhNCO-008	-2664.229014	+2.48	-2664.798967	-2660.078380	+4.18	-2660.585576
6ac-PhNCO-007	-2664.228727	+3.23	-2664.799036	-2660.078380	+4.18	-2660.587442
6ac-PhNCO-006	-2664.229117	+2.21	-2664.799422	-2660.078486	+3.90	-2660.588508
6ac-PhNCO-005	-2664.229566	+1.03	-2664.799284	-2660.078786	+3.11	-2660.587006
6ac-PhNCO-004	-2664.229314	+1.69	-2664.799504	-2660.078974	+2.62	-2660.588446
6ac-PhNCO-003	-2664.229355	+1.58	-2664.799304	-2660.079015	+2.51	-2660.587967
6ac-PhNCO-002	-2664.228622	+3.51	-2664.798741	-2660.079053	+2.41	-2660.589797
6ac-PhNCO-001	-2664.229957	+0.00	-2664.800153	-2660.079971	+0.00	-2660.589197

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
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6ah-106	-1846.614343	+26.53	-1847.020271
6ah-105	-1846.616314	+21.35	-1847.022156
6ah-104	-1846.617052	+19.42	-1847.023371

6ah-103	-1846.617089	+19.32	-1847.022574
6ah-102	-1846.617217	+18.98	-1847.023560
6ah-101	-1846.617246	+18.91	-1847.023443
6ah-100	-1846.617528	+18.17	-1847.023218
6ah-099	-1846.617674	+17.78	-1847.023950
6ah-098	-1846.617799	+17.45	-1847.023773
6ah-097	-1846.618031	+16.85	-1847.023826
6ah-096	-1846.618208	+16.38	-1847.024025
6ah-095	-1846.618262	+16.24	-1847.024024
6ah-094	-1846.618489	+15.64	-1847.024640
6ah-093	-1846.618741	+14.98	-1847.025003
6ah-092	-1846.618745	+14.97	-1847.024546
6ah-091	-1846.618802	+14.82	-1847.024941
6ah-090	-1846.618863	+14.66	-1847.024908
6ah-089	-1846.619008	+14.28	-1847.025429
6ah-088	-1846.619139	+13.94	-1847.025092
6ah-087	-1846.619153	+13.90	-1847.025031
6ah-086	-1846.619180	+13.83	-1847.025276
6ah-085	-1846.619200	+13.78	-1847.025712
6ah-084	-1846.619318	+13.47	-1847.025790
6ah-083	-1846.619633	+12.64	-1847.025739
6ah-082	-1846.619807	+12.18	-1847.025718
6ah-081	-1846.619863	+12.04	-1847.025546
6ah-080	-1846.619897	+11.95	-1847.026269
6ah-079	-1846.619905	+11.93	-1847.025752
6ah-078	-1846.620006	+11.66	-1847.025797
6ah-077	-1846.620048	+11.55	-1847.026209
6ah-076	-1846.620058	+11.52	-1847.026332
6ah-075	-1846.620071	+11.49	-1847.025860
6ah-074	-1846.620326	+10.82	-1847.026525
6ah-073	-1846.620345	+10.77	-1847.026844
6ah-072	-1846.620481	+10.41	-1847.026180
6ah-071	-1846.620483	+10.41	-1847.026680
6ah-070	-1846.620503	+10.35	-1847.026293
6ah-069	-1846.620576	+10.16	-1847.026462
6ah-068	-1846.620602	+10.10	-1847.026473
6ah-067	-1846.620755	+9.69	-1847.027056
6ah-066	-1846.620776	+9.64	-1847.026923
6ah-065	-1846.620791	+9.60	-1847.026392
6ah-064	-1846.620803	+9.57	-1847.026608
6ah-063	-1846.620872	+9.39	-1847.026628
6ah-062	-1846.620878	+9.37	-1847.026827
6ah-061	-1846.620889	+9.34	-1847.027206
6ah-060	-1846.620898	+9.32	-1847.026478
6ah-059	-1846.620904	+9.30	-1847.026766
6ah-058	-1846.620928	+9.24	-1847.027034
6ah-057	-1846.621028	+8.98	-1847.027115

6ah-056	-1846.621040	+8.95	-1847.027321
6ah-055	-1846.621044	+8.93	-1847.026768
6ah-054	-1846.621045	+8.93	-1847.026870
6ah-053	-1846.621087	+8.82	-1847.027107
6ah-052	-1846.621091	+8.81	-1847.027376
6ah-051	-1846.621105	+8.77	-1847.026785
6ah-050	-1846.621191	+8.55	-1847.027145
6ah-049	-1846.621202	+8.52	-1847.027288
6ah-048	-1846.621232	+8.44	-1847.027346
6ah-047	-1846.621377	+8.06	-1847.027426
6ah-046	-1846.621436	+7.91	-1847.027050
6ah-045	-1846.621451	+7.87	-1847.027387
6ah-044	-1846.621483	+7.78	-1847.027464
6ah-043	-1846.621581	+7.52	-1847.027792
6ah-042	-1846.621613	+7.44	-1847.027718
6ah-041	-1846.621630	+7.40	-1847.027142
6ah-040	-1846.621632	+7.39	-1847.027657
6ah-039	-1846.621657	+7.33	-1847.027449
6ah-038	-1846.621793	+6.97	-1847.028167
6ah-037	-1846.621997	+6.43	-1847.028142
6ah-036	-1846.622135	+6.07	-1847.028039
6ah-035	-1846.622200	+5.90	-1847.028107
6ah-034	-1846.622292	+5.66	-1847.028276
6ah-033	-1846.622326	+5.57	-1847.028300
6ah-032	-1846.622458	+5.22	-1847.028183
6ah-031	-1846.622512	+5.08	-1847.028420
6ah-030	-1846.622555	+4.97	-1847.028512
6ah-029	-1846.622624	+4.79	-1847.028177
6ah-028	-1846.622656	+4.70	-1847.028308
6ah-027	-1846.622748	+4.46	-1847.028527
6ah-026	-1846.622766	+4.41	-1847.028830
6ah-025	-1846.622767	+4.41	-1847.028657
6ah-024	-1846.622832	+4.24	-1847.028630
6ah-023	-1846.622859	+4.17	-1847.028533
6ah-022	-1846.622870	+4.14	-1847.028630
6ah-021	-1846.622929	+3.99	-1847.028922

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6ah-020	-1846.623190	+3.30	-1847.029405	-1844.001014	+7.44	-1844.366247
6ah-019	-1846.623067	+3.62	-1847.028789	-1844.001554	+6.03	-1844.363317
6ah-018	-1846.623163	+3.37	-1847.028988	-1844.001604	+5.89	-1844.362901
6ah-017	-1846.623386	+2.79	-1847.029030	-1844.001745	+5.52	-1844.362818
6ah-016	-1846.623396	+2.76	-1847.029200	-1844.002781	+2.80	-1844.364165
6ah-015	-1846.623089	+3.57	-1847.029022	-1844.002811	+2.73	-1844.364483
6ah-014	-1846.623199	+3.28	-1847.028917	-1844.002827	+2.68	-1844.364867
6ah-013	-1846.623246	+3.15	-1847.028903	-1844.002866	+2.58	-1844.364727

6ah-012	-1846.623397	+2.76	-1847.029126	-1844.002877	+2.55	-1844.364045
6ah-011	-1846.623397	+2.76	-1847.029009	-1844.002907	+2.47	-1844.361562
6ah-010	-1846.623055	+3.65	-1847.028738	-1844.002933	+2.40	-1844.363476
6ah-009	-1846.623270	+3.09	-1847.029013	-1844.002955	+2.35	-1844.364486
6ah-008	-1846.623772	+1.77	-1847.029762	-1844.002967	+2.32	-1844.367014
6ah-007	-1846.623319	+2.96	-1847.029098	-1844.003067	+2.05	-1844.365298
6ah-006	-1846.623755	+1.82	-1847.029626	-1844.003140	+1.86	-1844.364601
6ah-005	-1846.623277	+3.07	-1847.029064	-1844.003146	+1.85	-1844.365472
6ah-004	-1846.623239	+3.17	-1847.028954	-1844.003187	+1.74	-1844.361991
6ah-003	-1846.623396	+2.76	-1847.028962	-1844.003342	+1.33	-1844.363811
6ah-002	-1846.623463	+2.58	-1847.028989	-1844.003578	+0.71	-1844.364833
6ah-001	-1846.624447	+0.00	-1847.030103	-1844.003849	+0.00	-1844.367460

Nr.	$H_{298K}(DFT)/\text{Hartree}$	$\Delta H_{298K}(DFT)/\text{kJ mol}^{-1}$	$E_{298K}(DFT)/\text{Hartree}$
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6ah-Me2-138	-1886.324279	+31.98	-1886.774277
6ah-Me2-137	-1886.324326	+31.86	-1886.773078
6ah-Me2-136	-1886.324346	+31.81	-1886.773728
6ah-Me2-135	-1886.324371	+31.74	-1886.773726
6ah-Me2-134	-1886.325564	+28.61	-1886.774800
6ah-Me2-133	-1886.326023	+27.40	-1886.775277
6ah-Me2-132	-1886.328842	+20.00	-1886.778193
6ah-Me2-131	-1886.329133	+19.24	-1886.778491
6ah-Me2-130	-1886.329386	+18.58	-1886.778865
6ah-Me2-129	-1886.329432	+18.45	-1886.779014
6ah-Me2-128	-1886.329436	+18.44	-1886.778586
6ah-Me2-127	-1886.329635	+17.92	-1886.779742
6ah-Me2-126	-1886.329654	+17.87	-1886.779422
6ah-Me2-125	-1886.329705	+17.74	-1886.778860
6ah-Me2-124	-1886.329726	+17.68	-1886.778955
6ah-Me2-123	-1886.329951	+17.09	-1886.778808
6ah-Me2-122	-1886.330122	+16.64	-1886.779332
6ah-Me2-121	-1886.330139	+16.60	-1886.779242
6ah-Me2-120	-1886.330170	+16.52	-1886.779229
6ah-Me2-119	-1886.330542	+15.54	-1886.779821
6ah-Me2-118	-1886.330549	+15.52	-1886.779845
6ah-Me2-117	-1886.330704	+15.11	-1886.779867
6ah-Me2-116	-1886.330762	+14.96	-1886.780721
6ah-Me2-115	-1886.331082	+14.12	-1886.780257
6ah-Me2-114	-1886.331102	+14.07	-1886.780160
6ah-Me2-113	-1886.331110	+14.05	-1886.780001
6ah-Me2-112	-1886.331116	+14.03	-1886.780345
6ah-Me2-111	-1886.331177	+13.87	-1886.780234
6ah-Me2-110	-1886.331264	+13.64	-1886.780343
6ah-Me2-109	-1886.331288	+13.58	-1886.780093
6ah-Me2-108	-1886.331319	+13.50	-1886.780240
6ah-Me2-107	-1886.331331	+13.47	-1886.780321

6ah-Me2-106	-1886.331358	+13.40	-1886.780406
6ah-Me2-105	-1886.331375	+13.35	-1886.780460
6ah-Me2-104	-1886.331393	+13.31	-1886.781111
6ah-Me2-103	-1886.331419	+13.24	-1886.780463
6ah-Me2-102	-1886.331467	+13.11	-1886.780869
6ah-Me2-101	-1886.331491	+13.05	-1886.780212
6ah-Me2-100	-1886.331620	+12.71	-1886.781083
6ah-Me2-099	-1886.331672	+12.57	-1886.781306
6ah-Me2-098	-1886.331714	+12.46	-1886.781293
6ah-Me2-097	-1886.331805	+12.22	-1886.781090
6ah-Me2-096	-1886.331828	+12.16	-1886.780971
6ah-Me2-095	-1886.331878	+12.03	-1886.781376
6ah-Me2-094	-1886.331894	+11.99	-1886.781547
6ah-Me2-093	-1886.331922	+11.92	-1886.781137
6ah-Me2-092	-1886.331939	+11.87	-1886.781363
6ah-Me2-091	-1886.331999	+11.72	-1886.781203
6ah-Me2-090	-1886.332192	+11.21	-1886.781701
6ah-Me2-089	-1886.332195	+11.20	-1886.781879
6ah-Me2-088	-1886.332205	+11.17	-1886.781660
6ah-Me2-087	-1886.332237	+11.09	-1886.781339
6ah-Me2-086	-1886.332239	+11.08	-1886.781208
6ah-Me2-085	-1886.332270	+11.00	-1886.782262
6ah-Me2-084	-1886.332312	+10.89	-1886.781326
6ah-Me2-083	-1886.332330	+10.85	-1886.781434
6ah-Me2-082	-1886.332382	+10.71	-1886.781781
6ah-Me2-081	-1886.332384	+10.70	-1886.781402
6ah-Me2-080	-1886.332444	+10.55	-1886.781956
6ah-Me2-079	-1886.332485	+10.44	-1886.781405
6ah-Me2-078	-1886.332566	+10.23	-1886.782235
6ah-Me2-077	-1886.332608	+10.12	-1886.782226
6ah-Me2-076	-1886.332611	+10.11	-1886.782084
6ah-Me2-075	-1886.332640	+10.03	-1886.782415
6ah-Me2-074	-1886.332675	+9.94	-1886.782135
6ah-Me2-073	-1886.332693	+9.89	-1886.782293
6ah-Me2-072	-1886.332707	+9.86	-1886.782386
6ah-Me2-071	-1886.332771	+9.69	-1886.782125
6ah-Me2-070	-1886.332826	+9.54	-1886.782550
6ah-Me2-069	-1886.332854	+9.47	-1886.782251
6ah-Me2-068	-1886.332855	+9.47	-1886.782034
6ah-Me2-067	-1886.332863	+9.45	-1886.782065
6ah-Me2-066	-1886.332886	+9.39	-1886.782395
6ah-Me2-065	-1886.332887	+9.38	-1886.782468
6ah-Me2-064	-1886.332939	+9.25	-1886.782284
6ah-Me2-063	-1886.332942	+9.24	-1886.782243
6ah-Me2-062	-1886.332946	+9.23	-1886.782078
6ah-Me2-061	-1886.333018	+9.04	-1886.782740
6ah-Me2-060	-1886.333034	+9.00	-1886.782401

6ah-Me2-059	-1886.333126	+8.76	-1886.782366
6ah-Me2-058	-1886.333138	+8.72	-1886.782884
6ah-Me2-057	-1886.333139	+8.72	-1886.782502
6ah-Me2-056	-1886.333160	+8.67	-1886.782397
6ah-Me2-055	-1886.333165	+8.65	-1886.782952
6ah-Me2-054	-1886.333206	+8.55	-1886.782868
6ah-Me2-053	-1886.333227	+8.49	-1886.782498
6ah-Me2-052	-1886.333252	+8.43	-1886.782893
6ah-Me2-051	-1886.333314	+8.26	-1886.782513
6ah-Me2-050	-1886.333324	+8.24	-1886.782437
6ah-Me2-049	-1886.333340	+8.19	-1886.782689
6ah-Me2-048	-1886.333435	+7.94	-1886.782768
6ah-Me2-047	-1886.333443	+7.92	-1886.782603
6ah-Me2-046	-1886.333450	+7.91	-1886.782365
6ah-Me2-045	-1886.333489	+7.80	-1886.783374
6ah-Me2-044	-1886.333516	+7.73	-1886.783042
6ah-Me2-043	-1886.333532	+7.69	-1886.782621
6ah-Me2-042	-1886.333546	+7.65	-1886.782398
6ah-Me2-041	-1886.333648	+7.39	-1886.783495
6ah-Me2-040	-1886.333683	+7.29	-1886.782862
6ah-Me2-039	-1886.333713	+7.21	-1886.783172
6ah-Me2-038	-1886.333809	+6.96	-1886.783466
6ah-Me2-037	-1886.333848	+6.86	-1886.783569
6ah-Me2-036	-1886.333931	+6.64	-1886.783490
6ah-Me2-035	-1886.333980	+6.51	-1886.783747
6ah-Me2-034	-1886.334138	+6.10	-1886.783496
6ah-Me2-033	-1886.334305	+5.66	-1886.783659
6ah-Me2-032	-1886.334340	+5.57	-1886.784161
6ah-Me2-031	-1886.334345	+5.56	-1886.783410
6ah-Me2-030	-1886.334353	+5.53	-1886.783991
6ah-Me2-029	-1886.334401	+5.41	-1886.784341
6ah-Me2-028	-1886.334454	+5.27	-1886.784139
6ah-Me2-027	-1886.334551	+5.01	-1886.783716
6ah-Me2-026	-1886.334576	+4.95	-1886.783817
6ah-Me2-025	-1886.334586	+4.92	-1886.783553
6ah-Me2-024	-1886.334603	+4.88	-1886.783783
6ah-Me2-023	-1886.334652	+4.75	-1886.784099
6ah-Me2-022	-1886.334663	+4.72	-1886.783657
6ah-Me2-021	-1886.334719	+4.57	-1886.784287

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6ah-Me2-020	-1886.334967	+3.92	-1886.784244	-1883.640702	+6.38	-1884.011443
6ah-Me2-019	-1886.335016	+3.79	-1886.784254	-1883.640867	+5.95	-1884.011690
6ah-Me2-018	-1886.334884	+4.14	-1886.784834	-1883.640900	+5.86	-1884.011998
6ah-Me2-017	-1886.334977	+3.90	-1886.784758	-1883.640941	+5.75	-1884.012202
6ah-Me2-016	-1886.334726	+4.56	-1886.783878	-1883.641055	+5.45	-1884.012451

6ah-Me2-015	-1886.335085	+3.61	-1886.784936	-1883.641201	+5.07	-1884.012520
6ah-Me2-014	-1886.334735	+4.53	-1886.784254	-1883.641225	+5.01	-1884.011748
6ah-Me2-013	-1886.334799	+4.36	-1886.783986	-1883.641261	+4.91	-1884.011589
6ah-Me2-012	-1886.334759	+4.47	-1886.784535	-1883.641442	+4.44	-1884.010850
6ah-Me2-011	-1886.335416	+2.74	-1886.785039	-1883.641493	+4.30	-1884.012794
6ah-Me2-010	-1886.335106	+3.56	-1886.784532	-1883.641515	+4.25	-1884.011731
6ah-Me2-009	-1886.335711	+1.97	-1886.785168	-1883.641654	+3.88	-1884.013500
6ah-Me2-008	-1886.335715	+1.96	-1886.785125	-1883.641706	+3.74	-1884.013473
6ah-Me2-007	-1886.335029	+3.76	-1886.784697	-1883.641714	+3.72	-1884.011986
6ah-Me2-006	-1886.334831	+4.28	-1886.784502	-1883.641753	+3.62	-1884.011748
6ah-Me2-005	-1886.335826	+1.67	-1886.784969	-1883.641775	+3.56	-1884.013682
6ah-Me2-004	-1886.335112	+3.54	-1886.784345	-1883.642032	+2.89	-1884.011620
6ah-Me2-003	-1886.335528	+2.45	-1886.784573	-1883.642253	+2.31	-1884.012076
6ah-Me2-002	-1886.335624	+2.20	-1886.784498	-1883.642681	+1.18	-1884.011947
6ah-Me2-001	-1886.336461	+0.00	-1886.785935	-1883.643132	+0.00	-1884.014248

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
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6ah-Me-124	-1886.332150	+50.98	-1886.782121
6ah-Me-123	-1886.341265	+27.05	-1886.790925
6ah-Me-122	-1886.342224	+24.53	-1886.791948
6ah-Me-121	-1886.342995	+22.51	-1886.792801
6ah-Me-120	-1886.343438	+21.34	-1886.793550
6ah-Me-119	-1886.343845	+20.27	-1886.794389
6ah-Me-118	-1886.344810	+17.74	-1886.794822
6ah-Me-117	-1886.345429	+16.12	-1886.795570
6ah-Me-116	-1886.346015	+14.58	-1886.795604
6ah-Me-115	-1886.346046	+14.50	-1886.795883
6ah-Me-114	-1886.346402	+13.56	-1886.796710
6ah-Me-113	-1886.346499	+13.31	-1886.796290
6ah-Me-112	-1886.346540	+13.20	-1886.796872
6ah-Me-111	-1886.346954	+12.11	-1886.797093
6ah-Me-110	-1886.346970	+12.07	-1886.797102
6ah-Me-109	-1886.347239	+11.36	-1886.796953
6ah-Me-108	-1886.347369	+11.02	-1886.797373
6ah-Me-107	-1886.347401	+10.94	-1886.797521
6ah-Me-106	-1886.347414	+10.90	-1886.797540
6ah-Me-105	-1886.347470	+10.76	-1886.796510
6ah-Me-104	-1886.347518	+10.63	-1886.796695
6ah-Me-103	-1886.347549	+10.55	-1886.797551
6ah-Me-102	-1886.347602	+10.41	-1886.797515
6ah-Me-101	-1886.347729	+10.08	-1886.797553
6ah-Me-100	-1886.347796	+9.90	-1886.797621
6ah-Me-099	-1886.348066	+9.19	-1886.798542
6ah-Me-098	-1886.348253	+8.70	-1886.798372
6ah-Me-097	-1886.348276	+8.64	-1886.797805
6ah-Me-096	-1886.348339	+8.48	-1886.797926

6ah-Me-095	-1886.348348	+8.45	-1886.798170
6ah-Me-094	-1886.348389	+8.34	-1886.798643
6ah-Me-093	-1886.348393	+8.33	-1886.798267
6ah-Me-092	-1886.348431	+8.23	-1886.798497
6ah-Me-091	-1886.348544	+7.94	-1886.798692
6ah-Me-090	-1886.348636	+7.70	-1886.798218
6ah-Me-089	-1886.348637	+7.69	-1886.799100
6ah-Me-088	-1886.348756	+7.38	-1886.798686
6ah-Me-087	-1886.348771	+7.34	-1886.798309
6ah-Me-086	-1886.348772	+7.34	-1886.798672
6ah-Me-085	-1886.348788	+7.30	-1886.798282
6ah-Me-084	-1886.348792	+7.29	-1886.798626
6ah-Me-083	-1886.348796	+7.28	-1886.798547
6ah-Me-082	-1886.348844	+7.15	-1886.798106
6ah-Me-081	-1886.348862	+7.10	-1886.798292
6ah-Me-080	-1886.348985	+6.78	-1886.799251
6ah-Me-079	-1886.349007	+6.72	-1886.799035
6ah-Me-078	-1886.349070	+6.56	-1886.798874
6ah-Me-077	-1886.349109	+6.45	-1886.799210
6ah-Me-076	-1886.349138	+6.38	-1886.798770
6ah-Me-075	-1886.349191	+6.24	-1886.799120
6ah-Me-074	-1886.349243	+6.10	-1886.799094
6ah-Me-073	-1886.349308	+5.93	-1886.799156
6ah-Me-072	-1886.349308	+5.93	-1886.799151
6ah-Me-071	-1886.349398	+5.69	-1886.799380
6ah-Me-070	-1886.349407	+5.67	-1886.799654
6ah-Me-069	-1886.349471	+5.50	-1886.799042
6ah-Me-068	-1886.349476	+5.49	-1886.799486
6ah-Me-067	-1886.349480	+5.48	-1886.799442
6ah-Me-066	-1886.349498	+5.43	-1886.799491
6ah-Me-065	-1886.349514	+5.39	-1886.799832
6ah-Me-064	-1886.349649	+5.04	-1886.799694
6ah-Me-063	-1886.349761	+4.74	-1886.799307
6ah-Me-062	-1886.349827	+4.57	-1886.799138
6ah-Me-061	-1886.349929	+4.30	-1886.799873
6ah-Me-060	-1886.349990	+4.14	-1886.800229
6ah-Me-059	-1886.350006	+4.10	-1886.799521
6ah-Me-058	-1886.350088	+3.88	-1886.800208
6ah-Me-057	-1886.350105	+3.84	-1886.799938
6ah-Me-056	-1886.350119	+3.80	-1886.799657
6ah-Me-055	-1886.350167	+3.68	-1886.799811
6ah-Me-054	-1886.350210	+3.56	-1886.799913
6ah-Me-053	-1886.350224	+3.53	-1886.799881
6ah-Me-052	-1886.350232	+3.51	-1886.800012
6ah-Me-051	-1886.350254	+3.45	-1886.800205
6ah-Me-050	-1886.350272	+3.40	-1886.799827
6ah-Me-049	-1886.350277	+3.39	-1886.799629

6ah-Me-048	-1886.350328	+3.25	-1886.800089
6ah-Me-047	-1886.350333	+3.24	-1886.800201
6ah-Me-046	-1886.350337	+3.23	-1886.799837
6ah-Me-045	-1886.350355	+3.18	-1886.799817
6ah-Me-044	-1886.350365	+3.16	-1886.800027
6ah-Me-043	-1886.350395	+3.08	-1886.800459
6ah-Me-042	-1886.350407	+3.05	-1886.799912
6ah-Me-041	-1886.350479	+2.86	-1886.800270
6ah-Me-040	-1886.350481	+2.85	-1886.800194
6ah-Me-039	-1886.350498	+2.81	-1886.800026
6ah-Me-038	-1886.350521	+2.75	-1886.800064
6ah-Me-037	-1886.350539	+2.70	-1886.800229
6ah-Me-036	-1886.350596	+2.55	-1886.800733
6ah-Me-035	-1886.350600	+2.54	-1886.800513
6ah-Me-034	-1886.350608	+2.52	-1886.800753
6ah-Me-033	-1886.350627	+2.47	-1886.799991
6ah-Me-032	-1886.350652	+2.40	-1886.799984
6ah-Me-031	-1886.350663	+2.37	-1886.800736
6ah-Me-030	-1886.350693	+2.29	-1886.800640
6ah-Me-029	-1886.350694	+2.29	-1886.800336
6ah-Me-028	-1886.350721	+2.22	-1886.800088
6ah-Me-027	-1886.350731	+2.19	-1886.800319
6ah-Me-026	-1886.350734	+2.19	-1886.800465
6ah-Me-025	-1886.350735	+2.18	-1886.800951
6ah-Me-024	-1886.350791	+2.04	-1886.800181
6ah-Me-023	-1886.350816	+1.97	-1886.800924
6ah-Me-022	-1886.350817	+1.97	-1886.800039
6ah-Me-021	-1886.350823	+1.95	-1886.799970

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6ah-Me-020	-1886.350883	+1.80	-1886.800811	-1883.651510	+3.64	-1884.021937
6ah-Me-019	-1886.351029	+1.41	-1886.800658	-1883.652027	+2.28	-1884.019754
6ah-Me-018	-1886.351096	+1.24	-1886.800638	-1883.652067	+2.18	-1884.019750
6ah-Me-017	-1886.351035	+1.40	-1886.800663	-1883.652089	+2.12	-1884.021072
6ah-Me-016	-1886.350900	+1.75	-1886.800418	-1883.652119	+2.04	-1884.022713
6ah-Me-015	-1886.351031	+1.41	-1886.800693	-1883.652128	+2.02	-1884.020075
6ah-Me-014	-1886.351086	+1.26	-1886.800798	-1883.652237	+1.73	-1884.020057
6ah-Me-013	-1886.351076	+1.29	-1886.800747	-1883.652311	+1.54	-1884.020112
6ah-Me-012	-1886.351229	+0.89	-1886.800917	-1883.652408	+1.28	-1884.020201
6ah-Me-011	-1886.350902	+1.75	-1886.800510	-1883.652439	+1.20	-1884.022267
6ah-Me-010	-1886.350844	+1.90	-1886.800483	-1883.652440	+1.20	-1884.019444
6ah-Me-009	-1886.351115	+1.19	-1886.800678	-1883.652466	+1.13	-1884.021553
6ah-Me-008	-1886.351519	+0.13	-1886.800859	-1883.652609	+0.76	-1884.020259
6ah-Me-007	-1886.351484	+0.22	-1886.800756	-1883.652610	+0.75	-1884.020175
6ah-Me-006	-1886.351270	+0.78	-1886.800537	-1883.652636	+0.69	-1884.019966
6ah-Me-005	-1886.351387	+0.47	-1886.800615	-1883.652712	+0.49	-1884.020929

6ah-Me-004	-1886.351567	+0.00	-1886.800826	-1883.652720	+0.46	-1884.020504
6ah-Me-003	-1886.351510	+0.15	-1886.800847	-1883.652843	+0.14	-1884.021548
6ah-Me-002	-1886.351544	+0.06	-1886.800839	-1883.652893	+0.01	-1884.021202
6ah-Me-001	-1886.351472	+0.25	-1886.800870	-1883.652897	+0.00	-1884.021205

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
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6ah-PhNCO2-082	-2246.257749	+50.05	-2246.778281
6ah-PhNCO2-081	-2246.259195	+46.25	-2246.779256
6ah-PhNCO2-080	-2246.259977	+44.20	-2246.779834
6ah-PhNCO2-079	-2246.260048	+44.01	-2246.780407
6ah-PhNCO2-078	-2246.260052	+44.00	-2246.780418
6ah-PhNCO2-077	-2246.260912	+41.75	-2246.781136
6ah-PhNCO2-076	-2246.261735	+39.58	-2246.782123
6ah-PhNCO2-075	-2246.262637	+37.22	-2246.782957
6ah-PhNCO2-074	-2246.262896	+36.54	-2246.783172
6ah-PhNCO2-073	-2246.262906	+36.51	-2246.783049
6ah-PhNCO2-072	-2246.263023	+36.20	-2246.783253
6ah-PhNCO2-071	-2246.263077	+36.06	-2246.782680
6ah-PhNCO2-070	-2246.263340	+35.37	-2246.783370
6ah-PhNCO2-069	-2246.263382	+35.26	-2246.783373
6ah-PhNCO2-068	-2246.263532	+34.87	-2246.783816
6ah-PhNCO2-067	-2246.263555	+34.81	-2246.783815
6ah-PhNCO2-066	-2246.263555	+34.81	-2246.783816
6ah-PhNCO2-065	-2246.263769	+34.24	-2246.783650
6ah-PhNCO2-064	-2246.263888	+33.93	-2246.783929
6ah-PhNCO2-063	-2246.264116	+33.33	-2246.783636
6ah-PhNCO2-062	-2246.264195	+33.13	-2246.783958
6ah-PhNCO2-061	-2246.264200	+33.11	-2246.784398
6ah-PhNCO2-060	-2246.264295	+32.86	-2246.783929
6ah-PhNCO2-059	-2246.264305	+32.84	-2246.784429
6ah-PhNCO2-058	-2246.264465	+32.42	-2246.784641
6ah-PhNCO2-057	-2246.264698	+31.81	-2246.784778
6ah-PhNCO2-056	-2246.264780	+31.59	-2246.785197
6ah-PhNCO2-055	-2246.264971	+31.09	-2246.785225
6ah-PhNCO2-054	-2246.267704	+23.91	-2246.787779
6ah-PhNCO2-053	-2246.268410	+22.06	-2246.788414
6ah-PhNCO2-052	-2246.268695	+21.31	-2246.788736
6ah-PhNCO2-051	-2246.269256	+19.84	-2246.789576
6ah-PhNCO2-050	-2246.269361	+19.56	-2246.789595
6ah-PhNCO2-049	-2246.269443	+19.35	-2246.789431
6ah-PhNCO2-048	-2246.269730	+18.59	-2246.790213
6ah-PhNCO2-047	-2246.270076	+17.69	-2246.790477
6ah-PhNCO2-046	-2246.270297	+17.11	-2246.790858
6ah-PhNCO2-045	-2246.271466	+14.04	-2246.791651
6ah-PhNCO2-044	-2246.271628	+13.61	-2246.792148
6ah-PhNCO2-043	-2246.271816	+13.12	-2246.791954

6ah-PhNCO2-042	-2246.271833	+13.07	-2246.792169
6ah-PhNCO2-041	-2246.271908	+12.88	-2246.792263
6ah-PhNCO2-040	-2246.272133	+12.28	-2246.792108
6ah-PhNCO2-039	-2246.272182	+12.16	-2246.792363
6ah-PhNCO2-038	-2246.272264	+11.94	-2246.792816
6ah-PhNCO2-037	-2246.272300	+11.85	-2246.792357
6ah-PhNCO2-036	-2246.272434	+11.49	-2246.793097
6ah-PhNCO2-035	-2246.272600	+11.06	-2246.792954
6ah-PhNCO2-034	-2246.272614	+11.02	-2246.792929
6ah-PhNCO2-033	-2246.272632	+10.97	-2246.793016
6ah-PhNCO2-032	-2246.272683	+10.84	-2246.793003
6ah-PhNCO2-031	-2246.272884	+10.31	-2246.793281
6ah-PhNCO2-030	-2246.273097	+9.75	-2246.793287
6ah-PhNCO2-029	-2246.273120	+9.69	-2246.793489
6ah-PhNCO2-028	-2246.273180	+9.54	-2246.793485
6ah-PhNCO2-027	-2246.273209	+9.46	-2246.793420
6ah-PhNCO2-026	-2246.273290	+9.25	-2246.793437
6ah-PhNCO2-025	-2246.273467	+8.78	-2246.793482
6ah-PhNCO2-024	-2246.273623	+8.37	-2246.793943
6ah-PhNCO2-023	-2246.273639	+8.33	-2246.794166
6ah-PhNCO2-022	-2246.273648	+8.31	-2246.793800
6ah-PhNCO2-021	-2246.273827	+7.84	-2246.793881

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6ah-PhNCO2-020	-2246.273990	+7.41	-2246.794719	-2242.939500	+9.33	-2243.413168
6ah-PhNCO2-019	-2246.273879	+7.70	-2246.794383	-2242.939529	+9.25	-2243.413330
6ah-PhNCO2-018	-2246.274032	+7.30	-2246.794345	-2242.940031	+7.93	-2243.410943
6ah-PhNCO2-017	-2246.274122	+7.06	-2246.794304	-2242.940299	+7.23	-2243.411813
6ah-PhNCO2-016	-2246.274074	+7.19	-2246.794068	-2242.940380	+7.02	-2243.410280
6ah-PhNCO2-015	-2246.274297	+6.60	-2246.794376	-2242.940413	+6.93	-2243.412544
6ah-PhNCO2-014	-2246.274360	+6.44	-2246.794608	-2242.940462	+6.80	-2243.410393
6ah-PhNCO2-013	-2246.274494	+6.09	-2246.794961	-2242.940706	+6.16	-2243.411154
6ah-PhNCO2-012	-2246.274970	+4.84	-2246.795555	-2242.940749	+6.05	-2243.413646
6ah-PhNCO2-011	-2246.274322	+6.54	-2246.794427	-2242.940818	+5.87	-2243.410686
6ah-PhNCO2-010	-2246.274112	+7.09	-2246.794198	-2242.941030	+5.31	-2243.408351
6ah-PhNCO2-009	-2246.274750	+5.41	-2246.795196	-2242.941044	+5.27	-2243.412959
6ah-PhNCO2-008	-2246.274431	+6.25	-2246.794425	-2242.941229	+4.79	-2243.411660
6ah-PhNCO2-007	-2246.275449	+3.58	-2246.795316	-2242.941277	+4.66	-2243.410564
6ah-PhNCO2-006	-2246.275955	+2.25	-2246.796331	-2242.941475	+4.14	-2243.414420
6ah-PhNCO2-005	-2246.274555	+5.93	-2246.794299	-2242.941506	+4.06	-2243.412517
6ah-PhNCO2-004	-2246.274928	+4.95	-2246.795236	-2242.941602	+3.81	-2243.413247
6ah-PhNCO2-003	-2246.276812	+0.00	-2246.797100	-2242.942768	+0.75	-2243.417327
6ah-PhNCO2-002	-2246.276164	+1.70	-2246.796606	-2242.942792	+0.68	-2243.418863
6ah-PhNCO2-001	-2246.276751	+0.16	-2246.796816	-2242.943052	+0.00	-2243.417962

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
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6ah-PhNCO-126	-2246.285877	+17.76	-2246.807125
6ah-PhNCO-125	-2246.286576	+15.92	-2246.807587
6ah-PhNCO-124	-2246.286625	+15.79	-2246.807966
6ah-PhNCO-123	-2246.286690	+15.62	-2246.807572
6ah-PhNCO-122	-2246.286713	+15.56	-2246.807558
6ah-PhNCO-121	-2246.287072	+14.62	-2246.808114
6ah-PhNCO-120	-2246.287207	+14.26	-2246.808483
6ah-PhNCO-119	-2246.287351	+13.89	-2246.808197
6ah-PhNCO-118	-2246.287467	+13.58	-2246.808575
6ah-PhNCO-117	-2246.287476	+13.56	-2246.808650
6ah-PhNCO-116	-2246.287516	+13.45	-2246.808462
6ah-PhNCO-115	-2246.287574	+13.30	-2246.808731
6ah-PhNCO-114	-2246.287574	+13.30	-2246.808465
6ah-PhNCO-113	-2246.287645	+13.11	-2246.808797
6ah-PhNCO-112	-2246.287888	+12.48	-2246.809407
6ah-PhNCO-111	-2246.287904	+12.43	-2246.809087
6ah-PhNCO-110	-2246.287905	+12.43	-2246.809053
6ah-PhNCO-109	-2246.287941	+12.34	-2246.808972
6ah-PhNCO-108	-2246.288081	+11.97	-2246.808707
6ah-PhNCO-107	-2246.288125	+11.85	-2246.809028
6ah-PhNCO-106	-2246.288135	+11.83	-2246.809253
6ah-PhNCO-105	-2246.288188	+11.69	-2246.808882
6ah-PhNCO-104	-2246.288231	+11.58	-2246.809436
6ah-PhNCO-103	-2246.288317	+11.35	-2246.809334
6ah-PhNCO-102	-2246.288326	+11.33	-2246.809190
6ah-PhNCO-101	-2246.288336	+11.30	-2246.809206
6ah-PhNCO-100	-2246.288413	+11.10	-2246.808958
6ah-PhNCO-099	-2246.288457	+10.98	-2246.809123
6ah-PhNCO-098	-2246.288487	+10.90	-2246.809195
6ah-PhNCO-097	-2246.288766	+10.17	-2246.809783
6ah-PhNCO-096	-2246.288776	+10.14	-2246.810075
6ah-PhNCO-095	-2246.288810	+10.06	-2246.809817
6ah-PhNCO-094	-2246.289030	+9.48	-2246.809868
6ah-PhNCO-093	-2246.289109	+9.27	-2246.810434
6ah-PhNCO-092	-2246.289109	+9.27	-2246.809658
6ah-PhNCO-091	-2246.289242	+8.92	-2246.810790
6ah-PhNCO-090	-2246.289276	+8.83	-2246.810139
6ah-PhNCO-089	-2246.289285	+8.81	-2246.810964
6ah-PhNCO-088	-2246.289345	+8.65	-2246.809973
6ah-PhNCO-087	-2246.289378	+8.56	-2246.810749
6ah-PhNCO-086	-2246.289386	+8.54	-2246.810175
6ah-PhNCO-085	-2246.289432	+8.42	-2246.810409
6ah-PhNCO-084	-2246.289490	+8.27	-2246.810514
6ah-PhNCO-083	-2246.289532	+8.16	-2246.810172
6ah-PhNCO-082	-2246.289540	+8.14	-2246.810584
6ah-PhNCO-081	-2246.289552	+8.11	-2246.809870

6ah-PhNCO-080	-2246.289605	+7.97	-2246.810562
6ah-PhNCO-079	-2246.289608	+7.96	-2246.810077
6ah-PhNCO-078	-2246.289623	+7.92	-2246.810108
6ah-PhNCO-077	-2246.289663	+7.82	-2246.810731
6ah-PhNCO-076	-2246.289687	+7.75	-2246.810777
6ah-PhNCO-075	-2246.289723	+7.66	-2246.810665
6ah-PhNCO-074	-2246.289795	+7.47	-2246.810959
6ah-PhNCO-073	-2246.289807	+7.44	-2246.811018
6ah-PhNCO-072	-2246.289832	+7.37	-2246.810814
6ah-PhNCO-071	-2246.289845	+7.34	-2246.810369
6ah-PhNCO-070	-2246.289846	+7.34	-2246.810816
6ah-PhNCO-069	-2246.289851	+7.32	-2246.810697
6ah-PhNCO-068	-2246.289925	+7.13	-2246.810593
6ah-PhNCO-067	-2246.289957	+7.04	-2246.811383
6ah-PhNCO-066	-2246.289966	+7.02	-2246.810809
6ah-PhNCO-065	-2246.289975	+7.00	-2246.811211
6ah-PhNCO-064	-2246.290004	+6.92	-2246.811225
6ah-PhNCO-063	-2246.290023	+6.87	-2246.810568
6ah-PhNCO-062	-2246.290035	+6.84	-2246.810930
6ah-PhNCO-061	-2246.290057	+6.78	-2246.810811
6ah-PhNCO-060	-2246.290061	+6.77	-2246.810862
6ah-PhNCO-059	-2246.290080	+6.72	-2246.810801
6ah-PhNCO-058	-2246.290110	+6.64	-2246.811192
6ah-PhNCO-057	-2246.290117	+6.62	-2246.811299
6ah-PhNCO-056	-2246.290133	+6.58	-2246.811230
6ah-PhNCO-055	-2246.290140	+6.56	-2246.810936
6ah-PhNCO-054	-2246.290181	+6.46	-2246.811328
6ah-PhNCO-053	-2246.290197	+6.41	-2246.811550
6ah-PhNCO-052	-2246.290215	+6.37	-2246.811559
6ah-PhNCO-051	-2246.290226	+6.34	-2246.811313
6ah-PhNCO-050	-2246.290243	+6.29	-2246.811095
6ah-PhNCO-049	-2246.290248	+6.28	-2246.811198
6ah-PhNCO-048	-2246.290262	+6.24	-2246.811157
6ah-PhNCO-047	-2246.290409	+5.86	-2246.811141
6ah-PhNCO-046	-2246.290434	+5.79	-2246.811940
6ah-PhNCO-045	-2246.290510	+5.59	-2246.811739
6ah-PhNCO-044	-2246.290513	+5.58	-2246.810805
6ah-PhNCO-043	-2246.290524	+5.56	-2246.811138
6ah-PhNCO-042	-2246.290541	+5.51	-2246.811357
6ah-PhNCO-041	-2246.290553	+5.48	-2246.811492
6ah-PhNCO-040	-2246.290568	+5.44	-2246.811626
6ah-PhNCO-039	-2246.290595	+5.37	-2246.811345
6ah-PhNCO-038	-2246.290606	+5.34	-2246.811245
6ah-PhNCO-037	-2246.290607	+5.34	-2246.811973
6ah-PhNCO-036	-2246.290608	+5.34	-2246.811753
6ah-PhNCO-035	-2246.290647	+5.23	-2246.811658
6ah-PhNCO-034	-2246.290673	+5.16	-2246.811242

6ah-PhNCO-033	-2246.290685	+5.13	-2246.811790
6ah-PhNCO-032	-2246.290698	+5.10	-2246.811801
6ah-PhNCO-031	-2246.290718	+5.05	-2246.811703
6ah-PhNCO-030	-2246.290728	+5.02	-2246.811456
6ah-PhNCO-029	-2246.290744	+4.98	-2246.811414
6ah-PhNCO-028	-2246.290856	+4.68	-2246.812009
6ah-PhNCO-027	-2246.290869	+4.65	-2246.812289
6ah-PhNCO-026	-2246.290884	+4.61	-2246.811950
6ah-PhNCO-025	-2246.290886	+4.61	-2246.811880
6ah-PhNCO-024	-2246.290940	+4.46	-2246.811689
6ah-PhNCO-023	-2246.290963	+4.40	-2246.811780
6ah-PhNCO-022	-2246.290985	+4.35	-2246.811603
6ah-PhNCO-021	-2246.291015	+4.27	-2246.812014

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6ah-PhNCO-020	-2246.291136	+3.95	-2246.811967	-2242.954757	+4.96	-2243.422272
6ah-PhNCO-019	-2246.291064	+4.14	-2246.812074	-2242.955120	+4.01	-2243.421114
6ah-PhNCO-018	-2246.291221	+3.73	-2246.811895	-2242.955126	+3.99	-2243.417626
6ah-PhNCO-017	-2246.291053	+4.17	-2246.811726	-2242.955233	+3.71	-2243.419863
6ah-PhNCO-016	-2246.291289	+3.55	-2246.812045	-2242.955277	+3.60	-2243.420511
6ah-PhNCO-015	-2246.291241	+3.67	-2246.812145	-2242.955355	+3.39	-2243.418501
6ah-PhNCO-014	-2246.291341	+3.41	-2246.812172	-2242.955401	+3.27	-2243.420250
6ah-PhNCO-013	-2246.291992	+1.70	-2246.812839	-2242.955402	+3.27	-2243.421276
6ah-PhNCO-012	-2246.291527	+2.92	-2246.812400	-2242.955404	+3.26	-2243.422829
6ah-PhNCO-011	-2246.291549	+2.86	-2246.812569	-2242.955547	+2.89	-2243.420466
6ah-PhNCO-010	-2246.291456	+3.11	-2246.812395	-2242.955701	+2.48	-2243.419572
6ah-PhNCO-009	-2246.291077	+4.10	-2246.811680	-2242.955719	+2.44	-2243.418997
6ah-PhNCO-008	-2246.291117	+4.00	-2246.811848	-2242.955786	+2.26	-2243.419149
6ah-PhNCO-007	-2246.291720	+2.42	-2246.812374	-2242.955940	+1.86	-2243.420427
6ah-PhNCO-006	-2246.292640	+0.00	-2246.813677	-2242.955972	+1.77	-2243.423831
6ah-PhNCO-005	-2246.292009	+1.66	-2246.812627	-2242.956058	+1.55	-2243.419323
6ah-PhNCO-004	-2246.292016	+1.64	-2246.812490	-2242.956083	+1.48	-2243.421038
6ah-PhNCO-003	-2246.292054	+1.54	-2246.812568	-2242.956086	+1.47	-2243.420989
6ah-PhNCO-002	-2246.291832	+2.12	-2246.812438	-2242.956355	+0.77	-2243.419413
6ah-PhNCO-001	-2246.292145	+1.30	-2246.812853	-2242.956647	+0.00	-2243.421062

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6a-Me2-002	-1228.439305	+3.45	-1228.602584	-1226.813734	+3.37	-1226.962686
6a-Me2-001	-1228.440619	+0.00	-1228.603784	-1226.815017	+0.00	-1226.964188

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6a-Me-001	-1228.453362	+0.00	-1228.616700	-1226.822428	+0.00	-1226.956484

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6a-PhNCO2-004	-1588.348686	+26.95	-1588.582178	-1586.082124	+23.13	-1586.248265
6a-PhNCO2-003	-1588.358949	+0.00	-1588.593173	-1586.090619	+0.83	-1586.260225
6a-PhNCO2-002	-1588.355809	+8.24	-1588.589548	-1586.090692	+0.64	-1586.258426
6a-PhNCO2-001	-1588.357859	+2.86	-1588.591873	-1586.090935	+0.00	-1586.259767
Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree			
6a-PhNCO-011	-1588.368969	+28.67	-1588.602984			
6a-PhNCO-010	-1588.369070	+28.41	-1588.603106			
6a-PhNCO-009	-1588.370158	+25.55	-1588.604452			
6a-PhNCO-008	-1588.370242	+25.33	-1588.604491			
6a-PhNCO-007	-1588.370269	+25.26	-1588.604584			
Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6a-PhNCO-006	-1588.370343	+25.06	-1588.604634	-1586.101420	+22.87	-1586.269587
6a-PhNCO-005	-1588.378436	+3.81	-1588.612952	-1586.107847	+6.00	-1586.282446
6a-PhNCO-004	-1588.378390	+3.94	-1588.612939	-1586.107864	+5.95	-1586.282534
6a-PhNCO-003	-1588.378508	+3.63	-1588.613056	-1586.108188	+5.10	-1586.282580
6a-PhNCO-002	-1588.379889	+0.00	-1588.614515	-1586.110109	+0.06	-1586.284253
6a-PhNCO-001	-1588.379837	+0.14	-1588.614343	-1586.110132	+0.00	-1586.284137
Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree			
6bc-Me2-032	-2237.527374	+20.07	-2238.133790			
6bc-Me2-031	-2237.528907	+16.04	-2238.135043			
6bc-Me2-030	-2237.528939	+15.96	-2238.135120			
6bc-Me2-029	-2237.529614	+14.19	-2238.135810			
6bc-Me2-028	-2237.530097	+12.92	-2238.135878			
6bc-Me2-027	-2237.530279	+12.44	-2238.136421			
6bc-Me2-026	-2237.530344	+12.27	-2238.135891			
6bc-Me2-025	-2237.530511	+11.83	-2238.136946			
6bc-Me2-024	-2237.530528	+11.79	-2238.136620			
6bc-Me2-023	-2237.530705	+11.32	-2238.137313			
6bc-Me2-022	-2237.530807	+11.06	-2238.137253			
Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6bc-Me2-021	-2237.527792	+18.97	-2238.134222	-2233.873463	+24.26	-2234.392819
6bc-Me2-020	-2237.528473	+17.18	-2238.134972	-2233.874929	+20.41	-2234.392120
6bc-Me2-019	-2237.529113	+15.50	-2238.135009	-2233.875291	+19.46	-2234.392961
6bc-Me2-018	-2237.528076	+18.23	-2238.134750	-2233.875624	+18.59	-2234.390201
6bc-Me2-017	-2237.530307	+12.37	-2238.136423	-2233.876163	+17.17	-2234.393593

6bc-Me2-016	-2237.529437	+14.65	-2238.135726	-2233.877530	+13.58	-2234.393773
6bc-Me2-015	-2237.530167	+12.74	-2238.136694	-2233.878429	+11.22	-2234.396664
6bc-Me2-014	-2237.531678	+8.77	-2238.137546	-2233.878627	+10.70	-2234.399876
6bc-Me2-013	-2237.531654	+8.83	-2238.137316	-2233.878680	+10.56	-2234.399433
6bc-Me2-012	-2237.531751	+8.58	-2238.137836	-2233.878718	+10.46	-2234.400373
6bc-Me2-011	-2237.531473	+9.31	-2238.137535	-2233.878899	+9.99	-2234.398782
6bc-Me2-010	-2237.531620	+8.92	-2238.137564	-2233.878982	+9.77	-2234.400670
6bc-Me2-009	-2237.531824	+8.39	-2238.137737	-2233.879084	+9.50	-2234.398976
6bc-Me2-008	-2237.531262	+9.86	-2238.137623	-2233.879188	+9.23	-2234.398157
6bc-Me2-007	-2237.532009	+7.90	-2238.137852	-2233.879625	+8.08	-2234.397708
6bc-Me2-006	-2237.531860	+8.29	-2238.137828	-2233.879626	+8.08	-2234.397353
6bc-Me2-005	-2237.532068	+7.75	-2238.138244	-2233.879794	+7.64	-2234.398717
6bc-Me2-004	-2237.532087	+7.70	-2238.137872	-2233.879982	+7.14	-2234.397630
6bc-Me2-003	-2237.531941	+8.08	-2238.137853	-2233.880660	+5.36	-2234.398387
6bc-Me2-002	-2237.534993	+0.07	-2238.140952	-2233.882549	+0.40	-2234.403825
6bc-Me2-001	-2237.535018	+0.00	-2238.140970	-2233.882703	+0.00	-2234.403916

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
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6bc-Me-068	-2237.523241	+37.90	-2238.129465
6bc-Me-067	-2237.524461	+34.69	-2238.131084
6bc-Me-066	-2237.524788	+33.83	-2238.130900
6bc-Me-065	-2237.524862	+33.64	-2238.130916
6bc-Me-064	-2237.525543	+31.85	-2238.131456
6bc-Me-063	-2237.525590	+31.73	-2238.131790
6bc-Me-062	-2237.528081	+25.19	-2238.134070
6bc-Me-061	-2237.528331	+24.53	-2238.134470
6bc-Me-060	-2237.528479	+24.14	-2238.135656
6bc-Me-059	-2237.529556	+21.32	-2238.135919
6bc-Me-058	-2237.531022	+17.47	-2238.137120
6bc-Me-057	-2237.531547	+16.09	-2238.137605
6bc-Me-056	-2237.531796	+15.44	-2238.138086
6bc-Me-055	-2237.531977	+14.96	-2238.138382
6bc-Me-054	-2237.532094	+14.65	-2238.137736
6bc-Me-053	-2237.532139	+14.53	-2238.138229
6bc-Me-052	-2237.532601	+13.32	-2238.138687
6bc-Me-051	-2237.533069	+12.09	-2238.139311
6bc-Me-050	-2237.533419	+11.17	-2238.139407
6bc-Me-049	-2237.533422	+11.17	-2238.139361
6bc-Me-048	-2237.533437	+11.13	-2238.139530
6bc-Me-047	-2237.533687	+10.47	-2238.139457
6bc-Me-046	-2237.533805	+10.16	-2238.140410
6bc-Me-045	-2237.533837	+10.08	-2238.140419
6bc-Me-044	-2237.533949	+9.78	-2238.140417
6bc-Me-043	-2237.534027	+9.58	-2238.140191
6bc-Me-042	-2237.534153	+9.25	-2238.140438
6bc-Me-041	-2237.534355	+8.72	-2238.140887

6bc-Me-040	-2237.534483	+8.38	-2238.140608
6bc-Me-039	-2237.534588	+8.10	-2238.140529
6bc-Me-038	-2237.534609	+8.05	-2238.140545
6bc-Me-037	-2237.534614	+8.04	-2238.140425
6bc-Me-036	-2237.534697	+7.82	-2238.141042
6bc-Me-035	-2237.534963	+7.12	-2238.141032
6bc-Me-034	-2237.535028	+6.95	-2238.140996
6bc-Me-033	-2237.535038	+6.92	-2238.141431
6bc-Me-032	-2237.535049	+6.89	-2238.141232
6bc-Me-031	-2237.535068	+6.84	-2238.141600
6bc-Me-030	-2237.535125	+6.70	-2238.141330
6bc-Me-029	-2237.535145	+6.64	-2238.141585
6bc-Me-028	-2237.535194	+6.51	-2238.141125
6bc-Me-027	-2237.535211	+6.47	-2238.141284
6bc-Me-026	-2237.535263	+6.33	-2238.141087
6bc-Me-025	-2237.535312	+6.20	-2238.141743
6bc-Me-024	-2237.535335	+6.14	-2238.141739
6bc-Me-023	-2237.535353	+6.10	-2238.141674
6bc-Me-022	-2237.535376	+6.04	-2238.141518
6bc-Me-021	-2237.535473	+5.78	-2238.141481
6bc-Me-020	-2237.535475	+5.78	-2238.141248
6bc-Me-019	-2237.535673	+5.26	-2238.141130
6bc-Me-018	-2237.535720	+5.13	-2238.142119
6bc-Me-017	-2237.535763	+5.02	-2238.142090
6bc-Me-016	-2237.535825	+4.86	-2238.141917
6bc-Me-015	-2237.535867	+4.75	-2238.141970
6bc-Me-014	-2237.535871	+4.74	-2238.141759
6bc-Me-013	-2237.535961	+4.50	-2238.142184

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6bc-Me-012	-2237.536063	+4.23	-2238.142324	-2233.879233	+8.19	-2234.393263
6bc-Me-011	-2237.536041	+4.29	-2238.142118	-2233.879250	+8.15	-2234.392839
6bc-Me-010	-2237.536384	+3.39	-2238.141945	-2233.879527	+7.42	-2234.393995
6bc-Me-009	-2237.536726	+2.49	-2238.142672	-2233.879613	+7.20	-2234.390022
6bc-Me-008	-2237.536547	+2.96	-2238.142315	-2233.879827	+6.63	-2234.396891
6bc-Me-007	-2237.536745	+2.44	-2238.142602	-2233.879861	+6.55	-2234.390129
6bc-Me-006	-2237.536716	+2.52	-2238.142447	-2233.880206	+5.64	-2234.397280
6bc-Me-005	-2237.536931	+1.95	-2238.143018	-2233.880540	+4.76	-2234.397161
6bc-Me-004	-2237.536882	+2.08	-2238.143142	-2233.880704	+4.33	-2234.397543
6bc-Me-003	-2237.537454	+0.58	-2238.143235	-2233.881546	+2.12	-2234.394192
6bc-Me-002	-2237.537662	+0.03	-2238.143210	-2233.882328	+0.07	-2234.398077
6bc-Me-001	-2237.537675	+0.00	-2238.143271	-2233.882354	+0.00	-2234.398132

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
6bc-PhNCO2-033	-2597.456582	+31.44	-2598.133052

6bc-PhNCO2-032	-2597.457613	+28.73	-2598.134824
6bc-PhNCO2-031	-2597.458557	+26.25	-2598.135576
6bc-PhNCO2-030	-2597.460225	+21.88	-2598.136675
6bc-PhNCO2-029	-2597.460807	+20.35	-2598.137580
6bc-PhNCO2-028	-2597.461228	+19.24	-2598.138169
6bc-PhNCO2-027	-2597.461567	+18.35	-2598.138578
6bc-PhNCO2-026	-2597.461578	+18.32	-2598.138582
6bc-PhNCO2-025	-2597.461705	+17.99	-2598.138547
6bc-PhNCO2-024	-2597.461714	+17.97	-2598.138234
6bc-PhNCO2-023	-2597.461714	+17.97	-2598.138449
6bc-PhNCO2-022	-2597.461849	+17.61	-2598.138616
6bc-PhNCO2-021	-2597.462447	+16.04	-2598.138847
6bc-PhNCO2-020	-2597.462526	+15.83	-2598.138938
6bc-PhNCO2-019	-2597.462617	+15.60	-2598.139553
6bc-PhNCO2-018	-2597.463081	+14.38	-2598.140108
6bc-PhNCO2-017	-2597.463108	+14.31	-2598.139636
6bc-PhNCO2-016	-2597.463139	+14.22	-2598.140244
6bc-PhNCO2-015	-2597.463266	+13.89	-2598.139816
6bc-PhNCO2-014	-2597.463324	+13.74	-2598.139832
6bc-PhNCO2-013	-2597.463394	+13.56	-2598.139845

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6bc-PhNCO2-012	-2597.464294	+11.19	-2598.141206	-2593.173423	+11.05	-2593.786493
6bc-PhNCO2-011	-2597.464070	+11.78	-2598.140614	-2593.173476	+10.91	-2593.781810
6bc-PhNCO2-010	-2597.464247	+11.32	-2598.141405	-2593.173785	+10.10	-2593.785219
6bc-PhNCO2-009	-2597.464428	+10.84	-2598.141355	-2593.173885	+9.84	-2593.785202
6bc-PhNCO2-008	-2597.464599	+10.39	-2598.141636	-2593.174150	+9.14	-2593.785340
6bc-PhNCO2-007	-2597.465292	+8.57	-2598.142695	-2593.174461	+8.33	-2593.784867
6bc-PhNCO2-006	-2597.464355	+11.03	-2598.141150	-2593.175054	+6.77	-2593.782144
6bc-PhNCO2-005	-2597.464182	+11.49	-2598.141471	-2593.175087	+6.68	-2593.781393
6bc-PhNCO2-004	-2597.464690	+10.15	-2598.141603	-2593.175562	+5.43	-2593.786850
6bc-PhNCO2-003	-2597.468370	+0.49	-2598.144913	-2593.177386	+0.65	-2593.790269
6bc-PhNCO2-002	-2597.468557	+0.00	-2598.144986	-2593.177455	+0.46	-2593.790524
6bc-PhNCO2-001	-2597.468487	+0.18	-2598.144961	-2593.177632	+0.00	-2593.790599

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
6bc-PhNCO-049	-2597.457408	+57.48	-2598.134824
6bc-PhNCO-048	-2597.463740	+40.86	-2598.140759
6bc-PhNCO-047	-2597.469547	+25.61	-2598.147113
6bc-PhNCO-046	-2597.472002	+19.16	-2598.149630
6bc-PhNCO-045	-2597.472526	+17.79	-2598.149792
6bc-PhNCO-044	-2597.474231	+13.31	-2598.151728
6bc-PhNCO-043	-2597.474456	+12.72	-2598.151780
6bc-PhNCO-042	-2597.474518	+12.56	-2598.152020
6bc-PhNCO-041	-2597.474536	+12.51	-2598.151917

6bc-PhNCO-040	-2597.474552	+12.47	-2598.151937
6bc-PhNCO-039	-2597.474584	+12.38	-2598.151893
6bc-PhNCO-038	-2597.474607	+12.32	-2598.151523
6bc-PhNCO-037	-2597.474648	+12.22	-2598.151918
6bc-PhNCO-036	-2597.474698	+12.09	-2598.152068
6bc-PhNCO-035	-2597.474807	+11.80	-2598.152075
6bc-PhNCO-034	-2597.474830	+11.74	-2598.152128
6bc-PhNCO-033	-2597.474990	+11.32	-2598.152056
6bc-PhNCO-032	-2597.475004	+11.28	-2598.151868
6bc-PhNCO-031	-2597.475038	+11.19	-2598.152063
6bc-PhNCO-030	-2597.475112	+11.00	-2598.152083
6bc-PhNCO-029	-2597.475208	+10.75	-2598.152483
6bc-PhNCO-028	-2597.475234	+10.68	-2598.152616
6bc-PhNCO-027	-2597.475243	+10.65	-2598.152129
6bc-PhNCO-026	-2597.475562	+9.82	-2598.152317
6bc-PhNCO-025	-2597.475632	+9.63	-2598.152587
6bc-PhNCO-024	-2597.475738	+9.35	-2598.152983
6bc-PhNCO-023	-2597.476085	+8.44	-2598.153652
6bc-PhNCO-022	-2597.476123	+8.34	-2598.153470

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6bc-PhNCO-021	-2597.464320	+39.33	-2598.141709	-2593.169353	+45.14	-2593.762534
6bc-PhNCO-020	-2597.470397	+23.38	-2598.147567	-2593.177392	+24.03	-2593.777797
6bc-PhNCO-019	-2597.472913	+16.77	-2598.150092	-2593.178231	+21.83	-2593.784664
6bc-PhNCO-018	-2597.473275	+15.82	-2598.150211	-2593.178604	+20.85	-2593.785181
6bc-PhNCO-017	-2597.472729	+17.25	-2598.149840	-2593.179144	+19.43	-2593.785001
6bc-PhNCO-016	-2597.473379	+15.55	-2598.150559	-2593.179777	+17.77	-2593.786310
6bc-PhNCO-015	-2597.474572	+12.42	-2598.151947	-2593.180164	+16.76	-2593.787081
6bc-PhNCO-014	-2597.474686	+12.12	-2598.152065	-2593.181422	+13.45	-2593.788872
6bc-PhNCO-013	-2597.473614	+14.93	-2598.150544	-2593.181645	+12.87	-2593.783056
6bc-PhNCO-012	-2597.477672	+4.28	-2598.154550	-2593.184237	+6.06	-2593.794372
6bc-PhNCO-011	-2597.477741	+4.10	-2598.154546	-2593.184340	+5.79	-2593.794295
6bc-PhNCO-010	-2597.476584	+7.13	-2598.154390	-2593.184349	+5.77	-2593.786838
6bc-PhNCO-009	-2597.476491	+7.38	-2598.153922	-2593.184546	+5.25	-2593.792159
6bc-PhNCO-008	-2597.477241	+5.41	-2598.154598	-2593.184673	+4.92	-2593.787500
6bc-PhNCO-007	-2597.477754	+4.06	-2598.155000	-2593.184750	+4.72	-2593.789499
6bc-PhNCO-006	-2597.477157	+5.63	-2598.154393	-2593.184789	+4.61	-2593.791187
6bc-PhNCO-005	-2597.477195	+5.53	-2598.154458	-2593.184804	+4.57	-2593.788638
6bc-PhNCO-004	-2597.477284	+5.30	-2598.154616	-2593.184858	+4.43	-2593.787537
6bc-PhNCO-003	-2597.477263	+5.35	-2598.154531	-2593.184883	+4.37	-2593.786854
6bc-PhNCO-002	-2597.477190	+5.54	-2598.154589	-2593.184917	+4.28	-2593.786779
6bc-PhNCO-001	-2597.479301	+0.00	-2598.156824	-2593.186546	+0.00	-2593.790060

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
6bc-064	-2197.786207	+39.56	-2198.348805

6bc-063	-2197.786327	+39.24	-2198.348742
6bc-062	-2197.788378	+33.86	-2198.351057
6bc-061	-2197.789987	+29.63	-2198.352063
6bc-060	-2197.790005	+29.59	-2198.351950
6bc-059	-2197.790544	+28.17	-2198.352450
6bc-058	-2197.790707	+27.74	-2198.352963
6bc-057	-2197.791173	+26.52	-2198.353233
6bc-056	-2197.791493	+25.68	-2198.353654
6bc-055	-2197.791565	+25.49	-2198.354113
6bc-054	-2197.792556	+22.89	-2198.354654
6bc-053	-2197.792843	+22.14	-2198.354957
6bc-052	-2197.794228	+18.50	-2198.356641
6bc-051	-2197.794379	+18.10	-2198.356606
6bc-050	-2197.794402	+18.04	-2198.356601
6bc-049	-2197.794417	+18.00	-2198.356980
6bc-048	-2197.794521	+17.73	-2198.356406
6bc-047	-2197.795108	+16.19	-2198.357448
6bc-046	-2197.795628	+14.82	-2198.358123
6bc-045	-2197.795812	+14.34	-2198.358170
6bc-044	-2197.796472	+12.61	-2198.358827
6bc-043	-2197.796552	+12.40	-2198.359159
6bc-042	-2197.796978	+11.28	-2198.359097
6bc-041	-2197.797249	+10.57	-2198.359420
6bc-040	-2197.797270	+10.51	-2198.359328
6bc-039	-2197.797340	+10.33	-2198.359475
6bc-038	-2197.797446	+10.05	-2198.359520
6bc-037	-2197.797655	+9.50	-2198.359475
6bc-036	-2197.797739	+9.28	-2198.359462
6bc-035	-2197.797845	+9.00	-2198.360161
6bc-034	-2197.797870	+8.94	-2198.360256
6bc-033	-2197.797887	+8.89	-2198.359865
6bc-032	-2197.797932	+8.77	-2198.359908
6bc-031	-2197.798223	+8.01	-2198.360257
6bc-030	-2197.798441	+7.44	-2198.360575
6bc-029	-2197.798666	+6.85	-2198.360586
6bc-028	-2197.798684	+6.80	-2198.360585
6bc-027	-2197.798812	+6.46	-2198.360901
6bc-026	-2197.798895	+6.25	-2198.360824
6bc-025	-2197.799023	+5.91	-2198.361042
6bc-024	-2197.799288	+5.21	-2198.361254
6bc-023	-2197.799342	+5.07	-2198.361832
6bc-022	-2197.799363	+5.02	-2198.361464
6bc-021	-2197.799418	+4.87	-2198.361474
6bc-020	-2197.799447	+4.80	-2198.361665
6bc-019	-2197.799599	+4.40	-2198.361683
6bc-018	-2197.799622	+4.34	-2198.361819
6bc-017	-2197.799655	+4.25	-2198.361981

6bc-016	-2197.799801	+3.87	-2198.362166
6bc-015	-2197.799833	+3.78	-2198.361778
6bc-014	-2197.799883	+3.65	-2198.361921
6bc-013	-2197.799899	+3.61	-2198.362315

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6bc-012	-2197.801254	+0.05	-2198.363329	-2194.220632	+8.11	-2194.720117
6bc-011	-2197.800734	+1.42	-2198.362922	-2194.220633	+8.11	-2194.721645
6bc-010	-2197.800044	+3.23	-2198.361947	-2194.220872	+7.48	-2194.722723
6bc-009	-2197.801274	+0.00	-2198.363182	-2194.221148	+6.76	-2194.720399
6bc-008	-2197.800646	+1.65	-2198.363254	-2194.221326	+6.29	-2194.720246
6bc-007	-2197.800471	+2.11	-2198.362530	-2194.221541	+5.72	-2194.720531
6bc-006	-2197.800551	+1.90	-2198.362541	-2194.221570	+5.65	-2194.719717
6bc-005	-2197.800640	+1.66	-2198.362649	-2194.221731	+5.22	-2194.721602
6bc-004	-2197.799930	+3.53	-2198.361951	-2194.222651	+2.81	-2194.722926
6bc-003	-2197.800641	+1.66	-2198.362519	-2194.222726	+2.61	-2194.723242
6bc-002	-2197.801097	+0.46	-2198.363536	-2194.222996	+1.90	-2194.719771
6bc-001	-2197.801258	+0.04	-2198.363480	-2194.223721	+0.00	-2194.730857

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6b-Me2-003	-1161.695475	+10.14	-1161.965524	-1159.924792	+12.56	-1160.170543
6b-Me2-002	-1161.699337	+0.00	-1161.969786	-1159.929551	+0.06	-1160.176041
6b-Me2-001	-1161.699311	+0.07	-1161.969760	-1159.929575	+0.00	-1160.176083

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6b-Me-003	-1161.700049	+0.16	-1161.970467	-1159.925395	+4.42	-1160.160618
6b-Me-002	-1161.700056	+0.14	-1161.970433	-1159.925433	+4.32	-1160.160625
6b-Me-001	-1161.700109	+0.00	-1161.970457	-1159.927079	+0.00	-1160.159289

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
6b-PhNCO2-006	-1521.603386	+18.44	-1521.944168

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6b-PhNCO2-005	-1521.604275	+16.11	-1521.945245	-1519.194842	+14.70	-1519.455527
6b-PhNCO2-004	-1521.604404	+15.77	-1521.945246	-1519.195366	+13.32	-1519.453916
6b-PhNCO2-003	-1521.607866	+6.68	-1521.949030	-1519.199344	+2.88	-1519.461704
6b-PhNCO2-002	-1521.610411	+0.00	-1521.951600	-1519.199910	+1.39	-1519.463732
6b-PhNCO2-001	-1521.610334	+0.20	-1521.951407	-1519.200441	+0.00	-1519.464158

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
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6b-PhNCO-012	-1521.613520	+29.09	-1521.954939
6b-PhNCO-011	-1521.614771	+25.81	-1521.956266
6b-PhNCO-010	-1521.614784	+25.77	-1521.956282
6b-PhNCO-009	-1521.615006	+25.19	-1521.956359
6b-PhNCO-008	-1521.615046	+25.09	-1521.956380
6b-PhNCO-007	-1521.615121	+24.89	-1521.956727

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6b-PhNCO-006	-1521.617107	+19.68	-1521.958558	-1519.205486	+17.51	-1519.467576
6b-PhNCO-005	-1521.623102	+3.94	-1521.964938	-1519.208918	+8.50	-1519.477063
6b-PhNCO-004	-1521.623205	+3.67	-1521.964960	-1519.209015	+8.24	-1519.477055
6b-PhNCO-003	-1521.624542	+0.15	-1521.966188	-1519.211930	+0.59	-1519.479265
6b-PhNCO-002	-1521.624572	+0.08	-1521.966175	-1519.211970	+0.48	-1519.479328
6b-PhNCO-001	-1521.624601	+0.00	-1521.966338	-1519.212154	+0.00	-1519.479488

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6b-002	-1121.948210	+5.62	-1122.174923	-1120.249087	+11.09	-1120.401708
6b-001	-1121.950352	+0.00	-1122.177274	-1120.253312	+0.00	-1120.406034

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
6cg-Me2-029	-2504.431113	+11.12	-2505.099675
6cg-Me2-028	-2504.431152	+11.02	-2505.099591
6cg-Me2-027	-2504.431482	+10.15	-2505.100443
6cg-Me2-026	-2504.431512	+10.07	-2505.100490
6cg-Me2-025	-2504.431712	+9.55	-2505.100648
6cg-Me2-024	-2504.431927	+8.98	-2505.100189
6cg-Me2-023	-2504.431933	+8.97	-2505.100592
6cg-Me2-022	-2504.431967	+8.88	-2505.100653
6cg-Me2-021	-2504.432137	+8.43	-2505.100514
6cg-Me2-020	-2504.432147	+8.40	-2505.100663
6cg-Me2-019	-2504.432276	+8.07	-2505.101249
6cg-Me2-018	-2504.432464	+7.57	-2505.101234
6cg-Me2-017	-2504.432595	+7.23	-2505.101335
6cg-Me2-016	-2504.433020	+6.11	-2505.101697
6cg-Me2-015	-2504.433124	+5.84	-2505.101973
6cg-Me2-014	-2504.433341	+5.27	-2505.101757

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6cg-Me2-013	-2504.434494	+2.24	-2505.102870	-2500.308515	+6.45	-2500.891399
6cg-Me2-012	-2504.434061	+3.38	-2505.102594	-2500.308650	+6.09	-2500.889675
6cg-Me2-011	-2504.434659	+1.81	-2505.102945	-2500.308817	+5.66	-2500.891771

6cg-Me2-010	-2504.434062	+3.38	-2505.102931	-2500.309238	+4.55	-2500.891996
6cg-Me2-009	-2504.433870	+3.88	-2505.102134	-2500.309518	+3.81	-2500.889366
6cg-Me2-008	-2504.433665	+4.42	-2505.102136	-2500.309525	+3.80	-2500.889417
6cg-Me2-007	-2504.434291	+2.78	-2505.102887	-2500.309693	+3.36	-2500.891825
6cg-Me2-006	-2504.435348	+0.00	-2505.103967	-2500.309726	+3.27	-2500.892800
6cg-Me2-005	-2504.434507	+2.21	-2505.102774	-2500.309733	+3.25	-2500.891625
6cg-Me2-004	-2504.433680	+4.38	-2505.102320	-2500.309752	+3.20	-2500.890209
6cg-Me2-003	-2504.435206	+0.37	-2505.104005	-2500.309781	+3.12	-2500.892815
6cg-Me2-002	-2504.434671	+1.78	-2505.103542	-2500.310638	+0.87	-2500.891178
6cg-Me2-001	-2504.435012	+0.88	-2505.103661	-2500.310971	+0.00	-2500.891321

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
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6cg-Me-030	-2504.433951	+8.03	-2505.103531
6cg-Me-029	-2504.434191	+7.40	-2505.102494
6cg-Me-028	-2504.434231	+7.30	-2505.103156
6cg-Me-027	-2504.434395	+6.87	-2505.103098
6cg-Me-026	-2504.434543	+6.48	-2505.103171
6cg-Me-025	-2504.434565	+6.42	-2505.102965
6cg-Me-024	-2504.434697	+6.07	-2505.103022
6cg-Me-023	-2504.434725	+6.00	-2505.102967
6cg-Me-022	-2504.434891	+5.56	-2505.103921
6cg-Me-021	-2504.434931	+5.46	-2505.103520
6cg-Me-020	-2504.434950	+5.41	-2505.104079
6cg-Me-019	-2504.435014	+5.24	-2505.103728
6cg-Me-018	-2504.435190	+4.78	-2505.104470
6cg-Me-017	-2504.435203	+4.74	-2505.103510
6cg-Me-016	-2504.435247	+4.63	-2505.103827
6cg-Me-015	-2504.435252	+4.62	-2505.104440
6cg-Me-014	-2504.435271	+4.57	-2505.104457

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
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6cg-Me-013	-2504.435546	+3.84	-2505.104169	-2500.305556	+9.13	-2500.877462
6cg-Me-012	-2504.435405	+4.21	-2505.103888	-2500.305621	+8.96	-2500.881642
6cg-Me-011	-2504.435714	+3.40	-2505.104061	-2500.305845	+8.37	-2500.877082
6cg-Me-010	-2504.436414	+1.56	-2505.105631	-2500.306659	+6.23	-2500.879546
6cg-Me-009	-2504.436787	+0.59	-2505.105689	-2500.306705	+6.11	-2500.879713
6cg-Me-008	-2504.437010	+0.00	-2505.105323	-2500.307011	+5.31	-2500.881710
6cg-Me-007	-2504.435262	+4.59	-2505.104197	-2500.307369	+4.37	-2500.882757
6cg-Me-006	-2504.435476	+4.03	-2505.104209	-2500.307685	+3.54	-2500.883084
6cg-Me-005	-2504.435630	+3.62	-2505.104710	-2500.307948	+2.85	-2500.873535
6cg-Me-004	-2504.436141	+2.28	-2505.104509	-2500.308369	+1.74	-2500.882663
6cg-Me-003	-2504.435850	+3.05	-2505.104762	-2500.308584	+1.18	-2500.873236
6cg-Me-002	-2504.436243	+2.01	-2505.104986	-2500.308597	+1.14	-2500.882114
6cg-Me-001	-2504.435971	+2.73	-2505.105275	-2500.309033	+0.00	-2500.877225

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
6cg-031	-2464.692230	+21.24	-2465.316886
6cg-030	-2464.695073	+13.78	-2465.319762
6cg-029	-2464.696153	+10.94	-2465.320930
6cg-028	-2464.696852	+9.11	-2465.321936
6cg-027	-2464.697045	+8.60	-2465.321716
6cg-026	-2464.697127	+8.38	-2465.321762
6cg-025	-2464.697197	+8.20	-2465.321877
6cg-024	-2464.697303	+7.92	-2465.321800
6cg-023	-2464.697600	+7.14	-2465.322709
6cg-022	-2464.697629	+7.07	-2465.322308
6cg-021	-2464.697682	+6.93	-2465.322448
6cg-020	-2464.697825	+6.55	-2465.322529
6cg-019	-2464.697897	+6.36	-2465.322483
6cg-018	-2464.698030	+6.01	-2465.322798
6cg-017	-2464.698041	+5.98	-2465.322810
6cg-016	-2464.698056	+5.94	-2465.322657
6cg-015	-2464.698237	+5.47	-2465.323278
6cg-014	-2464.698557	+4.63	-2465.323872
6cg-013	-2464.698577	+4.58	-2465.323290

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6cg-012	-2464.698756	+4.11	-2465.323507	-2460.648034	+6.53	-2461.208119
6cg-011	-2464.699027	+3.39	-2465.323686	-2460.648036	+6.52	-2461.206428
6cg-010	-2464.698590	+4.54	-2465.323401	-2460.648144	+6.24	-2461.211209
6cg-009	-2464.699267	+2.76	-2465.324142	-2460.648196	+6.10	-2461.205062
6cg-008	-2464.698904	+3.72	-2465.323500	-2460.648323	+5.77	-2461.208642
6cg-007	-2464.698602	+4.51	-2465.323151	-2460.648492	+5.32	-2461.212032
6cg-006	-2464.699018	+3.42	-2465.323716	-2460.648527	+5.23	-2461.207068
6cg-005	-2464.699043	+3.35	-2465.323649	-2460.648692	+4.80	-2461.207238
6cg-004	-2464.699133	+3.12	-2465.323761	-2460.648701	+4.78	-2461.209375
6cg-003	-2464.698966	+3.55	-2465.324040	-2460.649512	+2.65	-2461.206798
6cg-002	-2464.700214	+0.28	-2465.325314	-2460.650518	+0.01	-2461.206242
6cg-001	-2464.700320	+0.00	-2465.325436	-2460.650520	+0.00	-2461.205993

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
6cg-PhNCO2-026	-2864.360599	+14.32	-2865.100707
6cg-PhNCO2-025	-2864.361144	+12.89	-2865.100477
6cg-PhNCO2-024	-2864.361156	+12.86	-2865.100585
6cg-PhNCO2-023	-2864.361299	+12.48	-2865.100728
6cg-PhNCO2-022	-2864.361345	+12.36	-2865.101079
6cg-PhNCO2-021	-2864.361365	+12.31	-2865.101087
6cg-PhNCO2-020	-2864.361478	+12.01	-2865.100664
6cg-PhNCO2-019	-2864.361535	+11.86	-2865.100743

6cg-PhNCO2-018	-2864.361670	+11.51	-2865.100711
6cg-PhNCO2-017	-2864.361704	+11.42	-2865.100992
6cg-PhNCO2-016	-2864.361706	+11.41	-2865.101149
6cg-PhNCO2-015	-2864.362085	+10.42	-2865.101407
6cg-PhNCO2-014	-2864.362104	+10.37	-2865.101591
6cg-PhNCO2-013	-2864.362163	+10.21	-2865.101334

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6cg-PhNCO2-012	-2864.363113	+7.72	-2865.102186	-2859.597056	+16.05	-2860.267368
6cg-PhNCO2-011	-2864.362761	+8.64	-2865.102061	-2859.597592	+14.64	-2860.269075
6cg-PhNCO2-010	-2864.363561	+6.54	-2865.102905	-2859.598953	+11.07	-2860.274943
6cg-PhNCO2-009	-2864.362770	+8.62	-2865.102527	-2859.599259	+10.26	-2860.263361
6cg-PhNCO2-008	-2864.362721	+8.75	-2865.102029	-2859.599269	+10.24	-2860.272700
6cg-PhNCO2-007	-2864.363086	+7.79	-2865.102664	-2859.599534	+9.54	-2860.262741
6cg-PhNCO2-006	-2864.362274	+9.92	-2865.101252	-2859.600069	+8.14	-2860.264075
6cg-PhNCO2-005	-2864.363600	+6.44	-2865.102784	-2859.600586	+6.78	-2860.264279
6cg-PhNCO2-004	-2864.362955	+8.13	-2865.101451	-2859.600703	+6.47	-2860.270722
6cg-PhNCO2-003	-2864.362227	+10.05	-2865.101696	-2859.601081	+5.48	-2860.264493
6cg-PhNCO2-002	-2864.363990	+5.42	-2865.103645	-2859.602546	+1.63	-2860.268759
6cg-PhNCO2-001	-2864.366053	+0.00	-2865.105728	-2859.603168	+0.00	-2860.269136

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
6cg-PhNCO-046	-2864.367662	+32.54	-2865.107452
6cg-PhNCO-045	-2864.368046	+31.53	-2865.108251
6cg-PhNCO-044	-2864.369547	+27.59	-2865.109837
6cg-PhNCO-043	-2864.371143	+23.40	-2865.111310
6cg-PhNCO-042	-2864.371757	+21.79	-2865.111727
6cg-PhNCO-041	-2864.372121	+20.83	-2865.111786
6cg-PhNCO-040	-2864.372212	+20.59	-2865.112215
6cg-PhNCO-039	-2864.372407	+20.08	-2865.112205
6cg-PhNCO-038	-2864.372516	+19.79	-2865.112814
6cg-PhNCO-037	-2864.372763	+19.15	-2865.112543
6cg-PhNCO-036	-2864.373145	+18.14	-2865.112828
6cg-PhNCO-035	-2864.373929	+16.08	-2865.113739
6cg-PhNCO-034	-2864.373989	+15.93	-2865.113934
6cg-PhNCO-033	-2864.374018	+15.85	-2865.113842
6cg-PhNCO-032	-2864.374037	+15.80	-2865.114143
6cg-PhNCO-031	-2864.374334	+15.02	-2865.114183
6cg-PhNCO-030	-2864.374896	+13.54	-2865.115060
6cg-PhNCO-029	-2864.374956	+13.39	-2865.114667
6cg-PhNCO-028	-2864.375427	+12.15	-2865.115167
6cg-PhNCO-027	-2864.375437	+12.12	-2865.115265
6cg-PhNCO-026	-2864.375468	+12.04	-2865.115375
6cg-PhNCO-025	-2864.375519	+11.91	-2865.115347
6cg-PhNCO-024	-2864.375578	+11.75	-2865.115407

6cg-PhNCO-023	-2864.375638	+11.60	-2865.115550
6cg-PhNCO-022	-2864.375714	+11.40	-2865.115549
6cg-PhNCO-021	-2864.375762	+11.27	-2865.115580
6cg-PhNCO-020	-2864.375771	+11.25	-2865.115880
6cg-PhNCO-019	-2864.375875	+10.97	-2865.115507
6cg-PhNCO-018	-2864.375903	+10.90	-2865.115658
6cg-PhNCO-017	-2864.375910	+10.88	-2865.115666
6cg-PhNCO-016	-2864.375950	+10.78	-2865.115576
6cg-PhNCO-015	-2864.376303	+9.85	-2865.116252
6cg-PhNCO-014	-2864.376471	+9.41	-2865.116366
6cg-PhNCO-013	-2864.376660	+8.91	-2865.116423

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6cg-PhNCO-012	-2864.377039	+7.92	-2865.116942	-2859.610896	+10.09	-2860.281790
6cg-PhNCO-011	-2864.376993	+8.04	-2865.116954	-2859.611015	+9.78	-2860.281970
6cg-PhNCO-010	-2864.377722	+6.13	-2865.117593	-2859.611086	+9.59	-2860.280331
6cg-PhNCO-009	-2864.377082	+7.81	-2865.116909	-2859.611319	+8.98	-2860.281042
6cg-PhNCO-008	-2864.377175	+7.56	-2865.116924	-2859.611762	+7.82	-2860.281226
6cg-PhNCO-007	-2864.377268	+7.32	-2865.117056	-2859.612614	+5.58	-2860.276212
6cg-PhNCO-006	-2864.378784	+3.34	-2865.118861	-2859.613304	+3.77	-2860.278836
6cg-PhNCO-005	-2864.380055	+0.00	-2865.120685	-2859.613990	+1.97	-2860.278112
6cg-PhNCO-004	-2864.380028	+0.07	-2865.120133	-2859.613998	+1.95	-2860.277209
6cg-PhNCO-003	-2864.379959	+0.25	-2865.120062	-2859.614028	+1.87	-2860.277233
6cg-PhNCO-002	-2864.379668	+1.02	-2865.119881	-2859.614390	+0.92	-2860.274752
6cg-PhNCO-001	-2864.379681	+0.98	-2865.119504	-2859.614739	+0.00	-2860.277311

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6c-Me2-004	-1236.900657	+10.60	-1237.176659	-1235.033197	+12.23	-1235.284493
6c-Me2-003	-1236.901039	+9.60	-1237.176928	-1235.033366	+11.79	-1235.284723
6c-Me2-002	-1236.904689	+0.01	-1237.180899	-1235.037852	+0.01	-1235.289634
6c-Me2-001	-1236.904694	+0.00	-1237.181015	-1235.037855	+0.00	-1235.289938

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6c-Me-004	-1236.904780	+0.10	-1237.181211	-1235.033172	+4.62	-1235.274012
6c-Me-003	-1236.904755	+0.17	-1237.181260	-1235.034360	+1.50	-1235.272363
6c-Me-002	-1236.904787	+0.08	-1237.181174	-1235.034929	+0.00	-1235.272560
6c-Me-001	-1236.904819	+0.00	-1237.181224	-1235.034930	+0.00	-1235.272536

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6c-003	-1197.152648	+6.12	-1197.385457	-1195.356524	+11.46	-1195.514467

6c-002	-1197.154557	+1.11	-1197.387538	-1195.360264	+1.64	-1195.518226
6c-001	-1197.154978	+0.00	-1197.387692	-1195.360890	+0.00	-1195.518706

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
6c-PhNCO2-012	-1596.807857	+19.45	-1597.154659
6c-PhNCO2-011	-1596.808159	+18.65	-1597.155175
6c-PhNCO2-010	-1596.808343	+18.17	-1597.155178
6c-PhNCO2-009	-1596.808389	+18.05	-1597.155188

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6c-PhNCO2-008	-1596.809359	+15.50	-1597.156310	-1594.301989	+16.46	-1594.565569
6c-PhNCO2-007	-1596.809045	+16.33	-1597.156085	-1594.302685	+14.63	-1594.568502
6c-PhNCO2-006	-1596.809632	+14.79	-1597.156386	-1594.303097	+13.55	-1594.568920
6c-PhNCO2-005	-1596.812581	+7.04	-1597.159881	-1594.306847	+3.70	-1594.574707
6c-PhNCO2-004	-1596.812910	+6.18	-1597.160069	-1594.307264	+2.61	-1594.575080
6c-PhNCO2-003	-1596.815264	+0.00	-1597.162533	-1594.307795	+1.22	-1594.577544
6c-PhNCO2-002	-1596.815033	+0.61	-1597.162321	-1594.308145	+0.30	-1594.577089
6c-PhNCO2-001	-1596.815236	+0.07	-1597.162553	-1594.308258	+0.00	-1594.577475

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
6c-PhNCO-022	-1596.818108	+29.31	-1597.165491
6c-PhNCO-021	-1596.818134	+29.24	-1597.165490
6c-PhNCO-020	-1596.818255	+28.93	-1597.165656
6c-PhNCO-019	-1596.818265	+28.90	-1597.165699
6c-PhNCO-018	-1596.819474	+25.72	-1597.166915
6c-PhNCO-017	-1596.819513	+25.62	-1597.166857
6c-PhNCO-016	-1596.819568	+25.48	-1597.166817
6c-PhNCO-015	-1596.819625	+25.33	-1597.167104
6c-PhNCO-014	-1596.819699	+25.13	-1597.167224
6c-PhNCO-013	-1596.819886	+24.64	-1597.167387
6c-PhNCO-012	-1596.820091	+24.10	-1597.167474
6c-PhNCO-011	-1596.820200	+23.82	-1597.167535
6c-PhNCO-010	-1596.822184	+18.61	-1597.169736
6c-PhNCO-009	-1596.822350	+18.17	-1597.170017

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
6c-PhNCO-008	-1596.827827	+3.79	-1597.175633	-1594.316610	+8.27	-1594.589905
6c-PhNCO-007	-1596.827851	+3.73	-1597.175510	-1594.316724	+7.97	-1594.589867
6c-PhNCO-006	-1596.828915	+0.94	-1597.176818	-1594.319229	+1.40	-1594.591833
6c-PhNCO-005	-1596.828924	+0.91	-1597.176642	-1594.319316	+1.17	-1594.591695
6c-PhNCO-004	-1596.829122	+0.39	-1597.176932	-1594.319456	+0.80	-1594.592327
6c-PhNCO-003	-1596.829053	+0.57	-1597.176805	-1594.319517	+0.64	-1594.592047
6c-PhNCO-002	-1596.829033	+0.63	-1597.176843	-1594.319571	+0.50	-1594.592230

6c-PhNCO-001 -1596.829272 +0.00 -1597.176951 -1594.319761 +0.00 -1594.592363

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
8a-005	-1189.159822	+22.18	-1189.293242	-1187.614175	+9.01	-1187.733044
8a-004	-1189.159903	+21.97	-1189.293216	-1187.614344	+8.56	-1187.733053
8a-003	-1189.160022	+21.66	-1189.293312	-1187.614621	+7.84	-1187.733587
8a-002	-1189.167846	+1.11	-1189.301506	-1187.617563	+0.11	-1187.722982
8a-001	-1189.168270	+0.00	-1189.302174	-1187.617606	+0.00	-1187.722020

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
10h-Me-066	-1879.918598	+40.24	-1880.537559
10h-Me-065	-1879.923221	+28.10	-1880.542733
10h-Me-064	-1879.923682	+26.89	-1880.543334
10h-Me-063	-1879.923718	+26.80	-1880.543419
10h-Me-062	-1879.923921	+26.27	-1880.542659
10h-Me-061	-1879.924272	+25.34	-1880.543325
10h-Me-060	-1879.924725	+24.15	-1880.544200
10h-Me-059	-1879.924874	+23.76	-1880.544487
10h-Me-058	-1879.925247	+22.78	-1880.544334
10h-Me-057	-1879.925497	+22.13	-1880.544476
10h-Me-056	-1879.925850	+21.20	-1880.544815
10h-Me-055	-1879.926089	+20.57	-1880.544729
10h-Me-054	-1879.926423	+19.70	-1880.545396
10h-Me-053	-1879.926472	+19.57	-1880.545813
10h-Me-052	-1879.926923	+18.38	-1880.546278
10h-Me-051	-1879.926937	+18.35	-1880.545644
10h-Me-050	-1879.926951	+18.31	-1880.545923
10h-Me-049	-1879.927000	+18.18	-1880.545987
10h-Me-048	-1879.927003	+18.17	-1880.546028
10h-Me-047	-1879.927095	+17.93	-1880.546125
10h-Me-046	-1879.927271	+17.47	-1880.546627
10h-Me-045	-1879.927358	+17.24	-1880.546160
10h-Me-044	-1879.927390	+17.16	-1880.546107
10h-Me-043	-1879.928059	+15.40	-1880.546849
10h-Me-042	-1879.928194	+15.05	-1880.547006
10h-Me-041	-1879.928427	+14.44	-1880.547020
10h-Me-040	-1879.928516	+14.20	-1880.547326
10h-Me-039	-1879.928858	+13.30	-1880.547701
10h-Me-038	-1879.929116	+12.63	-1880.548356
10h-Me-037	-1879.929336	+12.05	-1880.548516
10h-Me-036	-1879.929431	+11.80	-1880.548570
10h-Me-035	-1879.929796	+10.84	-1880.548234
10h-Me-034	-1879.929802	+10.82	-1880.548468
10h-Me-033	-1879.929918	+10.52	-1880.548522

10h-Me-032	-1879.929947	+10.44	-1880.548600
10h-Me-031	-1879.930027	+10.23	-1880.548694
10h-Me-030	-1879.930206	+9.76	-1880.548871
10h-Me-029	-1879.930251	+9.65	-1880.549161
10h-Me-028	-1879.930447	+9.13	-1880.549393
10h-Me-027	-1879.930447	+9.13	-1880.549065
10h-Me-026	-1879.930480	+9.04	-1880.549626
10h-Me-025	-1879.930578	+8.79	-1880.549422
10h-Me-024	-1879.930743	+8.35	-1880.549764
10h-Me-023	-1879.930749	+8.34	-1880.549540
10h-Me-022	-1879.930909	+7.92	-1880.549755
10h-Me-021	-1879.931282	+6.94	-1880.550075

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
10h-Me-020	-1879.931299	+6.89	-1880.550800	-1876.798215	+5.85	-1877.331858
10h-Me-019	-1879.931808	+5.56	-1880.550629	-1876.798287	+5.66	-1877.333654
10h-Me-018	-1879.931452	+6.49	-1880.550038	-1876.798322	+5.57	-1877.331814
10h-Me-017	-1879.932860	+2.80	-1880.551069	-1876.798819	+4.26	-1877.331922
10h-Me-016	-1879.931483	+6.41	-1880.550185	-1876.798841	+4.20	-1877.331902
10h-Me-015	-1879.931472	+6.44	-1880.549626	-1876.799143	+3.41	-1877.331433
10h-Me-014	-1879.931866	+5.41	-1880.551312	-1876.799172	+3.33	-1877.332686
10h-Me-013	-1879.931949	+5.19	-1880.551220	-1876.799177	+3.32	-1877.332612
10h-Me-012	-1879.931894	+5.33	-1880.551336	-1876.799181	+3.31	-1877.332687
10h-Me-011	-1879.932413	+3.97	-1880.551402	-1876.799338	+2.90	-1877.334159
10h-Me-010	-1879.932767	+3.04	-1880.551904	-1876.799559	+2.32	-1877.332792
10h-Me-009	-1879.932952	+2.55	-1880.551570	-1876.799635	+2.12	-1877.333466
10h-Me-008	-1879.932296	+4.28	-1880.550984	-1876.799637	+2.11	-1877.333855
10h-Me-007	-1879.932906	+2.68	-1880.551116	-1876.799754	+1.81	-1877.331089
10h-Me-006	-1879.933218	+1.86	-1880.551977	-1876.799896	+1.43	-1877.332677
10h-Me-005	-1879.933733	+0.50	-1880.552829	-1876.800181	+0.69	-1877.334166
10h-Me-004	-1879.933191	+1.93	-1880.551700	-1876.800241	+0.53	-1877.332837
10h-Me-003	-1879.933824	+0.27	-1880.552786	-1876.800340	+0.27	-1877.334450
10h-Me-002	-1879.933925	+0.00	-1880.552832	-1876.800417	+0.07	-1877.334526
10h-Me-001	-1879.933350	+1.51	-1880.552313	-1876.800442	+0.00	-1877.334254

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
10h-PhNCO-034	-2239.867479	+10.22	-2240.558082
10h-PhNCO-033	-2239.867854	+9.24	-2240.557936
10h-PhNCO-032	-2239.868091	+8.61	-2240.558358
10h-PhNCO-031	-2239.868138	+8.49	-2240.558352
10h-PhNCO-030	-2239.868167	+8.41	-2240.557937
10h-PhNCO-029	-2239.868204	+8.32	-2240.558498
10h-PhNCO-028	-2239.868209	+8.30	-2240.558335
10h-PhNCO-027	-2239.868221	+8.27	-2240.558140
10h-PhNCO-026	-2239.868319	+8.02	-2240.558033

10h-PhNCO-025	-2239.868322	+8.01	-2240.558331
10h-PhNCO-024	-2239.868397	+7.81	-2240.558373
10h-PhNCO-023	-2239.868403	+7.80	-2240.558395
10h-PhNCO-022	-2239.868404	+7.79	-2240.558229
10h-PhNCO-021	-2239.868442	+7.69	-2240.558060
10h-PhNCO-020	-2239.868459	+7.65	-2240.558387
10h-PhNCO-019	-2239.868488	+7.57	-2240.558490
10h-PhNCO-018	-2239.868498	+7.55	-2240.558494
10h-PhNCO-017	-2239.868553	+7.40	-2240.558201
10h-PhNCO-016	-2239.868638	+7.18	-2240.558788
10h-PhNCO-015	-2239.868641	+7.17	-2240.558756
10h-PhNCO-014	-2239.868667	+7.10	-2240.558725
10h-PhNCO-013	-2239.868796	+6.76	-2240.558787

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
10h-PhNCO-012	-2239.868822	+6.70	-2240.558834	-2236.096784	+10.90	-2236.718851
10h-PhNCO-011	-2239.868820	+6.70	-2240.558687	-2236.097037	+10.24	-2236.717837
10h-PhNCO-010	-2239.869020	+6.18	-2240.558770	-2236.097149	+9.95	-2236.718122
10h-PhNCO-009	-2239.869239	+5.60	-2240.559924	-2236.097163	+9.91	-2236.723991
10h-PhNCO-008	-2239.869124	+5.90	-2240.558823	-2236.097427	+9.22	-2236.719444
10h-PhNCO-007	-2239.869339	+5.34	-2240.558858	-2236.097601	+8.76	-2236.719455
10h-PhNCO-006	-2239.868947	+6.37	-2240.559031	-2236.098053	+7.57	-2236.723896
10h-PhNCO-005	-2239.869489	+4.94	-2240.560273	-2236.098928	+5.27	-2236.724603
10h-PhNCO-004	-2239.870572	+2.10	-2240.560437	-2236.099060	+4.93	-2236.730061
10h-PhNCO-003	-2239.869623	+4.59	-2240.559938	-2236.099392	+4.06	-2236.726203
10h-PhNCO-002	-2239.869059	+6.07	-2240.559313	-2236.099658	+3.36	-2236.724545
10h-PhNCO-001	-2239.871372	+0.00	-2240.561421	-2236.100937	+0.00	-2236.727281

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
10h-066	-1840.178096	+43.63	-1840.752907
10h-065	-1840.178546	+42.45	-1840.753770
10h-064	-1840.178986	+41.29	-1840.753965
10h-063	-1840.181035	+35.91	-1840.756490
10h-062	-1840.181078	+35.80	-1840.756129
10h-061	-1840.181313	+35.18	-1840.755978
10h-060	-1840.184063	+27.96	-1840.759668
10h-059	-1840.184370	+27.16	-1840.759028
10h-058	-1840.184724	+26.23	-1840.760119
10h-057	-1840.185276	+24.78	-1840.761033
10h-056	-1840.185395	+24.47	-1840.760429
10h-055	-1840.185399	+24.46	-1840.760515
10h-054	-1840.185421	+24.40	-1840.760496
10h-053	-1840.185673	+23.74	-1840.760471
10h-052	-1840.185676	+23.73	-1840.760776
10h-051	-1840.185907	+23.12	-1840.761217

10h-050	-1840.186037	+22.78	-1840.761289
10h-049	-1840.186073	+22.69	-1840.761529
10h-048	-1840.186653	+21.16	-1840.761873
10h-047	-1840.186711	+21.01	-1840.762050
10h-046	-1840.186898	+20.52	-1840.761879
10h-045	-1840.186992	+20.27	-1840.762042
10h-044	-1840.187064	+20.09	-1840.762238
10h-043	-1840.187068	+20.07	-1840.762474
10h-042	-1840.187172	+19.80	-1840.762871
10h-041	-1840.187192	+19.75	-1840.762373
10h-040	-1840.187376	+19.27	-1840.762545
10h-039	-1840.187398	+19.21	-1840.762426
10h-038	-1840.187693	+18.43	-1840.762639
10h-037	-1840.187708	+18.39	-1840.762956
10h-036	-1840.187982	+17.67	-1840.762757
10h-035	-1840.188226	+17.03	-1840.763727
10h-034	-1840.188861	+15.37	-1840.764058
10h-033	-1840.189095	+14.75	-1840.764938
10h-032	-1840.189264	+14.31	-1840.764177
10h-031	-1840.189766	+12.99	-1840.764882
10h-030	-1840.189981	+12.43	-1840.765003
10h-029	-1840.190031	+12.30	-1840.765000
10h-028	-1840.191404	+8.69	-1840.765966
10h-027	-1840.191453	+8.56	-1840.766393
10h-026	-1840.191587	+8.21	-1840.766572
10h-025	-1840.191758	+7.76	-1840.766845
10h-024	-1840.191800	+7.65	-1840.766831
10h-023	-1840.191829	+7.57	-1840.767030
10h-022	-1840.191846	+7.53	-1840.766850
10h-021	-1840.191863	+7.49	-1840.766937

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
10h-020	-1840.191925	+7.32	-1840.767031	-1837.137040	+7.56	-1837.659592
10h-019	-1840.191963	+7.22	-1840.766821	-1837.137198	+7.14	-1837.658860
10h-018	-1840.192619	+5.50	-1840.767529	-1837.137202	+7.13	-1837.661148
10h-017	-1840.192460	+5.92	-1840.767746	-1837.137251	+7.00	-1837.659925
10h-016	-1840.192410	+6.05	-1840.767704	-1837.137336	+6.78	-1837.660748
10h-015	-1840.192213	+6.57	-1840.767031	-1837.137405	+6.60	-1837.657221
10h-014	-1840.192269	+6.42	-1840.767127	-1837.137567	+6.17	-1837.657850
10h-013	-1840.192644	+5.43	-1840.767427	-1837.137674	+5.89	-1837.660721
10h-012	-1840.192221	+6.55	-1840.767070	-1837.138021	+4.98	-1837.658615
10h-011	-1840.192700	+5.29	-1840.767947	-1837.138129	+4.70	-1837.660144
10h-010	-1840.192728	+5.21	-1840.767934	-1837.138177	+4.57	-1837.660110
10h-009	-1840.193193	+3.99	-1840.768166	-1837.138399	+3.99	-1837.661443
10h-008	-1840.193224	+3.91	-1840.768189	-1837.138605	+3.45	-1837.661737
10h-007	-1840.193657	+2.78	-1840.768833	-1837.138877	+2.73	-1837.661656

10h-006	-1840.193837	+2.30	-1840.768990	-1837.138914	+2.64	-1837.661544
10h-005	-1840.193989	+1.90	-1840.768912	-1837.139152	+2.01	-1837.661763
10h-004	-1840.193616	+2.88	-1840.768906	-1837.139205	+1.87	-1837.664243
10h-003	-1840.194215	+1.31	-1840.768876	-1837.139338	+1.52	-1837.660513
10h-002	-1840.194543	+0.45	-1840.769386	-1837.139842	+0.20	-1837.662204
10h-001	-1840.194714	+0.00	-1840.769421	-1837.139918	+0.00	-1837.663197

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
10-Me2-004	-1222.029868	+4.00	-1222.362562	-1219.968062	+8.67	-1220.269215
10-Me2-003	-1222.030102	+3.39	-1222.362973	-1219.968967	+6.30	-1220.271118
10-Me2-002	-1222.029867	+4.01	-1222.362573	-1219.969643	+4.52	-1220.270540
10-Me2-001	-1222.031393	+0.00	-1222.364044	-1219.971366	+0.00	-1220.273934

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
10-Me-003	-1222.029131	+0.81	-1222.361626	-1219.964723	+0.96	-1220.259742
10-Me-002	-1222.029376	+0.17	-1222.361759	-1219.965023	+0.17	-1220.259963
10-Me-001	-1222.029439	+0.00	-1222.361727	-1219.965088	+0.00	-1220.259723

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
10-PhNCO2-009	-1581.939963	+16.81	-1582.343515
10-PhNCO2-008	-1581.940273	+15.99	-1582.344005
10-PhNCO2-007	-1581.940404	+15.65	-1582.344020

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
10-PhNCO2-006	-1581.941408	+13.01	-1582.345198	-1579.241687	+13.42	-1579.564215
10-PhNCO2-005	-1581.943125	+8.50	-1582.347175	-1579.243399	+8.92	-1579.566577
10-PhNCO2-004	-1581.943105	+8.56	-1582.347163	-1579.243414	+8.88	-1579.566634
10-PhNCO2-003	-1581.944659	+4.48	-1582.348154	-1579.245524	+3.34	-1579.564640
10-PhNCO2-002	-1581.946364	+0.00	-1582.350175	-1579.246582	+0.57	-1579.572014
10-PhNCO2-001	-1581.946310	+0.14	-1582.350137	-1579.246798	+0.00	-1579.571959

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
10-PhNCO-017	-1581.941762	+25.74	-1582.345475
10-PhNCO-016	-1581.941830	+25.56	-1582.345489
10-PhNCO-015	-1581.941845	+25.52	-1582.345609
10-PhNCO-014	-1581.941878	+25.44	-1582.345546
10-PhNCO-013	-1581.942468	+23.89	-1582.346032
10-PhNCO-012	-1581.942474	+23.87	-1582.346109
10-PhNCO-011	-1581.942494	+23.82	-1582.346052
10-PhNCO-010	-1581.942537	+23.71	-1582.346174

10-PhNCO-009 -1581.943051 +22.36 -1582.346740

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
10-PhNCO-008	-1581.943073	+22.30	-1582.346640	-1579.240611	+18.98	-1579.561761
10-PhNCO-007	-1581.946645	+12.92	-1582.350518	-1579.242579	+13.81	-1579.566499
10-PhNCO-006	-1581.946731	+12.69	-1582.350627	-1579.242674	+13.56	-1579.566570
10-PhNCO-005	-1581.951449	+0.31	-1582.355471	-1579.247455	+1.01	-1579.574785
10-PhNCO-004	-1581.951409	+0.41	-1582.355329	-1579.247515	+0.85	-1579.574670
10-PhNCO-003	-1581.951435	+0.34	-1582.355359	-1579.247643	+0.51	-1579.574778
10-PhNCO-002	-1581.951437	+0.34	-1582.355401	-1579.247824	+0.04	-1579.574742
10-PhNCO-001	-1581.951566	+0.00	-1582.355376	-1579.247839	+0.00	-1579.574568

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
10-002	-1182.273833	+0.00	-1182.562834	-1180.286039	+0.03	-1180.499782
10-001	-1182.273806	+0.07	-1182.562746	-1180.286051	+0.00	-1180.499646

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
11-004	-1182.738869	+47.64	-1183.041973	-1180.754574	+54.02	-1181.014846
11-003	-1182.745220	+30.97	-1183.048135	-1180.760959	+37.26	-1181.026740
11-002	-1182.753586	+9.00	-1183.056661	-1180.770657	+11.80	-1181.042220
11-001	-1182.757014	+0.00	-1183.059680	-1180.775150	+0.00	-1181.046302

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
14-005	-1175.376657	+37.56	-1175.588973	-1173.604534	+45.69	-1173.773945
14-004	-1175.375986	+39.32	-1175.587831	-1173.607772	+37.19	-1173.791691
14-003	-1175.385480	+14.40	-1175.598500	-1173.610772	+29.32	-1173.782332
14-002	-1175.382951	+21.04	-1175.595685	-1173.613902	+21.10	-1173.794445
14-001	-1175.390964	+0.00	-1175.603813	-1173.621938	+0.00	-1173.800258

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
15g-Me2-025	-2482.192298	+13.06	-2482.827216
15g-Me2-024	-2482.192337	+12.95	-2482.827045
15g-Me2-023	-2482.192409	+12.77	-2482.827033
15g-Me2-022	-2482.192445	+12.67	-2482.827287
15g-Me2-021	-2482.192533	+12.44	-2482.827502
15g-Me2-020	-2482.192537	+12.43	-2482.827501
15g-Me2-019	-2482.192968	+11.30	-2482.827375
15g-Me2-018	-2482.193006	+11.20	-2482.827837
15g-Me2-017	-2482.193070	+11.03	-2482.827576

15g-Me2-016	-2482.193115	+10.91	-2482.827431
15g-Me2-015	-2482.193287	+10.46	-2482.827581

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
15g-Me2-014	-2482.192972	+11.29	-2482.828197	-2478.087575	+10.34	-2478.624789
15g-Me2-013	-2482.193585	+9.68	-2482.828234	-2478.087984	+9.27	-2478.629823
15g-Me2-012	-2482.193323	+10.37	-2482.828074	-2478.088180	+8.75	-2478.627840
15g-Me2-011	-2482.193623	+9.58	-2482.827933	-2478.088291	+8.46	-2478.630894
15g-Me2-010	-2482.193218	+10.64	-2482.828102	-2478.088324	+8.38	-2478.626061
15g-Me2-009	-2482.193328	+10.35	-2482.827911	-2478.088479	+7.97	-2478.625684
15g-Me2-008	-2482.193814	+9.08	-2482.828341	-2478.088502	+7.91	-2478.630232
15g-Me2-007	-2482.193510	+9.87	-2482.828392	-2478.088577	+7.71	-2478.626812
15g-Me2-006	-2482.194381	+7.59	-2482.829210	-2478.088632	+7.57	-2478.628778
15g-Me2-005	-2482.193982	+8.64	-2482.828509	-2478.088845	+7.01	-2478.626482
15g-Me2-004	-2482.194637	+6.92	-2482.829349	-2478.089146	+6.22	-2478.628190
15g-Me2-003	-2482.194037	+8.49	-2482.828644	-2478.089679	+4.82	-2478.628039
15g-Me2-002	-2482.194662	+6.85	-2482.829474	-2478.090792	+1.90	-2478.626891
15g-Me2-001	-2482.197271	+0.00	-2482.832034	-2478.091514	+0.00	-2478.632736

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
15g-Me-034	-2482.197633	+14.00	-2482.832856
15g-Me-033	-2482.198170	+12.59	-2482.833128
15g-Me-032	-2482.198230	+12.43	-2482.832659
15g-Me-031	-2482.198299	+12.25	-2482.833153
15g-Me-030	-2482.198376	+12.05	-2482.832897
15g-Me-029	-2482.198378	+12.05	-2482.833361
15g-Me-028	-2482.198481	+11.78	-2482.832921
15g-Me-027	-2482.198539	+11.62	-2482.833014
15g-Me-026	-2482.198628	+11.39	-2482.832967
15g-Me-025	-2482.198649	+11.33	-2482.833420
15g-Me-024	-2482.198681	+11.25	-2482.833385
15g-Me-023	-2482.198692	+11.22	-2482.832936
15g-Me-022	-2482.198974	+10.48	-2482.834316
15g-Me-021	-2482.199013	+10.38	-2482.833089
15g-Me-020	-2482.199043	+10.30	-2482.833546
15g-Me-019	-2482.199048	+10.29	-2482.833595
15g-Me-018	-2482.199097	+10.16	-2482.833767
15g-Me-017	-2482.199178	+9.95	-2482.833755
15g-Me-016	-2482.199246	+9.77	-2482.833909
15g-Me-015	-2482.199273	+9.70	-2482.833747
15g-Me-014	-2482.199468	+9.18	-2482.833998
15g-Me-013	-2482.199500	+9.10	-2482.834283

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
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15g-Me-012	-2482.199503	+9.09	-2482.834406	-2478.086953	+12.21	-2478.622434
15g-Me-011	-2482.200006	+7.77	-2482.834341	-2478.087874	+9.79	-2478.624155
15g-Me-010	-2482.200448	+6.61	-2482.834441	-2478.088319	+8.62	-2478.627853
15g-Me-009	-2482.200668	+6.03	-2482.835598	-2478.088452	+8.27	-2478.623334
15g-Me-008	-2482.199598	+8.84	-2482.833955	-2478.088483	+8.19	-2478.624872
15g-Me-007	-2482.199511	+9.07	-2482.833911	-2478.088484	+8.19	-2478.624865
15g-Me-006	-2482.201305	+4.36	-2482.835877	-2478.089716	+4.95	-2478.623471
15g-Me-005	-2482.200767	+5.77	-2482.835384	-2478.090016	+4.17	-2478.624875
15g-Me-004	-2482.199672	+8.65	-2482.834439	-2478.090145	+3.83	-2478.618649
15g-Me-003	-2482.201298	+4.38	-2482.835916	-2478.090343	+3.31	-2478.624872
15g-Me-002	-2482.201731	+3.24	-2482.836278	-2478.091197	+1.07	-2478.625218
15g-Me-001	-2482.202966	+0.00	-2482.837558	-2478.091603	+0.00	-2478.625475

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
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15g-PhNCO2-028	-2842.126785	+19.83	-2842.832806
15g-PhNCO2-027	-2842.127259	+18.59	-2842.832984
15g-PhNCO2-026	-2842.127555	+17.81	-2842.833437
15g-PhNCO2-025	-2842.128232	+16.03	-2842.833762
15g-PhNCO2-024	-2842.128265	+15.94	-2842.834001
15g-PhNCO2-023	-2842.128425	+15.52	-2842.833893
15g-PhNCO2-022	-2842.128653	+14.93	-2842.834069
15g-PhNCO2-021	-2842.128678	+14.86	-2842.834056
15g-PhNCO2-020	-2842.128916	+14.24	-2842.834793
15g-PhNCO2-019	-2842.128924	+14.21	-2842.834702
15g-PhNCO2-018	-2842.128956	+14.13	-2842.834583
15g-PhNCO2-017	-2842.128991	+14.04	-2842.834816
15g-PhNCO2-016	-2842.129267	+13.31	-2842.835178
15g-PhNCO2-015	-2842.129515	+12.66	-2842.835491
15g-PhNCO2-014	-2842.129626	+12.37	-2842.835487
15g-PhNCO2-013	-2842.129704	+12.17	-2842.835415

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
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15g-PhNCO2-012	-2842.129783	+11.96	-2842.835438	-2837.386811	+13.38	-2838.021714
15g-PhNCO2-011	-2842.130766	+9.38	-2842.836752	-2837.387063	+12.72	-2838.020653
15g-PhNCO2-010	-2842.130905	+9.01	-2842.836908	-2837.388399	+9.21	-2838.027616
15g-PhNCO2-009	-2842.131163	+8.34	-2842.837065	-2837.388655	+8.54	-2838.028500
15g-PhNCO2-008	-2842.131461	+7.55	-2842.836710	-2837.388976	+7.69	-2838.027079
15g-PhNCO2-007	-2842.131376	+7.78	-2842.836710	-2837.389124	+7.30	-2838.027537
15g-PhNCO2-006	-2842.132384	+5.13	-2842.838270	-2837.389476	+6.38	-2838.028020
15g-PhNCO2-005	-2842.132033	+6.05	-2842.838094	-2837.389508	+6.30	-2838.027140
15g-PhNCO2-004	-2842.132423	+5.03	-2842.838245	-2837.389571	+6.13	-2838.027999
15g-PhNCO2-003	-2842.134338	+0.00	-2842.840059	-2837.389717	+5.75	-2838.024982
15g-PhNCO2-002	-2842.134072	+0.70	-2842.839893	-2837.389754	+5.65	-2838.027854
15g-PhNCO2-001	-2842.134092	+0.65	-2842.839578	-2837.391906	+0.00	-2838.029333

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
15g-PhNCO-029	-2842.140774	+16.87	-2842.846539
15g-PhNCO-028	-2842.140857	+16.65	-2842.846662
15g-PhNCO-027	-2842.140867	+16.62	-2842.846858
15g-PhNCO-026	-2842.141226	+15.68	-2842.847100
15g-PhNCO-025	-2842.141389	+15.25	-2842.847078
15g-PhNCO-024	-2842.141540	+14.86	-2842.847191
15g-PhNCO-023	-2842.141631	+14.62	-2842.847273
15g-PhNCO-022	-2842.141876	+13.97	-2842.847808
15g-PhNCO-021	-2842.142086	+13.42	-2842.848088
15g-PhNCO-020	-2842.142533	+12.25	-2842.848264
15g-PhNCO-019	-2842.142581	+12.12	-2842.848050
15g-PhNCO-018	-2842.142596	+12.08	-2842.848622
15g-PhNCO-017	-2842.142810	+11.52	-2842.848697
15g-PhNCO-016	-2842.142823	+11.49	-2842.848685
15g-PhNCO-015	-2842.142849	+11.42	-2842.848612
15g-PhNCO-014	-2842.142873	+11.36	-2842.848505
15g-PhNCO-013	-2842.143805	+8.91	-2842.849412

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
15g-PhNCO-012	-2842.143848	+8.80	-2842.849770	-2837.393325	+10.49	-2838.029344
15g-PhNCO-011	-2842.144160	+7.98	-2842.849680	-2837.394123	+8.39	-2838.030888
15g-PhNCO-010	-2842.144133	+8.05	-2842.849875	-2837.394588	+7.17	-2838.031605
15g-PhNCO-009	-2842.144340	+7.50	-2842.849722	-2837.394841	+6.51	-2838.032374
15g-PhNCO-008	-2842.144382	+7.39	-2842.850238	-2837.395218	+5.52	-2838.030619
15g-PhNCO-007	-2842.144548	+6.96	-2842.849917	-2837.395326	+5.24	-2838.031567
15g-PhNCO-006	-2842.145432	+4.64	-2842.851177	-2837.395711	+4.22	-2838.034539
15g-PhNCO-005	-2842.145077	+5.57	-2842.850640	-2837.395921	+3.67	-2838.034148
15g-PhNCO-004	-2842.145739	+3.83	-2842.851365	-2837.396406	+2.40	-2838.036621
15g-PhNCO-003	-2842.145642	+4.09	-2842.851319	-2837.396895	+1.12	-2838.035066
15g-PhNCO-002	-2842.147040	+0.41	-2842.852595	-2837.397131	+0.50	-2838.035548
15g-PhNCO-001	-2842.147198	+0.00	-2842.852904	-2837.397320	+0.00	-2838.035695

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
15g-026	-2442.462912	+27.47	-2443.053503
15g-025	-2442.463386	+26.23	-2443.053950
15g-024	-2442.467042	+16.63	-2443.057839
15g-023	-2442.467463	+15.52	-2443.058088
15g-022	-2442.468316	+13.28	-2443.059152
15g-021	-2442.468336	+13.23	-2443.059181
15g-020	-2442.468867	+11.84	-2443.059518
15g-019	-2442.469232	+10.88	-2443.059729
15g-018	-2442.469270	+10.78	-2443.059889
15g-017	-2442.469372	+10.51	-2443.060175

15g-016	-2442.469424	+10.37	-2443.060205
15g-015	-2442.469752	+9.51	-2443.060281
15g-014	-2442.469757	+9.50	-2443.060735
15g-013	-2442.469825	+9.32	-2443.060547

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
15g-012	-2442.470137	+8.50	-2443.060770	-2438.436131	+11.71	-2438.963516
15g-011	-2442.470178	+8.39	-2443.060667	-2438.436473	+10.81	-2438.963323
15g-010	-2442.470444	+7.70	-2443.061271	-2438.436775	+10.02	-2438.964503
15g-009	-2442.470568	+7.37	-2443.061216	-2438.436967	+9.52	-2438.964379
15g-008	-2442.470032	+8.78	-2443.060797	-2438.438221	+6.23	-2438.965605
15g-007	-2442.471497	+4.93	-2443.062254	-2438.438414	+5.72	-2438.967012
15g-006	-2442.471516	+4.88	-2443.062098	-2438.438560	+5.34	-2438.965147
15g-005	-2442.470485	+7.59	-2443.061286	-2438.438596	+5.24	-2438.962376
15g-004	-2442.471516	+4.88	-2443.061933	-2438.438686	+5.00	-2438.964781
15g-003	-2442.472064	+3.44	-2443.062598	-2438.439042	+4.07	-2438.964730
15g-002	-2442.471411	+5.16	-2443.062155	-2438.439447	+3.01	-2438.964696
15g-001	-2442.473375	+0.00	-2443.064301	-2438.440592	+0.00	-2438.968677

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
15-Me2-001	-1214.659964	+0.00	-1214.902365	-1212.812682	+0.00	-1213.020212

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
15-Me-002	-1214.660753	+25.73	-1214.902927	-1212.807894	+20.89	-1213.006719
15-Me-001	-1214.670553	+0.00	-1214.912884	-1212.815851	+0.00	-1213.016854

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
15-PhNCO2-005	-1574.574119	+19.18	-1574.887096	-1572.087610	+18.11	-1572.318155
15-PhNCO2-004	-1574.574700	+17.65	-1574.887631	-1572.088231	+16.48	-1572.319265
15-PhNCO2-003	-1574.577749	+9.65	-1574.891149	-1572.092927	+4.15	-1572.328809
15-PhNCO2-002	-1574.579225	+5.77	-1574.892680	-1572.094046	+1.21	-1572.330245
15-PhNCO2-001	-1574.581424	+0.00	-1574.894792	-1572.094508	+0.00	-1572.333003

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree
15-PhNCO-007	-1574.577502	+47.69	-1574.890640
15-PhNCO-006	-1574.577582	+47.48	-1574.890567

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
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15-PhNCO-005	-1574.578226	+45.79	-1574.891483	-1572.085926	+42.31	-1572.318806
15-PhNCO-004	-1574.579396	+42.72	-1574.892548	-1572.086900	+39.75	-1572.320613
15-PhNCO-003	-1574.586121	+25.06	-1574.899370	-1572.093594	+22.18	-1572.328377
15-PhNCO-002	-1574.587243	+22.12	-1574.900549	-1572.093860	+21.48	-1572.332481
15-PhNCO-001	-1574.595667	+0.00	-1574.909289	-1572.102041	+0.00	-1572.342492

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
15-002	-1174.916634	+25.36	-1175.115188	-1173.139543	+22.93	-1173.264526
15-001	-1174.926292	+0.00	-1175.125207	-1173.148275	+0.00	-1173.276290

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
22-Me-001	-1075.816070	+0.00	-1076.149411	-1073.934962	+0.00	-1074.192507

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
22-002	-1036.087156	+0.01	-1036.377953	-1034.279856	+0.04	-1034.548855
22-001	-1036.087159	+0.00	-1036.377950	-1034.279872	+0.00	-1034.548874

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
22-PhNCO-002	-1435.733666	+17.90	-1436.138498	-1433.210924	+16.54	-1433.577970
22-PhNCO-001	-1435.740483	+0.00	-1436.145378	-1433.217222	+0.00	-1433.583981

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
23-001	-401.825524	+0.00	-401.969205	-401.056657	+0.00	-401.185707

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
23-Me-001	-441.539916	+0.00	-441.727628	-440.692172	+0.00	-440.803142

Nr.	H _{298K} (DFT)/Hartree	ΔH _{298K} (DFT)/kJ mol ⁻¹	E _{298K} (DFT)/Hartree	H _{298K} (CC)/Hartree	ΔH _{298K} (CC)/kJ mol ⁻¹	E _{298K} (CC)/Hartree
23-PhNCO-003	-801.473861	+22.94	-801.731823	-799.990234	+19.23	-800.210840
23-PhNCO-002	-801.473416	+24.10	-801.731281	-799.990311	+19.02	-800.210499
23-PhNCO-001	-801.482597	+0.00	-801.740914	-799.997557	+0.00	-800.223110

Table of Structural Data

1a-001

1N	-2.678736	0.000017	-0.000122
2C	-1.958779	1.137117	0.010569
3C	-0.570675	1.201411	0.010702
4C	0.186293	-0.000025	0.000081
5C	-0.570711	-1.201451	-0.010535
6C	-1.958811	-1.137109	-0.010628
7N	1.553315	0.000000	0.000261
8C	2.285580	-1.260676	0.018590
9C	2.285499	1.260699	-0.018808
10H	-2.530891	2.063792	0.020446
11H	-0.091890	2.173351	0.022842
12H	-0.091983	-2.173416	-0.022371
13H	-2.530958	-2.063762	-0.020539
14H	2.025879	-1.863606	0.899372
15H	2.085237	-1.858241	-0.881752
16H	3.355677	-1.052094	0.057620
17H	2.025483	1.863322	-0.899710
18H	2.085399	1.858547	0.881391
19H	3.355605	1.052188	-0.058107

1a-Me-001

1N	-2.127404	-0.000220	-0.025500
2C	-1.436762	-1.172636	-0.028609
3C	-0.067156	-1.211074	-0.017157
4C	0.693058	-0.000225	0.000837
5C	-0.067446	1.210559	0.010631
6C	-1.436920	1.172083	0.000347
7N	2.037707	0.000123	0.004983
8C	2.780747	-1.263972	0.030930
9C	2.780394	1.264541	-0.020276
10C	-3.600423	0.000435	0.029395
11H	-2.033659	-2.077487	-0.045869
12H	0.410670	-2.181194	-0.033498
13H	0.409974	2.180820	0.028438
14H	-2.033892	2.077025	0.010000
15H	3.846756	-1.046051	0.084910
16H	2.508295	-1.860835	0.909124
17H	2.590150	-1.850558	-0.876013
18H	3.846760	1.046886	-0.067687
19H	2.512468	1.858627	-0.901824
20H	2.584416	1.853767	0.883726
21H	-3.977923	0.886924	-0.482328
22H	-3.978163	-0.890532	-0.474055
23H	-3.930920	0.005022	1.072117

1a-Me-002

1N	2.127837	0.011708	-0.002042
2C	1.439534	-1.163324	-0.013104
3C	0.071095	-1.207049	-0.008510
4C	-0.693561	0.001956	0.004043
5C	0.062894	1.213986	0.020479
6C	1.433667	1.180710	0.018027
7N	-2.038216	-0.003490	-0.000077
8C	-2.776877	-1.270329	0.023244
9C	-2.785020	1.258157	-0.030979
10C	3.602484	-0.012927	-0.005893
11H	2.040830	-2.065621	-0.027178
12H	-0.403497	-2.178783	-0.023013
13H	-0.417242	2.182877	0.041143
14H	2.022721	2.090332	0.033315
15H	-3.843968	-1.055929	0.069252
16H	-2.577901	-1.858414	-0.880896
17H	-2.508661	-1.864212	0.904775
18H	-3.850301	1.037201	-0.086930
19H	-2.598309	1.847695	0.874805
20H	-2.511840	1.853492	-0.910074
21H	3.980669	1.008775	-0.041527
22H	3.961551	-0.503371	0.902612
23H	3.953306	-0.558658	-0.885300

1a-PhNCO-001

1N	0.602418	0.448322	0.018823
2C	1.510798	1.455902	0.005839
3C	2.863502	1.222700	-0.003483

4C	3.366004	-0.112602	0.000954
5C	2.380898	-1.146900	0.022828
6C	1.044918	-0.836744	0.028542
7N	4.688605	-0.382566	-0.014427
8C	5.664403	0.708457	-0.053337
9C	5.161352	-1.768291	0.015893
10C	-0.892601	0.805064	0.018448
11O	-1.111111	2.028484	0.026654
12N	-1.619302	-0.278196	0.006812
13C	-3.016314	-0.238189	-0.000433
14C	-3.829563	0.921352	0.001693
15C	-5.223602	0.811603	-0.008290
16C	-5.852217	-0.437705	-0.020312
17C	-5.059086	-1.593116	-0.022414
18C	-3.669037	-1.493428	-0.012475
19H	1.089007	2.452722	0.003191
20H	3.524671	2.078991	-0.012403
21H	2.656206	-2.193405	0.030421
22H	0.266926	-1.588068	0.039362
23H	5.506023	1.344436	-0.932172
24H	6.668230	0.287905	-0.113162
25H	5.601958	1.327304	0.850365
26H	4.817294	-2.322189	-0.866096
27H	6.251161	-1.772888	0.019947
28H	4.811704	-2.284466	0.918057
29H	-3.362352	1.897796	0.011068
30H	-5.823710	1.719757	-0.006378
31H	-6.937113	-0.511246	-0.028062
32H	-5.526396	-2.575828	-0.031951
33H	-3.053499	-2.390233	-0.014596

1a-PhNCO-002

1N	0.010149	1.356472	-0.187267
2C	0.220499	0.335373	-1.053463
3C	1.389241	-0.384752	-1.060092
4C	2.423251	-0.087715	-0.122393
5C	2.172035	1.006431	0.760593
6C	0.986125	1.694675	0.688446
7N	3.572965	-0.794169	-0.079207
8C	3.799768	-1.895180	-1.017295
9C	4.618516	-0.448900	0.885579
10C	-1.309943	2.191825	-0.207277
11O	-1.088734	3.408972	-0.181446
12N	-2.424358	1.526560	-0.291599
13C	-2.578797	0.174163	0.011213
14C	-3.367641	-0.628950	-0.840289
15C	-3.591970	-1.976416	-0.554743
16C	-3.047332	-2.562643	0.595405
17C	-2.281298	-1.772462	1.460190
18C	-2.051839	-0.423799	1.179022
19H	-0.583425	0.121069	-1.745889
20H	1.492017	-1.177756	-1.788820
21H	2.901551	1.323614	1.494084
22H	0.769784	2.543081	1.326702
23H	4.769841	-2.345628	-0.808217
24H	3.031008	-2.669784	-0.909555
25H	3.800994	-1.537544	-2.054366
26H	5.454546	-1.137342	0.764292
27H	4.985884	0.571904	0.723284
28H	4.249452	-0.533753	1.914914
29H	-3.795972	-0.174036	-1.730454
30H	-4.199508	-2.572241	-1.232950
31H	-3.228266	-3.610869	0.819813
32H	-1.864537	-2.205807	2.367398
33H	-1.468471	0.181358	1.868459

1b-Me-001

1N	-2.494929	-0.002176	-0.027275
2C	-1.808599	1.167023	0.096312
3C	-0.438242	1.219206	0.127796
4C	0.305028	-0.000261	-0.000413
5C	-0.434042	-1.220187	-0.140581
6C	-1.805240	-1.170682	-0.129950
7N	1.652073	0.001397	0.006339
8C	0.298518	2.526953	0.284235
9C	1.641938	2.446857	-0.447617
10C	2.437913	1.246343	0.051987
11C	2.441110	-1.241777	-0.033987
12C	1.642142	-2.445752	0.452304
13C	0.306924	-2.525874	-0.294508
14C	-3.966439	-0.001906	0.036443
15H	-2.410696	2.065876	0.176685

16H	-2.403324	-2.071171	-0.217791
17H	0.477357	2.721928	1.351341
18H	-0.310491	3.354369	-0.095090
19H	2.228849	3.355847	-0.280902
20H	1.472529	2.353152	-1.527875
21H	3.326399	1.090843	-0.569229
22H	2.779586	1.406115	1.084256
23H	3.321956	-1.086422	0.598054
24H	2.795194	-1.397230	-1.062722
25H	1.460768	-2.356601	1.530982
26H	2.232737	-3.352909	0.288655
27H	0.497657	-2.716658	-1.360306
28H	-0.304537	-3.355998	0.075019
29H	-4.293399	0.003115	1.080602
30H	-4.348182	0.884686	-0.473537
31H	-4.348476	-0.893138	-0.463718

1b-Me-002

1N	2.494785	0.021681	0.008570
2C	1.814341	-1.152741	0.121539
3C	0.444696	-1.214314	0.138357
4C	-0.305285	0.000710	0.000894
5C	0.427016	1.224641	-0.132101
6C	1.799004	1.184371	-0.109815
7N	-1.652361	-0.009809	-0.002030
8C	-0.285575	-2.525912	0.292095
9C	-1.622668	-2.455657	-0.452438
10C	-2.430716	-1.259574	0.038170
11C	-2.448638	1.228565	-0.045605
12C	-1.660558	2.436107	0.449828
13C	-0.320528	2.526681	-0.287052
14C	3.967835	0.004308	-0.012927
15H	2.423292	-2.046709	0.207456
16H	2.388928	2.090249	-0.196070
17H	-0.473108	-2.718866	1.358061
18H	0.332034	-3.350722	-0.078994
19H	-2.205148	-3.368237	-0.289828
20H	-1.443939	-2.362472	-1.531241
21H	-3.314488	-1.110450	-0.591307
22H	-2.780843	-1.420239	1.067465
23H	-3.333377	1.066397	0.579269
24H	-2.795700	1.384559	-1.076656
25H	-1.486316	2.344736	1.529514
26H	-2.255691	3.340002	0.284681
27H	-0.504747	2.720491	-1.353427
28H	0.283164	3.358942	0.090327
29H	4.339877	1.029013	-0.002805
30H	4.338828	-0.521930	0.870030
31H	4.316730	-0.500986	-0.917924

1b-PhNCO-001

1N	0.114831	-0.493806	-0.008323
2C	-0.316141	0.794722	0.054107
3C	-1.647547	1.126472	0.076311
4C	-2.624456	0.083158	-0.003435
5C	-2.153333	-1.264715	-0.080055
6C	-0.799410	-1.496004	-0.065953
7N	-3.947030	0.363566	-0.004048
8C	-2.101067	2.563576	0.169105
9C	-3.429940	2.727586	-0.575644
10C	-4.457968	1.742648	-0.028155
11C	-4.972228	-0.690666	0.020697
12C	-4.431621	-2.005191	0.574271
13C	-3.148527	-2.397122	-0.166402
14C	1.601619	-0.857734	-0.023944
15O	1.818547	-2.079494	-0.108835
16N	2.340621	0.215805	0.063671
17C	3.735996	0.164597	0.038842
18C	4.402236	1.389597	0.280334
19C	5.792899	1.480450	0.265533
20C	6.574031	0.346843	0.003105
21C	5.932479	-0.871899	-0.240385
22C	4.537892	-0.973829	-0.221816
23H	0.469969	1.536957	0.094640
24H	-0.381373	-2.493922	-0.109906
25H	-1.333453	3.230035	-0.238251
26H	-2.240087	2.841439	1.224052
27H	-3.279763	2.545159	-1.647587
28H	-3.818647	3.745195	-0.463417
29H	-4.760298	2.025111	0.990830
30H	-5.360026	1.745220	-0.650505
31H	-5.361808	-0.829441	-0.998364

32H	-5.799009	-0.326377	0.640903
33H	-5.198934	-2.779109	0.464961
34H	-4.221905	-1.894179	1.646062
35H	-2.716291	-3.313893	0.248834
36H	-3.386204	-2.603088	-1.220250
37H	3.796172	2.270880	0.478490
38H	6.270380	2.439437	0.457071
39H	7.659326	0.413691	-0.010929
40H	6.523180	-1.762815	-0.446242
41H	4.061946	-1.928228	-0.407907

1b-PhNCO-002

1N	0.114535	-0.492821	-0.092901
2C	-0.798923	-1.495640	-0.083128
3C	-2.154088	-1.266946	-0.090853
4C	-2.627404	0.082537	-0.090805
5C	-1.649581	1.127885	-0.136725
6C	-0.317305	0.795453	-0.122511
7N	-3.952883	0.362940	-0.038831
8C	-3.133232	-2.418982	-0.100693
9C	-4.454320	-1.991542	0.543178
10C	-4.959695	-0.705664	-0.104813
11C	-4.445364	1.743529	-0.147451
12C	-3.458397	2.738619	0.456197
13C	-2.085533	2.574238	-0.199978
14C	1.602331	-0.857248	-0.064188
15O	1.818828	-2.081915	-0.078269
16N	2.339770	0.219975	-0.025866
17C	3.735091	0.167478	0.010097
18C	4.398330	1.417514	0.036741
19C	5.788502	1.506440	0.076537
20C	6.572794	0.344986	0.090986
21C	5.934483	-0.899218	0.065359
22C	4.540125	-0.998266	0.024786
23H	-0.380788	-2.494424	-0.068100
24H	0.468271	1.539308	-0.134685
25H	-2.703615	-3.282402	0.418921
26H	-3.318875	-2.732528	-1.138060
27H	-5.213218	-2.772955	0.427947
28H	-4.310392	-1.822711	1.618046
29H	-5.232262	-0.884268	-1.156203
30H	-5.855012	-0.345400	0.410677
31H	-5.405099	1.791481	0.375647
32H	-4.633200	1.980465	-1.205830
33H	-3.839492	3.754774	0.309581
34H	-3.382389	2.563899	1.537140
35H	-2.146462	2.892301	-1.250672
36H	-1.338798	3.214336	0.282184
37H	3.789965	2.319203	0.026224
38H	6.263010	2.485618	0.096355
39H	7.657839	0.410112	0.122042
40H	6.527339	-1.812135	0.076468
41H	4.065727	-1.971046	0.005243

1b-PhNCO-003

1N	0.115596	-0.489512	0.044976
2C	-0.797614	-1.491245	0.095248
3C	-2.152393	-1.261284	0.127621
4C	-2.625364	0.087587	0.079605
5C	-1.647343	1.132855	0.043966
6C	-0.315595	0.799008	0.021035
7N	-3.951966	0.366625	0.055945
8C	-3.129403	-2.411987	0.220539
9C	-4.478253	-2.012115	-0.382279
10C	-4.952362	-0.695887	0.227392
11C	-4.443528	1.750991	0.099987
12C	-3.473293	2.712708	-0.580261
13C	-2.082313	2.580847	0.044442
14C	1.603105	-0.854411	0.017034
15O	1.818749	-2.078319	-0.027006
16N	2.342133	0.221429	0.060330
17C	3.737278	0.167173	0.019525
18C	4.410593	1.387106	0.265379
19C	5.801489	1.472304	0.236022
20C	6.574783	0.338516	-0.047638
21C	5.925597	-0.874759	-0.298498
22C	4.531004	-0.971198	-0.264199
23H	-0.380058	-2.490294	0.111137
24H	0.470163	1.542043	-0.012820
25H	-3.270780	-2.685771	1.275893
26H	-2.720310	-3.294745	-0.283026
27H	-5.230678	-2.785814	-0.195373

28H	-4.384870	-1.894710	-1.469632
29H	-5.874104	-0.359718	-0.256433
30H	-5.168756	-0.822800	1.299189
31H	-4.607846	2.045855	1.147799
32H	-5.414895	1.768968	-0.403689
33H	-3.850686	3.735315	-0.474200
34H	-3.427205	2.484447	-1.652839
35H	-1.350075	3.194758	-0.491081
36H	-2.113277	2.952444	1.078707
37H	3.810351	2.268492	0.480037
38H	6.285189	2.426988	0.433324
39H	7.660143	0.401013	-0.072382
40H	6.510324	-1.765462	-0.521513
41H	4.048705	-1.921523	-0.455332

1b-PhNCO-004

1N	-0.493993	1.360197	-0.561995
2C	-0.351286	0.131320	-1.117632
3C	0.792815	-0.613996	-0.971606
4C	1.854431	-0.094936	-0.165611
5C	1.684719	1.203635	0.412492
6C	0.520557	1.889589	0.164040
7N	2.986773	-0.805876	0.036459
8C	0.942473	-1.968683	-1.618930
9C	1.810464	-2.861447	-0.725726
10C	3.149654	-2.182372	-0.455623
11C	4.141391	-0.254317	0.761211
12C	4.139787	1.271174	0.770599
13C	2.784922	1.789560	1.263723
14C	-1.788963	2.190760	-0.753396
15O	-1.554457	3.367866	-1.059857
16N	-2.922119	1.560092	-0.618755
17C	-3.091582	0.355759	0.061791
18C	-3.953953	-0.620806	-0.482875
19C	-4.194797	-1.823213	0.183762
20C	-3.592590	-2.087324	1.421006
21C	-2.753079	-1.119039	1.984206
22C	-2.508542	0.085968	1.322220
23H	-1.190924	-0.230241	-1.698283
24H	0.348490	2.888494	0.548068
25H	1.423165	-1.861645	-2.602104
26H	-0.042245	-2.416776	-1.789459
27H	1.993745	-3.830579	-1.201612
28H	1.292955	-3.048777	0.223747
29H	3.712021	-2.735185	0.305635
30H	3.763903	-2.160466	-1.367620
31H	5.044757	-0.632470	0.269319
32H	4.136043	-0.648539	1.787751
33H	4.951868	1.623404	1.415359
34H	4.332749	1.645241	-0.243023
35H	2.642611	1.490449	2.312291
36H	2.744552	2.883756	1.235030
37H	-4.427508	-0.416711	-1.440449
38H	-4.860371	-2.558180	-0.264541
39H	-3.784525	-3.022367	1.941468
40H	-2.289696	-1.297647	2.952788
41H	-1.869082	0.834637	1.782618

1b-PhNCO-005

1N	0.530727	-1.271521	0.667819
2C	-0.476962	-1.905192	0.019882
3C	-1.677576	-1.295545	-0.252069
4C	-1.869338	0.061668	0.159957
5C	-0.798781	0.708758	0.854259
6C	0.358190	0.006226	1.088233
7N	-3.028456	0.710918	-0.093588
8C	-2.789892	-2.018236	-0.971955
9C	-3.602439	-1.011754	-1.793515
10C	-4.107718	0.110106	-0.891989
11C	-3.299704	2.062625	0.419704
12C	-2.438932	2.400487	1.632976
13C	-0.963772	2.135548	1.316747
14C	1.843106	-2.047965	0.946020
15O	1.632246	-3.193488	1.368413
16N	2.964213	-1.410434	0.756314
17C	3.118123	-0.276639	-0.038275
18C	3.965278	0.759651	0.412053
19C	4.191085	1.895998	-0.365709
20C	3.588313	2.032195	-1.623337
21C	2.763467	1.003099	-2.092515
22C	2.533773	-0.136806	-1.319032
23H	-0.276975	-2.932637	-0.261577

24H	1.190071	0.451010	1.620131
25H	-3.449783	-2.505295	-0.239476
26H	-2.379406	-2.809440	-1.608304
27H	-2.975340	-0.590340	-2.589747
28H	-4.460674	-1.497951	-2.269341
29H	-4.553261	0.911323	-1.492543
30H	-4.886403	-0.262167	-0.210385
31H	-4.362974	2.103690	0.682240
32H	-3.131404	2.788847	-0.388815
33H	-2.599631	3.450171	1.900509
34H	-2.750856	1.787002	2.488132
35H	-0.632724	2.820058	0.522476
36H	-0.330029	2.328725	2.188806
37H	4.438369	0.654468	1.385713
38H	4.845231	2.679684	0.011323
39H	3.769384	2.916075	-2.229908
40H	2.300588	1.082110	-3.074441
41H	1.905120	-0.935515	-1.704537

1b-PhNCO-006

1N	0.520060	1.356389	-0.622064
2C	0.365044	0.116718	-1.146908
3C	-0.796987	-0.603639	-1.007511
4C	-1.870798	-0.039082	-0.248681
5C	-1.703349	1.288871	0.259398
6C	-0.507043	1.931751	0.046716
7N	-3.008176	-0.740218	-0.016019
8C	-0.940507	-1.970781	-1.635231
9C	-1.925136	-2.817286	-0.825227
10C	-3.232909	-2.054295	-0.634921
11C	-4.162080	-0.119942	0.649943
12C	-3.723749	0.923409	1.673994
13C	-2.828684	1.968860	1.004780
14C	1.841903	2.153530	-0.790922
15O	1.643270	3.327401	-1.132760
16N	2.954814	1.502201	-0.603796
17C	3.078054	0.304895	0.098661
18C	3.936588	-0.695584	-0.407256
19C	4.134491	-1.892688	0.282138
20C	3.491408	-2.127458	1.504700
21C	2.654666	-1.135597	2.029616
22C	2.452669	0.064488	1.344438
23H	1.212720	-0.280294	-1.691563
24H	-0.324839	2.938257	0.405490
25H	0.037956	-2.458786	-1.700426
26H	-1.314186	-1.864985	-2.663779
27H	-1.496036	-3.055780	0.156257
28H	-2.134229	-3.763165	-1.336210
29H	-3.743568	-1.918353	-1.600500
30H	-3.909212	-2.612627	0.019370
31H	-4.728335	-0.919433	1.137120
32H	-4.817675	0.335973	-0.107798
33H	-3.178764	0.426706	2.487123
34H	-4.612134	1.394526	2.108004
35H	-3.427396	2.561869	0.298571
36H	-2.423121	2.670034	1.742230
37H	4.441882	-0.513298	-1.352940
38H	4.798571	-2.646297	-0.136480
39H	3.650147	-3.058586	2.043044
40H	2.159446	-1.292122	2.986183
41H	1.814238	0.831531	1.775176

1b-PhNCO-007

1N	0.508401	1.284379	-0.608959
2C	0.354907	0.015436	-1.058013
3C	-0.784641	-0.717403	-0.825801
4C	-1.852594	-0.115345	-0.087938
5C	-1.666201	1.222459	0.386464
6C	-0.494279	1.874190	0.083741
7N	-3.010800	-0.784288	0.138942
8C	-0.901907	-2.139714	-1.324516
9C	-2.373083	-2.517892	-1.509530
10C	-3.157074	-2.196702	-0.240120
11C	-4.063797	-0.213693	0.990705
12C	-4.111237	1.307594	0.877983
13C	-2.739141	1.899157	1.208711
14C	1.798318	2.098621	-0.895161
15O	1.551258	3.246714	-1.289089
16N	2.936272	1.483541	-0.737183
17C	3.127862	0.332304	0.024178
18C	3.985108	-0.675212	-0.469508
19C	4.246157	-1.827724	0.272938

20C	3.669607	-2.008790	1.537106
21C	2.836005	-1.007754	2.049508
22C	2.571542	0.148151	1.311703
23H	1.185170	-0.396571	-1.618261
24H	-0.311856	2.898450	0.387912
25H	-0.440093	-2.817521	-0.592582
26H	-0.344890	-2.258521	-2.260439
27H	-2.472911	-3.585574	-1.732092
28H	-2.803089	-1.960647	-2.351657
29H	-4.223692	-2.387538	-0.391093
30H	-2.821056	-2.834329	0.591863
31H	-3.893041	-0.517813	2.034810
32H	-5.015715	-0.649440	0.672772
33H	-4.874181	1.693948	1.562206
34H	-4.405813	1.586618	-0.141810
35H	-2.723304	2.980096	1.030802
36H	-2.527945	1.749801	2.277270
37H	4.437392	-0.535341	-1.448657
38H	4.906926	-2.588795	-0.137343
39H	3.877177	-2.905283	2.116070
40H	2.393722	-1.121341	3.037554
41H	1.936717	0.924557	1.731087

1b-001

1N	0.000149	2.927530	0.020875
2C	-1.138329	2.212740	-0.001247
3C	-1.214838	0.823423	-0.040782
4C	0.000021	0.087083	-0.041304
5C	1.214875	0.823288	-0.040698
6C	1.138481	2.212681	-0.001353
7N	-0.000041	-1.293651	-0.009901
8C	-2.551351	0.112620	-0.091145
9C	-2.424850	-1.325108	0.422202
10C	-1.245538	-2.019278	-0.257796
11C	1.245331	-2.019324	-0.258078
12C	2.424709	-1.325412	0.421985
13C	2.551393	0.112481	-0.090848
14H	-2.063925	2.788615	0.013364
15H	2.064198	2.788373	0.013482
16H	-3.296355	0.668790	0.490843
17H	-2.919139	0.092659	-1.127829
18H	-3.343627	-1.889416	0.224732
19H	-2.261061	-1.324545	1.507797
20H	-1.431368	-2.104363	-1.342881
21H	-1.123756	-3.035265	0.132804
22H	1.431036	-2.104118	-1.343212
23H	1.123578	-3.035405	0.132293
24H	3.343455	-1.889707	0.224296
25H	2.260993	-1.325257	1.507597
26H	2.919632	0.092921	-1.127386
27H	3.296168	0.668414	0.491655

1b-002

1N	0.000001	2.929437	0.000000
2C	1.133538	2.213258	-0.112929
3C	1.206806	0.824763	-0.139636
4C	0.000000	0.087699	0.000000
5C	-1.206806	0.824764	0.139635
6C	-1.133536	2.213258	0.112930
7N	0.000000	-1.283571	-0.000001
8C	2.515655	0.086511	-0.292749
9C	2.442059	-1.252855	0.450137
10C	1.241091	-2.060082	-0.039404
11C	-1.241092	-2.060081	0.039405
12C	-2.442060	-1.252854	-0.450137
13C	-2.515655	0.086512	0.292748
14H	2.055957	2.788629	-0.196374
15H	-2.055955	2.788630	0.196375
16H	2.721956	-0.104310	-1.356943
17H	3.343902	0.698953	0.083565
18H	2.344968	-1.070489	1.528577
19H	3.354077	-1.840374	0.294097
20H	1.102200	-2.946082	0.593162
21H	1.417413	-2.419544	-1.066108
22H	-1.417414	-2.419541	1.066110
23H	-1.102202	-2.946083	-0.593160
24H	-3.354078	-1.840372	-0.294097
25H	-2.344969	-1.070489	-1.528577
26H	-2.721957	-0.104307	1.356943
27H	-3.343902	0.698954	-0.083567

1c-Me-001

1N	-2.842580	-0.001140	-0.025275
2C	-2.150898	-1.171640	-0.099885
3C	-0.781793	-1.210035	-0.093262
4C	-0.024289	-0.000145	-0.003370
5C	-0.783995	1.209527	0.077249
6C	-2.152562	1.169667	0.067332
7N	1.312601	0.000562	0.001790
8C	2.141446	-1.223649	0.009006
9C	3.550070	-0.702209	0.316272
10C	3.551160	0.702570	-0.304607
11C	2.141981	1.224512	-0.000955
12C	-4.314955	0.001333	0.037525
13H	-2.747325	-2.073925	-0.172654
14H	-0.295894	-2.173662	-0.177174
15H	-0.299850	2.174128	0.159958
16H	-2.751357	2.071130	0.133777
17H	2.090335	-1.707830	-0.975204
18H	1.776461	-1.928382	0.762781
19H	4.324878	-1.355986	-0.093844
20H	3.695468	-0.637750	1.401432
21H	3.699177	0.638030	-1.389410
22H	4.325211	1.356013	0.107461
23H	2.088234	1.707247	0.983806
24H	1.779835	1.930532	-0.754861
25H	-4.695459	0.878025	-0.489672
26H	-4.696269	-0.899456	-0.445404
27H	-4.640577	0.026349	1.081578

1c-Me-002

1N	-2.842578	0.010299	0.006204
2C	-2.153363	-1.162467	0.090962
3C	-0.785484	-1.205558	0.090468
4C	-0.024067	0.003199	0.002724
5C	-0.779789	1.213583	-0.082906
6C	-2.149709	1.178307	-0.081526
7N	1.312867	-0.000466	0.001636
8C	2.139633	-1.226084	-0.007636
9C	3.548443	-0.706089	-0.316637
10C	3.552908	0.697002	0.308066
11C	2.144096	1.222014	0.008062
12C	-4.316401	-0.015430	-0.012530
13H	-2.755341	-2.061755	0.161681
14H	-0.302104	-2.170432	0.175189
15H	-0.293137	2.176801	-0.166819
16H	-2.741157	2.083678	-0.154325
17H	1.772703	-1.929597	-0.761575
18H	2.089697	-1.711117	0.976182
19H	3.691313	-0.638793	-1.401982
20H	4.323211	-1.362185	0.089825
21H	4.327389	1.350275	-0.103452
22H	3.702637	0.629177	1.392422
23H	1.783487	1.925458	0.765212
24H	2.089767	1.708902	-0.974631
25H	-4.694623	1.006703	0.010820
26H	-4.662591	-0.512238	-0.922899
27H	-4.680874	-0.554571	0.865188

1c-PhNCO-001

1N	0.119941	0.531389	-0.021137
2C	-0.753527	1.570626	-0.055988
3C	-2.112638	1.384178	-0.049533
4C	-2.657569	0.065985	-0.007921
5C	-1.710813	-1.003160	0.027453
6C	-0.365893	-0.738685	0.020654
7N	-3.980713	-0.156631	0.000880
8C	-4.995674	0.912976	0.059173
9C	-6.296993	0.157071	0.354386
10C	-6.074082	-1.206497	-0.317035
11C	-4.594309	-1.498265	-0.040607
12C	1.624528	0.835504	-0.025615
13O	1.886844	2.050252	-0.056235
14N	2.314762	-0.271563	0.005697
15C	3.712184	-0.279447	0.009511
16C	4.565266	0.850985	-0.018989
17C	5.954743	0.693258	-0.011682
18C	6.540051	-0.576498	0.023544
19C	5.707458	-1.703429	0.052008
20C	4.321655	-1.555935	0.044846
21H	-0.296513	2.551154	-0.091730

22H	-2.753318	2.256407	-0.085429
23H	-2.031561	-2.036384	0.072943
24H	0.387492	-1.514060	0.051776
25H	-5.037735	1.439755	-0.903942
26H	-4.742905	1.638505	0.838570
27H	-7.174339	0.688055	-0.025964
28H	-6.416032	0.030841	1.437481
29H	-6.242283	-1.128576	-1.398165
30H	-6.726576	-1.992429	0.074289
31H	-4.450600	-2.003655	0.924392
32H	-4.130496	-2.108753	-0.821680
33H	4.131751	1.842426	-0.047150
34H	6.585870	1.579810	-0.034723
35H	7.621743	-0.687373	0.028810
36H	6.140655	-2.701243	0.079870
37H	3.675845	-2.430866	0.067234

1c-PhNCO-002

1N	-0.766654	1.449969	-0.182233
2C	-0.411451	0.454790	-1.033503
3C	0.851100	-0.081962	-1.038913
4C	1.836140	0.392414	-0.120979
5C	1.430148	1.448894	0.750581
6C	0.154081	1.947854	0.679425
7N	3.075547	-0.120556	-0.083272
8C	4.102492	0.274442	0.899807
9C	5.187021	-0.796799	0.734625
10C	5.081738	-1.178937	-0.749782
11C	3.571962	-1.149902	-1.017072
12C	-2.190141	2.086104	-0.210835
13O	-2.146350	3.322704	-0.178432
14N	-3.200665	1.272396	-0.313255
15C	-3.177125	-0.085619	-0.000769
16C	-3.856406	-0.989630	-0.846248
17C	-3.903367	-2.353212	-0.553501
18C	-3.285824	-2.857989	0.598430
19C	-2.629034	-1.969944	1.458238
20C	-2.577747	-0.604160	1.170350
21H	-1.180802	0.109023	-1.711836
22H	1.071840	-0.874462	-1.742604
23H	2.118714	1.886365	1.462821
24H	-0.183818	2.767026	1.302843
25H	3.678286	0.295902	1.908513
26H	4.480511	1.278121	0.661662
27H	4.954660	-1.662864	1.366471
28H	6.176415	-0.424568	1.015744
29H	5.583908	-0.426708	-1.370258
30H	5.518637	-2.155584	-0.976895
31H	3.331195	-0.878801	-2.050084
32H	3.097828	-2.115077	-0.792819
33H	-4.340773	-0.599197	-1.738243
34H	-4.428923	-3.026376	-1.227819
35H	-3.327363	-3.919869	0.827726
36H	-2.159124	-2.340678	2.367227
37H	-2.079505	0.075392	1.857193

1c-PhNCO-003

1N	-0.758682	1.451680	-0.185822
2C	-0.409059	0.448431	-1.030023
3C	0.850524	-0.095424	-1.031308
4C	1.839605	0.382114	-0.119047
5C	1.440125	1.449057	0.742651
6C	0.165576	1.951766	0.670606
7N	3.076337	-0.137417	-0.080275
8C	4.164327	0.377699	0.773693
9C	5.410092	-0.337571	0.237192
10C	4.857389	-1.680236	-0.264803
11C	3.509242	-1.296016	-0.885765
12C	-2.178621	2.095609	-0.216561
13O	-2.127668	3.332080	-0.187813
14N	-3.193885	1.287619	-0.316096
15C	-3.179204	-0.069462	0.000321
16C	-3.865669	-0.971051	-0.841928
17C	-3.921941	-2.333419	-0.545278
18C	-3.306851	-2.839285	0.607506
19C	-2.642980	-1.953455	1.464167
20C	-2.582342	-0.588863	1.172389
21H	-1.178095	0.107472	-1.711164
22H	1.073477	-0.878971	-1.744363
23H	2.123450	1.876546	1.465658
24H	-0.170089	2.771455	1.294488
25H	3.967205	0.121241	1.823681

26H	4.234404	1.467017	0.691152
27H	6.181527	-0.446995	1.004947
28H	5.836298	0.232607	-0.597351
29H	5.513998	-2.175641	-0.985820
30H	4.697471	-2.363046	0.578657
31H	3.614582	-0.999583	-1.938466
32H	2.769857	-2.100920	-0.825279
33H	-4.348257	-0.579642	-1.734456
34H	-4.452999	-3.004700	-1.217147
35H	-3.355808	-3.900169	0.839907
36H	-2.174875	-2.324923	2.373788
37H	-2.078465	0.089058	1.856741

1c-001

1N	3.387413	-0.000019	-0.000157
2C	2.667936	1.135092	0.084666
3C	1.280302	1.199623	0.089325
4C	0.525668	0.000003	0.000153
5C	1.280256	-1.199624	-0.089174
6C	2.667902	-1.135105	-0.084805
7N	-0.833497	0.000023	0.000153
8C	-1.650856	-1.220094	0.008011
9C	-3.064552	-0.703570	0.308765
10C	-3.064436	0.703572	-0.309169
11C	-1.650901	1.220111	-0.007730
12H	3.241392	2.058240	0.157313
13H	0.793735	2.165148	0.173949
14H	0.793672	-2.165148	-0.173698
15H	3.241316	-2.058269	-0.157600
16H	-1.601591	-1.723272	-0.969556
17H	-1.292578	-1.924117	0.768186
18H	-3.213784	-0.638946	1.393946
19H	-3.839926	-1.356995	-0.103018
20H	-3.840039	1.356969	0.102229
21H	-3.213093	0.638944	-1.394432
22H	-1.602087	1.723029	0.970005
23H	-1.292346	1.924347	-0.767555

1d-001

1N	-4.147575	-1.574945	-1.386155
2C	-2.822081	-1.823217	-1.372059
3C	-1.871431	-1.113941	-0.625820
4C	-2.348912	-0.049880	0.206111
5C	-3.739044	0.184246	0.205492
6C	-4.577733	-0.584130	-0.597188
7N	-1.477206	0.693175	0.959659
8N	-0.491639	-1.406012	-0.683483
9C	0.240844	-1.022885	0.535954
10C	-0.037947	0.473092	0.867150
11C	-0.154070	-2.714853	-1.245999
12C	-1.916342	1.819525	1.784671
13C	-2.407237	1.386029	3.168742
14C	0.628657	1.478884	-0.064431
15C	0.119359	1.733947	-1.346436
16C	0.757475	2.641282	-2.195766
17C	1.910356	3.313294	-1.772834
18C	2.415534	3.076644	-0.490901
19C	1.774846	2.166138	0.355058
20C	1.738501	-1.268679	0.461064
21C	2.398275	-1.797676	1.577674
22C	3.786219	-1.975964	1.573242
23C	4.530981	-1.634953	0.440938
24C	3.879196	-1.113485	-0.682936
25C	2.495813	-0.927930	-0.670726
26H	-2.506682	-2.638883	-2.012401
27H	-4.173721	0.957260	0.827804
28H	-5.649010	-0.390119	-0.597088
29H	-0.150998	-1.594542	1.394655
30H	0.375621	0.621440	1.872123
31H	-0.670744	-3.537445	-0.723355
32H	-0.421475	-2.748444	-2.306240
33H	0.919001	-2.883005	-1.175240
34H	-2.690594	2.384831	1.253845
35H	-1.063615	2.498136	1.886024
36H	-2.713217	2.261163	3.755797
37H	-3.262569	0.705521	3.093566
38H	-1.609675	0.868386	3.715910
39H	-0.776105	1.222651	-1.684417
40H	0.353383	2.823856	-3.188727
41H	2.405145	4.019874	-2.434881
42H	3.306492	3.598061	-0.149164
43H	2.178220	1.976936	1.347747

44H	1.823487	-2.072120	2.460167
45H	4.280198	-2.388441	2.449740
46H	5.608880	-1.777492	0.431224
47H	4.449287	-0.846320	-1.569484
48H	1.996089	-0.519757	-1.543734

1d-002

1N	-4.084833	-1.868409	-1.125357
2C	-2.752226	-2.071032	-1.133663
3C	-1.812980	-1.329371	-0.402816
4C	-2.314450	-0.288310	0.444617
5C	-3.708632	-0.085152	0.445958
6C	-4.535292	-0.885512	-0.338278
7N	-1.456258	0.450870	1.225095
8N	-0.428345	-1.574750	-0.498258
9C	0.355735	-1.114004	0.656600
10C	-0.017499	0.361103	0.997121
11C	-0.055517	-2.882665	-1.040901
12C	-1.936028	1.514695	2.109669
13C	-2.236773	2.851054	1.418571
14C	0.499105	1.396891	0.003914
15C	-0.099906	1.581740	-1.250881
16C	0.399387	2.533363	-2.143471
17C	1.505544	3.317003	-1.794921
18C	2.105461	3.143719	-0.544169
19C	1.601815	2.190405	0.345899
20C	1.859121	-1.231132	0.465349
21C	2.652188	-1.621054	1.552002
22C	4.046328	-1.667143	1.442487
23C	4.663661	-1.330829	0.234410
24C	3.878260	-0.947653	-0.859197
25C	2.488197	-0.892835	-0.742370
26H	-2.419925	-2.877768	-1.776881
27H	-4.156555	0.698564	1.044532
28H	-5.611084	-0.718942	-0.331316
29H	0.083751	-1.701470	1.549797
30H	0.466298	0.558982	1.959946
31H	-0.539604	-3.709416	-0.495073
32H	-0.332549	-2.948966	-2.097420
33H	1.023288	-3.014477	-0.978299
34H	-1.163807	1.662475	2.872562
35H	-2.824712	1.150754	2.637923
36H	-2.658319	3.555398	2.147224
37H	-1.327956	3.293193	0.999575
38H	-2.959288	2.728756	0.604601
39H	-0.962609	0.988663	-1.534785
40H	-0.078167	2.663664	-3.111829
41H	1.892234	4.058214	-2.490216
42H	2.964133	3.747829	-0.260762
43H	2.077385	2.055025	1.315277
44H	2.175673	-1.891329	2.492574
45H	4.645638	-1.971667	2.297191
46H	5.746495	-1.369408	0.143518
47H	4.349107	-0.684043	-1.803198
48H	1.883644	-0.587690	-1.590891

1d-003

1N	4.631127	0.200692	-0.172134
2C	3.651554	0.671540	0.622098
3C	2.327018	0.206155	0.631809
4C	1.969960	-0.814925	-0.305411
5C	3.006215	-1.300890	-1.121579
6C	4.294127	-0.773922	-1.022649
7N	0.652205	-1.250667	-0.419493
8N	1.378000	0.695730	1.530168
9C	-0.029677	0.548105	1.165523
10C	-0.257659	-0.916141	0.689837
11C	1.703492	1.857983	2.343859
12C	0.402836	-2.530860	-1.105407
13C	0.856588	-3.763218	-0.314609
14C	-1.726021	-1.141441	0.365898
15C	-2.305337	-0.702523	-0.834699
16C	-3.672018	-0.866623	-1.065793
17C	-4.484725	-1.466444	-0.096305
18C	-3.917462	-1.907030	1.102441
19C	-2.545406	-1.747201	1.326888
20C	-0.542714	1.639188	0.230144
21C	-1.682586	2.370299	0.593468
22C	-2.193590	3.371903	-0.237287
23C	-1.560907	3.664421	-1.449226
24C	-0.415029	2.950699	-1.816600
25C	0.089213	1.946953	-0.985488

26H	3.945753	1.465942	1.299695
27H	2.827877	-2.090628	-1.840252
28H	5.084685	-1.160310	-1.663329
29H	-0.601850	0.627783	2.096037
30H	-0.010671	-1.541125	1.560445
31H	2.569821	1.648143	2.980404
32H	1.917299	2.754917	1.741115
33H	0.852944	2.076256	2.994778
34H	0.883679	-2.496836	-2.086787
35H	-0.667333	-2.598061	-1.301795
36H	0.659642	-4.672396	-0.896105
37H	1.927604	-3.728403	-0.086647
38H	0.308376	-3.843995	0.631391
39H	-1.681152	-0.234686	-1.589685
40H	-4.103995	-0.520591	-2.001724
41H	-5.549617	-1.591352	-0.276939
42H	-4.537397	-2.379839	1.860411
43H	-2.107601	-2.097081	2.260081
44H	-2.184128	2.143621	1.532261
45H	-3.082932	3.921592	0.061766
46H	-1.952882	4.443035	-2.099161
47H	0.089186	3.172497	-2.754340
48H	0.976154	1.405059	-1.292870

1d-004

1N	-4.192979	-1.680742	-1.100633
2C	-2.883231	-1.989730	-1.028971
3C	-1.913928	-1.258316	-0.326881
4C	-2.358765	-0.112042	0.407954
5C	-3.724834	0.213325	0.307479
6C	-4.586905	-0.588680	-0.438954
7N	-1.471130	0.613686	1.183379
8N	-0.553779	-1.610254	-0.363660
9C	0.271656	-1.053947	0.713997
10C	-0.041879	0.458068	0.913271
11C	-0.259715	-2.994052	-0.741774
12C	-1.921249	1.873092	1.795882
13C	-0.961109	2.442187	2.838375
14C	0.470857	1.384963	-0.184681
15C	-0.169287	1.502299	-1.427433
16C	0.342863	2.349030	-2.414832
17C	1.502858	3.093415	-2.175489
18C	2.142567	2.991416	-0.936290
19C	1.625504	2.145409	0.048454
20C	1.763776	-1.242711	0.488552
21C	2.583644	-1.547754	1.582124
22C	3.970309	-1.656118	1.429625
23C	4.551429	-1.467043	0.172486
24C	3.737949	-1.170468	-0.927680
25C	2.355635	-1.055449	-0.769682
26H	-2.592947	-2.875453	-1.582377
27H	-4.129791	1.086794	0.802651
28H	-5.642362	-0.330331	-0.504319
29H	0.011233	-1.536419	1.671044
30H	0.490494	0.718282	1.829963
31H	-0.824396	-3.715530	-0.129006
32H	-0.499183	-3.164949	-1.795808
33H	0.803444	-3.190991	-0.612782
34H	-2.873709	1.672433	2.294825
35H	-2.112187	2.626379	1.014299
36H	-1.446954	3.296099	3.324715
37H	-0.727478	1.702609	3.613780
38H	-0.025475	2.804256	2.400915
39H	-1.069303	0.933606	-1.633997
40H	-0.165686	2.424449	-3.373159
41H	1.900709	3.750208	-2.945358
42H	3.043347	3.566844	-0.736024
43H	2.133653	2.064089	1.007008
44H	2.134267	-1.701801	2.561451
45H	4.591495	-1.893868	2.289869
46H	5.628153	-1.554041	0.048500
47H	4.181366	-1.022667	-1.909411
48H	1.727649	-0.820190	-1.623586

1d-005

1N	-4.683757	-0.157085	0.009318
2C	-3.730741	0.489967	-0.688282
3C	-2.375428	0.126651	-0.730410
4C	-1.958308	-0.991547	0.060967
5C	-2.965615	-1.656248	0.781929
6C	-4.288233	-1.214013	0.724710
7N	-0.619841	-1.363664	0.120282

8N	-1.454853	0.803652	-1.528993
9C	-0.038565	0.670833	-1.196642
10C	0.262794	-0.832845	-0.933356
11C	-1.846075	2.054585	-2.162345
12C	-0.297319	-2.701503	0.653160
13C	-0.108237	-2.729218	2.172161
14C	1.741452	-1.042607	-0.649175
15C	2.318779	-0.725826	0.589413
16C	3.690267	-0.884422	0.796157
17C	4.510320	-1.352715	-0.236896
18C	3.945850	-1.666293	-1.476629
19C	2.569257	-1.515572	-1.675999
20C	0.436261	1.641892	-0.120066
21C	-0.218229	1.775040	1.114774
22C	0.258603	2.665597	2.080710
23C	1.397665	3.438395	1.829778
24C	2.050617	3.321423	0.599112
25C	1.568424	2.431872	-0.365228
26H	-4.074522	1.347861	-1.256230
27H	-2.737325	-2.511477	1.404583
28H	-5.056561	-1.739170	1.289202
29H	0.517774	0.906671	-2.110231
30H	0.033697	-1.342693	-1.881846
31H	-2.678510	1.890713	-2.855616
32H	-2.141435	2.825942	-1.433814
33H	-0.997942	2.433799	-2.737930
34H	0.623720	-3.037955	0.173471
35H	-1.078430	-3.411390	0.349119
36H	0.017245	-3.765511	2.511226
37H	0.782272	-2.164797	2.465561
38H	-0.965726	-2.300009	2.700271
39H	1.692418	-0.346867	1.389208
40H	4.120040	-0.633722	1.763021
41H	5.578785	-1.472887	-0.075201
42H	4.571880	-2.034653	-2.285807
43H	2.132971	-1.771143	-2.639841
44H	-1.102690	1.186503	1.331300
45H	-0.261062	2.753526	3.032007
46H	1.768317	4.128648	2.583794
47H	2.934841	3.918741	0.389276
48H	2.088163	2.338874	-1.316828

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1N	-4.150160	-0.996422	-0.690316
2C	-2.877255	-1.492166	-0.746078
3C	-1.790344	-0.833153	-0.192565
4C	-2.034661	0.426926	0.477646
5C	-3.378776	0.864293	0.557283
6C	-4.398046	0.155835	-0.036554
7N	-1.012111	1.138450	0.990851
8N	-0.499792	-1.343919	-0.277654
9C	0.418878	-0.867838	0.776111
10C	0.375463	0.684137	0.843208
11C	-0.393677	-2.747862	-0.680804
12C	-1.196915	2.448803	1.637277
13C	-1.556726	2.328257	3.118261
14C	1.077093	1.412769	-0.295067
15C	2.340946	1.973378	-0.071421
16C	3.027817	2.622014	-1.101352
17C	2.451012	2.720922	-2.370927
18C	1.182519	2.175986	-2.599064
19C	0.498458	1.528641	-1.566944
20C	1.854294	-1.335114	0.607711
21C	2.578357	-1.709718	1.746469
22C	3.927596	-2.067001	1.650358
23C	4.564072	-2.063609	0.406303
24C	3.844478	-1.700942	-0.738023
25C	2.502069	-1.332590	-0.637147
26C	-5.226161	-1.744424	-1.363120
27H	-2.780382	-2.431902	-1.269376
28H	-3.636195	1.771509	1.085661
29H	-5.426806	0.491233	-0.001926
30H	0.058234	-1.224341	1.753829
31H	0.889500	0.941984	1.775440
32H	0.641229	-3.074469	-0.615742
33H	-1.005195	-3.402752	-0.040070
34H	-0.712786	-2.865736	-1.721267
35H	-1.950773	3.021135	1.088348
36H	-0.255190	2.990422	1.517377
37H	-1.660998	3.327013	3.558252
38H	-2.499875	1.789965	3.263070
39H	-0.771033	1.794943	3.666597
40H	2.795822	1.890462	0.913050
41H	4.009576	3.048557	-0.911691
42H	2.980950	3.225523	-3.174783

43H	0.723472	2.256890	-3.581313
44H	-0.487005	1.116397	-1.760081
45H	2.085896	-1.721663	2.716741
46H	4.475647	-2.352738	2.544682
47H	5.610953	-2.345673	0.326847
48H	4.331032	-1.695987	-1.710098
49H	1.953290	-1.041078	-1.527429
50H	-5.254503	-2.767835	-0.980964
51H	-6.181165	-1.256726	-1.163779
52H	-5.042200	-1.757164	-2.440892

1d-Me-002

1N	4.122516	-1.125045	0.567142
2C	2.839470	-1.577322	0.696013
3C	1.755227	-0.935056	0.116819
4C	2.017003	0.240984	-0.688750
5C	3.366297	0.653269	-0.805071
6C	4.381973	-0.031491	-0.176348
7N	1.003087	0.894254	-1.295872
8N	0.454725	-1.387787	0.297211
9C	-0.486530	-1.002049	-0.771942
10C	-0.391478	0.532099	-1.010240
11C	0.307180	-2.714992	0.894955
12C	1.227496	2.087100	-2.131753
13C	1.402220	3.386325	-1.339704
14C	-0.996278	1.405093	0.080546
15C	-2.238328	2.012595	-0.140856
16C	-2.833132	2.804645	0.845463
17C	-2.186121	2.999931	2.069035
18C	-0.940626	2.403107	2.295239
19C	-0.349176	1.613135	1.306813
20C	-1.926986	-1.406511	-0.512379
21C	-2.554469	-1.204081	0.726670
22C	-3.899574	-1.533467	0.901128
23C	-4.640898	-2.059953	-0.163132
24C	-4.024716	-2.262548	-1.400952
25C	-2.673935	-1.940750	-1.569947
26C	5.200177	-1.864575	1.247398
27H	2.731386	-2.470496	1.293370
28H	3.634911	1.532651	-1.373731
29H	5.416015	0.282349	-0.247013
30H	-0.171378	-1.474406	-1.715500
31H	-0.949932	0.712816	-1.932986
32H	-0.744583	-2.987482	0.931967
33H	0.845832	-3.485369	0.320647
34H	0.683118	-2.705764	1.923163
35H	0.361682	2.167563	-2.795373
36H	2.093753	1.897963	-2.773313
37H	1.637394	4.203622	-2.031885
38H	0.487500	3.644879	-0.799167
39H	2.216876	3.310095	-0.611272
40H	-2.749677	1.855951	-1.088173
41H	-3.798415	3.267955	0.657223
42H	-2.644386	3.616412	2.838222
43H	-0.427037	2.555198	3.241505
44H	0.621548	1.166528	1.496552
45H	-1.988130	-0.790061	1.555062
46H	-4.371292	-1.372964	1.867269
47H	-5.689182	-2.313209	-0.026290
48H	-4.589480	-2.675776	-2.232815
49H	-2.196822	-2.106477	-2.533870
50H	6.152243	-1.371314	1.049796
51H	5.011995	-1.873987	2.324207
52H	5.234972	-2.889552	0.868996

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1N	4.305052	-0.079692	-0.182775
2C	3.367904	0.507979	0.616582
3C	2.043656	0.091387	0.642794
4C	1.634250	-0.958373	-0.265231
5C	2.648841	-1.529972	-1.064620
6C	3.953664	-1.083580	-1.007351
7N	0.329609	-1.339940	-0.340589
8N	1.132329	0.644292	1.514030
9C	-0.289894	0.552527	1.175649
10C	-0.598033	-0.904912	0.731856
11C	1.533920	1.766242	2.351909
12C	-0.021544	-2.566998	-1.086099
13C	0.301700	-3.849669	-0.315988
14C	-2.067554	-1.057814	0.377742
15C	-2.604275	-0.593547	-0.833290
16C	-3.972022	-0.698910	-1.088571

17C	-4.826604	-1.259271	-0.131830
18C	-4.301918	-1.720054	1.078299
19C	-2.928482	-1.622193	1.327067
20C	-0.757586	1.657139	0.234108
21C	-0.113139	1.930557	-0.982134
22C	-0.582199	2.942032	-1.824374
23C	-1.704041	3.696214	-1.464108
24C	-2.347922	3.436911	-0.250763
25C	-1.872717	2.427291	0.590785
26C	5.692646	0.411285	-0.114592
27H	3.732073	1.314906	1.235461
28H	2.435866	-2.346054	-1.740466
29H	4.737114	-1.521417	-1.612922
30H	-0.836922	0.672258	2.115673
31H	-0.400642	-1.530087	1.612007
32H	0.705398	2.017841	3.016641
33H	2.393836	1.485713	2.970252
34H	1.790409	2.659083	1.761954
35H	0.486605	-2.538420	-2.052447
36H	-1.086984	-2.527955	-1.304261
37H	0.032469	-4.721212	-0.923973
38H	1.366603	-3.920505	-0.067945
39H	-0.273394	-3.897660	0.615780
40H	-1.949902	-0.153841	-1.579512
41H	-4.371500	-0.337510	-2.032754
42H	-5.892313	-1.337800	-0.331309
43H	-4.956078	-2.160786	1.826257
44H	-2.525053	-1.987390	2.269552
45H	0.754673	1.355431	-1.286837
46H	-0.071672	3.138196	-2.764224
47H	-2.069731	4.480643	-2.121866
48H	-3.219155	4.018077	0.040767
49H	-2.383233	2.224608	1.529860
50H	6.303284	-0.136951	-0.832269
51H	5.712472	1.476576	-0.359001
52H	6.084933	0.256009	0.893901

1d-Me-004

1N	-4.333662	-0.285381	0.044067
2C	-3.419218	0.427365	-0.676597
3C	-2.075932	0.077532	-0.731021
4C	-1.629465	-1.059768	0.046451
5C	-2.620468	-1.751607	0.777468
6C	-3.942899	-1.356109	0.759025
7N	-0.318073	-1.420499	0.059233
8N	-1.182265	0.772607	-1.513586
9C	0.244382	0.668947	-1.198295
10C	0.586441	-0.825715	-0.955712
11C	-1.615387	1.986104	-2.194656
12C	0.069221	-2.719663	0.655818
13C	0.251093	-2.676156	2.174183
14C	2.062439	-1.011458	-0.648751
15C	2.627457	-0.658780	0.585727
16C	3.998022	-0.804931	0.805526
17C	4.827231	-1.293567	-0.210305
18C	4.274735	-1.640115	-1.446420
19C	2.899057	-1.503432	-1.659488
20C	0.696621	1.653587	-0.125677
21C	0.059742	1.753729	1.120984
22C	0.518773	2.656949	2.083434
23C	1.621449	3.474855	1.814624
24C	2.256237	3.389377	0.572275
25C	1.792540	2.486723	-0.388776
26C	-5.740707	0.151662	0.020129
27H	-3.816977	1.276564	-1.213454
28H	-2.375588	-2.615643	1.377441
29H	-4.708591	-1.886614	1.311330
30H	0.779541	0.921120	-2.118356
31H	0.382918	-1.331682	-1.908992
32H	-2.437366	1.761674	-2.883505
33H	-1.939968	2.766365	-1.490565
34H	-0.779600	2.375520	-2.778720
35H	1.005942	-3.022156	0.187454
36H	-0.676248	-3.471992	0.371016
37H	0.435976	-3.691737	2.544184
38H	1.106226	-2.053152	2.449667
39H	-0.631632	-2.283391	2.688703
40H	1.996223	-0.263430	1.373621
41H	4.419540	-0.528540	1.768714
42H	5.894936	-1.403058	-0.038017
43H	4.909197	-2.022727	-2.241889
44H	2.472196	-1.783777	-2.620673
45H	-0.794288	1.127629	1.356204
46H	0.015619	2.719251	3.045343
47H	1.979154	4.175009	2.565322

48H	3.112508	4.021333	0.350199
49H	2.299156	2.418079	-1.349269
50H	-5.805576	1.184540	0.371592
51H	-6.126013	0.082750	-1.000605
52H	-6.327456	-0.492204	0.675581

1d-Me-005

1N	4.210642	-0.939169	0.525205
2C	2.962547	-1.494282	0.542257
3C	1.845447	-0.848153	0.031685
4C	2.039173	0.443983	-0.594065
5C	3.348569	0.978984	-0.565265
6C	4.400590	0.279379	-0.014263
7N	0.999745	1.092934	-1.172203
8N	0.580685	-1.407766	0.121618
9C	-0.410387	-0.906612	-0.846316
10C	-0.372442	0.647012	-0.896342
11C	0.517217	-2.825518	0.481122
12C	1.200705	2.439982	-1.750273
13C	0.085441	2.902413	-2.682120
14C	-0.978706	1.365116	0.303406
15C	-2.270858	1.896689	0.193991
16C	-2.880448	2.528961	1.280265
17C	-2.197312	2.644347	2.494674
18C	-0.901999	2.129109	2.609822
19C	-0.296383	1.495184	1.521085
20C	-1.824949	-1.384395	-0.568136
21C	-2.632058	-1.766890	-1.646063
22C	-3.962852	-2.147680	-1.442213
23C	-4.495521	-2.159023	-0.150329
24C	-3.691749	-1.786561	0.933630
25C	-2.367907	-1.397063	0.725555
26C	5.328331	-1.713185	1.093260
27H	2.910638	-2.471946	0.997166
28H	3.560844	1.959267	-0.966555
29H	5.406990	0.678616	0.009204
30H	-0.132017	-1.244561	-1.856585
31H	-0.973201	0.896620	-1.771854
32H	-0.512068	-3.172097	0.428203
33H	1.127852	-3.444151	-0.194885
34H	0.862571	-2.970833	1.510046
35H	2.129964	2.411099	-2.324709
36H	1.333241	3.162340	-0.932464
37H	0.396277	3.852579	-3.130624
38H	-0.083190	2.188049	-3.496116
39H	-0.858703	3.080590	-2.159390
40H	-2.809734	1.802355	-0.746141
41H	-3.885954	2.929177	1.177700
42H	-2.667304	3.136411	3.342402
43H	-0.360819	2.220171	3.548470
44H	0.709643	1.103759	1.633391
45H	-2.218900	-1.767557	-2.652909
46H	-4.576627	-2.440532	-2.290314
47H	-5.527660	-2.458787	0.012771
48H	-4.098106	-1.792792	1.941838
49H	-1.750566	-1.102577	1.568747
50H	5.446907	-2.644662	0.533305
51H	6.244743	-1.127211	1.021635
52H	5.120982	-1.936098	2.143130

1d-PhNCO-001

1N	-2.387332	-1.290086	-0.253697
2C	-1.520562	-0.238581	-0.258225
3C	-0.149980	-0.396487	-0.369014
4C	0.369734	-1.735643	-0.506222
5C	-0.573613	-2.791542	-0.533564
6C	-1.920871	-2.545810	-0.399501
7N	1.701185	-1.950102	-0.598472
8N	0.722945	0.699012	-0.344362
9C	1.988499	0.460845	-1.062780
10C	2.653320	-0.838785	-0.524094
11C	0.092440	2.008135	-0.533006
12C	2.285465	-3.293837	-0.713623
13C	2.315483	-3.795773	-2.158021
14C	3.269690	-0.733512	0.864640
15C	2.475804	-0.751170	2.020426
16C	3.060431	-0.622072	3.282827
17C	4.447385	-0.480879	3.406133
18C	5.246726	-0.477705	2.259106
19C	4.658216	-0.605284	0.997717
20C	2.973962	1.614061	-0.989171
21C	3.704001	1.953114	-2.135241

22C	4.675902	2.958842	-2.092833
23C	4.920464	3.644468	-0.899848
24C	4.189696	3.316728	0.248323
25C	3.229436	2.304824	0.205363
26C	-3.901584	-1.078807	-0.107005
27O	-4.560612	-2.131054	-0.166641
28N	-4.174828	0.188004	0.048645
29C	-5.480524	0.659492	0.200457
30C	-6.666364	-0.115239	0.212590
31C	-7.913279	0.496808	0.375831
32C	-8.026333	1.882342	0.529900
33C	-6.860920	2.660719	0.519402
34C	-5.614179	2.059618	0.357293
35H	-2.005724	0.718019	-0.154343
36H	-0.256508	-3.817709	-0.660368
37H	-2.668940	-3.327273	-0.405651
38H	1.773675	0.270083	-2.127030
39H	3.455820	-1.064930	-1.235010
40H	-0.503335	2.048128	-1.459309
41H	-0.557005	2.237331	0.317357
42H	0.855656	2.781732	-0.580086
43H	1.742087	-3.984520	-0.061868
44H	3.300448	-3.230921	-0.311420
45H	2.777866	-4.789220	-2.199869
46H	1.306128	-3.868274	-2.577613
47H	2.901520	-3.119416	-2.791751
48H	1.399246	-0.864204	1.940075
49H	2.432224	-0.632480	4.170211
50H	4.901078	-0.381718	4.389161
51H	6.325798	-0.375416	2.344245
52H	5.282449	-0.591963	0.106854
53H	3.512472	1.427529	-3.068797
54H	5.233621	3.208670	-2.992099
55H	5.670853	4.430498	-0.864465
56H	4.372339	3.844501	1.181098
57H	2.671962	2.049238	1.101080
58H	-6.599995	-1.189530	0.096036
59H	-8.808079	-0.123027	0.381876
60H	-9.000941	2.347948	0.655839
61H	-6.924728	3.740670	0.637498
62H	-4.709557	2.663674	0.349523

1d-PhNCO-002

1N	-2.376513	-1.235206	-0.449621
2C	-1.521637	-0.183014	-0.315814
3C	-0.153290	-0.300220	-0.494731
4C	0.372635	-1.586587	-0.885539
5C	-0.557731	-2.645515	-1.018794
6C	-1.901638	-2.446936	-0.796799
7N	1.697438	-1.747947	-1.120833
8N	0.705958	0.788309	-0.306875
9C	1.952546	0.708200	-1.087980
10C	2.641168	-0.663422	-0.829112
11C	0.058168	2.099045	-0.223441
12C	2.268431	-3.046771	-1.512199
13C	2.480936	-4.019937	-0.347603
14C	3.289983	-0.823387	0.539228
15C	4.685310	-0.775290	0.645974
16C	5.313360	-0.902611	1.888471
17C	4.546204	-1.084372	3.042721
18C	3.151218	-1.143387	2.943545
19C	2.527566	-1.016045	1.700327
20C	2.927156	1.841421	-0.816563
21C	3.591551	2.436409	-1.896465
22C	4.544692	3.439212	-1.686735
23C	4.835858	3.865357	-0.388084
24C	4.169847	3.282304	0.696419
25C	3.226046	2.276212	0.484190
26C	-3.888328	-1.072522	-0.230216
27O	-4.528095	-2.130356	-0.358940
28N	-4.181459	0.169866	0.042140
29C	-5.492243	0.595870	0.269909
30C	-5.654332	1.978081	0.526010
31C	-6.909299	2.533495	0.768451
32C	-8.054275	1.725256	0.764404
33C	-7.912675	0.356643	0.513529
34C	-6.657609	-0.209503	0.268455
35H	-2.013277	0.738812	-0.051128
36H	-0.235679	-3.642346	-1.287014
37H	-2.638118	-3.234536	-0.883387
38H	1.711655	0.722840	-2.163413
39H	3.431847	-0.728794	-1.583107
40H	-0.561314	2.308984	-1.110148
41H	-0.572975	2.147528	0.669025
42H	0.812687	2.877785	-0.135871

43H	3.224803	-2.834110	-1.999003
44H	1.622885	-3.490773	-2.277325
45H	2.832334	-4.983012	-0.737596
46H	3.227313	-3.638326	0.355001
47H	1.552121	-4.193747	0.205950
48H	5.285387	-0.627709	-0.249430
49H	6.397899	-0.860087	1.952835
50H	5.030005	-1.185416	4.011093
51H	2.547236	-1.291150	3.835550
52H	1.445628	-1.070414	1.640426
53H	3.361773	2.116015	-2.910760
54H	5.049642	3.890302	-2.537380
55H	5.571661	4.648192	-0.221194
56H	4.387821	3.608482	1.710383
57H	2.714865	1.827343	1.329918
58H	-4.765599	2.605249	0.528610
59H	-6.995393	3.600933	0.961699
60H	-9.035223	2.154771	0.953397
61H	-8.791115	-0.286104	0.506570
62H	-6.569770	-1.270938	0.074790

1d-PhNCO-003

1N	2.393307	0.034883	-0.160842
2C	1.277361	-0.734938	-0.047053
3C	-0.000079	-0.245974	-0.264769
4C	-0.139538	1.137530	-0.644776
5C	1.054581	1.888275	-0.786464
6C	2.284312	1.326728	-0.536037
7N	-1.363547	1.675514	-0.846138
8N	-1.135921	-1.053892	-0.118289
9C	-2.275841	-0.621362	-0.948140
10C	-2.581090	0.878580	-0.669983
11C	-0.876339	-2.494587	-0.056386
12C	-1.565529	3.082491	-1.219874
13C	-1.457578	3.307029	-2.729383
14C	-3.247354	1.175030	0.666225
15C	-4.622312	1.439249	0.708274
16C	-5.266730	1.682150	1.924619
17C	-4.536539	1.667160	3.116760
18C	-3.159792	1.417591	3.082044
19C	-2.518891	1.175739	1.864261
20C	-3.533397	-1.451690	-0.758997
21C	-3.996573	-1.832760	0.509820
22C	-5.190907	-2.541804	0.645291
23C	-5.948130	-2.871289	-0.485129
24C	-5.496082	-2.494148	-1.752552
25C	-4.291944	-1.793961	-1.885415
26C	3.749487	-0.622958	0.135127
27O	3.661518	-1.804169	0.513143
28N	4.723076	0.219020	-0.080283
29C	6.062771	-0.121056	0.122902
30C	7.004737	0.900498	-0.145725
31C	8.373242	0.694255	0.018403
32C	8.854783	-0.545664	0.459820
33C	7.938286	-1.567160	0.729386
34C	6.563178	-1.369703	0.567424
35H	1.482749	-1.753872	0.241289
36H	1.028230	2.924405	-1.095945
37H	3.215314	1.868646	-0.624902
38H	-1.994829	-0.678321	-2.012679
39H	-3.270453	1.181057	-1.465860
40H	-0.316846	-2.734442	0.852580
41H	-1.817644	-3.038047	-0.015968
42H	-0.305553	-2.847395	-0.930603
43H	-0.857771	3.710726	-0.670961
44H	-2.561063	3.363105	-0.864509
45H	-1.645772	4.361163	-2.966034
46H	-0.462708	3.041851	-3.103564
47H	-2.196752	2.699228	-3.264905
48H	-5.196326	1.441020	-0.216135
49H	-6.335456	1.881391	1.939837
50H	-5.034159	1.854661	4.065098
51H	-2.583619	1.410354	4.004130
52H	-1.450720	0.984243	1.851186
53H	-3.417606	-1.575849	1.391247
54H	-5.533083	-2.832491	1.635430
55H	-6.879955	-3.420907	-0.377244
56H	-6.072286	-2.749928	-2.638331
57H	-3.939153	-1.510769	-2.875300
58H	6.631726	1.863135	-0.488508
59H	9.067337	1.503854	-0.198306
60H	9.921787	-0.710772	0.589050
61H	8.294191	-2.536943	1.072629
62H	5.871301	-2.173911	0.782971

1d-PhNCO-004

1N	-2.270791	-1.217706	0.396093
2C	-1.564753	-0.348861	-0.377801
3C	-0.190666	-0.442149	-0.537077
4C	0.523668	-1.456364	0.197275
5C	-0.260130	-2.336348	0.975934
6C	-1.630238	-2.197590	1.059259
7N	1.887795	-1.528518	0.146720
8N	0.499450	0.405426	-1.392047
9C	1.911471	0.646233	-1.097372
10C	2.606535	-0.726837	-0.867516
11C	-0.217284	1.505507	-2.025506
12C	2.561214	-2.754403	0.623759
13C	2.395836	-3.939723	-0.331417
14C	4.079845	-0.532433	-0.549968
15C	4.524540	-0.137082	0.720828
16C	5.879842	0.096127	0.956535
17C	6.811275	-0.053390	-0.078071
18C	6.377342	-0.446398	-1.346848
19C	5.018367	-0.688540	-1.577003
20C	2.143687	1.708545	-0.026092
21C	1.479906	1.693046	1.210344
22C	1.731480	2.680860	2.166506
23C	2.652197	3.700435	1.903864
24C	3.311032	3.731385	0.671181
25C	3.053037	2.744417	-0.283690
26C	-3.797654	-1.102336	0.546395
27O	-4.293715	-1.972513	1.281728
28N	-4.249052	-0.090845	-0.143311
29C	-5.605251	0.242092	-0.180916
30C	-5.936246	1.388824	-0.941067
31C	-7.252797	1.829353	-1.062773
32C	-8.292642	1.137890	-0.426733
33C	-7.983912	0.001721	0.328202
34C	-6.665650	-0.447162	0.456929
35H	-2.170342	0.402724	-0.858443
36H	0.190579	-3.147873	1.529657
37H	-2.255650	-2.854181	1.648990
38H	2.358782	1.020411	-2.023495
39H	2.536801	-1.251727	-1.829243
40H	0.471523	2.029529	-2.692553
41H	-1.046570	1.120051	-2.627747
42H	-0.614009	2.227094	-1.295210
43H	2.190681	-2.990669	1.624490
44H	3.618679	-2.523055	0.742735
45H	2.908790	-4.818372	0.077420
46H	1.342035	-4.197617	-0.483072
47H	2.837583	-3.714788	-1.309100
48H	3.806652	-0.014319	1.526023
49H	6.208218	0.401158	1.947010
50H	7.866581	0.132065	0.106115
51H	7.092876	-0.571100	-2.155819
52H	4.685376	-1.000683	-2.565015
53H	0.759392	0.915683	1.439589
54H	1.206140	2.651462	3.118006
55H	2.847444	4.466887	2.649719
56H	4.024304	4.522174	0.451825
57H	3.574447	2.771714	-1.238071
58H	-5.129273	1.926136	-1.434362
59H	-7.469199	2.716079	-1.655356
60H	-9.321291	1.478174	-0.518883
61H	-8.779002	-0.547914	0.828788
62H	-6.447943	-1.328346	1.047019

1d-PhNCO-005

1N	2.343975	-0.220724	0.284884
2C	1.360951	0.424817	0.965339
3C	0.028696	0.042077	0.897212
4C	-0.329737	-1.047705	0.027659
5C	0.731437	-1.681252	-0.657928
6C	2.035961	-1.258909	-0.517258
7N	-1.635680	-1.421692	-0.128959
8N	-0.947216	0.668704	1.658106
9C	-2.322743	0.609302	1.166282
10C	-2.648679	-0.865782	0.793425
11C	-0.591636	1.848885	2.436099
12C	-1.937403	-2.740016	-0.724907
13C	-1.631311	-3.908067	0.216499
14C	-4.069906	-0.982353	0.267519
15C	-5.079975	-1.400917	1.142003
16C	-6.413507	-1.454028	0.721129
17C	-6.747328	-1.096150	-0.587711

18C	-5.741791	-0.684231	-1.470680
19C	-4.414313	-0.623719	-1.044733
20C	-2.646545	1.657108	0.104696
21C	-1.835996	1.869127	-1.020992
22C	-2.182074	2.828975	-1.976390
23C	-3.344381	3.591897	-1.822877
24C	-4.153591	3.395068	-0.699971
25C	-3.801447	2.437902	0.255057
26C	3.788973	0.276611	0.468881
27O	3.894714	1.220375	1.270704
28N	4.606523	-0.415411	-0.275436
29C	5.983282	-0.179952	-0.290601
30C	6.691483	0.764124	0.492706
31C	8.079957	0.884991	0.376740
32C	8.806139	0.084896	-0.511321
33C	8.117711	-0.853088	-1.292491
34C	6.734580	-0.982139	-1.182133
35H	1.710598	1.247133	1.570504
36H	0.550115	-2.523775	-1.310216
37H	2.869406	-1.724372	-1.023917
38H	-2.965556	0.815875	2.027374
39H	-2.593285	-1.422565	1.737832
40H	-0.247497	2.682781	1.805700
41H	-1.473348	2.175877	2.992167
42H	0.194249	1.603846	3.158483
43H	-1.390175	-2.833389	-1.666215
44H	-2.993988	-2.746516	-0.988444
45H	-1.879855	-4.855056	-0.277152
46H	-0.573337	-3.936817	0.499249
47H	-2.228628	-3.837169	1.132799
48H	-4.823656	-1.686402	2.160557
49H	-7.185675	-1.780904	1.413203
50H	-7.781672	-1.139677	-0.919613
51H	-5.992290	-0.403723	-2.490701
52H	-3.639952	-0.297462	-1.732461
53H	-0.928923	1.291931	-1.163755
54H	-1.541649	2.979038	-2.842227
55H	-3.612816	4.336211	-2.568509
56H	-5.057731	3.984088	-0.566256
57H	-4.440858	2.284292	1.121827
58H	6.148873	1.394806	1.185501
59H	8.598102	1.618419	0.991962
60H	9.885477	0.188247	-0.593764
61H	8.661545	-1.487105	-1.989993
62H	6.200765	-1.711586	-1.787252

1d-PhNCO-006

1N	-2.366636	-1.305000	-0.351240
2C	-1.529894	-0.231614	-0.393522
3C	-0.158705	-0.353817	-0.553723
4C	0.385276	-1.675900	-0.750110
5C	-0.523769	-2.757692	-0.682591
6C	-1.871864	-2.549028	-0.485370
7N	1.714037	-1.849610	-0.987399
8N	0.674867	0.763981	-0.508954
9C	1.992302	0.596526	-1.135877
10C	2.635246	-0.748440	-0.686175
11C	0.020211	2.063399	-0.679697
12C	2.261831	-3.214635	-1.123388
13C	3.669524	-3.276365	-1.709223
14C	3.136055	-0.792700	0.753187
15C	4.511232	-0.685095	1.002235
16C	5.006738	-0.687874	2.308785
17C	4.127080	-0.804441	3.389274
18C	2.753920	-0.924809	3.150988
19C	2.262298	-0.920204	1.842857
20C	2.951090	1.740308	-0.847808
21C	3.801305	2.186435	-1.867179
22C	4.751870	3.183129	-1.620655
23C	4.852847	3.752560	-0.348227
24C	4.000517	3.317875	0.673717
25C	3.060578	2.315895	0.427028
26C	-3.878790	-1.132299	-0.128567
27O	-4.496615	-2.207268	-0.045345
28N	-4.190963	0.133379	-0.073647
29C	-5.498985	0.573576	0.140826
30C	-6.642459	-0.235283	0.351581
31C	-7.895171	0.348233	0.566852
32C	-8.055860	1.737516	0.577894
33C	-6.932968	2.549248	0.367630
34C	-5.680513	1.976815	0.154017
35H	-2.034968	0.712746	-0.274146
36H	-0.183110	-3.779837	-0.769325
37H	-2.592851	-3.352966	-0.422026
38H	1.873895	0.517955	-2.228714

39H	3.499514	-0.860960	-1.341904
40H	-0.623785	2.281534	0.178214
41H	-0.585982	2.096581	-1.598694
42H	0.772617	2.847750	-0.732969
43H	1.594091	-3.766044	-1.790961
44H	2.240942	-3.713231	-0.143390
45H	3.918597	-4.330026	-1.878693
46H	3.729266	-2.759326	-2.674011
47H	4.427043	-2.865005	-1.035424
48H	5.199945	-0.585992	0.166153
49H	6.076428	-0.598134	2.481260
50H	4.507553	-0.806757	4.407671
51H	2.061268	-1.019996	3.983667
52H	1.193453	-1.012425	1.682391
53H	3.720457	1.753475	-2.862420
54H	5.403910	3.517895	-2.423728
55H	5.585980	4.531653	-0.154280
56H	4.071312	3.755562	1.666379
57H	2.406216	1.977203	1.224571
58H	-6.539891	-1.313040	0.345694
59H	-8.756683	-0.297251	0.727906
60H	-9.034619	2.180491	0.745816
61H	-7.034185	3.632714	0.371207
62H	-4.808287	2.606424	-0.007363

1d-PhNCO-007

1N	-2.367025	-0.184252	-0.373620
2C	-1.390793	0.576340	-0.935408
3C	-0.055947	0.196254	-0.940217
4C	0.312386	-1.026709	-0.273782
5C	-0.740924	-1.772357	0.302817
6C	-2.049201	-1.342026	0.237611
7N	1.618511	-1.419269	-0.201729
8N	0.910550	0.952765	-1.585449
9C	2.296064	0.801262	-1.140143
10C	2.612859	-0.717226	-1.044187
11C	0.545787	2.255981	-2.126080
12C	1.931487	-2.806408	0.207411
13C	2.031033	-3.003440	1.721897
14C	4.049850	-0.959738	-0.611114
15C	4.987714	-1.353339	-1.575233
16C	6.331126	-1.542279	-1.233813
17C	6.750503	-1.345794	0.084776
18C	5.820408	-0.955290	1.054575
19C	4.482202	-0.759686	0.708456
20C	2.641287	1.647233	0.081330
21C	3.758656	2.491894	0.027173
22C	4.125886	3.273003	1.126403
23C	3.369097	3.225827	2.300827
24C	2.243430	2.397321	2.361574
25C	1.882144	1.615106	1.261394
26C	-3.815273	0.331386	-0.456735
27O	-3.925751	1.417269	-1.051060
28N	-4.629853	-0.503139	0.127959
29C	-6.007630	-0.281604	0.189688
30C	-6.717909	0.803589	-0.379909
31C	-8.106736	0.893973	-0.242907
32C	-8.831008	-0.076783	0.456496
33C	-8.140620	-1.155841	1.024882
34C	-6.756905	-1.255153	0.892173
35H	-1.748795	1.488419	-1.387715
36H	-0.552234	-2.701785	0.820946
37H	-2.876828	-1.890452	0.664368
38H	2.924435	1.154047	-1.964281
39H	2.508311	-1.098632	-2.069271
40H	-0.244598	2.148429	-2.876824
41H	0.203110	2.955191	-1.348236
42H	1.421711	2.686176	-2.617025
43H	2.882106	-3.073226	-0.256950
44H	1.178706	-3.477773	-0.223255
45H	2.143322	-4.072086	1.942691
46H	2.899015	-2.478703	2.129898
47H	1.141047	-2.639713	2.245420
48H	4.666043	-1.516329	-2.602059
49H	7.043650	-1.849058	-1.995482
50H	7.792571	-1.496114	0.356009
51H	6.136800	-0.796189	2.082551
52H	3.773303	-0.445467	1.466391
53H	4.355395	2.528123	-0.881833
54H	5.000127	3.916434	1.064076
55H	3.648776	3.832683	3.158418
56H	1.643471	2.357858	3.267509
57H	1.005165	0.981700	1.335486
58H	-6.175805	1.566252	-0.924290
59H	-8.626435	1.738851	-0.691140

60H	-9.910715	0.003953	0.557415
61H	-8.683464	-1.923180	1.573262
62H	-6.221290	-2.093262	1.332556

1d-PhNCO-008

1N	3.129480	0.829162	-1.113287
2C	2.045776	0.035551	-1.312584
3C	0.747274	0.474343	-1.101873
4C	0.560942	1.837214	-0.665648
5C	1.719668	2.640883	-0.540184
6C	2.974293	2.118644	-0.768268
7N	-0.684744	2.306712	-0.403297
8N	-0.343813	-0.374857	-1.276749
9C	-1.634382	0.300617	-1.476429
10C	-1.823355	1.381882	-0.371855
11C	-0.088497	-1.604925	-2.028684
12C	-0.918541	3.680904	0.066644
13C	-0.641339	3.894470	1.558654
14C	-2.095378	0.841507	1.026921
15C	-3.389564	0.933391	1.554385
16C	-3.683475	0.429983	2.825067
17C	-2.678316	-0.173646	3.586035
18C	-1.380602	-0.263385	3.069630
19C	-1.090024	0.242470	1.800843
20C	-2.825132	-0.642305	-1.493868
21C	-3.842535	-0.431357	-2.432805
22C	-4.987285	-1.236023	-2.440857
23C	-5.121577	-2.269492	-1.509713
24C	-4.105645	-2.491904	-0.572764
25C	-2.968365	-1.682820	-0.562925
26C	4.570011	0.245585	-1.220318
27O	5.320726	0.957608	-1.898918
28N	4.777522	-0.898637	-0.631906
29C	3.961757	-1.439134	0.362544
30C	3.500153	-0.694637	1.472465
31C	2.699336	-1.286272	2.451329
32C	2.346469	-2.637910	2.364952
33C	2.824719	-3.394907	1.287545
34C	3.626106	-2.808902	0.306028
35H	2.269079	-0.972957	-1.621379
36H	1.651287	3.675334	-0.231770
37H	3.881432	2.700960	-0.665166
38H	-1.622774	0.848708	-2.432348
39H	-2.699794	1.958061	-0.683207
40H	0.377160	-1.396256	-3.004875
41H	0.567388	-2.267460	-1.455057
42H	-1.023816	-2.133437	-2.199263
43H	-1.964971	3.912221	-0.152871
44H	-0.316825	4.363232	-0.542852
45H	-0.786641	4.952840	1.808088
46H	-1.321050	3.298278	2.174237
47H	0.385486	3.619489	1.822460
48H	-4.176790	1.393546	0.960897
49H	-4.694625	0.507792	3.216937
50H	-2.901835	-0.566899	4.574674
51H	-0.591656	-0.730157	3.654138
52H	-0.076809	0.163668	1.422615
53H	-3.740249	0.366697	-3.165690
54H	-5.766733	-1.058660	-3.177767
55H	-6.007637	-2.899494	-1.515589
56H	-4.199476	-3.294351	0.154702
57H	-2.184268	-1.861438	0.166035
58H	3.773505	0.354060	1.557062
59H	2.353347	-0.685360	3.290234
60H	1.722122	-3.095750	3.128160
61H	2.571603	-4.450413	1.210521
62H	3.993675	-3.398717	-0.530514

1d-PhNCO-009

1N	2.824326	-1.499698	-0.637024
2C	1.927140	-0.500271	-0.842114
3C	0.674484	-0.482609	-0.249315
4C	0.332826	-1.571820	0.632548
5C	1.306790	-2.583674	0.820992
6C	2.519632	-2.530213	0.171650
7N	-0.874840	-1.607555	1.241203
8N	-0.238321	0.549751	-0.492427
9C	-1.217693	0.753735	0.589985
10C	-1.896117	-0.598759	0.948801
11C	0.330765	1.763786	-1.088629
12C	-1.272390	-2.686270	2.156810
13C	-0.752667	-2.462944	3.578041

14C	-2.908582	-1.114815	-0.065790
15C	-4.278035	-0.994292	0.203202
16C	-5.230453	-1.428902	-0.723146
17C	-4.819830	-1.995279	-1.933428
18C	-3.453655	-2.132309	-2.204283
19C	-2.504656	-1.697808	-1.275653
20C	-2.278320	1.793355	0.268494
21C	-2.909481	1.853235	-0.983509
22C	-3.925345	2.780004	-1.221875
23C	-4.335791	3.653587	-0.207933
24C	-3.714193	3.599889	1.042567
25C	-2.688495	2.676773	1.274591
26C	4.229957	-1.464350	-1.309187
27O	4.539096	-2.556401	-1.803275
28N	4.860855	-0.324917	-1.306085
29C	4.588127	0.747345	-0.458959
30C	4.602888	2.054278	-0.992797
31C	4.364164	3.165794	-0.183638
32C	4.118063	3.011271	1.187087
33C	4.129751	1.723264	1.735470
34C	4.367764	0.606919	0.930694
35H	2.259996	0.281337	-1.505365
36H	1.120749	-3.421409	1.479432
37H	3.276624	-3.297172	0.277843
38H	-0.689613	1.078182	1.501821
39H	-2.426548	-0.407128	1.887730
40H	-0.432308	2.537191	-1.143206
41H	1.179346	2.148856	-0.502786
42H	0.665717	1.559559	-2.110221
43H	-0.939230	-3.648297	1.755827
44H	-2.365368	-2.716337	2.151933
45H	-1.084650	-3.278159	4.231985
46H	0.342017	-2.426567	3.602707
47H	-1.134273	-1.519042	3.985481
48H	-4.603040	-0.545160	1.139336
49H	-6.289186	-1.324134	-0.498974
50H	-5.556751	-2.334895	-2.657044
51H	-3.124864	-2.577769	-3.140075
52H	-1.449452	-1.812699	-1.501184
53H	-2.601170	1.173627	-1.771888
54H	-4.401976	2.814939	-2.198379
55H	-5.129754	4.372675	-0.393921
56H	-4.019559	4.277978	1.835652
57H	-2.202103	2.645384	2.247521
58H	4.794368	2.176833	-2.056259
59H	4.371665	4.159846	-0.626075
60H	3.934723	3.878484	1.816533
61H	3.960244	1.584671	2.801592
62H	4.387596	-0.386183	1.372451

1d-PhNCO-010

1N	2.778833	-1.543365	-0.443726
2C	1.927525	-0.507844	-0.662790
3C	0.676055	-0.424931	-0.070717
4C	0.285352	-1.484879	0.826585
5C	1.211343	-2.538094	1.025555
6C	2.427516	-2.547021	0.379575
7N	-0.920993	-1.451349	1.445108
8N	-0.186270	0.642209	-0.336919
9C	-1.196081	0.888034	0.704599
10C	-1.916172	-0.444717	1.062434
11C	0.436664	1.826436	-0.938062
12C	-1.359294	-2.513066	2.364307
13C	-1.897633	-3.770479	1.673470
14C	-2.885365	-0.961604	0.006779
15C	-2.438203	-1.563257	-1.178356
16C	-3.352389	-2.009164	-2.135613
17C	-4.727562	-1.863390	-1.920194
18C	-5.181653	-1.273926	-0.736877
19C	-4.263315	-0.828332	0.218309
20C	-2.224026	1.940493	0.324549
21C	-2.665353	2.839780	1.303056
22C	-3.668438	3.772558	1.017654
23C	-4.235734	3.819527	-0.258804
24C	-3.793117	2.930374	-1.245283
25C	-2.799011	1.994927	-0.954362
26C	4.160211	-1.615134	-1.168005
27O	4.394387	-2.748331	-1.607007
28N	4.843487	-0.510993	-1.261428
29C	4.672843	0.616447	-0.461107
30C	4.717480	1.892575	-1.063419
31C	4.583105	3.053563	-0.300984
32C	4.414873	2.980491	1.088141
33C	4.397409	1.722415	1.702088
34C	4.529683	0.556790	0.944368

35H	2.291361	0.246355	-1.341078
36H	0.976600	-3.371870	1.673118
37H	3.143899	-3.351455	0.488572
38H	-0.696262	1.219632	1.629357
39H	-2.493147	-0.221256	1.964836
40H	1.297892	2.177763	-0.349791
41H	0.768368	1.602936	-1.956955
42H	-0.292719	2.631248	-1.001092
43H	-2.138335	-2.074909	2.995305
44H	-0.524830	-2.760653	3.028189
45H	-2.145008	-4.523252	2.431886
46H	-2.802049	-3.548490	1.099929
47H	-1.160381	-4.204406	0.989596
48H	-1.376511	-1.692195	-1.360832
49H	-2.989191	-2.472056	-3.049990
50H	-5.437459	-2.212436	-2.665976
51H	-6.247648	-1.159687	-0.555816
52H	-4.622305	-0.364224	1.134470
53H	-2.222000	2.811995	2.296664
54H	-3.999040	4.463172	1.789545
55H	-5.012506	4.545496	-0.486116
56H	-4.227147	2.960498	-2.241627
57H	-2.464485	1.303566	-1.721621
58H	4.849204	1.951871	-2.141248
59H	4.611565	4.022853	-0.794717
60H	4.313942	3.886293	1.680814
61H	4.287828	1.645956	2.782260
62H	4.529584	-0.413042	1.435763

1d-PhNCO-011

1N	-2.655127	-1.606271	0.197583
2C	-1.420411	-1.804467	-0.331517
3C	-0.284441	-1.188489	0.171402
4C	-0.435369	-0.348489	1.335908
5C	-1.730784	-0.243802	1.897286
6C	-2.811829	-0.853763	1.301176
7N	0.631804	0.304448	1.851435
8N	0.967545	-1.353483	-0.427930
9C	2.111161	-1.111715	0.468632
10C	1.934298	0.258483	1.184120
11C	1.080809	-2.483469	-1.354665
12C	0.535458	1.177488	3.029720
13C	0.639405	0.396772	4.340789
14C	2.152566	1.488935	0.311597
15C	3.362804	2.189639	0.394844
16C	3.602663	3.302825	-0.415627
17C	2.626298	3.732750	-1.319074
18C	1.408641	3.047521	-1.398418
19C	1.172303	1.934985	-0.586915
20C	3.458569	-1.160675	-0.230887
21C	4.537388	-1.775096	0.416781
22C	5.811485	-1.777294	-0.161644
23C	6.015962	-1.169965	-1.403670
24C	4.940639	-0.560791	-2.061257
25C	3.673450	-0.551408	-1.476643
26C	-3.868452	-2.286380	-0.498940
27O	-3.685425	-3.494346	-0.698449
28N	-4.900965	-1.529219	-0.737150
29C	-4.874189	-0.135323	-0.777658
30C	-3.871881	0.604158	-1.448016
31C	-3.921963	1.998604	-1.500262
32C	-4.975545	2.699035	-0.901221
33C	-5.987406	1.977118	-0.254952
34C	-5.941738	0.583267	-0.197837
35H	-1.400645	-2.469988	-1.181105
36H	-1.905675	0.332101	2.796016
37H	-3.818091	-0.755597	1.687435
38H	2.116559	-1.869947	1.268693
39H	2.692384	0.264072	1.974648
40H	0.761885	-3.428855	-0.888019
41H	0.470855	-2.303188	-2.245534
42H	2.112994	-2.591075	-1.680772
43H	-0.392620	1.755076	2.980860
44H	1.350100	1.903003	2.953418
45H	0.577839	1.083970	5.193011
46H	-0.166856	-0.339372	4.432939
47H	1.595641	-0.136930	4.398732
48H	4.130332	1.854057	1.088969
49H	4.549678	3.831545	-0.340146
50H	2.808570	4.598911	-1.950402
51H	0.640010	3.379680	-2.092114
52H	0.219627	1.419733	-0.657968
53H	4.381895	-2.258292	1.379390
54H	6.637975	-2.259587	0.354450
55H	7.003296	-1.174405	-1.858829

56H	5.089708	-0.085903	-3.027831
57H	2.843753	-0.072923	-1.987741
58H	-3.056807	0.074363	-1.934225
59H	-3.135172	2.540500	-2.021710
60H	-5.014196	3.784517	-0.947389
61H	-6.820785	2.503083	0.206403
62H	-6.730996	0.025177	0.300540

1d-PhNCO-012

1N	-2.609872	-1.722134	0.377963
2C	-1.358912	-1.974918	-0.083359
3C	-0.235764	-1.327117	0.411815
4C	-0.426586	-0.377073	1.481980
5C	-1.740392	-0.213681	1.978808
6C	-2.802904	-0.875668	1.404172
7N	0.630533	0.314176	1.978952
8N	1.031779	-1.563621	-0.118979
9C	2.164996	-1.145425	0.717595
10C	1.912354	0.288791	1.269216
11C	1.186967	-2.807119	-0.879713
12C	0.476721	1.293142	3.065783
13C	-0.071565	2.653497	2.620975
14C	2.036685	1.407958	0.241197
15C	1.037404	1.659805	-0.710423
16C	1.194261	2.681245	-1.650075
17C	2.350636	3.469273	-1.650531
18C	3.347405	3.230911	-0.699997
19C	3.187210	2.206908	0.238094
20C	3.500982	-1.184915	-0.005949
21C	3.637880	-0.775892	-1.340868
22C	4.893007	-0.756538	-1.951222
23C	6.032807	-1.132832	-1.231193
24C	5.905920	-1.539227	0.100160
25C	4.644715	-1.569011	0.704971
26C	-3.806124	-2.409714	-0.341253
27O	-3.659529	-3.634542	-0.444094
28N	-4.789135	-1.633383	-0.698510
29C	-4.706235	-0.244533	-0.808408
30C	-5.769497	0.542949	-0.317273
31C	-5.750763	1.933665	-0.436614
32C	-4.676760	2.582980	-1.059209
33C	-3.626812	1.813002	-1.572999
34C	-3.641664	0.421429	-1.459139
35H	-1.314577	-2.703955	-0.878775
36H	-1.947830	0.465397	2.794452
37H	-3.823243	-0.732925	1.735338
38H	2.234408	-1.799071	1.601987
39H	2.689111	0.441635	2.024474
40H	0.806266	-3.674879	-0.319692
41H	0.655093	-2.740529	-1.834567
42H	2.239287	-2.974277	-1.100245
43H	1.466073	1.418715	3.515616
44H	-0.160829	0.850843	3.838296
45H	-0.228759	3.287676	3.502006
46H	0.628480	3.160821	1.950956
47H	-1.028053	2.550936	2.097824
48H	0.127490	1.069526	-0.722990
49H	0.409766	2.862650	-2.380800
50H	2.469594	4.264735	-2.381972
51H	4.249030	3.838318	-0.687813
52H	3.970180	2.019755	0.969841
53H	2.757801	-0.473764	-1.900253
54H	4.981721	-0.440147	-2.987605
55H	7.010381	-1.113964	-1.706619
56H	6.783802	-1.840098	0.666648
57H	4.550217	-1.894604	1.739254
58H	-6.605087	0.041798	0.165958
59H	-6.581524	2.514750	-0.041229
60H	-4.664301	3.666114	-1.151686
61H	-2.790848	2.297717	-2.073845
62H	-2.826380	-0.163453	-1.877040

1d-PhNCO-013

1N	2.600926	-0.131623	-1.382813
2C	1.440134	0.573151	-1.402700
3C	0.340294	0.226589	-0.633001
4C	0.452459	-0.935442	0.216065
5C	1.684802	-1.632393	0.201442
6C	2.726677	-1.215668	-0.596324
7N	-0.592206	-1.331402	0.978859
8N	-0.850899	0.958726	-0.670565
9C	-1.639510	0.870514	0.573818

10C	-1.875428	-0.624388	0.932895
11C	-0.761761	2.275159	-1.306534
12C	-0.537089	-2.516695	1.846849
13C	0.106731	-2.218748	3.202355
14C	-2.878958	-1.361229	0.056250
15C	-4.171009	-1.604251	0.539458
16C	-5.121055	-2.252697	-0.254813
17C	-4.783919	-2.670181	-1.545845
18C	-3.491204	-2.442715	-2.031450
19C	-2.543893	-1.795241	-1.234473
20C	-2.962958	1.613413	0.520855
21C	-3.829148	1.518694	-0.579778
22C	-5.062012	2.172544	-0.570427
23C	-5.453170	2.924749	0.543564
24C	-4.597892	3.024240	1.644139
25C	-3.358258	2.375476	1.627455
26C	3.760041	0.349104	-2.302697
27O	3.379548	0.568654	-3.460413
28N	4.946597	0.416393	-1.771034
29C	5.212873	0.465656	-0.403383
30C	6.297093	-0.282353	0.104693
31C	6.638347	-0.230131	1.456950
32C	5.916917	0.578654	2.344827
33C	4.852678	1.342332	1.851369
34C	4.506073	1.293915	0.499376
35H	1.441403	1.413551	-2.080127
36H	1.838378	-2.507161	0.818444
37H	3.676112	-1.733863	-0.624541
38H	-1.050464	1.289122	1.406151
39H	-2.264076	-0.612929	1.957154
40H	0.021840	2.900275	-0.848262
41H	-0.548131	2.161375	-2.373539
42H	-1.713341	2.793752	-1.215610
43H	-0.017096	-3.327094	1.326292
44H	-1.568005	-2.855131	1.982188
45H	0.097637	-3.119402	3.827789
46H	1.145673	-1.889757	3.090446
47H	-0.445406	-1.430623	3.728224
48H	-4.439802	-1.269573	1.539253
49H	-6.120878	-2.429714	0.133908
50H	-5.519701	-3.174722	-2.167237
51H	-3.218849	-2.769151	-3.032166
52H	-1.544797	-1.627523	-1.623715
53H	-3.532768	0.935576	-1.446177
54H	-5.719738	2.090896	-1.432146
55H	-6.414610	3.432231	0.550070
56H	-4.887523	3.611844	2.511821
57H	-2.692618	2.465422	2.483667
58H	6.861620	-0.907817	-0.582882
59H	7.475673	-0.823100	1.819415
60H	6.187036	0.622094	3.396989
61H	4.290892	1.989779	2.522096
62H	3.687095	1.905401	0.129076

1d-PhNCO-014

1N	-2.824547	-1.839098	-0.170849
2C	-2.095725	-1.020049	-0.969913
3C	-0.709539	-0.955192	-0.903384
4C	-0.035884	-1.748692	0.094549
5C	-0.845999	-2.589304	0.890580
6C	-2.217429	-2.625583	0.731092
7N	1.319814	-1.664671	0.250236
8N	0.016367	-0.164402	-1.776855
9C	1.368261	0.229652	-1.379889
10C	2.101357	-1.027300	-0.835062
11C	-0.692872	0.761997	-2.651670
12C	2.005057	-2.640591	1.123664
13C	1.991069	-2.252389	2.603807
14C	3.538400	-0.711506	-0.454501
15C	4.567495	-1.135760	-1.306313
16C	5.903242	-0.830066	-1.025407
17C	6.226119	-0.100105	0.121807
18C	5.205728	0.323571	0.980612
19C	3.872979	0.024722	0.692055
20C	1.398618	1.472311	-0.496550
21C	2.215597	2.549249	-0.867612
22C	2.287717	3.703211	-0.082499
23C	1.532174	3.798272	1.089708
24C	0.701123	2.736177	1.461198
25C	0.631778	1.584097	0.673605
26C	-4.380220	-1.895969	-0.301876
27O	-4.797520	-3.058282	-0.374459
28N	-5.005330	-0.756195	-0.367039
29C	-4.482609	0.464954	0.058794
30C	-4.670448	1.609720	-0.744624

31C	-4.197709	2.858842	-0.338606
32C	-3.537193	3.008568	0.887589
33C	-3.370856	1.886841	1.707591
34C	-3.836518	0.633678	1.304822
35H	-2.665037	-0.423761	-1.665679
36H	-0.416695	-3.227507	1.649605
37H	-2.858565	-3.274688	1.314275
38H	1.901967	0.474453	-2.304053
39H	2.132639	-1.729799	-1.678972
40H	0.040505	1.286981	-3.267770
41H	-1.366841	0.214209	-3.319338
42H	-1.275015	1.506895	-2.089505
43H	3.036671	-2.718775	0.779559
44H	1.556052	-3.630242	0.974617
45H	2.443149	-3.057208	3.196270
46H	2.567364	-1.338497	2.773146
47H	0.976788	-2.083139	2.979010
48H	4.324090	-1.714256	-2.195282
49H	6.687310	-1.168859	-1.698030
50H	7.263299	0.135548	0.346871
51H	5.445632	0.894467	1.874224
52H	3.090491	0.367424	1.359301
53H	2.810615	2.480014	-1.775757
54H	2.931702	4.524689	-0.386933
55H	1.583244	4.693894	1.703904
56H	0.100866	2.804345	2.364901
57H	-0.027905	0.780271	0.980744
58H	-5.185446	1.496903	-1.695806
59H	-4.346913	3.722142	-0.983959
60H	-3.169336	3.981906	1.202191
61H	-2.876119	1.986514	2.671760
62H	-3.710770	-0.227248	1.956538

1d-PhNCO-015

1N	2.798372	-1.321581	0.715814
2C	1.770266	-1.048305	1.555615
3C	0.445465	-1.093678	1.143381
4C	0.164487	-1.431133	-0.229778
5C	1.273101	-1.750075	-1.043938
6C	2.563272	-1.670808	-0.559200
7N	-1.117411	-1.413210	-0.706367
8N	-0.599927	-0.835313	2.016252
9C	-1.834304	-0.315129	1.426427
10C	-2.236750	-1.239333	0.242777
11C	-0.293982	-0.382472	3.367305
12C	-1.423942	-2.114188	-1.970505
13C	-1.391411	-3.638810	-1.835118
14C	-3.509537	-0.725158	-0.411655
15C	-3.499570	0.325156	-1.341801
16C	-4.695091	0.826321	-1.858268
17C	-5.920688	0.290967	-1.444293
18C	-5.939754	-0.756650	-0.519809
19C	-4.738442	-1.262667	-0.010827
20C	-1.792235	1.182042	1.127979
21C	-0.775709	1.777736	0.364297
22C	-0.786160	3.152189	0.112922
23C	-1.813140	3.956217	0.617973
24C	-2.826626	3.374650	1.385201
25C	-2.809739	2.000329	1.638438
26C	4.251324	-1.205511	1.269177
27O	4.421630	-1.882028	2.291151
28N	5.071651	-0.466341	0.580531
29C	4.675246	0.486820	-0.359095
30C	3.679968	1.456836	-0.099473
31C	3.351372	2.421895	-1.053689
32C	4.010129	2.458745	-2.288231
33C	5.014548	1.517274	-2.548307
34C	5.347223	0.550177	-1.598145
35H	2.059679	-0.797301	2.565435
36H	1.144555	-2.053955	-2.073186
37H	3.427256	-1.881537	-1.176121
38H	-2.620712	-0.471281	2.171211
39H	-2.458160	-2.215098	0.695283
40H	0.231937	0.584638	3.379975
41H	-1.231829	-0.274139	3.916718
42H	0.319159	-1.127671	3.884864
43H	-0.733538	-1.766916	-2.743439
44H	-2.415548	-1.795791	-2.288908
45H	-0.407765	-4.000365	-1.516297
46H	-2.135481	-3.980735	-1.106375
47H	-1.627883	-4.099687	-2.801631
48H	-2.552329	0.748875	-1.661192
49H	-4.670158	1.640276	-2.578636
50H	-6.851812	0.684755	-1.844074
51H	-6.885637	-1.184534	-0.196952

52H	-4.759101	-2.081226	0.706197
53H	0.031215	1.181281	-0.045096
54H	0.009877	3.592601	-0.482618
55H	-1.820604	5.024865	0.418295
56H	-3.629971	3.987840	1.786293
57H	-3.605952	1.554168	2.230788
58H	3.172946	1.451612	0.862044
59H	2.581092	3.155978	-0.824725
60H	3.755649	3.213650	-3.028018
61H	5.545555	1.537703	-3.497849
62H	6.129815	-0.177294	-1.800954

1d-PhNCO-016

1N	2.604496	0.056598	1.258669
2C	1.448880	-0.655520	1.286332
3C	0.348843	-0.332269	0.505309
4C	0.461306	0.805179	-0.376887
5C	1.681882	1.521655	-0.354862
6C	2.723446	1.129537	0.456394
7N	-0.568685	1.152118	-1.187869
8N	-0.836382	-1.069293	0.566107
9C	-1.661354	-0.996102	-0.652260
10C	-1.872631	0.493879	-1.050903
11C	-0.741910	-2.373533	1.225635
12C	-0.490545	2.305831	-2.097908
13C	-0.730624	3.662265	-1.425946
14C	-2.822091	1.281104	-0.157322
15C	-2.444098	1.713459	1.122083
16C	-3.342398	2.418699	1.925967
17C	-4.630462	2.705898	1.460018
18C	-5.011801	2.286480	0.182163
19C	-4.109923	1.579932	-0.619200
20C	-3.002152	-1.699578	-0.528906
21C	-3.820460	-1.556249	0.602314
22C	-5.070912	-2.173903	0.656101
23C	-5.526504	-2.939317	-0.423798
24C	-4.718442	-3.087974	-1.554186
25C	-3.461865	-2.474149	-1.601255
26C	3.755182	-0.385954	2.212607
27O	3.347037	-0.622815	3.357108
28N	4.959696	-0.405602	1.719656
29C	5.277017	-0.452326	0.363355
30C	6.360304	0.321876	-0.106325
31C	6.752549	0.276105	-1.444845
32C	6.085155	-0.552147	-2.356624
33C	5.023418	-1.342214	-1.900540
34C	4.625780	-1.300465	-0.562451
35H	1.452494	-1.481682	1.980854
36H	1.823365	2.402236	-0.966142
37H	3.662965	1.664945	0.489097
38H	-1.114842	-1.456083	-1.491489
39H	-2.309640	0.460133	-2.053430
40H	0.045057	-3.002100	0.778527
41H	-0.530549	-2.242415	2.291251
42H	-1.691122	-2.897774	1.140965
43H	-1.241086	2.141128	-2.876745
44H	0.484297	2.285931	-2.596477
45H	-0.590888	4.462338	-2.163193
46H	-1.747940	3.730956	-1.030567
47H	-0.033001	3.834425	-0.599480
48H	-1.447657	1.506102	1.497538
49H	-3.034850	2.745069	2.916512
50H	-5.328193	3.255924	2.086654
51H	-6.008777	2.507555	-0.191172
52H	-4.414283	1.247087	-1.609368
53H	-3.473460	-0.963320	1.442692
54H	-5.691093	-2.053857	1.540941
55H	-6.501113	-3.419230	-0.381297
56H	-5.058528	-3.686570	-2.395686
57H	-2.833272	-2.601005	-2.480542
58H	6.883099	0.962415	0.600083
59H	7.587488	0.889519	-1.777486
60H	6.394585	-0.590059	-3.398110
61H	4.503594	-2.004917	-2.589949
62H	3.809646	-1.932172	-0.221145

1e-Me-001

1N	0.398014	2.414592	-0.079637
2C	1.227516	1.338655	-0.211371
3C	0.754837	0.037440	-0.196230
4C	-0.662494	-0.166719	0.005851
5C	-1.485844	0.976250	0.192759

6C	-0.924690	2.234449	0.126010
7N	-1.181968	-1.413910	-0.005746
8N	1.561836	-1.071378	-0.398840
9C	1.093369	-2.296500	0.250772
10C	-0.333005	-2.592509	-0.181874
11C	-2.627709	-1.666819	0.102860
12C	-3.451839	-0.456231	-0.322578
13C	-2.967794	0.792679	0.421610
14C	3.013764	-0.930232	-0.549038
15C	3.776402	-0.687161	0.759564
16C	0.984334	3.764940	-0.113349
17H	2.272492	1.577198	-0.346416
18H	-1.522446	3.130876	0.240206
19H	1.144765	-2.211657	1.346969
20H	1.741513	-3.121470	-0.054975
21H	-0.360205	-2.909861	-1.232474
22H	-0.743567	-3.403198	0.430481
23H	-2.857154	-1.950383	1.139810
24H	-2.854798	-2.528788	-0.533369
25H	-4.507486	-0.652077	-0.108651
26H	-3.353073	-0.305332	-1.405024
27H	-3.514876	1.683094	0.093343
28H	-3.164246	0.673002	1.496647
29H	3.209813	-0.129538	-1.270604
30H	3.367835	-1.855909	-1.015484
31H	4.848008	-0.583698	0.551422
32H	3.438805	0.223550	1.266615
33H	3.647690	-1.527330	1.451493
34H	0.181525	4.503198	-0.127810
35H	1.607226	3.918893	0.772619
36H	1.591932	3.874848	-1.015162

1e-Me-002

1N	0.414491	2.416478	-0.100728
2C	1.243463	1.337404	-0.194890
3C	0.763659	0.036387	-0.228799
4C	-0.666592	-0.157403	-0.117326
5C	-1.494720	0.990864	-0.021747
6C	-0.920598	2.246599	-0.010134
7N	-1.187098	-1.409265	-0.109682
8N	1.589103	-1.062541	-0.391280
9C	1.063954	-2.344870	0.073788
10C	-0.344074	-2.549815	-0.462009
11C	-2.636349	-1.643814	-0.041676
12C	-3.349981	-0.513766	0.693541
13C	-2.996716	0.831116	0.053055
14C	3.048273	-0.919586	-0.384363
15C	3.659510	-0.732604	1.009525
16C	1.011653	3.762598	-0.089316
17H	2.297033	1.571507	-0.239069
18H	-1.520421	3.146030	0.063392
19H	1.057376	-2.402973	1.172570
20H	1.713927	-3.138927	-0.304284
21H	-0.324125	-2.681356	-1.552829
22H	-0.780404	-3.449142	-0.018451
23H	-2.787057	-2.596772	0.475920
24H	-3.032910	-1.752156	-1.062125
25H	-3.049214	-0.516452	1.749033
26H	-4.429760	-0.690060	0.655546
27H	-3.421322	0.875683	-0.959708
28H	-3.434930	1.660841	0.618247
29H	3.322079	-0.091043	-1.046533
30H	3.451330	-1.826558	-0.846483
31H	4.747268	-0.620211	0.928861
32H	3.260913	0.156681	1.511081
33H	3.455551	-1.601318	1.645874
34H	0.219526	4.502714	0.026863
35H	1.711117	3.845419	0.746930
36H	1.539666	3.936730	-1.030891

1e-Me-003

1N	-0.466237	2.392019	-0.059724
2C	-1.267659	1.290687	-0.132910
3C	-0.755968	0.000565	-0.106152
4C	0.677600	-0.152039	0.024280
5C	1.476919	1.018148	0.083514
6C	0.872443	2.259312	0.031059
7N	1.227982	-1.390875	0.075392
8N	-1.563802	-1.117175	-0.177065
9C	-0.922615	-2.381959	-0.530048
10C	0.364774	-2.554906	0.258817
11C	2.668406	-1.576718	0.293670

12C	3.469021	-0.435784	-0.326321
13C	2.979586	0.905458	0.225643
14C	-2.997178	-0.989663	-0.467867
15C	-3.840239	-0.714078	0.779764
16C	-1.098134	3.721961	-0.076814
17H	-2.325501	1.496583	-0.203333
18H	1.449086	3.175819	0.069485
19H	-0.710905	-2.430669	-1.609648
20H	-1.605542	-3.197363	-0.279452
21H	0.143700	-2.697485	1.326106
22H	0.898178	-3.439350	-0.100722
23H	2.944827	-2.534530	-0.157642
24H	2.867445	-1.646133	1.373875
25H	3.351544	-0.459882	-1.417061
26H	4.530880	-0.580092	-0.102658
27H	3.252893	0.984587	1.287277
28H	3.467202	1.740393	-0.289555
29H	-3.160665	-0.216799	-1.233214
30H	-3.315503	-1.933359	-0.918201
31H	-3.533400	0.206316	1.288647
32H	-3.748612	-1.539943	1.494662
33H	-4.896849	-0.613472	0.503205
34H	-1.762016	3.822436	0.786159
35H	-1.671687	3.842522	-0.999815
36H	-0.322423	4.486741	-0.028147

1e-Me-004

1N	-0.522689	2.375833	-0.114013
2C	-1.303441	1.256330	-0.148403
3C	-0.765372	-0.020255	-0.128667
4C	0.675429	-0.145049	-0.087876
5C	1.454650	1.043403	-0.096964
6C	0.823097	2.269551	-0.093153
7N	1.254117	-1.364079	-0.030962
8N	-1.541743	-1.169519	-0.130233
9C	-0.891111	-2.351833	-0.699043
10C	0.448222	-2.583534	-0.020710
11C	2.709990	-1.541954	0.085482
12C	3.386924	-0.314770	0.686715
13C	2.961987	0.943044	-0.077664
14C	-2.999449	-1.070178	-0.281946
15C	-3.710925	-0.736587	1.031855
16C	-1.181996	3.691816	-0.095296
17H	-2.367074	1.442409	-0.163849
18H	1.382671	3.197101	-0.072492
19H	-0.751929	-2.241983	-1.786665
20H	-1.528636	-3.220629	-0.522623
21H	0.303262	-2.918776	1.014751
22H	1.000227	-3.362669	-0.557695
23H	3.117464	-1.763422	-0.910960
24H	2.881161	-2.421726	0.714368
25H	4.472351	-0.449509	0.641698
26H	3.106101	-0.220678	1.743414
27H	3.394174	1.842282	0.374255
28H	3.341724	0.887446	-1.107793
29H	-3.257043	-0.342919	-1.068099
30H	-3.349550	-2.041284	-0.640481
31H	-3.358583	0.203724	1.468940
32H	-3.543220	-1.531705	1.767116
33H	-4.790311	-0.647653	0.859493
34H	-1.815296	3.796863	-0.980387
35H	-1.791652	3.784199	0.807829
36H	-0.421662	4.473371	-0.100329

1e-Me-005

1N	-0.535010	2.484171	0.015033
2C	0.631839	1.775508	0.039894
3C	0.657673	0.391784	-0.031064
4C	-0.608665	-0.307493	-0.062928
5C	-1.800504	0.465169	-0.103206
6C	-1.719978	1.841671	-0.055881
7N	-0.644697	-1.659635	-0.059914
8N	1.839238	-0.338913	-0.086679
9C	1.743393	-1.675911	0.503086
10C	0.591390	-2.434788	-0.135721
11C	-1.908419	-2.394056	-0.212584
12C	-3.073140	-1.623587	0.401206
13C	-3.145062	-0.220451	-0.205340
14C	3.108030	0.389461	0.058090
15C	4.345433	-0.458640	-0.226622
16C	-0.464032	3.954345	0.076722
17H	1.527978	2.374489	0.106810

18H	-2.609542	2.460841	-0.074531
19H	1.606736	-1.618961	1.594909
20H	2.662674	-2.225631	0.304458
21H	0.824140	-2.667477	-1.183805
22H	0.436884	-3.378404	0.397591
23H	-1.783781	-3.363902	0.277611
24H	-2.088735	-2.582674	-1.281084
25H	-2.933772	-1.557433	1.487636
26H	-4.002635	-2.172068	0.216743
27H	-3.436897	-0.295563	-1.262375
28H	-3.912149	0.381692	0.293291
29H	3.088851	1.212462	-0.663968
30H	3.181247	0.835716	1.065214
31H	4.255387	-0.981642	-1.186065
32H	4.546794	-1.194265	0.558868
33H	5.216447	0.203907	-0.282391
34H	0.065204	4.332801	-0.802076
35H	0.065344	4.255996	0.984521
36H	-1.474639	4.362675	0.095655

1e-Me-006

1N	-0.995696	2.262597	-0.252554
2C	-1.552183	1.034922	-0.425617
3C	-0.810393	-0.122295	-0.354999
4C	0.610984	-0.026268	-0.165444
5C	1.174783	1.278929	-0.008853
6C	0.343370	2.371773	-0.035965
7N	1.377655	-1.133377	-0.135135
8N	-1.439409	-1.385204	-0.508059
9C	-0.512841	-2.327557	-1.153167
10C	0.806658	-2.459439	-0.392903
11C	2.823813	-1.080433	0.130619
12C	3.210302	0.176041	0.904872
13C	2.664340	1.421635	0.197418
14C	-2.073506	-1.933312	0.720529
15C	-3.251455	-1.111382	1.232865
16C	-1.858141	3.456736	-0.238903
17H	-2.616912	1.007010	-0.619682
18H	0.724701	3.377672	0.100151
19H	-0.316408	-1.967641	-2.169728
20H	-0.994656	-3.305487	-1.232065
21H	1.529343	-3.031316	-0.986407
22H	0.666650	-2.986196	0.559924
23H	3.359520	-1.130278	-0.827828
24H	3.080423	-1.979303	0.701075
25H	4.301070	0.223681	0.983716
26H	2.805312	0.118273	1.923321
27H	2.883180	2.328454	0.771285
28H	3.159787	1.531309	-0.777897
29H	-1.331638	-2.052350	1.527867
30H	-2.424273	-2.934830	0.450684
31H	-3.726346	-1.644720	2.065083
32H	-2.939936	-0.130672	1.608697
33H	-4.002320	-0.963556	0.447643
34H	-1.258932	4.335189	-0.481879
35H	-2.306621	3.578455	0.751675
36H	-2.644176	3.342097	-0.988112

1e-Me-007

1N	-0.847064	2.302437	-0.237419
2C	-1.460912	1.109561	-0.443426
3C	-0.796660	-0.091931	-0.322483
4C	0.614455	-0.077456	-0.040076
5C	1.231272	1.192481	0.190530
6C	0.474521	2.333700	0.082361
7N	1.325906	-1.223893	-0.004454
8N	-1.495087	-1.308386	-0.529256
9C	-0.584638	-2.334842	-1.053592
10C	0.652251	-2.514321	-0.172187
11C	2.754026	-1.238743	0.348185
12C	3.440610	0.065375	-0.047897
13C	2.695479	1.257500	0.559172
14C	-2.317004	-1.789236	0.613417
15C	-3.468204	-0.866342	1.000365
16C	-1.629327	3.549110	-0.304113
17H	-2.506951	1.143217	-0.718310
18H	0.903018	3.316458	0.244428
19H	-0.272065	-2.035794	-2.060869
20H	-1.122892	-3.282160	-1.137127
21H	0.380355	-2.924394	0.810229
22H	1.354552	-3.209361	-0.642964
23H	2.854805	-1.418808	1.428205

24H	3.209501	-2.086155	-0.172033
25H	3.457738	0.151008	-1.141694
26H	4.478327	0.041357	0.299790
27H	2.797049	1.230735	1.653192
28H	3.128084	2.205380	0.222553
29H	-1.685940	-1.977545	1.497995
30H	-2.726586	-2.753245	0.295158
31H	-4.082648	-1.365838	1.758914
32H	-3.118848	0.076780	1.434103
33H	-4.105137	-0.642616	0.136682
34H	-2.389560	3.456998	-1.082289
35H	-2.110413	3.735729	0.660827
36H	-0.963883	4.378010	-0.550413

1e-PhNCO-001

1N	0.198343	-0.855460	-0.084441
2C	-0.248651	0.426388	-0.182882
3C	-1.597077	0.737260	-0.224628
4C	-2.547038	-0.341729	-0.110164
5C	-2.044623	-1.665256	-0.013639
6C	-0.680629	-1.874929	-0.000521
7N	-3.883092	-0.085074	-0.098059
8N	-2.063483	2.037514	-0.406220
9C	-3.401323	2.302090	0.113496
10C	-4.371011	1.254419	-0.412752
11C	-4.867031	-1.173314	-0.092335
12C	-4.338556	-2.391523	0.660108
13C	-3.001532	-2.835157	0.061582
14C	-1.131725	3.168357	-0.400659
15C	-0.620568	3.576102	0.987205
16C	1.697598	-1.177193	-0.048494
17O	1.949679	-2.394386	-0.012709
18N	2.405584	-0.079359	-0.058485
19C	3.801712	-0.091547	-0.030946
20C	4.639829	-1.233699	-0.008967
21C	6.031097	-1.094731	0.016108
22C	6.634053	0.167280	0.021085
23C	5.816883	1.305760	0.000041
24C	4.429486	1.177004	-0.025829
25H	0.538379	1.161735	-0.228072
26H	-0.243246	-2.862052	0.075404
27H	-3.717403	3.290892	-0.231061
28H	-3.418754	2.303709	1.214941
29H	-5.348369	1.384713	0.063068
30H	-4.500847	1.367555	-1.498673
31H	-5.122095	-1.442366	-1.129203
32H	-5.776324	-0.790859	0.382754
33H	-5.077398	-3.197942	0.601051
34H	-4.208652	-2.134973	1.719398
35H	-2.557403	-3.642883	0.653708
36H	-3.169714	-3.238055	-0.947362
37H	-1.662010	4.010068	-0.860622
38H	-0.295458	2.932311	-1.067105
39H	0.090998	4.405487	0.893707
40H	-1.444999	3.909466	1.628791
41H	-0.109612	2.748676	1.491398
42H	4.192554	-2.219368	-0.011485
43H	6.649770	-1.990251	0.032489
44H	7.717023	0.263428	0.041068
45H	6.263619	2.298061	0.003606
46H	3.795667	2.060901	-0.042547

1e-PhNCO-002

1N	-0.200598	-0.840977	0.069494
2C	0.248555	0.437106	-0.074601
3C	1.595376	0.741132	-0.143019
4C	2.544642	-0.336174	-0.020241
5C	2.041928	-1.649613	0.178771
6C	0.679332	-1.857315	0.198158
7N	3.875112	-0.095164	-0.111551
8N	2.078841	2.032988	-0.357458
9C	3.392571	2.284212	0.233466
10C	4.390049	1.261331	-0.286077
11C	4.874130	-1.172637	-0.083535
12C	4.275891	-2.515908	-0.491442
13C	3.012881	-2.797210	0.329269
14C	1.155175	3.172099	-0.372527
15C	0.638501	3.608597	1.004960
16C	-1.697471	-1.162003	0.101787
17O	-1.950775	-2.364648	0.293250
18N	-2.407634	-0.080810	-0.083808
19C	-3.803716	-0.095664	-0.086813

20C	-4.431815	1.147194	-0.340717
21C	-5.819468	1.273502	-0.366006
22C	-6.636670	0.158276	-0.136029
23C	-6.033563	-1.077997	0.116819
24C	-4.642015	-1.214716	0.142307
25H	-0.536749	1.172463	-0.146455
26H	0.240181	-2.839069	0.319068
27H	3.355955	2.244803	1.334092
28H	3.720209	3.285989	-0.057157
29H	4.607408	1.440662	-1.347757
30H	5.329674	1.346231	0.272673
31H	5.305137	-1.230253	0.926860
32H	5.680194	-0.888229	-0.769165
33H	5.025139	-3.299991	-0.338741
34H	4.027105	-2.496921	-1.560251
35H	2.540594	-3.734048	0.015089
36H	3.287851	-2.916370	1.387281
37H	0.321594	2.930974	-1.040325
38H	1.694622	4.002181	-0.843032
39H	-0.065123	4.442105	0.890782
40H	0.117081	2.796152	1.522378
41H	1.460975	3.947849	1.645908
42H	-3.797897	2.013373	-0.517418
43H	-6.266598	2.245539	-0.564845
44H	-7.719844	0.252506	-0.154125
45H	-6.652236	-1.955284	0.297478
46H	-4.195000	-2.180997	0.337733

1e-PhNCO-003

1N	0.324240	0.128415	-0.127842
2C	-0.659332	1.064538	-0.186777
3C	-2.003225	0.728725	-0.208245
4C	-2.352656	-0.666554	-0.128504
5C	-1.299376	-1.617230	-0.071740
6C	0.009780	-1.183997	-0.067376
7N	-3.658061	-1.050272	-0.108650
8N	-3.013980	1.678659	-0.339681
9C	-4.318938	1.284284	0.181608
10C	-4.707691	-0.073958	-0.383712
11C	-4.038291	-2.467022	-0.129773
12C	-2.998840	-3.330027	0.580162
13C	-1.617680	-3.096203	-0.037126
14C	-2.702326	3.109557	-0.287270
15C	-2.411407	3.655377	1.116882
16C	1.777876	0.620767	-0.130086
17O	1.891912	1.851601	-0.268170
18N	2.603893	-0.378882	0.023084
19C	3.989807	-0.207557	0.021917
20C	4.695913	0.992685	-0.238830
21C	6.094177	1.012517	-0.225266
22C	6.833364	-0.142850	0.048572
23C	6.147572	-1.336794	0.309817
24C	4.754459	-1.367066	0.294322
25H	-0.297478	2.080429	-0.222267
26H	0.851098	-1.861819	-0.020363
27H	-5.056339	2.029151	-0.131002
28H	-4.323785	1.240845	1.282153
29H	-5.631262	-0.420427	0.091043
30H	-4.886331	0.000464	-1.466078
31H	-4.164669	-2.797553	-1.172603
32H	-5.011947	-2.551557	0.363832
33H	-3.288775	-4.382773	0.494898
34H	-2.981682	-3.075084	1.647586
35H	-0.843040	-3.631850	0.522460
36H	-1.604727	-3.497436	-1.060560
37H	-3.566605	3.630823	-0.714642
38H	-1.861666	3.306815	-0.960664
39H	-2.182448	4.726540	1.060380
40H	-3.278842	3.529973	1.775694
41H	-1.556192	3.151503	1.580569
42H	4.142562	1.899191	-0.448355
43H	6.610175	1.948831	-0.430568
44H	7.920429	-0.115547	0.058047
45H	6.701675	-2.248732	0.523731
46H	4.222804	-2.295179	0.492248

1e-PhNCO-004

1N	-0.322116	0.127056	-0.061248
2C	0.662550	1.058489	-0.176362
3C	2.003760	0.720918	-0.177074
4C	2.354880	-0.665459	-0.014463
5C	1.302634	-1.606824	0.149851

6C	-0.005611	-1.177809	0.102503
7N	3.652728	-1.054298	-0.040807
8N	3.028806	1.649633	-0.364897
9C	4.282222	1.293219	0.299062
10C	4.734940	-0.080732	-0.170198
11C	4.052876	-2.465921	0.031621
12C	2.932405	-3.400556	-0.414632
13C	1.640568	-3.067179	0.339034
14C	2.719903	3.081543	-0.432794
15C	2.394649	3.742433	0.913149
16C	-1.773623	0.614941	-0.115912
17O	-1.886749	1.839895	-0.302088
18N	-2.603182	-0.379942	0.051746
19C	-3.988613	-0.207772	0.026861
20C	-4.758199	-1.365435	0.293945
21C	-6.151333	-1.333966	0.291006
22C	-6.832746	-0.140263	0.017360
23C	-6.088905	1.013390	-0.250921
24C	-4.690572	0.992167	-0.247181
25H	0.301797	2.069602	-0.285274
26H	-0.846896	-1.850948	0.195541
27H	4.173860	1.298120	1.395640
28H	5.043141	2.031577	0.031903
29H	5.070474	-0.038292	-1.215154
30H	5.577349	-0.420413	0.444325
31H	4.361958	-2.694497	1.062306
32H	4.932161	-2.589459	-0.610467
33H	3.237772	-4.435946	-0.229466
34H	2.770352	-3.289081	-1.494382
35H	0.810807	-3.692876	-0.006498
36H	1.779241	-3.281423	1.408743
37H	1.896131	3.220476	-1.140551
38H	3.594867	3.567618	-0.879555
39H	3.249843	3.689602	1.597228
40H	2.153798	4.801002	0.757327
41H	1.536956	3.270498	1.404629
42H	-4.230204	-2.293261	0.502733
43H	-6.708916	-2.244659	0.501214
44H	-7.919823	-0.111859	0.013092
45H	-6.601259	1.949626	-0.465597
46H	-4.133778	1.897177	-0.453718

1e-PhNCO-005

1N	0.181254	-0.852866	-0.076619
2C	-0.258795	0.435858	-0.117591
3C	-1.603101	0.756316	-0.097153
4C	-2.560151	-0.320541	-0.072289
5C	-2.067148	-1.652697	-0.062730
6C	-0.706117	-1.870391	-0.049619
7N	-3.888399	-0.058231	-0.047145
8N	-2.072237	2.072477	-0.089222
9C	-3.366308	2.235848	-0.752968
10C	-4.391434	1.311927	-0.114718
11C	-4.897342	-1.120245	0.059189
12C	-4.325329	-2.385953	0.690382
13C	-3.044741	-2.805216	-0.040171
14C	-1.113379	3.175148	-0.239712
15C	-0.398823	3.526197	1.068037
16C	1.676574	-1.183229	-0.060471
17O	1.923653	-2.402304	-0.065317
18N	2.390985	-0.089170	-0.042807
19C	3.786804	-0.107894	-0.029250
20C	4.620260	-1.253700	-0.029548
21C	6.012302	-1.120695	-0.015512
22C	6.620686	0.138661	-0.000836
23C	5.808154	1.280724	0.000269
24C	4.420114	1.157984	-0.013649
25H	0.532985	1.166774	-0.140031
26H	-0.274621	-2.862607	-0.019736
27H	-3.291008	2.029067	-1.833979
28H	-3.699289	3.268561	-0.627137
29H	-4.646453	1.661316	0.894980
30H	-5.308657	1.311376	-0.715870
31H	-5.297457	-1.332273	-0.943404
32H	-5.721103	-0.728673	0.666263
33H	-5.079164	-3.179215	0.643747
34H	-4.103581	-2.198707	1.748789
35H	-2.586307	-3.676333	0.440296
36H	-3.294025	-3.102233	-1.069220
37H	-1.683158	4.046456	-0.574384
38H	-0.386141	2.954357	-1.037510
39H	0.297008	4.357087	0.898918
40H	-1.127289	3.833558	1.827585
41H	0.175524	2.686322	1.471718
42H	4.168589	-2.237335	-0.041026

43H	6.627381	-2.018855	-0.016391
44H	7.704202	0.230116	0.009883
45H	6.259081	2.271095	0.012028
46H	3.789702	2.044486	-0.012409

1e-PhNCO-006

1N	0.183011	-0.848043	-0.077653
2C	-0.258132	0.440949	-0.095461
3C	-1.603096	0.758988	-0.075430
4C	-2.558933	-0.319093	-0.084202
5C	-2.064492	-1.650641	-0.096811
6C	-0.703357	-1.866854	-0.075200
7N	-3.887658	-0.058577	-0.065166
8N	-2.075004	2.073469	-0.038051
9C	-3.361625	2.252131	-0.712113
10C	-4.392352	1.312049	-0.107347
11C	-4.896348	-1.123489	0.011629
12C	-4.327820	-2.401150	0.621447
13C	-3.041270	-2.803870	-0.107916
14C	-1.116524	3.181392	-0.141740
15C	-0.419430	3.489205	1.186131
16C	1.678562	-1.177847	-0.056988
17O	1.925616	-2.396164	-0.020413
18N	2.393441	-0.084820	-0.094519
19C	3.788922	-0.104899	-0.061897
20C	4.429912	1.136042	-0.290070
21C	5.818361	1.255816	-0.269173
22C	6.622123	0.136950	-0.011718
23C	6.005374	-1.096555	0.221851
24C	4.613384	-1.227595	0.196150
25H	0.532974	1.173211	-0.100846
26H	-0.270730	-2.858874	-0.058898
27H	-3.274329	2.071852	-1.796924
28H	-3.697219	3.281232	-0.564952
29H	-4.659251	1.637670	0.907215
30H	-5.302871	1.323748	-0.718543
31H	-5.288486	-1.315274	-0.998164
32H	-5.725246	-0.744937	0.620028
33H	-5.080386	-3.194037	0.553173
34H	-4.114253	-2.235197	1.685110
35H	-2.586302	-3.685468	0.356423
36H	-3.282060	-3.077401	-1.145512
37H	-1.683016	4.062573	-0.455473
38H	-0.378566	2.986958	-0.936512
39H	0.286778	4.317789	1.052350
40H	-1.156976	3.780910	1.943040
41H	0.140617	2.632244	1.573701
42H	3.805919	2.005691	-0.484159
43H	6.276421	2.225862	-0.452295
44H	7.705715	0.226368	0.006521
45H	6.613767	-1.976069	0.425086
46H	4.156475	-2.192913	0.373808

1e-PhNCO-007

1N	-0.178340	-0.856673	-0.008923
2C	0.259241	0.429103	-0.097124
3C	1.604731	0.755780	-0.075845
4C	2.561598	-0.318395	0.026036
5C	2.069043	-1.645894	0.117631
6C	0.707098	-1.868919	0.087663
7N	3.896118	-0.053659	0.022463
8N	2.051614	2.073709	-0.124913
9C	3.417331	2.260316	-0.606047
10C	4.360417	1.325447	0.135958
11C	4.882007	-1.117363	0.241109
12C	4.395752	-2.444911	-0.332928
13C	3.032377	-2.804257	0.263567
14C	1.098675	3.159612	-0.386445
15C	0.357502	3.621864	0.871440
16C	-1.675458	-1.189868	-0.013178
17O	-1.919683	-2.409090	0.003336
18N	-2.390582	-0.096730	-0.029356
19C	-3.786654	-0.117067	-0.032661
20C	-4.421570	1.147919	-0.040984
21C	-5.809895	1.268718	-0.043386
22C	-6.620708	0.125498	-0.037975
23C	-6.010545	-1.133085	-0.030138
24C	-4.618281	-1.264087	-0.027186
25H	-0.534137	1.154807	-0.167773
26H	0.277107	-2.860347	0.148004
27H	3.717890	3.292693	-0.410493
28H	3.491192	2.081473	-1.691671

29H	5.361161	1.389535	-0.303044
30H	4.431756	1.618190	1.193650
31H	5.085323	-1.214680	1.318965
32H	5.812591	-0.806445	-0.244223
33H	5.133315	-3.223719	-0.111548
34H	4.317541	-2.360633	-1.424575
35H	2.618737	-3.696986	-0.218561
36H	3.154168	-3.047870	1.328636
37H	0.387533	2.867017	-1.173866
38H	1.674186	3.997407	-0.790347
39H	-0.346095	4.423796	0.615784
40H	-0.211623	2.811602	1.338716
41H	1.067795	4.007859	1.612264
42H	-3.792416	2.035303	-0.044477
43H	-6.262261	2.258477	-0.049155
44H	-7.704408	0.215401	-0.039521
45H	-6.624377	-2.032073	-0.025539
46H	-4.165143	-2.247104	-0.019845

1e-PhNCO-008

1N	0.312928	0.126590	-0.082501
2C	-0.668317	1.068730	-0.104925
3C	-2.011105	0.738331	-0.083299
4C	-2.367579	-0.656004	-0.084769
5C	-1.317788	-1.614899	-0.094342
6C	-0.008721	-1.187320	-0.075276
7N	-3.668198	-1.033524	-0.066406
8N	-3.033819	1.690383	-0.052860
9C	-4.251563	1.255415	-0.738669
10C	-4.744629	-0.047578	-0.129306
11C	-4.076731	-2.442341	0.009022
12C	-2.988591	-3.315638	0.626067
13C	-1.659288	-3.087172	-0.101225
14C	-2.691563	3.115242	-0.148583
15C	-2.224669	3.702871	1.185827
16C	1.766470	0.611736	-0.079590
17O	1.884887	1.848067	-0.151565
18N	2.591522	-0.396976	0.008679
19C	3.977669	-0.227931	-0.002398
20C	4.682752	0.974121	-0.257496
21C	6.081071	0.991200	-0.262977
22C	6.821565	-0.168400	-0.011199
23C	6.136862	-1.363959	0.245238
24C	4.743539	-1.391840	0.246477
25H	-0.301551	2.083265	-0.119358
26H	0.830159	-1.869738	-0.057777
27H	-4.077229	1.124812	-1.820101
28H	-5.022929	2.017809	-0.608776
29H	-5.144059	0.127321	0.878771
30H	-5.551129	-0.458736	-0.748523
31H	-4.330269	-2.793475	-1.002394
32H	-4.991733	-2.485425	0.610466
33H	-3.294077	-4.365340	0.560586
34H	-2.877746	-3.066492	1.689263
35H	-0.852556	-3.662067	0.365983
36H	-1.746791	-3.443515	-1.137860
37H	-3.597195	3.638735	-0.467265
38H	-1.940735	3.285480	-0.936789
39H	-1.968918	4.761754	1.056892
40H	-3.022292	3.627878	1.934399
41H	-1.341473	3.191111	1.581542
42H	4.128571	1.884219	-0.448839
43H	6.596136	1.928842	-0.464576
44H	7.908717	-0.142985	-0.014992
45H	6.691847	-2.279136	0.442443
46H	4.212833	-2.321537	0.439566

1e-PhNCO-009

1N	-0.312675	0.129344	0.019253
2C	0.669669	1.062734	-0.087510
3C	2.014208	0.729201	-0.077176
4C	2.364655	-0.663728	0.033768
5C	1.313038	-1.609493	0.163067
6C	0.003418	-1.178233	0.139794
7N	3.668142	-1.051402	0.008666
8N	3.024143	1.686463	-0.147856
9C	4.295144	1.209722	-0.685019
10C	4.728036	-0.048587	0.052289
11C	4.052815	-2.447811	0.242882
12C	2.990917	-3.409361	-0.284026
13C	1.632173	-3.078305	0.338922
14C	2.680503	3.092288	-0.394471

15C	2.277954	3.839301	0.880078
16C	-1.766488	0.619131	-0.007994
17O	-1.879815	1.857370	-0.038994
18N	-2.593525	-0.391260	0.000363
19C	-3.979368	-0.222847	-0.019594
20C	-4.687160	1.004779	-0.032902
21C	-6.085444	1.019244	-0.054115
22C	-6.823648	-0.168691	-0.062781
23C	-6.136564	-1.390101	-0.049288
24C	-4.743469	-1.414540	-0.027278
25H	0.304899	2.074744	-0.167899
26H	-0.837476	-1.853448	0.220602
27H	5.051811	1.983649	-0.534327
28H	4.224449	1.004331	-1.766157
29H	5.617619	-0.467867	-0.429229
30H	4.983661	0.190980	1.094525
31H	4.215545	-2.607484	1.320093
32H	5.009300	-2.613968	-0.263271
33H	3.286882	-4.436641	-0.045571
34H	2.934374	-3.324072	-1.376854
35H	0.839048	-3.688744	-0.106494
36H	1.655116	-3.321372	1.410863
37H	1.890934	3.168258	-1.157432
38H	3.567420	3.567688	-0.823278
39H	2.021814	4.878441	0.639128
40H	1.410427	3.384539	1.369649
41H	3.106960	3.843623	1.597796
42H	-4.136063	1.936669	-0.027882
43H	-6.601982	1.977467	-0.064367
44H	-7.910714	-0.145219	-0.079970
45H	-6.689280	-2.327551	-0.055865
46H	-4.211169	-2.363221	-0.016968

1e-PhNCO-010

1N	-0.322225	-1.502479	-0.752767
2C	-0.260473	-0.173415	-1.017570
3C	0.866405	0.583513	-0.733019
4C	1.983256	-0.080530	-0.108315
5C	1.883661	-1.473817	0.143995
6C	0.722918	-2.140739	-0.194231
7N	3.100913	0.623012	0.224985
8N	0.964431	1.932573	-1.060564
9C	1.927253	2.705002	-0.280606
10C	3.268451	1.988009	-0.264072
11C	4.294459	-0.051851	0.746124
12C	3.916935	-1.268880	1.585418
13C	3.046837	-2.220346	0.760384
14C	-0.218797	2.665974	-1.522662
15C	-1.234920	2.994185	-0.422147
16C	-1.590336	-2.327586	-1.107385
17O	-1.310626	-3.393722	-1.671821
18N	-2.749364	-1.801608	-0.827003
19C	-2.992798	-0.796955	0.105480
20C	-3.998166	0.154052	-0.179467
21C	-4.345421	1.139221	0.745146
22C	-3.705398	1.208435	1.989081
23C	-2.714290	0.267319	2.290913
24C	-2.362940	-0.722705	1.370659
25H	-1.146036	0.250471	-1.464345
26H	0.600005	-3.205461	-0.036889
27H	1.579836	2.864432	0.752056
28H	2.046055	3.684113	-0.753588
29H	3.709914	1.981363	-1.271227
30H	3.957194	2.511434	0.406587
31H	4.845614	0.677171	1.349059
32H	4.943688	-0.349253	-0.092259
33H	3.370495	-0.938778	2.478101
34H	4.829993	-1.771842	1.921106
35H	3.655215	-2.671591	-0.035971
36H	2.675181	-3.044681	1.379005
37H	-0.690857	2.092655	-2.327649
38H	0.149013	3.590788	-1.980667
39H	-1.600995	2.092337	0.077997
40H	-0.793461	3.649942	0.337613
41H	-2.099620	3.512282	-0.853806
42H	-4.502972	0.098430	-1.141160
43H	-5.122083	1.858197	0.492252
44H	-3.978680	1.974487	2.710400
45H	-2.213555	0.295975	3.256897
46H	-1.605031	-1.456493	1.632142

1e-001

1N	-0.120381	2.805745	-0.194729
2C	-1.051885	1.838107	-0.285346
3C	-0.780209	0.462493	-0.256838
4C	0.585918	0.068807	-0.094077
5C	1.564351	1.080228	-0.013892
6C	1.151386	2.414586	-0.061970
7N	0.920969	-1.275027	0.011950
8N	-1.770789	-0.515108	-0.420155
9C	-1.442462	-1.852831	0.061031
10C	-0.059272	-2.253850	-0.432451
11C	2.324437	-1.667005	-0.096346
12C	3.217077	-0.689271	0.665446
13C	3.032791	0.725854	0.107967
14C	-3.186986	-0.150854	-0.363780
15C	-3.715362	0.178338	1.039519
16H	-2.073923	2.187556	-0.386433
17H	1.897896	3.205090	0.012476
18H	-2.186449	-2.553658	-0.332130
19H	-1.468927	-1.912837	1.161323
20H	0.211414	-3.229396	-0.013783
21H	-0.064761	-2.345510	-1.531679
22H	2.632018	-1.711652	-1.156592
23H	2.418486	-2.678297	0.314964
24H	4.262842	-1.006398	0.580975
25H	2.947483	-0.713649	1.729438
26H	3.509269	0.788714	-0.881700
27H	3.542829	1.460534	0.742987
28H	-3.745286	-0.999326	-0.776690
29H	-3.362069	0.689405	-1.044122
30H	-4.779421	0.441775	0.989292
31H	-3.612045	-0.681450	1.712118
32H	-3.176668	1.022220	1.484517

1e-002

1N	0.129329	2.798277	-0.066305
2C	1.055795	1.824080	-0.133365
3C	0.769574	0.449117	-0.129179
4C	-0.607151	0.069859	-0.035468
5C	-1.575369	1.087839	0.050909
6C	-1.149700	2.420041	0.017258
7N	-0.961267	-1.277351	-0.059777
8N	1.764261	-0.525630	-0.180663
9C	1.362430	-1.900256	-0.449035
10C	0.079086	-2.231552	0.298106
11C	-2.321690	-1.642421	0.333198
12C	-3.334315	-0.680657	-0.284638
13C	-3.046556	0.749183	0.185126
14C	3.148607	-0.169796	-0.494880
15C	3.970594	0.192179	0.746531
16H	2.084292	2.165574	-0.182862
17H	-1.891105	3.217249	0.066590
18H	2.157594	-2.570017	-0.104678
19H	1.217199	-2.073761	-1.528721
20H	-0.257565	-3.234728	0.016122
21H	0.266760	-2.228847	1.385649
22H	-2.419984	-1.636442	1.434092
23H	-2.502075	-2.668130	-0.007374
24H	-4.348912	-0.984300	-0.001816
25H	-3.262108	-0.740643	-1.378519
26H	-3.350716	0.852011	1.237022
27H	-3.649151	1.469665	-0.381734
28H	3.172898	0.650438	-1.225926
29H	3.604193	-1.033009	-0.992037
30H	3.534196	1.041744	1.282938
31H	4.013311	-0.657258	1.439142
32H	4.997074	0.457669	0.461941

1e-003

1N	0.120183	2.810847	-0.124147
2C	1.044370	1.838586	-0.258830
3C	0.767117	0.467625	-0.233764
4C	-0.589130	0.070561	-0.013659
5C	-1.554505	1.086645	0.161099
6C	-1.143882	2.417573	0.078829
7N	-0.936378	-1.259301	-0.002608
8N	1.726006	-0.537997	-0.445972
9C	1.442070	-1.778689	0.272850
10C	0.070519	-2.302772	-0.130140
11C	-2.325107	-1.697719	0.134927
12C	-3.310908	-0.619574	-0.312580
13C	-2.998145	0.704829	0.394459
14C	3.142599	-0.186377	-0.559209

15C	3.840638	0.172444	0.760815
16H	2.062439	2.183815	-0.408281
17H	-1.886296	3.208212	0.187044
18H	1.476535	-1.629949	1.365312
19H	2.203159	-2.519738	0.010632
20H	0.100070	-2.682500	-1.162626
21H	-0.204909	-3.139533	0.526261
22H	-2.520935	-1.980974	1.182192
23H	-2.453095	-2.601418	-0.473839
24H	-4.331083	-0.953109	-0.090818
25H	-3.234638	-0.484282	-1.399480
26H	-3.191857	0.590462	1.471911
27H	-3.661126	1.502709	0.039198
28H	3.235001	0.635704	-1.276525
29H	3.645060	-1.049187	-1.013729
30H	3.850554	-0.681087	1.449356
31H	4.882075	0.458332	0.566651
32H	3.346572	1.008896	1.267041

1e-004

1N	0.387069	2.884888	0.026289
2C	-0.694625	2.080651	0.028412
3C	-0.650145	0.681001	-0.035035
4C	0.643748	0.067916	-0.037712
5C	1.777053	0.907760	-0.066797
6C	1.583195	2.290396	-0.028460
7N	0.770485	-1.308482	0.016469
8N	-1.802562	-0.124731	-0.119169
9C	-1.630490	-1.473263	0.417280
10C	-0.408877	-2.124029	-0.216796
11C	2.067624	-1.929431	-0.237931
12C	3.191583	-1.115150	0.400624
13C	3.170077	0.317081	-0.143034
14C	-3.098455	0.522828	0.115604
15C	-4.303168	-0.376576	-0.158938
16H	-1.647213	2.595832	0.075492
17H	2.452086	2.948517	-0.035231
18H	-2.504833	-2.076276	0.169264
19H	-1.523935	-1.461484	1.516318
20H	-0.244617	-3.108931	0.235341
21H	-0.585966	-2.272570	-1.294933
22H	2.241390	-2.026962	-1.324082
23H	2.038596	-2.941523	0.181090
24H	4.154360	-1.595963	0.192740
25H	3.052205	-1.105863	1.489620
26H	3.510827	0.310375	-1.189141
27H	3.875901	0.950318	0.408136
28H	-3.162452	1.380001	-0.561476
29H	-3.155565	0.919223	1.146078
30H	-4.230234	-0.844478	-1.148433
31H	-4.428978	-1.164086	0.591886
32H	-5.211630	0.237041	-0.141104

1e-005

1N	0.201596	2.783956	-0.214856
2C	1.108800	1.786259	-0.203424
3C	0.794877	0.425591	-0.121165
4C	-0.588951	0.067650	-0.078312
5C	-1.542867	1.108609	-0.118640
6C	-1.088252	2.426395	-0.169696
7N	-0.967722	-1.249270	0.017283
8N	1.752058	-0.606134	-0.073541
9C	1.294490	-1.831307	-0.730893
10C	0.012349	-2.321868	-0.072667
11C	-2.369943	-1.646796	0.132189
12C	-3.230363	-0.527996	0.716402
13C	-3.015006	0.767525	-0.075472
14C	3.168558	-0.269494	-0.250349
15C	3.821166	0.243182	1.036994
16H	2.144874	2.104854	-0.243181
17H	-1.816179	3.237646	-0.178884
18H	2.062463	-2.601473	-0.623884
19H	1.123104	-1.666920	-1.809559
20H	-0.411460	-3.137848	-0.674387
21H	0.232486	-2.722435	0.928100
22H	-2.414682	-2.534277	0.776067
23H	-2.753004	-1.944625	-0.858152
24H	-2.955064	-0.367544	1.767112
25H	-4.282244	-0.834718	0.691701
26H	-3.580678	1.594735	0.369781
27H	-3.403474	0.633761	-1.096571
28H	3.304190	0.453796	-1.071504

29H	3.680386	-1.185639	-0.560286
30H	3.316356	1.130817	1.431651
31H	3.792306	-0.531989	1.812083
32H	4.869940	0.505495	0.847904

1e-006

1N	-0.233718	2.893589	-0.143583
2C	0.802660	2.076822	-0.387031
3C	0.734219	0.676793	-0.401161
4C	-0.535848	0.078474	-0.143683
5C	-1.633234	0.934093	0.108858
6C	-1.420284	2.311632	0.088711
7N	-0.682635	-1.301096	-0.165515
8N	1.868214	-0.108246	-0.693050
9C	1.600730	-1.520462	-0.963312
10C	0.528721	-2.097283	-0.038025
11C	-1.912750	-1.891822	0.357152
12C	-3.128220	-1.078807	-0.083523
13C	-3.001093	0.361274	0.423734
14C	3.134881	0.194903	-0.008297
15C	3.172202	-0.196776	1.474220
16H	1.751919	2.565709	-0.591357
17H	-2.259292	2.982321	0.272463
18H	2.531191	-2.083462	-0.851086
19H	1.263497	-1.635686	-2.002409
20H	0.297473	-3.128313	-0.328517
21H	0.889933	-2.109136	1.003293
22H	-1.876569	-1.947304	1.460105
23H	-1.973797	-2.918410	-0.021113
24H	-4.041221	-1.546045	0.302833
25H	-3.186850	-1.089519	-1.179726
26H	-3.164790	0.375737	1.511260
27H	-3.781455	0.995788	-0.014018
28H	3.346080	1.262316	-0.112348
29H	3.928799	-0.327169	-0.554995
30H	3.047347	-1.278196	1.605117
31H	4.135712	0.088101	1.916033
32H	2.377094	0.310502	2.033654

1e-007

1N	0.195515	2.807391	-0.396945
2C	1.093796	1.822234	-0.553381
3C	0.822491	0.463686	-0.387004
4C	-0.516378	0.074594	-0.095668
5C	-1.470864	1.108542	0.091154
6C	-1.053095	2.425367	-0.072460
7N	-0.876239	-1.252423	-0.036448
8N	1.858474	-0.511297	-0.544155
9C	1.292062	-1.782793	-1.013904
10C	0.153516	-2.279227	-0.117690
11C	-2.188966	-1.637478	0.477063
12C	-3.262642	-0.647738	0.023882
13C	-2.896150	0.770635	0.475168
14C	2.736351	-0.688839	0.638511
15C	3.606518	0.521332	0.966886
16H	2.101792	2.119960	-0.832276
17H	-1.780342	3.227213	0.055081
18H	2.086136	-2.534006	-1.061306
19H	0.909394	-1.633309	-2.030869
20H	-0.291890	-3.186387	-0.543415
21H	0.535510	-2.537097	0.883468
22H	-2.166357	-1.694270	1.578971
23H	-2.411029	-2.642818	0.102908
24H	-4.231925	-0.947834	0.438259
25H	-3.342925	-0.684320	-1.070378
26H	-3.010077	0.840374	1.567208
27H	-3.586943	1.505058	0.043899
28H	3.387295	-1.539335	0.405260
29H	2.149276	-0.964858	1.532188
30H	4.195132	0.832069	0.095591
31H	3.013267	1.375843	1.307584
32H	4.299598	0.256139	1.775322

1f-Me-001

1N	-1.281119	-2.232158	-1.127044
2C	-0.743408	-1.578148	-0.057418
3C	-1.456544	-0.634853	0.660357
4C	-2.824814	-0.379563	0.280070
5C	-3.365033	-1.112912	-0.811844

6C	-2.562443	-2.004312	-1.492698
7N	-3.553357	0.547571	0.938390
8N	-0.905853	0.096712	1.704332
9C	-1.868752	0.503485	2.728979
10C	-3.003078	1.279754	2.079689
11C	-4.917622	0.913831	0.527898
12C	-5.176342	0.587882	-0.939336
13C	-4.796101	-0.868125	-1.229704
14C	0.459118	-0.193113	2.141605
15C	1.519325	0.180632	1.115046
16C	1.335988	1.265305	0.251946
17C	2.313341	1.607820	-0.692063
18C	3.487975	0.843621	-0.743439
19C	3.702902	-0.243961	0.114848
20C	2.699500	-0.567257	1.039971
21C	4.985884	-1.059809	0.030887
22C	5.779979	-1.008536	1.349493
23C	4.705961	-2.517980	-0.379295
24C	2.101109	2.774206	-1.647183
25C	1.977831	4.111840	-0.894477
26C	0.878546	2.543759	-2.555494
27C	-0.435613	-3.192778	-1.856469
28H	0.286616	-1.818032	0.161397
29H	-2.927577	-2.556622	-2.350993
30H	-1.365296	1.151345	3.449695
31H	-2.264683	-0.370210	3.271079
32H	-3.807727	1.432266	2.807807
33H	-2.652093	2.265193	1.746242
34H	-5.633237	0.390134	1.177536
35H	-5.033736	1.987937	0.707367
36H	-4.584870	1.259416	-1.574720
37H	-6.233579	0.765362	-1.161632
38H	-4.924577	-1.102844	-2.291642
39H	-5.464974	-1.536955	-0.669431
40H	0.625340	0.386530	3.055285
41H	0.567387	-1.255055	2.420955
42H	0.410937	1.832616	0.305955
43H	4.253548	1.099682	-1.474225
44H	2.834776	-1.416527	1.707395
45H	5.610237	-0.609003	-0.752084
46H	6.003498	0.025169	1.639645
47H	5.218640	-1.475064	2.169073
48H	6.730884	-1.546453	1.247053
49H	4.161920	-2.567668	-1.330753
50H	5.645476	-3.072630	-0.496222
51H	4.105678	-3.033887	0.380996
52H	2.987900	2.835127	-2.292354
53H	2.858144	4.298671	-0.267783
54H	1.881079	4.944296	-1.602931
55H	1.093507	4.119923	-0.244472
56H	0.968811	1.602065	-3.110935
57H	-0.048723	2.501809	-1.969482
58H	0.778889	3.359817	-3.282269
59H	0.479899	-2.693869	-2.184553
60H	-0.980902	-3.559144	-2.726266
61H	-0.185133	-4.033000	-1.202693

1f-Me-002

1N	-1.294819	-2.313983	-0.937394
2C	-0.769455	-1.561228	0.070395
3C	-1.473964	-0.523288	0.658816
4C	-2.819913	-0.269148	0.198752
5C	-3.329605	-1.071768	-0.856294
6C	-2.544939	-2.076239	-1.387303
7N	-3.561282	0.713633	0.765151
8N	-0.924632	0.289728	1.636343
9C	-1.877006	0.942017	2.531865
10C	-2.949796	1.643552	1.712650
11C	-4.887195	1.068460	0.241326
12C	-5.595220	-0.150920	-0.340263
13C	-4.714790	-0.808431	-1.406024
14C	0.417970	0.012062	2.145918
15C	1.518436	0.275592	1.127283
16C	1.425815	1.352890	0.240663
17C	2.434118	1.601213	-0.699916
18C	3.545308	0.745623	-0.727690
19C	3.666508	-0.340428	0.150287
20C	2.637822	-0.561295	1.077884
21C	4.863904	-1.277407	0.071235
22C	5.651974	-1.322875	1.393091
23C	4.433413	-2.693784	-0.356659
24C	2.317409	2.761415	-1.678679
25C	2.263358	4.118155	-0.952490
26C	1.100796	2.591059	-2.607920
27C	-0.454567	-3.368229	-1.529823

28H	0.241160	-1.814205	0.353036
29H	-2.899673	-2.708262	-2.193116
30H	-1.343799	1.685810	3.128463
31H	-2.339968	0.218010	3.220385
32H	-3.733465	2.018217	2.378274
33H	-2.519247	2.499365	1.174552
34H	-4.776425	1.853242	-0.521965
35H	-5.462777	1.491585	1.070035
36H	-6.552244	0.161875	-0.770093
37H	-5.809206	-0.865602	0.464474
38H	-5.162894	-1.743635	-1.759295
39H	-4.640473	-0.142675	-2.277274
40H	0.565025	0.664951	3.011680
41H	0.491929	-1.022050	2.520235
42H	0.545012	1.989205	0.272322
43H	4.331519	0.924522	-1.459825
44H	2.699948	-1.406725	1.761037
45H	5.535976	-0.885706	-0.703839
46H	5.979017	-0.321118	1.696740
47H	5.044561	-1.739580	2.206621
48H	6.543368	-1.953403	1.285511
49H	3.896687	-2.674751	-1.313415
50H	5.308226	-3.346404	-0.470017
51H	3.772036	-3.147702	0.392829
52H	3.219038	2.754821	-2.305981
53H	3.140453	4.260904	-0.309815
54H	2.234679	4.941190	-1.677663
55H	1.367740	4.194819	-0.322690
56H	1.142013	1.635312	-3.144805
57H	0.161908	2.618392	-2.039773
58H	1.067925	3.398190	-3.350558
59H	-1.037300	-3.920653	-2.267158
60H	0.413413	-2.913573	-2.015216
61H	-0.121314	-4.052005	-0.745031

1f-Me-003

1N	-1.533634	2.360438	0.713500
2C	-1.036162	1.556750	-0.270858
3C	-1.720733	0.443146	-0.725303
4C	-3.019535	0.164039	-0.159173
5C	-3.527544	1.054949	0.824923
6C	-2.751850	2.114991	1.243961
7N	-3.716492	-0.924803	-0.549630
8N	-1.205695	-0.429369	-1.675005
9C	-2.219600	-1.101243	-2.489881
10C	-3.203250	-1.823556	-1.583237
11C	-5.000912	-1.301215	0.062315
12C	-5.160302	-0.711033	1.459370
13C	-4.889149	0.796741	1.425642
14C	0.078884	-0.129621	-2.310762
15C	1.265835	-0.256601	-1.366658
16C	2.322596	0.657243	-1.441053
17C	3.428450	0.558621	-0.583827
18C	3.452319	-0.482879	0.353532
19C	2.409148	-1.415962	0.447329
20C	1.321218	-1.290764	-0.426142
21C	2.445937	-2.531919	1.482831
22C	3.656486	-3.461821	1.282014
23C	2.419961	-1.969369	2.916442
24C	4.558075	1.578226	-0.652396
25C	5.914738	0.913707	-0.949807
26C	4.632747	2.416752	0.638120
27C	-0.700115	3.474527	1.195330
28H	-0.058521	1.831460	-0.637183
29H	-3.089892	2.795046	2.016853
30H	-1.727151	-1.834200	-3.132176
31H	-2.751432	-0.383348	-3.134810
32H	-4.051961	-2.184105	-2.175202
33H	-2.723246	-2.689902	-1.109343
34H	-5.032560	-2.395385	0.101771
35H	-5.814613	-0.969208	-0.597905
36H	-4.459232	-1.199678	2.147766
37H	-6.174398	-0.915579	1.817171
38H	-5.661923	1.291034	0.820014
39H	-4.946159	1.228076	2.430563
40H	0.068692	0.872939	-2.768963
41H	0.193986	-0.845089	-3.130997
42H	2.282360	1.468550	-2.166902
43H	4.297731	-0.564176	1.031565
44H	0.495304	-1.995781	-0.363166
45H	1.537645	-3.134712	1.345779
46H	3.626855	-4.290518	2.000660
47H	3.668365	-3.886851	0.270977
48H	4.601327	-2.924511	1.431441
49H	2.390892	-2.784853	3.650284

50H	1.541098	-1.332925	3.078536
51H	3.313760	-1.366913	3.121686
52H	4.332651	2.261606	-1.482411
53H	6.701719	1.672423	-1.043956
54H	6.206114	0.228631	-0.143959
55H	5.881315	0.340357	-1.884114
56H	3.679274	2.920229	0.842342
57H	4.872933	1.786948	1.504116
58H	5.412255	3.184906	0.555769
59H	-1.252632	4.037944	1.947863
60H	0.217636	3.078110	1.638334
61H	-0.450890	4.133366	0.359275

1f-Me-004

1N	1.388299	-2.461604	-0.644613
2C	0.877384	-1.625832	0.305205
3C	1.573179	-0.520084	0.762015
4C	2.896454	-0.283186	0.235446
5C	3.415649	-1.205654	-0.713226
6C	2.628904	-2.255122	-1.138696
7N	3.606309	0.795987	0.630148
8N	1.046607	0.381964	1.676106
9C	2.043501	1.055588	2.509333
10C	3.075679	1.732065	1.621056
11C	4.924201	1.123236	0.063054
12C	5.120554	0.502820	-1.315873
13C	4.805038	-0.995814	-1.267163
14C	-0.270187	0.129394	2.262797
15C	-1.409819	0.271125	1.263269
16C	-1.370515	1.257851	0.276475
17C	-2.418103	1.398560	-0.646972
18C	-3.507819	0.524086	-0.557753
19C	-3.578845	-0.472621	0.429530
20C	-2.515976	-0.586514	1.333984
21C	-4.769833	-1.418437	0.505068
22C	-6.082979	-0.659668	0.771538
23C	-4.885636	-2.282994	-0.764507
24C	-2.369479	2.477886	-1.719579
25C	-1.162897	2.294102	-2.658523
26C	-2.370613	3.887782	-1.099411
27C	0.542266	-3.562645	-1.135140
28H	-0.119158	-1.868825	0.641897
29H	2.976560	-2.957973	-1.886570
30H	2.535781	0.345950	3.193329
31H	1.543227	1.816668	3.111890
32H	2.632888	2.595965	1.108145
33H	3.909999	2.089788	2.234756
34H	5.701082	0.780201	0.760789
35H	4.990227	2.214841	0.005123
36H	6.153218	0.672338	-1.637227
37H	4.460672	0.998178	-2.039375
38H	4.887099	-1.446133	-2.261988
39H	5.539793	-1.501122	-0.624371
40H	-0.400482	0.862227	3.065229
41H	-0.308113	-0.864064	2.739462
42H	-0.503745	1.910822	0.219007
43H	-4.320243	0.621577	-1.274685
44H	-2.546197	-1.361117	2.099421
45H	-4.598073	-2.093804	1.354298
46H	-6.017098	-0.061740	1.688607
47H	-6.324090	0.018491	-0.056442
48H	-6.917820	-1.363049	0.882664
49H	-3.963770	-2.849683	-0.946431
50H	-5.711353	-2.999695	-0.670425
51H	-5.079774	-1.663067	-1.648889
52H	-3.280528	2.381305	-2.325437
53H	-1.170698	1.301667	-3.125795
54H	-1.179287	3.047057	-3.456529
55H	-0.215738	2.403496	-2.114830
56H	-3.244482	4.036843	-0.453707
57H	-1.471409	4.054339	-0.492686
58H	-2.391393	4.654251	-1.884534
59H	0.213771	-4.174088	-0.290609
60H	-0.328954	-3.151434	-1.652673
61H	1.118927	-4.180174	-1.824456

1f-Me-005

1N	-1.805921	1.243796	2.187387
2C	-1.044859	0.231156	1.684505
3C	-1.533181	-0.656605	0.737697
4C	-2.887014	-0.472696	0.268261
5C	-3.645418	0.595945	0.812915

6C	-3.070417	1.428608	1.752815
7N	-3.400614	-1.303484	-0.673288
8N	-0.774120	-1.700886	0.241693
9C	-1.181850	-2.268616	-1.041343
10C	-2.681743	-2.522582	-1.037822
11C	-4.803671	-1.199928	-1.095499
12C	-5.294177	0.242984	-1.031836
13C	-5.078229	0.808331	0.374407
14C	0.605500	-1.893161	0.668563
15C	1.637938	-0.910046	0.118568
16C	2.975729	-1.065140	0.506017
17C	3.969953	-0.192345	0.045564
18C	3.590691	0.855851	-0.808418
19C	2.261841	1.037686	-1.209079
20C	1.293175	0.137980	-0.737920
21C	1.869697	2.187742	-2.126315
22C	1.287025	1.681470	-3.459029
23C	0.888361	3.153037	-1.433839
24C	5.422702	-0.356016	0.472686
25C	5.985063	-1.740562	0.101892
26C	5.596885	-0.081096	1.978474
27C	-1.195006	2.162763	3.163484
28H	-0.030659	0.185459	2.054351
29H	-3.614653	2.260676	2.183952
30H	-0.656258	-3.216170	-1.183561
31H	-0.915699	-1.605297	-1.876832
32H	-3.004880	-2.824423	-2.038452
33H	-2.930992	-3.331950	-0.337493
34H	-5.423456	-1.847148	-0.456872
35H	-4.866294	-1.585342	-2.117386
36H	-6.355230	0.272069	-1.299846
37H	-4.748285	0.846075	-1.768395
38H	-5.326004	1.875053	0.408157
39H	-5.753823	0.302780	1.078694
40H	0.886803	-2.911833	0.380927
41H	0.632952	-1.876007	1.766088
42H	3.243000	-1.881867	1.174301
43H	4.351492	1.546233	-1.169465
44H	0.259998	0.267986	-1.042870
45H	2.783897	2.751478	-2.355503
46H	1.989287	1.013610	-3.972239
47H	0.352147	1.128633	-3.299114
48H	1.066852	2.523379	-4.127584
49H	1.307633	3.542491	-0.497861
50H	0.662289	4.005988	-2.086330
51H	-0.059588	2.653012	-1.195941
52H	6.009198	0.396394	-0.071403
53H	5.879281	-1.940044	-0.971415
54H	7.050942	-1.800893	0.355449
55H	5.468125	-2.540899	0.646388
56H	5.220152	0.913401	2.247747
57H	5.054986	-0.822365	2.579902
58H	6.656524	-0.131131	2.259673
59H	-1.957584	2.846518	3.537074
60H	-0.785229	1.588032	3.997566
61H	-0.396314	2.731561	2.679264

1f-Me-006

1N	1.531598	2.318845	0.711828
2C	1.042747	1.502375	-0.264579
3C	1.723598	0.372546	-0.688927
4C	3.013801	0.095884	-0.100586
5C	3.488428	0.969085	0.913486
6C	2.727480	2.060526	1.281899
7N	3.738142	-0.972911	-0.512638
8N	1.197938	-0.505864	-1.622457
9C	2.170754	-1.299857	-2.369680
10C	3.140592	-1.964521	-1.404489
11C	5.006546	-1.334978	0.134729
12C	5.730903	-0.099559	0.659981
13C	4.809505	0.687904	1.594882
14C	-0.076396	-0.200466	-2.272924
15C	-1.274180	-0.289869	-1.337027
16C	-1.329295	-1.264018	-0.334587
17C	-2.426312	-1.348522	0.532748
18C	-3.478564	-0.435358	0.370028
19C	-3.457423	0.542297	-0.634165
20C	-2.340261	0.604633	-1.480002
21C	-4.610083	1.524551	-0.795585
22C	-5.937542	0.799836	-1.085650
23C	-4.747312	2.442812	0.433567
24C	-2.465753	-2.403205	1.630333
25C	-3.656132	-3.363925	1.455122
26C	-2.482280	-1.760758	3.030181
27C	0.737298	3.495949	1.102144

28H	0.079428	1.785891	-0.660866
29H	3.059256	2.749664	2.049374
30H	2.722889	-0.679400	-3.092987
31H	1.636914	-2.076194	-2.923005
32H	2.624645	-2.736053	-0.816242
33H	3.944336	-2.446913	-1.968907
34H	5.616480	-1.854544	-0.610644
35H	4.805513	-2.043006	0.952597
36H	6.036775	0.530353	-0.185021
37H	6.637936	-0.413306	1.186447
38H	4.631829	0.103470	2.508707
39H	5.279661	1.627308	1.905491
40H	-0.194685	-0.925684	-3.084026
41H	-0.047270	0.793527	-2.748173
42H	-0.496480	-1.953914	-0.218794
43H	-4.333940	-0.487859	1.038766
44H	-2.301663	1.367684	-2.256865
45H	-4.380529	2.159587	-1.662156
46H	-6.740852	1.525237	-1.266177
47H	-5.854293	0.156194	-1.969723
48H	-6.239666	0.170739	-0.239006
49H	-3.817319	2.991908	0.627915
50H	-5.548680	3.176742	0.280372
51H	-4.991511	1.864502	1.333545
52H	-1.544412	-2.996218	1.548399
53H	-3.629587	-4.151208	2.219053
54H	-4.611804	-2.834161	1.553849
55H	-3.637831	-3.843740	0.469056
56H	-1.617627	-1.101328	3.175955
57H	-3.390378	-1.163804	3.181238
58H	-2.457295	-2.533510	3.808977
59H	0.708838	4.210844	0.274619
60H	-0.278622	3.180816	1.352836
61H	1.195477	3.965727	1.972871

1f-Me-007

1N	1.972497	1.993829	-1.427016
2C	1.206383	0.867638	-1.359215
3C	1.670245	-0.302362	-0.782674
4C	2.995808	-0.303020	-0.209696
5C	3.750394	0.899384	-0.269792
6C	3.214640	2.006875	-0.894373
7N	3.495503	-1.425046	0.354356
8N	0.923216	-1.466697	-0.732535
9C	1.228239	-2.371095	0.375225
10C	2.720082	-2.665083	0.397872
11C	4.870466	-1.495822	0.874818
12C	5.777987	-0.454854	0.227291
13C	5.138376	0.933899	0.326079
14C	-0.394528	-1.549831	-1.348663
15C	-1.552396	-0.891013	-0.603654
16C	-1.364963	-0.114785	0.539311
17C	-2.450593	0.505817	1.181824
18C	-3.732063	0.322104	0.655874
19C	-3.954233	-0.463290	-0.490170
20C	-2.851700	-1.060258	-1.108255
21C	-5.358056	-0.659212	-1.046019
22C	-6.276008	-1.362990	-0.029513
23C	-5.974657	0.673535	-1.510399
24C	-2.220787	1.372767	2.412088
25C	-1.377465	2.615711	2.068612
26C	-1.574808	0.575429	3.560402
27C	1.399708	3.195195	-2.057110
28H	0.211362	0.954405	-1.772574
29H	3.770164	2.933031	-0.983200
30H	0.679861	-3.303810	0.224559
31H	0.912114	-1.944837	1.338439
32H	2.976058	-3.195705	1.321679
33H	2.999551	-3.301887	-0.451851
34H	5.241751	-2.505993	0.673425
35H	4.841018	-1.363942	1.965548
36H	5.941956	-0.714887	-0.826236
37H	6.750893	-0.470449	0.729038
38H	5.079607	1.231933	1.382698
39H	5.749476	1.685663	-0.184445
40H	-0.614228	-2.614776	-1.484486
41H	-0.324208	-1.128540	-2.359841
42H	-0.365605	0.023925	0.938486
43H	-4.576574	0.799915	1.147965
44H	-3.003706	-1.669842	-1.998650
45H	-5.273944	-1.310947	-1.926432
46H	-7.266706	-1.542903	-0.465649
47H	-5.859307	-2.329119	0.280504
48H	-6.412403	-0.751176	0.870958
49H	-5.338268	1.168129	-2.254714

50H	-6.959691	0.504455	-1.963675
51H	-6.107672	1.363828	-0.668011
52H	-3.202874	1.721525	2.758048
53H	-1.261311	3.260012	2.949260
54H	-0.373721	2.329674	1.727518
55H	-1.848524	3.207420	1.274080
56H	-2.176888	-0.302626	3.824041
57H	-0.571413	0.225107	3.285165
58H	-1.474862	1.201135	4.456315
59H	1.194533	2.994819	-3.112262
60H	0.472595	3.467029	-1.545374
61H	2.112031	4.016383	-1.973148

1f-Me-008

1N	-3.934706	-1.820567	1.386618
2C	-2.615058	-1.638950	1.084478
3C	-2.184226	-0.612216	0.263956
4C	-3.182564	0.235408	-0.347556
5C	-4.548695	-0.005898	-0.037638
6C	-4.874837	-1.018217	0.839742
7N	-2.814011	1.233918	-1.175969
8N	-0.844513	-0.348925	0.000267
9C	-0.612625	0.157131	-1.357177
10C	-1.415442	1.429545	-1.561017
11C	-3.783003	2.176295	-1.755489
12C	-5.057909	2.265065	-0.922902
13C	-5.614873	0.860841	-0.665366
14C	0.170774	-1.257561	0.553988
15C	1.571156	-0.697583	0.425378
16C	1.908314	0.498263	1.078301
17C	3.189258	1.045002	0.964349
18C	4.136730	0.363466	0.178727
19C	3.830236	-0.829653	-0.482369
20C	2.531106	-1.351342	-0.347538
21C	4.872815	-1.535963	-1.337777
22C	5.206507	-2.935936	-0.790526
23C	4.434485	-1.616244	-2.812359
24C	3.544412	2.349480	1.664582
25C	3.849754	3.466150	0.648011
26C	4.714919	2.173421	2.649075
27C	-4.303217	-2.928993	2.283886
28H	-1.938001	-2.344240	1.544427
29H	-5.903159	-1.217657	1.117945
30H	-0.887911	-0.599570	-2.109360
31H	0.446950	0.384454	-1.476350
32H	-0.986575	2.251904	-0.974280
33H	-1.390920	1.715222	-2.618897
34H	-4.008511	1.860337	-2.784009
35H	-3.290592	3.153034	-1.810653
36H	-5.788842	2.880960	-1.456669
37H	-4.839849	2.760271	0.031885
38H	-6.498370	0.900550	-0.019320
39H	-5.933663	0.416269	-1.619052
40H	0.111202	-2.247614	0.072669
41H	-0.056846	-1.392776	1.617091
42H	1.154918	1.009188	1.675532
43H	5.139685	0.773783	0.080893
44H	2.263917	-2.273690	-0.858948
45H	5.790090	-0.933603	-1.296554
46H	5.544925	-2.886348	0.251551
47H	4.330377	-3.596021	-0.828723
48H	6.002276	-3.401864	-1.385310
49H	4.219296	-0.620319	-3.218784
50H	5.223812	-2.070535	-3.424487
51H	3.531182	-2.229668	-2.923789
52H	2.664374	2.658406	2.245524
53H	3.008043	3.621819	-0.038261
54H	4.047637	4.414182	1.164171
55H	4.733927	3.221360	0.046001
56H	4.501213	1.390382	3.386765
57H	5.638375	1.898796	2.124465
58H	4.904188	3.108963	3.190393
59H	-5.377578	-2.900232	2.468017
60H	-4.040335	-3.882269	1.816516
61H	-3.770713	-2.823534	3.232618

1f-Me-009

1N	-1.748726	0.244852	2.406907
2C	-1.094732	-0.474081	1.450085
3C	-1.675166	-0.767595	0.226742
4C	-3.014452	-0.288306	-0.023913
5C	-3.640368	0.502221	0.976353

6C	-2.987572	0.728319	2.170711
7N	-3.644532	-0.596087	-1.180161
8N	-1.029057	-1.505075	-0.749234
9C	-1.496767	-1.321327	-2.122150
10C	-3.009970	-1.460999	-2.174397
11C	-5.032682	-0.187395	-1.451726
12C	-5.809181	0.083842	-0.167052
13C	-5.025763	1.049985	0.727858
14C	0.321658	-2.007098	-0.530266
15C	1.445591	-0.974354	-0.464011
16C	1.257771	0.367722	-0.815873
17C	2.306847	1.292151	-0.729774
18C	3.559650	0.841576	-0.287172
19C	3.779787	-0.496144	0.065672
20C	2.705015	-1.393724	-0.023566
21C	5.151367	-0.959638	0.536541
22C	5.110608	-1.478649	1.985679
23C	5.746818	-2.021502	-0.406787
24C	2.079401	2.753573	-1.091876
25C	3.012124	3.218630	-2.225531
26C	2.223425	3.664282	0.141940
27C	-1.062492	0.500394	3.683956
28H	-0.092146	-0.783353	1.708412
29H	-3.444919	1.301053	2.968571
30H	-1.042685	-2.091999	-2.749461
31H	-1.199178	-0.341293	-2.522014
32H	-3.369675	-1.164339	-3.165150
33H	-3.307664	-2.503645	-1.999160
34H	-5.504820	-0.995992	-2.018742
35H	-5.017299	0.703986	-2.094632
36H	-5.978013	-0.860511	0.365820
37H	-6.788265	0.500251	-0.425096
38H	-4.953159	2.027970	0.231087
39H	-5.544315	1.212495	1.678801
40H	0.528675	-2.716168	-1.338638
41H	0.322117	-2.596811	0.396230
42H	0.280680	0.711460	-1.143837
43H	4.385161	1.546155	-0.212020
44H	2.850241	-2.436479	0.254733
45H	5.816596	-0.085999	0.515201
46H	6.117248	-1.755958	2.323241
47H	4.719670	-0.716832	2.671507
48H	4.473358	-2.368265	2.069770
49H	5.795346	-1.654466	-1.439185
50H	6.763397	-2.288326	-0.091339
51H	5.144355	-2.938875	-0.403200
52H	1.045472	2.842962	-1.453465
53H	2.783783	4.253516	-2.509989
54H	4.064224	3.182616	-1.916551
55H	2.901589	2.588422	-3.116371
56H	1.538174	3.360461	0.943161
57H	3.244643	3.626994	0.541412
58H	2.002329	4.707081	-0.118768
59H	-0.868748	-0.447513	4.193421
60H	-0.117935	1.017193	3.494050
61H	-1.697536	1.127080	4.310963

1f-Me-010

1N	0.882776	1.006362	1.963516
2C	0.541369	-0.184114	1.409297
3C	1.391317	-0.873668	0.573239
4C	2.707594	-0.354042	0.338574
5C	3.059731	0.878444	0.974145
6C	2.123446	1.522015	1.745297
7N	3.573286	-1.005632	-0.463519
8N	0.964118	-2.083738	-0.030041
9C	2.112230	-2.972345	-0.258688
10C	3.223666	-2.296810	-1.063314
11C	4.900959	-0.464273	-0.793025
12C	4.949422	1.052588	-0.634470
13C	4.437604	1.455412	0.753418
14C	0.098565	-1.932739	-1.240749
15C	-1.126202	-1.088999	-0.983353
16C	-1.134947	0.261963	-1.337245
17C	-2.225064	1.089518	-1.021576
18C	-3.314595	0.521968	-0.352973
19C	-3.341630	-0.837818	0.006974
20C	-2.234428	-1.629774	-0.314039
21C	-4.537920	-1.428315	0.741099
22C	-4.725901	-0.777314	2.124699
23C	-5.828256	-1.323213	-0.092629
24C	-2.199580	2.572749	-1.361999
25C	-2.055172	2.816635	-2.874851
26C	-1.084757	3.297463	-0.582334
27C	-0.062430	1.682627	2.868622

28H	-0.446756	-0.560481	1.638558
29H	2.336426	2.470653	2.225262
30H	1.770479	-3.869109	-0.782266
31H	2.502283	-3.281105	0.717927
32H	4.121687	-2.925257	-1.065210
33H	2.923644	-2.142400	-2.108373
34H	5.118862	-0.749160	-1.827781
35H	5.649170	-0.949374	-0.150670
36H	4.331659	1.522738	-1.410262
37H	5.979772	1.391769	-0.780455
38H	5.123184	1.065384	1.519255
39H	4.416616	2.544509	0.866238
40H	-0.191358	-2.949195	-1.525174
41H	0.671130	-1.500500	-2.075397
42H	-0.269980	0.681634	-1.846596
43H	-4.165335	1.154396	-0.107130
44H	-2.224657	-2.681292	-0.031781
45H	-4.330193	-2.495058	0.900120
46H	-3.823024	-0.880072	2.739564
47H	-4.951895	0.292610	2.032311
48H	-5.557371	-1.249225	2.663096
49H	-5.709204	-1.804046	-1.071125
50H	-6.662336	-1.810650	0.427590
51H	-6.106822	-0.275975	-0.264170
52H	-3.159875	3.000751	-1.044507
53H	-2.860030	2.327060	-3.436060
54H	-2.090774	3.890885	-3.095873
55H	-1.099467	2.430188	-3.251068
56H	-1.198535	3.153073	0.498844
57H	-0.094672	2.921390	-0.870459
58H	-1.106997	4.375467	-0.786230
59H	-1.079248	1.537171	2.500170
60H	0.028899	1.266929	3.876762
61H	0.163341	2.749598	2.890489

1f-PhNCO-001

1N	-1.022332	-2.068509	0.229955
2C	-1.066901	-0.977391	-0.582313
3C	-2.237110	-0.281590	-0.812386
4C	-3.452978	-0.775782	-0.224647
5C	-3.376389	-1.935927	0.592945
6C	-2.151106	-2.529063	0.811117
7N	-4.625760	-0.131726	-0.432727
8N	-2.289870	0.890974	-1.572606
9C	-3.547647	1.049348	-2.303121
10C	-4.710809	1.025088	-1.322013
11C	-5.873894	-0.538426	0.226077
12C	-5.609533	-1.324550	1.507228
13C	-4.637150	-2.475493	1.227179
14C	-1.072957	1.340106	-2.255490
15C	-0.009073	1.867231	-1.303708
16C	1.325391	1.475007	-1.445737
17C	2.318596	1.942074	-0.572734
18C	1.943095	2.827572	0.445963
19C	0.613052	3.244148	0.609333
20C	-0.354332	2.751826	-0.275507
21C	0.221717	4.195843	1.732465
22C	0.951018	5.547633	1.621091
23C	0.456795	3.561326	3.116253
24C	3.762161	1.481278	-0.725134
25C	4.683481	2.647062	-1.131095
26C	4.283518	0.789221	0.547521
27C	0.306128	-2.766305	0.528991
28O	0.238783	-3.623612	1.427228
29N	1.247175	-2.312915	-0.255788
30C	2.579107	-2.705472	-0.123177
31C	3.429517	-2.412338	-1.214168
32C	4.791202	-2.706599	-1.177097
33C	5.357855	-3.296422	-0.039620
34C	4.531646	-3.588673	1.051322
35C	3.162656	-3.307869	1.017156
36H	-0.109317	-0.696666	-0.987579
37H	-2.025588	-3.392925	1.451536
38H	-3.672782	0.258595	-3.062005
39H	-3.538985	2.013713	-2.816578
40H	-4.725785	1.946826	-0.724915
41H	-5.655974	0.963584	-1.875165
42H	-6.470882	-1.134291	-0.480086
43H	-6.439193	0.374333	0.446138
44H	-6.561272	-1.702791	1.895121
45H	-5.183059	-0.655252	2.265474
46H	-4.393667	-3.016312	2.147997
47H	-5.115216	-3.197517	0.549279
48H	-1.379612	2.143298	-2.933575
49H	-0.650495	0.538843	-2.884340

50H	1.594461	0.767283	-2.228034
51H	2.699689	3.191057	1.136761
52H	-1.395935	3.042011	-0.152406
53H	-0.855153	4.390971	1.634645
54H	0.776747	6.016318	0.644645
55H	0.601152	6.239387	2.398276
56H	2.034365	5.426479	1.746290
57H	-0.081795	2.610849	3.213770
58H	1.522711	3.360806	3.282898
59H	0.112894	4.233499	3.913190
60H	3.784534	0.739434	-1.534064
61H	4.341742	3.121126	-2.059650
62H	4.710813	3.418348	-0.350642
63H	5.710013	2.291015	-1.287651
64H	3.643128	-0.051212	0.835406
65H	5.295409	0.398814	0.383252
66H	4.327990	1.490308	1.390758
67H	2.992491	-1.940279	-2.090971
68H	5.415001	-2.467671	-2.036328
69H	6.420842	-3.523000	-0.005000
70H	4.955445	-4.045055	1.944115
71H	2.538204	-3.546986	1.869611

1f-PhNCO-002

1N	-0.607172	-2.183137	0.180421
2C	-0.788130	-1.102027	-0.626590
3C	-2.038292	-0.565848	-0.862982
4C	-3.183343	-1.214261	-0.283518
5C	-2.962040	-2.363743	0.522572
6C	-1.671188	-2.792295	0.747259
7N	-4.427949	-0.724031	-0.494551
8N	-2.242375	0.593628	-1.615671
9C	-3.500175	0.585163	-2.361552
10C	-4.659743	0.407943	-1.391035
11C	-5.615445	-1.292479	0.156905
12C	-5.255724	-2.049429	1.432421
13C	-4.145538	-3.066404	1.144666
14C	-1.088395	1.237006	-2.248618
15C	-0.159204	1.901413	-1.242849
16C	1.224278	1.696179	-1.307900
17C	2.090459	2.280020	-0.375974
18C	1.537005	3.096619	0.622572
19C	0.157541	3.325884	0.708708
20C	-0.681946	2.717555	-0.236299
21C	-0.417207	4.207148	1.810163
22C	-1.399194	3.429937	2.706661
23C	-1.084903	5.470033	1.234854
24C	3.585969	2.001409	-0.430784
25C	4.396451	3.282441	-0.699311
26C	4.076990	1.295485	0.846526
27C	0.797395	-2.706618	0.488020
28O	0.830022	-3.580892	1.371883
29N	1.681827	-2.120669	-0.274450
30C	3.051844	-2.342728	-0.135889
31C	3.697108	-2.953668	0.966412
32C	5.091056	-3.052438	1.009256
33C	5.884400	-2.566031	-0.035424
34C	5.257892	-1.967152	-1.136440
35C	3.869782	-1.854552	-1.181690
36H	0.126603	-0.694535	-1.022765
37H	-1.439132	-3.637290	1.382883
38H	-3.512658	-0.215714	-3.119942
39H	-3.614304	1.541969	-2.876604
40H	-4.804451	1.321460	-0.798851
41H	-5.583227	0.216968	-1.951703
42H	-6.129685	-1.953722	-0.556209
43H	-6.293156	-0.461564	0.383257
44H	-6.152864	-2.547196	1.815496
45H	-4.916470	-1.338588	2.196866
46H	-3.838130	-3.583506	2.060005
47H	-4.527631	-3.833985	0.456212
48H	-1.490223	1.996451	-2.927233
49H	-0.523461	0.523791	-2.871686
50H	1.632177	1.039943	-2.074777
51H	2.192170	3.554719	1.361394
52H	-1.758665	2.858261	-0.178284
53H	0.421080	4.532304	2.440938
54H	-0.926808	2.535843	3.131210
55H	-1.745757	4.060069	3.535972
56H	-2.282538	3.106339	2.141487
57H	-0.380231	6.051780	0.628025
58H	-1.940193	5.209681	0.598139
59H	-1.452462	6.115927	2.042723
60H	3.756797	1.314351	-1.269785
61H	4.072051	3.773329	-1.625298

62H	4.282161	4.003131	0.120650
63H	5.464800	3.048670	-0.792830
64H	3.520329	0.369272	1.025036
65H	5.139757	1.037871	0.758806
66H	3.958326	1.940836	1.726477
67H	3.101357	-3.342270	1.783297
68H	5.560615	-3.519519	1.873174
69H	6.967752	-2.650654	0.006343
70H	5.854896	-1.579445	-1.959745
71H	3.384473	-1.375757	-2.028815

1f-PhNCO-003

1N	-0.980517	-2.043955	0.310078
2C	-1.043391	-0.977841	-0.531998
3C	-2.220796	-0.290087	-0.762563
4C	-3.423920	-0.769142	-0.133738
5C	-3.318223	-1.873476	0.752324
6C	-2.090833	-2.475492	0.942978
7N	-4.618073	-0.171269	-0.389077
8N	-2.273906	0.856896	-1.553328
9C	-3.559904	1.101661	-2.198346
10C	-4.664915	1.073716	-1.151240
11C	-5.833989	-0.556730	0.335766
12C	-5.812022	-2.037555	0.705879
13C	-4.541520	-2.361578	1.496765
14C	-1.067161	1.300814	-2.254536
15C	-0.012596	1.877961	-1.320850
16C	-0.369676	2.828388	-0.357133
17C	0.584058	3.363529	0.517045
18C	1.911689	2.920737	0.411241
19C	2.298800	1.971495	-0.543455
20C	1.319840	1.465778	-1.411158
21C	3.731773	1.461033	-0.611048
22C	4.109748	0.694925	0.670409
23C	4.736242	2.593741	-0.891282
24C	0.182128	4.386306	1.571802
25C	0.368035	3.828537	2.995752
26C	0.941313	5.715200	1.402879
27C	0.349929	-2.754904	0.576826
28O	0.299395	-3.599531	1.487767
29N	1.271122	-2.324489	-0.243374
30C	2.600238	-2.738838	-0.151719
31C	3.208809	-3.354270	0.968409
32C	4.574427	-3.652976	0.961069
33C	5.372284	-3.366113	-0.152075
34C	4.780399	-2.764194	-1.270265
35C	3.422055	-2.452462	-1.266342
36H	-0.096992	-0.715359	-0.973441
37H	-1.950616	-3.318033	1.608145
38H	-3.768527	0.358263	-2.985399
39H	-3.536358	2.090588	-2.662998
40H	-4.567105	1.935418	-0.475397
41H	-5.640342	1.136674	-1.644181
42H	-6.687404	-0.333136	-0.312952
43H	-5.932712	0.064433	1.239505
44H	-5.847697	-2.641093	-0.210048
45H	-6.705446	-2.272871	1.294132
46H	-4.589960	-1.871181	2.479694
47H	-4.462003	-3.437917	1.684518
48H	-1.387011	2.073794	-2.960525
49H	-0.632363	0.485272	-2.854786
50H	-1.410039	3.138145	-0.275402
51H	2.655673	3.312344	1.100696
52H	1.597033	0.709790	-2.143952
53H	3.787323	0.749959	-1.445802
54H	3.409187	-0.124294	0.862327
55H	5.114557	0.264070	0.579402
56H	4.104567	1.360981	1.543063
57H	4.489820	3.127577	-1.817719
58H	4.747533	3.327184	-0.075082
59H	5.751882	2.189752	-0.990633
60H	-0.887619	4.595563	1.433549
61H	-0.192787	2.896133	3.133619
62H	1.424889	3.617152	3.201673
63H	0.017876	4.552069	3.743368
64H	0.799739	6.130688	0.397499
65H	0.587337	6.456670	2.130780
66H	2.018599	5.580554	1.561503
67H	2.607375	-3.587340	1.838839
68H	5.018168	-4.118462	1.839359
69H	6.432946	-3.605866	-0.149286
70H	5.381865	-2.529954	-2.146540
71H	2.966161	-1.970587	-2.128120

1f-PhNCO-004

1N	0.276022	-2.170231	-0.407617
2C	0.588261	-1.185053	0.477081
3C	1.897149	-0.843454	0.765094
4C	2.953248	-1.599735	0.143056
5C	2.590710	-2.598325	-0.798634
6C	1.255278	-2.850811	-1.038473
7N	4.252495	-1.355627	0.459953
8N	2.228427	0.211022	1.611455
9C	3.499108	0.064985	2.312396
10C	4.604517	-0.214943	1.302337
11C	5.348853	-2.035634	-0.239825
12C	4.939113	-3.438880	-0.679575
13C	3.667047	-3.370571	-1.529081
14C	1.167905	0.997915	2.244400
15C	0.467603	1.929255	1.265009
16C	1.225116	2.832680	0.505033
17C	0.614515	3.702019	-0.403529
18C	-0.783198	3.647271	-0.539891
19C	-1.565792	2.754072	0.199801
20C	-0.919241	1.899084	1.108672
21C	-3.064598	2.663637	-0.056670
22C	-3.899421	2.504754	1.224578
23C	-3.358776	1.517687	-1.046387
24C	1.446376	4.668422	-1.236445
25C	1.360264	4.333409	-2.737723
26C	1.053400	6.135701	-0.983684
27C	-1.181018	-2.542334	-0.694332
28O	-1.325730	-3.309438	-1.662264
29N	-1.978110	-1.978083	0.174244
30C	-3.364665	-2.129686	0.123853
31C	-4.083771	-1.581042	1.211981
32C	-5.474844	-1.630192	1.268463
33C	-6.204321	-2.230888	0.233648
34C	-5.510172	-2.780501	-0.849274
35C	-4.113690	-2.739100	-0.911887
36H	-0.268412	-0.700538	0.913301
37H	0.921046	-3.606327	-1.737901
38H	3.460559	-0.743527	3.061191
39H	3.723606	0.999314	2.832800
40H	4.782485	0.674664	0.681499
41H	5.533934	-0.452186	1.831039
42H	6.198734	-2.080434	0.448588
43H	5.656764	-1.434049	-1.108975
44H	4.763618	-4.060296	0.208009
45H	5.760484	-3.891074	-1.245620
46H	3.893513	-2.873792	-2.483099
47H	3.306550	-4.375560	-1.774289
48H	1.648843	1.591339	3.028015
49H	0.432953	0.351835	2.749901
50H	2.307906	2.846641	0.618559
51H	-1.275300	4.307255	-1.251991
52H	-1.500163	1.181142	1.681893
53H	-3.367565	3.605128	-0.535822
54H	-3.675134	3.296148	1.950683
55H	-4.969127	2.552977	0.986097
56H	-3.721112	1.536773	1.707184
57H	-2.828595	1.669891	-1.994747
58H	-3.038108	0.555156	-0.633448
59H	-4.433364	1.452005	-1.260127
60H	2.494016	4.547186	-0.928309
61H	1.665575	3.298303	-2.933536
62H	0.335769	4.455631	-3.110839
63H	2.010986	4.997983	-3.320877
64H	1.131062	6.393274	0.079688
65H	1.708921	6.811790	-1.547561
66H	0.021300	6.330486	-1.300936
67H	-3.518781	-1.105068	2.010040
68H	-5.992557	-1.193655	2.120305
69H	-7.290427	-2.268659	0.271894
70H	-6.060396	-3.251108	-1.662146
71H	-3.595303	-3.171165	-1.758552

1f-PhNCO-005

1N	-2.099668	0.630409	-0.667681
2C	-1.030638	0.445019	-1.476400
3C	0.172405	1.095256	-1.278758
4C	0.278799	2.021124	-0.187145
5C	-0.874184	2.220415	0.628576
6C	-2.023852	1.515913	0.358366
7N	1.441160	2.679202	0.054943
8N	1.256651	0.851469	-2.143636
9C	2.301852	1.873771	-2.083902

10C	2.655030	2.275956	-0.650215
11C	1.595441	3.553505	1.222254
12C	0.273317	4.221509	1.589837
13C	-0.804497	3.157597	1.814653
14C	1.719532	-0.550886	-2.293034
15C	2.495903	-1.056113	-1.091561
16C	1.815275	-1.416839	0.079915
17C	2.511428	-1.743535	1.250155
18C	3.914735	-1.722943	1.216449
19C	4.625129	-1.396027	0.053023
20C	3.894963	-1.061963	-1.097547
21C	6.147691	-1.381599	0.047245
22C	6.694875	0.034848	-0.213384
23C	6.724692	-2.386002	-0.967214
24C	1.766899	-2.112709	2.525718
25C	0.808800	-0.992950	2.974173
26C	1.009892	-3.444808	2.368501
27C	-3.364017	-0.195006	-0.944570
28O	-3.241393	-0.997499	-1.886413
29N	-4.316650	0.129984	-0.113302
30C	-5.571598	-0.483225	-0.140842
31C	-5.991357	-1.520429	-1.009899
32C	-7.284411	-2.045371	-0.917801
33C	-8.197015	-1.564968	0.026899
34C	-7.795408	-0.538054	0.891832
35C	-6.508609	-0.009491	0.808279
36H	-1.184386	-0.258867	-2.282770
37H	-2.924670	1.612782	0.948843
38H	1.955529	2.762592	-2.626323
39H	3.193513	1.498515	-2.590954
40H	3.142152	1.446146	-0.123455
41H	3.343806	3.127243	-0.659891
42H	2.352528	4.303673	0.971490
43H	1.978727	2.966035	2.071059
44H	-0.029443	4.897792	0.780135
45H	0.415297	4.825172	2.492550
46H	-0.563983	2.582857	2.720470
47H	-1.782966	3.619866	1.983838
48H	2.339647	-0.587543	-3.194562
49H	0.844448	-1.177850	-2.479324
50H	0.728441	-1.425196	0.077982
51H	4.468446	-1.974762	2.120362
52H	4.420277	-0.788254	-2.010302
53H	6.482682	-1.688641	1.047353
54H	6.310670	0.751288	0.523240
55H	7.790900	0.042923	-0.157898
56H	6.408178	0.391501	-1.210938
57H	6.363340	-3.402415	-0.769080
58H	6.440216	-2.122316	-1.993727
59H	7.820997	-2.397190	-0.917143
60H	2.517652	-2.245208	3.316605
61H	1.334406	-0.035104	3.075271
62H	-0.007591	-0.854934	2.254956
63H	0.358028	-1.239459	3.943746
64H	1.690864	-4.259078	2.092383
65H	0.511873	-3.719629	3.307138
66H	0.240703	-3.370619	1.589528
67H	-5.301653	-1.906565	-1.749534
68H	-7.579085	-2.842642	-1.597865
69H	-9.199941	-1.980563	0.089070
70H	-8.488329	-0.148021	1.634821
71H	-6.197024	0.787044	1.480366

1f-PhNCO-006

1N	-2.132356	0.694828	-0.682940
2C	-1.125749	0.619415	-1.584687
3C	0.101286	1.216538	-1.376488
4C	0.297000	1.994260	-0.187594
5C	-0.787116	2.070433	0.737341
6C	-1.961235	1.412896	0.457332
7N	1.475353	2.623028	0.047740
8N	1.138597	1.032805	-2.315545
9C	2.178980	2.059008	-2.231804
10C	2.634398	2.341340	-0.797206
11C	1.725726	3.341900	1.301969
12C	0.437334	3.918717	1.882577
13C	-0.606435	2.810222	2.043381
14C	1.607910	-0.362488	-2.519877
15C	2.411947	-0.912707	-1.355649
16C	1.773068	-1.245278	-0.155185
17C	2.507782	-1.612826	0.981231
18C	3.903944	-1.672166	0.881619
19C	4.574087	-1.379515	-0.317601
20C	3.809693	-0.994458	-1.426262
21C	6.092037	-1.458845	-0.410000

22C	6.606600	-2.883101	-0.131161
23C	6.770936	-0.439752	0.524280
24C	1.803139	-1.911049	2.297617
25C	1.082802	-0.658688	2.834746
26C	0.823206	-3.092113	2.174572
27C	-3.431980	-0.064236	-0.983558
28O	-3.425449	-0.655701	-2.077090
29N	-4.280659	0.072298	-0.000915
30C	-5.537219	-0.537496	-0.009194
31C	-6.060653	-1.391084	-1.011459
32C	-7.340007	-1.940776	-0.879839
33C	-8.136653	-1.665167	0.236214
34C	-7.631475	-0.821667	1.234805
35C	-6.357204	-0.270710	1.113117
36H	-1.340548	0.036793	-2.470438
37H	-2.810304	1.417845	1.127069
38H	1.785669	2.985463	-2.668365
39H	3.035568	1.744022	-2.832540
40H	3.195940	1.491908	-0.390577
41H	3.288496	3.220201	-0.782829
42H	2.441804	4.140746	1.082626
43H	2.201423	2.658590	2.021726
44H	0.054209	4.700367	1.214179
45H	0.658777	4.386693	2.847723
46H	-0.270148	2.103300	2.815316
47H	-1.565256	3.217795	2.381241
48H	2.208566	-0.366719	-3.435268
49H	0.727934	-0.982753	-2.709114
50H	0.689308	-1.198823	-0.098335
51H	4.480040	-1.958249	1.759729
52H	4.312041	-0.741492	-2.358938
53H	6.370113	-1.200503	-1.441164
54H	6.144212	-3.611920	-0.807773
55H	7.694416	-2.933804	-0.267093
56H	6.383169	-3.191082	0.897872
57H	6.431633	0.581956	0.312630
58H	6.548175	-0.657469	1.576462
59H	7.860998	-0.468587	0.399714
60H	2.575130	-2.192544	3.026439
61H	1.780683	0.178876	2.957132
62H	0.288087	-0.337792	2.150937
63H	0.623556	-0.864151	3.810121
64H	1.330059	-3.992731	1.807333
65H	0.378378	-3.324666	3.150405
66H	0.003656	-2.860821	1.482683
67H	-5.461116	-1.617164	-1.883991
68H	-7.716182	-2.594098	-1.665082
69H	-9.130208	-2.097595	0.327461
70H	-8.233090	-0.593107	2.112381
71H	-5.965027	0.382780	1.889246

1f-PhNCO-007

1N	-1.923805	1.481091	-0.096182
2C	-1.190507	0.928844	-1.095083
3C	0.134425	1.248906	-1.298002
4C	0.750295	2.221292	-0.440410
5C	-0.068691	2.846712	0.545977
6C	-1.371201	2.433791	0.695788
7N	2.065163	2.517096	-0.555497
8N	0.872229	0.610427	-2.316806
9C	2.054224	1.369564	-2.725326
10C	2.905023	1.848426	-1.547988
11C	2.748562	3.434952	0.367269
12C	2.014081	3.557821	1.699249
13C	0.537179	3.888054	1.455931
14C	1.001369	-0.866749	-2.225521
15C	1.738449	-1.345781	-0.988941
16C	3.115213	-1.597779	-1.022113
17C	3.822505	-1.920001	0.145289
18C	3.115586	-1.977398	1.355581
19C	1.732835	-1.751089	1.418910
20C	1.055699	-1.448697	0.230722
21C	0.980384	-1.841789	2.739358
22C	-0.000940	-3.029247	2.741305
23C	0.246201	-0.528438	3.069920
24C	5.320824	-2.189540	0.105521
25C	5.657466	-3.403184	-0.780363
26C	6.108886	-0.946554	-0.349312
27C	-3.361471	1.037202	0.188937
28O	-3.938106	1.723804	1.050626
29N	-3.675189	0.000945	-0.541981
30C	-4.932866	-0.602973	-0.479160
31C	-6.027905	-0.202517	0.325724
32C	-7.236246	-0.905418	0.283295
33C	-7.398944	-2.018486	-0.547804

34C	-6.323306	-2.426290	-1.348355
35C	-5.115674	-1.731643	-1.313314
36H	-1.708382	0.192101	-1.692429
37H	-2.026681	2.835182	1.457830
38H	1.717244	2.244188	-3.296811
39H	2.662015	0.752782	-3.391631
40H	3.431650	1.011142	-1.076122
41H	3.654256	2.567904	-1.901009
42H	2.845529	4.417935	-0.116362
43H	3.759820	3.044247	0.524416
44H	2.494867	4.336869	2.300388
45H	2.095889	2.612089	2.250092
46H	-0.017313	3.934973	2.399199
47H	0.460595	4.880212	0.988032
48H	1.511170	-1.195850	-3.136243
49H	-0.006972	-1.289895	-2.251862
50H	3.643027	-1.531296	-1.971493
51H	3.654545	-2.217518	2.271585
52H	-0.017713	-1.281480	0.252611
53H	1.722382	-2.018113	3.530126
54H	0.518463	-3.974182	2.539800
55H	-0.502506	-3.115846	3.713635
56H	-0.775978	-2.900074	1.975477
57H	0.939001	0.322027	3.084930
58H	-0.536684	-0.312255	2.333029
59H	-0.234328	-0.593798	4.054204
60H	5.638996	-2.427687	1.129565
61H	5.119868	-4.299158	-0.447282
62H	5.385506	-3.217510	-1.827093
63H	6.733334	-3.618006	-0.747377
64H	5.900666	-0.084227	0.295991
65H	7.188567	-1.141210	-0.317656
66H	5.850698	-0.669290	-1.379364
67H	-5.922310	0.655956	0.976561
68H	-8.060797	-0.574409	0.912169
69H	-8.342905	-2.557720	-0.572695
70H	-6.426675	-3.289630	-2.002716
71H	-4.281509	-2.047749	-1.935751

1f-PhNCO-008

1N	1.257688	1.957236	0.002113
2C	0.553011	1.314679	0.965900
3C	-0.810566	1.485108	1.127032
4C	-1.491334	2.380093	0.229055
5C	-0.715454	3.076381	-0.736913
6C	0.640227	2.838487	-0.815841
7N	-2.841254	2.539881	0.309342
8N	-1.507568	0.791979	2.118759
9C	-2.874862	1.240220	2.370263
10C	-3.615641	1.568535	1.075527
11C	-3.565086	3.355675	-0.670108
12C	-2.712109	4.529440	-1.142147
13C	-1.388379	4.015875	-1.715022
14C	-1.156726	-0.617722	2.397137
15C	-1.342725	-1.522097	1.192977
16C	-2.625536	-1.948170	0.821957
17C	-2.834570	-2.677773	-0.354950
18C	-1.722145	-2.976013	-1.158372
19C	-0.426058	-2.573419	-0.810056
20C	-0.251842	-1.853493	0.381336
21C	0.760503	-2.870468	-1.715828
22C	1.835154	-3.712068	-1.003083
23C	1.372608	-1.567949	-2.267734
24C	-4.230855	-3.130255	-0.761047
25C	-4.835233	-4.107437	0.264397
26C	-5.170662	-1.931176	-0.989780
27C	2.746630	1.665234	-0.223032
28O	3.295275	2.434976	-1.029923
29N	3.119173	0.632694	0.485348
30C	4.416507	0.120255	0.437105
31C	4.679293	-0.969735	1.300569
32C	5.926944	-1.589438	1.335988
33C	6.963058	-1.142679	0.504672
34C	6.720922	-0.067045	-0.356034
35C	5.472761	0.562438	-0.396773
36H	1.143254	0.653601	1.580089
37H	1.277151	3.318342	-1.547726
38H	-2.856577	2.137128	3.004247
39H	-3.411098	0.459466	2.913462
40H	-3.774668	0.657102	0.483310
41H	-4.591796	2.008870	1.303245
42H	-4.481623	3.710758	-0.187393
43H	-3.860772	2.727795	-1.525656
44H	-2.520517	5.201619	-0.296006
45H	-3.266217	5.096248	-1.897910

46H	-1.581262	3.484587	-2.657834
47H	-0.717344	4.848492	-1.954117
48H	-1.790950	-0.936353	3.228871
49H	-0.124581	-0.670086	2.757697
50H	-3.470851	-1.697449	1.459127
51H	-1.872814	-3.534595	-2.081473
52H	0.745202	-1.530601	0.667444
53H	0.386571	-3.455252	-2.567489
54H	1.419629	-4.655031	-0.625976
55H	2.654101	-3.950455	-1.693477
56H	2.267257	-3.167210	-0.155078
57H	0.621178	-0.968137	-2.796417
58H	1.788420	-0.954336	-1.459930
59H	2.186911	-1.792100	-2.968363
60H	-4.137348	-3.665365	-1.715633
61H	-4.185904	-4.978288	0.415113
62H	-4.976644	-3.621895	1.238360
63H	-5.814902	-4.467119	-0.075769
64H	-4.757899	-1.237284	-1.732458
65H	-6.150679	-2.271099	-1.348414
66H	-5.332074	-1.372724	-0.058828
67H	3.872592	-1.319632	1.941028
68H	6.091726	-2.425950	2.012258
69H	7.937719	-1.624289	0.527985
70H	7.514226	0.292606	-1.008953
71H	5.305121	1.393396	-1.070046

1f-PhNCO-009

1N	-1.946168	1.423909	0.081635
2C	-1.276840	0.990341	-1.015940
3C	0.028937	1.348303	-1.269807
4C	0.690857	2.244307	-0.364996
5C	-0.061913	2.743137	0.739326
6C	-1.345841	2.291923	0.934194
7N	1.987223	2.583976	-0.547000
8N	0.704259	0.819212	-2.389941
9C	1.834524	1.645888	-2.812964
10C	2.762231	2.043475	-1.663590
11C	2.717336	3.431005	0.406830
12C	2.093265	3.391015	1.798546
13C	0.593123	3.694016	1.712715
14C	0.876212	-0.656317	-2.426690
15C	1.699446	-1.214004	-1.280395
16C	3.081192	-1.418772	-1.412829
17C	3.865120	-1.817705	-0.324250
18C	3.233151	-2.007743	0.916479
19C	1.853876	-1.830751	1.077405
20C	1.096503	-1.445123	-0.039126
21C	1.189772	-2.033291	2.432104
22C	0.129782	-3.149206	2.391808
23C	0.576517	-0.719073	2.952959
24C	5.364894	-2.029662	-0.481929
25C	6.171504	-1.053345	0.394886
26C	5.769422	-3.486215	-0.188255
27C	-3.361186	0.936278	0.409555
28O	-3.850890	1.461391	1.424813
29N	-3.753370	0.046609	-0.462328
30C	-5.004004	-0.570262	-0.390629
31C	-6.005607	-0.350088	0.586801
32C	-7.215876	-1.049122	0.534533
33C	-7.471909	-1.981555	-0.476076
34C	-6.489767	-2.208583	-1.449741
35C	-5.280764	-1.517062	-1.405663
36H	-1.828907	0.316070	-1.654905
37H	-1.948422	2.595837	1.780400
38H	1.433786	2.556892	-3.275903
39H	2.403137	1.109564	-3.576763
40H	3.350293	1.186496	-1.316427
41H	3.458412	2.820520	-2.003184
42H	2.743248	4.460423	0.020685
43H	3.749448	3.066220	0.442420
44H	2.602199	4.119557	2.438593
45H	2.245417	2.396817	2.237717
46H	0.118955	3.611718	2.696497
47H	0.450668	4.730193	1.373139
48H	1.335886	-0.895059	-3.390663
49H	-0.121396	-1.105841	-2.426390
50H	3.554677	-1.252846	-2.379555
51H	3.826360	-2.308906	1.777770
52H	0.023478	-1.308315	0.063260
53H	1.973143	-2.340781	3.138346
54H	0.561754	-4.097014	2.048002
55H	-0.296554	-3.309923	3.390181
56H	-0.695289	-2.890147	1.716808
57H	1.327635	0.079328	2.997618

58H	-0.238279	-0.376915	2.303096
59H	0.163775	-0.857592	3.960311
60H	5.615959	-1.819737	-1.531027
61H	5.913758	-0.010317	0.172417
62H	5.978341	-1.227353	1.460948
63H	7.248227	-1.180888	0.224398
64H	5.214158	-4.188434	-0.821891
65H	6.841160	-3.633524	-0.373487
66H	5.570828	-3.748994	0.858387
67H	-5.826778	0.366720	1.378177
68H	-7.967509	-0.859594	1.298756
69H	-8.416452	-2.519409	-0.506815
70H	-6.666745	-2.928720	-2.246184
71H	-4.518596	-1.693969	-2.161349

1f-PhNCO-010

1N	-2.096771	0.834672	-0.618406
2C	-1.088442	0.813123	-1.522714
3C	0.135351	1.401973	-1.279861
4C	0.330665	2.102064	-0.043682
5C	-0.773723	2.171833	0.858752
6C	-1.937104	1.509773	0.550522
7N	1.524142	2.661526	0.259378
8N	1.169882	1.312416	-2.235423
9C	2.174024	2.366212	-2.089711
10C	2.662194	2.542716	-0.650751
11C	1.779868	3.319576	1.548500
12C	0.838773	2.819718	2.640779
13C	-0.615442	2.912241	2.165750
14C	1.664587	-0.044911	-2.574313
15C	2.421000	-0.734866	-1.453067
16C	3.823145	-0.723697	-1.418383
17C	4.528474	-1.274111	-0.341569
18C	3.793886	-1.841833	0.712891
19C	2.394161	-1.882280	0.701772
20C	1.720223	-1.327664	-0.396841
21C	1.620839	-2.508235	1.854887
22C	0.768352	-3.702773	1.388461
23C	0.747280	-1.465256	2.577020
24C	6.050809	-1.249202	-0.313951
25C	6.583371	-0.417532	0.867933
26C	6.644608	-2.669979	-0.293807
27C	-3.385786	0.075129	-0.952335
28O	-3.362339	-0.491920	-2.058864
29N	-4.249443	0.185558	0.020880
30C	-5.501812	-0.430868	-0.016699
31C	-6.002985	-1.275807	-1.037520
32C	-7.281230	-1.834162	-0.934185
33C	-8.098990	-1.575329	0.170584
34C	-7.616077	-0.740259	1.187170
35C	-6.342864	-0.181400	1.094076
36H	-1.299905	0.276421	-2.437985
37H	-2.790278	1.484213	1.214402
38H	1.732590	3.310741	-2.432972
39H	3.023054	2.139294	-2.739115
40H	3.290540	1.699059	-0.342725
41H	3.258527	3.459841	-0.573272
42H	1.682026	4.407151	1.417808
43H	2.820810	3.111670	1.818181
44H	0.992338	3.418501	3.544878
45H	1.083442	1.778406	2.884534
46H	-1.301160	2.504354	2.916019
47H	-0.883246	3.969597	2.026345
48H	2.301838	0.063199	-3.457587
49H	0.801877	-0.646479	-2.873710
50H	4.372527	-0.270578	-2.242724
51H	4.323588	-2.273568	1.559872
52H	0.634231	-1.350576	-0.428835
53H	2.357174	-2.885754	2.577673
54H	1.385430	-4.460748	0.890707
55H	0.268940	-4.176037	2.243398
56H	-0.009257	-3.384721	0.683058
57H	1.350688	-0.625210	2.942187
58H	-0.021555	-1.061096	1.907431
59H	0.237069	-1.917618	3.436928
60H	6.386677	-0.762442	-1.239800
61H	6.189679	0.606333	0.843885
62H	6.298421	-0.864748	1.828599
63H	7.679063	-0.361367	0.837512
64H	6.292468	-3.259812	-1.148863
65H	7.740705	-2.630097	-0.334602
66H	6.363549	-3.205352	0.621889
67H	-5.387201	-1.488292	-1.902150
68H	-7.639928	-2.480787	-1.733053
69H	-9.091589	-2.014043	0.239406

70H	-8.234192	-0.524235	2.056434
71H	-5.967830	0.465767	1.883914

1f-001

1N	3.513035	0.409180	-2.226444
2C	2.460272	-0.410581	-2.360774
3C	1.778254	-1.015499	-1.301267
4C	2.252805	-0.783150	0.020889
5C	3.361128	0.087341	0.173112
6C	3.934953	0.637158	-0.970101
7N	1.662564	-1.400232	1.106214
8N	0.645869	-1.832157	-1.552239
9C	0.305430	-2.716626	-0.435242
10C	0.353172	-2.013681	0.925177
11C	2.003792	-0.969255	2.460170
12C	3.492162	-0.642986	2.569712
13C	3.864880	0.443576	1.555747
14C	-0.505504	-1.180333	-2.224850
15C	-1.303774	-0.251995	-1.325954
16C	-2.529889	-0.659521	-0.788512
17C	-3.218194	0.135538	0.140458
18C	-2.640289	1.352400	0.527607
19C	-1.416496	1.793875	0.000778
20C	-0.766001	0.983343	-0.937252
21C	-0.797906	3.109054	0.455394
22C	-0.623475	4.095858	-0.713510
23C	0.545681	2.872412	1.172262
24C	-4.542593	-0.320592	0.737465
25C	-4.360563	-1.580752	1.605198
26C	-5.613174	-0.553695	-0.344007
27H	2.120368	-0.598391	-3.377714
28H	4.791504	1.302702	-0.864689
29H	-0.692245	-3.131694	-0.602448
30H	1.017953	-3.551258	-0.424466
31H	0.203242	-2.748380	1.725456
32H	-0.446159	-1.263456	0.998941
33H	1.401298	-0.089079	2.743663
34H	1.736244	-1.783010	3.143670
35H	3.718336	-0.315159	3.590792
36H	4.074677	-1.553217	2.375754
37H	4.950341	0.598530	1.533131
38H	3.419427	1.398814	1.871364
39H	-1.149433	-1.979030	-2.608795
40H	-0.118972	-0.635271	-3.089389
41H	-2.945936	-1.619239	-1.088962
42H	-3.157351	1.974184	1.257730
43H	0.184233	1.301894	-1.356198
44H	-1.487632	3.565923	1.178436
45H	0.086665	3.709055	-1.454986
46H	-1.576609	4.280597	-1.223993
47H	-0.237580	5.057364	-0.350909
48H	0.425381	2.195431	2.026905
49H	0.958810	3.819521	1.542575
50H	1.281436	2.426488	0.492434
51H	-4.901182	0.485521	1.392146
52H	-3.622892	-1.413910	2.399885
53H	-5.309677	-1.867683	2.075964
54H	-4.016275	-2.429303	1.000318
55H	-5.763217	0.344595	-0.955070
56H	-5.329251	-1.373609	-1.015733
57H	-6.573812	-0.817812	0.116475

1f-002

1N	-3.596874	0.556282	-2.088560
2C	-2.661469	-0.392927	-2.238376
3C	-1.974652	-1.010449	-1.189650
4C	-2.315953	-0.644053	0.142840
5C	-3.297778	0.364723	0.311555
6C	-3.888520	0.911155	-0.824571
7N	-1.723385	-1.263911	1.224867
8N	-0.960607	-1.965214	-1.461549
9C	-0.652481	-2.825838	-0.316719
10C	-0.519570	-2.053710	0.999999
11C	-1.896645	-0.703978	2.563566
12C	-3.321235	-0.188129	2.759393
13C	-3.644411	0.867778	1.696942
14C	0.211444	-1.479568	-2.232170
15C	1.149478	-0.582116	-1.442640
16C	0.761729	0.721114	-1.109907
17C	1.544779	1.518720	-0.262677
18C	2.748518	0.992470	0.224074
19C	3.182211	-0.299573	-0.115455

20C	2.364627	-1.075448	-0.946720
21C	4.492213	-0.856259	0.426500
22C	4.452204	-0.998262	1.960020
23C	5.702366	-0.009956	-0.010048
24C	1.078383	2.910947	0.143186
25C	-0.215489	2.839434	0.978113
26C	0.890114	3.836600	-1.072770
27H	-2.425096	-0.682238	-3.260777
28H	-4.648246	1.683469	-0.706182
29H	-1.458582	-3.563577	-0.212578
30H	0.273545	-3.370209	-0.521942
31H	0.372096	-1.412578	0.981668
32H	-0.411432	-2.759534	1.832563
33H	-1.670674	-1.496921	3.285308
34H	-1.172927	0.111976	2.730983
35H	-4.022829	-1.028793	2.679712
36H	-3.420085	0.232625	3.766618
37H	-3.065543	1.779224	1.908548
38H	-4.702428	1.153151	1.740917
39H	-0.167270	-0.953962	-3.112359
40H	0.749408	-2.363625	-2.591388
41H	-0.176130	1.109046	-1.496648
42H	3.361750	1.606669	0.881012
43H	2.671714	-2.088945	-1.202054
44H	4.620505	-1.861881	0.002781
45H	5.378166	-1.457293	2.329694
46H	4.346411	-0.019677	2.445321
47H	3.610468	-1.624293	2.280859
48H	5.758479	0.071188	-1.102340
49H	5.645034	1.006215	0.399798
50H	6.636959	-0.461888	0.346627
51H	1.861688	3.348208	0.777553
52H	-0.078626	2.211280	1.866886
53H	-0.516742	3.841133	1.311122
54H	-1.039991	2.416437	0.392119
55H	0.094598	3.469861	-1.733223
56H	0.611811	4.847020	-0.746706
57H	1.810857	3.911783	-1.664112

1f-003

1N	-2.037102	0.336560	2.807776
2C	-1.308620	-0.436617	1.982272
3C	-1.724283	-0.852257	0.708708
4C	-2.995608	-0.389175	0.248039
5C	-3.764521	0.411232	1.116391
6C	-3.233482	0.740180	2.366755
7N	-3.429896	-0.698836	-1.036209
8N	-0.958469	-1.696777	-0.101619
9C	-1.279588	-1.734819	-1.523142
10C	-2.789146	-1.819972	-1.707843
11C	-4.828510	-0.452646	-1.383436
12C	-5.294065	0.888981	-0.821305
13C	-5.138998	0.897201	0.703032
14C	0.386871	-2.091483	0.280519
15C	1.490368	-1.053470	0.082021
16C	1.214505	0.264500	-0.279746
17C	2.245797	1.205985	-0.438582
18C	3.565359	0.793674	-0.232471
19C	3.876461	-0.529968	0.128176
20C	2.825703	-1.439705	0.280583
21C	5.320049	-0.966409	0.341706
22C	5.988068	-0.190492	1.491949
23C	6.147239	-0.843603	-0.951872
24C	1.923092	2.647482	-0.808433
25C	1.109875	3.340555	0.301749
26C	1.191676	2.742801	-2.160137
27H	-0.331493	-0.726123	2.355197
28H	-3.812737	1.369792	3.041815
29H	-0.892281	-0.852188	-2.055621
30H	-0.807935	-2.621231	-1.959525
31H	-3.160712	-2.783896	-1.320667
32H	-3.030813	-1.768777	-2.775138
33H	-4.905307	-0.462166	-2.476331
34H	-5.470154	-1.266098	-0.999287
35H	-4.690661	1.691133	-1.266220
36H	-6.338195	1.062640	-1.105929
37H	-5.907342	0.248013	1.147919
38H	-5.315289	1.903055	1.103336
39H	0.634856	-2.987289	-0.301868
40H	0.376777	-2.414462	1.328801
41H	0.185519	0.573421	-0.429274
42H	4.367953	1.518710	-0.352749
43H	3.046669	-2.469713	0.560909
44H	5.301826	-2.027883	0.624714
45H	7.003618	-0.566770	1.670838

46H	6.063992	0.878960	1.258773
47H	5.417986	-0.291320	2.423492
48H	5.696833	-1.420468	-1.768942
49H	6.218316	0.201395	-1.279008
50H	7.167958	-1.215561	-0.794562
51H	2.877804	3.182056	-0.907990
52H	1.643019	3.314486	1.259912
53H	0.921085	4.390866	0.044290
54H	0.139387	2.849776	0.446707
55H	1.019447	3.792222	-2.431920
56H	1.774170	2.273550	-2.962651
57H	0.214526	2.245386	-2.118255

1f-004

1N	-2.031349	0.056640	2.843720
2C	-1.248023	-0.606273	1.973959
3C	-1.620152	-0.942306	0.663938
4C	-2.909626	-0.516599	0.217890
5C	-3.735596	0.168424	1.131668
6C	-3.242566	0.426592	2.413558
7N	-3.305427	-0.744411	-1.095242
8N	-0.792651	-1.672918	-0.196663
9C	-1.097096	-1.624597	-1.622211
10C	-2.596959	-1.777460	-1.836142
11C	-4.705778	-0.533116	-1.457772
12C	-5.250094	0.729637	-0.793134
13C	-5.128536	0.608845	0.729369
14C	0.584126	-1.975206	0.160610
15C	1.593505	-0.835515	0.019355
16C	1.194630	0.482156	-0.216433
17C	2.135389	1.516451	-0.330959
18C	3.493789	1.199124	-0.210860
19C	3.927183	-0.115992	0.021693
20C	2.960360	-1.123327	0.136505
21C	5.412545	-0.430236	0.142977
22C	5.882414	-1.397178	-0.959854
23C	5.767176	-0.978566	1.537640
24C	1.681082	2.948411	-0.578627
25C	0.767403	3.457945	0.552140
26C	0.984217	3.089166	-1.945191
27H	-0.261219	-0.868050	2.341800
28H	-3.866406	0.966988	3.125198
29H	-0.572288	-2.450365	-2.113862
30H	-0.752253	-0.686240	-2.083636
31H	-2.920334	-2.785630	-1.525888
32H	-2.827975	-1.661347	-2.900508
33H	-5.316366	-1.405854	-1.164359
34H	-4.756201	-0.448914	-2.549155
35H	-6.295168	0.876852	-1.088847
36H	-4.678662	1.596957	-1.149168
37H	-5.865079	-0.122694	1.093378
38H	-5.373683	1.562022	1.213608
39H	0.903105	-2.809344	-0.476109
40H	0.609134	-2.362000	1.186442
41H	0.138759	0.713132	-0.305766
42H	4.234613	1.992808	-0.300362
43H	3.270302	-2.151614	0.317338
44H	5.956608	0.514699	0.009908
45H	5.389657	-2.373321	-0.866411
46H	6.965690	-1.562061	-0.893852
47H	5.657965	-1.001685	-1.958086
48H	5.275900	-1.942514	1.721342
49H	5.454702	-0.286099	2.328756
50H	6.850134	-1.133956	1.627181
51H	2.579105	3.581061	-0.593553
52H	1.260889	3.380303	1.528440
53H	0.500651	4.509822	0.386985
54H	-0.163552	2.879626	0.602893
55H	1.634216	2.749024	-2.760817
56H	0.062111	2.494960	-1.979215
57H	0.715277	4.135979	-2.137105

1f-005

1N	-1.592977	-1.647262	2.180727
2C	-0.980591	-1.391502	1.009385
3C	-1.605598	-0.808410	-0.102770
4C	-2.985517	-0.458506	0.025324
5C	-3.621570	-0.706591	1.257607
6C	-2.882699	-1.309404	2.280050
7N	-3.674872	0.077100	-1.056464
8N	-0.920792	-0.536107	-1.291907
9C	-1.728584	-0.274159	-2.477592

10C	-2.879003	0.658531	-2.127309
11C	-4.986770	0.677900	-0.824965
12C	-5.808935	-0.183127	0.131936
13C	-5.072658	-0.323623	1.468460
14C	0.395709	-1.118520	-1.513759
15C	1.538115	-0.403320	-0.800753
16C	1.407009	0.911325	-0.347773
17C	2.471713	1.565298	0.289277
18C	3.680073	0.873917	0.450061
19C	3.842287	-0.445142	0.000437
20C	2.753248	-1.074069	-0.617611
21C	5.161713	-1.178477	0.202989
22C	5.763352	-1.659450	-1.130296
23C	5.007194	-2.354881	1.185625
24C	2.315418	2.990045	0.803214
25C	1.204857	3.090825	1.866032
26C	2.063360	3.984912	-0.345142
27H	0.071123	-1.653118	0.965775
28H	-3.369610	-1.523517	3.231275
29H	-2.128776	-1.206624	-2.910546
30H	-1.094920	0.205152	-3.230407
31H	-3.521258	0.791569	-3.004372
32H	-2.485666	1.648796	-1.841076
33H	-5.487133	0.765542	-1.795866
34H	-4.877563	1.698259	-0.415168
35H	-5.961963	-1.171774	-0.320227
36H	-6.795288	0.271569	0.278531
37H	-5.566602	-1.068051	2.105009
38H	-5.125125	0.631649	2.011163
39H	0.582931	-1.083660	-2.592818
40H	0.404472	-2.186143	-1.239316
41H	0.454446	1.417008	-0.477285
42H	4.513386	1.370270	0.945909
43H	2.846358	-2.104157	-0.957912
44H	5.868545	-0.464381	0.647388
45H	5.121317	-2.409570	-1.608916
46H	6.746064	-2.119644	-0.964837
47H	5.890211	-0.827340	-1.833648
48H	4.315740	-3.109922	0.790422
49H	4.616995	-2.016919	2.153277
50H	5.975235	-2.842997	1.358524
51H	3.262352	3.271055	1.284060
52H	1.387480	2.401493	2.699129
53H	1.150187	4.110033	2.270217
54H	0.223937	2.845434	1.440109
55H	2.865285	3.942645	-1.092526
56H	1.116298	3.767810	-0.855565
57H	2.009286	5.011983	0.038648

1f-006

1N	1.726252	-1.709204	2.155209
2C	1.110393	-1.473722	0.981574
3C	1.712135	-0.844332	-0.118578
4C	3.067210	-0.414530	0.028784
5C	3.706384	-0.644079	1.262715
6C	2.994006	-1.301172	2.270735
7N	3.731126	0.182404	-1.037935
8N	1.024160	-0.600253	-1.310644
9C	1.818731	-0.251672	-2.482523
10C	2.904366	0.742743	-2.096964
11C	4.996265	0.866859	-0.778276
12C	5.866352	0.043153	0.169008
13C	5.129507	-0.177079	1.494565
14C	-0.256479	-1.249703	-1.552800
15C	-1.447973	-0.586973	-0.869360
16C	-2.662407	-1.284796	-0.786676
17C	-3.791352	-0.707152	-0.196915
18C	-3.677408	0.592391	0.327846
19C	-2.476964	1.307216	0.266339
20C	-1.365839	0.702091	-0.344781
21C	-2.374219	2.710663	0.848024
22C	-2.127624	3.758998	-0.253231
23C	-1.290744	2.800898	1.938928
24C	-5.105245	-1.472842	-0.112542
25C	-6.237988	-0.746049	-0.861346
26C	-5.506154	-1.748374	1.348872
27H	0.074776	-1.791725	0.926125
28H	3.483938	-1.499831	3.223751
29H	2.280498	-1.143236	-2.939418
30H	1.159102	0.207449	-3.225662
31H	2.445601	1.696023	-1.783807
32H	3.540955	0.943964	-2.965001
33H	5.498954	1.010541	-1.741277
34H	4.812615	1.867804	-0.347512
35H	6.091793	-0.922074	-0.302925

36H	6.817722	0.561061	0.336351
37H	5.116923	0.765502	2.061245
38H	5.664894	-0.904456	2.117222
39H	-0.215583	-2.313487	-1.267574
40H	-0.425456	-1.236342	-2.635302
41H	-2.724928	-2.297249	-1.185118
42H	-4.541315	1.054446	0.801646
43H	-0.418207	1.229547	-0.399324
44H	-3.339721	2.942502	1.318098
45H	-2.915016	3.726691	-1.016404
46H	-2.106510	4.770718	0.172161
47H	-1.166359	3.585721	-0.753905
48H	-0.291362	2.619487	1.524132
49H	-1.287561	3.799360	2.395004
50H	-1.460860	2.062983	2.732094
51H	-4.951939	-2.443375	-0.604009
52H	-5.968539	-0.559967	-1.908248
53H	-7.157209	-1.345904	-0.847558
54H	-6.464380	0.221463	-0.395837
55H	-4.717618	-2.293943	1.881357
56H	-5.690491	-0.812288	1.891177
57H	-6.425207	-2.347236	1.391718

1f-007

1N	2.251327	0.270854	2.813897
2C	1.522506	-0.485976	1.973613
3C	1.910384	-0.825302	0.669099
4C	3.148888	-0.294047	0.192522
5C	3.919233	0.488473	1.075795
6C	3.418948	0.736581	2.357192
7N	3.546642	-0.519880	-1.120562
8N	1.148936	-1.658053	-0.156921
9C	1.426928	-1.626576	-1.587591
10C	2.931779	-1.637165	-1.822128
11C	4.917489	-0.192390	-1.508200
12C	5.352458	1.132419	-0.884859
13C	5.260618	1.043872	0.642039
14C	-0.168907	-2.119972	0.244608
15C	-1.321514	-1.128840	0.090792
16C	-2.634516	-1.589683	0.261351
17C	-3.731108	-0.726933	0.143262
18C	-3.489560	0.623208	-0.154734
19C	-2.189598	1.111926	-0.335039
20C	-1.113397	0.220181	-0.209188
21C	-1.936378	2.579127	-0.655614
22C	-2.419931	3.499236	0.480635
23C	-2.570863	2.987716	-1.998105
24C	-5.151044	-1.246705	0.326582
25C	-5.976215	-1.109900	-0.966853
26C	-5.863380	-0.554246	1.503299
27H	0.567610	-0.825892	2.361175
28H	3.998869	1.351354	3.045286
29H	0.984103	-0.742659	-2.072208
30H	0.980615	-2.516050	-2.044420
31H	3.135776	-1.528989	-2.892883
32H	3.356634	-2.599637	-1.490591
33H	4.946876	-0.133759	-2.601926
34H	5.608156	-0.998540	-1.201470
35H	4.699316	1.933531	-1.255179
36H	6.376015	1.366188	-1.199556
37H	5.421346	2.029195	1.096335
38H	6.066438	0.395216	1.016025
39H	-0.121999	-2.466072	1.284208
40H	-0.391089	-3.012594	-0.352965
41H	-2.806044	-2.641422	0.491046
42H	-4.331978	1.304381	-0.249517
43H	-0.102185	0.593498	-0.342154
44H	-0.849607	2.709943	-0.747693
45H	-1.949178	3.231797	1.434261
46H	-3.507444	3.430813	0.611310
47H	-2.174300	4.546096	0.260168
48H	-3.664539	2.905609	-1.961149
49H	-2.214120	2.350945	-2.817118
50H	-2.321629	4.028770	-2.241496
51H	-5.079854	-2.316853	0.564438
52H	-6.976753	-1.541597	-0.834339
53H	-6.100523	-0.056341	-1.247133
54H	-5.491122	-1.624881	-1.805198
55H	-5.987183	0.519644	1.314995
56H	-5.295904	-0.667976	2.434917
57H	-6.861572	-0.984173	1.657080

1f-008

1N	-1.762212	-1.530813	2.211041
2C	-1.157010	-1.305392	1.029631
3C	-1.775036	-0.705594	-0.077460
4C	-3.137912	-0.300429	0.068112
5C	-3.766350	-0.518708	1.309992
6C	-3.036845	-1.143953	2.325624
7N	-3.820554	0.257874	-1.006110
8N	-1.096970	-0.470887	-1.279408
9C	-1.914263	-0.185728	-2.453855
10C	-3.017451	0.798173	-2.092688
11C	-5.104068	0.911736	-0.760313
12C	-5.946861	0.087991	0.211414
13C	-5.198405	-0.078241	1.538284
14C	0.178950	-1.132321	-1.522296
15C	1.379234	-0.476918	-0.848968
16C	1.366793	0.875942	-0.488318
17C	2.488109	1.479115	0.093406
18C	3.635072	0.696576	0.304629
19C	3.677064	-0.657693	-0.048553
20C	2.531816	-1.233393	-0.621289
21C	4.932866	-1.485399	0.192399
22C	5.508749	-2.043575	-1.122482
23C	4.680985	-2.620980	1.201927
24C	2.456333	2.948835	0.492265
25C	3.506657	3.771786	-0.276993
26C	2.627834	3.127886	2.012310
27H	-0.116428	-1.606561	0.973343
28H	-3.518463	-1.334672	3.284503
29H	-2.361458	-1.104394	-2.870253
30H	-1.273960	0.258546	-3.222454
31H	-3.666837	0.953489	-2.960717
32H	-2.576925	1.772003	-1.819353
33H	-5.613512	1.014902	-1.725017
34H	-4.949213	1.928818	-0.357130
35H	-6.146555	-0.894953	-0.234968
36H	-6.911719	0.583026	0.370196
37H	-5.713279	-0.800426	2.183859
38H	-5.205249	0.879876	2.078412
39H	0.342661	-1.121427	-2.605770
40H	0.131234	-2.194923	-1.233570
41H	0.462410	1.457439	-0.650774
42H	4.514778	1.148040	0.759309
43H	2.535251	-2.288459	-0.889976
44H	5.687677	-0.815650	0.626823
45H	4.810214	-2.745631	-1.595045
46H	6.446777	-2.581954	-0.934528
47H	5.715524	-1.240107	-1.840251
48H	3.943414	-3.336734	0.817439
49H	4.303856	-2.230666	2.154868
50H	5.609036	-3.171886	1.402130
51H	1.465239	3.338166	0.222218
52H	3.379960	3.665745	-1.361452
53H	3.421564	4.837132	-0.026415
54H	4.525155	3.450546	-0.024732
55H	1.862699	2.571131	2.566637
56H	3.610732	2.770750	2.345085
57H	2.545998	4.187313	2.288241

1f-009

1N	1.990469	-0.371995	2.780248
2C	1.296188	-0.860544	1.736541
3C	1.775094	-0.913335	0.418608
4C	3.078033	-0.381615	0.170638
5C	3.809455	0.120755	1.264489
6C	3.214982	0.103585	2.529743
7N	3.578541	-0.338003	-1.127175
8N	1.040537	-1.470539	-0.629911
9C	1.453820	-1.161101	-1.992618
10C	2.971696	-1.234164	-2.100947
11C	4.999332	-0.051135	-1.319618
12C	5.454433	1.067015	-0.384061
13C	5.213274	0.657601	1.072574
14C	-0.313060	-1.954442	-0.425638
15C	-1.414541	-0.902660	-0.294821
16C	-2.726802	-1.332688	-0.071851
17C	-3.782350	-0.416504	0.047330
18C	-3.492815	0.950206	-0.059917
19C	-2.185541	1.411484	-0.277635
20C	-1.155474	0.468799	-0.393917
21C	-1.883841	2.900175	-0.389222
22C	-2.254741	3.658110	0.898816
23C	-2.578719	3.527474	-1.612351
24C	-5.207313	-0.890958	0.301951
25C	-5.336159	-1.565968	1.680744

26C	-5.711145	-1.828403	-0.810916
27H	0.297161	-1.216404	1.966122
28H	3.765703	0.501426	3.381775
29H	1.006050	-1.899322	-2.665966
30H	1.110355	-0.164565	-2.311750
31H	3.283177	-0.919273	-3.102699
32H	3.308008	-2.274116	-1.950934
33H	5.603017	-0.959704	-1.142643
34H	5.140049	0.237834	-2.367144
35H	6.515686	1.279351	-0.556884
36H	4.890884	1.979931	-0.617453
37H	5.383624	1.506562	1.745906
38H	5.943523	-0.114434	1.356795
39H	-0.328504	-2.604691	0.458609
40H	-0.549976	-2.605542	-1.275617
41H	-2.926356	-2.399855	0.013857
42H	-4.305720	1.667829	0.033564
43H	-0.137279	0.813324	-0.549035
44H	-0.799695	3.003959	-0.533145
45H	-1.745428	3.231540	1.771347
46H	-1.968159	4.714881	0.819413
47H	-3.335223	3.617970	1.086716
48H	-2.296382	3.011114	-2.538145
49H	-3.670767	3.474403	-1.517552
50H	-2.302105	4.584906	-1.713784
51H	-5.852605	-0.001943	0.304194
52H	-5.002835	-0.897566	2.483817
53H	-6.379007	-1.845244	1.879685
54H	-4.728950	-2.478875	1.730185
55H	-5.128519	-2.757873	-0.842204
56H	-6.761034	-2.098912	-0.639956
57H	-5.638356	-1.353059	-1.796737

1f-010

1N	-2.244542	0.215675	2.806873
2C	-1.461331	-0.467948	1.952780
3C	-1.826024	-0.815890	0.643740
4C	-3.103705	-0.374915	0.177878
5C	-3.930165	0.329571	1.076051
6C	-3.446910	0.595057	2.360413
7N	-3.487907	-0.610078	-1.137297
8N	-1.007631	-1.575173	-0.197536
9C	-1.284690	-1.526987	-1.627531
10C	-2.783721	-1.654676	-1.866072
11C	-4.881049	-0.383684	-1.518095
12C	-5.417748	0.890543	-0.869406
13C	-5.313962	0.781134	0.655291
14C	0.333437	-1.968353	0.199397
15C	1.431579	-0.915478	0.055333
16C	1.146397	0.433661	-0.186648
17C	2.170915	1.382144	-0.301425
18C	3.499693	0.951293	-0.167091
19C	3.816803	-0.391862	0.072696
20C	2.766489	-1.316044	0.178781
21C	5.268497	-0.834974	0.197404
22C	5.677560	-1.756699	-0.967091
23C	5.550126	-1.511019	1.551891
24C	1.840683	2.847205	-0.553944
25C	2.449270	3.352848	-1.874970
26C	2.279932	3.735663	0.625240
27H	-0.481550	-0.739196	2.332927
28H	-4.071464	1.150408	3.059852
29H	-0.915080	-0.596463	-2.085697
30H	-0.766300	-2.363597	-2.107146
31H	-3.127651	-2.657328	-1.560259
32H	-2.996262	-1.535693	-2.934079
33H	-4.917395	-0.307052	-2.610578
34H	-5.505818	-1.246821	-1.226055
35H	-4.832444	1.748222	-1.226194
36H	-6.457781	1.047252	-1.177695
37H	-6.062095	0.060397	1.017298
38H	-5.554348	1.740779	1.128965
39H	0.603391	-2.841898	-0.406887
40H	0.304517	-2.326696	1.235381
41H	0.113967	0.756597	-0.282916
42H	4.308576	1.674365	-0.252771
43H	2.989248	-2.366466	0.360545
44H	5.891188	0.068232	0.140970
45H	5.511723	-1.270838	-1.936573
46H	6.740602	-2.021516	-0.896030
47H	5.097468	-2.688431	-0.954136
48H	5.270442	-0.858734	2.388150
49H	4.987658	-2.447633	1.653370
50H	6.616929	-1.750458	1.648009
51H	0.748294	2.926269	-0.638878

52H	2.125718	2.738110	-2.723997
53H	2.143051	4.389118	-2.068172
54H	3.545982	3.329074	-1.842038
55H	1.824858	3.400863	1.565196
56H	3.369732	3.714081	0.752791
57H	1.982953	4.778544	0.454631

1g-Me-001

1N	0.000000	0.861314	0.000000
2C	1.173111	0.181865	0.000000
3C	1.189446	-1.201826	0.000000
4C	-0.021947	-1.899584	0.000000
5C	-1.219469	-1.182835	0.000000
6C	-1.182595	0.203298	0.000000
7C	0.044699	2.343512	0.000000
8H	2.074866	0.783663	0.000000
9H	2.142865	-1.718118	0.000000
10H	-0.030805	-2.985212	0.000000
11H	-2.181534	-1.682820	0.000000
12H	-2.079551	0.811073	0.000000
13H	-0.970227	2.738348	0.000000
14H	0.572457	2.678647	0.895326
15H	0.572457	2.678647	-0.895326

1g-PhNCO-001

1N	-1.865554	-0.166525	0.000051
2C	-2.162067	1.152150	0.000138
3C	-3.480102	1.579973	0.000174
4C	-4.508588	0.632794	0.000113
5C	-4.179580	-0.723642	0.000026
6C	-2.842814	-1.096293	0.000000
7C	-0.373906	-0.678419	0.000001
8O	-0.290791	-1.912717	-0.000007
9N	0.430586	0.339157	-0.000011
10C	1.822551	0.189319	-0.000040
11C	2.535405	-1.032808	-0.000031
12C	3.933615	-1.035874	-0.000072
13C	4.659373	0.159640	-0.000121
14C	3.963735	1.375746	-0.000132
15C	2.570073	1.388723	-0.000093
16H	-1.307240	1.815326	0.000179
17H	-3.690026	2.644223	0.000249
18H	-5.547818	0.947914	0.000138
19H	-4.943456	-1.493962	-0.000022
20H	-2.502245	-2.124024	-0.000066
21H	1.992139	-1.969688	0.000001
22H	4.459172	-1.988836	-0.000069
23H	5.746627	0.145556	-0.000152
24H	4.509301	2.317051	-0.000167
25H	2.028480	2.331896	-0.000098

1g-PhNCO-002

1N	1.395041	0.424058	-0.124216
2C	1.087380	-0.406392	-1.138237
3C	1.715786	-1.638553	-1.258985
4C	2.662478	-2.012790	-0.302744
5C	2.967765	-1.132688	0.739298
6C	2.321796	0.094470	0.793886
7C	0.696307	1.891149	-0.012998
8O	1.555274	2.765385	0.081775
9N	-0.590938	1.900562	-0.086467
10C	-1.432695	0.796239	0.069987
11C	-2.483086	0.608945	-0.851622
12C	-3.374397	-0.456079	-0.714411
13C	-3.250637	-1.355631	0.352214
14C	-2.226136	-1.165815	1.286319
15C	-1.329777	-0.102223	1.153697
16H	0.335130	-0.058226	-1.835304
17H	1.459206	-2.287115	-2.089692
18H	3.160339	-2.975504	-0.370951
19H	3.700026	-1.384783	1.498839
20H	2.522837	0.839962	1.554457
21H	-2.581788	1.310720	-1.676331
22H	-4.172128	-0.582204	-1.443219
23H	-3.948706	-2.181913	0.459746
24H	-2.126536	-1.845588	2.129963
25H	-0.547997	0.045426	1.894656

1g-001

1N	0.000060	-1.420882	-0.000004
2C	1.147371	-0.723004	-0.000001
3C	1.201001	0.673488	0.000001
4C	-0.000066	1.386555	0.000001
5C	-1.201060	0.673388	-0.000003
6C	-1.147300	-0.723109	0.000012
7H	2.064714	-1.308850	-0.000002
8H	2.160528	1.183266	0.000001
9H	-0.000097	2.473799	-0.000001
10H	-2.160638	1.183072	-0.000015
11H	-2.064599	-1.309023	-0.000013

6ac-001

1C	3.050092	1.918620	0.327352
2C	3.150874	3.097694	1.060639
3N	2.404078	3.399493	2.137411
4C	1.512371	2.461730	2.510732
5C	1.329806	1.250661	1.856849
6C	2.104688	0.942602	0.715951
7N	1.831694	-0.276375	0.110815
8S	2.520318	-0.812078	-1.195056
9O	1.779029	-2.005791	-1.669265
10O	2.936027	0.168013	-2.228436
11C	4.172859	-1.573081	-0.656633
12F	3.985748	-2.506216	0.298849
13F	4.800332	-2.162111	-1.694815
14F	4.994790	-0.626509	-0.155397
15H	3.684058	1.770807	-0.538352
16H	3.876589	3.851264	0.757417
17H	0.905740	2.699159	3.383680
18H	0.586932	0.539872	2.205665
19P	-1.999913	-0.461671	-0.553307
20C	-1.456127	-1.470632	-1.954140
21C	-1.322515	1.210169	-0.680192
22C	-3.814716	-0.364758	-0.605198
23C	-1.502246	-1.237962	1.005400
24C	-1.772459	2.193187	0.217969
25C	-1.213712	3.469550	0.185256
26C	-0.204550	3.767460	-0.736818
27C	0.236469	2.792907	-1.635157
28C	-0.321144	1.512909	-1.613664
29C	-4.581059	-1.415125	-0.072219
30C	-5.971953	-1.387326	-0.186781
31C	-6.602459	-0.317764	-0.831451
32C	-5.840731	0.725112	-1.366765
33C	-4.448410	0.705088	-1.257151
34C	-2.120455	-0.835715	2.202300
35C	-1.693875	-1.370647	3.417122
36C	-0.654907	-2.308970	3.442270
37C	-0.042771	-2.709163	2.252377
38C	-0.456817	-2.173026	1.030590
39H	-0.369010	-1.593892	-1.961816
40H	-1.935279	-2.451161	-1.872299
41H	-1.786701	-0.985990	-2.877631
42H	-2.548695	1.960907	0.942467
43H	-1.553289	4.225101	0.888119
44H	0.246976	4.755654	-0.744472
45H	1.030856	3.015822	-2.341067
46H	0.046313	0.764885	-2.307001
47H	-4.100801	-2.248105	0.433395
48H	-6.561488	-2.199287	0.230232
49H	-7.685824	-0.297539	-0.915917
50H	-6.327073	1.557257	-1.868423
51H	-3.866030	1.520838	-1.674873
52H	-2.930894	-0.112840	2.191541
53H	-2.171602	-1.056198	4.341097
54H	-0.320773	-2.721715	4.390601
55H	0.774393	-3.424885	2.268818
56H	0.062998	-2.458844	0.123795

6ac-002

1C	-1.568537	1.006432	2.139175
2C	-1.769168	2.179361	2.853946
3N	-2.526058	3.208232	2.425788
4C	-3.115241	3.039634	1.228724
5C	-2.984121	1.908579	0.427661
6C	-2.177180	0.837922	0.874217
7N	-1.890697	-0.352636	0.222345
8S	-2.463368	-0.785171	-1.174710

9O	-2.758077	0.262127	-2.182285
10O	-1.714635	-1.974327	-1.648772
11C	-4.179624	-1.514502	-0.826112
12F	-4.728190	-2.034394	-1.943178
13F	-4.112608	-2.493839	0.098251
14F	-5.012455	-0.560187	-0.357345
15H	-0.937821	0.215867	2.535206
16H	-1.292092	2.307768	3.824738
17H	-3.731716	3.867444	0.880642
18H	-3.483762	1.870168	-0.532634
19P	2.009812	-0.446191	-0.572364
20C	1.519595	-1.481045	-1.975647
21C	1.173770	1.155473	-0.641756
22C	1.647744	-1.307250	0.980036
23C	3.805499	-0.184857	-0.675428
24C	1.305482	2.036542	0.444485
25C	0.699634	3.291278	0.396035
26C	-0.045696	3.664782	-0.726899
27C	-0.187955	2.782990	-1.801471
28C	0.421687	1.527928	-1.765611
29C	2.423820	-1.047904	2.123339
30C	2.110202	-1.674352	3.329956
31C	1.030291	-2.561954	3.397876
32C	0.261896	-2.821365	2.259595
33C	0.560878	-2.194039	1.048234
34C	4.341362	1.069511	-1.001948
35C	5.725686	1.222123	-1.121863
36C	6.573418	0.130201	-0.918048
37C	6.039179	-1.122768	-0.595075
38C	4.659000	-1.283599	-0.472880
39H	1.841717	-0.996297	-2.901930
40H	2.030417	-2.444341	-1.880703
41H	0.436530	-1.636889	-1.988021
42H	1.864733	1.741331	1.328056
43H	0.787810	3.965575	1.242754
44H	-0.534651	4.634627	-0.752469
45H	-0.791324	3.058412	-2.661390
46H	0.283990	0.847473	-2.598729
47H	3.271768	-0.370736	2.075297
48H	2.709590	-1.471118	4.213326
49H	0.788349	-3.049898	4.338617
50H	-0.583621	-3.501640	2.311238
51H	-0.069571	-2.375140	0.184989
52H	3.690053	1.923276	-1.161243
53H	6.137700	2.195702	-1.372964
54H	7.649329	0.253377	-1.009906
55H	6.696145	-1.973100	-0.434068
56H	4.251643	-2.256786	-0.211268

6ac-003

1C	-1.854146	1.157734	2.034058
2C	-2.071099	2.419093	2.572596
3N	-2.765325	3.396404	1.959452
4C	-3.272036	3.081248	0.754407
5C	-3.113361	1.852970	0.118834
6C	-2.371018	0.834409	0.758547
7N	-2.069799	-0.437882	0.285419
8S	-2.586407	-1.036430	-1.077848
9O	-2.817557	-0.113774	-2.215248
10O	-1.839390	-2.281619	-1.366948
11C	-4.332087	-1.686196	-0.719072
12F	-4.871590	-2.265530	-1.810734
13F	-4.317147	-2.599970	0.271523
14F	-5.143396	-0.675767	-0.338552
15H	-1.278377	0.418874	2.582253
16H	-1.662501	2.664426	3.552004
17H	-3.839046	3.866494	0.256135
18H	-3.543567	1.699958	-0.862964
19P	2.093967	-0.495108	-0.386952
20C	1.424912	-1.829865	-1.411665
21C	1.169055	1.033428	-0.652854
22C	1.987184	-0.979458	1.356159
23C	3.833333	-0.245065	-0.842710
24C	1.175797	2.025340	0.342209
25C	0.511115	3.231557	0.120586
26C	-0.167591	3.445264	-1.082540
27C	-0.186120	2.452495	-2.066548
28C	0.483244	1.246333	-1.859116
29C	3.094400	-0.873707	2.212134
30C	2.967779	-1.245198	3.552966
31C	1.745085	-1.720959	4.036736
32C	0.641472	-1.818976	3.182108
33C	0.753665	-1.447671	1.841609
34C	4.333226	1.036515	-1.117403
35C	5.676853	1.196244	-1.466881

36C	6.520341	0.084577	-1.541855
37C	6.022050	-1.194706	-1.269137
38C	4.682016	-1.363329	-0.920016
39H	1.581681	-1.596838	-2.468714
40H	1.956884	-2.753978	-1.166140
41H	0.356061	-1.961828	-1.217856
42H	1.683788	1.854640	1.287698
43H	0.501174	3.991630	0.896204
44H	-0.702160	4.377297	-1.243269
45H	-0.738678	2.605611	-2.988946
46H	0.447846	0.478792	-2.625783
47H	4.047922	-0.509003	1.842039
48H	3.824641	-1.163105	4.216197
49H	1.650861	-2.011189	5.079989
50H	-0.313240	-2.177902	3.557046
51H	-0.121802	-1.488396	1.197620
52H	3.683215	1.904561	-1.067996
53H	6.059780	2.189885	-1.682818
54H	7.564324	0.212073	-1.815813
55H	6.675743	-2.060613	-1.328161
56H	4.304690	-2.359459	-0.704454

6ac-004

1C	-2.198680	1.120322	2.231798
2C	-2.531378	2.352878	2.778056
3N	-3.175056	3.329412	2.109673
4C	-3.508669	3.041926	0.838784
5C	-3.226570	1.842190	0.191461
6C	-2.533984	0.827728	0.889989
7N	-2.123251	-0.412880	0.421254
8S	-2.391214	-0.961529	-1.028429
9O	-2.461313	0.000374	-2.154339
10O	-1.565927	-2.175095	-1.239522
11C	-4.146672	-1.678662	-0.990510
12F	-4.468788	-2.250360	-2.169074
13F	-4.268733	-2.614383	-0.028329
14F	-5.049765	-0.706150	-0.739802
15H	-1.670928	0.378086	2.823863
16H	-2.264247	2.575546	3.810256
17H	-4.033611	3.826695	0.295665
18H	-3.517675	1.711363	-0.843469
19P	2.127863	-0.460404	-0.496472
20C	1.635139	-1.627179	-1.791291
21C	1.178029	1.072211	-0.628764
22C	1.882898	-1.214582	1.130829
23C	3.890326	-0.078175	-0.705840
24C	0.864682	1.803063	0.528045
25C	0.204770	3.027117	0.415382
26C	-0.146509	3.520512	-0.843731
27C	0.156868	2.788051	-1.995609
28C	0.821193	1.565539	-1.894190
29C	2.836596	-1.030116	2.145434
30C	2.617884	-1.585296	3.407689
31C	1.453522	-2.319315	3.657481
32C	0.504964	-2.499853	2.645473
33C	0.711464	-1.950024	1.379099
34C	4.349536	1.246812	-0.665860
35C	5.713791	1.512481	-0.811803
36C	6.618148	0.462912	-0.994621
37C	6.160836	-0.859537	-1.032834
38C	4.800452	-1.133833	-0.888749
39H	1.894673	-1.214651	-2.770403
40H	2.174028	-2.567514	-1.640629
41H	0.556980	-1.808594	-1.736541
42H	1.115490	1.414900	1.510650
43H	-0.058875	3.579761	1.311893
44H	-0.675861	4.465808	-0.925607
45H	-0.135988	3.158956	-2.973818
46H	1.045549	1.003445	-2.795590
47H	3.743393	-0.463639	1.954036
48H	3.356214	-1.444447	4.192514
49H	1.285426	-2.749940	4.641341
50H	-0.404105	-3.062719	2.838741
51H	-0.044276	-2.076100	0.610899
52H	3.653355	2.068199	-0.525645
53H	6.065785	2.540050	-0.783222
54H	7.678336	0.673407	-1.108486
55H	6.862515	-1.676983	-1.174626
56H	4.455138	-2.164037	-0.914949

6ac-005

1C	3.788880	1.287287	0.463401
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2C	4.075879	2.451196	1.172837
3N	3.220992	3.473801	1.349872
4C	2.011280	3.327858	0.776943
5C	1.619728	2.212134	0.049591
6C	2.512978	1.132282	-0.123761
7N	2.016941	0.031973	-0.817709
8S	2.907262	-1.157713	-1.345132
9O	2.102210	-1.974243	-2.280132
10O	4.311099	-0.861474	-1.712272
11C	3.123954	-2.373520	0.103033
12F	1.932681	-2.884489	0.493580
13F	3.915539	-3.405830	-0.245149
14F	3.675795	-1.769115	1.178020
15H	4.547702	0.520168	0.371428
16H	5.057674	2.565783	1.630151
17H	1.313219	4.152196	0.914471
18H	0.623448	2.158212	-0.375112
19P	-1.869809	-0.416275	-0.120926
20C	-1.004860	-1.879053	-0.742130
21C	-1.985917	0.818641	-1.442717
22C	-3.546754	-0.915850	0.364627
23C	-1.014212	0.289024	1.308324
24C	-3.103485	1.666175	-1.525739
25C	-3.157305	2.645458	-2.519158
26C	-2.103487	2.779650	-3.429344
27C	-0.990716	1.937223	-3.344139
28C	-0.922664	0.957482	-2.351679
29C	-3.944983	-0.921337	1.709549
30C	-5.225920	-1.364853	2.050809
31C	-6.106018	-1.802349	1.057607
32C	-5.708060	-1.799717	-0.284543
33C	-4.432082	-1.358425	-0.634008
34C	-1.451878	1.526479	1.811184
35C	-0.806678	2.096000	2.907253
36C	0.280966	1.441416	3.496883
37C	0.717637	0.213579	2.994451
38C	0.071173	-0.369728	1.902329
39H	0.019826	-1.632399	-1.025987
40H	-1.008643	-2.653533	0.029703
41H	-1.547626	-2.245111	-1.619093
42H	-3.930543	1.562033	-0.829257
43H	-4.022824	3.299511	-2.582103
44H	-2.149326	3.541423	-4.203407
45H	-0.166846	2.043326	-4.044499
46H	-0.035894	0.336005	-2.273987
47H	-3.267376	-0.586161	2.488589
48H	-5.531917	-1.367255	3.093354
49H	-7.101620	-2.144969	1.327001
50H	-6.390748	-2.139089	-1.058766
51H	-4.132428	-1.350440	-1.678777
52H	-2.281676	2.049281	1.343581
53H	-1.140927	3.056580	3.289397
54H	0.796475	1.897956	4.337388
55H	1.573939	-0.286115	3.438243
56H	0.434167	-1.311959	1.510092

6ac-006

1C	-1.821064	0.004452	1.624412
2C	-1.381564	0.141476	2.937589
3N	-1.591939	1.221844	3.710517
4C	-2.298140	2.217003	3.139075
5C	-2.779689	2.187775	1.836873
6C	-2.535275	1.062433	1.017363
7N	-3.019967	1.138636	-0.281918
8S	-2.760098	0.063974	-1.399372
9O	-3.088981	0.621275	-2.726349
10O	-1.517448	-0.748835	-1.305628
11C	-4.097255	-1.263212	-1.173380
12F	-5.333080	-0.737627	-1.264282
13F	-3.986489	-2.230308	-2.109806
14F	-3.983017	-1.849553	0.039573
15H	-1.591901	-0.901858	1.081498
16H	-0.819092	-0.671547	3.394437
17H	-2.481377	3.092173	3.761024
18H	-3.330639	3.032142	1.432568
19P	1.975280	-0.310695	-0.716785
20C	1.489325	-0.980662	-2.329358
21C	1.141698	1.264128	-0.406950
22C	1.616125	-1.518659	0.587411
23C	3.772529	-0.037221	-0.750322
24C	1.225361	1.846886	0.869507
25C	0.623887	3.080973	1.106760
26C	-0.067341	3.732978	0.079719
27C	-0.157848	3.150401	-1.186168
28C	0.445411	1.915771	-1.435186

29C	2.365015	-1.507970	1.776822
30C	2.055310	-2.405246	2.799471
31C	1.007083	-3.317570	2.638286
32C	0.267271	-3.333214	1.452094
33C	0.565130	-2.435254	0.425240
34C	4.305260	1.259098	-0.808697
35C	5.689096	1.436655	-0.894450
36C	6.539401	0.328181	-0.922424
37C	6.008365	-0.965761	-0.864825
38C	4.628713	-1.152182	-0.778289
39H	1.862483	-0.313218	-3.111834
40H	1.955592	-1.963000	-2.449875
41H	0.401870	-1.064660	-2.394838
42H	1.741186	1.340429	1.680003
43H	0.675298	3.520402	2.098459
44H	-0.552840	4.685627	0.273468
45H	-0.718291	3.640135	-1.977015
46H	0.348467	1.466430	-2.417457
47H	3.187036	-0.809595	1.905713
48H	2.632607	-2.390884	3.719776
49H	0.766896	-4.014032	3.437231
50H	-0.550697	-4.037067	1.326046
51H	-0.035627	-2.437018	-0.476961
52H	3.652033	2.125970	-0.786727
53H	6.098734	2.442056	-0.937014
54H	7.614875	0.470390	-0.987270
55H	6.667799	-1.829196	-0.883327
56H	4.225191	-2.159867	-0.723363

6ac-007

1C	3.649826	-1.565965	0.612360
2C	4.099015	-2.850873	0.904125
3N	3.839847	-3.944617	0.165272
4C	3.101070	-3.737455	-0.941977
5C	2.604382	-2.499669	-1.329458
6C	2.858206	-1.354753	-0.539426
7N	2.282150	-0.172768	-0.985719
8S	2.381266	1.207062	-0.230066
9O	1.423062	2.157012	-0.842327
10O	2.463974	1.196693	1.248971
11C	4.048559	1.959600	-0.731871
12F	4.133033	2.108460	-2.068379
13F	4.225500	3.171079	-0.165920
14F	5.065999	1.163464	-0.338788
15H	3.891822	-0.752531	1.284782
16H	4.701254	-3.011679	1.797340
17H	2.894592	-4.616686	-1.550740
18H	2.013565	-2.401652	-2.236076
19P	-2.073938	0.041849	-0.376274
20C	-1.123486	0.185926	-1.912303
21C	-1.058171	-0.720728	0.910253
22C	-2.617846	1.684334	0.158957
23C	-3.530003	-0.996009	-0.689016
24C	-0.996093	-0.165594	2.197213
25C	-0.219679	-0.785901	3.178210
26C	0.488758	-1.952388	2.879252
27C	0.426911	-2.504839	1.595585
28C	-0.344767	-1.893183	0.609401
29C	-3.939369	1.895782	0.583170
30C	-4.330285	3.163817	1.019165
31C	-3.408830	4.215456	1.033414
32C	-2.090768	4.000594	0.615956
33C	-1.686950	2.737947	0.178803
34C	-3.903571	-2.000375	0.216940
35C	-5.041609	-2.771800	-0.033567
36C	-5.806372	-2.543357	-1.180919
37C	-5.436166	-1.539963	-2.083580
38C	-4.301815	-0.764931	-1.841263
39H	-0.837996	-0.813294	-2.252520
40H	-1.742470	0.670717	-2.673048
41H	-0.222945	0.778548	-1.731146
42H	-1.533495	0.748352	2.431168
43H	-0.159943	-0.347691	4.170560
44H	1.104450	-2.423897	3.640493
45H	0.998387	-3.395952	1.354116
46H	-0.372831	-2.320101	-0.388878
47H	-4.660185	1.083469	0.573530
48H	-5.354178	3.327430	1.344406
49H	-3.716835	5.201591	1.371263
50H	-1.370684	4.814240	0.631269
51H	-0.656722	2.579069	-0.128698
52H	-3.311505	-2.186662	1.107960
53H	-5.326376	-3.551603	0.667422
54H	-6.689572	-3.146533	-1.374411
55H	-6.028635	-1.360314	-2.976543

56H -4.027640 0.015447 -2.545885

6ac-008

1C -3.717783 1.459696 -0.096278
2C -4.027179 2.760304 -0.488171
3N -3.138580 3.764211 -0.591562
4C -1.866831 3.451657 -0.277682
5C -1.447829 2.190737 0.124848
6C -2.380109 1.133640 0.221616
7N -1.863698 -0.104943 0.587608
8S -2.736851 -1.345076 1.003589
9O -1.858525 -2.356500 1.637114
10O -4.056559 -1.094563 1.627051
11C -3.211041 -2.233471 -0.609661
12F -2.110146 -2.690399 -1.252613
13F -4.014093 -3.289049 -0.375811
14F -3.854748 -1.398424 -1.453771
15H -4.506786 0.719807 -0.038637
16H -5.057988 3.008774 -0.737084
17H -1.140767 4.259787 -0.355539
18H -0.405668 2.008762 0.361201
19P 1.877209 -0.525233 0.017126
20C 1.146886 -2.176024 0.138068
21C 1.587938 0.403065 1.544488
22C 3.668591 -0.709826 -0.224793
23C 1.198833 0.354917 -1.413926
24C 2.256034 1.625728 1.735831
25C 2.002404 2.382824 2.878306
26C 1.085054 1.923963 3.831770
27C 0.424537 0.707947 3.642127
28C 0.668635 -0.056830 2.498593
29C 4.185583 -0.853642 -1.522906
30C 5.551737 -1.076220 -1.705417
31C 6.403819 -1.157089 -0.599341
32C 5.889437 -1.018379 0.693779
33C 4.524226 -0.796252 0.885476
34C 1.805058 1.548742 -1.843894
35C 1.249542 2.265657 -2.902943
36C 0.092577 1.797273 -3.536779
37C -0.503514 0.606470 -3.116029
38C 0.044741 -0.117361 -2.055066
39H 0.077296 -2.122865 0.351237
40H 1.320402 -2.702963 -0.804995
41H 1.650335 -2.714814 0.946637
42H 2.970893 1.982466 0.999364
43H 2.518164 3.328074 3.024205
44H 0.883967 2.517599 4.719762
45H -0.296216 0.354113 4.374003
46H 0.118944 -0.978863 2.351786
47H 3.531132 -0.786505 -2.387207
48H 5.948647 -1.182716 -2.711269
49H 7.467381 -1.327016 -0.744865
50H 6.549384 -1.079878 1.554762
51H 4.134641 -0.684760 1.893107
52H 2.705957 1.917143 -1.360312
53H 1.717036 3.190069 -3.230874
54H -0.344911 2.363905 -4.354349
55H -1.406401 0.243266 -3.598785
56H -0.444510 -1.024367 -1.724454

6ac-009

1C 4.121624 1.252200 0.072652
2C 4.566445 2.421583 0.685027
3N 3.769887 3.411209 1.125950
4C 2.449568 3.219837 0.943930
5C 1.896569 2.094116 0.348332
6C 2.734153 1.054599 -0.114544
7N 2.087924 -0.036817 -0.688092
8S 2.825849 -1.293833 -1.292042
9O 1.846064 -2.107537 -2.044728
10O 4.164896 -1.102938 -1.895167
11C 3.199549 -2.416501 0.192930
12F 2.059502 -2.761290 0.834426
13F 3.814559 -3.552463 -0.189917
14F 3.995622 -1.789981 1.085146
15H 4.843962 0.515075 -0.255230
16H 5.635685 2.570271 0.829308
17H 1.795975 4.014107 1.301691
18H 0.821180 2.002891 0.245575
19P -2.009080 -0.380112 -0.099703
20C -1.141813 -1.863874 -0.664914
21C -1.985655 0.871418 -1.410660

22C	-3.724926	-0.834549	0.274943
23C	-1.201517	0.304334	1.366450
24C	-3.132537	1.621077	-1.716203
25C	-3.064446	2.619733	-2.690654
26C	-1.860354	2.869491	-3.356520
27C	-0.717990	2.123372	-3.046740
28C	-0.771509	1.123825	-2.074148
29C	-4.283623	-0.614159	1.542128
30C	-5.601866	-1.004206	1.795321
31C	-6.360005	-1.611892	0.791185
32C	-5.802377	-1.833607	-0.473600
33C	-4.488033	-1.447684	-0.735015
34C	-1.536464	1.605703	1.779567
35C	-0.914069	2.159056	2.897696
36C	0.053035	1.425882	3.594613
37C	0.393632	0.136949	3.176776
38C	-0.233824	-0.431309	2.065939
39H	-0.096689	-1.635922	-0.885291
40H	-1.208087	-2.641277	0.101802
41H	-1.631236	-2.216904	-1.577629
42H	-4.071757	1.430849	-1.205287
43H	-3.952586	3.199120	-2.928448
44H	-1.811424	3.646759	-4.114859
45H	0.220974	2.318798	-3.557478
46H	0.131398	0.570929	-1.822821
47H	-3.701066	-0.147306	2.330300
48H	-6.031914	-0.834266	2.778531
49H	-7.384285	-1.914471	0.992206
50H	-6.389672	-2.306703	-1.255775
51H	-4.062967	-1.618653	-1.720729
52H	-2.265288	2.188889	1.222604
53H	-1.169965	3.167006	3.212440
54H	0.552599	1.867346	4.452680
55H	1.160267	-0.424709	3.702915
56H	0.056622	-1.424534	1.742036

6ac-010

1C	-4.106001	1.272439	-0.118427
2C	-4.541376	2.413500	-0.788375
3N	-3.736434	3.368922	-1.285796
4C	-2.417305	3.171591	-1.102240
5C	-1.872978	2.071744	-0.452681
6C	-2.719594	1.067041	0.068177
7N	-2.083102	-0.002831	0.691468
8S	-2.830923	-1.224500	1.352501
9O	-1.857757	-2.011199	2.141623
10O	-4.168529	-0.995961	1.945726
11C	-3.214190	-2.409978	-0.079862
12F	-2.076628	-2.807231	-0.694847
13F	-3.853569	-3.514466	0.352043
14F	-3.991619	-1.812393	-1.007799
15H	-4.834386	0.561920	0.252203
16H	-5.609807	2.567468	-0.933156
17H	-1.757098	3.938451	-1.504866
18H	-0.797887	1.974274	-0.352838
19P	2.011721	-0.371200	0.128631
20C	1.150461	-1.816658	0.792848
21C	1.984489	0.957959	1.361229
22C	3.728780	-0.841153	-0.224806
23C	1.200156	0.208961	-1.378821
24C	3.131718	1.718741	1.636031
25C	3.061533	2.764607	2.559423
26C	1.854493	3.050739	3.204975
27C	0.710840	2.295637	2.923253
28C	0.766836	1.248474	2.002437
29C	4.259434	-0.747722	-1.519832
30C	5.574484	-1.155106	-1.761199
31C	6.358573	-1.653258	-0.717555
32C	5.829518	-1.748154	0.575098
33C	4.517877	-1.345533	0.825003
34C	1.549583	1.468548	-1.896504
35C	0.919697	1.943962	-3.045642
36C	-0.067153	1.174152	-3.672157
37C	-0.418812	-0.074383	-3.153453
38C	0.214314	-0.564198	-2.008715
39H	0.107126	-1.576569	1.010836
40H	1.210450	-2.639913	0.075305
41H	1.650516	-2.113341	1.720138
42H	4.073322	1.501506	1.140671
43H	3.950601	3.351482	2.774198
44H	1.803989	3.863782	3.924679
45H	-0.230866	2.519701	3.416930
46H	-0.136657	0.686852	1.773460
47H	3.656973	-0.366150	-2.338250
48H	5.981781	-1.083405	-2.765919

49H	7.380811	-1.968680	-0.909041
50H	6.437156	-2.135326	1.388364
51H	4.116697	-1.419134	1.832682
52H	2.297869	2.079596	-1.398011
53H	1.186392	2.920173	-3.441096
54H	-0.572044	1.556142	-4.555301
55H	-1.198814	-0.664078	-3.626506
56H	-0.086036	-1.524998	-1.606263

6ac-011

1C	3.744267	1.508020	0.379524
2C	4.069124	2.633057	1.134179
3N	3.178000	3.433101	1.745800
4C	1.884769	3.090532	1.590382
5C	1.448232	1.992865	0.861115
6C	2.385926	1.148154	0.225121
7N	1.858119	0.059709	-0.459212
8S	2.691896	-0.919877	-1.362085
9O	1.755662	-1.750492	-2.156748
10O	3.888485	-0.392309	-2.058348
11C	3.441336	-2.215144	-0.191929
12F	2.475689	-2.852674	0.509682
13F	4.137444	-3.147308	-0.871977
14F	4.275534	-1.637042	0.697822
15H	4.535522	0.930061	-0.082232
16H	5.116487	2.906889	1.253766
17H	1.156017	3.734451	2.080971
18H	0.389543	1.775177	0.777925
19P	-1.972379	-0.532653	-0.241079
20C	-1.323908	-2.017803	-1.044929
21C	-1.579354	0.935809	-1.224904
22C	-3.779527	-0.683506	-0.127686
23C	-1.290693	-0.375009	1.429042
24C	-2.210853	2.153274	-0.913318
25C	-1.875267	3.308225	-1.617748
26C	-0.911478	3.253186	-2.632130
27C	-0.287252	2.043002	-2.942724
28C	-0.615156	0.879537	-2.241811
29C	-4.368264	-1.295461	0.990769
30C	-5.751911	-1.479594	1.032878
31C	-6.549442	-1.058766	-0.036039
32C	-5.963481	-0.453634	-1.152585
33C	-4.581191	-0.264912	-1.202761
34C	-1.854169	0.558431	2.316770
35C	-1.285592	0.749074	3.575439
36C	-0.154832	0.014422	3.951579
37C	0.403167	-0.914611	3.070298
38C	-0.159331	-1.111777	1.807469
39H	-0.238062	-1.965988	-1.166422
40H	-1.597652	-2.886836	-0.438809
41H	-1.792963	-2.106797	-2.029766
42H	-2.962691	2.199801	-0.129443
43H	-2.363103	4.248446	-1.375343
44H	-0.645932	4.155967	-3.176041
45H	0.469099	1.999553	-3.721484
46H	-0.097516	-0.043341	-2.474925
47H	-3.756919	-1.621114	1.827426
48H	-6.204809	-1.949184	1.901823
49H	-7.626245	-1.201372	0.001198
50H	-6.580737	-0.124931	-1.984277
51H	-4.134389	0.211364	-2.070863
52H	-2.730737	1.132909	2.028845
53H	-1.720638	1.472777	4.259208
54H	0.293942	0.172194	4.928704
55H	1.288326	-1.477421	3.352967
56H	0.304086	-1.813067	1.125232

6ac-012

1C	4.111860	1.176336	0.386260
2C	4.535338	2.195766	1.235976
3N	3.739184	3.148435	1.752514
4C	2.442966	3.081411	1.394204
5C	1.912631	2.111309	0.553892
6C	2.748986	1.106284	0.017335
7N	2.119972	0.161150	-0.788895
8S	2.873079	-0.992153	-1.561512
9O	1.940940	-1.610455	-2.529072
10O	4.262518	-0.741567	-2.007979
11C	3.089376	-2.393468	-0.298053
12F	1.888787	-2.839594	0.133507
13F	3.751024	-3.438850	-0.831088
14F	3.779029	-1.969551	0.783394

15H	4.833205	0.458272	0.016404
16H	5.585629	2.246763	1.519572
17H	1.790744	3.851062	1.804806
18H	0.858146	2.121496	0.303304
19P	-2.020354	-0.270011	-0.289781
20C	-1.174616	-1.421387	-1.401809
21C	-1.621251	1.435905	-0.739322
22C	-3.806936	-0.555064	-0.415289
23C	-1.469262	-0.559562	1.412276
24C	-1.925328	2.463769	0.170695
25C	-1.600148	3.783209	-0.141355
26C	-0.965040	4.079325	-1.353119
27C	-0.659870	3.057107	-2.255360
28C	-0.987453	1.732742	-1.955126
29C	-4.304772	-1.837920	-0.124099
30C	-5.670123	-2.095915	-0.243666
31C	-6.542304	-1.081360	-0.655438
32C	-6.047664	0.191914	-0.949449
33C	-4.680828	0.459896	-0.831679
34C	-2.380117	-0.630127	2.477434
35C	-1.904363	-0.809960	3.778807
36C	-0.530107	-0.915400	4.016149
37C	0.375430	-0.836820	2.952538
38C	-0.087054	-0.656531	1.648875
39H	-0.107721	-1.190479	-1.446630
40H	-1.314644	-2.438217	-1.023562
41H	-1.608569	-1.345747	-2.403162
42H	-2.397539	2.234395	1.122378
43H	-1.828583	4.576048	0.565490
44H	-0.696770	5.106093	-1.586972
45H	-0.149735	3.283249	-3.187309
46H	-0.721369	0.947158	-2.654448
47H	-3.634774	-2.629720	0.200331
48H	-6.051812	-3.087384	-0.015754
49H	-7.605694	-1.285905	-0.747671
50H	-6.722175	0.979950	-1.272882
51H	-4.305946	1.451340	-1.066077
52H	-3.448360	-0.550371	2.299829
53H	-2.608712	-0.867309	4.604369
54H	-0.164523	-1.055260	5.030108
55H	1.444351	-0.909966	3.133202
56H	0.623470	-0.578569	0.830264

6a-001

1C	1.663595	0.559345	0.775526
2C	2.956737	1.073612	0.825660
3N	3.988792	0.641477	0.079377
4C	3.708836	-0.367308	-0.769235
5C	2.457121	-0.953134	-0.904365
6C	1.370981	-0.496703	-0.120265
7N	0.157350	-1.135958	-0.334947
8S	-1.175961	-0.802229	0.441298
9O	-2.190217	-1.834512	0.146946
10O	-1.066101	-0.335118	1.845928
11C	-1.908021	0.721161	-0.425882
12F	-2.085240	0.497107	-1.743757
13F	-3.106983	1.050679	0.101404
14F	-1.093084	1.792483	-0.297089
15H	0.900612	0.969487	1.425241
16H	3.175783	1.889104	1.514022
17H	4.538971	-0.725165	-1.376954
18H	2.299812	-1.763619	-1.610751

6a-002

1C	2.366027	1.416485	0.000050
2C	3.741611	1.233084	0.000002
3N	4.352745	0.030505	-0.000048
4C	3.532538	-1.035945	-0.000049
5C	2.142689	-0.970986	-0.000002
6C	1.501805	0.293600	0.000049
7N	0.146844	0.540467	0.000106
8S	-0.922005	-0.630560	0.000032
9O	-1.043337	-1.418534	-1.254053
10O	-1.043487	-1.418552	1.254092
11C	-2.448483	0.468428	-0.000034
12F	-3.548278	-0.315003	-0.000100
13F	-2.503405	1.254518	1.090963
14F	-2.503299	1.254552	-1.091010
15H	1.941285	2.416666	0.000088
16H	4.399564	2.101190	0.000003
17H	4.018016	-2.011244	-0.000087
18H	1.568408	-1.892378	-0.000005

6ac-Me-001

1C	-1.489940	1.771662	-0.382971
2C	-2.007223	2.985530	-0.746079
3N	-3.333173	3.266887	-0.605070
4C	-4.159197	2.318761	-0.091231
5C	-3.702422	1.081764	0.295466
6C	-2.323316	0.746928	0.156958
7N	-1.695664	-0.417542	0.465701
8S	-2.415455	-1.674330	1.146438
9O	-1.368499	-2.593554	1.627661
10O	-3.564576	-1.396833	2.031373
11C	-3.184756	-2.615481	-0.306617
12F	-2.247246	-2.949190	-1.213913
13F	-4.106886	-1.847617	-0.920916
14F	-3.780480	-3.738113	0.121750
15C	-3.852862	4.570967	-1.055553
16H	-0.430566	1.585821	-0.504761
17H	-1.393677	3.777073	-1.161326
18H	-5.204459	2.591459	-0.001888
19H	-4.414071	0.379306	0.707347
20H	-4.864159	4.707045	-0.671038
21H	-3.211302	5.366886	-0.671050
22H	-3.868158	4.600903	-2.148776
23P	2.201106	-0.568260	0.133246
24C	1.760350	-2.254766	0.617281
25C	1.641800	0.618233	1.384354
26C	4.005671	-0.449894	-0.013329
27C	1.445244	-0.165106	-1.463145
28C	2.076002	1.953049	1.293706
29C	1.611973	2.898071	2.207540
30C	0.715978	2.517170	3.213971
31C	0.288998	1.190444	3.307215
32C	0.746462	0.236649	2.394149
33C	4.636731	-0.763193	-1.228647
34C	6.030400	-0.744349	-1.309985
35C	6.795256	-0.418131	-0.185355
36C	6.167382	-0.111669	1.026198
37C	4.774482	-0.126514	1.117294
38C	1.857182	0.990367	-2.150497
39C	1.221730	1.354549	-3.337320
40C	0.174633	0.572334	-3.839892
41C	-0.233400	-0.576387	-3.157187
42C	0.396903	-0.947893	-1.967517
43H	0.680179	-2.363405	0.749485
44H	2.116763	-2.940646	-0.157238
45H	2.266081	-2.486473	1.559649
46H	2.777635	2.252716	0.519838
47H	1.952499	3.927603	2.137630
48H	0.354930	3.254713	3.925971
49H	-0.407951	0.891332	4.085088
50H	0.385805	-0.782418	2.469866
51H	4.050754	-1.015243	-2.108013
52H	6.516999	-0.982307	-2.251865
53H	7.879745	-0.402292	-0.253190
54H	6.759755	0.141327	1.901199
55H	4.293724	0.117717	2.060342
56H	2.671637	1.597272	-1.764601
57H	1.545170	2.244115	-3.870862
58H	-0.320631	0.857849	-4.764220
59H	-1.047736	-1.183996	-3.541803
60H	0.055318	-1.829798	-1.439281

6ac-Me-002

1C	-2.927314	1.246357	-1.674433
2C	-3.857810	2.200979	-1.991312
3N	-4.840356	2.553435	-1.117116
4C	-4.896623	1.943282	0.097314
5C	-3.995450	0.980234	0.475742
6C	-2.950485	0.582030	-0.413070
7N	-1.971057	-0.336190	-0.214034
8S	-1.842432	-1.255053	1.093946
9O	-0.486280	-1.824320	1.134937
10O	-2.416977	-0.737043	2.352806
11C	-2.930872	-2.745275	0.674518
12F	-2.505805	-3.343469	-0.450237
13F	-4.206423	-2.349830	0.489410
14F	-2.903569	-3.641697	1.673749
15C	-5.816356	3.605999	-1.451804
16H	-2.158656	0.990566	-2.394849
17H	-3.857544	2.714797	-2.945140
18H	-5.699418	2.263479	0.752337

19H	-4.093763	0.537783	1.457578
20H	-6.825566	3.244118	-1.243174
21H	-5.612065	4.499609	-0.855483
22H	-5.732455	3.847267	-2.511939
23P	2.589835	-0.152101	0.538736
24C	2.571169	-1.155270	2.047522
25C	2.335259	-1.222181	-0.899283
26C	1.298018	1.114538	0.622524
27C	4.203241	0.665651	0.369408
28C	1.083628	-1.296090	-1.528061
29C	0.903721	-2.179230	-2.595178
30C	1.959517	-2.984468	-3.031337
31C	3.206850	-2.911832	-2.399952
32C	3.399031	-2.032427	-1.334484
33C	1.125138	1.979163	-0.471434
34C	0.146105	2.970170	-0.422866
35C	-0.659139	3.104685	0.713806
36C	-0.483182	2.249318	1.803367
37C	0.494809	1.252757	1.762800
38C	4.646815	1.073398	-0.900188
39C	5.853124	1.763412	-1.026487
40C	6.620049	2.050850	0.107440
41C	6.181001	1.644919	1.371084
42C	4.973457	0.956200	1.507369
43H	3.383545	-1.886022	1.987854
44H	2.701410	-0.533748	2.937292
45H	1.612747	-1.678037	2.097858
46H	0.248028	-0.697607	-1.182825
47H	-0.068703	-2.242076	-3.076095
48H	1.812234	-3.671482	-3.860583
49H	4.029304	-3.536741	-2.737047
50H	4.371821	-1.971871	-0.853801
51H	1.749271	1.879262	-1.355071
52H	0.009347	3.633731	-1.272251
53H	-1.426171	3.874128	0.747164
54H	-1.115490	2.340391	2.681556
55H	0.604956	0.582566	2.608000
56H	4.065771	0.843878	-1.788518
57H	6.194260	2.072468	-2.010727
58H	7.560317	2.586002	0.005113
59H	6.776121	1.862815	2.253622
60H	4.647998	0.649235	2.496754

6ac-Me-003

1C	-1.707594	1.379276	1.286514
2C	-1.940085	2.685438	1.618197
3N	-2.865462	3.437383	0.956700
4C	-3.575245	2.871572	-0.055511
5C	-3.388623	1.568030	-0.441263
6C	-2.419205	0.751274	0.219280
7N	-2.071439	-0.522339	-0.063447
8S	-2.778919	-1.444239	-1.169515
9O	-1.854757	-1.768776	-2.275288
10O	-4.184488	-1.145904	-1.508360
11C	-2.859938	-3.039980	-0.171120
12F	-1.628042	-3.456650	0.179930
13F	-3.434713	-3.998278	-0.913967
14F	-3.585495	-2.868489	0.945224
15C	-3.023464	4.864232	1.286115
16H	-0.960713	0.815772	1.832852
17H	-1.400628	3.184528	2.414897
18H	-4.297288	3.513479	-0.547760
19H	-3.986764	1.181933	-1.255583
20H	-3.996394	5.209093	0.934892
21H	-2.966113	4.993911	2.368694
22H	-2.231000	5.443141	0.802209
23P	2.007459	-0.420494	-0.316145
24C	1.354591	-1.833840	-1.239145
25C	1.181041	1.103005	-0.845532
26C	1.746129	-0.670116	1.460956
27C	3.787149	-0.292542	-0.643054
28C	1.491577	2.308394	-0.192170
29C	0.863688	3.490390	-0.582888
30C	-0.077839	3.473905	-1.618504
31C	-0.389688	2.274824	-2.263996
32C	0.237654	1.085848	-1.883510
33C	2.613655	-0.071459	2.390683
34C	2.370997	-0.216280	3.757721
35C	1.270109	-0.957638	4.200520
36C	0.407474	-1.553130	3.275130
37C	0.638361	-1.410861	1.905343
38C	4.291566	0.692535	-1.506210
39C	5.657524	0.722760	-1.798917
40C	6.517778	-0.224874	-1.237648
41C	6.014401	-1.210288	-0.380700

42C	4.652514	-1.248173	-0.081626
43H	1.640198	-1.729521	-2.290037
44H	1.801302	-2.746844	-0.834973
45H	0.266487	-1.884007	-1.165308
46H	2.214244	2.327196	0.619529
47H	1.106477	4.421171	-0.077327
48H	-0.570827	4.395013	-1.918335
49H	-1.127806	2.256280	-3.060883
50H	-0.034000	0.161039	-2.380629
51H	3.477902	0.495199	2.056005
52H	3.045900	0.243294	4.474577
53H	1.086429	-1.072810	5.265542
54H	-0.450018	-2.127786	3.614395
55H	-0.056383	-1.855017	1.202463
56H	3.630467	1.430562	-1.950126
57H	6.045795	1.487291	-2.466102
58H	7.579574	-0.197653	-1.467378
59H	6.681458	-1.948070	0.056468
60H	4.271864	-2.012900	0.590103

6ac-Me-004

1C	3.178874	1.196885	-1.027718
2C	4.371025	1.856907	-0.896784
3N	5.280241	1.502281	0.054974
4C	4.988770	0.477880	0.899457
5C	3.810894	-0.223679	0.821219
6C	2.838692	0.108081	-0.169762
7N	1.633580	-0.467846	-0.403304
8S	1.045642	-1.715234	0.420183
9O	-0.395629	-1.810240	0.149777
10O	1.510807	-1.886055	1.812263
11C	1.771854	-3.210713	-0.484208
12F	1.406470	-3.215564	-1.777054
13F	1.346755	-4.350106	0.085156
14F	3.118967	-3.179686	-0.425185
15C	6.534136	2.263371	0.198391
16H	2.480793	1.502803	-1.798899
17H	4.649224	2.684599	-1.539453
18H	5.743951	0.241841	1.640363
19H	3.642303	-1.028025	1.524206
20H	6.357425	3.154483	0.807904
21H	7.285974	1.633533	0.676275
22H	6.890849	2.557695	-0.790368
23P	-2.708103	1.426569	0.030550
24C	-3.793207	2.883633	0.074154
25C	-3.524014	0.057975	0.885318
26C	-2.376238	0.998341	-1.695150
27C	-1.158287	1.846735	0.868901
28C	-3.527824	-1.228132	0.325789
29C	-4.148920	-2.275246	1.010085
30C	-4.758180	-2.043596	2.246078
31C	-4.746296	-0.761596	2.808529
32C	-4.129542	0.291485	2.133426
33C	-1.109131	0.519760	-2.061410
34C	-0.869051	0.153972	-3.387552
35C	-1.881451	0.267554	-4.344397
36C	-3.145496	0.744006	-3.976934
37C	-3.399064	1.108266	-2.653997
38C	-0.634606	1.019423	1.871722
39C	0.572349	1.360056	2.486849
40C	1.252480	2.518559	2.105704
41C	0.730308	3.344360	1.102853
42C	-0.472398	3.011215	0.480954
43H	-3.962881	3.177539	1.113834
44H	-3.314410	3.706089	-0.465462
45H	-4.753356	2.646009	-0.392448
46H	-3.040323	-1.419084	-0.624135
47H	-4.147447	-3.271919	0.577972
48H	-5.239403	-2.861956	2.775024
49H	-5.215246	-0.582663	3.772250
50H	-4.111976	1.280945	2.583826
51H	-0.316789	0.411312	-1.328524
52H	0.110621	-0.225944	-3.664934
53H	-1.690198	-0.018008	-5.375542
54H	-3.934794	0.829756	-4.718853
55H	-4.386738	1.468469	-2.380217
56H	-1.146530	0.107557	2.159359
57H	0.985173	0.704836	3.247600
58H	2.193417	2.775713	2.585007
59H	1.261338	4.243601	0.802742
60H	-0.871669	3.650547	-0.302085

6ac-Me-005

1C	-1.588587	1.813913	0.012931
2C	-2.137605	3.025577	-0.308957
3N	-3.487422	3.200852	-0.375454
4C	-4.305654	2.149296	-0.112570
5C	-3.817947	0.908004	0.219057
6C	-2.412194	0.681806	0.288144
7N	-1.750994	-0.471418	0.569392
8S	-2.462754	-1.822378	1.049909
9O	-1.423583	-2.708666	1.603472
10O	-3.737664	-1.684509	1.781128
11C	-2.958786	-2.694075	-0.557660
12F	-1.870707	-3.008661	-1.286596
13F	-3.742626	-1.889226	-1.303531
14F	-3.632641	-3.822511	-0.294006
15C	-4.032191	4.511623	-0.772590
16H	-0.511670	1.711398	0.059882
17H	-1.532792	3.898601	-0.527317
18H	-5.370073	2.342856	-0.179562
19H	-4.527579	0.118276	0.425195
20H	-5.106078	4.525164	-0.585925
21H	-3.552904	5.296117	-0.182679
22H	-3.842682	4.679867	-1.836529
23P	2.162046	-0.483106	0.055447
24C	1.636473	-2.195458	0.306178
25C	1.787391	0.503877	1.528414
26C	3.951966	-0.460686	-0.237624
27C	1.318678	0.219458	-1.387312
28C	2.417468	1.749111	1.703399
29C	2.080714	2.548944	2.795153
30C	1.119320	2.111307	3.713992
31C	0.498408	0.871204	3.543030
32C	0.826639	0.062787	2.451849
33C	4.455000	-0.484897	-1.548658
34C	5.833602	-0.555351	-1.760206
35C	6.709567	-0.603438	-0.671578
36C	6.208698	-0.583843	0.634549
37C	4.832556	-0.513747	0.856341
38C	1.669882	1.508616	-1.824115
39C	1.005564	2.079734	-2.908588
40C	-0.013669	1.371726	-3.557097
41C	-0.366487	0.092632	-3.119697
42C	0.296345	-0.487395	-2.035089
43H	0.562413	-2.262730	0.496575
44H	1.899307	-2.775800	-0.583574
45H	2.181415	-2.596709	1.166350
46H	3.174343	2.087635	1.001238
47H	2.573511	3.507690	2.932233
48H	0.859978	2.735045	4.565471
49H	-0.247079	0.527370	4.254657
50H	0.319366	-0.886236	2.325042
51H	3.782251	-0.447767	-2.400475
52H	6.220516	-0.571484	-2.775236
53H	7.781763	-0.655791	-0.840500
54H	6.888298	-0.620900	1.481472
55H	4.452363	-0.495480	1.873801
56H	2.458042	2.063086	-1.322642
57H	1.284408	3.073910	-3.247218
58H	-0.530821	1.818870	-4.402004
59H	-1.161512	-0.457123	-3.615855
60H	0.000334	-1.472629	-1.697605

6ac-Me-006

1C	-1.604905	1.799689	-0.067972
2C	-2.148242	2.990924	-0.466971
3N	-3.496817	3.164797	-0.555978
4C	-4.319503	2.128691	-0.247984
5C	-3.837514	0.908125	0.159845
6C	-2.432965	0.687526	0.267713
7N	-1.776843	-0.442916	0.640167
8S	-2.503433	-1.763642	1.182966
9O	-1.481833	-2.616349	1.814425
10O	-3.796473	-1.581369	1.871551
11C	-2.963397	-2.724821	-0.383780
12F	-1.861579	-3.076101	-1.074196
13F	-3.734584	-1.963426	-1.186477
14F	-3.640038	-3.839258	-0.071604
15C	-4.036094	4.455180	-1.021812
16H	-0.528622	1.701830	-0.002699
17H	-1.538768	3.849098	-0.727215
18H	-5.382896	2.318277	-0.340635
19H	-4.550177	0.130954	0.399591
20H	-5.106143	4.491513	-0.815715
21H	-3.538961	5.268300	-0.488056
22H	-3.864743	4.557926	-2.097109

23P	2.152321	-0.462659	0.105213
24C	1.593470	-2.127742	0.538831
25C	1.834708	0.680074	1.476210
26C	3.937595	-0.518659	-0.212794
27C	1.305330	0.114904	-1.389834
28C	2.539875	1.895450	1.535808
29C	2.254790	2.814829	2.545101
30C	1.271512	2.525912	3.498562
31C	0.577323	1.314152	3.444801
32C	0.852400	0.387575	2.436066
33C	4.422542	-0.625323	-1.526087
34C	5.795763	-0.749317	-1.749632
35C	6.683769	-0.769057	-0.670263
36C	6.200712	-0.666339	0.638936
37C	4.830545	-0.542100	0.872469
38C	1.635949	1.374806	-1.920158
39C	0.972236	1.848589	-3.050810
40C	-0.025211	1.073084	-3.654366
41C	-0.354643	-0.178041	-3.127451
42C	0.307888	-0.661507	-1.996032
43H	0.518182	-2.155813	0.730975
44H	1.847918	-2.806319	-0.280640
45H	2.129904	-2.441637	1.439718
46H	3.314808	2.118865	0.807852
47H	2.804265	3.751153	2.590319
48H	1.052796	3.242532	4.285791
49H	-0.184396	1.085117	4.184874
50H	0.288749	-0.537023	2.398536
51H	3.740251	-0.609726	-2.370901
52H	6.168611	-0.828871	-2.767015
53H	7.751701	-0.862976	-0.848318
54H	6.890076	-0.680253	1.478645
55H	4.465762	-0.457439	1.892268
56H	2.406938	1.983706	-1.455574
57H	1.233965	2.820335	-3.460550
58H	-0.543377	1.445213	-4.534281
59H	-1.130958	-0.781218	-3.589958
60H	0.029516	-1.627374	-1.592573

6ac-Me-007

1C	-3.718469	1.880354	-1.106832
2C	-4.583364	2.769405	-0.527138
3N	-5.049415	2.585923	0.740998
4C	-4.646486	1.494853	1.442712
5C	-3.779704	0.567355	0.918986
6C	-3.275028	0.718574	-0.406059
7N	-2.424523	-0.091811	-1.088426
8S	-1.862949	-1.479448	-0.516664
9O	-0.769814	-1.938073	-1.391392
10O	-1.667953	-1.587516	0.943991
11C	-3.252064	-2.714842	-0.876767
12F	-3.528424	-2.760861	-2.189100
13F	-4.373538	-2.355619	-0.219556
14F	-2.895098	-3.944280	-0.469747
15C	-6.016709	3.544084	1.304592
16H	-3.367080	2.055942	-2.117533
17H	-4.942059	3.654551	-1.040818
18H	-5.046745	1.395778	2.445072
19H	-3.488942	-0.270525	1.537482
20H	-6.172661	3.319412	2.360102
21H	-5.624115	4.558625	1.204521
22H	-6.967208	3.460589	0.770466
23P	2.603419	0.037038	-0.511847
24C	2.196172	-0.596133	-2.161853
25C	1.260937	1.111905	0.055567
26C	2.825632	-1.341155	0.641268
27C	4.140010	0.992487	-0.608685
28C	0.746981	0.996890	1.355100
29C	-0.264039	1.864078	1.776202
30C	-0.758920	2.839401	0.907718
31C	-0.251803	2.948230	-0.391817
32C	0.756587	2.087200	-0.821673
33C	3.894774	-1.338929	1.551951
34C	4.028370	-2.390207	2.461499
35C	3.102225	-3.437895	2.464426
36C	2.036853	-3.437068	1.557621
37C	1.892088	-2.392270	0.644074
38C	4.284647	2.186497	0.114524
39C	5.491977	2.887155	0.059910
40C	6.551717	2.400488	-0.711034
41C	6.408832	1.208113	-1.429516
42C	5.207148	0.500650	-1.380488
43H	2.192493	0.233132	-2.875818
44H	2.942103	-1.336026	-2.464996
45H	1.205409	-1.058040	-2.127599

46H	1.117988	0.232548	2.030740
47H	-0.668732	1.766616	2.779611
48H	-1.547727	3.509687	1.238608
49H	-0.645420	3.697004	-1.073380
50H	1.143570	2.174731	-1.833184
51H	4.619690	-0.530247	1.553710
52H	4.856658	-2.389154	3.164897
53H	3.209614	-4.253792	3.174438
54H	1.312263	-4.246810	1.561156
55H	1.053364	-2.394800	-0.045048
56H	3.463958	2.571581	0.712749
57H	5.601624	3.812898	0.618031
58H	7.489010	2.948874	-0.753108
59H	7.232008	0.828239	-2.028354
60H	5.109897	-0.427786	-1.936325

6ac-Me-008

1C	1.547307	1.381899	-1.434921
2C	1.607434	2.705701	-1.771557
3N	2.363026	3.591590	-1.061398
4C	3.087253	3.142095	-0.003013
5C	3.063620	1.828663	0.394777
6C	2.267062	0.874616	-0.309818
7N	2.082257	-0.431208	-0.021248
8S	2.857516	-1.226623	1.136610
9O	1.953330	-1.606347	2.243091
10O	4.215074	-0.762877	1.485444
11C	3.124759	-2.845049	0.212000
12F	1.949655	-3.420576	-0.103949
13F	3.812033	-3.689984	0.996634
14F	3.820977	-2.646429	-0.917684
15C	2.414969	5.002957	-1.478830
16H	0.936220	0.709884	-2.023398
17H	1.061925	3.115192	-2.614285
18H	3.681926	3.884558	0.516858
19H	3.653659	1.541733	1.254922
20H	2.878193	5.592353	-0.686904
21H	3.002026	5.095967	-2.396951
22H	1.399213	5.366479	-1.650967
23P	-1.962001	-0.570230	0.358577
24C	-1.349131	-1.991376	1.298704
25C	-1.450215	-0.702478	-1.375248
26C	-3.775286	-0.561225	0.434968
27C	-1.339759	0.968198	1.090400
28C	-1.919863	0.247485	-2.299882
29C	-1.517117	0.177121	-3.632740
30C	-0.647570	-0.838466	-4.049925
31C	-0.181678	-1.782756	-3.131942
32C	-0.579103	-1.718710	-1.793671
33C	-4.415505	-0.001507	1.553879
34C	-5.805935	-0.061344	1.657939
35C	-6.559110	-0.677416	0.652861
36C	-5.922240	-1.237501	-0.458790
37C	-4.531336	-1.182593	-0.572369
38C	-1.924898	2.192919	0.722409
39C	-1.424537	3.385305	1.244368
40C	-0.348285	3.361748	2.138988
41C	0.226050	2.144118	2.511882
42C	-0.263077	0.943936	1.990037
43H	-0.257212	-2.037592	1.288473
44H	-1.700682	-1.898105	2.330541
45H	-1.767587	-2.902160	0.860373
46H	-2.596458	1.036986	-1.984964
47H	-1.884533	0.910286	-4.345580
48H	-0.334935	-0.891631	-5.089342
49H	0.498217	-2.568059	-3.449854
50H	-0.193113	-2.449685	-1.093227
51H	-3.837616	0.484417	2.335329
52H	-6.299061	0.375662	2.521780
53H	-7.641828	-0.719654	0.735904
54H	-6.505787	-1.716030	-1.240428
55H	-4.045864	-1.618145	-1.440768
56H	-2.772055	2.218143	0.042240
57H	-1.882013	4.329688	0.962002
58H	0.036847	4.291984	2.548427
59H	1.059528	2.120974	3.208367
60H	0.209689	0.012156	2.279226

6ac-Me-009

1C	4.285296	1.745869	0.982864
2C	5.047088	2.539029	0.166475
3N	5.116727	2.318654	-1.176510

4C	4.420411	1.281983	-1.713349
5C	3.636533	0.452507	-0.950184
6C	3.534624	0.651355	0.459107
7N	2.814158	-0.054310	1.367570
8S	1.865636	-1.290466	0.997536
9O	0.982483	-1.567925	2.140880
10O	1.266377	-1.299903	-0.355378
11C	3.037824	-2.776750	0.967513
12F	3.647393	-2.936679	2.151492
13F	3.983776	-2.601454	0.022303
14F	2.354086	-3.898282	0.681035
15C	6.001190	3.145825	-2.017205
16H	4.248607	1.953417	2.046675
17H	5.625271	3.373993	0.545789
18H	4.517910	1.146063	-2.784583
19H	3.095058	-0.341478	-1.445553
20H	5.644871	3.119695	-3.047752
21H	5.981504	4.175373	-1.655670
22H	7.022707	2.757419	-1.969996
23P	-2.609170	-0.106015	0.352347
24C	-2.234350	-1.239898	1.714581
25C	-1.235789	1.041763	0.096670
26C	-2.860266	-1.084355	-1.150288
27C	-4.114291	0.824888	0.744146
28C	-0.935387	1.501208	-1.195323
29C	0.092421	2.427782	-1.376408
30C	0.821151	2.890171	-0.276395
31C	0.523713	2.428172	1.008946
32C	-0.506126	1.507169	1.201302
33C	-4.085295	-1.073448	-1.833663
34C	-4.245307	-1.867290	-2.972804
35C	-3.191414	-2.666331	-3.425163
36C	-1.969184	-2.672987	-2.742450
37C	-1.796571	-1.884559	-1.604634
38C	-4.264511	2.146468	0.293626
39C	-5.445881	2.840053	0.563529
40C	-6.475460	2.221670	1.279829
41C	-6.325424	0.906277	1.731306
42C	-5.148408	0.204301	1.465556
43H	-2.197719	-0.696759	2.662869
44H	-3.014513	-2.005961	1.757082
45H	-1.265554	-1.711201	1.531146
46H	-1.488513	1.132760	-2.054561
47H	0.327896	2.779401	-2.377227
48H	1.626273	3.605712	-0.421016
49H	1.101906	2.769562	1.862211
50H	-0.719318	1.145725	2.202408
51H	-4.908500	-0.455583	-1.487201
52H	-5.193343	-1.859424	-3.503591
53H	-3.320821	-3.282586	-4.311032
54H	-1.148005	-3.290893	-3.095544
55H	-0.839840	-1.878546	-1.089145
56H	-3.465620	2.636120	-0.255618
57H	-5.557894	3.864151	0.218286
58H	-7.392427	2.765662	1.490565
59H	-7.122439	0.425600	2.291808
60H	-5.044022	-0.815843	1.823435

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1C	-2.265430	1.293128	1.536346
2C	-2.600542	2.597369	1.781465
3N	-3.287804	3.341473	0.869074
4C	-3.647853	2.772197	-0.312772
5C	-3.342719	1.471944	-0.621592
6C	-2.617862	0.660164	0.305284
7N	-2.212303	-0.616196	0.142856
8S	-2.608002	-1.530054	-1.119526
9O	-1.490668	-1.706463	-2.068471
10O	-3.960853	-1.336315	-1.678110
11C	-2.686731	-3.171341	-0.201087
12F	-1.497598	-3.470833	0.354212
13F	-3.006040	-4.145189	-1.068523
14F	-3.615433	-3.137198	0.766256
15C	-3.584217	4.761941	1.122442
16H	-1.718616	0.733616	2.286402
17H	-2.338325	3.098492	2.706250
18H	-4.187468	3.411286	-1.002593
19H	-3.659340	1.084864	-1.581241
20H	-4.557817	5.007719	0.694443
21H	-3.611228	4.937932	2.198613
22H	-2.812395	5.389407	0.666287
23P	2.122867	-0.399318	-0.265611
24C	1.630692	-1.961088	-1.041600
25C	1.106422	0.965773	-0.881268
26C	1.887675	-0.543755	1.524932

27C	3.866957	-0.081791	-0.639319
28C	0.899966	2.090824	-0.066278
29C	0.174787	3.177432	-0.557081
30C	-0.353557	3.139820	-1.850818
31C	-0.159791	2.013782	-2.656973
32C	0.573436	0.926633	-2.179443
33C	2.905438	-0.207255	2.429910
34C	2.672839	-0.323822	3.803147
35C	1.434590	-0.774893	4.270088
36C	0.419614	-1.105860	3.364602
37C	0.638983	-0.989362	1.991897
38C	4.290743	1.179822	-1.083946
39C	5.643570	1.398360	-1.356108
40C	6.570428	0.366365	-1.185188
41C	6.148066	-0.891922	-0.740776
42C	4.799471	-1.120296	-0.467220
43H	1.842065	-1.925793	-2.114233
44H	2.204851	-2.772447	-0.584684
45H	0.562816	-2.129728	-0.888280
46H	1.296319	2.118342	0.944748
47H	0.018176	4.047708	0.074062
48H	-0.923651	3.984022	-2.229361
49H	-0.582852	1.976291	-3.656788
50H	0.708320	0.055868	-2.811424
51H	3.871609	0.137966	2.073842
52H	3.461508	-0.065234	4.504259
53H	1.259600	-0.868969	5.338671
54H	-0.544316	-1.455517	3.724585
55H	-0.164405	-1.221266	1.298227
56H	3.576328	1.985335	-1.223009
57H	5.969835	2.374515	-1.704168
58H	7.621415	0.539788	-1.400549
59H	6.867283	-1.695492	-0.608981
60H	4.480004	-2.098826	-0.118714

6ac-Me-011

1C	2.331250	2.014757	-0.191653
2C	3.112534	3.105261	0.089878
3N	4.470300	3.039559	0.031141
4C	5.062598	1.864611	-0.312046
5C	4.337694	0.737302	-0.607186
6C	2.911014	0.766292	-0.556573
7N	2.031542	-0.241253	-0.807935
8S	2.471859	-1.708394	-1.290692
9O	1.266633	-2.414501	-1.755659
10O	3.701955	-1.805047	-2.100427
11C	2.914857	-2.610808	0.314841
12F	1.886388	-2.580513	1.180598
13F	3.977729	-2.026905	0.903391
14F	3.218846	-3.892578	0.058868
15C	5.311612	4.213728	0.326060
16H	1.254116	2.102774	-0.127663
17H	2.687058	4.061387	0.370641
18H	6.146688	1.872413	-0.339564
19H	4.874813	-0.160703	-0.880252
20H	5.907416	4.465126	-0.554999
21H	4.671687	5.057968	0.583623
22H	5.971026	3.987107	1.167743
23P	-2.276212	0.109218	-0.385252
24C	-1.339168	-0.137675	-1.916430
25C	-2.311667	-1.419526	0.580577
26C	-1.482769	1.425007	0.582472
27C	-3.965212	0.632204	-0.787068
28C	-3.315398	-1.607533	1.546769
29C	-3.314081	-2.763895	2.326751
30C	-2.319044	-3.731722	2.145595
31C	-1.323945	-3.543910	1.182449
32C	-1.313464	-2.389168	0.396027
33C	-1.505133	2.741567	0.089169
34C	-0.889341	3.762894	0.813492
35C	-0.249300	3.475196	2.025099
36C	-0.218028	2.164631	2.508935
37C	-0.834025	1.135565	1.791654
38C	-4.670055	1.491043	0.072736
39C	-5.987583	1.843373	-0.226274
40C	-6.603259	1.344126	-1.378262
41C	-5.901895	0.489863	-2.235526
42C	-4.585055	0.130287	-1.943904
43H	-1.711360	-1.012392	-2.456776
44H	-1.453269	0.757009	-2.536151
45H	-0.281976	-0.276284	-1.672417
46H	-4.095677	-0.865327	1.688261
47H	-4.091836	-2.910645	3.071101
48H	-2.322724	-4.632984	2.752875
49H	-0.550324	-4.292759	1.038514

50H	-0.532618	-2.261370	-0.346364
51H	-2.010217	2.972871	-0.845319
52H	-0.915307	4.781173	0.435385
53H	0.224734	4.273514	2.590215
54H	0.284948	1.938516	3.445059
55H	-0.806665	0.119558	2.173433
56H	-4.196319	1.888733	0.965596
57H	-6.529583	2.509060	0.439839
58H	-7.628187	1.621634	-1.609507
59H	-6.378084	0.102621	-3.131987
60H	-4.051994	-0.535595	-2.616392

6ac-PhNCO-001

1C	1.751799	-1.781353	0.763710
2C	0.409607	-2.051055	0.677348
3N	-0.102434	-2.861587	-0.286200
4C	0.742342	-3.449978	-1.174311
5C	2.093815	-3.220906	-1.140660
6C	2.663614	-2.336639	-0.180718
7N	4.004443	-2.116234	-0.293383
8S	4.826397	-1.105110	0.635180
9O	6.264371	-1.311319	0.407460
10O	4.357378	-0.921289	2.026978
11C	4.507354	0.594840	-0.142408
12F	3.197187	0.919160	-0.054197
13F	4.851324	0.615436	-1.441908
14F	5.213369	1.545297	0.497393
15C	-1.602966	-3.060703	-0.459670
16O	-1.916764	-3.770723	-1.428692
17N	-2.266612	-2.414941	0.464569
18C	-3.655564	-2.304536	0.421812
19C	-4.453579	-2.390050	-0.744873
20C	-5.827840	-2.140228	-0.689480
21C	-6.454876	-1.814563	0.518394
22C	-5.680248	-1.744589	1.684037
23C	-4.306554	-1.979549	1.634937
24H	2.093091	-1.126212	1.551387
25H	-0.317923	-1.627087	1.355272
26H	0.267303	-4.086285	-1.909312
27H	2.736500	-3.695728	-1.874152
28H	-3.990386	-2.657824	-1.687118
29H	-6.414764	-2.208890	-1.603544
30H	-7.525562	-1.629119	0.553643
31H	-6.149537	-1.504847	2.636184
32H	-3.704623	-1.918916	2.538063
33P	-1.700706	1.722889	-0.114446
34C	-3.486571	1.418528	-0.148296
35C	-1.399570	3.496672	-0.358150
36C	-1.017079	1.223307	1.488063
37C	-0.908483	0.822776	-1.471762
38C	-1.168526	4.342312	0.738288
39C	-0.995587	5.712993	0.531091
40C	-1.054436	6.241429	-0.761700
41C	-1.290555	5.399824	-1.854355
42C	-1.463279	4.029361	-1.657566
43C	0.355531	1.406069	1.734051
44C	0.903635	0.998842	2.948918
45C	0.089787	0.406298	3.921252
46C	-1.274836	0.227870	3.679526
47C	-1.834024	0.636212	2.466029
48C	0.394692	1.173317	-1.865410
49C	1.032528	0.451218	-2.872724
50C	0.372810	-0.614186	-3.495132
51C	-0.925640	-0.957944	-3.110417
52C	-1.569888	-0.245511	-2.096788
53H	-3.869308	1.722096	-1.127100
54H	-3.712171	0.362150	0.022390
55H	-3.962520	2.028760	0.624746
56H	-1.114755	3.940753	1.745764
57H	-0.809303	6.363928	1.380801
58H	-0.913983	7.307505	-0.919237
59H	-1.334392	5.807808	-2.860327
60H	-1.636613	3.380925	-2.512090
61H	1.000617	1.851842	0.982814
62H	1.966878	1.129183	3.129187
63H	0.522651	0.078364	4.862461
64H	-1.907076	-0.239211	4.429456
65H	-2.890894	0.470764	2.288244
66H	0.910268	2.003015	-1.391145
67H	2.044967	0.715608	-3.164522
68H	0.875464	-1.180697	-4.274381
69H	-1.434477	-1.795300	-3.577546
70H	-2.570269	-0.537702	-1.796818

6ac-PhNCO-002

1C	3.155114	2.458277	-0.697063
2C	1.853233	2.777965	-0.420568
3N	1.146231	2.111823	0.535363
4C	1.752989	1.117512	1.232298
5C	3.054124	0.745141	0.999379
6C	3.822608	1.405669	-0.003532
7N	5.103344	1.161797	-0.396249
8S	6.034183	0.019489	0.233289
9O	5.789699	-0.352218	1.644046
10O	7.421424	0.245223	-0.198451
11C	5.530834	-1.540743	-0.717079
12F	4.229200	-1.829097	-0.492612
13F	6.267238	-2.594125	-0.321823
14F	5.696141	-1.381365	-2.041808
15C	-0.303484	2.436351	0.833501
16O	-0.784089	1.803725	1.797206
17N	-0.788304	3.288363	-0.026429
18C	-2.108664	3.734590	0.080419
19C	-2.795946	3.949032	1.296461
20C	-4.110641	4.419718	1.297327
21C	-4.781111	4.684532	0.096576
22C	-4.106006	4.488363	-1.114425
23C	-2.787356	4.029733	-1.121528
24H	3.688935	3.007407	-1.465161
25H	1.309661	3.557746	-0.935833
26H	1.134321	0.637149	1.978457
27H	3.475219	-0.056099	1.590849
28H	-2.294187	3.736761	2.234036
29H	-4.617292	4.579771	2.247177
30H	-5.806543	5.045755	0.104915
31H	-4.605860	4.699967	-2.057546
32H	-2.257777	3.889420	-2.061177
33P	-2.786985	-0.971049	0.102100
34C	-3.576758	0.578408	0.602034
35C	-1.271912	-0.634465	-0.825649
36C	-2.376088	-1.933294	1.582197
37C	-3.932342	-1.915014	-0.940514
38C	-0.171274	-1.499607	-0.707765
39C	0.978758	-1.261420	-1.461144
40C	1.033643	-0.165651	-2.328353
41C	-0.063263	0.692511	-2.446986
42C	-1.218911	0.462986	-1.699545
43C	-2.752330	-3.279755	1.698308
44C	-2.401508	-3.998150	2.844531
45C	-1.678647	-3.377336	3.867258
46C	-1.301544	-2.034583	3.747422
47C	-1.645202	-1.306459	2.607823
48C	-3.472712	-2.574443	-2.090831
49C	-4.365205	-3.316842	-2.868045
50C	-5.711320	-3.403260	-2.501704
51C	-6.170732	-2.745668	-1.354997
52C	-5.286124	-2.002631	-0.572318
53H	-3.891968	1.140436	-0.281063
54H	-4.449662	0.351124	1.221555
55H	-2.856865	1.166611	1.176984
56H	-0.203699	-2.343465	-0.024575
57H	1.835519	-1.920412	-1.359416
58H	1.937999	0.027676	-2.898778
59H	-0.014343	1.557295	-3.102279
60H	-2.055796	1.148766	-1.785187
61H	-3.313546	-3.767457	0.906811
62H	-2.692939	-5.041100	2.934622
63H	-1.407927	-3.938922	4.757628
64H	-0.737981	-1.551806	4.541273
65H	-1.339216	-0.267403	2.513015
66H	-2.429727	-2.507720	-2.385197
67H	-4.006599	-3.823771	-3.759709
68H	-6.403594	-3.979484	-3.109869
69H	-7.217221	-2.809769	-1.069818
70H	-5.652760	-1.499807	0.318217

6ac-PhNCO-003

1C	1.924353	-1.901976	0.508263
2C	0.594415	-2.170938	0.302021
3N	0.115078	-2.542480	-0.913569
4C	0.981720	-2.698911	-1.950692
5C	2.324625	-2.472430	-1.801734
6C	2.858399	-2.012554	-0.562768
7N	4.189557	-1.720315	-0.563458
8S	4.963883	-1.080521	0.683728
9O	6.409373	-1.120909	0.417210
10O	4.490480	-1.441932	2.038532

11C	4.549789	0.766203	0.568679
12F	3.225194	0.962601	0.751561
13F	4.883262	1.270650	-0.631525
14F	5.207998	1.459349	1.516156
15C	-1.376813	-2.669521	-1.173747
16O	-1.694283	-2.490438	-2.367646
17N	-2.026088	-2.898667	-0.064920
18C	-3.420503	-2.957510	-0.012345
19C	-4.320371	-2.815654	-1.097133
20C	-5.702160	-2.862675	-0.884843
21C	-6.232639	-3.051714	0.395379
22C	-5.353099	-3.203601	1.476067
23C	-3.975196	-3.158129	1.273847
24H	2.236334	-1.583692	1.492604
25H	-0.148113	-2.080627	1.082693
26H	0.533463	-2.991631	-2.891242
27H	2.988618	-2.603102	-2.649172
28H	-3.930270	-2.675076	-2.097104
29H	-6.370668	-2.753272	-1.736798
30H	-7.308403	-3.088422	0.548663
31H	-5.743697	-3.360856	2.479443
32H	-3.290064	-3.277237	2.109165
33P	-1.705230	1.529934	-0.332177
34C	-3.050803	0.629367	-1.144090
35C	-2.274270	3.214427	0.027948
36C	-1.239720	0.710715	1.213207
37C	-0.277397	1.618500	-1.441471
38C	-2.418977	3.662188	1.349044
39C	-2.887981	4.956216	1.592667
40C	-3.212869	5.797742	0.525545
41C	-3.068508	5.350130	-0.793273
42C	-2.600208	4.061172	-1.046149
43C	0.051090	0.901860	1.734413
44C	0.408738	0.299499	2.939908
45C	-0.515670	-0.494823	3.626652
46C	-1.799793	-0.685826	3.107755
47C	-2.167945	-0.086217	1.902048
48C	0.652439	2.662689	-1.295536
49C	1.796435	2.687117	-2.093411
50C	2.010339	1.683074	-3.043365
51C	1.075969	0.655790	-3.200482
52C	-0.066948	0.612835	-2.399388
53H	-3.289296	1.139421	-2.082472
54H	-2.764187	-0.402957	-1.354699
55H	-3.934110	0.642459	-0.500415
56H	-2.167268	3.013637	2.182798
57H	-2.996940	5.303099	2.616554
58H	-3.575659	6.803788	0.718937
59H	-3.317857	6.004528	-1.623992
60H	-2.479129	3.722918	-2.072373
61H	0.782637	1.497341	1.198143
62H	1.413006	0.436217	3.330799
63H	-0.231171	-0.973615	4.559772
64H	-2.513989	-1.315255	3.630318
65H	-3.161017	-0.264651	1.503268
66H	0.486644	3.449704	-0.565087
67H	2.521744	3.486434	-1.969892
68H	2.906127	1.700853	-3.658102
69H	1.238533	-0.123788	-3.938652
70H	-0.770068	-0.206066	-2.525122

6ac-PhNCO-004

1C	2.388666	2.759961	-0.870211
2C	1.098754	3.011836	-0.486628
3N	0.572533	2.455232	0.640318
4C	1.363089	1.674366	1.420373
5C	2.659300	1.372638	1.084238
6C	3.222392	1.876591	-0.124160
7N	4.440573	1.607689	-0.672072
8S	5.490888	0.573506	-0.043406
9O	5.523260	0.452157	1.430495
10O	6.767370	0.699099	-0.761970
11C	4.846174	-1.122811	-0.598681
12F	3.625416	-1.366073	-0.070795
13F	5.677952	-2.098723	-0.194918
14F	4.736314	-1.187989	-1.938263
15C	-0.890297	2.618782	1.016773
16O	-1.197464	2.091510	2.107058
17N	-1.553350	3.234020	0.077754
18C	-2.928321	3.463473	0.176433
19C	-3.700913	3.436359	1.362070
20C	-5.074819	3.690307	1.321763
21C	-5.723650	3.969531	0.113883
22C	-4.969257	4.006608	-1.066101
23C	-3.596126	3.764862	-1.032959

24H	2.770627	3.203565	-1.783221
25H	0.418471	3.631222	-1.054240
26H	0.893056	1.294534	2.316340
27H	3.228732	0.733130	1.744713
28H	-3.218753	3.215809	2.306271
29H	-5.643525	3.668494	2.249586
30H	-6.793366	4.163147	0.092506
31H	-5.452084	4.230623	-2.015241
32H	-3.008198	3.802258	-1.947219
33P	-2.172372	-1.349171	0.196762
34C	-3.356184	-0.162408	0.886802
35C	-1.132987	-0.542178	-1.044285
36C	-1.132048	-2.020976	1.518684
37C	-3.082446	-2.711079	-0.582606
38C	0.248446	-0.792647	-1.085847
39C	1.025419	-0.211372	-2.088618
40C	0.431144	0.616828	-3.044865
41C	-0.941989	0.875867	-2.996453
42C	-1.728278	0.299886	-1.998464
43C	-0.715561	-3.361473	1.472883
44C	0.136300	-3.854854	2.463026
45C	0.570664	-3.017397	3.495501
46C	0.152760	-1.683406	3.540696
47C	-0.696639	-1.177501	2.554941
48C	-2.759639	-3.146135	-1.876570
49C	-3.458182	-4.216249	-2.441902
50C	-4.472509	-4.851768	-1.720770
51C	-4.793386	-4.419371	-0.428450
52C	-4.101116	-3.352278	0.144044
53H	-3.995105	0.213722	0.083160
54H	-3.973410	-0.666877	1.636614
55H	-2.818108	0.668815	1.351304
56H	0.718891	-1.427994	-0.341598
57H	2.094664	-0.394783	-2.112601
58H	1.043025	1.074094	-3.817735
59H	-1.401385	1.536015	-3.726777
60H	-2.792731	0.514125	-1.964665
61H	-1.050479	-4.017175	0.674170
62H	0.459365	-4.891553	2.426195
63H	1.234548	-3.403998	4.264240
64H	0.489412	-1.031631	4.342508
65H	-0.998644	-0.134417	2.589334
66H	-1.974185	-2.656016	-2.443706
67H	-3.207237	-4.549517	-3.445192
68H	-5.013851	-5.683385	-2.164093
69H	-5.581487	-4.913162	0.133329
70H	-4.350204	-3.027158	1.150956

6ac-PhNCO-005

1C	2.002364	-1.871374	0.531118
2C	0.679929	-2.175312	0.325048
3N	0.217594	-2.596966	-0.880763
4C	1.095764	-2.769770	-1.905995
5C	2.431834	-2.506717	-1.756395
6C	2.946334	-1.993899	-0.530025
7N	4.269417	-1.668195	-0.533399
8S	5.012926	-0.951893	0.690796
9O	6.461882	-0.964267	0.441547
10O	4.534147	-1.263951	2.055924
11C	4.546399	0.874539	0.483465
12F	3.210024	1.034201	0.606774
13F	4.910616	1.341170	-0.722795
14F	5.144323	1.626060	1.426371
15C	-1.269534	-2.766320	-1.150097
16O	-1.575092	-2.650016	-2.354427
17N	-1.927964	-2.952345	-0.038358
18C	-3.321549	-3.039753	-0.000072
19C	-4.208258	-2.982134	-1.103217
20C	-5.591530	-3.048193	-0.906671
21C	-6.136233	-3.174226	0.375400
22C	-5.269478	-3.243707	1.474655
23C	-3.889972	-3.178805	1.288235
24H	2.300779	-1.515869	1.506746
25H	-0.070281	-2.073049	1.097139
26H	0.661476	-3.105373	-2.838787
27H	3.104944	-2.651435	-2.594357
28H	-3.806980	-2.888965	-2.104208
29H	-6.249997	-3.003310	-1.772176
30H	-7.213071	-3.225922	0.516320
31H	-5.671166	-3.351668	2.480149
32H	-3.214562	-3.234144	2.138004
33P	-1.769574	1.479749	-0.328928
34C	-3.045219	0.484068	-1.146208
35C	-2.464166	3.115662	0.030399
36C	-1.233995	0.701305	1.214725

37C	-0.346058	1.665776	-1.432750
38C	-2.421928	3.652393	1.325447
39C	-2.966336	4.916814	1.567382
40C	-3.550473	5.641036	0.524809
41C	-3.592181	5.104948	-0.767947
42C	-3.050858	3.844519	-1.019010
43C	0.065349	0.940504	1.692864
44C	0.476716	0.373682	2.898869
45C	-0.402096	-0.434116	3.627777
46C	-1.695327	-0.672341	3.151967
47C	-2.117752	-0.106503	1.947928
48C	0.415563	2.845807	-1.403609
49C	1.565159	2.946313	-2.189154
50C	1.953039	1.878641	-3.004356
51C	1.187307	0.709233	-3.041674
52C	0.039762	0.594094	-2.255861
53H	-3.336636	0.993554	-2.069951
54H	-2.669809	-0.511734	-1.387728
55H	-3.918479	0.400463	-0.494385
56H	-1.969500	3.094071	2.139517
57H	-2.933426	5.331865	2.570901
58H	-3.973608	6.623463	0.717110
59H	-4.045320	5.667392	-1.579598
60H	-3.079632	3.436712	-2.026282
61H	0.761492	1.548130	1.123908
62H	1.487355	0.548803	3.256663
63H	-0.075420	-0.885623	4.560705
64H	-2.374344	-1.311328	3.708926
65H	-3.117667	-0.318375	1.584717
66H	0.118185	3.679164	-0.773513
67H	2.157997	3.856303	-2.160188
68H	2.853329	1.956174	-3.607820
69H	1.486741	-0.121012	-3.673913
70H	-0.536563	-0.325673	-2.288887

6ac-PhNCO-006

1C	-1.796090	-2.864340	-1.027000
2C	-0.505106	-3.022633	-0.600881
3N	-0.103298	-2.575136	0.621956
4C	-1.020414	-2.018804	1.454308
5C	-2.324882	-1.814269	1.079071
6C	-2.760268	-2.185999	-0.225709
7N	-3.967121	-1.961794	-0.817457
8S	-5.132376	-1.083950	-0.155779
9O	-5.258608	-1.117850	1.317660
10O	-6.352605	-1.227838	-0.963319
11C	-4.588223	0.701556	-0.497967
12F	-3.423634	0.972418	0.132241
13F	-5.513999	1.572356	-0.059271
14F	-4.402264	0.909859	-1.814864
15C	1.356895	-2.576856	1.045055
16O	1.557087	-2.093315	2.179343
17N	2.122316	-3.031872	0.092521
18C	3.514223	-3.061708	0.204557
19C	4.276250	-2.831235	1.376037
20C	5.672822	-2.888237	1.337565
21C	6.354141	-3.167954	0.148356
22C	5.612136	-3.404798	-1.016523
23C	4.219320	-3.354774	-0.986434
24H	-2.078064	-3.207457	-2.016129
25H	0.271633	-3.470477	-1.204230
26H	-0.643122	-1.729162	2.424375
27H	-2.998598	-1.345876	1.783329
28H	3.768902	-2.614232	2.307321
29H	6.233343	-2.711760	2.253850
30H	7.440555	-3.208327	0.129751
31H	6.121327	-3.631709	-1.951039
32H	3.641400	-3.544031	-1.888191
33P	1.726118	1.567066	0.238563
34C	3.104925	0.663303	0.990095
35C	1.016406	0.618625	-1.130007
36C	0.455564	1.909030	1.480606
37C	2.357100	3.143904	-0.400423
38C	-0.358388	0.706795	-1.406887
39C	-0.883922	0.051889	-2.520969
40C	-0.045371	-0.692193	-3.356237
41C	1.319151	-0.795505	-3.070916
42C	1.855881	-0.142428	-1.960131
43C	-0.363344	3.043987	1.348819
44C	-1.391121	3.265038	2.266643
45C	-1.599980	2.364199	3.316465
46C	-0.778208	1.241514	3.452008
47C	0.248907	1.005604	2.535844
48C	2.223677	3.486995	-1.753418
49C	2.728977	4.707597	-2.210285

50C	3.362567	5.581485	-1.323049
51C	3.493986	5.239340	0.028453
52C	2.992962	4.023644	0.493109
53H	3.893994	0.522240	0.246510
54H	3.499516	1.258648	1.819206
55H	2.768354	-0.306773	1.364117
56H	-1.020058	1.271093	-0.757667
57H	-1.949153	0.109793	-2.724081
58H	-0.460263	-1.206848	-4.218851
59H	1.968672	-1.392138	-3.705210
60H	2.916729	-0.234646	-1.749621
61H	-0.201814	3.750097	0.539074
62H	-2.028311	4.138527	2.160170
63H	-2.403423	2.537159	4.027462
64H	-0.938490	0.541319	4.267333
65H	0.864147	0.116666	2.638629
66H	1.732125	2.812725	-2.448287
67H	2.624850	4.972120	-3.259029
68H	3.753418	6.529971	-1.681889
69H	3.984287	5.919206	0.719766
70H	3.089651	3.766383	1.544850

6ac-PhNCO-007

1C	3.256358	1.446643	0.227533
2C	2.019726	2.038988	0.285396
3N	1.082167	1.668715	1.197674
4C	1.382110	0.689796	2.093773
5C	2.594309	0.051613	2.081334
6C	3.595152	0.391089	1.125340
7N	4.740377	-0.343755	1.184788
8S	5.975279	-0.162222	0.179433
9O	7.130229	-0.903633	0.707051
10O	6.202124	1.189171	-0.376913
11C	5.467233	-1.175758	-1.339990
12F	4.345618	-0.665690	-1.896369
13F	5.218673	-2.456012	-1.010998
14F	6.439942	-1.157638	-2.267653
15C	-0.300100	2.295860	1.233730
16O	-1.013645	1.900245	2.180523
17N	-0.485341	3.097965	0.223245
18C	-1.684700	3.792636	0.047710
19C	-2.634166	4.087266	1.055115
20C	-3.792732	4.807492	0.751990
21C	-4.049425	5.248706	-0.551116
22C	-3.112351	4.973243	-1.555278
23C	-1.948308	4.264343	-1.258307
24H	3.958325	1.791439	-0.519174
25H	1.712142	2.823219	-0.392482
26H	0.598443	0.453876	2.800383
27H	2.794576	-0.733127	2.802845
28H	-2.458450	3.747978	2.068690
29H	-4.503534	5.024785	1.547174
30H	-4.955283	5.805748	-0.777854
31H	-3.285886	5.317432	-2.572857
32H	-1.214456	4.060806	-2.034568
33P	-2.869863	-0.881973	0.060570
34C	-3.629898	0.691381	0.535128
35C	-2.535910	-1.868672	1.543202
36C	-4.006794	-1.787837	-1.022981
37C	-1.319676	-0.574848	-0.819442
38C	-2.801405	-3.246987	1.557853
39C	-2.498944	-3.996872	2.697001
40C	-1.933971	-3.376953	3.815629
41C	-1.669600	-2.002978	3.798499
42C	-1.966810	-1.242683	2.666334
43C	-3.524260	-2.480703	-2.143895
44C	-4.411145	-3.198882	-2.949684
45C	-5.773901	-3.228219	-2.640228
46C	-6.255513	-2.538877	-1.521595
47C	-5.376958	-1.819605	-0.710432
48C	-0.165975	-1.313028	-0.511156
49C	1.010574	-1.088196	-1.227875
50C	1.038176	-0.133156	-2.247795
51C	-0.110241	0.604393	-2.552329
52C	-1.290299	0.388956	-1.841344
53H	-2.915779	1.265187	1.132418
54H	-3.894217	1.253521	-0.364667
55H	-4.531397	0.498278	1.124207
56H	-3.242315	-3.735172	0.693750
57H	-2.706401	-5.063434	2.708160
58H	-1.700264	-3.963067	4.700617
59H	-1.229999	-1.519580	4.666932
60H	-1.743475	-0.178845	2.656269
61H	-2.467395	-2.459199	-2.392638
62H	-4.035162	-3.731915	-3.818680

63H	-6.461795	-3.785285	-3.270788
64H	-7.314718	-2.559715	-1.280390
65H	-5.761507	-1.293017	0.158808
66H	-0.177452	-2.050089	0.286137
67H	1.906720	-1.648775	-0.979752
68H	1.959259	0.047240	-2.794407
69H	-0.084439	1.359910	-3.332491
70H	-2.173578	0.975396	-2.077917

6ac-PhNCO-008

1C	1.875499	-1.889204	0.582641
2C	0.561161	-2.228596	0.384494
3N	0.124110	-2.779483	-0.779378
4C	1.021847	-3.033774	-1.769624
5C	2.350548	-2.728066	-1.628859
6C	2.841101	-2.105422	-0.444387
7N	4.164994	-1.784434	-0.447012
8S	4.888897	-0.974031	0.729629
9O	6.344604	-1.047933	0.537120
10O	4.354824	-1.135996	2.100362
11C	4.478393	0.831263	0.326257
12F	3.140025	1.014251	0.320532
13F	4.953275	1.186095	-0.879611
14F	5.007906	1.656587	1.248898
15C	-1.357366	-3.035989	-1.045886
16O	-1.615964	-3.325902	-2.227118
17N	-2.057688	-2.866475	0.045161
18C	-3.452051	-2.929652	0.055376
19C	-4.302930	-2.954454	-1.076416
20C	-5.692580	-2.942675	-0.921074
21C	-6.279490	-2.913193	0.348469
22C	-5.448761	-2.896629	1.477062
23C	-4.062424	-2.900680	1.331453
24H	2.152670	-1.441702	1.526090
25H	-0.204288	-2.064618	1.130021
26H	0.606689	-3.473821	-2.667100
27H	3.038077	-2.938229	-2.440975
28H	-3.868628	-2.986812	-2.067754
29H	-6.322804	-2.961724	-1.808306
30H	-7.361201	-2.909900	0.457892
31H	-5.883662	-2.880484	2.474366
32H	-3.415853	-2.882728	2.205386
33P	-1.638222	1.513521	-0.294794
34C	-2.893014	0.426372	-1.020526
35C	-0.220731	1.633502	-1.416758
36C	-2.352436	3.162403	-0.059958
37C	-1.091892	0.841549	1.293821
38C	0.538881	2.813732	-1.468629
39C	1.674686	2.869335	-2.278429
40C	2.052822	1.755843	-3.034608
41C	1.291636	0.583755	-2.989042
42C	0.156077	0.516633	-2.181108
43C	-2.321049	3.792255	1.192539
44C	-2.884563	5.062681	1.341273
45C	-3.477305	5.699936	0.248032
46C	-3.508426	5.070398	-1.002228
47C	-2.947297	3.803554	-1.160896
48C	0.195737	1.147489	1.764190
49C	0.629605	0.630530	2.984655
50C	-0.217503	-0.190434	3.736703
51C	-1.500977	-0.491796	3.269849
52C	-1.944724	0.021236	2.049756
53H	-2.522163	-0.599611	-1.044448
54H	-3.804438	0.467417	-0.418589
55H	-3.116508	0.765422	-2.036072
56H	0.249084	3.682382	-0.884046
57H	2.265164	3.780618	-2.313597
58H	2.943178	1.799095	-3.655881
59H	1.584591	-0.282791	-3.573990
60H	-0.423723	-0.400103	-2.151300
61H	-1.864797	3.300087	2.046084
62H	-2.859686	5.550208	2.311907
63H	-3.915700	6.687190	0.367628
64H	-3.968687	5.565442	-1.852866
65H	-2.968302	3.323863	-2.136226
66H	0.865369	1.767460	1.176633
67H	1.633326	0.853011	3.335606
68H	0.127581	-0.604031	4.680503
69H	-2.154222	-1.141668	3.845192
70H	-2.933394	-0.244728	1.690176

6ac-PhNCO-009

1C	-3.188553	1.578413	-0.250916
2C	-1.951451	2.170044	-0.313537
3N	-1.007728	1.781208	-1.212399
4C	-1.303662	0.786319	-2.092342
5C	-2.520981	0.158615	-2.082719
6C	-3.526491	0.514296	-1.138737
7N	-4.671842	-0.221444	-1.192404
8S	-5.937096	0.019455	-0.238905
9O	-7.082620	-0.734063	-0.770516
10O	-6.164008	1.399485	0.241171
11C	-5.503617	-0.926191	1.346370
12F	-4.363482	-0.446765	1.890281
13F	-5.322901	-2.236118	1.093701
14F	-6.485607	-0.804471	2.255747
15C	0.371775	2.416939	-1.261201
16O	1.140842	1.899173	-2.098859
17N	0.483184	3.372503	-0.381620
18C	1.650555	4.126473	-0.242321
19C	2.745302	4.159115	-1.139190
20C	3.858934	4.961133	-0.872250
21C	3.923208	5.749416	0.281707
22C	2.839709	5.736973	1.170282
23C	1.723139	4.944787	0.908542
24H	-3.892959	1.935828	0.487639
25H	-1.650141	2.972063	0.346347
26H	-0.512815	0.531911	-2.784720
27H	-2.718839	-0.637650	-2.791347
28H	2.718262	3.550267	-2.033978
29H	4.687512	4.965722	-1.578080
30H	4.796049	6.365792	0.482617
31H	2.864581	6.347999	2.070229
32H	0.882135	4.933968	1.597910
33P	2.632306	-1.535096	-0.492256
34C	2.866025	-0.847160	-2.152498
35C	3.307626	-0.399175	0.743728
36C	0.864713	-1.799030	-0.197016
37C	3.485301	-3.132831	-0.374474
38C	3.842784	-0.906031	1.940091
39C	4.333135	-0.024655	2.904757
40C	4.295121	1.355375	2.677744
41C	3.761605	1.858593	1.487718
42C	3.261383	0.986676	0.518445
43C	0.169844	-2.707122	-1.016386
44C	-1.185167	-2.943678	-0.791546
45C	-1.851490	-2.277105	0.242895
46C	-1.163549	-1.369324	1.050962
47C	0.196151	-1.127636	0.837182
48C	2.956754	-4.163833	0.419132
49C	3.650875	-5.369149	0.543787
50C	4.868389	-5.550077	-0.119230
51C	5.395668	-4.524046	-0.910588
52C	4.710197	-3.314967	-1.038791
53H	3.920532	-0.606822	-2.315741
54H	2.535076	-1.585458	-2.889226
55H	2.261944	0.062249	-2.245471
56H	3.883314	-1.976347	2.119896
57H	4.748507	-0.417145	3.828957
58H	4.681369	2.039660	3.428658
59H	3.726336	2.928360	1.308910
60H	2.834349	1.394039	-0.392854
61H	0.682638	-3.233711	-1.817398
62H	-1.723628	-3.642590	-1.425542
63H	-2.908670	-2.457819	0.407123
64H	-1.684312	-0.841340	1.844045
65H	0.722981	-0.417837	1.468092
66H	2.009027	-4.034825	0.933211
67H	3.237220	-6.165014	1.157025
68H	5.404561	-6.490377	-0.021968
69H	6.339920	-4.663654	-1.429760
70H	5.133534	-2.525501	-1.652810

6ac-PhNCO-010

1C	-2.335183	-0.702493	1.867586
2C	-1.047947	-1.156494	1.950817
3N	-0.547411	-2.062620	1.064155
4C	-1.364905	-2.561450	0.096687
5C	-2.662431	-2.142626	-0.044095
6C	-3.201781	-1.144692	0.825050
7N	-4.421691	-0.568657	0.758817
8S	-5.425971	-0.831283	-0.469170
9O	-6.324041	-1.992647	-0.308221
10O	-4.849188	-0.604677	-1.813901
11C	-6.523815	0.666989	-0.169466
12F	-7.491758	0.682645	-1.103770
13F	-5.822603	1.810559	-0.272154

14F	-7.101840	0.625785	1.040333
15C	0.909902	-2.461726	1.176155
16O	1.523705	-1.894108	2.105761
17N	1.250107	-3.299206	0.235998
18C	2.535961	-3.839398	0.157874
19C	3.486970	-3.886871	1.204832
20C	4.733959	-4.486896	1.005696
21C	5.078548	-5.045380	-0.230241
22C	4.143205	-5.009662	-1.272841
23C	2.893155	-4.423921	-1.078521
24H	-2.692352	0.033401	2.579433
25H	-0.351933	-0.819653	2.706778
26H	-0.908283	-3.293796	-0.554988
27H	-3.254192	-2.569693	-0.845266
28H	3.243744	-3.451297	2.165992
29H	5.445872	-4.512600	1.828646
30H	6.052829	-5.505327	-0.376643
31H	4.387697	-5.444042	-2.240052
32H	2.164523	-4.402117	-1.885582
33P	2.207574	1.844125	0.490440
34C	2.273303	1.280471	2.210717
35C	3.380995	0.890748	-0.506273
36C	0.524574	1.635096	-0.145447
37C	2.640996	3.604408	0.406654
38C	3.953586	1.475620	-1.648858
39C	4.832621	0.733402	-2.438271
40C	5.143538	-0.585740	-2.090420
41C	4.572780	-1.167097	-0.954853
42C	3.688055	-0.435747	-0.159142
43C	-0.508199	2.427480	0.387684
44C	-1.809875	2.278457	-0.089206
45C	-2.087274	1.343341	-1.092448
46C	-1.061489	0.553577	-1.617079
47C	0.247025	0.695013	-1.148896
48C	2.086660	4.417896	-0.595811
49C	2.463801	5.758994	-0.689335
50C	3.389800	6.292334	0.212454
51C	3.943779	5.483127	1.209764
52C	3.575679	4.140048	1.308713
53H	3.295043	1.353583	2.593895
54H	1.606743	1.905140	2.813248
55H	1.944776	0.236096	2.256292
56H	3.722704	2.501409	-1.920715
57H	5.276031	1.187144	-3.320549
58H	5.829401	-1.162246	-2.705775
59H	4.804148	-2.192806	-0.687218
60H	3.238291	-0.910689	0.708159
61H	-0.299150	3.161032	1.162311
62H	-2.610321	2.883249	0.327788
63H	-3.103581	1.209132	-1.449444
64H	-1.281041	-0.183026	-2.384020
65H	1.037907	0.073436	-1.558000
66H	1.360558	4.013799	-1.295139
67H	2.030474	6.385037	-1.464477
68H	3.678035	7.337696	0.139983
69H	4.662586	5.895470	1.912504
70H	4.020418	3.523425	2.084498

6ac-PhNCO-011

1C	1.585494	-3.391125	-0.702282
2C	0.246583	-3.684552	-0.675704
3N	-0.638436	-2.922061	0.022028
4C	-0.176680	-1.871339	0.747963
5C	1.147850	-1.520337	0.759894
6C	2.094859	-2.248758	-0.019846
7N	3.407058	-1.954105	-0.189199
8S	4.034498	-0.594638	0.387274
9O	4.212982	-0.525643	1.853165
10O	3.544501	0.640669	-0.272095
11C	5.765478	-0.840031	-0.304748
12F	6.521371	0.212845	0.061388
13F	5.751593	-0.900734	-1.646325
14F	6.334638	-1.955726	0.173649
15C	-2.131266	-3.227421	-0.091118
16O	-2.394643	-4.189210	-0.833423
17N	-2.827956	-2.374393	0.612622
18C	-4.221900	-2.380638	0.630788
19C	-5.077974	-3.264966	-0.071459
20C	-6.467200	-3.139056	0.029408
21C	-7.050634	-2.144178	0.820799
22C	-6.215941	-1.263583	1.522370
23C	-4.830605	-1.380805	1.427519
24H	2.260079	-4.009357	-1.284816
25H	-0.188944	-4.513767	-1.217863
26H	-0.933590	-1.329281	1.294309

27H	1.443599	-0.664496	1.354965
28H	-4.646792	-4.043996	-0.687305
29H	-7.100209	-3.833664	-0.519934
30H	-8.132136	-2.057392	0.892569
31H	-6.647484	-0.483834	2.147012
32H	-4.182486	-0.699330	1.974521
33P	0.028229	2.478150	-0.493014
34C	1.565853	3.165380	-1.162903
35C	0.266759	1.975565	1.229557
36C	-1.255836	3.757766	-0.580055
37C	-0.484393	1.053633	-1.486803
38C	-0.804438	1.361040	1.902099
39C	-0.636979	0.916711	3.212019
40C	0.596703	1.080846	3.853901
41C	1.659859	1.694361	3.186819
42C	1.500298	2.146638	1.874297
43C	-1.833029	4.063715	-1.824898
44C	-2.768945	5.093968	-1.919894
45C	-3.129096	5.822493	-0.780619
46C	-2.552531	5.521177	0.456391
47C	-1.615460	4.490267	0.561664
48C	-1.840212	0.691205	-1.555817
49C	-2.216113	-0.450844	-2.263344
50C	-1.248048	-1.228623	-2.905228
51C	0.101010	-0.868906	-2.835526
52C	0.490317	0.265530	-2.122211
53H	2.387899	2.452124	-1.066005
54H	1.401270	3.402922	-2.218216
55H	1.808900	4.085398	-0.623332
56H	-1.756727	1.211411	1.401154
57H	-1.462209	0.429429	3.723736
58H	0.730329	0.719856	4.870146
59H	2.622273	1.806600	3.676988
60H	2.343171	2.595540	1.361654
61H	-1.565699	3.497187	-2.713108
62H	-3.219226	5.323867	-2.881625
63H	-3.861107	6.622171	-0.857626
64H	-2.832054	6.084227	1.342665
65H	-1.175556	4.259715	1.527195
66H	-2.601930	1.286562	-1.061753
67H	-3.262527	-0.737983	-2.302352
68H	-1.544867	-2.123697	-3.444710
69H	0.857183	-1.480224	-3.319001
70H	1.544933	0.511064	-2.046369

6ac-PhNCO-012

1C	-1.292741	-3.047646	1.210467
2C	0.068105	-3.193884	1.277276
3N	0.865039	-2.961617	0.198268
4C	0.290793	-2.668531	-0.998373
5C	-1.063157	-2.502932	-1.130420
6C	-1.918948	-2.609856	0.007629
7N	-3.241957	-2.327536	0.056183
8S	-3.964757	-1.563738	-1.158331
9O	-4.459961	-2.419947	-2.255266
10O	-3.328325	-0.281173	-1.548188
11C	-5.509255	-1.053943	-0.215661
12F	-6.327609	-0.400231	-1.059893
13F	-5.207247	-0.226166	0.800610
14F	-6.164034	-2.115991	0.274772
15C	2.377234	-2.941487	0.392717
16O	2.761729	-3.440651	1.463157
17N	2.954057	-2.355966	-0.626137
18C	4.333105	-2.145290	-0.685592
19C	5.263234	-2.331874	0.365509
20C	6.611937	-2.008713	0.185705
21C	7.080530	-1.503262	-1.031775
22C	6.172007	-1.325032	-2.083832
23C	4.825242	-1.637768	-1.911140
24H	-1.893578	-3.203453	2.099149
25H	0.590981	-3.462117	2.186144
26H	0.980892	-2.553673	-1.822715
27H	-1.458073	-2.263267	-2.110910
28H	4.920466	-2.721723	1.315728
29H	7.304300	-2.156866	1.012291
30H	8.131827	-1.257604	-1.161048
31H	6.514135	-0.935851	-3.040637
32H	4.117873	-1.486953	-2.723512
33P	0.350293	1.881591	-0.172802
34C	0.074892	0.848357	-1.635198
35C	-0.544724	3.447260	-0.367820
36C	-0.283153	1.030074	1.293919
37C	2.119516	2.212022	0.021889
38C	-1.201378	4.028104	0.728836
39C	-1.854565	5.253215	0.577274

40C	-1.855925	5.899839	-0.661917
41C	-1.200203	5.323065	-1.754946
42C	-0.542398	4.100812	-1.612234
43C	0.528384	0.835666	2.422301
44C	-0.009132	0.231756	3.561712
45C	-1.347994	-0.169176	3.577442
46C	-2.152351	0.017103	2.448263
47C	-1.625575	0.612922	1.303065
48C	2.560714	3.492242	0.394604
49C	3.923936	3.722729	0.590334
50C	4.843322	2.682995	0.418064
51C	4.403485	1.407643	0.048464
52C	3.042917	1.165946	-0.150391
53H	0.398366	1.382646	-2.532825
54H	0.659865	-0.067404	-1.532119
55H	-0.988241	0.598728	-1.707464
56H	-1.210730	3.530461	1.693831
57H	-2.364741	5.697549	1.427454
58H	-2.370080	6.850271	-0.777999
59H	-1.201377	5.822327	-2.719913
60H	-0.032862	3.668728	-2.468544
61H	1.568207	1.147679	2.417608
62H	0.620782	0.074397	4.432942
63H	-1.763194	-0.638747	4.465430
64H	-3.185137	-0.315936	2.448155
65H	-2.255385	0.738191	0.426842
66H	1.851574	4.303574	0.528925
67H	4.264648	4.714325	0.875884
68H	5.903867	2.865588	0.570818
69H	5.113099	0.597202	-0.085776
70H	2.719611	0.165267	-0.424661

6ah-001

1C	1.205754	2.085910	-0.707857
2C	0.725402	3.367052	-0.965451
3N	0.022166	4.115041	-0.096558
4C	-0.196987	3.556031	1.109276
5C	0.236651	2.287420	1.473684
6C	0.951775	1.490450	0.549525
7N	1.297208	0.219038	0.986816
8S	1.905495	-0.907715	0.062291
9O	1.830067	-2.204604	0.762712
10O	1.517127	-0.885456	-1.371804
11C	3.774331	-0.595371	-0.009392
12F	4.308686	-0.582773	1.226293
13F	4.394871	-1.555502	-0.723842
14F	4.041630	0.594292	-0.589325
15H	1.745800	1.555719	-1.482147
16H	0.915477	3.819464	-1.937697
17H	-0.754890	4.160647	1.823047
18H	0.024444	1.894580	2.464016
19P	-2.676070	-0.748050	-0.141625
20C	-1.951611	-0.625579	1.525437
21C	-2.576125	-1.580360	2.550136
22C	-4.435610	-0.256796	-0.081972
23C	-1.765631	0.358175	-1.267277
24C	-2.594648	-2.466141	-0.753033
25C	-2.386731	0.483865	-2.664173
26C	-1.176794	-3.055103	-0.760135
27C	-4.661599	1.187611	0.386129
28H	-2.073722	0.419126	1.833190
29H	-0.873559	-0.791395	1.424481
30H	-2.083524	-1.437677	3.518136
31H	-3.646998	-1.392703	2.688770
32H	-2.442065	-2.629141	2.263658
33H	-4.942245	-0.970782	0.578268
34H	-4.839573	-0.411170	-1.089182
35H	-0.743744	-0.030223	-1.327180
36H	-1.704668	1.332975	-0.772186
37H	-3.025049	-2.458310	-1.761843
38H	-3.268835	-3.057536	-0.121951
39H	-1.755465	1.138545	-3.274954
40H	-2.449841	-0.483945	-3.173528
41H	-3.389464	0.923796	-2.629392
42H	-1.215991	-4.082401	-1.139428
43H	-0.498379	-2.483228	-1.399422
44H	-0.738798	-3.082607	0.242129
45H	-5.734058	1.410749	0.374516
46H	-4.298748	1.344158	1.408047
47H	-4.161876	1.910345	-0.268147

6ah-002

1C	1.886127	1.777839	-0.964854
2C	1.954792	3.130909	-1.288013
3N	1.837805	4.140320	-0.407341
4C	1.654954	3.776044	0.876439
5C	1.572173	2.459289	1.311477
6C	1.677956	1.398590	0.381960
7N	1.536319	0.119818	0.906640
8S	1.490214	-1.201642	0.046419
9O	0.977227	-2.310258	0.879087
10O	0.953384	-1.101635	-1.334514
11C	3.294967	-1.705676	-0.241165
12F	3.937541	-1.890846	0.927062
13F	3.374019	-2.851262	-0.947853
14F	3.949114	-0.745211	-0.928851
15H	1.978341	1.036887	-1.749068
16H	2.111461	3.420160	-2.326393
17H	1.568152	4.588009	1.597018
18H	1.423884	2.232787	2.363662
19P	-2.930893	-0.133659	0.091790
20C	-2.362402	-1.837351	-0.226881
21C	-3.332342	-2.925909	0.250593
22C	-3.058417	0.157316	1.890788
23C	-1.728438	1.021673	-0.643655
24C	-4.589149	0.132593	-0.628238
25C	-2.034793	2.504165	-0.400473
26C	-4.666443	-0.110776	-2.141945
27C	-1.716852	0.090008	2.632977
28H	-1.387906	-1.940026	0.262192
29H	-2.177397	-1.913800	-1.304406
30H	-2.893631	-3.908493	0.046042
31H	-3.516276	-2.864630	1.328960
32H	-4.296030	-2.875412	-0.268509
33H	-3.762810	-0.588785	2.278185
34H	-3.531470	1.138704	2.016351
35H	-1.678664	0.791256	-1.713664
36H	-0.758368	0.748930	-0.223511
37H	-4.874656	1.162292	-0.381051
38H	-5.279269	-0.526266	-0.088042
39H	-1.243714	3.110705	-0.853558
40H	-2.988521	2.805787	-0.847739
41H	-2.061682	2.742857	0.668102
42H	-5.690481	0.069494	-2.486694
43H	-4.003901	0.562637	-2.696704
44H	-4.402798	-1.141926	-2.401083
45H	-1.887267	0.270661	3.700095
46H	-1.237068	-0.888308	2.529452
47H	-1.012565	0.845401	2.271839

6ah-003

1C	1.861613	1.769040	-0.949117
2C	1.911880	3.122203	-1.275355
3N	1.764438	4.131716	-0.399583
4C	1.567450	3.767634	0.882134
5C	1.500876	2.450849	1.319897
6C	1.639457	1.389540	0.395420
7N	1.511841	0.109413	0.921467
8S	1.515781	-1.214534	0.061777
9O	1.039134	-2.338054	0.895655
10O	0.981740	-1.134249	-1.321347
11C	3.337124	-1.660356	-0.221206
12F	3.985440	-1.813868	0.948417
13F	3.451875	-2.809489	-0.917167
14F	3.961038	-0.686753	-0.918421
15H	1.977257	1.028032	-1.730172
16H	2.078938	3.411222	-2.312182
17H	1.455427	4.579881	1.598898
18H	1.339988	2.224919	2.370271
19P	-2.937493	-0.149621	0.068214
20C	-4.545284	-0.009574	-0.792391
21C	-4.489348	-0.379062	-2.280877
22C	-1.713889	0.953778	-0.707960
23C	-3.188817	0.331320	1.811864
24C	-2.328117	-1.865114	-0.031018
25C	-1.890073	0.397031	2.628664
26C	-3.295547	-2.907086	0.545714
27C	-2.043738	2.447355	-0.600177
28H	-4.884073	1.024155	-0.655728
29H	-5.251763	-0.651188	-0.252372
30H	-5.486243	-0.267620	-2.721235
31H	-3.805474	0.273748	-2.834218
32H	-4.171604	-1.416601	-2.431857
33H	-1.617021	0.637898	-1.752371
34H	-0.759950	0.728296	-0.227880
35H	-3.890704	-0.394918	2.238966
36H	-3.700303	1.301323	1.801737

37H	-1.364481	-1.898638	0.488229
38H	-2.115649	-2.060552	-1.088075
39H	-2.128601	0.660371	3.665012
40H	-1.362558	-0.561689	2.638019
41H	-1.202378	1.153584	2.238328
42H	-2.844718	-3.901029	0.453523
43H	-3.495108	-2.731730	1.608743
44H	-4.252070	-2.923369	0.011194
45H	-1.250897	3.023039	-1.088882
46H	-2.992064	2.697309	-1.089236
47H	-2.093694	2.776591	0.442969

6ah-004

1C	-1.217559	1.888134	0.876242
2C	-0.679885	3.120329	1.237521
3N	-0.040619	3.957048	0.400481
4C	0.049632	3.544442	-0.878710
5C	-0.450131	2.336176	-1.348568
6C	-1.100863	1.445092	-0.462716
7N	-1.530808	0.246399	-1.013420
8S	-2.045195	-0.981162	-0.160418
9O	-2.080286	-2.188155	-1.009601
10O	-1.490106	-1.132831	1.209048
11C	-3.886615	-0.667852	0.168111
12F	-4.561718	-0.514573	-0.986678
13F	-4.439474	-1.696224	0.842088
14F	-4.060838	0.452122	0.902799
15H	-1.698398	1.277627	1.629879
16H	-0.764032	3.453070	2.271134
17H	0.557273	4.220752	-1.565036
18H	-0.338019	2.062265	-2.393953
19P	2.841705	-0.632159	0.015402
20C	1.443033	-1.510003	-0.750524
21C	1.847827	-2.628066	-1.718274
22C	3.927981	0.075746	-1.271935
23C	2.176135	0.697803	1.069518
24C	3.834581	-1.798913	1.011242
25C	3.237799	1.524480	1.805448
26C	3.064115	-2.425550	2.181961
27C	3.203989	1.020294	-2.241275
28H	0.829804	-0.755674	-1.254104
29H	0.834077	-1.900271	0.072140
30H	0.940577	-3.097531	-2.112683
31H	2.421210	-2.243036	-2.568560
32H	2.440399	-3.406495	-1.224236
33H	4.379659	-0.769093	-1.805396
34H	4.740481	0.592719	-0.747967
35H	1.482689	0.221536	1.771057
36H	1.569271	1.333413	0.417341
37H	4.716100	-1.251830	1.366463
38H	4.193273	-2.568758	0.317595
39H	2.736937	2.276276	2.424704
40H	3.858586	0.906152	2.463321
41H	3.894517	2.056158	1.107749
42H	3.720373	-3.119823	2.718036
43H	2.724050	-1.667092	2.895354
44H	2.189243	-2.988336	1.839414
45H	3.920165	1.406533	-2.974878
46H	2.407094	0.505064	-2.788329
47H	2.763364	1.876511	-1.720530

6ah-005

1C	-1.880523	1.801941	0.926280
2C	-1.956023	3.159638	1.227587
3N	-1.865210	4.154776	0.327852
4C	-1.703635	3.769855	-0.952790
5C	-1.616172	2.446612	-1.366670
6C	-1.694203	1.401178	-0.417491
7N	-1.547587	0.114479	-0.922368
8S	-1.477391	-1.190386	-0.037354
9O	-0.980741	-2.315292	-0.856080
10O	-0.907229	-1.058720	1.327906
11C	-3.273800	-1.691767	0.306088
12F	-3.946466	-1.895550	-0.842052
13F	-3.331596	-2.827184	1.031181
14F	-3.912351	-0.722760	0.996469
15H	-1.949779	1.074274	1.725050
16H	-2.095184	3.465075	2.263844
17H	-1.638111	4.569974	-1.688702
18H	-1.485996	2.204050	-2.417710
19P	2.915677	-0.128082	-0.100694
20C	4.596086	0.291958	0.482814

21C	4.747718	0.281028	2.009777
22C	1.711546	1.073297	0.553302
23C	2.925157	-0.066692	-1.926167
24C	2.447421	-1.796189	0.471545
25C	1.613942	-0.534820	-2.573625
26C	3.405646	-2.901925	0.010764
27C	2.024719	2.535951	0.216605
28H	4.831391	1.280021	0.069120
29H	5.282898	-0.421812	0.012951
30H	5.776236	0.549125	2.275270
31H	4.079041	1.003599	2.490432
32H	4.541375	-0.709690	2.429077
33H	1.656348	0.915481	1.635980
34H	0.742634	0.777522	0.147283
35H	3.773696	-0.675164	-2.261108
36H	3.151144	0.971923	-2.196766
37H	1.429341	-1.979877	0.111716
38H	2.388953	-1.749553	1.565036
39H	1.685138	-0.406647	-3.659594
40H	1.415308	-1.591607	-2.371341
41H	0.747696	0.032975	-2.220853
42H	3.038435	-3.868406	0.372361
43H	3.465911	-2.958553	-1.081852
44H	4.417346	-2.758680	0.406584
45H	1.228356	3.172129	0.616722
46H	2.972358	2.863941	0.658051
47H	2.068353	2.703657	-0.864967

6ah-006

1C	2.268383	1.588453	-0.921103
2C	2.515940	2.902771	-1.308155
3N	2.285504	3.986312	-0.545797
4C	1.791145	3.740945	0.682566
5C	1.508161	2.471884	1.172497
6C	1.732312	1.335052	0.362234
7N	1.378597	0.112703	0.921465
8S	1.394649	-1.261041	0.143841
9O	0.674373	-2.277461	0.937598
10O	1.107362	-1.221793	-1.313569
11C	3.182442	-1.891020	0.200888
12F	3.608050	-2.015281	1.472283
13F	3.288602	-3.095182	-0.395781
14F	4.012619	-1.036758	-0.434279
15H	2.470797	0.781880	-1.614588
16H	2.922804	3.095887	-2.299822
17H	1.609194	4.613765	1.307991
18H	1.108464	2.343816	2.174624
19P	-2.961329	0.041307	-0.104204
20C	-2.029457	0.275252	1.443482
21C	-2.395680	1.551486	2.211786
22C	-2.748950	1.481254	-1.206317
23C	-2.357331	-1.471653	-0.924136
24C	-4.743341	-0.123189	0.267242
25C	-3.133485	-1.860860	-2.189340
26C	-5.085866	-1.356185	1.114496
27C	-1.282492	1.799836	-1.527558
28H	-0.963522	0.264250	1.188274
29H	-2.209354	-0.619558	2.051111
30H	-1.798049	1.599617	3.128427
31H	-2.179207	2.452479	1.627290
32H	-3.452562	1.571654	2.501168
33H	-3.241992	2.331060	-0.719489
34H	-3.319156	1.260728	-2.116750
35H	-2.398733	-2.269775	-0.174093
36H	-1.297454	-1.311867	-1.149279
37H	-5.270805	-0.144731	-0.693746
38H	-5.043338	0.800173	0.777285
39H	-2.703788	-2.780610	-2.601106
40H	-4.192829	-2.050115	-1.982606
41H	-3.064745	-1.089586	-2.964371
42H	-6.163813	-1.377266	1.308878
43H	-4.818904	-2.286916	0.602405
44H	-4.572195	-1.338799	2.081857
45H	-1.236849	2.628210	-2.242697
46H	-0.731569	2.100834	-0.632632
47H	-0.763555	0.943695	-1.969920

6ah-007

1C	1.910739	1.765566	-0.955409
2C	2.032010	3.116325	-1.272853
3N	1.999465	4.123087	-0.382233
4C	1.851463	3.757355	0.905707

5C	1.721813	2.442775	1.335423
6C	1.738546	1.385610	0.396287
7N	1.554385	0.110447	0.918256
8S	1.446808	-1.203807	0.052352
9O	0.926149	-2.305094	0.888147
10O	0.872667	-1.076818	-1.312198
11C	3.227562	-1.755357	-0.293749
12F	3.901003	-1.961517	0.853454
13F	3.251753	-2.901170	-1.004317
14F	3.887311	-0.812642	-1.000353
15H	1.936405	1.028047	-1.747749
16H	2.160271	3.405845	-2.315083
17H	1.833141	4.566694	1.634188
18H	1.603691	2.215657	2.391332
19P	-2.936130	-0.080315	0.094593
20C	-4.611641	0.353865	-0.495593
21C	-4.765121	0.334214	-2.022193
22C	-1.713270	1.106549	-0.552495
23C	-2.961520	-0.030698	1.919897
24C	-2.484817	-1.751174	-0.483823
25C	-1.648558	-0.475695	2.580199
26C	-3.466066	-2.845699	-0.045596
27C	-1.899843	2.549879	-0.069621
28H	-4.841286	1.345371	-0.087909
29H	-5.303205	-0.352685	-0.021543
30H	-5.795501	0.596008	-2.286882
31H	-4.101601	1.058274	-2.507439
32H	-4.554817	-0.657395	-2.437462
33H	-1.758234	1.040647	-1.645512
34H	-0.734614	0.720045	-0.262751
35H	-3.799602	-0.661300	2.240209
36H	-3.214973	0.999970	2.196555
37H	-1.475184	-1.952438	-0.110169
38H	-2.408414	-1.697171	-1.575819
39H	-1.746830	-0.384528	3.667771
40H	-1.408392	-1.517914	2.349384
41H	-0.795537	0.132423	2.265053
42H	-3.108625	-3.814691	-0.410283
43H	-3.541874	-2.910323	1.045592
44H	-4.470160	-2.683888	-0.453394
45H	-1.123181	3.178200	-0.517752
46H	-2.873901	2.959521	-0.360598
47H	-1.800409	2.628706	1.017836

6ah-008

1C	-1.169377	2.543409	1.273181
2C	-1.217681	3.857209	0.823931
3N	-1.488555	4.215051	-0.446051
4C	-1.732630	3.202154	-1.295904
5C	-1.708560	1.851527	-0.956531
6C	-1.409253	1.477598	0.374618
7N	-1.290015	0.200154	0.907854
8S	-1.548634	-1.134537	0.107619
9O	-1.246093	-1.136303	-1.347108
10O	-1.041868	-2.277495	0.895093
11C	-3.424428	-1.405524	0.135336
12F	-3.759219	-2.551540	-0.490617
13F	-3.885736	-1.469622	1.398399
14F	-4.056127	-0.388472	-0.488585
15H	-0.950366	2.323769	2.314034
16H	-1.029733	4.672296	1.521356
17H	-1.961113	3.486091	-2.322351
18H	-1.907898	1.107359	-1.717437
19P	2.842042	-0.331176	-0.104276
20C	4.434605	0.544845	0.097136
21C	5.451105	-0.193561	0.978695
22C	1.693519	0.733769	-1.036972
23C	3.138823	-1.887228	-1.014287
24C	2.135372	-0.717626	1.534108
25C	1.872679	-2.719640	-1.266169
26C	1.988253	0.502058	2.452762
27C	2.225406	1.197928	-2.399010
28H	4.199528	1.532855	0.511487
29H	4.834908	0.705676	-0.910546
30H	5.074130	-0.343223	1.996085
31H	5.715285	-1.171769	0.562288
32H	6.370400	0.398532	1.047055
33H	1.461032	1.588157	-0.392183
34H	0.768006	0.164158	-1.159365
35H	3.871417	-2.453964	-0.427072
36H	3.627096	-1.612272	-1.956995
37H	2.786439	-1.477203	1.984299
38H	1.161779	-1.188358	1.358736
39H	2.144096	-3.626448	-1.818101
40H	1.391015	-3.023118	-0.331890

41H	1.129972	-2.172451	-1.854094
42H	1.361611	1.276541	2.000385
43H	1.501780	0.190539	3.383114
44H	2.959049	0.941762	2.707884
45H	1.461775	1.815060	-2.884682
46H	3.133403	1.803188	-2.302583
47H	2.440328	0.352181	-3.061821

6ah-009

1C	-2.060812	1.700555	0.997706
2C	-2.319602	3.029304	1.325894
3N	-2.372407	4.044069	0.445428
4C	-2.163222	3.709900	-0.842585
5C	-1.899255	2.419072	-1.282837
6C	-1.834964	1.353713	-0.354898
7N	-1.533968	0.105119	-0.887114
8S	-1.374498	-1.214630	-0.039049
9O	-0.759660	-2.265407	-0.877684
10O	-0.854435	-1.082071	1.346043
11C	-3.126972	-1.883367	0.237001
12F	-3.755156	-2.094218	-0.934748
13F	-3.097826	-3.050365	0.912037
14F	-3.863042	-1.006086	0.952303
15H	-2.028429	0.954340	1.781777
16H	-2.494130	3.293425	2.368141
17H	-2.210279	4.525555	-1.562690
18H	-1.742394	2.216391	-2.338689
19P	2.975054	-0.013122	-0.109280
20C	2.500241	-1.670747	0.486984
21C	3.512159	-2.770679	0.140623
22C	3.045090	-0.004784	-1.934247
23C	1.748962	1.200688	0.481403
24C	4.637677	0.420640	0.514610
25C	1.994491	2.634610	-0.004959
26C	4.749439	0.431156	2.044750
27C	1.692511	-0.271263	-2.610466
28H	1.518161	-1.892196	0.056543
29H	2.354612	-1.588453	1.569807
30H	3.132987	-3.731587	0.504782
31H	3.659664	-2.861979	-0.941234
32H	4.487120	-2.596092	0.609269
33H	3.787903	-0.759501	-2.219859
34H	3.451329	0.969612	-2.230251
35H	1.749354	1.143408	1.575802
36H	0.772342	0.837008	0.151575
37H	4.885513	1.402364	0.094247
38H	5.336286	-0.299889	0.073280
39H	1.229925	3.292566	0.420692
40H	2.974271	3.013968	0.307175
41H	1.924667	2.708840	-1.095525
42H	5.773298	0.694421	2.332251
43H	4.075793	1.167644	2.496070
44H	4.522949	-0.550249	2.475407
45H	1.832648	-0.295849	-3.696854
46H	1.256127	-1.225763	-2.301241
47H	0.963592	0.511684	-2.381743

6ah-010

1C	-1.352464	1.886899	1.030846
2C	-1.151841	3.240272	1.293561
3N	-0.787631	4.157952	0.380792
4C	-0.631566	3.699441	-0.875820
5C	-0.807504	2.374174	-1.252267
6C	-1.171582	1.404396	-0.287819
7N	-1.248824	0.097417	-0.746786
8S	-1.791055	-1.131208	0.081907
9O	-1.350527	-2.388345	-0.557991
10O	-1.713579	-1.070160	1.563036
11C	-3.659312	-1.127360	-0.230948
12F	-3.934801	-1.237317	-1.544809
13F	-4.263692	-2.148804	0.408680
14F	-4.203985	0.025584	0.213465
15H	-1.638722	1.221007	1.835265
16H	-1.288873	3.607937	2.309677
17H	-0.345933	4.438604	-1.622898
18H	-0.668115	2.071428	-2.286499
19P	2.833792	-0.405241	0.036248
20C	2.034102	-0.370600	-1.601609
21C	2.970193	0.014985	-2.753438
22C	3.609033	1.205821	0.410099
23C	1.570989	-0.789419	1.291429
24C	4.148161	-1.675562	0.060141

25C	2.120293	-0.949587	2.713952
26C	3.634134	-3.107356	-0.143092
27C	2.639114	2.392777	0.334945
28H	1.185752	0.315493	-1.523320
29H	1.601764	-1.365989	-1.754290
30H	2.405699	-0.000005	-3.692184
31H	3.379267	1.023809	-2.627552
32H	3.806344	-0.685942	-2.857008
33H	4.443933	1.330382	-0.289715
34H	4.042994	1.112709	1.412909
35H	1.063204	-1.700169	0.958865
36H	0.831963	0.016093	1.247283
37H	4.668134	-1.575744	1.020227
38H	4.865691	-1.398884	-0.721259
39H	1.288010	-1.171164	3.390588
40H	2.838646	-1.773490	2.786110
41H	2.605852	-0.034278	3.070444
42H	4.479021	-3.804348	-0.118631
43H	2.934113	-3.402257	0.646006
44H	3.130639	-3.226387	-1.108674
45H	3.167668	3.313336	0.605030
46H	2.235654	2.521135	-0.673599
47H	1.797142	2.276672	1.024696

6ah-011

1C	-0.781609	1.506897	1.040364
2C	-0.011742	2.533144	1.581306
3N	0.431674	3.604803	0.901353
4C	0.065928	3.663818	-0.394264
5C	-0.697914	2.697871	-1.036728
6C	-1.142651	1.556165	-0.327911
7N	-1.863768	0.628045	-1.063941
8S	-2.310509	-0.784929	-0.517676
9O	-2.759891	-1.631782	-1.638562
10O	-1.440568	-1.423565	0.505505
11C	-3.920471	-0.497000	0.443190
12F	-4.864986	0.046410	-0.346890
13F	-4.402200	-1.656253	0.935434
14F	-3.716275	0.342226	1.482377
15H	-1.082654	0.680375	1.671338
16H	0.269295	2.486290	2.632833
17H	0.411175	4.534344	-0.949909
18H	-0.952280	2.803886	-2.087628
19P	2.870850	-0.716730	-0.110049
20C	4.608708	-1.005100	0.379087
21C	5.030835	-0.263031	1.654533
22C	2.624155	1.048608	-0.492334
23C	2.527815	-1.736524	-1.583349
24C	1.748841	-1.175327	1.249774
25C	1.083831	-1.627081	-2.091868
26C	1.811212	-2.656239	1.646352
27C	3.475827	1.568903	-1.657075
28H	5.228526	-0.705987	-0.474536
29H	4.731047	-2.088268	0.496214
30H	6.090341	-0.457664	1.854013
31H	4.902786	0.820753	1.557899
32H	4.460634	-0.600901	2.526512
33H	2.832685	1.603780	0.428775
34H	1.558082	1.176761	-0.701757
35H	2.770568	-2.770548	-1.310961
36H	3.248218	-1.430566	-2.351327
37H	0.736592	-0.912819	0.926849
38H	1.998737	-0.523937	2.095818
39H	0.961324	-2.263301	-2.974991
40H	0.365135	-1.959872	-1.338131
41H	0.825225	-0.603119	-2.380772
42H	1.109689	-2.834239	2.468300
43H	1.515651	-3.307776	0.816828
44H	2.809915	-2.955246	1.985258
45H	3.265392	2.633563	-1.804896
46H	4.548798	1.464372	-1.460404
47H	3.243411	1.050702	-2.593969

6ah-012

1C	-1.958055	1.682956	0.917282
2C	-2.112330	3.009210	1.314415
3N	-2.115075	4.066407	0.483791
4C	-1.967382	3.780472	-0.824304
5C	-1.806139	2.497084	-1.330849
6C	-1.788718	1.386609	-0.455478
7N	-1.588844	0.148409	-1.052968
8S	-1.404927	-1.204267	-0.263319

9O	-0.881180	-2.240401	-1.176896
10O	-0.792328	-1.130905	1.089150
11C	-3.151313	-1.839962	0.112214
12F	-3.861229	-2.000955	-1.020204
13F	-3.107439	-3.027098	0.750652
14F	-3.817006	-0.967812	0.899499
15H	-1.958884	0.900650	1.666064
16H	-2.239366	3.234447	2.372526
17H	-1.976324	4.631060	-1.504227
18H	-1.689607	2.335353	-2.398929
19P	2.928954	-0.044646	0.052100
20C	3.888782	0.185515	1.590194
21C	3.074097	-0.082628	2.863432
22C	1.530169	1.118308	0.021176
23C	4.039096	0.275330	-1.363958
24C	2.287643	-1.748419	-0.031566
25C	3.347733	0.157745	-2.729748
26C	3.371206	-2.832354	0.029593
27C	1.938814	2.594747	0.079841
28H	4.271077	1.212918	1.576226
29H	4.756456	-0.481839	1.527105
30H	3.707987	0.078128	3.742268
31H	2.213320	0.590120	2.943708
32H	2.704040	-1.112785	2.899852
33H	0.880901	0.847473	0.859813
34H	0.961564	0.900537	-0.888775
35H	4.869433	-0.435864	-1.279862
36H	4.459835	1.277487	-1.218420
37H	1.701319	-1.821274	-0.953806
38H	1.568629	-1.851236	0.787323
39H	4.077510	0.349277	-3.524061
40H	2.931864	-0.842710	-2.890583
41H	2.536063	0.885188	-2.838337
42H	2.895239	-3.815866	-0.047005
43H	4.089341	-2.745571	-0.793897
44H	3.925494	-2.802652	0.974371
45H	1.036633	3.215018	0.062197
46H	2.488033	2.830352	0.998105
47H	2.558916	2.881584	-0.776828

6ah-013

1C	1.742432	1.755136	-0.934945
2C	1.724267	3.096172	-1.310050
3N	1.698487	4.134386	-0.456044
4C	1.705310	3.813326	0.852134
5C	1.724642	2.512234	1.338169
6C	1.735110	1.420162	0.439593
7N	1.725107	0.157957	1.019702
8S	1.563790	-1.190444	0.219702
9O	1.287369	-2.297609	1.156135
10O	0.746214	-1.146808	-1.022319
11C	3.285116	-1.639414	-0.437222
12F	4.174613	-1.735172	0.568775
13F	3.260765	-2.820608	-1.087695
14F	3.732337	-0.700228	-1.298477
15H	1.750225	0.989309	-1.700484
16H	1.727288	3.350445	-2.369212
17H	1.691688	4.648853	1.550468
18H	1.728358	2.321543	2.407792
19P	-2.946673	-0.156421	0.082973
20C	-4.661409	0.276239	-0.379616
21C	-4.919634	0.292749	-1.892619
22C	-1.783201	1.053797	-0.625419
23C	-2.848420	-0.141982	1.905266
24C	-2.525387	-1.811561	-0.558003
25C	-1.456393	-0.478386	2.454406
26C	-3.440088	-2.931099	-0.045038
27C	-1.897823	2.465814	-0.038745
28H	-4.867850	1.257283	0.064443
29H	-5.316170	-0.444418	0.124380
30H	-5.968142	0.548903	-2.080154
31H	-4.297922	1.037600	-2.401418
32H	-4.727781	-0.684675	-2.348964
33H	-1.960088	1.056919	-1.708064
34H	-0.782316	0.640432	-0.480187
35H	-3.602763	-0.852357	2.264490
36H	-3.171953	0.856476	2.224644
37H	-1.478608	-1.991715	-0.291539
38H	-2.556856	-1.742387	-1.651873
39H	-1.481552	-0.443701	3.549391
40H	-1.127067	-1.479094	2.159007
41H	-0.696429	0.229736	2.113174
42H	-3.117379	-3.884456	-0.477166
43H	-3.389894	-3.028343	1.044922
44H	-4.485856	-2.770720	-0.330608

45H	-1.163707	3.115517	-0.525559
46H	-2.891739	2.899463	-0.199155
47H	-1.684421	2.476691	1.034821

6ah-014

1C	1.756139	1.755735	-0.937756
2C	1.750160	3.097788	-1.309563
3N	1.723558	4.133985	-0.453102
4C	1.716753	3.809593	0.854226
5C	1.722640	2.507166	1.337098
6C	1.733337	1.417403	0.435791
7N	1.705677	0.153730	1.012302
8S	1.546975	-1.191610	0.206535
9O	1.246574	-2.298685	1.135862
10O	0.750194	-1.139635	-1.048345
11C	3.275195	-1.651692	-0.424093
12F	4.148093	-1.758009	0.595313
13F	3.251966	-2.830336	-1.079233
14F	3.742709	-0.712913	-1.274993
15H	1.765746	0.991633	-1.704972
16H	1.764407	3.354675	-2.368003
17H	1.702766	4.643440	1.554558
18H	1.715444	2.313854	2.406225
19P	-2.940285	-0.151208	0.084956
20C	-4.650952	0.275965	-0.398474
21C	-4.890076	0.290288	-1.914661
22C	-1.773123	1.058970	-0.617158
23C	-2.858066	-0.127976	1.908052
24C	-2.509975	-1.809261	-0.542741
25C	-1.469044	-0.457471	2.469959
26C	-3.433180	-2.925626	-0.038408
27C	-1.903433	2.475324	-0.044520
28H	-4.866081	1.256616	0.042382
29H	-5.309394	-0.446680	0.097808
30H	-5.937618	0.540298	-2.115499
31H	-4.266451	1.038543	-2.416016
32H	-4.686759	-0.686325	-2.367753
33H	-1.933648	1.051878	-1.702238
34H	-0.772397	0.652720	-0.454593
35H	-3.612563	-0.839712	2.264229
36H	-3.187579	0.870520	2.220947
37H	-1.467867	-1.989505	-0.259338
38H	-2.524534	-1.745071	-1.637132
39H	-1.505374	-0.426274	3.564728
40H	-1.130164	-1.454751	2.173776
41H	-0.710481	0.256552	2.137921
42H	-3.100591	-3.882155	-0.455809
43H	-3.404533	-3.013654	1.053160
44H	-4.473209	-2.769490	-0.346325
45H	-1.166405	3.124806	-0.527390
46H	-2.897491	2.901759	-0.222106
47H	-1.704505	2.496853	1.031716

6ah-015

1C	2.104393	1.742508	-0.934308
2C	2.344475	3.087524	-1.205503
3N	2.279876	4.079448	-0.300080
4C	1.967643	3.703724	0.955059
5C	1.710615	2.393359	1.338169
6C	1.768797	1.351987	0.383058
7N	1.462013	0.080424	0.855063
8S	1.404579	-1.214478	-0.045700
9O	0.770718	-2.311718	0.715179
10O	0.976712	-1.048739	-1.457968
11C	3.194321	-1.814981	-0.219377
12F	3.744869	-2.051216	0.986236
13F	3.256460	-2.954452	-0.937613
14F	3.946709	-0.885019	-0.845367
15H	2.169559	1.017259	-1.735763
16H	2.603280	3.385144	-2.220779
17H	1.920654	4.500730	1.695781
18H	1.468218	2.157773	2.370739
19P	-2.964848	-0.032916	0.104877
20C	-2.495665	-1.716373	-0.414069
21C	-3.499895	-2.799041	0.002583
22C	-3.034064	0.064634	1.927894
23C	-1.732619	1.149937	-0.534192
24C	-4.622116	0.389642	-0.540169
25C	-2.062745	2.619647	-0.245834
26C	-4.721110	0.353862	-2.070866
27C	-1.757972	-0.424403	2.628528
28H	-1.507069	-1.913595	0.015177

29H	-2.364462	-1.690480	-1.501671
30H	-3.121588	-3.777567	-0.312098
31H	-3.636979	-2.830756	1.089378
32H	-4.479645	-2.652368	-0.465529
33H	-3.908834	-0.515369	2.245362
34H	-3.241906	1.113752	2.170902
35H	-1.640009	0.965568	-1.610332
36H	-0.776770	0.869440	-0.084653
37H	-4.864974	1.385456	-0.150567
38H	-5.328013	-0.312737	-0.081414
39H	-1.264550	3.250739	-0.650012
40H	-3.003666	2.928332	-0.714712
41H	-2.128310	2.817298	0.829667
42H	-5.737996	0.623415	-2.376598
43H	-4.031383	1.064507	-2.539169
44H	-4.506150	-0.644322	-2.467532
45H	-1.855111	-0.260554	3.707545
46H	-1.589308	-1.492935	2.463489
47H	-0.864894	0.105232	2.283121

6ah-016

1C	1.961586	1.714728	-0.883804
2C	2.101406	3.052584	-1.245655
3N	2.061968	4.089622	-0.390739
4C	1.885101	3.770106	0.905921
5C	1.735193	2.472213	1.377957
6C	1.762157	1.382990	0.476540
7N	1.570478	0.127383	1.039233
8S	1.415253	-1.205983	0.211145
9O	0.897503	-2.273912	1.091474
10O	0.814133	-1.104161	-1.144375
11C	3.173658	-1.809044	-0.161220
12F	3.870651	-1.995798	0.975187
13F	3.152182	-2.976760	-0.835565
14F	3.839084	-0.906191	-0.913284
15H	1.995980	0.950392	-1.650142
16H	2.252246	3.305127	-2.294417
17H	1.859729	4.604246	1.605574
18H	1.593664	2.282715	2.438447
19P	-2.922370	-0.061813	-0.034582
20C	-4.002340	0.181590	-1.487891
21C	-3.273667	0.027972	-2.830252
22C	-1.535978	1.116526	-0.083807
23C	-3.922686	0.227307	1.467874
24C	-2.258610	-1.758541	-0.023634
25C	-3.148719	0.001941	2.774063
26C	-3.331406	-2.852610	0.047558
27C	-1.957604	2.585673	-0.207321
28H	-4.443470	1.180558	-1.389903
29H	-4.822390	-0.540562	-1.397785
30H	-3.983283	0.185955	-3.649747
31H	-2.466186	0.759966	-2.940183
32H	-2.843792	-0.972702	-2.947223
33H	-0.891151	0.812249	-0.914189
34H	-0.957261	0.947042	0.829773
35H	-4.793033	-0.436352	1.404811
36H	-4.297633	1.255702	1.403263
37H	-1.568393	-1.824457	0.823878
38H	-1.639075	-1.857939	-0.920895
39H	-3.805706	0.207835	3.626148
40H	-2.795741	-1.030825	2.863982
41H	-2.280530	0.665149	2.853226
42H	-2.841146	-3.832025	0.040801
43H	-3.924229	-2.784614	0.966521
44H	-4.014933	-2.816222	-0.808381
45H	-1.061086	3.214415	-0.204064
46H	-2.497461	2.779495	-1.140742
47H	-2.589639	2.901463	0.630382

6ah-017

1C	-3.710331	0.587761	-0.019616
2C	-4.599613	1.605371	-0.356941
3N	-4.311000	2.918616	-0.337706
4C	-3.060160	3.235223	0.046332
5C	-2.093080	2.304043	0.403183
6C	-2.394603	0.922946	0.374286
7N	-1.353592	0.069053	0.723070
8S	-1.467368	-1.503442	0.782843
9O	-0.243192	-2.052822	1.404519
10O	-2.764546	-2.093860	1.184120
11C	-1.284124	-2.102633	-1.010842
12F	-0.109489	-1.687673	-1.538871

13F	-1.312790	-3.448082	-1.081850
14F	-2.273700	-1.621520	-1.791705
15H	-4.039462	-0.443227	-0.058970
16H	-5.611629	1.344291	-0.662965
17H	-2.819821	4.297334	0.067714
18H	-1.101249	2.630329	0.701667
19P	2.838501	0.602492	0.082166
20C	1.393501	1.205133	-0.848435
21C	1.351328	2.728546	-1.025226
22C	2.833568	1.293063	1.773410
23C	2.774147	-1.217929	0.140488
24C	4.381807	1.156126	-0.726848
25C	3.928833	-1.863696	0.917687
26C	4.502519	0.737488	-2.198411
27C	1.688550	0.781633	2.658654
28H	0.508270	0.837978	-0.314075
29H	1.411558	0.698020	-1.820088
30H	0.456197	2.998967	-1.594771
31H	1.300572	3.249238	-0.062495
32H	2.223278	3.103459	-1.573303
33H	2.789857	2.383187	1.657710
34H	3.810502	1.059372	2.213072
35H	2.754936	-1.565669	-0.898828
36H	1.805629	-1.479036	0.581886
37H	5.210146	0.752222	-0.132733
38H	4.419915	2.247146	-0.624198
39H	3.791424	-2.950406	0.923505
40H	4.902950	-1.652350	0.462281
41H	3.953816	-1.528928	1.960607
42H	5.462629	1.081629	-2.598177
43H	4.462896	-0.351101	-2.316450
44H	3.708072	1.178045	-2.810514
45H	1.728910	1.292432	3.627223
46H	0.706493	0.966323	2.213107
47H	1.768277	-0.294761	2.839668

6ah-018

1C	3.731295	0.558031	0.010906
2C	4.636440	1.559265	0.355082
3N	4.360898	2.875377	0.370388
4C	3.106572	3.212571	0.016308
5C	2.124143	2.299008	-0.343977
6C	2.412269	0.914823	-0.352108
7N	1.357345	0.079770	-0.704976
8S	1.452521	-1.492475	-0.795902
9O	0.218878	-2.016432	-1.420808
10O	2.739835	-2.091462	-1.215742
11C	1.272050	-2.119826	0.988191
12F	0.110590	-1.690452	1.533526
13F	1.274101	-3.466702	1.035431
14F	2.277915	-1.672525	1.768246
15H	4.050947	-0.476647	0.021237
16H	5.651001	1.281609	0.637173
17H	2.876497	4.277146	0.022828
18H	1.130500	2.641104	-0.617479
19P	-2.835713	0.636111	-0.075062
20C	-1.398938	1.233135	0.872880
21C	-1.338703	2.757394	1.038858
22C	-2.820220	1.339028	-1.761227
23C	-2.769484	-1.182973	-0.142403
24C	-4.387773	1.171111	0.728893
25C	-3.930889	-1.822549	-0.914683
26C	-4.596736	0.582287	2.130955
27C	-1.662569	0.842608	-2.638715
28H	-0.510193	0.851942	0.354190
29H	-1.437288	0.733839	1.847982
30H	-0.446886	3.019673	1.617318
31H	-1.269035	3.269759	0.072819
32H	-2.211716	3.149085	1.573378
33H	-2.788838	2.428971	-1.640005
34H	-3.790373	1.097150	-2.211115
35H	-2.747421	-1.531145	0.896942
36H	-1.803886	-1.445566	-0.588527
37H	-5.206962	0.886535	0.058125
38H	-4.367765	2.266977	0.759643
39H	-3.803786	-2.910486	-0.916037
40H	-4.902135	-1.599098	-0.458845
41H	-3.954184	-1.491678	-1.958896
42H	-5.530583	0.968153	2.554091
43H	-4.668832	-0.510445	2.102699
44H	-3.783451	0.853994	2.812919
45H	-1.702797	1.353621	-3.607174
46H	-0.685800	1.038855	-2.186660
47H	-1.727240	-0.234667	-2.820323

6ah-019

1C	-3.564311	0.886304	0.460617
2C	-4.478354	1.910958	0.226764
3N	-4.167714	3.124135	-0.263011
4C	-2.865303	3.324756	-0.538012
5C	-1.870121	2.374459	-0.346437
6C	-2.196797	1.099331	0.170240
7N	-1.131890	0.217298	0.326155
8S	-1.270264	-1.254295	0.881876
9O	0.076631	-1.803214	1.149236
10O	-2.325386	-1.527142	1.885353
11C	-1.828598	-2.303892	-0.598583
12F	-0.949373	-2.201824	-1.619655
13F	-1.924153	-3.606761	-0.266485
14F	-3.033097	-1.898084	-1.051957
15H	-3.912009	-0.054928	0.867695
16H	-5.530742	1.742964	0.451042
17H	-2.605195	4.304480	-0.936690
18H	-0.838867	2.603845	-0.596791
19P	2.907739	0.466900	-0.087919
20C	1.862158	-0.514003	-1.211888
21C	2.469724	-0.734790	-2.602609
22C	3.287863	2.088641	-0.841854
23C	2.050964	0.709184	1.501581
24C	4.498711	-0.390903	0.189949
25C	2.802058	1.616714	2.483470
26C	4.354426	-1.810497	0.756765
27C	2.047853	2.952870	-1.107044
28H	0.895603	-0.002937	-1.263203
29H	1.669088	-1.460833	-0.699357
30H	1.781164	-1.343219	-3.199376
31H	2.627579	0.208006	-3.138358
32H	3.425867	-1.268407	-2.555327
33H	3.833847	1.887811	-1.771235
34H	3.985181	2.595669	-0.164564
35H	1.884981	-0.289269	1.916486
36H	1.053611	1.094690	1.265114
37H	5.084526	0.245417	0.864099
38H	5.023756	-0.402800	-0.772304
39H	2.223605	1.693827	3.410748
40H	3.789680	1.217671	2.741804
41H	2.932935	2.630865	2.089591
42H	5.349223	-2.248625	0.894219
43H	3.850139	-1.814408	1.729366
44H	3.791993	-2.462964	0.080180
45H	2.355708	3.907450	-1.547830
46H	1.359167	2.468115	-1.807008
47H	1.502537	3.170847	-0.183135

6ah-020

1C	-3.692716	0.644037	0.258284
2C	-4.631494	1.633592	-0.024793
3N	-4.340163	2.919552	-0.288022
4C	-3.032153	3.237069	-0.268217
5C	-2.012718	2.332304	0.000130
6C	-2.320118	0.980734	0.277234
7N	-1.231215	0.152175	0.531995
8S	-1.328325	-1.397484	0.807354
9O	-0.006210	-1.883411	1.263062
10O	-2.523843	-1.917611	1.508302
11C	-1.468303	-2.208843	-0.903624
12F	-0.418902	-1.867891	-1.686091
13F	-1.491252	-3.552773	-0.810193
14F	-2.594127	-1.812621	-1.531553
15H	-4.027369	-0.364756	0.466586
16H	-5.688535	1.371925	-0.039287
17H	-2.787960	4.276800	-0.481622
18H	-0.976489	2.655866	-0.004352
19P	2.703596	0.386449	0.082340
20C	1.536519	0.946528	-1.208724
21C	1.595908	2.440045	-1.558981
22C	2.935882	-1.411977	-0.129246
23C	4.308785	1.236916	-0.117924
24C	2.078801	0.707357	1.767669
25C	5.019166	0.927413	-1.442469
26C	1.732829	2.168192	2.084299
27C	3.887025	-2.056273	0.887581
28H	0.542073	0.660951	-0.844967
29H	1.747624	0.336944	-2.095560
30H	0.849580	2.651122	-2.332734
31H	1.369965	3.078007	-0.699595
32H	2.575882	2.731485	-1.952333

33H	3.294883	-1.557537	-1.154826
34H	1.936520	-1.854031	-0.060172
35H	4.928956	0.948995	0.739040
36H	4.112323	2.310601	-0.019975
37H	2.855637	0.336146	2.447422
38H	1.201980	0.062791	1.886425
39H	5.950709	1.501397	-1.499980
40H	5.275519	-0.134431	-1.525580
41H	4.405508	1.199106	-2.308401
42H	1.446263	2.242658	3.139173
43H	2.579980	2.843556	1.918937
44H	0.883480	2.516196	1.489676
45H	3.978607	-3.125278	0.666040
46H	3.506494	-1.962927	1.910055
47H	4.891750	-1.619492	0.847763

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1C	2.293990	1.882038	-1.214836
2C	1.643891	3.092841	-1.463598
3N	1.038363	3.819961	-0.513414
4C	1.077888	3.350573	0.742908
5C	1.709521	2.159734	1.104761
6C	2.321867	1.410367	0.098855
7N	3.002405	0.184280	0.428275
8S	2.092880	-1.148261	0.797988
9O	0.838527	-0.714637	1.411926
10O	2.949326	-2.165448	1.399256
11C	1.582071	-1.886502	-0.871349
12F	2.674475	-2.171143	-1.592021
13F	0.831604	-1.004818	-1.553001
14F	0.874235	-3.004925	-0.678434
15C	4.384615	-0.008931	-0.073078
16H	2.758440	1.329645	-2.024928
17H	1.603121	3.489293	-2.475444
18H	0.585597	3.955971	1.500435
19H	1.724584	1.824614	2.135653
20H	4.407738	-0.146366	-1.158032
21H	4.952114	0.882744	0.201352
22H	4.826681	-0.875121	0.419738
23P	-2.907972	-0.027067	0.139081
24C	-2.120118	-1.668897	0.048588
25C	-3.049850	-2.828170	0.430408
26C	-3.346726	0.351590	1.870028
27C	-1.744331	1.232958	-0.486273
28C	-4.444067	-0.014728	-0.845286
29C	-2.299924	2.662401	-0.417727
30C	-4.243415	-0.357766	-2.327839
31C	-2.135669	0.495367	2.801492
32H	-1.249175	-1.623719	0.709136
33H	-1.742953	-1.788877	-0.972702
34H	-2.487410	-3.767233	0.387063
35H	-3.439793	-2.721513	1.448639
36H	-3.897643	-2.914493	-0.257485
37H	-4.011673	-0.452337	2.206578
38H	-3.941218	1.272430	1.848958
39H	-1.495024	0.954858	-1.516605
40H	-0.827762	1.131502	0.105320
41H	-4.881869	0.983268	-0.726500
42H	-5.128228	-0.723430	-0.364033
43H	-1.562991	3.358512	-0.828188
44H	-3.224673	2.768037	-0.995877
45H	-2.503657	2.966252	0.614985
46H	-5.209051	-0.317988	-2.843213
47H	-3.571801	0.353141	-2.821562
48H	-3.835107	-1.365755	-2.458930
49H	-2.486117	0.706389	3.817661
50H	-1.534898	-0.419098	2.835099
51H	-1.483211	1.319186	2.494136

6ah-Me2-002

1C	1.162769	-2.107115	0.901937
2C	-0.090536	-2.714281	0.998627
3N	-0.891999	-2.935248	-0.054054
4C	-0.440304	-2.564528	-1.262498
5C	0.799921	-1.961414	-1.473318
6C	1.610475	-1.719855	-0.362901
7N	2.906193	-1.120231	-0.540278
8S	2.990644	0.498961	-0.892298
9O	1.741084	0.909267	-1.528394
10O	4.300164	0.802650	-1.460645
11C	2.991696	1.365592	0.795495
12F	1.967004	0.913676	1.539133

13F	2.864584	2.685365	0.628853
14F	4.136860	1.108477	1.439394
15C	4.080245	-1.768847	0.090740
16H	1.761193	-1.936810	1.790390
17H	-0.470295	-3.023660	1.969044
18H	-1.099423	-2.760010	-2.105157
19H	1.124646	-1.685556	-2.470327
20H	4.078843	-1.647418	1.178447
21H	4.037850	-2.829964	-0.163028
22H	4.992603	-1.342876	-0.328156
23P	-3.196058	0.572843	0.142164
24C	-3.737813	-0.980375	-0.646131
25C	-5.205675	-1.339601	-0.373141
26C	-3.383379	0.454526	1.954399
27C	-1.448564	0.881839	-0.284018
28C	-4.237685	1.955957	-0.437975
29C	-0.900950	2.192633	0.296236
30C	-4.228638	2.147930	-1.959862
31C	-2.517775	-0.635519	2.599565
32H	-3.066758	-1.768503	-0.288683
33H	-3.554037	-0.865063	-1.720989
34H	-5.446720	-2.277426	-0.885021
35H	-5.395012	-1.487443	0.695920
36H	-5.893789	-0.571235	-0.742321
37H	-4.448752	0.278122	2.146164
38H	-3.145273	1.444253	2.361596
39H	-1.383318	0.877675	-1.377595
40H	-0.873316	0.019522	0.071493
41H	-3.882320	2.856563	0.075900
42H	-5.251599	1.758789	-0.070105
43H	0.124456	2.335452	-0.053169
44H	-1.485468	3.059339	-0.031601
45H	-0.890630	2.178813	1.391638
46H	-4.871016	2.995584	-2.221531
47H	-3.222663	2.363293	-2.336838
48H	-4.611775	1.264844	-2.482679
49H	-2.701661	-0.652390	3.679230
50H	-2.752507	-1.628193	2.201771
51H	-1.450803	-0.448006	2.443198

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1C	-1.185192	2.073469	1.024927
2C	-0.006825	2.820474	1.005634
3N	0.607395	3.212802	-0.121061
4C	0.031628	2.877958	-1.286508
5C	-1.148987	2.140077	-1.382125
6C	-1.757252	1.717734	-0.198843
7N	-2.972155	0.947535	-0.248203
8S	-2.878755	-0.639294	-0.724770
9O	-1.780580	-0.788870	-1.675665
10O	-4.225221	-1.136256	-0.988668
11C	-2.310083	-1.596628	0.810121
12F	-1.090594	-1.175027	1.189296
13F	-2.249684	-2.902782	0.533545
14F	-3.168922	-1.394284	1.818563
15C	-4.110148	1.373953	0.600968
16H	-1.629691	1.771013	1.967072
17H	0.470274	3.105210	1.940072
18H	0.535871	3.214937	-2.188858
19H	-1.576082	1.891257	-2.346767
20H	-3.910431	1.212232	1.664438
21H	-4.271194	2.437072	0.409907
22H	-5.003908	0.824044	0.305348
23P	2.986302	-0.459934	-0.035438
24C	3.654356	1.232311	-0.173550
25C	4.876347	1.499719	0.715842
26C	1.381653	-0.546053	-0.897875
27C	4.166366	-1.635350	-0.785415
28C	2.739367	-0.900517	1.719427
29C	3.671635	-3.088717	-0.804656
30C	1.893943	0.117108	2.496496
31C	1.471074	-0.244065	-2.398856
32H	2.835505	1.921219	0.062937
33H	3.898520	1.381538	-1.231898
34H	4.631400	1.406846	1.779230
35H	5.705511	0.820073	0.490135
36H	5.228563	2.522427	0.543910
37H	0.714373	0.159400	-0.392324
38H	0.980307	-1.549646	-0.720434
39H	5.102549	-1.544609	-0.222096
40H	4.366906	-1.274224	-1.800942
41H	3.736024	-1.008060	2.163783
42H	2.271750	-1.892088	1.731909
43H	4.432270	-3.724576	-1.269971
44H	3.491110	-3.469869	0.206466

45H	2.747843	-3.193018	-1.384524
46H	0.891909	0.221204	2.070683
47H	1.784894	-0.218856	3.533410
48H	2.367105	1.104104	2.510244
49H	0.472638	-0.327544	-2.837150
50H	1.839900	0.769470	-2.587587
51H	2.126864	-0.953182	-2.915765

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1C	-1.576980	1.832104	1.390726
2C	-0.657407	2.834200	1.706527
3N	-0.128398	3.668957	0.798863
4C	-0.525085	3.531808	-0.475159
5C	-1.438617	2.564334	-0.899445
6C	-1.963939	1.695936	0.056120
7N	-2.919109	0.692322	-0.344190
8S	-2.358258	-0.725805	-0.974814
9O	-1.044904	-0.487130	-1.570468
10O	-3.438408	-1.402409	-1.686793
11C	-2.011808	-1.846113	0.511128
12F	-1.057824	-1.298817	1.284499
13F	-1.592133	-3.045095	0.092587
14F	-3.125303	-1.994052	1.240652
15C	-4.287065	0.760423	0.219480
16H	-1.970909	1.177681	2.161490
17H	-0.327142	2.965197	2.734273
18H	-0.091225	4.223285	-1.193391
19H	-1.727386	2.482197	-1.941722
20H	-4.284892	0.564087	1.296000
21H	-4.670502	1.764505	0.024752
22H	-4.923696	0.035437	-0.288879
23P	2.872595	-0.355897	-0.021204
24C	4.520789	-0.250553	-0.798803
25C	5.204985	1.111601	-0.619051
26C	2.100181	-1.949162	-0.463377
27C	3.070321	-0.220939	1.788549
28C	1.828525	1.015208	-0.612336
29C	1.756386	-0.322010	2.572992
30C	1.730498	1.094040	-2.141055
31C	2.909206	-3.178449	-0.026794
32H	4.383809	-0.485227	-1.861154
33H	5.126570	-1.054876	-0.365169
34H	4.619354	1.920902	-1.067643
35H	5.370085	1.349000	0.437598
36H	6.182168	1.092334	-1.113300
37H	1.956379	-1.936281	-1.549684
38H	1.102311	-1.952103	-0.013292
39H	3.562942	0.742003	1.968939
40H	3.774850	-1.003820	2.092927
41H	2.251936	1.934806	-0.193077
42H	0.839327	0.881728	-0.163615
43H	1.963648	-0.192740	3.640836
44H	1.045306	0.454885	2.273940
45H	1.278242	-1.297625	2.440628
46H	1.281482	0.190489	-2.563156
47H	1.090466	1.938175	-2.414654
48H	2.711059	1.251181	-2.603684
49H	2.360168	-4.086221	-0.299239
50H	3.885219	-3.216701	-0.522871
51H	3.070060	-3.196505	1.056949

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1C	2.632184	1.727499	-1.174286
2C	2.099151	2.934112	-1.633975
3N	1.362834	3.757732	-0.873411
4C	1.144695	3.395086	0.399912
5C	1.637031	2.216781	0.963908
6C	2.391271	1.368425	0.152467
7N	2.941832	0.153135	0.697621
8S	1.935972	-1.140357	0.908354
9O	0.593400	-0.652104	1.222626
10O	2.610146	-2.149408	1.719310
11C	1.756431	-1.935410	-0.801942
12F	1.115053	-1.093848	-1.628415
13F	1.055641	-3.069819	-0.703954
14F	2.967221	-2.202105	-1.308639
15C	4.403554	-0.064644	0.583115
16H	3.209700	1.090367	-1.836170
17H	2.266468	3.245261	-2.662526
18H	0.551274	4.079259	1.001881
19H	1.445744	1.967107	2.001717
20H	4.716470	-0.177923	-0.459047

21H	4.894179	0.804787	1.026163
22H	4.680523	-0.954006	1.149731
23P	-3.018058	0.026201	0.062964
24C	-4.552279	0.078333	-0.928140
25C	-5.687618	-0.794576	-0.374049
26C	-1.725349	1.007635	-0.773408
27C	-3.355969	0.725006	1.716925
28C	-2.463057	-1.702014	0.248125
29C	-2.109314	0.889718	2.596721
30C	-2.225314	-2.428237	-1.082667
31C	-2.093206	2.488077	-0.950335
32H	-4.281877	-0.224505	-1.946773
33H	-4.856539	1.130280	-0.977175
34H	-5.416598	-1.855900	-0.363095
35H	-5.969063	-0.499718	0.642809
36H	-6.571877	-0.681824	-1.010273
37H	-1.545339	0.531064	-1.744281
38H	-0.812775	0.889268	-0.179395
39H	-4.086221	0.059036	2.191785
40H	-3.855844	1.687722	1.558295
41H	-3.231247	-2.211703	0.841683
42H	-1.550174	-1.673634	0.850994
43H	-2.410232	1.283778	3.573589
44H	-1.592737	-0.061129	2.759396
45H	-1.394821	1.592376	2.156345
46H	-1.447658	-1.940893	-1.678569
47H	-1.895583	-3.452477	-0.880160
48H	-3.139485	-2.484561	-1.684216
49H	-1.272465	3.008859	-1.452289
50H	-2.994088	2.611799	-1.561249
51H	-2.259959	2.983221	0.012614

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1C	1.283652	-1.825015	1.315293
2C	0.067184	-2.445063	1.606948
3N	-0.759285	-2.934662	0.670335
4C	-0.373103	-2.832307	-0.611120
5C	0.821088	-2.232820	-1.012753
6C	1.657380	-1.712073	-0.025193
7N	2.906032	-1.099484	-0.398009
8S	2.882451	0.445435	-0.991352
9O	1.581445	0.692833	-1.608595
10O	4.143769	0.720830	-1.672523
11C	2.917223	1.566810	0.537502
12F	1.889034	1.263923	1.348389
13F	2.819547	2.846955	0.165838
14F	4.062419	1.385821	1.208497
15C	4.153089	-1.630266	0.199830
16H	1.911037	-1.436602	2.110862
17H	-0.260812	-2.540495	2.639075
18H	-1.051203	-3.245786	-1.352778
19H	1.093378	-2.170654	-2.060850
20H	4.195630	-1.442353	1.276921
21H	4.171997	-2.705706	0.009658
22H	5.011594	-1.171066	-0.291405
23P	-3.182928	0.498890	0.021580
24C	-4.248063	1.661197	-0.902031
25C	-5.751291	1.393333	-0.743581
26C	-1.436233	0.825897	-0.399447
27C	-3.439623	0.746271	1.813049
28C	-3.621932	-1.217029	-0.409464
29C	-2.499135	-0.089165	2.694415
30C	-3.480806	-1.542076	-1.903447
31C	-0.978529	2.244069	-0.028979
32H	-3.944883	1.601405	-1.954361
33H	-3.991017	2.667374	-0.551888
34H	-6.034916	0.414176	-1.143622
35H	-6.065306	1.441895	0.304653
36H	-6.312870	2.155126	-1.294862
37H	-1.331299	0.652422	-1.475918
38H	-0.829562	0.064749	0.104400
39H	-4.489247	0.506378	2.020261
40H	-3.310762	1.817890	2.005189
41H	-4.653160	-1.369546	-0.068982
42H	-2.981527	-1.867189	0.196879
43H	-2.721047	0.110725	3.748354
44H	-2.625796	-1.162881	2.523025
45H	-1.448649	0.166067	2.520324
46H	-2.455282	-1.391735	-2.256351
47H	-3.742373	-2.592343	-2.070153
48H	-4.148369	-0.929657	-2.519412
49H	0.046228	2.389708	-0.377571
50H	-1.601896	3.008272	-0.505362
51H	-0.998525	2.408339	1.053872

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1C	-1.480928	1.924958	1.416044
2C	-0.369001	2.663621	1.826643
3N	0.513681	3.211446	0.977396
4C	0.293222	3.045017	-0.336066
5C	-0.786613	2.328107	-0.854343
6C	-1.682182	1.750134	0.046046
7N	-2.814621	1.011252	-0.448707
8S	-2.582814	-0.536260	-0.985370
9O	-1.205275	-0.672882	-1.455161
10O	-3.732874	-0.944488	-1.786398
11C	-2.669131	-1.632982	0.557878
12F	-1.708057	-1.275074	1.425567
13F	-2.491321	-2.912515	0.213224
14F	-3.861724	-1.494286	1.152545
15C	-4.168327	1.440806	-0.028662
16H	-2.159576	1.494723	2.145333
17H	-0.175602	2.811342	2.886456
18H	1.011256	3.507961	-1.008812
19H	-0.926333	2.217960	-1.923960
20H	-4.329661	1.277164	1.040955
21H	-4.257232	2.504845	-0.258998
22H	-4.915002	0.892653	-0.603941
23P	3.014612	-0.474079	-0.081347
24C	4.120162	-1.779593	0.558327
25C	3.515697	-3.189710	0.484118
26C	3.743049	1.162125	0.264117
27C	2.813143	-0.704091	-1.880488
28C	1.393788	-0.583551	0.748814
29C	1.936925	0.357017	-2.559325
30C	1.493948	-0.595631	2.280515
31C	5.122632	1.387228	-0.369921
32H	4.363962	-1.509607	1.592876
33H	5.049868	-1.718743	-0.018692
34H	2.603347	-3.270605	1.085289
35H	3.277357	-3.475913	-0.546146
36H	4.238855	-3.914161	0.873657
37H	3.791654	1.258418	1.355286
38H	3.019974	1.907050	-0.086238
39H	2.392067	-1.706455	-2.021536
40H	3.823731	-0.716335	-2.305222
41H	0.900427	-1.485930	0.373487
42H	0.803633	0.266206	0.396117
43H	1.901850	0.156303	-3.635722
44H	0.911343	0.330463	-2.182977
45H	2.339060	1.366836	-2.422161
46H	1.990283	0.302476	2.663082
47H	0.487939	-0.629809	2.709834
48H	2.040890	-1.473264	2.641209
49H	5.481710	2.387210	-0.104203
50H	5.858951	0.660912	-0.008299
51H	5.084477	1.325857	-1.463118

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1C	-2.746633	1.711901	1.168161
2C	-2.237629	2.942643	1.589188
3N	-1.489605	3.742242	0.814887
4C	-1.239881	3.329638	-0.437444
5C	-1.708365	2.125720	-0.964997
6C	-2.469861	1.298465	-0.136581
7N	-2.990734	0.052901	-0.639091
8S	-1.933875	-1.192360	-0.913830
9O	-0.654773	-0.645042	-1.364328
10O	-2.625421	-2.257330	-1.632779
11C	-1.547983	-1.931159	0.787666
12F	-0.908839	-1.027024	1.547021
13F	-0.766107	-3.005869	0.638518
14F	-2.683770	-2.288923	1.400182
15C	-4.419338	-0.263716	-0.395603
16H	-3.334268	1.100128	1.844511
17H	-2.434266	3.293142	2.599784
18H	-0.641068	3.995480	-1.054472
19H	-1.491220	1.839979	-1.987766
20H	-4.618257	-0.484898	0.656709
21H	-4.995927	0.609957	-0.706039
22H	-4.707101	-1.114753	-1.012848
23P	2.967291	0.093948	-0.070395
24C	4.506430	0.172973	0.910417
25C	5.641025	-0.703389	0.360393
26C	1.659262	1.051146	0.771635
27C	3.283818	0.805197	-1.723158
28C	2.434187	-1.643525	-0.241948

29C	2.026429	0.981009	-2.585221
30C	2.396224	-2.412334	1.086539
31C	2.004493	2.534719	0.963092
32H	4.244667	-0.117741	1.934932
33H	4.804880	1.227048	0.943173
34H	5.370919	-1.764959	0.361768
35H	5.917585	-0.418463	-0.660617
36H	6.528171	-0.582760	0.991161
37H	1.479103	0.561636	1.735844
38H	0.751254	0.925908	0.172008
39H	4.008009	0.143710	-2.213148
40H	3.786583	1.765797	-1.560790
41H	3.124386	-2.117762	-0.949301
42H	1.448748	-1.621217	-0.718075
43H	2.315379	1.387290	-3.560688
44H	1.506340	0.033411	-2.753225
45H	1.318400	1.679145	-2.127152
46H	1.735412	-1.937036	1.818594
47H	2.017346	-3.423532	0.906804
48H	3.393586	-2.504051	1.528651
49H	1.171681	3.040697	1.460542
50H	2.897713	2.666823	1.583320
51H	2.173881	3.039148	0.005474

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1C	2.738469	1.738352	-1.154973
2C	2.224402	2.969698	-1.568279
3N	1.466818	3.758102	-0.791733
4C	1.211130	3.332439	0.454963
5C	1.684191	2.127030	0.974978
6C	2.457059	1.312177	0.144713
7N	2.986874	0.068187	0.640948
8S	1.941018	-1.187182	0.911761
9O	0.655037	-0.652482	1.357588
10O	2.640141	-2.245581	1.633047
11C	1.568641	-1.929394	-0.791028
12F	0.927222	-1.029965	-1.553915
13F	0.792845	-3.008957	-0.644979
14F	2.709767	-2.279862	-1.397845
15C	4.418651	-0.235344	0.399260
16H	3.334296	1.136382	-1.832935
17H	2.425468	3.330527	-2.574357
18H	0.604052	3.988931	1.073993
19H	1.462529	1.831548	1.994001
20H	4.621461	-0.451561	-0.653348
21H	4.987237	0.642214	0.713554
22H	4.712600	-1.085873	1.014298
23P	-2.971276	0.069605	0.058492
24C	-4.516256	0.143599	-0.913529
25C	-5.686111	-0.631306	-0.290186
26C	-1.664496	1.015028	-0.798858
27C	-3.275988	0.798604	1.705460
28C	-2.433314	-1.665510	0.244447
29C	-2.014525	0.975431	2.561406
30C	-2.374226	-2.441536	-1.079036
31C	-2.005808	2.496382	-1.010642
32H	-4.277900	-0.237522	-1.913586
33H	-4.766399	1.204852	-1.026845
34H	-5.456761	-1.696402	-0.175055
35H	-5.961321	-0.230028	0.690982
36H	-6.562014	-0.546872	-0.942215
37H	-1.483010	0.511459	-1.755313
38H	-0.757285	0.896930	-0.196452
39H	-4.003207	0.147503	2.204642
40H	-3.773317	1.760927	1.535263
41H	-3.127703	-2.140389	0.947125
42H	-1.452903	-1.634062	0.730717
43H	-2.297469	1.396116	3.532508
44H	-1.501338	0.025964	2.739643
45H	-1.302875	1.662220	2.092187
46H	-1.706117	-1.966281	-1.804469
47H	-1.993002	-3.449903	-0.888852
48H	-3.365066	-2.540107	-1.534815
49H	-1.170404	2.993700	-1.512401
50H	-2.896834	2.622947	-1.634921
51H	-2.176557	3.013255	-0.060009

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1C	1.479501	-2.206742	0.931150
2C	0.379150	-3.044065	1.129473
3N	-0.494338	-3.365804	0.162340
4C	-0.274213	-2.859289	-1.060855

5C	0.794460	-2.016228	-1.369221
6C	1.682674	-1.681455	-0.346687
7N	2.819992	-0.847161	-0.635966
8S	2.595587	0.781079	-0.829504
9O	1.216545	1.020036	-1.253551
10O	3.741500	1.348717	-1.532606
11C	2.700044	1.514887	0.914537
12F	1.850714	0.866681	1.728962
13F	2.370767	2.810243	0.880954
14F	3.943656	1.383050	1.390735
15C	4.167026	-1.344268	-0.268527
16H	2.151397	-1.973382	1.750463
17H	0.188447	-3.467154	2.112931
18H	-0.978401	-3.147336	-1.837504
19H	0.935897	-1.637575	-2.375333
20H	4.317169	-1.348309	0.815437
21H	4.253356	-2.360688	-0.657986
22H	4.923158	-0.719457	-0.745358
23P	-3.043658	0.453771	0.034442
24C	-3.440432	2.219690	-0.198757
25C	-4.743644	2.477379	-0.968126
26C	-1.440872	0.307204	0.892909
27C	-4.344966	-0.346097	1.037795
28C	-2.947982	-0.395435	-1.575749
29C	-3.991468	-1.779408	1.462421
30C	-1.937954	0.221710	-2.551896
31C	-1.467360	0.849265	2.328457
32H	-2.582164	2.667188	-0.714395
33H	-3.481046	2.664873	0.802391
34H	-4.707205	2.061094	-1.980544
35H	-5.612015	2.055094	-0.450882
36H	-4.902430	3.557417	-1.057142
37H	-0.697880	0.830013	0.281807
38H	-1.179383	-0.756375	0.875056
39H	-5.263198	-0.328165	0.439601
40H	-4.516256	0.293756	1.911403
41H	-3.960423	-0.391748	-1.996543
42H	-2.698249	-1.437332	-1.349263
43H	-4.822714	-2.202343	2.036580
44H	-3.816469	-2.429750	0.598718
45H	-3.098547	-1.805449	2.095762
46H	-0.927640	0.244099	-2.135046
47H	-1.911864	-0.373750	-3.471082
48H	-2.217180	1.245436	-2.825197
49H	-0.486001	0.705302	2.791058
50H	-1.692363	1.921034	2.351618
51H	-2.206478	0.327754	2.946107

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1C	-2.350307	1.982108	1.109479
2C	-1.671829	3.150256	1.464936
3N	-0.868598	3.827000	0.630893
4C	-0.725635	3.345931	-0.613189
5C	-1.363000	2.193345	-1.075919
6C	-2.189542	1.499544	-0.190721
7N	-2.904195	0.332580	-0.638305
8S	-2.069853	-1.075008	-0.883611
9O	-0.684617	-0.752984	-1.222869
10O	-2.882007	-1.984216	-1.686061
11C	-1.970151	-1.906642	0.815617
12F	-1.241995	-1.148903	1.651145
13F	-1.398061	-3.109174	0.703245
14F	-3.203231	-2.048282	1.320593
15C	-4.366372	0.271198	-0.399259
16H	-2.983639	1.473919	1.828996
17H	-1.775489	3.553885	2.469378
18H	-0.077570	3.911582	-1.278413
19H	-1.227179	1.848945	-2.094812
20H	-4.598934	0.163502	0.664133
21H	-4.794272	1.200337	-0.781710
22H	-4.786365	-0.566693	-0.956242
23P	2.995295	-0.084587	-0.030076
24C	4.396685	-0.425762	1.091067
25C	5.569072	-1.156139	0.421231
26C	1.607939	0.598855	0.940127
27C	3.521220	1.133257	-1.285843
28C	2.471705	-1.620434	-0.865601
29C	2.413976	1.511356	-2.279690
30C	2.040117	-2.733013	0.099066
31C	1.954856	1.899026	1.678323
32H	3.998195	-1.007008	1.931104
33H	4.716525	0.543011	1.492633
34H	5.278340	-2.152476	0.072103
35H	5.965970	-0.592724	-0.430450
36H	6.380398	-1.279739	1.146426

37H	1.303875	-0.182162	1.645516
38H	0.776039	0.741661	0.242420
39H	4.384557	0.701999	-1.805376
40H	3.878664	2.013790	-0.739294
41H	3.313909	-1.940704	-1.490999
42H	1.650695	-1.349641	-1.536579
43H	2.799294	2.252024	-2.988666
44H	2.070076	0.644001	-2.852932
45H	1.548784	1.948984	-1.771971
46H	1.197081	-2.421065	0.723141
47H	1.719256	-3.607024	-0.477518
48H	2.861437	-3.044755	0.753890
49H	1.078771	2.241822	2.236971
50H	2.773388	1.754533	2.391915
51H	2.236120	2.699401	0.985983

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1C	-1.420171	2.189743	1.219908
2C	-0.262779	2.944920	1.417219
3N	0.589468	3.274216	0.435909
4C	0.285876	2.857309	-0.803053
5C	-0.850748	2.112304	-1.116531
6C	-1.718582	1.762966	-0.077491
7N	-2.924893	1.031676	-0.347304
8S	-2.822140	-0.520768	-0.937123
9O	-1.602346	-0.660745	-1.727192
10O	-4.132170	-0.928740	-1.432326
11C	-2.521655	-1.590988	0.597638
12F	-1.448798	-1.125014	1.260761
13F	-2.296427	-2.857474	0.236320
14F	-3.585575	-1.542433	1.408494
15C	-4.157958	1.405564	0.387518
16H	-2.060900	1.945119	2.060016
17H	-0.007188	3.290028	2.416512
18H	0.978996	3.142109	-1.590596
19H	-1.057628	1.819875	-2.138906
20H	-4.141265	1.062097	1.426186
21H	-4.228494	2.494399	0.358672
22H	-5.020793	0.982608	-0.127180
23P	3.025662	-0.534764	0.015124
24C	1.759746	0.106445	1.162735
25C	1.533437	-0.770004	2.402249
26C	3.129079	0.575336	-1.433067
27C	4.640127	-0.591108	0.866284
28C	2.591744	-2.219851	-0.536628
29C	5.809134	-0.980978	-0.048965
30C	1.195153	-2.331135	-1.161956
31C	3.729722	1.953007	-1.119903
32H	0.836364	0.226959	0.585082
33H	2.085837	1.112942	1.446064
34H	1.201799	-1.778602	2.134176
35H	2.441677	-0.854549	3.008909
36H	0.756296	-0.317141	3.026724
37H	2.109863	0.669215	-1.824827
38H	3.720321	0.051185	-2.193010
39H	4.534724	-1.302062	1.693837
40H	4.798422	0.398642	1.310614
41H	2.684644	-2.871491	0.340475
42H	3.369990	-2.524384	-1.245895
43H	6.736624	-0.990174	0.533676
44H	5.674827	-1.980703	-0.476430
45H	5.937492	-0.267226	-0.869896
46H	1.086156	-1.689757	-2.042212
47H	1.020170	-3.365085	-1.478251
48H	0.410605	-2.064222	-0.449856
49H	3.727398	2.562175	-2.030109
50H	3.154805	2.488214	-0.357809
51H	4.767109	1.871333	-0.778866

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1C	-1.798700	2.259581	0.891205
2C	-0.795337	3.214228	1.073200
3N	0.069366	3.576683	0.114752
4C	-0.062210	2.992576	-1.086917
5C	-1.030684	2.031786	-1.378855
6C	-1.907372	1.650620	-0.360276
7N	-2.929373	0.672933	-0.623075
8S	-2.483454	-0.911345	-0.824018
9O	-1.097988	-0.957142	-1.287388
10O	-3.560007	-1.635378	-1.491906
11C	-2.426363	-1.642849	0.925900
12F	-1.673244	-0.860746	1.717935

13F	-1.888145	-2.866807	0.883623
14F	-3.660404	-1.717113	1.436547
15C	-4.317862	0.963981	-0.193850
16H	-2.464235	2.001064	1.707652
17H	-0.677975	3.700592	2.038727
18H	0.636921	3.310443	-1.856836
19H	-1.100949	1.591520	-2.367189
20H	-4.423965	0.932900	0.895093
21H	-4.566507	1.961511	-0.562300
22H	-4.992895	0.240218	-0.651813
23P	3.032980	-0.332862	0.049064
24C	3.794304	-1.808757	0.809946
25C	5.148441	-2.198792	0.200789
26C	1.410621	-0.024294	0.827416
27C	4.146873	1.091417	0.303516
28C	2.797786	-0.608042	-1.741966
29C	3.599293	2.426046	-0.219247
30C	2.086007	-1.924454	-2.085961
31C	1.491630	0.344381	2.315035
32H	3.067440	-2.623801	0.714096
33H	3.892366	-1.592666	1.880257
34H	5.064150	-2.423038	-0.867838
35H	5.895176	-1.408178	0.330558
36H	5.523557	-3.097603	0.701939
37H	0.819940	-0.932827	0.673496
38H	0.924103	0.767701	0.248949
39H	5.091722	0.834772	-0.189968
40H	4.351020	1.141872	1.379852
41H	3.793333	-0.565773	-2.199780
42H	2.233092	0.252784	-2.118581
43H	4.335534	3.215421	-0.032933
44H	3.414938	2.392834	-1.298731
45H	2.670053	2.713132	0.282351
46H	1.080875	-1.968483	-1.658413
47H	1.985544	-2.002939	-3.173967
48H	2.653848	-2.794685	-1.740322
49H	0.479755	0.463233	2.714978
50H	1.991596	-0.434503	2.901324
51H	2.023701	1.289230	2.467800

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1C	1.514036	2.241165	-0.885189
2C	0.423579	3.093779	-1.071426
3N	-0.463143	3.387966	-0.107983
4C	-0.268824	2.834797	1.099503
5C	0.789173	1.974026	1.395741
6C	1.694070	1.671891	0.377069
7N	2.827088	0.828558	0.654723
8S	2.599329	-0.802043	0.818058
9O	1.216853	-1.046312	1.226516
10O	3.739942	-1.383016	1.518946
11C	2.713949	-1.504381	-0.937611
12F	1.857102	-0.852236	-1.741157
13F	2.400366	-2.803882	-0.926425
14F	3.956166	-1.349700	-1.410901
15C	4.178717	1.332291	0.313261
16H	2.196341	2.029178	-1.701884
17H	0.252333	3.553023	-2.042262
18H	-0.987199	3.097767	1.872427
19H	0.911787	1.558662	2.389882
20H	4.340178	1.360460	-0.768629
21H	4.262149	2.339623	0.726275
22H	4.928567	0.695326	0.783773
23P	-3.038445	-0.442083	-0.057816
24C	-3.504723	-2.205523	-0.117891
25C	-4.846565	-2.522207	0.555753
26C	-1.424824	-0.227279	-0.882379
27C	-4.313120	0.546393	-0.915030
28C	-2.930250	0.112684	1.677469
29C	-3.989271	2.045631	-0.996169
30C	-2.026216	-0.758624	2.560042
31C	-1.461033	-0.528866	-2.386557
32H	-2.684727	-2.762168	0.351562
33H	-3.519537	-2.488932	-1.177021
34H	-4.840202	-2.260881	1.619854
35H	-5.675974	-1.992699	0.074957
36H	-5.045472	-3.596428	0.478027
37H	-0.711767	-0.874361	-0.361148
38H	-1.111367	0.805060	-0.699339
39H	-5.253089	0.374430	-0.377274
40H	-4.431701	0.113505	-1.915484
41H	-3.956865	0.134051	2.061795
42H	-2.577589	1.149511	1.650776
43H	-4.805343	2.563877	-1.510941
44H	-3.881590	2.494544	-0.003038

45H	-3.067115	2.233126	-1.556263
46H	-1.002694	-0.806820	2.178375
47H	-1.989176	-0.333252	3.568910
48H	-2.409443	-1.781133	2.644734
49H	-0.461378	-0.385421	-2.808200
50H	-1.763263	-1.562105	-2.589481
51H	-2.145341	0.142652	-2.916113

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1C	-2.366539	2.087523	1.015811
2C	-1.678050	3.265911	1.313350
3N	-0.831113	3.868737	0.466139
4C	-0.659429	3.302453	-0.738431
5C	-1.307486	2.135778	-1.145216
6C	-2.171514	1.512463	-0.241877
7N	-2.887658	0.328078	-0.634665
8S	-2.054331	-1.085842	-0.865929
9O	-0.660443	-0.774166	-1.178514
10O	-2.854174	-1.992546	-1.682692
11C	-1.985209	-1.911173	0.839046
12F	-1.467323	-1.053766	1.733318
13F	-1.211718	-3.001581	0.780670
14F	-3.215758	-2.259058	1.231089
15C	-4.338823	0.242624	-0.340183
16H	-3.030655	1.640223	1.747990
17H	-1.808454	3.738930	2.283790
18H	0.021073	3.808872	-1.418036
19H	-1.153215	1.727793	-2.137624
20H	-4.529994	0.080140	0.724855
21H	-4.787794	1.185605	-0.658018
22H	-4.774952	-0.569779	-0.922480
23P	2.990054	-0.106953	-0.008330
24C	2.286281	0.780818	-1.440103
25C	2.751631	2.239585	-1.550167
26C	2.190716	-1.737025	0.169978
27C	4.785156	-0.310980	-0.275244
28C	2.710213	0.866339	1.509631
29C	5.509452	-1.061180	0.850571
30C	1.224857	1.069648	1.840119
31C	2.351766	-2.657134	-1.047991
32H	1.197633	0.715258	-1.354721
33H	2.571592	0.209766	-2.331406
34H	2.398431	2.842702	-0.707570
35H	3.843347	2.318176	-1.597077
36H	2.348056	2.678885	-2.468564
37H	1.132112	-1.541267	0.364417
38H	2.610334	-2.195805	1.073355
39H	5.198059	0.696438	-0.405556
40H	4.902241	-0.830844	-1.233492
41H	3.217359	1.826356	1.358880
42H	3.229784	0.350570	2.325493
43H	6.575850	-1.131362	0.610597
44H	5.417268	-0.540499	1.809917
45H	5.126769	-2.080309	0.971588
46H	0.745370	0.127228	2.119476
47H	1.131382	1.758230	2.686121
48H	0.674435	1.500535	0.998695
49H	1.824494	-3.598179	-0.858011
50H	1.918646	-2.212177	-1.949721
51H	3.402707	-2.896001	-1.245214

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1C	-1.337178	1.684795	1.124326
2C	-0.623262	2.834087	1.460652
3N	-0.493271	3.900087	0.654683
4C	-1.099530	3.834201	-0.538944
5C	-1.825674	2.728347	-0.984654
6C	-1.943315	1.623896	-0.135361
7N	-2.704041	0.483294	-0.550245
8S	-2.025563	-1.037994	-0.516981
9O	-0.629296	-0.964433	-0.087897
10O	-2.432825	-1.788593	-1.702534
11C	-2.943068	-1.864429	0.914163
12F	-4.262813	-1.789016	0.711453
13F	-2.640027	-1.256315	2.067931
14F	-2.574318	-3.147262	0.983152
15C	-3.863242	0.673067	-1.457869
16H	-1.416048	0.868656	1.832087
17H	-0.140763	2.902682	2.432351
18H	-0.991354	4.702000	-1.185491
19H	-2.269965	2.737612	-1.973339
20H	-4.402101	1.556401	-1.111132

21H	-3.546512	0.803509	-2.496166
22H	-4.528184	-0.188156	-1.389549
23P	3.185811	-0.228815	-0.115529
24C	2.224421	-0.001250	1.418114
25C	2.607403	1.250468	2.217427
26C	4.958960	-0.426836	0.275042
27C	2.564123	-1.721114	-0.958744
28C	3.000723	1.231797	-1.192440
29C	3.230267	-1.996943	-2.312380
30C	1.549769	1.514378	-1.602903
31C	5.270085	-1.656746	1.138354
32H	2.364945	-0.911605	2.013218
33H	1.171620	0.024226	1.118261
34H	2.000356	1.298034	3.127730
35H	3.659782	1.235065	2.521358
36H	2.426067	2.167075	1.646636
37H	5.272654	0.496395	0.777104
38H	5.492703	-0.468914	-0.681749
39H	1.482028	-1.593386	-1.066009
40H	2.717386	-2.554932	-0.263184
41H	3.638684	1.060457	-2.067548
42H	3.427254	2.081401	-0.646473
43H	2.818686	-2.919425	-2.735838
44H	3.041073	-1.189414	-3.027832
45H	4.313797	-2.128603	-2.218335
46H	1.520860	2.405993	-2.237578
47H	1.115553	0.682691	-2.167579
48H	0.916893	1.700015	-0.732406
49H	6.344923	-1.691645	1.346047
50H	4.745335	-1.620354	2.099394
51H	4.995856	-2.588061	0.631495

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1C	-2.306981	2.151879	1.057657
2C	-1.527369	3.221411	1.503570
3N	-0.560948	3.795362	0.771757
4C	-0.361323	3.318770	-0.466533
5C	-1.091606	2.265059	-1.016912
6C	-2.072153	1.660116	-0.227650
7N	-2.838207	0.561798	-0.754642
8S	-2.084160	-0.899940	-0.970721
9O	-0.655132	-0.668316	-1.176301
10O	-2.879307	-1.727490	-1.872012
11C	-2.187482	-1.780412	0.706396
12F	-1.759002	-0.957640	1.675543
13F	-1.413472	-2.872318	0.685980
14F	-3.451144	-2.135163	0.963330
15C	-4.310089	0.571415	-0.580208
16H	-3.059822	1.714480	1.704494
17H	-1.679305	3.623489	2.502430
18H	0.415985	3.804365	-1.052029
19H	-0.901193	1.921705	-2.027321
20H	-4.601799	0.400316	0.460532
21H	-4.666224	1.550039	-0.907821
22H	-4.750183	-0.195117	-1.218990
23P	3.004002	-0.271095	0.038402
24C	4.823113	-0.399364	-0.061719
25C	5.539983	0.956160	-0.139323
26C	2.277538	-1.944346	0.062177
27C	2.539837	0.629526	1.558442
28C	2.360537	0.652732	-1.397361
29C	1.045566	0.528161	1.892595
30C	2.573576	-0.042292	-2.748716
31C	2.659383	-2.774390	1.294746
32H	5.051791	-1.017756	-0.937870
33H	5.144678	-0.962865	0.822178
34H	5.253692	1.517906	-1.035214
35H	5.331204	1.577331	0.738895
36H	6.621866	0.790904	-0.180847
37H	2.597722	-2.440749	-0.861293
38H	1.192897	-1.810787	-0.010821
39H	2.839403	1.673229	1.407990
40H	3.153844	0.231294	2.374139
41H	2.847298	1.634832	-1.373865
42H	1.294897	0.810444	-1.205707
43H	0.827016	1.150119	2.766591
44H	0.418407	0.876264	1.068234
45H	0.761018	-0.500719	2.131167
46H	2.048043	-1.001571	-2.794330
47H	2.173947	0.592703	-3.546847
48H	3.634815	-0.215037	-2.959959
49H	2.160733	-3.748102	1.239887
50H	3.738638	-2.954652	1.346176
51H	2.344131	-2.290730	2.225758

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1C	-2.297628	2.203464	0.911612
2C	-1.553332	3.346002	1.212583
3N	-0.634682	3.874673	0.389847
4C	-0.444299	3.266690	-0.791060
5C	-1.141161	2.128621	-1.197816
6C	-2.080170	1.583563	-0.320447
7N	-2.840536	0.426665	-0.713962
8S	-2.077220	-1.040748	-0.808402
9O	-0.654233	-0.822237	-1.063555
10O	-2.882177	-1.955725	-1.611190
11C	-2.147793	-1.752935	0.948799
12F	-1.694207	-0.841710	1.823835
13F	-1.384905	-2.849848	1.023888
14F	-3.409734	-2.067103	1.262352
15C	-4.309376	0.441967	-0.512979
16H	-3.016515	1.813754	1.624146
17H	-1.697486	3.851958	2.164238
18H	0.294243	3.714434	-1.451917
19H	-0.962826	1.679784	-2.168258
20H	-4.576218	0.376114	0.546020
21H	-4.681582	1.378858	-0.932015
22H	-4.753683	-0.390344	-1.059689
23P	2.994359	-0.228547	0.015659
24C	4.464398	0.535337	0.787946
25C	5.099924	-0.308590	1.901948
26C	2.321959	0.922372	-1.231060
27C	3.471925	-1.805670	-0.772345
28C	1.734203	-0.561431	1.291124
29C	2.341913	-2.470246	-1.572842
30C	1.159458	0.702967	1.945069
31C	3.244191	1.136924	-2.439143
32H	4.144721	1.513061	1.169010
33H	5.179408	0.724587	-0.021315
34H	4.404166	-0.473963	2.731680
35H	5.436855	-1.282892	1.531609
36H	5.974251	0.217982	2.299261
37H	2.133345	1.865374	-0.706011
38H	1.348766	0.525126	-1.535947
39H	3.822219	-2.462881	0.032783
40H	4.337113	-1.593133	-1.411802
41H	2.210273	-1.211641	2.034004
42H	0.945383	-1.143301	0.805550
43H	2.708793	-3.410957	-1.997325
44H	1.475024	-2.697188	-0.945549
45H	2.002758	-1.837210	-2.399061
46H	0.611182	1.314964	1.222767
47H	0.460960	0.415577	2.737003
48H	1.942834	1.320518	2.398552
49H	2.787233	1.863977	-3.119268
50H	4.223636	1.527522	-2.142032
51H	3.397425	0.208169	-2.999145

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1C	-2.299831	1.848980	1.293414
2C	-1.627609	2.987175	1.744791
3N	-0.927776	3.803981	0.942449
4C	-0.892300	3.506535	-0.365171
5C	-1.524914	2.393397	-0.921470
6C	-2.233280	1.548529	-0.067806
7N	-2.915519	0.401835	-0.614287
8S	-2.040612	-0.965551	-0.921478
9O	-0.642696	-0.587627	-1.131248
10O	-2.770087	-1.814466	-1.858606
11C	-2.032508	-1.951478	0.697494
12F	-1.605302	-1.171095	1.701962
13F	-1.211406	-3.001895	0.580258
14F	-3.268106	-2.381406	0.979026
15C	-4.379008	0.294851	-0.409829
16H	-2.846293	1.216852	1.985568
17H	-1.649014	3.248794	2.800151
18H	-0.333198	4.188488	-1.001030
19H	-1.470885	2.187990	-1.985386
20H	-4.625413	0.123893	0.642535
21H	-4.822948	1.234239	-0.746632
22H	-4.770061	-0.519117	-1.021631
23P	3.034476	-0.133687	-0.070299
24C	4.499011	0.149740	0.985489
25C	5.415220	-1.073205	1.124228
26C	1.980668	1.355470	-0.031381
27C	3.583397	-0.466840	-1.779952
28C	2.096618	-1.571428	0.546829

29C	2.431458	-0.664934	-2.776372
30C	1.625532	-1.423448	1.999894
31C	2.667312	2.607800	-0.593377
32H	4.125153	0.477029	1.963131
33H	5.038717	0.997761	0.548135
34H	4.905094	-1.908529	1.616073
35H	5.783717	-1.416773	0.151331
36H	6.284737	-0.808243	1.735280
37H	1.687360	1.505075	1.014288
38H	1.070027	1.111890	-0.588753
39H	4.222560	-1.356836	-1.736282
40H	4.221892	0.374676	-2.074476
41H	2.746493	-2.446969	0.426894
42H	1.246910	-1.698353	-0.130672
43H	2.846928	-0.850398	-3.772751
44H	1.802705	-1.519519	-2.507413
45H	1.789934	0.220290	-2.838234
46H	0.969839	-0.556005	2.126029
47H	1.058987	-2.314229	2.288978
48H	2.468653	-1.324206	2.692754
49H	1.985078	3.459302	-0.510879
50H	3.577650	2.858981	-0.038445
51H	2.928070	2.486772	-1.650631

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1C	2.193652	1.888746	-1.284753
2C	1.472973	3.008296	-1.706845
3N	0.770424	3.795904	-0.877816
4C	0.782508	3.488340	0.427935
5C	1.468017	2.392857	0.956487
6C	2.176714	1.576722	0.075449
7N	2.905553	0.444619	0.591908
8S	2.075535	-0.947600	0.911758
9O	0.673233	-0.608784	1.155685
10O	2.848987	-1.782059	1.826160
11C	2.053489	-1.925319	-0.712434
12F	1.595718	-1.144289	-1.703088
13F	1.247755	-2.987332	-0.586989
14F	3.288189	-2.338336	-1.020592
15C	4.365535	0.377341	0.350062
16H	2.739078	1.278312	-1.997134
17H	1.455144	3.278404	-2.760117
18H	0.219032	4.146482	1.084754
19H	1.450893	2.177201	2.019627
20H	4.590538	0.217284	-0.708877
21H	4.793214	1.326300	0.680557
22H	4.793470	-0.428595	0.947759
23P	-3.009118	-0.180728	0.047389
24C	-4.532873	0.151923	-0.904861
25C	-5.436567	-1.074286	-1.098256
26C	-2.062533	1.369256	0.221725
27C	-3.456739	-0.839404	1.692035
28C	-1.982264	-1.403012	-0.837209
29C	-2.264175	-1.040648	2.637643
30C	-1.534933	-0.938415	-2.230345
31C	-2.764651	2.438006	1.069235
32H	-4.210620	0.560692	-1.870268
33H	-5.065048	0.952929	-0.378259
34H	-4.915413	-1.887428	-1.615784
35H	-5.810084	-1.456478	-0.142436
36H	-6.303177	-0.792915	-1.706047
37H	-1.873952	1.736163	-0.793780
38H	-1.092999	1.093359	0.650305
39H	-3.982429	-1.785321	1.514989
40H	-4.188095	-0.143413	2.120831
41H	-2.568232	-2.327630	-0.896039
42H	-1.120005	-1.601767	-0.193151
43H	-2.627713	-1.435874	3.592379
44H	-1.535183	-1.748445	2.232572
45H	-1.743217	-0.099262	2.839067
46H	-0.915333	-0.037540	-2.176644
47H	-0.939116	-1.726628	-2.700924
48H	-2.389793	-0.730720	-2.883039
49H	-2.142040	3.338019	1.100243
50H	-3.735894	2.719364	0.648204
51H	-2.918289	2.100301	2.099654

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1C	2.473412	1.856174	0.155310
2C	3.669621	2.505519	0.310616
3N	4.855257	1.874910	0.087077
4C	4.850578	0.573172	-0.303477

5C	3.685938	-0.133893	-0.478243
6C	2.423208	0.490276	-0.251146
7N	1.177525	-0.043208	-0.366136
8S	0.885155	-1.569043	-0.771867
9O	-0.545667	-1.689571	-1.094319
10O	1.866196	-2.235843	-1.650224
11C	1.038995	-2.497624	0.872001
12F	0.173102	-2.006215	1.777286
13F	2.285427	-2.366398	1.367468
14F	0.781447	-3.803147	0.701352
15C	6.120790	2.623145	0.189108
16H	1.549137	2.387945	0.352615
17H	3.729923	3.542751	0.619724
18H	5.822544	0.121578	-0.469079
19H	3.753989	-1.166413	-0.792083
20H	6.931439	1.928057	0.410561
21H	6.321234	3.134885	-0.756856
22H	6.043315	3.354890	0.995399
23P	-3.307664	0.857858	-0.018143
24C	-4.760275	1.516258	0.874363
25C	-5.307020	0.582746	1.963763
26C	-3.726163	-0.711652	-0.845535
27C	-2.798309	2.107260	-1.248341
28C	-1.940270	0.559825	1.146847
29C	-1.658537	1.655454	-2.172734
30C	-1.595773	1.768870	2.026227
31C	-4.823890	-0.587431	-1.909615
32H	-5.526727	1.733500	0.121238
33H	-4.451141	2.478121	1.301245
34H	-6.142447	1.073139	2.475237
35H	-5.679872	-0.357376	1.543512
36H	-4.546814	0.346418	2.716611
37H	-4.017445	-1.412691	-0.054176
38H	-2.792549	-1.091024	-1.272785
39H	-2.514706	2.999949	-0.677866
40H	-3.694251	2.369943	-1.823515
41H	-1.080072	0.266106	0.538783
42H	-2.217544	-0.309158	1.754309
43H	-1.393545	2.480509	-2.843412
44H	-0.762819	1.367291	-1.613740
45H	-1.954912	0.802427	-2.791863
46H	-0.723515	1.525716	2.643064
47H	-1.342870	2.649798	1.424419
48H	-2.418616	2.036478	2.697992
49H	-5.009060	-1.572515	-2.351420
50H	-5.768454	-0.227770	-1.486578
51H	-4.529056	0.088903	-2.719391

6ah-Me-002

1C	2.471073	1.860933	0.154194
2C	3.669859	2.509084	0.293425
3N	4.851973	1.881854	0.040116
4C	4.840232	0.580954	-0.350952
5C	3.672455	-0.124672	-0.511339
6C	2.413951	0.496676	-0.258589
7N	1.166885	-0.037738	-0.358093
8S	0.875440	-1.563759	-0.765138
9O	-0.560869	-1.691341	-1.060941
10O	1.842290	-2.222648	-1.664839
11C	1.063877	-2.497283	0.872610
12F	0.201603	-2.021069	1.789563
13F	2.314181	-2.349466	1.353282
14F	0.823471	-3.805889	0.701158
15C	6.121968	2.601088	0.249399
16H	1.550128	2.392877	0.366160
17H	3.736738	3.543704	0.610537
18H	5.807503	0.126458	-0.532556
19H	3.736081	-1.153683	-0.837047
20H	6.924866	2.068021	-0.261114
21H	6.038489	3.608281	-0.163823
22H	6.339881	2.655577	1.319865
23P	-3.322966	0.856813	-0.001925
24C	-2.806541	2.091353	-1.243825
25C	-1.666788	1.625637	-2.161647
26C	-1.962838	0.543753	1.168484
27C	-4.771839	1.533663	0.885147
28C	-3.752234	-0.718711	-0.813248
29C	-5.339468	0.601527	1.964739
30C	-4.852825	-0.603101	-1.875072
31C	-1.466443	1.791425	1.908940
32H	-2.521783	2.991189	-0.684746
33H	-3.701660	2.347844	-1.823085
34H	-1.401504	2.441048	-2.843903
35H	-0.771208	1.344460	-1.598956
36H	-1.963747	0.764254	-2.768695

37H	-1.155786	0.095958	0.584103
38H	-2.318939	-0.220555	1.869227
39H	-5.529440	1.766153	0.127584
40H	-4.452296	2.488888	1.319668
41H	-4.042190	-1.411386	-0.013866
42H	-2.821258	-1.104528	-1.240651
43H	-6.173067	1.099154	2.472135
44H	-5.719652	-0.331779	1.535657
45H	-4.588433	0.351820	2.722310
46H	-5.040450	-1.592150	-2.306855
47H	-5.795865	-0.238402	-1.453035
48H	-4.559233	0.065181	-2.691998
49H	-0.639107	1.510579	2.569761
50H	-1.093582	2.549905	1.211770
51H	-2.250349	2.246024	2.525107

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1C	2.583300	1.866626	0.230601
2C	3.799907	2.484089	0.348826
3N	4.961865	1.825215	0.081523
4C	4.910722	0.524212	-0.303529
5C	3.722400	-0.151377	-0.445490
6C	2.483584	0.505292	-0.185311
7N	1.220625	0.007354	-0.276844
8S	0.881345	-1.480981	-0.775328
9O	-0.555612	-1.543802	-1.088560
10O	1.833436	-2.113330	-1.708935
11C	1.023348	-2.522138	0.800403
12F	0.168469	-2.078299	1.740429
13F	2.272931	-2.447862	1.298953
14F	0.741319	-3.807777	0.540412
15C	6.245718	2.540113	0.201532
16H	1.680287	2.423848	0.453806
17H	3.898814	3.519111	0.656508
18H	5.862795	0.042934	-0.494516
19H	3.757474	-1.184144	-0.763588
20H	7.059970	1.854508	-0.033901
21H	6.262010	3.376991	-0.501545
22H	6.363115	2.909596	1.223215
23P	-3.371728	0.847993	-0.003622
24C	-3.765535	-0.639752	-0.980608
25C	-4.743528	-0.389889	-2.136132
26C	-4.875187	1.448877	0.843424
27C	-2.096198	0.414589	1.223207
28C	-2.765538	2.181191	-1.093197
29C	-1.715424	1.557106	2.173110
30C	-1.570586	1.777738	-1.969157
31C	-5.431305	0.472578	1.889344
32H	-4.165878	-1.376122	-0.273534
33H	-2.810349	-1.033113	-1.341747
34H	-4.916756	-1.330713	-2.669664
35H	-5.713915	-0.022659	-1.783407
36H	-4.342740	0.331550	-2.856828
37H	-5.615713	1.652428	0.061046
38H	-4.619217	2.412282	1.300306
39H	-1.227263	0.076027	0.653510
40H	-2.477988	-0.451732	1.775887
41H	-2.510752	3.022482	-0.437093
42H	-3.616690	2.502439	-1.705494
43H	-0.954466	1.199112	2.875230
44H	-1.290545	2.408966	1.630389
45H	-2.571377	1.912216	2.757728
46H	-1.253399	2.642209	-2.563235
47H	-0.718728	1.438499	-1.372377
48H	-1.834104	0.971699	-2.661509
49H	-6.329965	0.901735	2.345589
50H	-5.710829	-0.487722	1.442014
51H	-4.707962	0.282373	2.689721

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1C	-2.351247	1.800020	0.178774
2C	-3.519237	2.489695	-0.012106
3N	-4.723797	1.854750	-0.041905
4C	-4.764580	0.505301	0.108898
5C	-3.630188	-0.244410	0.304246
6C	-2.350222	0.383158	0.349595
7N	-1.129338	-0.186403	0.535897
8S	-0.888065	-1.764070	0.714379
9O	0.465826	-1.971536	1.250370
10O	-1.996771	-2.557653	1.279408
11C	-0.751278	-2.378682	-1.072202
12F	0.280748	-1.784230	-1.702195

13F	-1.879475	-2.092359	-1.751800
14F	-0.558088	-3.705461	-1.100766
15C	-5.952894	2.627872	-0.297178
16H	-1.411818	2.340987	0.197908
17H	-3.543293	3.564849	-0.148596
18H	-5.747287	0.049471	0.070161
19H	-3.735952	-1.313397	0.428206
20H	-6.817696	2.043462	0.019215
21H	-5.918226	3.558062	0.273484
22H	-6.030542	2.851140	-1.365220
23P	3.128119	0.917974	0.108550
24C	2.886508	1.521383	1.815723
25C	1.724068	0.858411	2.566247
26C	1.646480	1.247406	-0.901273
27C	4.567664	1.805017	-0.584801
28C	3.434106	-0.880489	0.099882
29C	4.879427	1.451108	-2.045088
30C	4.611258	-1.324405	0.978161
31C	1.311506	2.737513	-1.056448
32H	2.746163	2.607047	1.744972
33H	3.838189	1.357646	2.336042
34H	1.658477	1.285070	3.573411
35H	0.766256	1.017061	2.062381
36H	1.865028	-0.221621	2.661492
37H	0.819292	0.706236	-0.428212
38H	1.821751	0.781090	-1.877753
39H	5.420011	1.576243	0.065526
40H	4.364078	2.876671	-0.474110
41H	3.596855	-1.160425	-0.948062
42H	2.500902	-1.355497	0.420133
43H	5.761230	2.011200	-2.374530
44H	5.096523	0.384323	-2.167432
45H	4.049464	1.711278	-2.711023
46H	4.726564	-2.410810	0.899743
47H	5.556093	-0.865199	0.665531
48H	4.442501	-1.085061	2.033819
49H	0.397832	2.842328	-1.651367
50H	1.139595	3.219632	-0.087742
51H	2.107867	3.283880	-1.574204

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1C	-2.357312	-1.862830	0.564619
2C	-3.496785	-2.622659	0.540176
3N	-4.637758	-2.174752	-0.054769
4C	-4.645710	-0.943862	-0.628849
5C	-3.535656	-0.134822	-0.642855
6C	-2.320297	-0.568777	-0.035944
7N	-1.130401	0.084018	0.046452
8S	-0.860077	1.533604	-0.589493
9O	0.593310	1.769442	-0.592744
10O	-1.630737	1.892402	-1.796478
11C	-1.495452	2.729126	0.733272
12F	-0.876375	2.512984	1.906685
13F	-2.819421	2.555671	0.915891
14F	-1.277868	4.000011	0.362474
15C	-5.853633	-3.008183	-0.023254
16H	-1.467273	-2.248138	1.049784
17H	-3.547860	-3.609207	0.986931
18H	-5.579647	-0.632466	-1.081552
19H	-3.609765	0.827320	-1.130651
20H	-6.576437	-2.618492	-0.740958
21H	-5.594642	-4.034079	-0.293558
22H	-6.285810	-2.987609	0.981052
23P	3.387742	-0.806115	-0.025137
24C	3.756224	0.766716	-0.869832
25C	4.814540	0.650145	-1.974625
26C	4.925402	-1.516182	0.660986
27C	2.213107	-0.479601	1.330933
28C	2.697038	-2.017482	-1.203251
29C	1.715514	-1.736875	2.054795
30C	1.393877	-1.570311	-1.879986
31C	5.689369	-0.562158	1.589260
32H	4.071822	1.470764	-0.090824
33H	2.804540	1.139230	-1.261235
34H	4.969197	1.634382	-2.429818
35H	5.778895	0.306744	-1.583938
36H	4.498978	-0.036140	-2.768129
37H	5.545802	-1.821033	-0.190120
38H	4.636368	-2.432058	1.190666
39H	1.377690	0.076839	0.896214
40H	2.728538	0.198569	2.022434
41H	2.550779	-2.945761	-0.637759
42H	3.480857	-2.218217	-1.943569
43H	1.023115	-1.439635	2.849870
44H	1.174364	-2.404885	1.376102

45H	2.532582	-2.302572	2.516815
46H	1.033816	-2.373199	-2.532965
47H	0.611402	-1.344557	-1.149958
48H	1.542883	-0.678332	-2.497238
49H	6.588588	-1.063264	1.963754
50H	6.007166	0.345970	1.065714
51H	5.087301	-0.267182	2.455743

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1C	2.463799	1.865123	0.230409
2C	3.662947	2.489337	0.452046
3N	4.847511	1.860276	0.214695
4C	4.836886	0.581116	-0.241934
5C	3.669082	-0.099116	-0.487998
6C	2.408125	0.526651	-0.260088
7N	1.161041	0.016200	-0.444867
8S	0.869550	-1.447012	-1.041588
9O	-0.551896	-1.514563	-1.415941
10O	1.873313	-2.003402	-1.969541
11C	0.972269	-2.580963	0.470564
12F	0.066363	-2.217917	1.397562
13F	2.196914	-2.509545	1.027841
14F	0.735506	-3.853979	0.119484
15C	6.116786	2.553627	0.501478
16H	1.541156	2.400960	0.424429
17H	3.728106	3.506623	0.821423
18H	5.805423	0.122622	-0.405043
19H	3.735487	-1.110598	-0.864296
20H	6.931533	2.033054	-0.003325
21H	6.059303	3.578469	0.129332
22H	6.296715	2.559482	1.580292
23P	-3.273296	0.849397	0.191091
24C	-4.866125	1.660834	-0.189082
25C	-5.335998	1.463581	-1.636938
26C	-1.971452	1.466734	-0.924026
27C	-2.844477	1.235895	1.925202
28C	-3.429830	-0.955325	-0.016524
29C	-1.585846	0.516812	2.432767
30C	-4.480116	-1.598764	0.898107
31C	-1.756504	2.983956	-0.854959
32H	-4.743350	2.724919	0.045822
33H	-5.598517	1.259951	0.521680
34H	-6.292878	1.976758	-1.781367
35H	-4.621494	1.878908	-2.355886
36H	-5.485896	0.404476	-1.873207
37H	-2.248286	1.149582	-1.936166
38H	-1.054500	0.926244	-0.669675
39H	-3.718576	0.974616	2.533504
40H	-2.730020	2.324736	1.983816
41H	-2.434039	-1.375458	0.152773
42H	-3.661222	-1.132436	-1.072897
43H	-1.380530	0.831485	3.461881
44H	-1.716596	-0.569495	2.435875
45H	-0.704215	0.748989	1.826527
46H	-4.511874	-2.676520	0.705237
47H	-4.238582	-1.457553	1.957447
48H	-5.483734	-1.197389	0.717513
49H	-0.944909	3.260635	-1.536902
50H	-2.649128	3.543934	-1.154872
51H	-1.470253	3.308617	0.152066

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1C	2.321175	-1.805477	0.162796
2C	3.480400	-2.509323	-0.032538
3N	4.690635	-1.887365	-0.076121
4C	4.748563	-0.538512	0.081356
5C	3.624348	0.224408	0.281341
6C	2.337179	-0.389191	0.332962
7N	1.123549	0.194640	0.519995
8S	0.897782	1.771793	0.721528
9O	-0.453706	1.981645	1.262502
10O	2.015765	2.544608	1.296879
11C	0.763727	2.418224	-1.053925
12F	-0.273519	1.843003	-1.692780
13F	1.888675	2.136107	-1.740509
14F	0.580664	3.746760	-1.057425
15C	5.927208	-2.678501	-0.211128
16H	1.375544	-2.335265	0.184002
17H	3.490324	-3.585324	-0.161927
18H	5.737818	-0.096982	0.039547
19H	3.741995	1.292869	0.399800
20H	6.689817	-2.072763	-0.702751

21H	6.277975	-2.982405	0.779484
22H	5.723556	-3.562401	-0.817592
23P	-3.113981	-0.930855	0.099935
24C	-2.795951	-1.631123	1.757353
25C	-1.698590	-0.908813	2.551273
26C	-1.652185	-1.147943	-0.966939
27C	-4.551423	-1.812521	-0.602819
28C	-3.477014	0.852627	0.210471
29C	-4.911271	-1.379341	-2.030244
30C	-4.683084	1.192904	1.096148
31C	-1.267211	-2.610222	-1.224132
32H	-2.544116	-2.686583	1.597075
33H	-3.752094	-1.611321	2.294035
34H	-1.562663	-1.413430	3.514429
35H	-0.740724	-0.909611	2.023326
36H	-1.962028	0.134468	2.748559
37H	-0.830641	-0.609771	-0.481507
38H	-1.870719	-0.626477	-1.906279
39H	-5.387297	-1.637295	0.084914
40H	-4.326053	-2.884793	-0.560700
41H	-3.630541	1.200845	-0.818275
42H	-2.563205	1.331359	0.578381
43H	-5.794952	-1.932349	-2.366532
44H	-5.145736	-0.310424	-2.083891
45H	-4.097611	-1.588706	-2.733244
46H	-4.822839	2.279157	1.111068
47H	-5.608628	0.742893	0.720032
48H	-4.533951	0.863915	2.130393
49H	-0.377000	-2.641848	-1.861761
50H	-1.031339	-3.139532	-0.293905
51H	-2.063045	-3.161057	-1.737753

6ah-Me-008

1C	2.434240	1.779577	-0.335431
2C	3.608847	2.437112	-0.083624
3N	4.773795	1.761133	0.121136
4C	4.766434	0.403626	0.079750
5C	3.622209	-0.315285	-0.169788
6C	2.383093	0.354527	-0.391211
7N	1.157681	-0.180733	-0.641536
8S	0.876566	-1.757405	-0.766469
9O	-0.466913	-1.943746	-1.335697
10O	1.981179	-2.595305	-1.271743
11C	0.665404	-2.321155	1.030444
12F	-0.370738	-1.683715	1.609426
13F	1.776262	-2.049280	1.743949
14F	0.434098	-3.641112	1.084704
15C	6.006908	2.510253	0.425699
16H	1.528345	2.352618	-0.498527
17H	3.670666	3.518477	-0.035881
18H	5.717388	-0.087157	0.252917
19H	3.693237	-1.393793	-0.200381
20H	6.863371	1.840666	0.342772
21H	6.118350	3.328622	-0.288886
22H	5.951171	2.909011	1.442441
23P	-3.116199	0.927012	-0.091307
24C	-4.506000	1.811324	0.699890
25C	-4.689431	1.478506	2.186622
26C	-3.372212	-0.873710	0.028852
27C	-3.046180	1.461446	-1.837341
28C	-1.554635	1.347797	0.749372
29C	-1.890024	0.851123	-2.641843
30C	-1.224197	2.846347	0.744693
31C	-4.652755	-1.369080	-0.657070
32H	-5.407694	1.565761	0.126304
33H	-4.318767	2.882007	0.555352
34H	-5.533372	2.051318	2.585969
35H	-4.905079	0.415381	2.340301
36H	-3.801763	1.738101	2.773905
37H	-3.381293	-1.113045	1.098989
38H	-2.481972	-1.345909	-0.399496
39H	-2.982399	2.556243	-1.819283
40H	-4.014599	1.206655	-2.282815
41H	-0.765218	0.773442	0.251316
42H	-1.635300	0.964622	1.773281
43H	-1.934314	1.223215	-3.671393
44H	-0.915027	1.119845	-2.223734
45H	-1.942700	-0.240771	-2.669698
46H	-0.285487	3.009386	1.285133
47H	-1.096314	3.230828	-0.273485
48H	-1.998617	3.441936	1.241295
49H	-4.733509	-2.453504	-0.526283
50H	-5.552200	-0.912724	-0.228252
51H	-4.640234	-1.165807	-1.733225

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1C	-2.496596	1.856108	-0.074605
2C	-3.701281	2.494720	-0.205470
3N	-4.878974	1.841940	-0.001685
4C	-4.856448	0.525499	0.333443
5C	-3.682345	-0.172349	0.481691
6C	-2.428208	0.474249	0.273347
7N	-1.175892	-0.049394	0.363055
8S	-0.868300	-1.591780	0.686410
9O	0.563480	-1.718183	1.000307
10O	-1.840762	-2.314741	1.529095
11C	-1.014438	-2.430036	-1.004659
12F	-0.151380	-1.882125	-1.880714
13F	-2.261458	-2.284004	-1.493663
14F	-0.744929	-3.740688	-0.905444
15C	-6.155370	2.548355	-0.214954
16H	-1.579120	2.408340	-0.244807
17H	-3.776473	3.541509	-0.477765
18H	-5.820810	0.052449	0.480412
19H	-3.737304	-1.215070	0.762822
20H	-6.954420	2.008908	0.294880
21H	-6.082168	3.557044	0.196182
22H	-6.371339	2.598768	-1.286118
23P	3.320992	0.852871	0.083225
24C	2.991547	1.560488	1.734579
25C	1.818219	0.913258	2.481953
26C	1.853471	1.038249	-0.981737
27C	4.743319	1.761917	-0.615127
28C	3.721185	-0.924397	0.190906
29C	5.124660	1.334806	-2.038712
30C	4.921811	-1.247737	1.089489
31C	1.351151	2.479488	-1.125595
32H	2.816692	2.631196	1.573363
33H	3.924768	1.475145	2.304300
34H	1.668895	1.433972	3.434495
35H	0.888800	0.969145	1.907871
36H	2.007212	-0.142439	2.696145
37H	1.074944	0.404238	-0.546402
38H	2.116573	0.608426	-1.955754
39H	5.577468	1.608753	0.080312
40H	4.491791	2.828420	-0.577703
41H	3.896663	-1.259649	-0.838725
42H	2.811849	-1.425384	0.537987
43H	6.001253	1.903632	-2.367088
44H	5.378733	0.270374	-2.089787
45H	4.313595	1.529691	-2.748845
46H	5.091606	-2.329826	1.087125
47H	5.840301	-0.765526	0.736561
48H	4.746445	-0.942475	2.126872
49H	0.485787	2.491055	-1.797122
50H	1.033630	2.891515	-0.161575
51H	2.110705	3.144421	-1.552290

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1C	2.355629	-1.842159	-0.228460
2C	3.548872	-2.493022	-0.399655
3N	4.736539	-1.888538	-0.118479
4C	4.734856	-0.607338	0.331962
5C	3.572964	0.099002	0.527657
6C	2.308029	-0.499247	0.250563
7N	1.064678	0.041455	0.377318
8S	0.800047	1.532085	0.923879
9O	-0.636610	1.673412	1.201494
10O	1.765572	2.061730	1.907060
11C	1.060970	2.628866	-0.598325
12F	0.222575	2.278354	-1.590914
13F	2.323890	2.506724	-1.053025
14F	0.840579	3.915882	-0.289915
15C	6.000169	-2.610260	-0.354707
16H	1.431449	-2.358374	-0.460162
17H	3.606599	-3.513117	-0.762517
18H	5.705549	-0.168747	0.532659
19H	3.648471	1.110535	0.901531
20H	6.810849	-2.092737	0.159718
21H	5.914578	-3.625593	0.037897
22H	6.208263	-2.643380	-1.427952
23P	-3.229482	-0.885184	-0.124248
24C	-2.898323	-2.636125	-0.524022
25C	-1.414682	-3.017090	-0.425067
26C	-2.224379	0.187367	-1.202230
27C	-5.008571	-0.574492	-0.401072
28C	-2.795205	-0.558457	1.616571

29C	-5.449000	0.861650	-0.084628
30C	-3.557086	-1.426727	2.625480
31C	-2.457501	-0.041265	-2.700633
32H	-3.281192	-2.813515	-1.535566
33H	-3.509100	-3.236077	0.159902
34H	-1.298589	-4.087229	-0.628558
35H	-0.815569	-2.466318	-1.157212
36H	-1.008199	-2.815472	0.571708
37H	-1.181343	0.004736	-0.926393
38H	-2.443953	1.220375	-0.913649
39H	-5.555560	-1.299010	0.213879
40H	-5.213141	-0.827509	-1.448487
41H	-2.974347	0.507444	1.788569
42H	-1.712600	-0.698500	1.697259
43H	-6.522550	0.961829	-0.277772
44H	-5.272542	1.119416	0.965335
45H	-4.928207	1.594656	-0.710283
46H	-3.231722	-1.167415	3.638799
47H	-4.639119	-1.262646	2.572833
48H	-3.363232	-2.495058	2.476556
49H	-1.813117	0.636055	-3.271725
50H	-2.210346	-1.066116	-2.999527
51H	-3.493913	0.161755	-2.991420

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1C	-3.040569	0.554905	-0.824071
2C	-4.063990	1.434539	-1.078340
3N	-4.507135	2.319371	-0.147198
4C	-3.917787	2.341963	1.080455
5C	-2.894149	1.488129	1.398305
6C	-2.401660	0.541530	0.452095
7N	-1.387518	-0.252698	0.887047
8S	-0.668107	-1.358085	-0.024946
9O	0.560292	-1.794169	0.660166
10O	-0.585365	-1.070756	-1.473394
11C	-1.798308	-2.873514	0.074080
12F	-1.301761	-3.869538	-0.676775
13F	-3.027241	-2.562940	-0.384719
14F	-1.914612	-3.304080	1.339030
15C	-5.559709	3.293842	-0.487130
16H	-2.738780	-0.120605	-1.612637
17H	-4.568809	1.460879	-2.037360
18H	-4.307883	3.066775	1.785813
19H	-2.456290	1.525090	2.389678
20H	-6.124136	3.541058	0.413375
21H	-5.102999	4.199406	-0.897143
22H	-6.233007	2.853648	-1.224459
23P	3.382020	0.731827	-0.030464
24C	4.314994	2.122780	-0.764385
25C	4.725021	3.205874	0.243632
26C	2.935678	-0.451601	-1.345225
27C	4.427606	-0.088289	1.224125
28C	1.876691	1.364663	0.785048
29C	3.840711	-1.401039	1.764357
30C	0.931614	2.131845	-0.149451
31C	4.142325	-1.044561	-2.085942
32H	3.683955	2.539957	-1.558730
33H	5.196720	1.689033	-1.250859
34H	3.855854	3.656931	0.734879
35H	5.389353	2.807176	1.018211
36H	5.264025	4.003249	-0.279365
37H	2.268707	0.078221	-2.034555
38H	2.339139	-1.233827	-0.866697
39H	4.570862	0.639957	2.031371
40H	5.408554	-0.254984	0.763309
41H	2.216754	2.001858	1.610234
42H	1.372285	0.499749	1.227682
43H	4.498065	-1.790936	2.549205
44H	2.844159	-1.260537	2.193828
45H	3.765096	-2.161303	0.980488
46H	0.572437	1.501986	-0.969147
47H	0.057105	2.463818	0.419192
48H	1.412568	3.018916	-0.577200
49H	3.784727	-1.753206	-2.840802
50H	4.727668	-0.274600	-2.600070
51H	4.808155	-1.590455	-1.408409

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1C	-2.429718	1.776626	0.372028
2C	-3.601569	2.439406	0.121028
3N	-4.766123	1.768283	-0.101109
4C	-4.761437	0.410303	-0.076162

5C	-3.620118	-0.313826	0.171504
6C	-2.381049	0.350946	0.407603
7N	-1.157586	-0.189712	0.655516
8S	-0.878137	-1.768674	0.755991
9O	0.465168	-1.964707	1.321594
10O	-1.984310	-2.612086	1.248570
11C	-0.668170	-2.306835	-1.048948
12F	0.365396	-1.658490	-1.620411
13F	-1.780640	-2.028722	-1.757507
14F	-0.432847	-3.625219	-1.121823
15C	-5.994979	2.523114	-0.409557
16H	-1.523723	2.345448	0.549488
17H	-3.661137	3.521371	0.087660
18H	-5.712136	-0.076727	-0.260970
19H	-3.693364	-1.392479	0.189017
20H	-6.855126	1.858077	-0.327256
21H	-6.103629	3.343013	0.303628
22H	-5.934934	2.920147	-1.426748
23P	3.105189	0.933065	0.088480
24C	3.043151	1.463756	1.836050
25C	1.983879	0.743401	2.681614
26C	1.538053	1.351169	-0.743708
27C	4.488332	1.826289	-0.704652
28C	3.367605	-0.866408	-0.041236
29C	4.662239	1.508191	-2.195677
30C	4.641044	-1.363536	0.656430
31C	1.207998	2.849898	-0.747666
32H	2.865608	2.546116	1.816305
33H	4.048737	1.314685	2.246370
34H	2.011223	1.138969	3.703012
35H	0.973919	0.887737	2.285924
36H	2.165746	-0.333993	2.728628
37H	0.751525	0.780269	-0.237401
38H	1.611697	0.961576	-1.765711
39H	5.393723	1.574509	-0.139706
40H	4.302595	2.895576	-0.547984
41H	3.389399	-1.097905	-1.112917
42H	2.473814	-1.343930	0.373798
43H	5.501821	2.087057	-2.595507
44H	4.879860	0.447213	-2.360743
45H	3.769945	1.770530	-2.774595
46H	4.725620	-2.446965	0.520047
47H	5.544718	-0.902695	0.241582
48H	4.614845	-1.166494	1.733517
49H	0.264866	3.008850	-1.281620
50H	1.088697	3.242871	0.268248
51H	1.978402	3.441248	-1.255493

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1C	2.125307	-1.814429	-0.280154
2C	3.282823	-2.535605	-0.415908
3N	4.491744	-2.011867	-0.072907
4C	4.551302	-0.740140	0.401177
5C	3.428747	0.033448	0.564918
6C	2.141565	-0.480280	0.225413
7N	0.930187	0.133107	0.317246
8S	0.730081	1.628227	0.876480
9O	-0.701757	1.843985	1.133795
10O	1.702928	2.100881	1.881240
11C	1.072542	2.717297	-0.633793
12F	0.247245	2.401785	-1.648633
13F	2.341227	2.544798	-1.054654
14F	0.895847	4.011084	-0.327050
15C	5.722559	-2.796633	-0.275960
16H	1.181157	-2.268561	-0.559662
17H	3.293178	-3.551150	-0.794841
18H	5.539166	-0.367923	0.647185
19H	3.548985	1.031177	0.963477
20H	6.492435	-2.439825	0.409954
21H	5.514422	-3.847573	-0.066967
22H	6.065410	-2.683761	-1.308588
23P	-3.072139	-0.904016	-0.116769
24C	-3.054971	-2.564826	-0.878441
25C	-1.641452	-3.135424	-1.056695
26C	-2.224735	0.274534	-1.218793
27C	-4.813719	-0.401884	0.112763
28C	-2.215933	-0.960243	1.491563
29C	-4.979760	0.954016	0.813892
30C	-2.806865	-1.979253	2.474123
31C	-2.799526	0.326837	-2.639752
32H	-3.568898	-2.473865	-1.842526
33H	-3.670009	-3.217379	-0.248242
34H	-1.701264	-4.111150	-1.551030
35H	-1.016483	-2.483883	-1.677354
36H	-1.142005	-3.279066	-0.092919

37H	-1.166751	-0.004840	-1.218491
38H	-2.278979	1.250190	-0.727371
39H	-5.305391	-1.201781	0.678964
40H	-5.269984	-0.389562	-0.884303
41H	-2.242468	0.055405	1.897335
42H	-1.162302	-1.165904	1.275583
43H	-6.046341	1.188247	0.900514
44H	-4.556119	0.943323	1.823853
45H	-4.504242	1.764542	0.250968
46H	-2.243033	-1.941690	3.412641
47H	-3.855020	-1.761427	2.708659
48H	-2.745869	-3.003486	2.089722
49H	-2.264143	1.090862	-3.214066
50H	-2.681398	-0.627662	-3.164678
51H	-3.862350	0.594234	-2.643710

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1C	-2.109128	-1.790753	0.353694
2C	-3.259710	-2.524846	0.486100
3N	-4.464207	-2.037053	0.083043
4C	-4.526056	-0.789212	-0.454442
5C	-3.411917	-0.004620	-0.615914
6C	-2.128641	-0.480897	-0.208889
7N	-0.924355	0.147567	-0.286066
8S	-0.726874	1.636058	-0.861419
9O	0.706893	1.859479	-1.100869
10O	-1.688551	2.092579	-1.884479
11C	-1.096782	2.733831	0.635612
12F	-0.277067	2.435679	1.660162
13F	-2.367379	2.549657	1.045732
14F	-0.932152	4.027132	0.320296
15C	-5.704585	-2.814040	0.265140
16H	-1.168572	-2.215266	0.686080
17H	-3.263100	-3.520557	0.913935
18H	-5.511760	-0.448226	-0.751590
19H	-3.532366	0.972962	-1.062035
20H	-6.292384	-2.774056	-0.654324
21H	-5.450900	-3.851785	0.485068
22H	-6.281383	-2.392877	1.093205
23P	3.066417	-0.908587	0.094322
24C	3.070402	-2.586377	0.817540
25C	1.664109	-3.168107	1.015848
26C	2.232099	0.244034	1.234286
27C	4.801513	-0.394196	-0.153973
28C	2.196016	-0.937399	-1.508049
29C	4.945962	1.022879	-0.727345
30C	2.778499	-1.942725	-2.509612
31C	2.825354	0.261769	2.648933
32H	3.606697	-2.515099	1.770823
33H	3.673595	-3.221545	0.158710
34H	1.740208	-4.158185	1.478361
35H	1.054201	-2.537366	1.672340
36H	1.138574	-3.283775	0.062160
37H	1.173383	-0.032422	1.240588
38H	2.283037	1.231438	0.766217
39H	5.257841	-1.136928	-0.819308
40H	5.303868	-0.482472	0.816769
41H	2.222410	0.083510	-1.899918
42H	1.143430	-1.144350	-1.288319
43H	6.007949	1.249949	-0.870422
44H	4.448268	1.121035	-1.697923
45H	4.529004	1.778020	-0.052502
46H	2.209392	-1.888728	-3.444141
47H	3.825596	-1.723245	-2.747151
48H	2.717006	-2.972688	-2.141187
49H	2.299100	1.013134	3.247894
50H	2.711922	-0.704263	3.153595
51H	3.888456	0.527333	2.645616

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1C	2.428428	1.881138	0.274871
2C	3.620109	2.521717	0.490063
3N	4.811315	1.917699	0.222688
4C	4.815225	0.647626	-0.258411
5C	3.655338	-0.048079	-0.498827
6C	2.387472	0.551000	-0.239432
7N	1.146007	0.021696	-0.411641
8S	0.875594	-1.437185	-1.028488
9O	-0.554962	-1.535308	-1.360229
10O	1.863804	-1.944529	-2.000346
11C	1.056284	-2.609197	0.447857
12F	0.158161	-2.315318	1.404997

13F	2.289286	-2.504961	0.981357
14F	0.864493	-3.879329	0.059953
15C	6.072216	2.628622	0.502875
16H	1.500309	2.397209	0.494105
17H	3.674179	3.532900	0.877584
18H	5.788594	0.208790	-0.445020
19H	3.734159	-1.050919	-0.895302
20H	6.892428	2.116720	-0.001815
21H	6.000713	3.651328	0.127044
22H	6.254910	2.640852	1.581127
23P	-3.285987	0.835623	0.183489
24C	-3.450560	-0.969932	0.001369
25C	-4.433491	-1.607296	0.991813
26C	-2.698076	1.244364	1.864854
27C	-2.103050	1.451298	-1.060218
28C	-4.916471	1.629593	-0.037517
29C	-1.860965	2.965107	-1.002094
30C	-5.552215	1.389217	-1.413353
31C	-1.419884	0.502240	2.278296
32H	-2.443333	-1.383882	0.107350
33H	-3.753438	-1.155134	-1.035672
34H	-4.474620	-2.686994	0.812108
35H	-4.120315	-1.455392	2.030862
36H	-5.448476	-1.210525	0.876918
37H	-3.524107	1.022547	2.550807
38H	-2.552325	2.330867	1.884371
39H	-2.494561	1.148848	-2.038492
40H	-1.171611	0.896745	-0.909471
41H	-4.779240	2.700306	0.153659
42H	-5.558740	1.244254	0.763171
43H	-1.139883	3.241387	-1.779076
44H	-2.777117	3.539301	-1.179259
45H	-1.443898	3.273662	-0.036963
46H	-6.520278	1.899836	-1.459264
47H	-4.929360	1.781802	-2.224586
48H	-5.726885	0.323687	-1.598728
49H	-1.094464	0.860674	3.261387
50H	-1.591894	-0.575456	2.355733
51H	-0.602076	0.662102	1.568524

6ah-Me-016

1C	3.192948	0.611864	0.765741
2C	4.305711	1.380033	1.007586
3N	4.955789	2.044813	0.017333
4C	4.487298	1.959140	-1.258909
5C	3.382226	1.209895	-1.566453
6C	2.677878	0.486339	-0.558950
7N	1.607074	-0.232828	-0.990553
8S	0.698595	-1.145138	-0.039247
9O	-0.528993	-1.509553	-0.765416
10O	0.553719	-0.716255	1.370306
11C	1.647294	-2.778023	0.082263
12F	0.962661	-3.657497	0.831758
13F	2.849277	-2.570441	0.655705
14F	1.843884	-3.310598	-1.133090
15C	6.114046	2.901836	0.326434
16H	2.725979	0.108502	1.601163
17H	4.718951	1.485324	2.004357
18H	5.041313	2.509949	-2.010451
19H	3.044346	1.154735	-2.595346
20H	6.821248	2.863531	-0.503849
21H	5.779333	3.931848	0.480578
22H	6.600424	2.532109	1.230032
23P	-3.597550	0.711304	0.074230
24C	-2.949148	-0.284402	1.458900
25C	-2.804317	0.500376	2.770132
26C	-3.479708	-0.222518	-1.486976
27C	-5.342853	1.122169	0.428052
28C	-2.647310	2.262071	-0.094017
29C	-6.049219	1.913828	-0.680341
30C	-1.138457	2.050126	-0.280935
31C	-4.280439	-1.531420	-1.493976
32H	-1.986502	-0.691763	1.137604
33H	-3.635406	-1.130842	1.581090
34H	-2.075599	1.312674	2.674688
35H	-3.757566	0.924152	3.105587
36H	-2.443485	-0.175602	3.552662
37H	-2.415240	-0.419858	-1.649649
38H	-3.818476	0.455635	-2.279615
39H	-5.344983	1.679250	1.372512
40H	-5.853339	0.170543	0.617898
41H	-2.856911	2.861937	0.799871
42H	-3.078524	2.796604	-0.948602
43H	-7.086733	2.104685	-0.385371
44H	-5.569573	2.883038	-0.856319

45H	-6.067745	1.360669	-1.625919
46H	-0.919198	1.451865	-1.170245
47H	-0.648105	3.022814	-0.398971
48H	-0.692307	1.549589	0.583009
49H	-4.158731	-2.021776	-2.465928
50H	-3.922187	-2.226155	-0.727144
51H	-5.351207	-1.359265	-1.336365

6ah-Me-017

1C	-3.616417	0.107942	-0.650329
2C	-4.754725	0.869877	-0.568886
3N	-4.758318	2.112761	-0.017028
4C	-3.596618	2.624276	0.472673
5C	-2.425235	1.913082	0.423453
6C	-2.377442	0.607826	-0.146912
7N	-1.159392	0.002710	-0.135920
8S	-0.880963	-1.463687	-0.727407
9O	0.576241	-1.645748	-0.826791
10O	-1.720915	-1.902784	-1.859610
11C	-1.378611	-2.627589	0.680994
12F	-1.101164	-3.899377	0.354585
13F	-2.701114	-2.523801	0.919144
14F	-0.721970	-2.322742	1.813182
15C	-6.010481	2.890857	0.009169
16H	-3.683964	-0.868903	-1.108948
17H	-5.708322	0.515002	-0.943667
18H	-3.650922	3.618833	0.899544
19H	-1.518820	2.350756	0.826562
20H	-5.858357	3.795794	0.598081
21H	-6.293223	3.161239	-1.011687
22H	-6.800251	2.290433	0.466234
23P	3.413514	0.768261	0.069893
24C	3.004377	0.669087	1.847436
25C	1.796370	-0.222988	2.165760
26C	4.871205	1.854149	-0.125436
27C	3.793563	-0.903022	-0.554068
28C	2.017868	1.472850	-0.868234
29C	4.197978	-0.938780	-2.033957
30C	1.516349	2.824001	-0.341288
31C	6.173088	1.253726	0.422719
32H	2.838411	1.699603	2.183647
33H	3.908193	0.309217	2.354180
34H	0.892859	0.110682	1.647274
35H	1.978384	-1.263727	1.882199
36H	1.602544	-0.196915	3.243881
37H	4.629991	2.794755	0.383787
38H	4.961579	2.081060	-1.194220
39H	2.898449	-1.508397	-0.382737
40H	4.589698	-1.301907	0.085960
41H	1.218618	0.726162	-0.846977
42H	2.357516	1.556334	-1.907576
43H	4.432399	-1.970422	-2.317382
44H	3.383090	-0.595102	-2.679602
45H	5.084121	-0.326006	-2.234180
46H	2.297306	3.592542	-0.358508
47H	0.693513	3.170537	-0.975720
48H	1.136387	2.740297	0.682959
49H	6.984778	1.980723	0.310400
50H	6.091804	1.007568	1.487254
51H	6.458921	0.346393	-0.119558

6ah-Me-018

1C	-2.361264	-1.890321	0.234248
2C	-3.540473	-2.538757	0.490458
3N	-4.743753	-1.938693	0.273210
4C	-4.772908	-0.666854	-0.203295
5C	-3.626609	0.036575	-0.483191
6C	-2.347024	-0.555746	-0.269694
7N	-1.115301	-0.017047	-0.477224
8S	-0.870322	1.454223	-1.074906
9O	0.550315	1.566871	-1.442541
10O	-1.888243	1.971855	-2.009808
11C	-1.017231	2.599507	0.426942
12F	-0.092819	2.291403	1.354555
13F	-2.235109	2.481838	0.991671
14F	-0.839463	3.876839	0.056803
15C	-5.989298	-2.655485	0.602363
16H	-1.422501	-2.402485	0.414239
17H	-3.574570	-3.552377	0.873763
18H	-5.755353	-0.233562	-0.351914
19H	-3.724529	1.040256	-0.873616
20H	-6.829124	-2.157077	0.117217

21H	-5.921441	-3.682301	0.237487
22H	-6.138586	-2.655097	1.685819
23P	3.225788	-0.827688	0.192395
24C	2.531484	-1.340106	1.803749
25C	1.280170	-0.554748	2.219852
26C	3.378547	0.987929	0.142955
27C	4.870313	-1.603198	0.030550
28C	2.143290	-1.379863	-1.166652
29C	5.565851	-1.330016	-1.309630
30C	2.016527	-2.905187	-1.275870
31C	4.210876	1.571826	1.292951
32H	3.332473	-1.224910	2.543771
33H	2.322077	-2.413472	1.726037
34H	0.884775	-0.970386	3.153542
35H	1.514176	0.499690	2.395124
36H	0.492392	-0.601807	1.462271
37H	2.357332	1.381153	0.143406
38H	3.808821	1.244681	-0.831706
39H	4.728342	-2.678569	0.190907
40H	5.471088	-1.232372	0.869174
41H	2.554272	-0.950259	-2.087689
42H	1.167706	-0.909162	-1.008645
43H	6.536672	-1.837233	-1.323871
44H	4.980793	-1.704922	-2.156365
45H	5.745830	-0.260281	-1.462807
46H	1.357409	-3.151248	-2.115516
47H	2.983072	-3.388333	-1.456924
48H	1.578767	-3.342585	-0.371168
49H	4.255148	2.661075	1.186687
50H	3.763293	1.350983	2.268364
51H	5.239803	1.194638	1.290199

6ah-Me-019

1C	-2.355496	-1.883631	0.254570
2C	-3.533026	-2.532288	0.517221
3N	-4.737597	-1.933953	0.302973
4C	-4.770424	-0.667368	-0.187221
5C	-3.625742	0.036637	-0.472736
6C	-2.344757	-0.552430	-0.258491
7N	-1.114164	-0.012542	-0.469797
8S	-0.872078	1.456293	-1.074507
9O	0.547279	1.568234	-1.447254
10O	-1.893423	1.969621	-2.008084
11C	-1.015271	2.607075	0.423431
12F	-0.086320	2.304878	1.348432
13F	-2.230559	2.488603	0.993564
14F	-0.842092	3.883387	0.047590
15C	-5.979991	-2.688375	0.548606
16H	-1.415443	-2.391425	0.440048
17H	-3.565728	-3.544106	0.905459
18H	-5.754472	-0.239000	-0.340459
19H	-3.725873	1.039275	-0.865330
20H	-6.821856	-1.996046	0.573358
21H	-6.128466	-3.419173	-0.251419
22H	-5.906490	-3.200808	1.509934
23P	3.222001	-0.829654	0.190663
24C	2.531095	-1.330391	1.807175
25C	1.285894	-0.536571	2.225494
26C	3.380859	0.985062	0.129823
27C	4.863854	-1.611267	0.029732
28C	2.134226	-1.385152	-1.162725
29C	5.555195	-1.353580	-1.315678
30C	2.004720	-2.910639	-1.266289
31C	4.216839	1.573078	1.275025
32H	3.335967	-1.215827	2.543126
33H	2.315799	-2.403019	1.735596
34H	0.893123	-0.945783	3.163137
35H	1.526047	0.517467	2.394831
36H	0.494020	-0.583243	1.472220
37H	2.360945	1.381800	0.129450
38H	3.810511	1.234269	-0.847040
39H	4.719808	-2.684617	0.201339
40H	5.468732	-1.233809	0.862401
41H	2.542891	-0.959517	-2.086653
42H	1.159997	-0.912170	-1.003026
43H	6.524888	-1.862979	-1.328094
44H	4.966123	-1.736181	-2.156181
45H	5.736699	-0.285890	-1.480955
46H	1.341942	-3.158541	-2.102504
47H	2.969838	-3.395719	-1.449648
48H	1.569885	-3.344484	-0.358485
49H	4.264094	2.661561	1.162439
50H	3.769995	1.359077	2.252364
51H	5.244633	1.192874	1.272837

6ah-Me-020

1C	-2.362786	1.839567	-0.146823
2C	-3.557580	2.500359	-0.259619
3N	-4.740220	1.884694	0.018200
4C	-4.733699	0.584306	0.410643
5C	-3.569902	-0.133611	0.545234
6C	-2.311963	0.474432	0.262610
7N	-1.068920	-0.075500	0.328521
8S	-0.783264	-1.605932	0.717859
9O	-1.721888	-2.254246	1.653727
10O	0.662678	-1.750573	0.959821
11C	-1.043078	-2.534754	-0.912130
12F	-2.304543	-2.357945	-1.351308
13F	-0.826788	-3.848158	-0.748182
14F	-0.199489	-2.076758	-1.855234
15C	-6.006924	2.615955	-0.169632
16H	-1.440927	2.361810	-0.378517
17H	-3.620791	3.535600	-0.575399
18H	-5.701408	0.140141	0.614066
19H	-3.636577	-1.162061	0.872519
20H	-6.806609	2.090240	0.353354
21H	-5.906930	3.622095	0.242502
22H	-6.241037	2.672974	-1.236505
23P	3.122430	0.670680	0.096587
24C	1.908492	0.713419	-1.272349
25C	1.597905	2.101755	-1.850383
26C	3.813137	-1.017945	0.176103
27C	4.462756	1.872676	-0.220385
28C	2.348856	1.058618	1.705505
29C	5.284249	1.576144	-1.482889
30C	1.587283	2.388769	1.773291
31C	4.803309	-1.241208	1.326264
32H	1.000513	0.247146	-0.878380
33H	2.304200	0.051563	-2.051974
34H	0.848469	1.995388	-2.642872
35H	1.191648	2.783080	-1.096751
36H	2.484088	2.569653	-2.291208
37H	4.285819	-1.206534	-0.795076
38H	2.953952	-1.692379	0.257662
39H	5.101065	1.881168	0.671093
40H	3.991411	2.860335	-0.282646
41H	3.161018	1.037653	2.442112
42H	1.682874	0.217301	1.924381
43H	6.030609	2.365386	-1.624617
44H	5.818365	0.623513	-1.402506
45H	4.657507	1.543891	-2.380664
46H	1.216079	2.534306	2.793803
47H	2.224388	3.244629	1.523968
48H	0.722752	2.386674	1.103492
49H	5.194726	-2.262768	1.270342
50H	4.320209	-1.123727	2.301935
51H	5.655086	-0.553303	1.275788

6ah-PhNCO2-001

1C	-3.932632	1.043817	-0.039845
2C	-5.022797	1.670153	0.564326
3N	-5.221665	1.699786	1.892551
4C	-4.309688	1.092818	2.667226
5C	-3.179691	0.444573	2.164939
6C	-2.994618	0.423716	0.784486
7N	-1.840044	-0.224397	0.222991
8S	-1.887329	-1.875501	0.005527
9O	-3.202873	-2.332811	0.464680
10O	-0.679056	-2.548346	0.486047
11C	-1.916207	-2.162591	-1.890654
12F	-2.771246	-3.174338	-2.124571
13F	-0.721749	-2.509908	-2.366372
14F	-2.364397	-1.073892	-2.526820
15C	-0.721230	0.540029	-0.373419
16O	0.059209	-0.150458	-1.067890
17N	-0.755459	1.799008	-0.017024
18C	0.125701	2.729923	-0.569214
19C	0.387098	3.892851	0.190797
20C	1.218467	4.905249	-0.289191
21C	1.812995	4.797671	-1.552915
22C	1.553560	3.658261	-2.324433
23C	0.729248	2.636812	-1.847177
24H	-3.810867	1.044010	-1.118101
25H	-5.773125	2.167801	-0.046016
26H	-4.488531	1.126720	3.739784
27H	-2.460823	-0.026972	2.827731
28H	-0.084820	3.983494	1.166599

29H	1.399557	5.785507	0.324639
30H	2.457619	5.587498	-1.931086
31H	1.998539	3.560697	-3.313252
32H	0.548447	1.758770	-2.456494
33P	3.333698	-0.850026	0.775089
34C	2.598127	-0.608525	2.430089
35C	1.120213	-0.196506	2.413800
36C	3.203160	0.675051	-0.209954
37C	5.089892	-1.289799	1.033103
38C	2.480001	-2.175201	-0.136140
39C	5.846575	-1.634445	-0.256595
40C	2.495769	-3.539765	0.561636
41C	3.753240	1.934268	0.468708
42H	3.215232	0.146937	2.931663
43H	2.740620	-1.548858	2.976241
44H	0.771638	-0.065335	3.444574
45H	0.963362	0.747983	1.885270
46H	0.497513	-0.959097	1.939651
47H	2.142104	0.779807	-0.456524
48H	3.720915	0.477189	-1.156370
49H	5.105266	-2.132469	1.734617
50H	5.555570	-0.440370	1.547073
51H	2.958798	-2.225909	-1.121791
52H	1.456644	-1.822277	-0.298767
53H	6.890380	-1.865400	-0.016550
54H	5.418237	-2.509888	-0.756433
55H	5.845264	-0.799272	-0.965994
56H	1.966316	-4.266647	-0.063354
57H	3.514128	-3.912781	0.722688
58H	1.981076	-3.504961	1.527314
59H	3.607799	2.788894	-0.199409
60H	3.225632	2.157485	1.401821
61H	4.824660	1.851098	0.685814

6ah-PhNCO2-002

1C	-3.689600	1.700410	-0.436756
2C	-4.712377	2.583385	-0.091543
3N	-5.143487	2.767184	1.167271
4C	-4.540256	2.058802	2.133979
5C	-3.500016	1.157798	1.898950
6C	-3.071697	0.977459	0.584746
7N	-1.995865	0.079448	0.276736
8S	-2.233682	-1.561815	0.387636
9O	-3.575804	-1.778385	0.936345
10O	-1.077970	-2.236620	0.981921
11C	-2.354901	-2.218594	-1.410179
12F	-3.309651	-3.166824	-1.422970
13F	-1.217205	-2.769566	-1.826977
14F	-2.723407	-1.237942	-2.243490
15C	-0.726439	0.558742	-0.324567
16O	-0.138123	-0.286223	-1.036490
17N	-0.436577	1.774740	0.063024
18C	0.665396	2.419705	-0.505149
19C	1.512026	3.164795	0.342495
20C	2.619490	3.850536	-0.162909
21C	2.906741	3.824426	-1.532907
22C	2.058214	3.109513	-2.389363
23C	0.956270	2.416032	-1.888067
24H	-3.374079	1.584132	-1.468629
25H	-5.212457	3.165912	-0.862147
26H	-4.900522	2.221445	3.147484
27H	-3.034751	0.615371	2.715280
28H	1.284272	3.192586	1.405791
29H	3.258148	4.411191	0.516990
30H	3.766246	4.360551	-1.928053
31H	2.259663	3.088955	-3.458737
32H	0.316081	1.853106	-2.560339
33P	3.241840	-1.035057	0.607670
34C	3.173237	-2.813064	0.193287
35C	1.950974	-3.207085	-0.649047
36C	1.820305	-0.590426	1.654532
37C	4.798646	-0.737229	1.518529
38C	3.192936	-0.034163	-0.910249
39C	4.955841	0.705628	2.018679
40C	4.257292	-0.406342	-1.950064
41C	1.812718	-1.265915	3.030465
42H	3.189528	-3.357804	1.145229
43H	4.108741	-3.051973	-0.326781
44H	1.976069	-4.286382	-0.837731
45H	1.012324	-2.971971	-0.140868
46H	1.947424	-2.695695	-1.616888
47H	0.934183	-0.868812	1.079687
48H	1.816456	0.501522	1.739705
49H	5.621321	-1.012698	0.847777
50H	4.814355	-1.448192	2.353401

51H	3.292632	1.011598	-0.599882
52H	2.177062	-0.140072	-1.305535
53H	5.904893	0.804404	2.557217
54H	4.963079	1.423453	1.191591
55H	4.149834	0.986283	2.705366
56H	4.152950	0.256648	-2.815897
57H	5.275544	-0.287166	-1.561848
58H	4.141042	-1.436457	-2.305107
59H	0.907671	-0.965612	3.569519
60H	1.796279	-2.358125	2.945340
61H	2.677551	-0.978602	3.639153

6ah-PhNCO2-003

1C	-2.564144	2.281981	1.013011
2C	-3.038975	2.984402	2.119485
3N	-3.044842	2.491688	3.369777
4C	-2.558164	1.253819	3.542499
5C	-2.046342	0.470984	2.506104
6C	-2.051770	0.998768	1.214866
7N	-1.517863	0.257127	0.110693
8S	-2.279259	-1.133904	-0.395163
9O	-3.340043	-1.439937	0.570361
10O	-1.306059	-2.164915	-0.761666
11C	-3.226141	-0.695747	-2.005316
12F	-4.400754	-1.351586	-1.967246
13F	-2.570984	-1.079896	-3.096648
14F	-3.476759	0.617461	-2.053512
15C	-0.455502	0.824517	-0.779247
16O	-0.503486	0.425103	-1.958588
17N	0.331926	1.620192	-0.096459
18C	1.383370	2.316326	-0.692452
19C	2.094328	3.199089	0.156077
20C	3.192373	3.925659	-0.298516
21C	3.627146	3.798855	-1.625367
22C	2.933579	2.936925	-2.480881
23C	1.828773	2.203989	-2.034010
24H	-2.577964	2.724788	0.022778
25H	-3.437500	3.988865	1.995591
26H	-2.570516	0.868196	4.559753
27H	-1.656083	-0.521581	2.700959
28H	1.759726	3.293313	1.186752
29H	3.713022	4.594007	0.384562
30H	4.484011	4.364280	-1.983725
31H	3.251716	2.830266	-3.516527
32H	1.304582	1.544118	-2.713622
33P	2.433575	-1.838374	0.689924
34C	2.474957	-3.654836	0.883824
35C	1.155984	-4.346852	0.510425
36C	1.161645	-1.128571	1.785952
37C	4.082070	-1.190875	1.139233
38C	2.046541	-1.406698	-1.035442
39C	4.192372	0.337542	1.050272
40C	2.954137	-2.081640	-2.071551
41C	1.444461	-1.325795	3.280308
42H	2.747830	-3.860601	1.925737
43H	3.300649	-4.017787	0.260077
44H	1.270686	-5.430642	0.622605
45H	0.332406	-4.027949	1.157382
46H	0.866682	-4.142568	-0.525232
47H	0.218013	-1.599588	1.492587
48H	1.070863	-0.067803	1.524857
49H	4.803476	-1.679112	0.473196
50H	4.294874	-1.545636	2.154731
51H	2.120419	-0.317748	-1.104368
52H	0.994907	-1.656870	-1.203139
53H	5.203985	0.646011	1.336493
54H	4.005074	0.702908	0.036164
55H	3.486623	0.835139	1.722590
56H	2.662448	-1.740734	-3.070819
57H	4.009184	-1.822785	-1.925930
58H	2.857294	-3.172896	-2.050281
59H	0.635508	-0.871934	3.862930
60H	1.498534	-2.385701	3.553932
61H	2.378509	-0.841785	3.585794

6ah-PhNCO2-004

1C	-2.342436	-1.898661	-2.027480
2C	-2.591046	-3.271766	-1.994500
3N	-2.785249	-3.969460	-0.864070
4C	-2.726542	-3.289698	0.291665
5C	-2.458953	-1.922837	0.372582
6C	-2.268828	-1.211978	-0.815324

7N	-1.946848	0.185752	-0.811562
8S	-3.027531	1.277010	-0.172687
9O	-4.276306	0.550437	0.086682
10O	-3.045967	2.522765	-0.934366
11C	-2.410405	1.747387	1.582825
12F	-1.607495	0.790689	2.079929
13F	-3.495374	1.829155	2.377566
14F	-1.788698	2.921793	1.614235
15C	-0.564114	0.622304	-1.202915
16O	-0.003450	-0.103878	-2.045200
17N	-0.198846	1.660469	-0.494268
18C	0.998201	2.326216	-0.753876
19C	1.621385	2.421137	-2.019950
20C	2.818987	3.121375	-2.175534
21C	3.437982	3.743343	-1.083324
22C	2.822360	3.671361	0.172592
23C	1.619378	2.981335	0.332723
24H	-2.193339	-1.376997	-2.964896
25H	-2.642008	-3.835534	-2.923385
26H	-2.890659	-3.865411	1.200206
27H	-2.406967	-1.429134	1.336141
28H	1.164032	1.933145	-2.873485
29H	3.275583	3.179074	-3.161949
30H	4.373153	4.283089	-1.211421
31H	3.278112	4.160065	1.031674
32H	1.137064	2.934695	1.306147
33P	2.570774	-1.676660	0.605425
34C	2.196579	-3.308822	-0.123063
35C	0.934831	-3.318641	-0.998612
36C	1.116390	-1.041979	1.506557
37C	3.975220	-1.878483	1.758036
38C	2.998757	-0.485472	-0.699942
39C	4.462447	-0.560233	2.376336
40C	4.211207	-0.887073	-1.548046
41C	0.604567	-1.967543	2.616804
42H	2.109609	-4.020621	0.706503
43H	3.082931	-3.598818	-0.700113
44H	0.810729	-4.311212	-1.444779
45H	0.038532	-3.103055	-0.410795
46H	0.987260	-2.581589	-1.804683
47H	0.343229	-0.861943	0.755175
48H	1.397701	-0.060866	1.904504
49H	4.778188	-2.369414	1.195770
50H	3.651153	-2.583732	2.532501
51H	3.164024	0.476468	-0.202570
52H	2.099986	-0.365337	-1.315329
53H	5.286959	-0.765429	3.067806
54H	4.830304	0.133279	1.612531
55H	3.669431	-0.056868	2.940006
56H	4.388927	-0.111341	-2.300579
57H	5.123148	-0.984528	-0.947681
58H	4.043293	-1.831149	-2.078219
59H	-0.257657	-1.502414	3.106422
60H	0.281502	-2.936899	2.222247
61H	1.365334	-2.144068	3.385352

6ah-PhNCO2-005

1C	-3.776837	1.675073	-0.441643
2C	-4.751517	2.612275	-0.101330
3N	-5.145772	2.852266	1.160511
4C	-4.552020	2.146488	2.134732
5C	-3.556988	1.194525	1.904410
6C	-3.166761	0.956465	0.587557
7N	-2.143141	-0.003130	0.287825
8S	-2.467633	-1.629202	0.476280
9O	-3.821675	-1.740243	1.028686
10O	-1.358783	-2.345063	1.106904
11C	-2.625572	-2.357595	-1.291406
12F	-3.636259	-3.246144	-1.264894
13F	-1.523432	-2.996837	-1.676288
14F	-2.931553	-1.397328	-2.172587
15C	-0.884011	0.375746	-0.393588
16O	-0.326408	-0.567801	-0.997505
17N	-0.582396	1.634285	-0.187813
18C	0.513503	2.221253	-0.818867
19C	1.033677	3.395665	-0.224603
20C	2.121379	4.072849	-0.776617
21C	2.724228	3.610788	-1.953845
22C	2.209099	2.462653	-2.566943
23C	1.128581	1.771174	-2.014276
24H	-3.490406	1.515071	-1.475957
25H	-5.243090	3.193467	-0.878376
26H	-4.882258	2.353544	3.150412
27H	-3.098576	0.655016	2.726635
28H	0.560852	3.761644	0.684053

29H	2.497879	4.969187	-0.287550
30H	3.569436	4.139158	-2.388401
31H	2.655161	2.094043	-3.489269
32H	0.754180	0.878705	-2.500578
33P	3.602163	-0.819153	0.725914
34C	2.661787	-1.074978	2.271080
35C	1.266594	-0.436533	2.258258
36C	3.849561	0.963061	0.436294
37C	5.221600	-1.644368	0.923896
38C	2.706951	-1.511391	-0.699946
39C	6.157022	-1.489415	-0.283629
40C	2.449580	-3.021589	-0.615782
41C	4.582675	1.691846	1.568542
42H	3.281495	-0.669069	3.080108
43H	2.598730	-2.158434	2.429134
44H	0.777959	-0.612639	3.222908
45H	1.314092	0.645338	2.098084
46H	0.634825	-0.873174	1.482002
47H	2.857486	1.394436	0.268142
48H	4.393423	1.055757	-0.509896
49H	5.010690	-2.701447	1.124733
50H	5.680148	-1.234724	1.831692
51H	3.292968	-1.254194	-1.590706
52H	1.756030	-0.968555	-0.772581
53H	7.091867	-2.027668	-0.092253
54H	5.714662	-1.904113	-1.196276
55H	6.408915	-0.439704	-0.470657
56H	1.886568	-3.334540	-1.501575
57H	3.379277	-3.601739	-0.583616
58H	1.845224	-3.278507	0.260760
59H	4.683257	2.750370	1.305667
60H	4.030075	1.636657	2.512911
61H	5.588909	1.290392	1.733074

6ah-PhNCO2-006

1C	-2.959752	2.113894	0.693684
2C	-3.561616	2.918071	1.660970
3N	-3.528042	2.651708	2.977552
4C	-2.870547	1.548370	3.364731
5C	-2.226016	0.681977	2.479879
6C	-2.274510	0.974735	1.117977
7N	-1.618404	0.126357	0.163213
8S	-2.294686	-1.350946	-0.202654
9O	-3.426816	-1.554178	0.707400
10O	-1.273768	-2.391815	-0.341583
11C	-3.107005	-1.168907	-1.931099
12F	-4.273563	-1.838362	-1.895600
13F	-2.357581	-1.689226	-2.898634
14F	-3.365841	0.118513	-2.189661
15C	-0.528541	0.638026	-0.718249
16O	-0.409810	0.027561	-1.799897
17N	0.110510	1.622519	-0.133654
18C	1.107533	2.347437	-0.784882
19C	1.862224	3.228207	0.026984
20C	2.891392	4.007853	-0.498774
21C	3.202360	3.945433	-1.863668
22C	2.458171	3.090220	-2.684413
23C	1.430113	2.298300	-2.164699
24H	-3.013032	2.369571	-0.359373
25H	-4.100523	3.815281	1.364911
26H	-2.854245	1.346203	4.433633
27H	-1.702047	-0.196216	2.841980
28H	1.615293	3.283532	1.084922
29H	3.450478	4.670896	0.158693
30H	4.002110	4.554339	-2.278380
31H	2.680790	3.033327	-3.748537
32H	0.876926	1.633169	-2.816003
33P	2.761169	-1.573011	0.764293
34C	2.884049	-3.394117	0.672734
35C	1.720239	-4.058916	-0.076344
36C	1.265245	-1.101011	1.688643
37C	4.246643	-0.956241	1.632272
38C	2.679301	-0.857106	-0.907423
39C	4.261271	0.565803	1.828543
40C	3.786776	-1.337686	-1.853440
41C	1.266827	-1.545253	3.156812
42H	2.947817	-3.758683	1.705144
43H	3.844220	-3.620497	0.193728
44H	1.879307	-5.142743	-0.100256
45H	0.759181	-3.868344	0.410035
46H	1.647837	-3.706342	-1.110572
47H	0.426119	-1.543987	1.144015
48H	1.158869	-0.015042	1.592341
49H	5.115920	-1.287587	1.051727
50H	4.288967	-1.478106	2.595722

51H	2.723036	0.229088	-0.778010
52H	1.683958	-1.073648	-1.309896
53H	5.166615	0.853123	2.374678
54H	4.262798	1.099694	0.873010
55H	3.397233	0.909606	2.407055
56H	3.680544	-0.819473	-2.812648
57H	4.786691	-1.114498	-1.464140
58H	3.721169	-2.414146	-2.045560
59H	0.327982	-1.233021	3.626933
60H	1.339161	-2.634102	3.256244
61H	2.086896	-1.090585	3.723154

6ah-PhNCO2-007

1C	-3.102867	1.995158	0.625308
2C	-3.745587	2.810687	1.555675
3N	-3.727960	2.587603	2.880745
4C	-3.044752	1.517557	3.313579
5C	-2.356820	0.644438	2.468676
6C	-2.388908	0.892142	1.096940
7N	-1.692645	0.035237	0.179806
8S	-2.289623	-1.495068	-0.109139
9O	-3.370233	-1.737035	0.852402
10O	-1.208141	-2.470915	-0.254030
11C	-3.178580	-1.425771	-1.809394
12F	-4.311570	-2.143006	-1.698258
13F	-2.443138	-1.957268	-2.781676
14F	-3.505484	-0.164408	-2.114406
15C	-0.671053	0.565313	-0.771812
16O	-0.567894	-0.087066	-1.830225
17N	-0.066990	1.614387	-0.266974
18C	0.888452	2.333640	-0.986240
19C	1.465318	3.433743	-0.306319
20C	2.457483	4.218104	-0.890987
21C	2.913128	3.936549	-2.186538
22C	2.347858	2.859871	-2.877874
23C	1.354324	2.064175	-2.297548
24H	-3.146097	2.216291	-0.435856
25H	-4.306261	3.680701	1.221262
26H	-3.041967	1.348951	4.388411
27H	-1.814442	-0.204882	2.869143
28H	1.113107	3.651467	0.699592
29H	2.876660	5.054642	-0.335188
30H	3.685581	4.547445	-2.647545
31H	2.682198	2.629987	-3.888178
32H	0.935076	1.232173	-2.848761
33P	3.019236	-1.348031	0.850645
34C	2.223613	-1.985719	2.366550
35C	0.803658	-1.449267	2.593600
36C	3.094496	0.470571	0.919717
37C	4.704924	-2.049281	0.783780
38C	2.083926	-1.843957	-0.631263
39C	5.503226	-1.637920	-0.460737
40C	2.064247	-3.356312	-0.887318
41C	3.831419	1.026728	2.144646
42H	2.888024	-1.719561	3.197811
43H	2.225249	-3.079675	2.293352
44H	0.422271	-1.825421	3.549422
45H	0.781116	-0.355211	2.627278
46H	0.124560	-1.782646	1.804770
47H	2.058002	0.820853	0.890766
48H	3.561997	0.805044	-0.013103
49H	4.592803	-3.138637	0.839161
50H	5.215673	-1.733743	1.700943
51H	2.527319	-1.303120	-1.475162
52H	1.066209	-1.461644	-0.519210
53H	6.494002	-2.104287	-0.428117
54H	5.011592	-1.961356	-1.384662
55H	5.646347	-0.552976	-0.510392
56H	1.448438	-3.557006	-1.769966
57H	3.068204	-3.753484	-1.076131
58H	1.624946	-3.906361	-0.048265
59H	3.834467	2.120711	2.091949
60H	3.336360	0.740838	3.079241
61H	4.874015	0.691440	2.188178

6ah-PhNCO2-008

1C	3.708165	1.765453	0.165421
2C	4.526782	2.765877	-0.358707
3N	4.600906	3.056575	-1.668188
4C	3.835458	2.337868	-2.503729
5C	2.975812	1.321727	-2.082327
6C	2.915937	1.035600	-0.720060

7N	2.036448	0.010706	-0.231021
8S	2.494568	-1.583540	-0.390784
9O	3.799767	-1.588571	-1.060654
10O	1.415151	-2.434314	-0.892847
11C	2.866876	-2.209066	1.384748
12F	3.966320	-2.981659	1.310893
13F	1.873363	-2.945412	1.876684
14F	3.126060	-1.182936	2.204400
15C	0.829877	0.323118	0.567707
16O	0.373173	-0.652072	1.204791
17N	0.464407	1.572032	0.410623
18C	-0.615634	2.108857	1.108948
19C	-1.123409	3.338297	0.623069
20C	-2.212925	3.967625	1.223735
21C	-2.832263	3.400142	2.345373
22C	-2.328644	2.197762	2.854461
23C	-1.243372	1.554485	2.253342
24H	3.678149	1.565152	1.231524
25H	5.155051	3.358535	0.302550
26H	3.909344	2.587062	-3.560166
27H	2.367499	0.769806	-2.791943
28H	-0.641353	3.782082	-0.245141
29H	-2.579411	4.908016	0.816561
30H	-3.680475	3.890040	2.817571
31H	-2.786932	1.748043	3.733863
32H	-0.878456	0.619011	2.658397
33P	-3.461375	-0.871066	-0.854109
34C	-2.463225	-1.073104	-2.369653
35C	-1.069757	-0.434736	-2.289279
36C	-3.713226	0.900033	-0.502022
37C	-5.077608	-1.668465	-1.161730
38C	-2.634927	-1.639489	0.573789
39C	-6.040872	-1.615266	0.031132
40C	-2.395800	-3.147763	0.426291
41C	-4.310644	1.695915	-1.669547
42H	-3.053757	-0.639794	-3.186109
43H	-2.390985	-2.150014	-2.562649
44H	-0.559456	-0.559468	-3.250984
45H	-1.120813	0.636675	-2.070551
46H	-0.455624	-0.915276	-1.524751
47H	-2.741337	1.307891	-0.208093
48H	-4.356165	0.952515	0.383664
49H	-4.866462	-2.704702	-1.451361
50H	-5.509933	-1.174257	-2.040137
51H	-3.255392	-1.417849	1.450909
52H	-1.681645	-1.115594	0.717184
53H	-6.971764	-2.131711	-0.227964
54H	-5.618929	-2.109241	0.913330
55H	-6.294462	-0.584736	0.302833
56H	-1.882905	-3.513685	1.322149
57H	-3.331167	-3.708912	0.318202
58H	-1.751910	-3.371714	-0.430719
59H	-4.458986	2.734356	-1.354531
60H	-3.640416	1.705620	-2.536048
61H	-5.282129	1.300095	-1.987196

6ah-PhNCO2-009

1C	-0.851012	-2.662270	-1.928870
2C	-0.361300	-3.968741	-1.896406
3N	-0.289613	-4.711013	-0.779594
4C	-0.719168	-4.146884	0.359680
5C	-1.210093	-2.843108	0.440350
6C	-1.278356	-2.087348	-0.731536
7N	-1.728564	-0.725212	-0.717806
8S	-3.332567	-0.399768	-0.404880
9O	-4.001074	-1.693548	-0.215315
10O	-3.895571	0.581164	-1.329886
11C	-3.402061	0.413029	1.330607
12F	-2.303737	0.123367	2.042866
13F	-4.463954	-0.117055	1.970041
14F	-3.573549	1.729560	1.269347
15C	-0.749657	0.379692	-0.933967
16O	0.310311	0.037652	-1.497002
17N	-1.187442	1.493219	-0.407645
18C	-0.505384	2.695103	-0.586658
19C	0.268847	3.029663	-1.723160
20C	0.871872	4.284329	-1.833176
21C	0.735252	5.240929	-0.819415
22C	-0.030649	4.923800	0.309292
23C	-0.645484	3.675685	0.421095
24H	-0.888824	-2.099105	-2.853990
25H	-0.013206	-4.441461	-2.812270
26H	-0.659117	-4.761350	1.255427
27H	-1.538707	-2.434026	1.389616
28H	0.387147	2.299289	-2.516004

29H	1.454776	4.516587	-2.722793
30H	1.210027	6.214949	-0.910314
31H	-0.156799	5.655668	1.104840
32H	-1.250770	3.435976	1.291895
33P	3.355944	-0.412079	0.563398
34C	5.117306	-0.687887	0.971130
35C	6.016192	-0.946438	-0.245253
36C	2.698320	-1.845537	-0.351388
37C	2.468280	-0.229456	2.148031
38C	3.182100	1.087986	-0.454293
39C	0.961498	0.017910	2.001438
40C	3.528583	2.389076	0.281055
41C	2.841943	-3.173825	0.402331
42H	5.152585	-1.530306	1.671743
43H	5.450693	0.198688	1.523718
44H	7.051059	-1.079984	0.088891
45H	5.720533	-1.853122	-0.784430
46H	5.999456	-0.108254	-0.950847
47H	3.225665	-1.875610	-1.312278
48H	1.653586	-1.609353	-0.580124
49H	2.954676	0.592161	2.687148
50H	2.667035	-1.144931	2.718634
51H	2.149129	1.091494	-0.819823
52H	3.829365	0.941102	-1.327662
53H	0.510191	0.096462	2.996554
54H	0.746332	0.943636	1.461653
55H	0.468877	-0.801481	1.470721
56H	3.436343	3.227567	-0.416236
57H	2.837525	2.578619	1.108843
58H	4.552556	2.386523	0.673273
59H	2.414763	-3.980902	-0.200559
60H	3.891099	-3.420487	0.601815
61H	2.304894	-3.159059	1.357011

6ah-PhNCO2-010

1C	-2.048521	-0.917648	2.349781
2C	-1.948669	-1.930157	3.302169
3N	-1.583137	-3.191940	3.015478
4C	-1.305676	-3.471993	1.733888
5C	-1.362444	-2.529714	0.705171
6C	-1.737675	-1.224427	1.023066
7N	-1.776752	-0.204035	0.016607
8S	-2.937091	-0.280835	-1.181700
9O	-3.648305	-1.553798	-1.017951
10O	-2.399961	0.094155	-2.487693
11C	-4.247682	1.047326	-0.734543
12F	-5.457204	0.520783	-1.001423
13F	-4.108129	2.155573	-1.455178
14F	-4.192126	1.335787	0.571810
15C	-0.998158	1.064135	0.148617
16O	-1.469397	2.029984	-0.479605
17N	0.045062	0.881625	0.924729
18C	0.919498	1.919420	1.243359
19C	1.820070	1.666769	2.306350
20C	2.791214	2.594856	2.679047
21C	2.902792	3.816123	2.000222
22C	2.015874	4.086406	0.952107
23C	1.036468	3.162855	0.573805
24H	-2.339970	0.088292	2.631768
25H	-2.176071	-1.720158	4.344947
26H	-1.015873	-4.497769	1.515734
27H	-1.123487	-2.807759	-0.315355
28H	1.733448	0.719996	2.834124
29H	3.461423	2.366690	3.505850
30H	3.658030	4.543220	2.288905
31H	2.082934	5.032384	0.417535
32H	0.360172	3.391336	-0.240523
33P	3.158983	-0.990207	-1.026513
34C	2.130192	-1.755575	-2.325771
35C	0.720098	-1.155730	-2.419321
36C	2.477346	-1.371111	0.618593
37C	4.851346	-1.662754	-1.179331
38C	3.186734	0.818388	-1.251828
39C	5.834134	-1.113278	-0.136464
40C	3.698146	1.269670	-2.625966
41C	2.410041	-2.868378	0.943006
42H	2.092382	-2.828460	-2.102262
43H	2.672569	-1.644564	-3.272275
44H	0.135534	-1.705734	-3.163909
45H	0.189619	-1.212809	-1.466193
46H	0.745376	-0.105663	-2.725576
47H	1.488623	-0.895235	0.666192
48H	3.104699	-0.840274	1.342829
49H	5.190630	-1.439351	-2.197697
50H	4.766070	-2.753510	-1.104441

51H	3.798185	1.231481	-0.442096
52H	2.164802	1.167780	-1.078763
53H	6.824518	-1.551470	-0.302129
54H	5.933966	-0.024478	-0.205747
55H	5.525291	-1.364667	0.884169
56H	3.674202	2.363653	-2.674372
57H	4.730097	0.949491	-2.807361
58H	3.069242	0.887120	-3.437531
59H	1.955927	-2.998898	1.930956
60H	1.793509	-3.416981	0.223101
61H	3.404318	-3.329837	0.966685

6ah-PhNCO2-011

1C	-2.234834	0.916279	2.327579
2C	-2.372395	0.836366	3.712431
3N	-1.951932	-0.208941	4.445379
4C	-1.366260	-1.220430	3.788070
5C	-1.167964	-1.235081	2.406131
6C	-1.613122	-0.142656	1.661917
7N	-1.416221	-0.090434	0.240429
8S	-2.322694	-1.090355	-0.741200
9O	-2.930787	-2.117308	0.111983
10O	-1.560658	-1.479051	-1.927120
11C	-3.816403	-0.058871	-1.363964
12F	-4.891148	-0.868201	-1.367255
13F	-3.636257	0.400367	-2.597834
14F	-4.052476	0.956321	-0.522859
15C	-0.778325	1.112935	-0.401003
16O	-1.241073	1.418241	-1.513927
17N	0.165147	1.582903	0.379781
18C	0.883701	2.736221	0.061877
19C	1.743365	3.223667	1.075594
20C	2.547269	4.344322	0.876128
21C	2.525878	5.022935	-0.350011
22C	1.680799	4.557062	-1.362819
23C	0.869457	3.434058	-1.171690
24H	-2.588205	1.784670	1.781843
25H	-2.846995	1.648177	4.258989
26H	-1.033820	-2.060945	4.393944
27H	-0.682586	-2.076048	1.925098
28H	1.759514	2.696672	2.026870
29H	3.193573	4.690750	1.680377
30H	3.151046	5.898244	-0.509583
31H	1.648388	5.073099	-2.320804
32H	0.224218	3.088112	-1.969177
33P	2.832233	-1.690931	-0.419830
34C	4.256803	-2.816297	-0.211448
35C	4.348277	-3.463955	1.176824
36C	2.881233	-0.384004	0.847693
37C	2.922232	-0.988155	-2.100966
38C	1.269742	-2.609834	-0.214295
39C	1.745548	-0.069791	-2.455548
40C	1.022318	-3.696736	-1.266227
41C	4.141478	0.489939	0.800749
42H	5.155939	-2.228297	-0.430678
43H	4.179081	-3.577894	-0.996528
44H	5.220072	-4.126408	1.212597
45H	4.464851	-2.715258	1.967876
46H	3.462337	-4.066956	1.404225
47H	2.788212	-0.893085	1.815237
48H	1.970968	0.217281	0.718594
49H	2.985862	-1.841044	-2.787786
50H	3.877084	-0.452639	-2.165605
51H	0.476640	-1.857273	-0.238530
52H	1.285234	-3.031491	0.797134
53H	1.867902	0.293195	-3.482006
54H	0.783612	-0.586786	-2.397168
55H	1.702776	0.802704	-1.798949
56H	0.059166	-4.177840	-1.066282
57H	0.975455	-3.277328	-2.276055
58H	1.796727	-4.471702	-1.244154
59H	4.103790	1.217540	1.617472
60H	5.059051	-0.098869	0.917364
61H	4.207044	1.055097	-0.134890

6ah-PhNCO2-012

1C	2.403313	-1.492712	2.061089
2C	2.677637	-1.592485	3.424476
3N	2.498964	-0.586160	4.297206
4C	2.028204	0.571544	3.810252
5C	1.710245	0.772660	2.465892
6C	1.901325	-0.284156	1.576064

7N	1.565071	-0.144705	0.188594
8S	2.499964	0.840371	-0.779073
9O	3.474661	1.512454	0.086898
10O	1.676627	1.629639	-1.697439
11C	3.561067	-0.320184	-1.878820
12F	4.792862	0.216430	-1.950448
13F	3.077447	-0.420477	-3.112998
14F	3.659918	-1.532220	-1.320547
15C	0.585851	-1.054565	-0.488243
16O	0.747276	-1.153293	-1.719753
17N	-0.269006	-1.532569	0.381570
18C	-1.333859	-2.347545	0.006901
19C	-2.156112	-2.810205	1.064359
20C	-3.294526	-3.577490	0.824035
21C	-3.659414	-3.916027	-0.486471
22C	-2.853806	-3.478580	-1.543073
23C	-1.708625	-2.709081	-1.312844
24H	2.559913	-2.335086	1.395766
25H	3.063329	-2.522892	3.835065
26H	1.893347	1.377919	4.528194
27H	1.330267	1.728543	2.121874
28H	-1.873235	-2.547178	2.081239
29H	-3.900642	-3.914600	1.662829
30H	-4.547492	-4.513742	-0.677246
31H	-3.115671	-3.739372	-2.567079
32H	-1.097874	-2.381660	-2.144816
33P	-2.533111	1.858789	-0.072604
34C	-4.347136	1.854606	-0.290876
35C	-4.948664	0.446890	-0.419092
36C	-1.736969	1.060168	-1.501513
37C	-1.971172	3.593148	0.051865
38C	-2.098695	0.957350	1.448986
39C	-0.477814	3.731104	0.382607
40C	-2.627759	1.603471	2.735669
41C	-2.146697	1.644152	-2.858769
42H	-4.558813	2.457274	-1.182339
43H	-4.774584	2.388956	0.565813
44H	-6.029287	0.527222	-0.580582
45H	-4.522893	-0.104171	-1.264371
46H	-4.787785	-0.147584	0.486400
47H	-1.971622	-0.006858	-1.443502
48H	-0.657347	1.154859	-1.358943
49H	-2.592467	4.079078	0.813409
50H	-2.207771	4.068932	-0.906814
51H	-1.009944	0.856927	1.465549
52H	-2.485473	-0.059302	1.327021
53H	-0.203541	4.791676	0.390990
54H	-0.247130	3.320296	1.371780
55H	0.154066	3.227267	-0.355724
56H	-2.328551	0.989184	3.591937
57H	-2.219943	2.608987	2.889019
58H	-3.721773	1.670874	2.740421
59H	-1.593075	1.120620	-3.645561
60H	-3.216371	1.513546	-3.056819
61H	-1.904537	2.710173	-2.937537

6ah-PhNCO2-013

1C	-2.437600	1.049512	2.231590
2C	-2.722680	0.976555	3.594222
3N	-2.495915	-0.113099	4.347481
4C	-1.960053	-1.179046	3.734753
5C	-1.624317	-1.206886	2.380165
6C	-1.871252	-0.067760	1.613358
7N	-1.529909	-0.026789	0.221309
8S	-2.359295	-0.988972	-0.857556
9O	-3.114469	-1.982485	-0.087163
10O	-1.483048	-1.412046	-1.949031
11C	-3.712494	0.108419	-1.658357
12F	-4.819448	-0.646822	-1.784644
13F	-3.358396	0.535493	-2.866263
14F	-3.998055	1.148198	-0.865067
15C	-0.735135	1.117482	-0.350486
16O	-1.092540	1.482529	-1.484794
17N	0.198564	1.478654	0.497145
18C	1.038935	2.565347	0.247154
19C	1.848716	2.980269	1.332302
20C	2.763088	4.024493	1.205140
21C	2.908814	4.694180	-0.017285
22C	2.117049	4.298315	-1.100512
23C	1.194762	3.253595	-0.981919
24H	-2.638465	1.954858	1.668635
25H	-3.159345	1.832419	4.104029
26H	-1.782822	-2.054703	4.355900
27H	-1.186702	-2.092544	1.934818
28H	1.737045	2.458027	2.279925

29H	3.364761	4.317834	2.063274
30H	3.621419	5.509010	-0.120277
31H	2.214810	4.808825	-2.057010
32H	0.592333	2.961797	-1.832685
33P	2.842017	-1.734187	-0.356685
34C	4.034521	-3.107319	-0.173257
35C	4.255896	-3.557910	1.276749
36C	3.444899	-0.256746	0.523053
37C	2.672454	-1.384614	-2.139764
38C	1.241415	-2.192563	0.381796
39C	1.783257	-0.176434	-2.462041
40C	0.592907	-3.444820	-0.218732
41C	4.728930	0.351346	-0.054143
42H	4.973199	-2.767349	-0.626796
43H	3.665082	-3.934734	-0.790680
44H	4.995367	-4.365964	1.296987
45H	4.636169	-2.742164	1.901472
46H	3.333171	-3.937096	1.729837
47H	3.578853	-0.549542	1.571506
48H	2.621237	0.463744	0.501965
49H	2.282708	-2.298494	-2.604405
50H	3.691901	-1.243189	-2.519077
51H	0.595913	-1.315404	0.274303
52H	1.427713	-2.313942	1.455571
53H	1.792398	-0.001891	-3.543794
54H	0.745649	-0.343082	-2.166291
55H	2.138839	0.736247	-1.974139
56H	-0.360188	-3.637315	0.286124
57H	0.373622	-3.314336	-1.282242
58H	1.222599	-4.332768	-0.092991
59H	5.014245	1.221818	0.545812
60H	5.564434	-0.358093	-0.037212
61H	4.584226	0.694744	-1.083957

6ah-PhNCO2-014

1C	-2.808279	1.444686	1.857386
2C	-3.222403	1.636329	3.175081
3N	-2.985294	0.760681	4.166253
4C	-2.305863	-0.352479	3.851607
5C	-1.836349	-0.635687	2.568059
6C	-2.095749	0.283735	1.552415
7N	-1.624090	0.056989	0.216921
8S	-2.326138	-1.131080	-0.710706
9O	-3.211665	-1.911540	0.159868
10O	-1.327946	-1.804972	-1.541525
11C	-3.519873	-0.253246	-1.928250
12F	-4.618718	-1.023186	-2.036493
13F	-2.988734	-0.113129	-3.139504
14F	-3.884477	0.939835	-1.443749
15C	-0.722963	1.039236	-0.471484
16O	-0.902367	1.134524	-1.699957
17N	0.096441	1.581474	0.397693
18C	1.030301	2.549990	0.026651
19C	1.742925	3.156869	1.089203
20C	2.742400	4.099396	0.855880
21C	3.073403	4.472847	-0.454205
22C	2.379228	3.885066	-1.516736
23C	1.371766	2.940911	-1.292554
24H	-3.025388	2.181333	1.090902
25H	-3.776303	2.532417	3.445932
26H	-2.122908	-1.051844	4.664758
27H	-1.286043	-1.547137	2.363934
28H	1.489452	2.861600	2.105021
29H	3.265292	4.546382	1.699234
30H	3.852781	5.207945	-0.640355
31H	2.620782	4.164142	-2.540922
32H	0.846977	2.497521	-2.129079
33P	2.851470	-1.736537	-0.046463
34C	4.060504	-2.994200	0.500048
35C	4.343147	-2.975534	2.008160
36C	3.491787	-0.066677	0.300592
37C	2.596166	-1.958863	-1.840819
38C	1.288350	-1.939436	0.870919
39C	1.833300	-0.814978	-2.522828
40C	0.657022	-3.331805	0.742774
41C	4.796813	0.281950	-0.424294
42H	4.976108	-2.815017	-0.076065
43H	3.671499	-3.969338	0.183466
44H	5.100758	-3.730154	2.246261
45H	4.724949	-2.003260	2.338913
46H	3.445724	-3.209242	2.591154
47H	3.607860	0.005710	1.388150
48H	2.694672	0.631203	0.028596
49H	2.066875	-2.911550	-1.962281
50H	3.593147	-2.089303	-2.279268

51H	0.615061	-1.156435	0.510506
52H	1.513599	-1.697895	1.916827
53H	1.740548	-1.036596	-3.592047
54H	0.823487	-0.696255	-2.124639
55H	2.358157	0.140878	-2.423566
56H	-0.280104	-3.361704	1.308718
57H	0.414807	-3.573270	-0.296349
58H	1.311963	-4.113465	1.143984
59H	5.078269	1.310269	-0.173464
60H	5.621228	-0.376834	-0.128789
61H	4.682925	0.226803	-1.512355

6ah-PhNCO2-015

1C	3.083426	1.990944	-1.003523
2C	3.689966	2.658027	-2.066719
3N	3.728130	2.181912	-3.322569
4C	3.135632	0.999099	-3.545413
5C	2.487878	0.255994	-2.557157
6C	2.466168	0.762935	-1.256908
7N	1.801011	0.067562	-0.195604
8S	2.354879	-1.409805	0.318276
9O	3.257269	-1.945238	-0.705683
10O	1.244410	-2.213826	0.828783
11C	3.502602	-1.092584	1.820218
12F	4.512962	-1.978726	1.751927
13F	2.874510	-1.264059	2.979940
14F	4.015789	0.142821	1.753726
15C	0.838781	0.793744	0.710651
16O	0.984447	0.570464	1.925611
17N	0.010400	1.506373	-0.015151
18C	-1.012889	2.264924	0.552343
19C	-1.767988	3.049321	-0.352827
20C	-2.868145	3.794191	0.067157
21C	-3.259435	3.783621	1.413017
22C	-2.518193	3.023385	2.324161
23C	-1.410579	2.274849	1.913002
24H	3.084150	2.418226	-0.005913
25H	4.175324	3.617114	-1.899833
26H	3.171827	0.626729	-4.567020
27H	2.016219	-0.689988	-2.795832
28H	-1.468412	3.048483	-1.398450
29H	-3.425001	4.384308	-0.658133
30H	-4.118441	4.362252	1.744057
31H	-2.803261	3.008734	3.374657
32H	-0.854048	1.687374	2.631949
33P	-3.119424	-1.396227	-0.492711
34C	-2.592571	-2.316733	0.994464
35C	-1.846875	-1.472808	2.035243
36C	-1.698163	-0.942511	-1.536588
37C	-4.237931	-2.497883	-1.431061
38C	-4.005094	0.121677	0.000815
39C	-4.724136	-1.919771	-2.766077
40C	-5.234669	-0.123811	0.886007
41C	-0.847084	-2.138544	-1.985457
42H	-1.970693	-3.148874	0.644353
43H	-3.503860	-2.757166	1.416860
44H	-1.569951	-2.110526	2.882098
45H	-0.924716	-1.046933	1.637155
46H	-2.468691	-0.657269	2.417860
47H	-1.094933	-0.212907	-0.981130
48H	-2.113600	-0.407519	-2.399796
49H	-5.082253	-2.722991	-0.768819
50H	-3.694336	-3.437895	-1.583589
51H	-4.278030	0.646049	-0.921686
52H	-3.274235	0.753929	0.515821
53H	-5.400324	-2.634846	-3.247450
54H	-5.274190	-0.982222	-2.627916
55H	-3.892787	-1.731443	-3.453764
56H	-5.684231	0.840836	1.144863
57H	-5.997305	-0.724745	0.377871
58H	-4.966758	-0.626735	1.822006
59H	-0.035823	-1.776163	-2.625090
60H	-0.389295	-2.649295	-1.133197
61H	-1.428398	-2.867085	-2.562516

6ah-PhNCO2-016

1C	-0.293171	-2.749281	-1.859004
2C	0.485778	-3.896412	-1.698519
3N	0.705871	-4.489896	-0.514270
4C	0.132466	-3.934341	0.565236
5C	-0.645575	-2.777047	0.518346
6C	-0.861673	-2.173104	-0.722795

7N	-1.595308	-0.946484	-0.845094
8S	-3.214859	-0.914185	-0.475768
9O	-3.644781	-2.306970	-0.298126
10O	-3.947155	-0.025295	-1.374383
11C	-3.414049	-0.148892	1.274346
12F	-2.276976	-0.250405	1.980889
13F	-4.361828	-0.861254	1.914913
14F	-3.812005	1.119213	1.230543
15C	-0.834043	0.326979	-1.076250
16O	0.193016	0.201051	-1.771269
17N	-1.390072	1.313673	-0.421338
18C	-0.919621	2.623737	-0.516090
19C	-0.037882	3.131254	-1.501622
20C	0.355470	4.472871	-1.483580
21C	-0.101588	5.347984	-0.492124
22C	-0.979361	4.860078	0.485205
23C	-1.382674	3.525738	0.470480
24H	-0.441953	-2.301805	-2.834548
25H	0.952648	-4.361243	-2.564104
26H	0.311927	-4.431116	1.516412
27H	-1.069363	-2.360378	1.425479
28H	0.332340	2.469561	-2.274834
29H	1.029345	4.836023	-2.257741
30H	0.212077	6.389133	-0.484602
31H	-1.353996	5.524062	1.261858
32H	-2.067862	3.149593	1.225599
33P	3.294960	-0.013633	0.521799
34C	4.221416	-0.643326	1.966101
35C	3.410938	-1.608688	2.843376
36C	1.815395	0.893184	1.075678
37C	4.394563	1.111487	-0.404757
38C	2.774538	-1.395127	-0.544478
39C	3.736780	1.734525	-1.644042
40C	3.935124	-2.172261	-1.177719
41C	2.104840	2.087368	1.992742
42H	4.541804	0.234609	2.539357
43H	5.129355	-1.125832	1.584545
44H	4.020880	-1.928772	3.695075
45H	2.506660	-1.133526	3.239196
46H	3.112133	-2.505618	2.289982
47H	1.157055	0.167507	1.566284
48H	1.308386	1.211583	0.161324
49H	5.284333	0.530696	-0.676145
50H	4.719923	1.884639	0.301160
51H	2.102865	-0.969236	-1.296988
52H	2.158433	-2.053088	0.078093
53H	4.460212	2.383845	-2.149393
54H	3.411512	0.970615	-2.357926
55H	2.865221	2.341199	-1.379802
56H	3.528660	-2.991060	-1.780759
57H	4.539152	-1.538864	-1.836733
58H	4.595323	-2.613512	-0.422419
59H	1.160018	2.587615	2.228848
60H	2.571585	1.780655	2.935882
61H	2.753843	2.824511	1.507065

6ah-PhNCO2-017

1C	-3.015108	2.102225	0.875019
2C	-3.572830	2.880963	1.887529
3N	-3.618587	2.507376	3.177636
4C	-3.087088	1.315417	3.487248
5C	-2.490251	0.465227	2.554701
6C	-2.456088	0.868570	1.219139
7N	-1.835685	0.060466	0.212489
8S	-2.460500	-1.435516	-0.162959
9O	-3.435286	-1.791941	0.872892
10O	-1.389380	-2.363654	-0.525664
11C	-3.528203	-1.216241	-1.741602
12F	-4.609451	-2.006494	-1.606762
13F	-2.881279	-1.582174	-2.844470
14F	-3.941668	0.052498	-1.849439
15C	-0.847166	0.649471	-0.752864
16O	-0.943828	0.231653	-1.921162
17N	-0.050342	1.481234	-0.124440
18C	0.971633	2.169042	-0.777320
19C	1.749025	3.027252	0.038199
20C	2.843599	3.724611	-0.468531
21C	3.205612	3.594516	-1.816331
22C	2.440217	2.763135	-2.641190
23C	1.339803	2.058486	-2.142324
24H	-3.005351	2.449910	-0.152578
25H	-4.009122	3.848765	1.650319
26H	-3.131412	1.024920	4.534852
27H	-2.069207	-0.484962	2.861576
28H	1.470842	3.123412	1.085351

29H	3.418344	4.372672	0.190375
30H	4.059983	4.136006	-2.215383
31H	2.701563	2.655741	-3.692487
32H	0.766221	1.413307	-2.795316
33P	3.177293	-1.328821	0.614067
34C	2.622975	-2.520602	-0.653086
35C	1.804284	-1.905584	-1.795640
36C	1.783048	-0.714707	1.610370
37C	4.364835	-2.209975	1.691756
38C	3.998000	0.093845	-0.177011
39C	4.912428	-1.372213	2.854599
40C	5.216828	-0.277422	-1.030170
41C	0.908814	-1.818384	2.219543
42H	2.047573	-3.289619	-0.124201
43H	3.528430	-3.009032	-1.034320
44H	1.500366	-2.700437	-2.485718
45H	0.893381	-1.418332	-1.442589
46H	2.388979	-1.173747	-2.362791
47H	1.185334	-0.047704	0.976897
48H	2.226135	-0.083369	2.390307
49H	5.176146	-2.555547	1.040321
50H	3.849977	-3.105424	2.060487
51H	4.271988	0.787386	0.625461
52H	3.235071	0.598280	-0.779098
53H	5.629078	-1.970653	3.427902
54H	5.434336	-0.476157	2.501047
55H	4.117446	-1.059106	3.539825
56H	5.633401	0.634269	-1.471972
57H	6.005627	-0.754966	-0.438027
58H	4.947398	-0.949833	-1.851962
59H	0.149715	-1.355168	2.858394
60H	0.385025	-2.388066	1.446124
61H	1.486982	-2.514228	2.839045

6ah-PhNCO2-018

1C	-2.864856	1.636885	1.612253
2C	-3.360529	1.995251	2.864841
3N	-3.293330	1.203880	3.948806
4C	-2.707185	0.007024	3.796185
5C	-2.165742	-0.443982	2.591092
6C	-2.247758	0.390697	1.476221
7N	-1.687155	0.001248	0.215156
8S	-2.363346	-1.253966	-0.640383
9O	-3.215475	-2.020396	0.274280
10O	-1.345481	-1.926839	-1.446806
11C	-3.599092	-0.484182	-1.888717
12F	-4.662796	-1.305113	-1.965833
13F	-3.076324	-0.364617	-3.105861
14F	-4.016512	0.709833	-1.448552
15C	-0.785636	0.944116	-0.539402
16O	-1.004909	1.019217	-1.761489
17N	0.075055	1.483836	0.290174
18C	1.024381	2.414739	-0.132228
19C	1.748075	3.067930	0.894500
20C	2.775583	3.964386	0.607496
21C	3.122775	4.243382	-0.721701
22C	2.413861	3.612443	-1.749516
23C	1.378133	2.714625	-1.471619
24H	-2.945780	2.313955	0.768119
25H	-3.840566	2.961534	3.002767
26H	-2.659988	-0.623225	4.681809
27H	-1.694455	-1.417429	2.523690
28H	1.484788	2.842266	1.925555
29H	3.309181	4.447809	1.423535
30H	3.925095	4.941028	-0.949742
31H	2.667252	3.819634	-2.787768
32H	0.843682	2.233805	-2.280947
33P	3.009380	-1.601875	0.122867
34C	2.637644	-1.993912	-1.622953
35C	1.834006	-0.917949	-2.364111
36C	1.503747	-1.646289	1.150903
37C	4.197646	-2.861913	0.708834
38C	3.755664	0.056749	0.248466
39C	4.688353	-2.649433	2.146778
40C	5.072710	0.213938	-0.522141
41C	0.745452	-2.978441	1.089300
42H	2.104910	-2.952455	-1.619378
43H	3.606401	-2.168542	-2.106883
44H	1.665397	-1.244581	-3.396415
45H	0.854345	-0.749608	-1.913683
46H	2.369021	0.036254	-2.397189
47H	0.877685	-0.804005	0.833741
48H	1.828772	-1.420766	2.174193
49H	5.035567	-2.850790	0.001713
50H	3.704084	-3.834994	0.599457

51H	3.890904	0.265395	1.316013
52H	3.003332	0.763219	-0.113940
53H	5.382360	-3.452887	2.417000
54H	5.219540	-1.697560	2.256533
55H	3.862735	-2.665699	2.866708
56H	5.422093	1.247211	-0.424010
57H	5.857225	-0.446029	-0.134775
58H	4.943745	0.008548	-1.590595
59H	-0.099233	-2.945906	1.785604
60H	0.339187	-3.164795	0.091447
61H	1.377786	-3.825717	1.379059

6ah-PhNCO2-019

1C	-3.089790	2.022663	0.951379
2C	-3.721563	2.684107	2.003410
3N	-3.786142	2.204035	3.256647
4C	-3.195176	1.022061	3.488380
5C	-2.522235	0.285204	2.512670
6C	-2.472815	0.796364	1.214585
7N	-1.773296	0.113481	0.169333
8S	-2.239995	-1.397809	-0.325733
9O	-3.138395	-1.963334	0.685429
10O	-1.076504	-2.150596	-0.795407
11C	-3.364805	-1.167817	-1.859666
12F	-4.311947	-2.122846	-1.814774
13F	-2.694382	-1.298639	-3.000802
14F	-3.964703	0.028598	-1.812639
15C	-0.808406	0.857993	-0.722441
16O	-0.947718	0.651268	-1.941169
17N	0.014202	1.561188	0.017910
18C	1.039330	2.329644	-0.534399
19C	1.800483	3.088471	0.387066
20C	2.904330	3.836210	-0.018012
21C	3.292090	3.855435	-1.364847
22C	2.543697	3.122174	-2.291935
23C	1.432786	2.370621	-1.895568
24H	-3.070784	2.453902	-0.044318
25H	-4.205611	3.642527	1.828950
26H	-3.252391	0.646145	4.507750
27H	-2.052155	-0.659787	2.756127
28H	1.503915	3.064597	1.433282
29H	3.466798	4.405495	0.719513
30H	4.154132	4.436156	-1.684155
31H	2.825707	3.130964	-3.343308
32H	0.870976	1.804340	-2.627210
33P	2.955177	-1.440067	0.513097
34C	1.619803	-0.915892	1.638401
35C	0.786463	-2.068264	2.212565
36C	2.319718	-2.345639	-0.946292
37C	3.881456	0.046043	-0.000401
38C	4.073043	-2.584758	1.397571
39C	5.151287	-0.244617	-0.809680
40C	4.666549	-2.011997	2.690392
41C	1.832124	-1.460989	-2.099903
42H	0.993983	-0.195531	1.096098
43H	2.113862	-0.352382	2.439594
44H	0.046620	-1.660691	2.909623
45H	0.244660	-2.603871	1.427572
46H	1.401539	-2.786622	2.767209
47H	1.510016	-2.989585	-0.584068
48H	3.133313	-3.005118	-1.272905
49H	4.115989	0.599718	0.915478
50H	3.183341	0.668162	-0.570394
51H	4.862367	-2.855960	0.686927
52H	3.498132	-3.497340	1.595541
53H	5.603183	0.704790	-1.116718
54H	5.893700	-0.795787	-0.221512
55H	4.935553	-0.818424	-1.717809
56H	5.339511	-2.749350	3.141749
57H	5.246167	-1.101515	2.501295
58H	3.887872	-1.776464	3.423798
59H	1.455264	-2.103070	-2.903753
60H	1.011424	-0.806609	-1.803461
61H	2.641855	-0.848494	-2.509386

6ah-PhNCO2-020

1C	-3.388725	1.943532	0.100340
2C	-4.184954	2.836344	0.816575
3N	-4.283724	2.837394	2.156447
4C	-3.560054	1.926859	2.825159
5C	-2.720182	0.998363	2.207910
6C	-2.639673	1.006588	0.815313

7N	-1.786238	0.094425	0.113724
8S	-2.098402	-1.537226	0.139430
9O	-3.179854	-1.775385	1.100558
10O	-0.855604	-2.306487	0.219098
11C	-2.873137	-1.978232	-1.558406
12F	-3.835425	-2.892024	-1.333631
13F	-1.982023	-2.508859	-2.392038
14F	-3.436609	-0.898108	-2.111793
15C	-0.719239	0.573898	-0.818995
16O	-0.536810	-0.160146	-1.812457
17N	-0.161865	1.666727	-0.358144
18C	0.848743	2.331868	-1.054883
19C	1.380291	3.478073	-0.415786
20C	2.425172	4.210303	-0.976179
21C	2.979354	3.828339	-2.205865
22C	2.458610	2.705716	-2.858241
23C	1.413203	1.961896	-2.301485
24H	-3.343246	1.980658	-0.983324
25H	-4.776575	3.581234	0.289037
26H	-3.648578	1.942225	3.909391
27H	-2.145053	0.291873	2.795383
28H	0.951011	3.772986	0.539205
29H	2.808204	5.084609	-0.453508
30H	3.793260	4.398125	-2.647839
31H	2.869485	2.398611	-3.818594
32H	1.030338	1.092221	-2.819621
33P	2.944335	-1.185225	0.887593
34C	1.778327	-1.657982	2.221109
35C	0.751902	-0.579990	2.594588
36C	3.305349	0.601263	0.949316
37C	4.483213	-2.135787	1.147458
38C	2.255088	-1.583661	-0.751966
39C	5.565300	-1.875527	0.091564
40C	2.094869	-3.084985	-1.021286
41C	4.067018	1.048726	2.203245
42H	2.384995	-1.939543	3.089975
43H	1.273237	-2.564958	1.871045
44H	0.027112	-1.007747	3.296042
45H	1.227288	0.278563	3.079757
46H	0.203014	-0.213526	1.726096
47H	2.342752	1.115801	0.864653
48H	3.866351	0.843276	0.039775
49H	4.198987	-3.194892	1.171916
50H	4.843541	-1.882198	2.151363
51H	2.920689	-1.119188	-1.488880
52H	1.290002	-1.077434	-0.836538
53H	6.448531	-2.483803	0.315887
54H	5.223233	-2.141047	-0.914850
55H	5.876567	-0.824903	0.081030
56H	1.619290	-3.217242	-1.999052
57H	3.059180	-3.605169	-1.039268
58H	1.447946	-3.564186	-0.280152
59H	4.173398	2.138900	2.186775
60H	3.536884	0.779643	3.123585
61H	5.072159	0.614708	2.244418

6ah-PhNCO-001

1C	1.430423	1.446546	1.545513
2C	0.190663	1.834167	1.110328
3N	-0.185851	1.675961	-0.189022
4C	0.706216	1.174547	-1.080028
5C	1.955512	0.744325	-0.703691
6C	2.365580	0.830926	0.660469
7N	3.525720	0.404948	1.229646
8S	4.661494	-0.405563	0.436924
9O	4.211122	-1.231840	-0.705538
10O	5.580603	-1.010472	1.412176
11C	5.711308	0.944856	-0.377098
12F	4.952785	1.694573	-1.203589
13F	6.704888	0.395473	-1.097512
14F	6.253408	1.755623	0.546043
15C	-1.616389	1.921582	-0.659527
16O	-1.733643	2.052772	-1.889355
17N	-2.436216	1.871896	0.358633
18C	-3.822354	1.951390	0.204421
19C	-4.537336	1.976451	-1.018282
20C	-5.936130	1.988295	-1.022106
21C	-6.664080	1.981827	0.171894
22C	-5.968380	1.966207	1.388414
23C	-4.575231	1.948974	1.402486
24H	1.699817	1.584313	2.587193
25H	-0.560794	2.256411	1.763136
26H	0.352962	1.117643	-2.101994
27H	2.603326	0.322810	-1.459684
28H	-3.992314	1.990566	-1.953568

29H	-6.460416	2.007839	-1.975784
30H	-7.751229	1.994215	0.157090
31H	-6.514608	1.966210	2.329455
32H	-4.034514	1.929926	2.346207
33P	-1.879192	-2.335059	-0.030515
34C	-2.311619	-1.276876	-1.449733
35C	-2.976193	-2.026663	-2.611556
36C	-0.740438	-3.662285	-0.557788
37C	-1.068338	-1.304815	1.236277
38C	-3.386079	-3.114217	0.646189
39C	-0.806568	-2.025428	2.564742
40C	-4.451902	-2.106702	1.099737
41C	0.549122	-3.155208	-1.217490
42H	-1.387834	-0.788042	-1.774880
43H	-2.966202	-0.487066	-1.067826
44H	-3.180138	-1.318748	-3.421894
45H	-2.332846	-2.818801	-3.010821
46H	-3.930464	-2.473409	-2.311592
47H	-1.303883	-4.312132	-1.237686
48H	-0.517179	-4.253762	0.338060
49H	-1.692490	-0.414521	1.372900
50H	-0.126993	-0.965921	0.790273
51H	-3.063869	-3.753498	1.476872
52H	-3.775341	-3.778253	-0.134792
53H	-0.280294	-1.344302	3.242166
54H	-1.738557	-2.330158	3.053346
55H	-0.177308	-2.912770	2.432461
56H	-5.308490	-2.647364	1.516669
57H	-4.071774	-1.432351	1.873969
58H	-4.814874	-1.496039	0.266879
59H	1.173064	-4.010684	-1.497655
60H	0.342943	-2.581503	-2.127469
61H	1.137600	-2.527434	-0.540666

6ah-PhNCO-002

1C	-1.348653	1.239168	-1.522433
2C	-0.114467	1.653357	-1.096941
3N	0.200874	1.697145	0.228602
4C	-0.750818	1.384119	1.144457
5C	-2.002742	0.948359	0.782629
6C	-2.346315	0.813090	-0.594871
7N	-3.493213	0.330287	-1.144792
8S	-4.655288	-0.377436	-0.295709
9O	-4.235564	-1.057996	0.949679
10O	-5.543520	-1.099091	-1.218783
11C	-5.735429	1.052355	0.317427
12F	-5.025179	1.866156	1.125704
13F	-6.786495	0.581132	1.011110
14F	-6.197062	1.781833	-0.711641
15C	1.623477	1.973193	0.720201
16O	1.722052	2.073957	1.954437
17N	2.456207	1.995386	-0.287498
18C	3.836153	2.132115	-0.113117
19C	4.532314	2.187852	1.118809
20C	5.928586	2.266572	1.141652
21C	6.672629	2.293241	-0.042307
22C	5.995286	2.244100	-1.268006
23C	4.604383	2.162841	-1.300783
24H	-1.565405	1.204336	-2.584722
25H	0.682072	1.938916	-1.769717
26H	-0.439548	1.474430	2.177388
27H	-2.700085	0.685591	1.565966
28H	3.974881	2.170833	2.046616
29H	6.438434	2.309145	2.102391
30H	7.757702	2.356335	-0.012421
31H	6.553513	2.268838	-2.201696
32H	4.078270	2.121489	-2.252017
33P	1.889298	-2.536408	-0.102983
34C	0.256983	-1.854337	0.337853
35C	-0.935252	-2.760711	0.008624
36C	2.010060	-2.741677	-1.913363
37C	3.162528	-1.366129	0.472305
38C	2.127143	-4.169746	0.675999
39C	4.602263	-1.789077	0.155062
40C	2.095782	-4.130648	2.210176
41C	1.786142	-1.443934	-2.702169
42H	0.181880	-0.905125	-0.199220
43H	0.291027	-1.615721	1.406810
44H	-1.862313	-2.259060	0.304724
45H	-1.001028	-2.973317	-1.064158
46H	-0.885058	-3.712800	0.547992
47H	1.278405	-3.507457	-2.196911
48H	3.003557	-3.160668	-2.112466
49H	3.013657	-1.239898	1.550961
50H	2.927216	-0.403028	0.008200

51H	3.083665	-4.560757	0.309061
52H	1.341371	-4.824628	0.280944
53H	5.289703	-1.035020	0.551966
54H	4.858291	-2.752514	0.610307
55H	4.775803	-1.856154	-0.924352
56H	2.232643	-5.143817	2.603050
57H	2.896596	-3.502734	2.615377
58H	1.138345	-3.752912	2.585797
59H	1.926300	-1.642308	-3.770305
60H	0.770575	-1.058630	-2.564241
61H	2.492161	-0.659661	-2.409855

6ah-PhNCO-003

1C	-1.112249	0.747504	-1.693142
2C	0.123771	1.242995	-1.373857
3N	0.386619	1.750956	-0.136715
4C	-0.619228	1.833959	0.770811
5C	-1.876590	1.339973	0.517794
6C	-2.163882	0.712656	-0.730174
7N	-3.302585	0.078737	-1.122168
8S	-4.507938	-0.270498	-0.122372
9O	-4.137886	-0.493285	1.293031
10O	-5.391739	-1.248476	-0.774277
11C	-5.568151	1.299229	-0.070173
12F	-4.872545	2.324262	0.463893
13F	-6.664991	1.098398	0.680797
14F	-5.956570	1.655219	-1.305860
15C	1.801449	2.137827	0.302749
16O	1.847346	2.760124	1.375579
17N	2.676958	1.672383	-0.549808
18C	4.053469	1.833138	-0.369786
19C	4.698459	2.414501	0.748471
20C	6.094236	2.477755	0.808592
21C	6.887850	1.973014	-0.226595
22C	6.261609	1.397084	-1.340031
23C	4.871327	1.328727	-1.407937
24H	-1.287311	0.338785	-2.682707
25H	0.960235	1.241982	-2.058795
26H	-0.348083	2.289297	1.715089
27H	-2.620378	1.406927	1.299542
28H	4.101555	2.813349	1.558719
29H	6.564185	2.931682	1.679030
30H	7.972217	2.029706	-0.170428
31H	6.859531	1.001972	-2.158887
32H	4.385057	0.882514	-2.272202
33P	1.525590	-2.559422	0.345210
34C	2.275446	-1.718293	-1.087585
35C	3.653420	-2.266650	-1.482863
36C	2.554680	-2.310436	1.833208
37C	-0.138265	-1.866720	0.615559
38C	1.410799	-4.354195	0.025756
39C	-0.927672	-2.516112	1.759583
40C	0.585077	-4.708402	-1.218713
41C	2.654670	-0.847659	2.288776
42H	2.338247	-0.649883	-0.842804
43H	1.560146	-1.816196	-1.912837
44H	4.026096	-1.709277	-2.348302
45H	4.383992	-2.147128	-0.676001
46H	3.610908	-3.325828	-1.761061
47H	3.544577	-2.718514	1.597282
48H	2.127414	-2.942251	2.621038
49H	-0.677928	-1.950363	-0.333765
50H	0.004406	-0.799389	0.804734
51H	0.981769	-4.808777	0.926304
52H	2.438553	-4.726263	-0.061831
53H	-1.898987	-2.017511	1.846840
54H	-1.113316	-3.579752	1.574371
55H	-0.408412	-2.415913	2.719187
56H	0.572998	-5.795850	-1.349698
57H	-0.453470	-4.372335	-1.126636
58H	1.010433	-4.267895	-2.127178
59H	3.324615	-0.783212	3.152818
60H	3.060309	-0.199596	1.506330
61H	1.680724	-0.452705	2.595706

6ah-PhNCO-004

1C	1.119139	-0.738789	-1.685474
2C	-0.117268	-1.233296	-1.366376
3N	-0.380434	-1.741855	-0.129667
4C	0.625324	-1.826426	0.777849
5C	1.883029	-1.333334	0.525079
6C	2.170995	-0.706074	-0.722727

7N	3.310663	-0.073843	-1.114815
8S	4.518172	0.270795	-0.116031
9O	4.151355	0.489489	1.300866
10O	5.402259	1.249467	-0.766533
11C	5.575750	-1.300770	-0.070692
12F	4.879292	-2.326064	0.461753
13F	6.674328	-1.103983	0.678824
14F	5.961284	-1.653900	-1.308102
15C	-1.795126	-2.131118	0.308298
16O	-1.840870	-2.751600	1.382322
17N	-2.670547	-1.670107	-0.546502
18C	-4.046565	-1.837365	-0.370232
19C	-4.691846	-2.435828	0.738846
20C	-6.087439	-2.505679	0.794860
21C	-6.880878	-1.990500	-0.235336
22C	-6.254485	-1.397693	-1.339767
23C	-4.864321	-1.323254	-1.403768
24H	1.294552	-0.329628	-2.674802
25H	-0.953770	-1.231461	-2.051249
26H	0.354009	-2.282820	1.721559
27H	2.627046	-1.401659	1.306496
28H	-4.095312	-2.841653	1.545881
29H	-6.557433	-2.972572	1.658385
30H	-7.965127	-2.052112	-0.182222
31H	-6.852148	-0.994263	-2.154747
32H	-4.378049	-0.864162	-2.261280
33P	-1.530801	2.561268	0.349210
34C	-2.271603	1.732021	-1.095142
35C	-3.649441	2.280775	-1.490461
36C	-2.588299	2.331882	1.820011
37C	0.117886	1.839874	0.644144
38C	-1.379583	4.353781	0.031115
39C	0.921355	2.496293	1.774539
40C	-0.541202	4.693099	-1.208995
41C	-2.819159	0.864273	2.205642
42H	-2.333081	0.661239	-0.861132
43H	-1.552577	1.840268	-1.915815
44H	-4.013407	1.737131	-2.368338
45H	-4.385180	2.143544	-0.691098
46H	-3.610613	3.344964	-1.749654
47H	-3.537398	2.836132	1.602385
48H	-2.112860	2.886705	2.637685
49H	0.661104	1.891948	-0.305204
50H	-0.049700	0.779939	0.854258
51H	-0.946649	4.799740	0.934238
52H	-2.399169	4.746278	-0.061388
53H	1.884264	1.982639	1.867558
54H	1.125542	3.552764	1.568803
55H	0.404713	2.423356	2.737940
56H	-0.497388	5.780765	-1.331202
57H	0.487012	4.326199	-1.118809
58H	-0.978426	4.272593	-2.121214
59H	-3.481166	0.820609	3.077208
60H	-3.293810	0.296088	1.400285
61H	-1.885155	0.361762	2.476723

6ah-PhNCO-005

1C	1.971142	-0.687941	-1.593814
2C	0.747604	-1.158326	-1.199265
3N	0.402493	-1.224594	0.118256
4C	1.307367	-0.844797	1.056621
5C	2.549655	-0.360840	0.726912
6C	2.935440	-0.239978	-0.641030
7N	4.096743	0.238752	-1.161851
8S	5.277762	0.877067	-0.283536
9O	4.886302	1.532390	0.983880
10O	6.199959	1.589094	-1.180739
11C	6.291377	-0.617031	0.289484
12F	5.542920	-1.421115	1.072913
13F	7.358889	-0.210897	0.999645
14F	6.726893	-1.338378	-0.756926
15C	-0.988476	-1.645241	0.572770
16O	-1.150798	-1.623589	1.806840
17N	-1.758328	-1.895410	-0.453919
18C	-3.087508	-2.300976	-0.311416
19C	-3.738521	-2.668288	0.890933
20C	-5.086437	-3.040366	0.883819
21C	-5.828767	-3.053824	-0.302035
22C	-5.193796	-2.702150	-1.500707
23C	-3.848594	-2.337220	-1.503367
24H	2.213412	-0.644486	-2.650259
25H	-0.012825	-1.493738	-1.890820
26H	0.971484	-0.937614	2.081141
27H	3.213640	-0.062842	1.526633
28H	-3.185515	-2.654512	1.821519

29H	-5.560987	-3.321590	1.822110
30H	-6.876866	-3.342990	-0.295476
31H	-5.747629	-2.717128	-2.437292
32H	-3.353891	-2.069239	-2.434077
33P	-3.246047	2.024882	0.097927
34C	-4.610281	3.228250	-0.073746
35C	-5.978519	2.578868	-0.325298
36C	-3.026217	1.121806	-1.469471
37C	-1.725496	2.942118	0.520188
38C	-3.634922	0.825915	1.413732
39C	-0.486195	2.044491	0.634655
40C	-3.948299	1.465756	2.772620
41C	-2.578233	2.000148	-2.644356
42H	-4.336751	3.901334	-0.895325
43H	-4.621382	3.830568	0.842107
44H	-6.736479	3.361185	-0.441787
45H	-5.977936	1.973652	-1.238541
46H	-6.283852	1.939220	0.509833
47H	-3.986095	0.637015	-1.678902
48H	-2.311779	0.313532	-1.275254
49H	-1.924775	3.463241	1.464176
50H	-1.591282	3.712909	-0.248158
51H	-2.781471	0.144567	1.493399
52H	-4.477692	0.227386	1.053054
53H	0.384238	2.651487	0.904583
54H	-0.614647	1.280168	1.406980
55H	-0.261883	1.542993	-0.312177
56H	-4.165136	0.672756	3.496553
57H	-3.098661	2.040646	3.157391
58H	-4.822094	2.125680	2.728036
59H	-2.503150	1.383043	-3.546459
60H	-3.291707	2.806066	-2.850317
61H	-1.594136	2.447248	-2.466286

6ah-PhNCO-006

1C	-1.381285	1.261771	-0.361867
2C	-0.055965	1.612052	-0.402571
3N	0.615668	2.019816	0.706513
4C	-0.064794	2.175811	1.873216
5C	-1.390472	1.836561	1.980070
6C	-2.094609	1.282971	0.873115
7N	-3.354173	0.830208	1.127096
8S	-4.168609	-0.098276	0.106524
9O	-5.278545	-0.740575	0.825449
10O	-3.350168	-0.932658	-0.804585
11C	-5.052518	1.101993	-1.062999
12F	-4.157544	1.868263	-1.720955
13F	-5.878031	1.913167	-0.382574
14F	-5.774099	0.422989	-1.972007
15C	2.134965	2.207897	0.709823
16O	2.572464	2.811515	1.701836
17N	2.652279	1.629418	-0.342926
18C	4.028979	1.569940	-0.568787
19C	5.049758	2.020705	0.302576
20C	6.396127	1.857373	-0.038590
21C	6.770678	1.249994	-1.241689
22C	5.769838	0.802239	-2.114296
23C	4.425358	0.958755	-1.781912
24H	-1.849162	0.927894	-1.276993
25H	0.534699	1.560043	-1.306397
26H	0.521346	2.549495	2.703446
27H	-1.895439	1.937990	2.934596
28H	4.779189	2.496822	1.236616
29H	7.161112	2.214626	0.648199
30H	7.820694	1.131841	-1.498014
31H	6.038733	0.331755	-3.057935
32H	3.647732	0.612743	-2.459212
33P	1.021789	-2.520876	0.305063
34C	0.591154	-4.207822	-0.248474
35C	1.684752	-4.895502	-1.077895
36C	-0.432900	-1.756217	1.093617
37C	2.395997	-2.614983	1.507058
38C	1.554330	-1.520208	-1.120222
39C	2.792411	-1.261482	2.114962
40C	0.525207	-1.453884	-2.256788
41C	-1.020270	-2.557251	2.263230
42H	-0.340980	-4.121390	-0.819495
43H	0.359942	-4.787923	0.652534
44H	1.888504	-4.357606	-2.009974
45H	2.624181	-4.987436	-0.521461
46H	1.355149	-5.906075	-1.342868
47H	-1.184670	-1.604503	0.311622
48H	-0.109918	-0.764973	1.426430
49H	3.242337	-3.068105	0.977999
50H	2.086977	-3.322337	2.285711

51H	2.497105	-1.959888	-1.467813
52H	1.797715	-0.518338	-0.743195
53H	3.634808	-1.407628	2.799593
54H	3.106517	-0.543614	1.350710
55H	1.971035	-0.819496	2.689397
56H	-0.435164	-1.054038	-1.917190
57H	0.902493	-0.794570	-3.046151
58H	0.345184	-2.438777	-2.702279
59H	-1.863383	-1.999139	2.684652
60H	-1.397871	-3.532487	1.938469
61H	-0.287765	-2.715725	3.062650

6ah-PhNCO-007

1C	-2.178041	0.485789	-0.203362
2C	-0.905893	0.994954	-0.133174
3N	-0.256214	1.160535	1.050460
4C	-0.901669	0.851329	2.207535
5C	-2.178657	0.354393	2.206626
6C	-2.878755	0.121268	0.986804
7N	-4.123676	-0.413039	1.109330
8S	-5.043244	-0.828968	-0.138297
9O	-6.160129	-1.650223	0.351483
10O	-4.340998	-1.260247	-1.367753
11C	-5.884859	0.786304	-0.660234
12F	-4.969505	1.672134	-1.105893
13F	-6.541547	1.344866	0.370063
14F	-6.764313	0.554845	-1.650936
15C	1.198154	1.610297	1.119956
16O	1.703391	1.528001	2.254105
17N	1.636777	1.944037	-0.065136
18C	2.942098	2.392742	-0.277216
19C	3.854297	2.825464	0.714133
20C	5.130441	3.270854	0.357852
21C	5.544467	3.289215	-0.978012
22C	4.649536	2.866350	-1.969750
23C	3.370688	2.431873	-1.624606
24H	-2.628406	0.361578	-1.178342
25H	-0.341473	1.284074	-1.008898
26H	-0.330082	1.013148	3.111984
27H	-2.663126	0.119611	3.148096
28H	3.556670	2.810197	1.755125
29H	5.810699	3.603608	1.139571
30H	6.541263	3.632650	-1.243614
31H	4.946989	2.882208	-3.016336
32H	2.670243	2.117066	-2.394897
33P	2.986956	-2.133039	-0.154802
34C	4.048490	-3.379413	-0.966192
35C	4.804088	-4.292588	0.008787
36C	2.183257	-1.120161	-1.441337
37C	1.732589	-2.993694	0.856779
38C	3.993887	-1.068531	0.933429
39C	0.694696	-2.054973	1.485805
40C	5.211963	-0.440628	0.242785
41C	1.080859	-1.846046	-2.224719
42H	4.745137	-2.825851	-1.606902
43H	3.396684	-3.961462	-1.628615
44H	5.465342	-3.720587	0.669238
45H	4.119003	-4.879335	0.630336
46H	5.425252	-4.995148	-0.557404
47H	2.982313	-0.781390	-2.111407
48H	1.793702	-0.222836	-0.946343
49H	2.282699	-3.546996	1.627138
50H	1.252463	-3.735872	0.207583
51H	4.299108	-1.691853	1.782893
52H	3.325888	-0.293704	1.328218
53H	0.000824	-2.637707	2.100566
54H	1.161593	-1.301133	2.126809
55H	0.108236	-1.541019	0.719452
56H	4.918859	0.205775	-0.589353
57H	5.749054	0.182226	0.964128
58H	5.906922	-1.202376	-0.128163
59H	0.666899	-1.162605	-2.974172
60H	1.459657	-2.728474	-2.752512
61H	0.257300	-2.161081	-1.575084

6ah-PhNCO-008

1C	1.350643	1.366534	1.505615
2C	0.105542	1.748024	1.080780
3N	-0.243774	1.687292	-0.235378
4C	0.683148	1.301583	-1.148324
5C	1.943524	0.892105	-0.785841
6C	2.323304	0.866473	0.588402

7N	3.483393	0.423407	1.144501
8S	4.641347	-0.316033	0.316692
9O	4.214295	-1.072485	-0.881700
10O	5.555463	-0.971460	1.263654
11C	5.687183	1.094365	-0.394332
12F	4.941811	1.867951	-1.210451
13F	6.717791	0.602057	-1.104085
14F	6.178196	1.869907	0.586166
15C	-1.673387	1.941821	-0.712769
16O	-1.788409	2.036822	-1.945968
17N	-2.494726	1.945541	0.304939
18C	-3.878878	2.053126	0.146193
19C	-4.591171	2.080700	-1.077684
20C	-5.988672	2.136082	-1.084199
21C	-6.718396	2.166927	0.108456
22C	-6.025451	2.145667	1.326312
23C	-4.633089	2.087429	1.343066
24H	1.595758	1.417281	2.561065
25H	-0.673236	2.087648	1.749661
26H	0.346650	1.316288	-2.177287
27H	2.620772	0.566429	-1.563206
28H	-4.044796	2.061549	-2.012056
29H	-6.510828	2.157638	-2.039000
30H	-7.804655	2.212035	0.091225
31H	-6.572568	2.174795	2.266438
32H	-4.095030	2.068809	2.288049
33P	-1.831787	-2.514528	0.101494
34C	-0.123492	-1.914273	0.313446
35C	0.730450	-2.758318	1.268746
36C	-2.696584	-2.518648	1.711049
37C	-2.702837	-1.400633	-1.051311
38C	-1.807990	-4.220590	-0.548880
39C	-4.097775	-1.886215	-1.466623
40C	-1.172211	-4.341683	-1.941205
41C	-2.583096	-1.191427	2.474227
42H	-0.202682	-0.883795	0.670831
43H	0.326321	-1.873800	-0.684465
44H	1.728017	-2.313998	1.346833
45H	0.302071	-2.794149	2.276475
46H	0.850915	-3.785017	0.906770
47H	-2.287340	-3.351122	2.295187
48H	-3.744331	-2.759981	1.495940
49H	-2.053096	-1.267078	-1.923496
50H	-2.766471	-0.431368	-0.547322
51H	-2.844744	-4.576651	-0.552577
52H	-1.263825	-4.825391	0.186065
53H	-4.549057	-1.142875	-2.131630
54H	-4.055786	-2.840267	-2.003520
55H	-4.761360	-2.001189	-0.602431
56H	-1.172132	-5.392526	-2.250125
57H	-1.729449	-3.771921	-2.692946
58H	-0.133915	-3.992800	-1.945017
59H	-3.185906	-1.246307	3.387216
60H	-1.549282	-0.983602	2.769519
61H	-2.944580	-0.344424	1.882581

6ah-PhNCO-009

1C	1.313958	0.905458	1.693975
2C	0.085574	1.403542	1.349987
3N	-0.221475	1.703032	0.056146
4C	0.731458	1.559670	-0.898999
5C	1.975743	1.045552	-0.622734
6C	2.312833	0.653007	0.706358
7N	3.453857	0.065312	1.159227
8S	4.653033	-0.404341	0.202435
9O	4.281157	-0.811911	-1.170682
10O	5.553545	-1.278957	0.968104
11C	5.684580	1.162241	-0.062697
12F	4.947013	2.112891	-0.673200
13F	6.752273	0.895901	-0.835259
14F	6.118833	1.656296	1.108441
15C	-1.627513	2.124051	-0.374521
16O	-1.692183	2.578541	-1.528057
17N	-2.484851	1.859585	0.576719
18C	-3.857898	2.072881	0.427919
19C	-4.530045	2.466907	-0.753916
20C	-5.923588	2.584159	-0.771357
21C	-6.687390	2.321161	0.370509
22C	-6.032910	1.937216	1.548736
23C	-4.645183	1.812890	1.573910
24H	1.525533	0.671077	2.731677
25H	-0.710813	1.567174	2.062868
26H	0.429953	1.857264	-1.895197
27H	2.675446	0.928902	-1.438693
28H	-3.955893	2.678244	-1.647228

29H	-6.415666	2.888528	-1.693238
30H	-7.770022	2.418766	0.346273
31H	-6.606870	1.732686	2.450325
32H	-4.136162	1.509561	2.486102
33P	-1.857393	-2.579239	-0.319894
34C	-3.109372	-1.495392	0.444095
35C	-4.487417	-1.545957	-0.228592
36C	-1.810121	-2.323781	-2.126610
37C	-0.237725	-2.167922	0.411877
38C	-2.260632	-4.333672	-0.013462
39C	0.914525	-3.083937	-0.017388
40C	-2.305252	-4.714536	1.472595
41C	-1.436173	-0.893814	-2.538644
42H	-2.704994	-0.475824	0.432368
43H	-3.172046	-1.794324	1.497716
44H	-5.177513	-0.900696	0.323794
45H	-4.446624	-1.175507	-1.257994
46H	-4.904523	-2.559781	-0.239102
47H	-2.801607	-2.598647	-2.506032
48H	-1.098714	-3.052643	-2.532656
49H	-0.369692	-2.179244	1.499971
50H	-0.034677	-1.130446	0.129404
51H	-1.509239	-4.924816	-0.549934
52H	-3.224602	-4.525465	-0.499648
53H	1.837560	-2.752304	0.469142
54H	0.738734	-4.125150	0.273712
55H	1.081951	-3.049275	-1.099204
56H	-2.536032	-5.781024	1.567904
57H	-1.343685	-4.536205	1.966306
58H	-3.078341	-4.155999	2.011428
59H	-1.481976	-0.806032	-3.629486
60H	-2.120095	-0.150596	-2.117790
61H	-0.417691	-0.641183	-2.228989

6ah-PhNCO-010

1C	-2.123838	0.527344	-0.185178
2C	-0.854099	1.043969	-0.128051
3N	-0.228157	1.298600	1.052369
4C	-0.895827	1.074635	2.216171
5C	-2.170494	0.571249	2.227363
6C	-2.846380	0.247975	1.014853
7N	-4.092647	-0.279941	1.152378
8S	-4.976538	-0.806593	-0.078253
9O	-6.107576	-1.583545	0.449802
10O	-4.236351	-1.345887	-1.241090
11C	-5.802877	0.752877	-0.768065
12F	-4.873012	1.606203	-1.246135
13F	-6.506003	1.389503	0.183028
14F	-6.637749	0.434063	-1.773101
15C	1.224023	1.763828	1.118625
16O	1.666522	1.887197	2.273770
17N	1.718483	1.900494	-0.084136
18C	3.026422	2.332848	-0.311579
19C	3.971451	2.727602	0.666029
20C	5.253156	3.139389	0.288158
21C	5.639581	3.166912	-1.055515
22C	4.713282	2.780620	-2.033286
23C	3.431892	2.373270	-1.666731
24H	-2.555485	0.333095	-1.157143
25H	-0.273283	1.271226	-1.011052
26H	-0.342309	1.307181	3.116511
27H	-2.671730	0.401090	3.174010
28H	3.693141	2.711669	1.712063
29H	5.958302	3.442014	1.060133
30H	6.639362	3.488149	-1.337262
31H	4.989317	2.802116	-3.085614
32H	2.709261	2.083621	-2.426319
33P	2.846872	-2.196258	-0.114298
34C	3.771847	-3.579216	-0.872526
35C	4.618406	-4.389058	0.119307
36C	2.008451	-1.243636	-1.423672
37C	1.637773	-2.895137	1.062160
38C	4.000255	-1.103196	0.784790
39C	0.695798	-1.859174	1.687452
40C	5.180058	-0.614093	-0.065925
41C	0.813393	-1.959639	-2.067823
42H	4.398739	-3.143527	-1.659273
43H	3.030383	-4.217312	-1.368032
44H	5.378802	-3.768048	0.604869
45H	4.002100	-4.852430	0.897593
46H	5.136075	-5.191839	-0.417146
47H	2.775346	-1.010587	-2.171978
48H	1.710595	-0.287701	-0.975062
49H	2.224899	-3.410051	1.831843
50H	1.074658	-3.664634	0.520453

51H	4.348862	-1.666020	1.659141
52H	3.414122	-0.255309	1.157998
53H	0.050633	-2.351133	2.422756
54H	1.245352	-1.063970	2.200580
55H	0.050472	-1.403180	0.932052
56H	4.844300	-0.011684	-0.914546
57H	5.825143	0.020681	0.548627
58H	5.784143	-1.447788	-0.440618
59H	0.377612	-1.309437	-2.834203
60H	1.106541	-2.896519	-2.554621
61H	0.028900	-2.180659	-1.336841

6ah-PhNCO-011

1C	1.270258	1.629034	1.517355
2C	0.011235	1.932865	1.069802
3N	-0.361323	1.690183	-0.217989
4C	0.554874	1.196257	-1.088184
5C	1.823764	0.845463	-0.696668
6C	2.230167	1.011368	0.660636
7N	3.408802	0.658959	1.242757
8S	4.542127	-0.196675	0.493832
9O	4.072830	-1.134927	-0.550168
10O	5.501009	-0.690091	1.493060
11C	5.543744	1.083851	-0.480286
12F	4.748985	1.734346	-1.355881
13F	6.526863	0.480659	-1.171433
14F	6.095623	1.992169	0.340192
15C	-1.805059	1.829396	-0.695265
16O	-1.933683	1.828357	-1.931916
17N	-2.618032	1.849531	0.328306
18C	-4.006938	1.895041	0.175305
19C	-4.725993	1.921681	-1.044631
20C	-6.124538	1.930681	-1.043718
21C	-6.848696	1.915596	0.152524
22C	-6.149072	1.895762	1.366547
23C	-4.755595	1.885205	1.375771
24H	1.534117	1.829513	2.550226
25H	-0.759366	2.347832	1.704776
26H	0.204165	1.080052	-2.105522
27H	2.491377	0.425397	-1.435727
28H	-4.184642	1.937996	-1.981928
29H	-6.651922	1.953291	-1.995625
30H	-7.935948	1.924673	0.141068
31H	-6.692111	1.889907	2.309431
32H	-4.211674	1.869965	2.317756
33P	-1.552667	-2.480310	0.010214
34C	-1.107416	-1.242657	1.269181
35C	-1.067860	-1.784258	2.703712
36C	-3.202069	-3.176234	0.371050
37C	-1.553750	-1.667909	-1.624274
38C	-0.323766	-3.832933	0.016922
39C	-1.982076	-2.579480	-2.781751
40C	1.122832	-3.354283	-0.182412
41C	-4.332410	-2.137224	0.338976
42H	-1.818827	-0.414049	1.171816
43H	-0.126581	-0.855390	0.976344
44H	-0.779908	-0.973100	3.381365
45H	-2.045301	-2.157212	3.028435
46H	-0.333131	-2.588759	2.818570
47H	-3.130521	-3.650558	1.356791
48H	-3.376766	-3.977558	-0.356423
49H	-0.536679	-1.292859	-1.780477
50H	-2.206225	-0.791852	-1.551936
51H	-0.620520	-4.532198	-0.773796
52H	-0.436160	-4.363119	0.969889
53H	-1.938582	-2.011732	-3.717485
54H	-1.321388	-3.447399	-2.886079
55H	-3.009537	-2.939137	-2.658758
56H	1.794391	-4.219277	-0.188016
57H	1.252829	-2.827806	-1.133614
58H	1.447730	-2.689227	0.623891
59H	-5.282858	-2.629112	0.572278
60H	-4.178795	-1.341941	1.075878
61H	-4.431600	-1.670206	-0.646411

6ah-PhNCO-012

1C	-1.970270	1.052876	-0.694215
2C	-0.664167	1.449676	-0.579451
3N	-0.137614	1.870038	0.604077
4C	-0.946366	1.941776	1.699203
5C	-2.261422	1.565247	1.650536
6C	-2.837952	1.064354	0.444139

7N	-4.122976	0.656539	0.495402
8S	-4.844291	0.003767	-0.790348
9O	-4.261212	-1.276746	-1.248826
10O	-5.253392	0.964712	-1.836087
11C	-6.442058	-0.475753	0.078380
12F	-6.215116	-1.349620	1.072281
13F	-7.252443	-1.060841	-0.822713
14F	-7.071897	0.596462	0.581319
15C	1.342903	2.169180	0.771875
16O	1.668398	2.517889	1.919627
17N	1.992625	1.947878	-0.343737
18C	3.381658	2.042513	-0.430801
19C	3.933168	1.803104	-1.712971
20C	5.309820	1.800141	-1.927396
21C	6.192805	2.038191	-0.865367
22C	5.665996	2.288571	0.405883
23C	4.285428	2.293194	0.631387
24H	-2.321429	0.725716	-1.666170
25H	0.024915	1.445148	-1.411970
26H	-0.465787	2.297367	2.601132
27H	-2.871525	1.627569	2.545252
28H	3.249001	1.614852	-2.536957
29H	5.696511	1.611123	-2.926672
30H	7.267525	2.036903	-1.029261
31H	6.336381	2.485014	1.240405
32H	3.898476	2.493057	1.622276
33P	2.897106	-1.874109	0.159047
34C	2.332308	-1.076952	1.701753
35C	0.842742	-1.249352	2.026578
36C	4.670915	-1.473951	-0.017369
37C	2.692540	-3.686113	0.289672
38C	1.976526	-1.264521	-1.298615
39C	3.511353	-4.330913	1.415913
40C	0.628598	-1.948323	-1.575025
41C	5.376265	-2.169118	-1.187346
42H	2.597558	-0.017270	1.617865
43H	2.956225	-1.497245	2.499979
44H	0.626431	-0.760797	2.982251
45H	0.205675	-0.787995	1.268106
46H	0.561851	-2.304567	2.117355
47H	5.142437	-1.737285	0.936796
48H	4.734702	-0.385370	-0.112766
49H	2.966248	-4.105914	-0.685691
50H	1.622424	-3.876361	0.427940
51H	2.647194	-1.392438	-2.155999
52H	1.853667	-0.185497	-1.142475
53H	3.323439	-5.410092	1.427548
54H	4.587222	-4.180659	1.275193
55H	3.234169	-3.934157	2.398727
56H	0.168635	-1.481433	-2.452837
57H	0.748137	-3.014732	-1.793867
58H	-0.073597	-1.846755	-0.742967
59H	6.426423	-1.858189	-1.205277
60H	4.935309	-1.893197	-2.151093
61H	5.349599	-3.260436	-1.093425

6ah-PhNCO-013

1C	-1.512193	1.157496	-0.322928
2C	-0.197311	1.543250	-0.376564
3N	0.470039	1.984472	0.721852
4C	-0.205413	2.127163	1.893794
5C	-1.519963	1.752709	2.013646
6C	-2.222308	1.181508	0.913996
7N	-3.479577	0.725831	1.172596
8S	-4.296630	-0.201555	0.151163
9O	-5.411830	-0.835225	0.869749
10O	-3.481075	-1.041259	-0.756647
11C	-5.173320	1.001168	-1.022407
12F	-4.274941	1.762878	-1.681239
13F	-5.997184	1.817178	-0.345623
14F	-5.895940	0.322675	-1.931156
15C	1.979802	2.228240	0.707571
16O	2.407661	2.833537	1.703318
17N	2.507486	1.689609	-0.361335
18C	3.883007	1.692279	-0.602132
19C	4.894707	2.147157	0.277607
20C	6.243241	2.038969	-0.075877
21C	6.629412	1.485057	-1.300926
22C	5.637638	1.035428	-2.182717
23C	4.290830	1.136632	-1.837784
24H	-1.977385	0.804328	-1.231898
25H	0.388177	1.498388	-1.283870
26H	0.376207	2.523219	2.716643
27H	-2.020580	1.850833	2.970777
28H	4.615450	2.579672	1.230007

29H	7.000628	2.396669	0.619100
30H	7.681030	1.408932	-1.566434
31H	5.915471	0.606757	-3.143535
32H	3.520838	0.786761	-2.521873
33P	1.293261	-2.481002	0.267172
34C	0.552361	-4.103489	-0.128846
35C	1.383003	-4.944970	-1.107139
36C	0.170280	-1.567986	1.378564
37C	2.901906	-2.744839	1.091186
38C	1.556234	-1.520101	-1.260303
39C	3.577032	-1.454005	1.575518
40C	0.338807	-1.488856	-2.195278
41C	-0.084152	-2.254946	2.726706
42H	-0.446891	-3.900182	-0.532772
43H	0.413560	-4.630256	0.822558
44H	1.532903	-4.428327	-2.061440
45H	2.365134	-5.198151	-0.693290
46H	0.856877	-5.883058	-1.314806
47H	-0.767028	-1.420998	0.832372
48H	0.618127	-0.579619	1.521888
49H	3.536805	-3.267930	0.366110
50H	2.724908	-3.437387	1.923080
51H	2.424136	-1.961210	-1.765051
52H	1.846667	-0.507144	-0.949943
53H	4.546147	-1.699114	2.023311
54H	3.757003	-0.754100	0.754500
55H	2.978161	-0.942808	2.336677
56H	-0.562011	-1.126071	-1.692310
57H	0.547518	-0.815559	-3.034100
58H	0.121018	-2.479070	-2.608921
59H	-0.750068	-1.625709	3.326987
60H	-0.570840	-3.228028	2.601448
61H	0.842504	-2.398493	3.293503

6ah-PhNCO-014

1C	-1.050247	1.400118	-0.253228
2C	0.296907	1.665165	-0.221898
3N	0.978531	1.798751	0.945590
4C	0.297241	1.748076	2.120490
5C	-1.048739	1.484910	2.158021
6C	-1.782143	1.239566	0.961759
7N	-3.084859	0.876006	1.126149
8S	-4.026619	0.385371	-0.073103
9O	-5.209389	-0.280848	0.491683
10O	-3.348053	-0.257860	-1.222266
11C	-4.730663	1.979811	-0.812704
12F	-3.733887	2.754178	-1.288418
13F	-5.405110	2.682710	0.111237
14F	-5.566483	1.696520	-1.827327
15C	2.509420	1.901945	0.989986
16O	2.960019	2.210676	2.105274
17N	3.012369	1.593359	-0.174937
18C	4.390359	1.542404	-0.401079
19C	5.411606	1.681670	0.570276
20C	6.757502	1.575627	0.205461
21C	7.132580	1.334403	-1.120189
22C	6.131845	1.196112	-2.091394
23C	4.787558	1.296112	-1.736603
24H	-1.527236	1.289083	-1.217071
25H	0.896974	1.756104	-1.116727
26H	0.897225	1.900731	3.008599
27H	-1.557660	1.425841	3.114007
28H	5.142546	1.874179	1.601101
29H	7.521879	1.687260	0.972321
30H	8.182452	1.258552	-1.392883
31H	6.400628	1.011233	-3.129556
32H	4.011189	1.189585	-2.491039
33P	0.363891	-3.000625	0.027434
34C	0.678008	-4.651860	0.743912
35C	0.257547	-5.816331	-0.163444
36C	0.811386	-1.715183	1.239649
37C	1.369365	-2.799458	-1.483666
38C	-1.399322	-2.816909	-0.399809
39C	1.303087	-1.387995	-2.086039
40C	-2.360117	-2.968704	0.786977
41C	2.301933	-1.655959	1.595767
42H	0.147739	-4.686467	1.702903
43H	1.750785	-4.697082	0.966748
44H	-0.817049	-5.799427	-0.374808
45H	0.797903	-5.803912	-1.116433
46H	0.483885	-6.764642	0.335969
47H	0.196463	-1.890214	2.129626
48H	0.475877	-0.772978	0.799706
49H	1.015978	-3.551602	-2.198541
50H	2.400048	-3.062764	-1.218174

51H	-1.616512	-3.553933	-1.182123
52H	-1.513332	-1.827982	-0.856085
53H	1.894205	-1.362941	-3.008055
54H	0.276521	-1.102615	-2.340577
55H	1.719736	-0.637579	-1.407498
56H	-2.177522	-2.213882	1.558657
57H	-3.387003	-2.832938	0.433818
58H	-2.289525	-3.960210	1.247833
59H	2.470444	-0.840066	2.305660
60H	2.643996	-2.584337	2.065853
61H	2.922661	-1.457933	0.716877

6ah-PhNCO-015

1C	1.577919	-1.201735	-1.609141
2C	0.336250	-1.604024	-1.195425
3N	-0.033097	-1.535371	0.115062
4C	0.869730	-1.103858	1.033028
5C	2.126784	-0.674613	0.681821
6C	2.532001	-0.676255	-0.686401
7N	3.700250	-0.243307	-1.231158
8S	4.851358	0.502173	-0.398086
9O	4.417469	1.267969	0.791585
10O	5.776652	1.146611	-1.341629
11C	5.883614	-0.907929	0.332348
12F	5.126064	-1.672607	1.145776
13F	6.908785	-0.415153	1.049748
14F	6.381909	-1.692446	-0.637312
15C	-1.462414	-1.811975	0.573676
16O	-1.619886	-1.750246	1.807051
17N	-2.249584	-1.991060	-0.452763
18C	-3.619844	-2.219784	-0.306189
19C	-4.308036	-2.493418	0.900552
20C	-5.691784	-2.695105	0.898516
21C	-6.432474	-2.626317	-0.286156
22C	-5.763084	-2.358371	-1.487570
23C	-4.382764	-2.163449	-1.496121
24H	1.837910	-1.262642	-2.660511
25H	-0.424377	-1.972547	-1.869615
26H	0.517332	-1.101927	2.056504
27H	2.785618	-0.321258	1.463032
28H	-3.754563	-2.543776	1.829560
29H	-6.195315	-2.908162	1.839687
30H	-7.508201	-2.783981	-0.275703
31H	-6.318043	-2.307192	-2.422146
32H	-3.860984	-1.963465	-2.429555
33P	-2.259484	2.399242	0.159344
34C	-3.364536	1.087357	0.774369
35C	-4.557464	1.602783	1.589796
36C	-1.496215	3.294745	1.557366
37C	-0.955068	1.637957	-0.863895
38C	-3.207853	3.600586	-0.836030
39C	-0.048508	2.639481	-1.589861
40C	-3.906352	2.977853	-2.052391
41C	-0.702431	2.393443	2.514601
42H	-2.750563	0.401375	1.368028
43H	-3.703043	0.523043	-0.100234
44H	-5.151449	0.746547	1.925997
45H	-4.237027	2.157018	2.478921
46H	-5.211394	2.249365	0.993857
47H	-2.304545	3.815578	2.083799
48H	-0.851264	4.065704	1.119910
49H	-1.454338	0.963903	-1.568012
50H	-0.368399	1.011677	-0.185962
51H	-2.503365	4.382887	-1.142057
52H	-3.932304	4.070177	-0.160150
53H	0.716672	2.090144	-2.148488
54H	-0.606256	3.254431	-2.304236
55H	0.469652	3.304250	-0.889980
56H	-4.449921	3.757655	-2.596901
57H	-3.187780	2.525436	-2.744600
58H	-4.628587	2.209078	-1.756927
59H	-0.275998	3.005250	3.316697
60H	-1.337190	1.628889	2.974926
61H	0.125740	1.890268	2.004052

6ah-PhNCO-016

1C	-0.781083	-1.585661	1.654490
2C	0.500021	-1.829058	1.232784
3N	0.821920	-1.827610	-0.090512
4C	-0.159694	-1.659219	-1.010619
5C	-1.458327	-1.387514	-0.652839
6C	-1.813560	-1.272149	0.722553

7N	-3.002319	-0.882117	1.261129
8S	-4.155287	-0.167832	0.407237
9O	-3.700323	0.592882	-0.779279
10O	-5.095985	0.482897	1.331057
11C	-5.184813	-1.577692	-0.328080
12F	-4.429467	-2.341792	-1.144005
13F	-6.211091	-1.084268	-1.042994
14F	-5.679944	-2.362589	0.642426
15C	2.271037	-1.902323	-0.578608
16O	2.384620	-2.131850	-1.794235
17N	3.087098	-1.638256	0.407268
18C	4.473334	-1.588489	0.235056
19C	5.189695	-1.858499	-0.956278
20C	6.584235	-1.757081	-0.983746
21C	7.307085	-1.389862	0.155919
22C	6.610209	-1.122532	1.341937
23C	5.220524	-1.221459	1.379094
24H	-1.004477	-1.576775	2.715940
25H	1.325864	-2.001150	1.909386
26H	0.162604	-1.724589	-2.042216
27H	-2.183223	-1.225568	-1.438186
28H	4.648774	-2.145468	-1.849115
29H	7.110385	-1.971912	-1.912057
30H	8.391473	-1.316809	0.123469
31H	7.152787	-0.840258	2.241966
32H	4.678728	-1.018191	2.300275
33P	0.666031	2.754934	-0.101964
34C	-0.771774	1.943405	0.668983
35C	-1.723330	2.894395	1.405993
36C	1.671389	3.589618	1.174272
37C	1.670227	1.485287	-0.942833
38C	0.103293	4.006131	-1.307947
39C	2.908587	2.033403	-1.665262
40C	-0.763254	3.429579	-2.437750
41C	2.256401	2.633537	2.223597
42H	-0.369827	1.182991	1.346639
43H	-1.302092	1.412893	-0.128251
44H	-2.527665	2.309486	1.863384
45H	-1.214813	3.446336	2.204368
46H	-2.185604	3.615050	0.722962
47H	1.025041	4.342318	1.641464
48H	2.466523	4.130982	0.648574
49H	1.003094	0.970866	-1.642498
50H	1.962633	0.756327	-0.179434
51H	1.004066	4.487577	-1.706970
52H	-0.443479	4.768114	-0.740046
53H	3.440454	1.202050	-2.139001
54H	2.640698	2.752536	-2.447160
55H	3.603366	2.516767	-0.970004
56H	-1.051583	4.236445	-3.120046
57H	-0.221829	2.675879	-3.020544
58H	-1.681302	2.972988	-2.053097
59H	2.846186	3.207810	2.946262
60H	1.470264	2.108163	2.777137
61H	2.916997	1.885829	1.771789

6ah-PhNCO-017

1C	-0.450305	1.329651	-1.733759
2C	0.843708	1.533738	-1.329661
3N	1.160439	1.686618	-0.014409
4C	0.166443	1.695074	0.907846
5C	-1.148397	1.477422	0.570226
6C	-1.512875	1.241657	-0.787301
7N	-2.738233	0.928458	-1.296276
8S	-3.990649	0.518842	-0.385021
9O	-3.661197	-0.132348	0.904473
10O	-5.015022	-0.104958	-1.235427
11C	-4.795220	2.155711	0.126789
12F	-3.928103	2.909232	0.833631
13F	-5.876319	1.927106	0.892364
14F	-5.177157	2.856366	-0.952952
15C	2.613974	1.742148	0.477770
16O	2.723170	1.995045	1.689473
17N	3.431628	1.462587	-0.500300
18C	4.817521	1.416097	-0.324353
19C	5.527852	1.665687	0.875167
20C	6.923001	1.573204	0.905874
21C	7.652422	1.234882	-0.238464
22C	6.961571	0.986319	-1.432070
23C	5.571423	1.076266	-1.472461
24H	-0.668391	1.200676	-2.788586
25H	1.683517	1.558412	-2.010588
26H	0.489039	1.856765	1.928586
27H	-1.883505	1.467680	1.362625
28H	4.981635	1.930637	1.771553

29H	7.444251	1.771911	1.840530
30H	8.737189	1.168528	-0.203532
31H	7.509282	0.725501	-2.335464
32H	5.034711	0.887246	-2.399545
33P	0.009223	-2.978573	0.308463
34C	1.401846	-1.816454	0.111862
35C	2.668736	-2.206883	0.883501
36C	-0.469626	-3.094564	2.067373
37C	-1.399808	-2.355124	-0.666332
38C	0.493733	-4.641506	-0.267075
39C	-2.604648	-3.302006	-0.722716
40C	0.861675	-4.696845	-1.756293
41C	-0.850955	-1.748549	2.700072
42H	1.027654	-0.843130	0.439169
43H	1.602752	-1.734370	-0.962093
44H	3.439449	-1.448492	0.713300
45H	2.486268	-2.261454	1.962234
46H	3.066445	-3.171532	0.549088
47H	0.371475	-3.558681	2.596150
48H	-1.306094	-3.802102	2.113661
49H	-1.025279	-2.125898	-1.670011
50H	-1.685077	-1.406382	-0.205233
51H	-0.344148	-5.311556	-0.041022
52H	1.336382	-4.959266	0.358274
53H	-3.407669	-2.821919	-1.291372
54H	-2.358487	-4.247938	-1.217258
55H	-2.995635	-3.520446	0.276826
56H	1.142586	-5.721483	-2.022808
57H	0.019363	-4.404823	-2.392835
58H	1.711607	-4.046056	-1.989038
59H	-1.133217	-1.911586	3.745957
60H	-0.012125	-1.044424	2.687903
61H	-1.702581	-1.284119	2.192304

6ah-PhNCO-018

1C	1.605838	-1.104480	-0.201601
2C	0.301294	-1.526731	-0.137853
3N	-0.363524	-1.640219	1.042756
4C	0.303541	-1.400541	2.203642
5C	1.607796	-0.978565	2.207834
6C	2.312986	-0.757749	0.989594
7N	3.566283	-0.241282	1.112737
8S	4.447428	0.245963	-0.135886
9O	5.567898	1.056887	0.362821
10O	3.698887	0.734360	-1.316429
11C	5.295729	-1.325552	-0.767573
12F	4.378768	-2.207505	-1.217272
13F	6.002677	-1.917058	0.208995
14F	6.129680	-1.031630	-1.780515
15C	-1.858839	-1.955029	1.109055
16O	-2.276068	-2.192809	2.254600
17N	-2.394452	-1.854420	-0.079306
18C	-3.760184	-2.047112	-0.303331
19C	-4.733339	-2.419336	0.655285
20C	-6.076312	-2.552433	0.287716
21C	-6.494234	-2.323299	-1.027148
22C	-5.539878	-1.959896	-1.986653
23C	-4.199510	-1.826001	-1.629903
24H	2.068745	-1.017094	-1.174356
25H	-0.280175	-1.767232	-1.017106
26H	-0.276213	-1.545025	3.106232
27H	2.102313	-0.774252	3.151171
28H	-4.430567	-2.602277	1.678511
29H	-6.803373	-2.842003	1.044125
30H	-7.540872	-2.430561	-1.301598
31H	-5.841505	-1.783121	-3.017144
32H	-3.458019	-1.548313	-2.375775
33P	-1.571274	2.654830	-0.092480
34C	-0.076323	2.158684	0.827661
35C	-0.198242	2.288453	2.351944
36C	-1.221125	2.591079	-1.884119
37C	-2.928587	1.512910	0.322218
38C	-2.046508	4.363183	0.348312
39C	-4.267065	1.835401	-0.355765
40C	-0.911542	5.387904	0.214307
41C	-0.815746	1.200706	-2.394111
42H	0.752515	2.764562	0.443005
43H	0.130662	1.124293	0.538005
44H	-0.392298	3.322238	2.658522
45H	-0.995560	1.653037	2.751606
46H	0.742861	1.973022	2.813525
47H	-0.428429	3.323506	-2.077407
48H	-2.124928	2.951271	-2.390534
49H	-3.028792	1.527008	1.414052
50H	-2.584604	0.508929	0.046248

51H	-2.429957	4.331914	1.375341
52H	-2.890687	4.626092	-0.300355
53H	-5.005351	1.083870	-0.058683
54H	-4.648449	2.819631	-0.061421
55H	-4.187520	1.803877	-1.447861
56H	-0.533569	5.444362	-0.812213
57H	-1.286796	6.380371	0.486707
58H	-0.071996	5.154220	0.877943
59H	-0.641203	1.249324	-3.474479
60H	0.108850	0.854317	-1.922512
61H	-1.597337	0.456271	-2.211362

6ah-PhNCO-019

1C	1.086534	-1.350447	-0.218929
2C	-0.260196	-1.617287	-0.211158
3N	-0.956193	-1.783185	0.943258
4C	-0.290937	-1.754336	2.127991
5C	1.054370	-1.491152	2.189282
6C	1.803294	-1.220074	1.008769
7N	3.101409	-0.851368	1.196773
8S	4.036447	-0.283299	0.026252
9O	5.210169	0.366687	0.627167
10O	3.342125	0.415468	-1.080388
11C	4.765482	-1.820492	-0.804196
12F	3.780980	-2.589453	-1.313234
13F	5.460968	-2.556479	0.077246
14F	5.587216	-1.467035	-1.807893
15C	-2.482326	-1.926002	0.961682
16O	-2.943578	-2.260700	2.065030
17N	-2.975199	-1.617949	-0.208195
18C	-4.350114	-1.604425	-0.455715
19C	-5.381410	-1.764137	0.501845
20C	-6.724114	-1.697657	0.116806
21C	-7.085898	-1.477278	-1.216109
22C	-6.075117	-1.318378	-2.173720
23C	-4.734017	-1.377625	-1.798413
24H	1.574473	-1.214815	-1.173971
25H	-0.848734	-1.690654	-1.115603
26H	-0.902177	-1.929004	3.004311
27H	1.550201	-1.449995	3.153066
28H	-5.122182	-1.943977	1.537477
29H	-7.496294	-1.824674	0.873364
30H	-8.133295	-1.433316	-1.504784
31H	-6.333657	-1.148957	-3.217080
32H	-3.949227	-1.254505	-2.541762
33P	-0.419474	2.904876	-0.000056
34C	1.072368	2.248805	0.817900
35C	2.275594	3.200349	0.816584
36C	-1.808783	1.742869	0.227437
37C	-0.845795	4.526315	0.725255
38C	-0.097504	3.119122	-1.784733
39C	-2.133859	5.145488	0.166174
40C	0.338318	1.832903	-2.502168
41C	-2.221812	1.531979	1.689758
42H	1.321893	1.322966	0.293319
43H	0.785528	1.977286	1.839936
44H	2.577825	3.473147	-0.199834
45H	2.071511	4.116761	1.380904
46H	3.126275	2.697521	1.287727
47H	-1.516334	0.795021	-0.233640
48H	-2.646638	2.131220	-0.363451
49H	0.012437	5.184680	0.547830
50H	-0.916953	4.375994	1.809047
51H	0.672637	3.895125	-1.871538
52H	-1.016553	3.525987	-2.223403
53H	-2.315383	6.107664	0.657361
54H	-2.060309	5.330155	-0.911068
55H	-3.006259	4.508727	0.348136
56H	-0.439058	1.062348	-2.460555
57H	0.526055	2.058213	-3.557785
58H	1.261033	1.423882	-2.079137
59H	-3.055777	0.824629	1.726148
60H	-1.405642	1.114300	2.288688
61H	-2.553210	2.465252	2.158649

6ah-PhNCO-020

1C	-0.672664	-2.137796	1.314148
2C	0.626887	-2.115032	0.877512
3N	0.954822	-1.618549	-0.348300
4C	-0.036993	-1.226459	-1.187538
5C	-1.356203	-1.215576	-0.806227
6C	-1.723643	-1.602293	0.514590

7N	-2.945028	-1.508655	1.112052
8S	-4.106350	-0.554334	0.559107
9O	-3.654436	0.603620	-0.247836
10O	-5.081382	-0.314146	1.633165
11C	-5.092245	-1.602383	-0.672708
12F	-4.311482	-1.993438	-1.701393
13F	-6.119820	-0.892820	-1.171657
14F	-5.582086	-2.701893	-0.077459
15C	2.407065	-1.362951	-0.764364
16O	2.512252	-0.722386	-1.828169
17N	3.231940	-1.832714	0.127627
18C	4.615008	-1.654739	0.033264
19C	5.318111	-1.043752	-1.033228
20C	6.710832	-0.924529	-0.988884
21C	7.444063	-1.401310	0.102397
22C	6.760314	-2.012200	1.162173
23C	5.372671	-2.137101	1.125970
24H	-0.897554	-2.506104	2.309303
25H	1.464057	-2.444628	1.477672
26H	0.290913	-0.893673	-2.163247
27H	-2.090303	-0.859691	-1.515553
28H	4.768527	-0.670598	-1.888028
29H	7.226527	-0.452784	-1.823280
30H	8.526793	-1.304333	0.126178
31H	7.311153	-2.394400	2.019187
32H	4.840982	-2.613436	1.946637
33P	0.475450	2.812708	0.190791
34C	-0.472838	1.588103	1.150858
35C	-0.775143	2.003690	2.595892
36C	2.131337	3.052183	0.923584
37C	0.646820	2.204426	-1.520949
38C	-0.399818	4.415196	0.216260
39C	1.293674	3.209901	-2.483531
40C	-1.835897	4.339665	-0.320805
41C	2.964853	1.765901	1.024640
42H	0.109009	0.661785	1.130080
43H	-1.398953	1.398459	0.597121
44H	-1.345417	1.204533	3.081564
45H	0.139787	2.164537	3.176944
46H	-1.379433	2.916277	2.638333
47H	1.976292	3.504623	1.910241
48H	2.639567	3.803292	0.307161
49H	-0.355786	1.919810	-1.859523
50H	1.246213	1.287978	-1.470345
51H	0.207002	5.118789	-0.365530
52H	-0.386802	4.764224	1.255266
53H	1.400971	2.742067	-3.468096
54H	0.685853	4.113064	-2.605732
55H	2.294105	3.506408	-2.149334
56H	-2.288086	5.336929	-0.290466
57H	-1.865099	3.990696	-1.358736
58H	-2.460335	3.671145	0.281012
59H	3.942871	2.000864	1.457865
60H	2.488319	1.020848	1.670152
61H	3.138400	1.310439	0.044904

6a-Me2-001

1C	-1.919957	-0.536610	-1.084215
2C	-3.171648	-1.037086	-0.721697
3N	-3.843407	-0.647220	0.371487
4C	-3.265461	0.285394	1.144312
5C	-2.025918	0.864675	0.869839
6C	-1.335106	0.435270	-0.266491
7N	-0.065851	1.015605	-0.616961
8S	1.237537	0.773873	0.390750
9O	0.804169	0.818296	1.783638
10O	2.357718	1.567757	-0.108031
11C	1.749563	-1.029084	0.108872
12F	0.780883	-1.851027	0.530919
13F	2.875789	-1.289507	0.780531
14F	1.959259	-1.238588	-1.200845
15C	0.209296	1.297415	-2.046914
16H	-1.424666	-0.904773	-1.976253
17H	-3.650397	-1.794216	-1.338624
18H	-3.824412	0.597250	2.023572
19H	-1.613243	1.625950	1.520872
20H	0.447512	0.391960	-2.613027
21H	-0.689523	1.763043	-2.455664
22H	1.035847	2.003959	-2.117090

6a-Me2-002

1C	-1.647666	-1.126227	-0.099902
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2C	-2.946618	-1.624124	-0.017635
3N	-4.048104	-0.856981	0.007471
4C	-3.858210	0.468666	-0.043972
5C	-2.603664	1.077051	-0.111943
6C	-1.466426	0.261386	-0.139391
7N	-0.169181	0.854782	-0.253596
8S	1.080007	0.378343	0.745868
9O	0.603998	-0.568924	1.748884
10O	1.897045	1.540837	1.088489
11C	2.169326	-0.633731	-0.423496
12F	2.563406	0.124731	-1.455166
13F	1.492364	-1.689499	-0.893717
14F	3.245013	-1.062658	0.244830
15C	-0.029132	2.178239	-0.906360
16H	-0.810534	-1.811913	-0.129794
17H	-3.106674	-2.699273	0.018215
18H	-4.753078	1.086822	-0.021574
19H	-2.532818	2.158263	-0.137241
20H	-0.635565	2.162444	-1.813883
21H	-0.352824	2.988435	-0.246896
22H	1.011310	2.341094	-1.186148

6a-Me-001

1C	1.927750	-1.202181	-0.951989
2C	3.214999	-0.747871	-0.854138
3N	3.562829	0.223130	0.037639
4C	2.605794	0.753319	0.843642
5C	1.297047	0.340818	0.796635
6C	0.890580	-0.671822	-0.124855
7N	-0.345050	-1.194562	-0.326627
8S	-1.656116	-0.734751	0.482924
9O	-2.729797	-1.706061	0.234738
10O	-1.450801	-0.246355	1.863399
11C	-2.221917	0.809743	-0.455040
12F	-2.489217	0.523339	-1.739512
13F	-1.254415	1.751359	-0.426108
14F	-3.328665	1.324779	0.106376
15C	4.947802	0.722887	0.069851
16H	1.687306	-1.977108	-1.671345
17H	4.015694	-1.131180	-1.476688
18H	2.933713	1.524550	1.531157
19H	0.590129	0.798469	1.474861
20H	5.104556	1.287612	0.989531
21H	5.639467	-0.122245	0.045659
22H	5.125652	1.370630	-0.793591

6a-PhNCO2-001

1C	0.547338	1.961490	1.219139
2C	0.664862	3.310267	1.551016
3N	1.038688	4.263226	0.679904
4C	1.300700	3.874733	-0.577504
5C	1.202201	2.553137	-1.016544
6C	0.820787	1.578196	-0.095595
7N	0.696750	0.204697	-0.489619
8S	2.075298	-0.670037	-0.810978
9O	3.211776	0.256739	-0.733972
10O	1.916945	-1.541455	-1.973751
11C	2.347812	-1.844954	0.681993
12F	3.674655	-1.882573	0.921139
13F	1.940396	-3.087064	0.435201
14F	1.740541	-1.371127	1.778372
15C	-0.592883	-0.542019	-0.349454
16O	-0.456052	-1.770804	-0.187647
17N	-1.609788	0.281593	-0.427436
18C	-2.921333	-0.139833	-0.216594
19C	-3.922482	0.846946	-0.394921
20C	-5.272894	0.565495	-0.197051
21C	-5.681837	-0.717253	0.193912
22C	-4.708012	-1.705305	0.375463
23C	-3.350922	-1.434320	0.173793
24H	0.238847	1.228627	1.957446
25H	0.453682	3.641277	2.565633
26H	1.599703	4.657263	-1.271807
27H	1.414700	2.289878	-2.047345
28H	-3.606101	1.843999	-0.693096
29H	-6.011114	1.351484	-0.346223
30H	-6.734808	-0.940882	0.349383
31H	-5.005073	-2.708775	0.676346
32H	-2.615855	-2.217335	0.309987

6a-PhNCO2-002

1C	-0.321306	1.913776	1.114352
2C	-1.028922	3.110107	1.006036
3N	-1.674536	3.498366	-0.105818
4C	-1.627708	2.666784	-1.158922
5C	-0.963737	1.440201	-1.153539
6C	-0.290287	1.057361	0.009473
7N	0.356543	-0.213479	0.117228
8S	1.631085	-0.593751	-0.850053
9O	1.590507	0.228473	-2.065588
10O	1.768693	-2.047810	-0.928073
11C	3.213205	0.016516	0.038045
12F	4.108609	0.380398	-0.901912
13F	3.767781	-0.927331	0.795491
14F	2.932236	1.092972	0.789130
15C	0.167324	-1.026985	1.441166
16O	1.215104	-1.215555	2.072397
17N	-1.068517	-1.316883	1.727516
18C	-2.114793	-1.250626	0.806234
19C	-3.294958	-0.562006	1.153851
20C	-4.379004	-0.504456	0.275897
21C	-4.320486	-1.142240	-0.969711
22C	-3.161232	-1.847328	-1.317760
23C	-2.074089	-1.906391	-0.444039
24H	0.185828	1.650563	2.036841
25H	-1.074094	3.791542	1.853025
26H	-2.162482	2.987689	-2.050317
27H	-0.983041	0.793878	-2.022050
28H	-3.336050	-0.058698	2.116884
29H	-5.272130	0.046738	0.563632
30H	-5.164656	-1.096503	-1.653690
31H	-3.102164	-2.357052	-2.277693
32H	-1.179118	-2.457655	-0.719037

6a-PhNCO2-003

1C	3.204980	1.075665	-1.036831
2C	4.362171	1.711737	-0.585063
3N	4.512697	2.188431	0.660648
4C	3.479816	2.032159	1.505093
5C	2.285962	1.399540	1.159546
6C	2.148487	0.910353	-0.141328
7N	0.927743	0.276496	-0.549229
8S	0.945028	-1.365812	-0.841238
9O	2.351591	-1.793188	-0.852601
10O	0.068325	-1.747220	-1.945926
11C	0.240624	-2.220775	0.728122
12F	0.325424	-1.409959	1.791678
13F	1.006439	-3.305148	0.968811
14F	-1.013644	-2.637730	0.570372
15C	-0.364655	1.024851	-0.376863
16O	-0.243425	2.260949	-0.435521
17N	-1.356441	0.188003	-0.189892
18C	-2.679775	0.609694	-0.091277
19C	-3.147852	1.948737	-0.099898
20C	-4.512973	2.229286	0.015148
21C	-5.456683	1.204670	0.144251
22C	-5.008696	-0.123707	0.154841
23C	-3.650393	-0.413961	0.039996
24H	3.127680	0.717506	-2.057636
25H	5.205117	1.849517	-1.258936
26H	3.615655	2.425689	2.510241
27H	1.481221	1.295756	1.879709
28H	-2.434754	2.757509	-0.197100
29H	-4.839160	3.268240	0.004180
30H	-6.516136	1.434065	0.233286
31H	-5.723507	-0.939075	0.251377
32H	-3.306538	-1.445011	0.044218

6a-PhNCO2-004

1C	-1.149327	1.887951	1.141255
2C	-2.228534	2.729210	0.868862
3N	-2.750963	2.897076	-0.356078
4C	-2.190898	2.204830	-1.361365
5C	-1.117440	1.329416	-1.196829
6C	-0.589594	1.167005	0.084409
7N	0.496162	0.253343	0.330542
8S	2.020052	0.842624	-0.080702
9O	2.759923	1.516829	0.989319
10O	1.881771	1.535417	-1.370449
11C	2.989761	-0.761902	-0.486998
12F	3.701164	-0.503270	-1.600791

13F	2.171459	-1.788129	-0.742926
14F	3.839470	-1.084544	0.482981
15C	0.421409	-0.766437	1.453985
16O	1.499224	-0.932489	2.050931
17N	-0.740030	-1.325986	1.671587
18C	-1.753983	-1.454471	0.729469
19C	-3.089296	-1.187811	1.103353
20C	-4.138787	-1.358985	0.199949
21C	-3.895160	-1.818732	-1.101003
22C	-2.578668	-2.111695	-1.477961
23C	-1.524444	-1.938552	-0.580305
24H	-0.766778	1.781198	2.150955
25H	-2.691463	3.296858	1.673274
26H	-2.628536	2.347794	-2.346967
27H	-0.709425	0.780840	-2.036940
28H	-3.281495	-0.825055	2.110371
29H	-5.155352	-1.128206	0.513031
30H	-4.714806	-1.951668	-1.803084
31H	-2.368976	-2.479148	-2.481102
32H	-0.506612	-2.169166	-0.883365

6a-PhNCO-001

1C	0.892577	0.104471	0.531968
2C	-0.475278	0.090796	0.402639
3N	-1.150104	-1.003987	-0.036015
4C	-0.451812	-2.125027	-0.357613
5C	0.915020	-2.174904	-0.255453
6C	1.661157	-1.049430	0.196620
7N	3.014158	-1.217843	0.245454
8S	4.040214	-0.098568	0.747656
9O	5.360511	-0.717639	0.947296
10O	3.554575	0.855201	1.769753
11C	4.311107	1.000536	-0.771599
12F	3.159878	1.604519	-1.133391
13F	4.752312	0.282201	-1.819622
14F	5.220108	1.957212	-0.503856
15C	-2.675167	-1.025409	-0.178181
16O	-3.132932	-2.132103	-0.512159
17N	-3.179376	0.152493	0.076167
18C	-4.553806	0.395616	0.040812
19C	-5.580754	-0.566221	-0.127335
20C	-6.924861	-0.180436	-0.120998
21C	-7.294465	1.158329	0.044712
22C	-6.288824	2.120432	0.211140
23C	-4.946789	1.744664	0.211778
24H	1.365128	1.005846	0.897820
25H	-1.095259	0.944803	0.639242
26H	-1.051829	-2.959884	-0.695686
27H	1.440059	-3.085107	-0.524481
28H	-5.316294	-1.607459	-0.260687
29H	-7.692177	-0.942015	-0.249277
30H	-8.342908	1.447331	0.045109
31H	-6.552369	3.168151	0.342708
32H	-4.167073	2.491227	0.345271

6a-PhNCO-002

1C	-0.492370	-1.571650	0.278155
2C	0.812401	-1.158638	0.207114
3N	1.148615	0.156097	0.324217
4C	0.167263	1.071772	0.519861
5C	-1.160675	0.723140	0.599380
6C	-1.553876	-0.640144	0.472683
7N	-2.808506	-1.175278	0.510228
8S	-4.144613	-0.318629	0.705467
9O	-4.045557	0.921696	1.506864
10O	-5.262947	-1.234759	0.981712
11C	-4.534880	0.323472	-1.034292
12F	-3.551240	1.138895	-1.469348
13F	-5.687028	1.020294	-1.033630
14F	-4.655826	-0.688953	-1.911323
15C	2.599902	0.641956	0.247932
16O	2.729696	1.866478	0.418839
17N	3.407896	-0.356746	0.011218
18C	4.789073	-0.188057	-0.100916
19C	5.514312	1.018417	0.061955
20C	6.905965	1.035733	-0.075640
21C	7.620038	-0.128301	-0.377905
22C	6.915319	-1.328511	-0.542983
23C	5.528866	-1.355950	-0.405799
24H	-0.725373	-2.626535	0.180369
25H	1.643448	-1.833598	0.055295
26H	0.507524	2.095566	0.608101

27H	-1.889883	1.504472	0.764611
28H	4.980951	1.931287	0.294335
29H	7.436612	1.977197	0.056024
30H	8.702172	-0.102724	-0.482979
31H	7.449357	-2.247261	-0.777916
32H	4.982248	-2.287735	-0.532840

6a-PhNCO-003

1C	-0.806947	1.844080	-0.054444
2C	0.560642	1.919750	-0.023367
3N	1.341204	0.804330	-0.024590
4C	0.745656	-0.418061	-0.059006
5C	-0.618319	-0.563535	-0.092307
6C	-1.471723	0.582937	-0.092182
7N	-2.824602	0.600783	-0.125913
8S	-3.692511	-0.751003	-0.162047
9O	-3.484065	-1.680564	0.970699
10O	-3.843100	-1.358886	-1.502287
11C	-5.357275	0.054946	0.177594
12F	-6.303881	-0.903573	0.177758
13F	-5.673232	0.956458	-0.766264
14F	-5.374750	0.662146	1.375446
15C	2.859985	0.972697	0.002072
16O	3.236317	2.158409	-0.002329
17N	3.454599	-0.190735	0.027095
18C	4.843918	-0.320040	0.036323
19C	5.797706	0.726331	-0.029911
20C	7.167170	0.441717	-0.025321
21C	7.635183	-0.874390	0.045871
22C	6.703053	-1.918930	0.114659
23C	5.336794	-1.645346	0.108683
24H	-1.395473	2.755348	-0.052866
25H	1.100772	2.857064	0.003150
26H	1.428477	-1.256644	-0.058722
27H	-1.026257	-1.567358	-0.116443
28H	5.457432	1.752819	-0.083098
29H	7.876673	1.265817	-0.078096
30H	8.702379	-1.083722	0.049054
31H	7.042566	-2.951440	0.171167
32H	4.613690	-2.456362	0.159347

6a-PhNCO-004

1C	0.951171	1.248738	-0.161964
2C	-0.399412	1.446529	-0.002696
3N	-1.303988	0.443788	-0.139928
4C	-0.861015	-0.806824	-0.452625
5C	0.471267	-1.072338	-0.623682
6C	1.455636	-0.048645	-0.476818
7N	2.742007	-0.422262	-0.682440
8S	4.025654	0.492571	-0.414841
9O	3.869062	1.639825	0.507143
10O	4.828108	0.699822	-1.635869
11C	5.044701	-0.743142	0.578393
12F	4.418938	-1.066042	1.725268
13F	6.235163	-0.193383	0.890026
14F	5.273346	-1.872575	-0.112968
15C	-2.786410	0.758925	0.060381
16O	-3.016973	1.950210	0.333013
17N	-3.513874	-0.314773	-0.103302
18C	-4.904066	-0.298489	0.018129
19C	-5.717710	0.819923	0.327801
20C	-7.107148	0.686715	0.414845
21C	-7.733077	-0.545421	0.200022
22C	-6.940671	-1.660258	-0.106676
23C	-5.555447	-1.537347	-0.195459
24H	1.615197	2.093876	-0.040403
25H	-0.822158	2.413299	0.238998
26H	-1.635368	-1.555003	-0.550598
27H	0.788276	-2.079491	-0.872431
28H	-5.253847	1.783407	0.495818
29H	-7.706291	1.563932	0.653011
30H	-8.814564	-0.637009	0.269267
31H	-7.405341	-2.629505	-0.277384
32H	-4.940895	-2.402960	-0.432277

6a-PhNCO-005

1C	0.447012	-1.115217	-0.442339
2C	-0.888757	-0.840156	-0.324470
3N	-1.337965	0.421162	-0.065171

4C	-0.435377	1.425888	0.072036
5C	0.918310	1.218088	-0.034068
6C	1.429346	-0.089150	-0.295382
7N	2.722665	-0.465203	-0.428337
8S	3.960629	0.537012	-0.240006
9O	3.877341	1.487782	0.891456
10O	4.514242	1.050341	-1.510558
11C	5.216824	-0.748323	0.318975
12F	6.404774	-0.141026	0.507805
13F	5.382454	-1.718214	-0.595132
14F	4.846045	-1.313874	1.480748
15C	-2.824571	0.745777	0.074657
16O	-3.062025	1.949295	0.279813
17N	-3.547931	-0.336630	-0.045762
18C	-4.942012	-0.310080	0.015488
19C	-5.585035	-1.571250	-0.001820
20C	-6.973343	-1.684876	0.038899
21C	-7.777570	-0.538126	0.092737
22C	-7.159949	0.716868	0.106953
23C	-5.767463	0.840539	0.072188
24H	0.768237	-2.130385	-0.649953
25H	-1.662703	-1.588373	-0.425813
26H	-0.862729	2.400314	0.271066
27H	1.580704	2.065216	0.091687
28H	-4.961315	-2.461049	-0.049105
29H	-7.431093	-2.672217	0.026330
30H	-8.861419	-0.622574	0.122745
31H	-7.767930	1.618998	0.148521
32H	-5.309591	1.821372	0.089907

6a-PhNCO-006

1C	0.201975	-0.792906	0.858617
2C	-1.165711	-0.922697	0.920795
3N	-1.858107	-1.683803	0.039272
4C	-1.187922	-2.365743	-0.923873
5C	0.173325	-2.263344	-1.057219
6C	0.937259	-1.449115	-0.171046
7N	2.277260	-1.401613	-0.424730
8S	3.319968	-0.533632	0.421885
9O	4.686342	-0.913566	0.028874
10O	3.034963	-0.348074	1.862289
11C	3.138295	1.216733	-0.283115
12F	4.014959	2.056431	0.299334
13F	1.893668	1.688297	-0.063272
14F	3.360976	1.230553	-1.609775
15C	-3.403503	-1.819816	0.106339
16O	-3.775903	-2.996293	-0.002354
17N	-4.091726	-0.730418	0.299898
18C	-3.633674	0.567732	0.079525
19C	-4.007092	1.579619	0.990794
20C	-3.614631	2.904912	0.797688
21C	-2.847227	3.267332	-0.317000
22C	-2.489095	2.279135	-1.241081
23C	-2.880320	0.951697	-1.054507
24H	0.697281	-0.181831	1.600706
25H	-1.751082	-0.422781	1.682181
26H	-1.798674	-2.982125	-1.572327
27H	0.680346	-2.802758	-1.850055
28H	-4.604142	1.300998	1.856172
29H	-3.910275	3.660368	1.523056
30H	-2.540499	4.299737	-0.465509
31H	-1.901871	2.541433	-2.118907
32H	-2.602277	0.200610	-1.789112

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1C	-4.294301	-1.583599	0.273853
2C	-4.296544	-2.856278	0.849614
3N	-3.677152	-3.919190	0.316240
4C	-3.032869	-3.728210	-0.847746
5C	-2.970812	-2.503378	-1.508954
6C	-3.611058	-1.398645	-0.933413
7N	-3.584336	-0.135516	-1.604604
8S	-2.093809	0.711178	-1.565919
9O	-2.220668	1.800522	-2.541931
10O	-1.040025	-0.302948	-1.715250
11C	-1.986279	1.414090	0.072184
12C	-2.407685	2.729090	0.288708
13C	-2.387363	3.236103	1.587356
14C	-1.959182	2.449748	2.670038
15C	-1.545527	1.131588	2.419178
16C	-1.558040	0.605278	1.128391
17C	-1.913851	3.023729	4.063925

18C	-4.770324	0.732413	-1.463078
19H	-4.811910	-0.766323	0.763880
20H	-4.817651	-3.023317	1.789947
21H	-2.546283	-4.601395	-1.277080
22H	-2.446719	-2.403943	-2.452121
23H	-2.732326	3.344743	-0.543653
24H	-2.707235	4.260605	1.761948
25H	-1.208349	0.506726	3.242589
26H	-1.232918	-0.411715	0.945671
27H	-1.925104	2.235310	4.823936
28H	-0.996612	3.610825	4.209784
29H	-2.760051	3.695021	4.248370
30H	-5.652073	0.118191	-1.658683
31H	-4.856391	1.183406	-0.466252
32H	-4.718707	1.520113	-2.215853
33P	2.358516	-0.470450	-0.680719
34C	2.049845	-1.206030	-2.308989
35C	4.151759	-0.469918	-0.393842
36C	1.753432	1.235584	-0.631240
37C	1.573282	-1.481873	0.604417
38C	4.890718	0.720784	-0.463050
39C	6.277389	0.685575	-0.293282
40C	6.925353	-0.529531	-0.055926
41C	6.188555	-1.717893	0.010847
42C	4.803934	-1.692938	-0.156494
43C	1.715804	1.917030	0.597567
44C	1.291929	3.244051	0.641406
45C	0.895777	3.892445	-0.533262
46C	0.923855	3.212774	-1.753101
47C	1.354931	1.885686	-1.808133
48C	0.476027	-2.301076	0.293009
49C	-0.148503	-3.034965	1.303737
50C	0.310910	-2.951318	2.621298
51C	1.407116	-2.139882	2.932017
52C	2.042964	-1.409195	1.927541
53H	2.382173	-2.247968	-2.282326
54H	0.989432	-1.154524	-2.565354
55H	2.640170	-0.666272	-3.055330
56H	4.394818	1.669745	-0.642772
57H	6.847126	1.609347	-0.343956
58H	8.003426	-0.552430	0.079002
59H	6.691113	-2.663027	0.197279
60H	4.237487	-2.618479	-0.092144
61H	2.006925	1.418079	1.517322
62H	1.259916	3.766669	1.592973
63H	0.553572	4.923013	-0.494366
64H	0.597489	3.706763	-2.663445
65H	1.356461	1.368443	-2.761288
66H	0.088704	-2.354257	-0.717980
67H	-1.001263	-3.661245	1.061651
68H	-0.182288	-3.521536	3.403980
69H	1.773007	-2.080051	3.953289
70H	2.905783	-0.797710	2.175015

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1C	-4.295976	-1.583920	0.269997
2C	-4.301078	-2.856673	0.845583
3N	-3.681694	-3.920268	0.313552
4C	-3.034400	-3.729911	-0.848869
5C	-2.969209	-2.505047	-1.509678
6C	-3.609432	-1.399611	-0.935470
7N	-3.579824	-0.136588	-1.606539
8S	-2.088819	0.708826	-1.565744
9O	-2.211759	1.795408	-2.545317
10O	-1.035390	-0.306562	-1.708685
11C	-1.986480	1.416087	0.070761
12C	-2.401412	2.732361	0.280260
13C	-2.380196	3.246251	1.578155
14C	-1.960161	2.463495	2.664057
15C	-1.549820	1.141072	2.419268
16C	-1.562418	0.609362	1.132658
17C	-1.947381	3.017268	4.066960
18C	-4.765283	0.732507	-1.468841
19H	-4.813956	-0.766074	0.758707
20H	-4.824665	-3.023270	1.784615
21H	-2.547936	-4.603638	-1.277232
22H	-2.442756	-2.406111	-2.451581
23H	-2.718411	3.347343	-0.555498
24H	-2.690821	4.274454	1.745981
25H	-1.211702	0.520683	3.246067
26H	-1.236989	-0.408266	0.953599
27H	-0.973892	2.857858	4.546919
28H	-2.162401	4.090713	4.078942
29H	-2.699033	2.516380	4.691145
30H	-5.647177	0.119055	-1.666168

31H	-4.853284	1.184604	-0.472670
32H	-4.710979	1.519532	-2.222144
33P	2.359240	-0.470602	-0.679532
34C	2.052982	-1.205689	-2.308550
35C	4.152137	-0.471129	-0.390080
36C	1.755573	1.235902	-0.631152
37C	1.572045	-1.481614	0.604788
38C	4.891816	0.719214	-0.457181
39C	6.278179	0.683238	-0.284928
40C	6.925107	-0.532328	-0.047222
41C	6.187597	-1.720390	0.017384
42C	4.803291	-1.694653	-0.152357
43C	1.717091	1.917802	0.597379
44C	1.295256	3.245500	0.640200
45C	0.901940	3.894139	-0.535274
46C	0.930721	3.214018	-1.754850
47C	1.359810	1.886273	-1.808834
48C	0.475456	-2.301186	0.292091
49C	-0.150408	-3.034808	1.302206
50C	0.307053	-2.950577	2.620400
51C	1.402660	-2.138803	2.932386
52C	2.039859	-1.408408	1.928541
53H	2.384450	-2.247890	-2.281604
54H	0.993235	-1.153158	-2.567442
55H	2.645529	-0.666194	-3.053346
56H	4.396757	1.668542	-0.637269
57H	6.848432	1.606785	-0.333876
58H	8.002917	-0.555855	0.089707
59H	6.689408	-2.665882	0.204018
60H	4.236286	-2.619967	-0.089645
61H	2.006025	1.418659	1.517743
62H	1.262345	3.768349	1.591565
63H	0.561294	4.925254	-0.497162
64H	0.606519	3.708239	-2.665848
65H	1.362227	1.368847	-2.761890
66H	0.089681	-2.354879	-0.719407
67H	-1.002641	-3.661441	1.059112
68H	-0.187125	-3.520646	3.402574
69H	1.767160	-2.078627	3.954136
70H	2.902296	-0.796794	2.177028

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1C	4.549258	1.374053	0.475825
2C	4.530825	2.732615	0.797670
3N	4.072829	3.690000	-0.022357
4C	3.624695	3.295917	-1.225920
5C	3.604796	1.969635	-1.652190
6C	4.067491	0.978354	-0.778432
7N	4.056578	-0.391726	-1.190015
8S	2.512126	-1.135081	-1.267010
9O	2.731499	-2.456497	-1.869435
10O	1.600432	-0.170524	-1.892465
11C	2.017432	-1.363815	0.438151
12C	2.174256	-2.614709	1.039871
13C	1.776092	-2.780994	2.366941
14C	1.244833	-1.711219	3.105942
15C	1.122319	-0.460224	2.478158
16C	1.502471	-0.275548	1.149974
17C	0.836420	-1.892436	4.546806
18C	5.112566	-1.271860	-0.650382
19H	4.921994	0.654105	1.195963
20H	4.895379	3.062635	1.768202
21H	3.269082	4.082460	-1.887924
22H	3.238436	1.706169	-2.637036
23H	2.575144	-3.447954	0.472243
24H	1.878254	-3.757809	2.833399
25H	0.715710	0.382217	3.031897
26H	1.376767	0.690054	0.674377
27H	0.007723	-1.228587	4.817451
28H	0.535730	-2.925069	4.753739
29H	1.673981	-1.655180	5.216846
30H	6.062666	-0.742259	-0.749339
31H	4.953605	-1.537799	0.402858
32H	5.151997	-2.181192	-1.250752
33P	-2.673801	-0.025378	0.520078
34C	-2.694098	-0.655944	2.221926
35C	-4.348615	0.508486	0.084008
36C	-1.518861	1.361352	0.400604
37C	-2.149963	-1.346242	-0.597856
38C	-4.590064	1.802095	-0.401284
39C	-5.893836	2.183994	-0.729683
40C	-6.949024	1.280671	-0.577865
41C	-6.706815	-0.011787	-0.096687
42C	-5.409935	-0.401953	0.235386
43C	-0.839719	1.589846	-0.806096

44C	0.060864	2.651600	-0.901503
45C	0.293919	3.476716	0.201676
46C	-0.387271	3.252078	1.403703
47C	-1.297950	2.200088	1.506997
48C	-1.164821	-2.258887	-0.184140
49C	-0.702505	-3.225037	-1.077272
50C	-1.213624	-3.283182	-2.377359
51C	-2.197089	-2.378056	-2.787346
52C	-2.668518	-1.407537	-1.901397
53H	-3.316219	-1.555228	2.258925
54H	-1.677743	-0.898619	2.543466
55H	-3.120366	0.102216	2.884883
56H	-3.773636	2.507859	-0.522490
57H	-6.080828	3.186660	-1.103912
58H	-7.961341	1.581001	-0.834775
59H	-7.526550	-0.715508	0.018297
60H	-5.227176	-1.409444	0.601342
61H	-0.978681	0.927962	-1.654502
62H	0.600930	2.811731	-1.828943
63H	1.015121	4.285959	0.131548
64H	-0.204651	3.892176	2.262364
65H	-1.821993	2.038417	2.444474
66H	-0.745127	-2.215090	0.815924
67H	0.070108	-3.918981	-0.761376
68H	-0.840769	-4.030993	-3.071888
69H	-2.595612	-2.422797	-3.797013
70H	-3.433417	-0.707312	-2.224829

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1C	-5.265183	-0.895594	-1.778400
2C	-6.536308	-0.323798	-1.753606
3N	-7.201246	-0.023197	-0.625484
4C	-6.585177	-0.296979	0.533528
5C	-5.308099	-0.854014	0.624540
6C	-4.626630	-1.159249	-0.560193
7N	-3.318997	-1.745309	-0.550203
8S	-2.049314	-0.718189	-1.075011
9O	-0.831238	-1.544052	-1.035506
10O	-2.473697	-0.101344	-2.337988
11C	-1.911238	0.561191	0.161717
12C	-2.727565	1.694326	0.068877
13C	-2.625051	2.675922	1.051984
14C	-1.721784	2.544846	2.121672
15C	-0.927337	1.390339	2.190778
16C	-1.020578	0.390622	1.222808
17C	-1.593730	3.639483	3.150339
18C	-2.962386	-2.583298	0.612718
19H	-4.780010	-1.129623	-2.718259
20H	-7.050734	-0.107615	-2.687372
21H	-7.133128	-0.051591	1.440844
22H	-4.866330	-1.031017	1.599000
23H	-3.415496	1.811431	-0.762149
24H	-3.250978	3.562758	0.985159
25H	-0.221282	1.270621	3.008476
26H	-0.395190	-0.492206	1.277848
27H	-2.577042	4.010389	3.462176
28H	-1.056899	3.295995	4.040677
29H	-1.042314	4.494549	2.736294
30H	-2.766419	-1.997748	1.520174
31H	-3.798822	-3.261210	0.796182
32H	-2.079981	-3.171912	0.362737
33P	2.791886	-0.516705	-0.703181
34C	2.348825	-1.492173	-2.164361
35C	2.090595	1.148278	-0.840854
36C	2.175228	-1.322157	0.798957
37C	4.598648	-0.377962	-0.608648
38C	2.639199	2.194087	-0.077843
39C	2.061614	3.462699	-0.125195
40C	0.944505	3.695350	-0.935115
41C	0.405589	2.658988	-1.701746
42C	0.971903	1.383669	-1.655605
43C	1.562382	-2.582252	0.747018
44C	1.063864	-3.156734	1.919239
45C	1.177794	-2.482437	3.137637
46C	1.797242	-1.228227	3.190812
47C	2.293425	-0.645446	2.025884
48C	5.330365	-1.127686	0.325065
49C	6.724500	-1.035915	0.346404
50C	7.387681	-0.202457	-0.558331
51C	6.658219	0.543166	-1.491615
52C	5.266181	0.458711	-1.520651
53H	2.684510	-0.952176	-3.054670
54H	2.868245	-2.453676	-2.116187
55H	1.268526	-1.651835	-2.207999
56H	3.515748	2.024681	0.541071

57H	2.487496	4.269372	0.465161
58H	0.495967	4.684593	-0.968537
59H	-0.464303	2.834173	-2.327941
60H	0.532362	0.587537	-2.246630
61H	1.448650	-3.110901	-0.192464
62H	0.581185	-4.129012	1.875073
63H	0.783812	-2.931582	4.045355
64H	1.887656	-0.701637	4.136830
65H	2.753449	0.337485	2.072290
66H	4.823950	-1.774902	1.034787
67H	7.288455	-1.614188	1.073062
68H	8.471801	-0.131184	-0.536143
69H	7.171746	1.193880	-2.193964
70H	4.707133	1.049055	-2.242129

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1C	5.070274	0.182240	-1.959217
2C	6.353865	-0.320503	-1.752495
3N	7.047070	-0.161690	-0.612595
4C	6.446770	0.523009	0.371354
5C	5.160074	1.056759	0.277091
6C	4.448807	0.881069	-0.916415
7N	3.132709	1.416858	-1.097104
8S	1.867951	0.258689	-1.189624
9O	0.644907	1.038154	-1.438273
10O	2.291146	-0.770437	-2.145803
11C	1.771745	-0.472005	0.437224
12C	2.527481	-1.617708	0.712015
13C	2.507059	-2.142021	2.001866
14C	1.751397	-1.538174	3.022554
15C	1.009625	-0.387713	2.715977
16C	1.015156	0.155244	1.430128
17C	1.740045	-2.130043	4.409647
18C	2.786116	2.628378	-0.328243
19H	4.562294	0.035713	-2.904510
20H	6.854683	-0.867958	-2.547907
21H	7.016181	0.647860	1.290007
22H	4.735342	1.585786	1.122632
23H	3.105932	-2.094012	-0.072499
24H	3.085043	-3.036782	2.221327
25H	0.413452	0.089907	3.489433
26H	0.428336	1.037935	1.203637
27H	2.756975	-2.197712	4.816049
28H	1.136329	-1.530733	5.098819
29H	1.331897	-3.148862	4.397044
30H	2.627646	2.432055	0.739831
31H	3.609993	3.336031	-0.444848
32H	1.883483	3.066685	-0.752916
33P	-2.729593	0.322010	-0.843727
34C	-2.499074	0.979286	-2.517385
35C	-1.841933	-1.250623	-0.676193
36C	-2.181702	1.547918	0.377108
37C	-4.500295	0.013237	-0.587737
38C	-1.993245	-2.010112	0.497861
39C	-1.318524	-3.222017	0.633860
40C	-0.492249	-3.684452	-0.396320
41C	-0.345042	-2.934580	-1.564807
42C	-1.016545	-1.718628	-1.709501
43C	-2.462751	1.337962	1.738562
44C	-2.004942	2.245913	2.692559
45C	-1.274819	3.371727	2.295256
46C	-1.013044	3.593070	0.940528
47C	-1.461525	2.684241	-0.021031
48C	-5.046662	-1.239566	-0.911981
49C	-6.422100	-1.447540	-0.791678
50C	-7.253127	-0.412819	-0.351034
51C	-6.709991	0.835561	-0.029856
52C	-5.336050	1.053317	-0.146626
53H	-2.905520	0.256356	-3.231015
54H	-3.060656	1.914305	-2.601895
55H	-1.440513	1.155254	-2.723801
56H	-2.636235	-1.667680	1.303244
57H	-1.435364	-3.801332	1.545507
58H	0.038567	-4.626023	-0.284526
59H	0.304466	-3.282321	-2.362445
60H	-0.874386	-1.143591	-2.617057
61H	-3.042747	0.476959	2.056844
62H	-2.222628	2.076515	3.743495
63H	-0.918093	4.078078	3.040127
64H	-0.455085	4.471410	0.628065
65H	-1.230706	2.862019	-1.064584
66H	-4.407435	-2.050424	-1.249329
67H	-6.841881	-2.418556	-1.039462
68H	-8.322698	-0.579923	-0.255933
69H	-7.353614	1.639908	0.315605

70H -4.922029 2.023478 0.113015

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1C	5.430731	-0.761078	0.539970
2C	6.678228	-0.151557	0.392482
3N	7.228283	0.149433	-0.792491
4C	6.524597	-0.177005	-1.889557
5C	5.278486	-0.800920	-1.858084
6C	4.707750	-1.092082	-0.612539
7N	3.431058	-1.738104	-0.541233
8S	2.088978	-0.788960	-1.027722
9O	0.924169	-1.687333	-0.970374
10O	2.442682	-0.136548	-2.294725
11C	1.895654	0.469450	0.223801
12C	1.043518	0.232000	1.306921
13C	0.897240	1.222729	2.274337
14C	1.600079	2.436625	2.186715
15C	2.468638	2.632047	1.101437
16C	2.622920	1.657613	0.114798
17C	1.411659	3.499347	3.240103
18C	3.166550	-2.577971	0.644818
19H	5.042607	-0.960385	1.532344
20H	7.256834	0.113968	1.274755
21H	6.986125	0.061090	-2.845346
22H	4.761910	-1.054461	-2.775727
23H	0.487091	-0.695520	1.375069
24H	0.217979	1.052722	3.105924
25H	3.021485	3.564335	1.017832
26H	3.276470	1.829642	-0.734231
27H	1.995064	4.397924	3.016589
28H	0.356285	3.790113	3.317651
29H	1.718122	3.132775	4.228241
30H	4.027474	-3.237380	0.775458
31H	3.016920	-1.992559	1.561077
32H	2.282885	-3.186408	0.453594
33P	-2.765571	-0.494828	-0.681983
34C	-2.227060	-1.463074	-2.115361
35C	-4.576246	-0.405703	-0.687790
36C	-2.191598	-1.277395	0.848284
37C	-2.106043	1.188842	-0.797420
38C	-5.342568	-1.086618	0.269599
39C	-6.737588	-1.025692	0.207960
40C	-7.364904	-0.292495	-0.802936
41C	-6.599557	0.384924	-1.759647
42C	-5.207113	0.331856	-1.705558
43C	-2.328315	-0.580665	2.061609
44C	-1.862602	-1.150160	3.245586
45C	-1.255489	-2.411138	3.225192
46C	-1.122077	-3.105479	2.019716
47C	-1.590449	-2.544632	0.828856
48C	-0.927083	1.437153	-1.517474
49C	-0.395311	2.727233	-1.551714
50C	-1.029859	3.766885	-0.867058
51C	-2.206732	3.521160	-0.151192
52C	-2.749854	2.236589	-0.116268
53H	-2.515953	-0.924186	-3.022680
54H	-1.144556	-1.613060	-2.094289
55H	-2.739192	-2.429535	-2.099907
56H	-4.862746	-1.656901	1.059251
57H	-7.330620	-1.550229	0.952072
58H	-8.449791	-0.246300	-0.845985
59H	-7.086150	0.957026	-2.544697
60H	-4.617172	0.870486	-2.443075
61H	-2.777711	0.407973	2.083611
62H	-1.967884	-0.608335	4.181375
63H	-0.884812	-2.849556	4.147849
64H	-0.647267	-4.082425	2.000446
65H	-1.460326	-3.087678	-0.100285
66H	-0.417893	0.640634	-2.049043
67H	0.519250	2.912111	-2.107335
68H	-0.609690	4.768773	-0.891582
69H	-2.706111	4.330068	0.374987
70H	-3.672518	2.058051	0.428712

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1C	-5.240800	-0.915370	-1.742289
2C	-6.538592	-0.410327	-1.680711
3N	-7.195988	-0.170215	-0.533834
4C	-6.544281	-0.438024	0.606897
5C	-5.239135	-0.931068	0.661391
6C	-4.566710	-1.174956	-0.542443
7N	-3.233508	-1.698736	-0.570087

8S	-2.020544	-0.607216	-1.099485
9O	-0.772397	-1.387213	-1.116231
10O	-2.504998	0.024701	-2.332728
11C	-1.894944	0.643361	0.167812
12C	-2.730294	1.764479	0.106219
13C	-2.635985	2.725908	1.109982
14C	-1.725331	2.584498	2.171702
15C	-0.915384	1.439132	2.212803
16C	-0.995766	0.462004	1.220779
17C	-1.602087	3.661598	3.219361
18C	-2.817029	-2.548007	0.564071
19H	-4.762523	-1.103247	-2.695906
20H	-7.081129	-0.199280	-2.599624
21H	-7.086088	-0.240631	1.529520
22H	-4.770326	-1.108083	1.622968
23H	-3.424645	1.889290	-0.718383
24H	-3.274765	3.604955	1.065814
25H	-0.205320	1.310611	3.025987
26H	-0.355336	-0.411376	1.253738
27H	-1.079968	3.299739	4.111193
28H	-1.036409	4.516927	2.825340
29H	-2.585627	4.037735	3.523647
30H	-2.641011	-1.979641	1.486358
31H	-3.612881	-3.275677	0.737282
32H	-1.907331	-3.079750	0.286758
33P	2.789347	-0.540288	-0.732881
34C	2.432551	-1.529100	-2.209289
35C	2.061360	1.111072	-0.897737
36C	2.146852	-1.371150	0.744735
37C	4.587494	-0.366506	-0.559407
38C	2.539174	2.155683	-0.086513
39C	1.943763	3.414719	-0.153789
40C	0.877154	3.639871	-1.031041
41C	0.408216	2.605396	-1.844420
42C	0.993353	1.339324	-1.779393
43C	1.415113	-2.563431	0.651158
44C	0.891374	-3.145107	1.808896
45C	1.092613	-2.542702	3.053152
46C	1.831429	-1.357153	3.148056
47C	2.360029	-0.771732	1.999081
48C	5.306943	-1.235683	0.276856
49C	6.697388	-1.129596	0.354102
50C	7.371429	-0.163681	-0.398939
51C	6.655576	0.699762	-1.235272
52C	5.265995	0.602318	-1.318585
53H	2.819193	-0.996817	-3.083350
54H	2.949640	-2.488943	-2.118849
55H	1.357625	-1.693357	-2.318594
56H	3.374319	1.991084	0.588680
57H	2.314796	4.219179	0.475295
58H	0.413145	4.621228	-1.080145
59H	-0.422909	2.773985	-2.522962
60H	0.602784	0.544433	-2.404484
61H	1.226459	-3.032139	-0.307715
62H	0.321474	-4.066892	1.733237
63H	0.676936	-2.995671	3.949246
64H	1.994061	-0.888304	4.114614
65H	2.930720	0.149895	2.079165
66H	4.792620	-1.986214	0.870099
67H	7.250646	-1.800052	1.005958
68H	8.453010	-0.081610	-0.332787
69H	7.176686	1.453216	-1.819354
70H	4.717469	1.284757	-1.962015

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1C	-4.926867	-0.914697	-0.191830
2C	-5.183732	-2.114250	-0.858606
3N	-4.838565	-2.351363	-2.132525
4C	-4.227375	-1.352711	-2.791571
5C	-3.935082	-0.112173	-2.228033
6C	-4.278725	0.112979	-0.888869
7N	-3.976388	1.369765	-0.273228
8S	-2.310905	1.665330	0.015444
9O	-2.226427	3.022797	0.572311
10O	-1.591790	1.322774	-1.215759
11C	-1.846756	0.499952	1.291641
12C	-1.851800	0.907365	2.630136
13C	-1.574334	-0.032840	3.622685
14C	-1.310058	-1.374614	3.299731
15C	-1.322478	-1.753246	1.947744
16C	-1.586190	-0.828447	0.938379
17C	-0.974101	-2.372837	4.378514
18C	-4.862771	1.821202	0.818619
19H	-5.217781	-0.803558	0.846721
20H	-5.682405	-2.927044	-0.334840

21H	-3.964326	-1.550688	-3.828391
22H	-3.447199	0.660288	-2.809654
23H	-2.061826	1.940951	2.886260
24H	-1.567383	0.279988	4.663986
25H	-1.112856	-2.784507	1.676659
26H	-1.575746	-1.132293	-0.102367
27H	-1.226243	-3.394433	4.074603
28H	0.101983	-2.351025	4.601139
29H	-1.503016	-2.148479	5.311252
30H	-5.892380	1.697699	0.475460
31H	-4.720623	1.257816	1.749997
32H	-4.678080	2.879433	1.003678
33P	2.520121	-0.081024	0.277889
34C	2.059043	-0.252398	2.025579
35C	2.355409	1.650576	-0.216720
36C	4.238750	-0.614192	0.068587
37C	1.432900	-1.120519	-0.728350
38C	3.264914	2.210508	-1.128982
39C	3.095203	3.531097	-1.549063
40C	2.022926	4.289651	-1.068013
41C	1.115635	3.730986	-0.162136
42C	1.280544	2.414536	0.267270
43C	4.608046	-1.428964	-1.012933
44C	5.946457	-1.794220	-1.177681
45C	6.912680	-1.348212	-0.271583
46C	6.544363	-0.534178	0.805920
47C	5.210843	-0.163284	0.978523
48C	1.250164	-2.467364	-0.367274
49C	0.400187	-3.274839	-1.120627
50C	-0.264092	-2.745971	-2.234959
51C	-0.071983	-1.411646	-2.599030
52C	0.774603	-0.593083	-1.847657
53H	1.009509	0.020379	2.159247
54H	2.208518	-1.290480	2.336077
55H	2.688886	0.405453	2.631913
56H	4.098560	1.626692	-1.508294
57H	3.800379	3.964741	-2.252675
58H	1.892378	5.315594	-1.401738
59H	0.269688	4.306846	0.200591
60H	0.565014	1.989266	0.963259
61H	3.862546	-1.779887	-1.720107
62H	6.230828	-2.425934	-2.014611
63H	7.952803	-1.634527	-0.402719
64H	7.294652	-0.186156	1.510376
65H	4.935731	0.474400	1.814101
66H	1.761758	-2.882337	0.497140
67H	0.252506	-4.313669	-0.838498
68H	-0.934746	-3.375293	-2.813859
69H	-0.592437	-0.996528	-3.456974
70H	0.896453	0.448983	-2.121794

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1C	4.948963	-2.240019	-0.830162
2C	6.145847	-2.500612	-0.164625
3N	7.029536	-1.551757	0.187271
4C	6.720242	-0.286085	-0.129476
5C	5.544076	0.088110	-0.782158
6C	4.631931	-0.912074	-1.140683
7N	3.411774	-0.611598	-1.828890
8S	1.975661	-0.793245	-0.908278
9O	0.875719	-0.547359	-1.856448
10O	2.068888	-2.077593	-0.206141
11C	2.001254	0.531160	0.287650
12C	2.731443	0.365027	1.470805
13C	2.824691	1.434252	2.357523
14C	2.200690	2.664676	2.085479
15C	1.475704	2.798733	0.892139
16C	1.375649	1.742321	-0.014405
17C	2.307661	3.803400	3.068214
18C	3.410537	0.569150	-2.716220
19H	4.277479	-3.045460	-1.101814
20H	6.412777	-3.524395	0.088031
21H	7.442671	0.474128	0.159785
22H	5.353034	1.134848	-0.990382
23H	3.206684	-0.583919	1.696189
24H	3.385257	1.310874	3.281301
25H	0.978633	3.738753	0.665920
26H	0.811064	1.854854	-0.933033
27H	3.357011	4.038631	3.285258
28H	1.825379	4.710498	2.689881
29H	1.834402	3.541228	4.023489
30H	3.394823	1.520177	-2.168125
31H	4.315326	0.520491	-3.325853
32H	2.542016	0.513494	-3.372783
33P	-2.807846	-0.627270	-0.460896

34C	-2.208468	-1.813512	-1.694782
35C	-1.714912	-0.621138	0.979846
36C	-2.866384	1.034555	-1.184049
37C	-4.482002	-1.109632	0.038361
38C	-1.639780	0.527496	1.785493
39C	-0.846683	0.515928	2.932556
40C	-0.126180	-0.632656	3.275000
41C	-0.195636	-1.772665	2.469951
42C	-0.990702	-1.773728	1.323143
43C	-3.921325	1.904997	-0.865960
44C	-3.930677	3.200965	-1.386805
45C	-2.894809	3.628435	-2.222865
46C	-1.844968	2.759681	-2.540569
47C	-1.823716	1.463570	-2.023364
48C	-4.810288	-1.299119	1.388660
49C	-6.110529	-1.675657	1.736842
50C	-7.077881	-1.859642	0.745407
51C	-6.749651	-1.669869	-0.602422
52C	-5.454912	-1.294812	-0.959998
53H	-2.322603	-2.828642	-1.304008
54H	-2.807549	-1.708139	-2.604012
55H	-1.155947	-1.618711	-1.916393
56H	-2.186513	1.427059	1.516609
57H	-0.783619	1.406824	3.550543
58H	0.501272	-0.633234	4.162006
59H	0.380272	-2.658143	2.722368
60H	-1.028327	-2.662944	0.702348
61H	-4.732625	1.576461	-0.223020
62H	-4.748698	3.872369	-1.140735
63H	-2.906570	4.636451	-2.628842
64H	-1.040665	3.089835	-3.192627
65H	-0.995088	0.804869	-2.262310
66H	-4.063734	-1.160784	2.164741
67H	-6.363873	-1.824236	2.782941
68H	-8.087784	-2.151807	1.020669
69H	-7.501499	-1.811788	-1.373767
70H	-5.207025	-1.143002	-2.007597

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1C	-4.192126	-2.582309	-1.300954
2C	-5.332721	-2.609970	-2.101567
3N	-6.509614	-2.065484	-1.750201
4C	-6.565142	-1.464430	-0.553019
5C	-5.481025	-1.365011	0.321182
6C	-4.259259	-1.933680	-0.060926
7N	-3.107716	-1.886958	0.788631
8S	-1.803413	-0.920555	0.229292
9O	-0.743759	-1.080435	1.238857
10O	-1.545090	-1.299676	-1.164880
11C	-2.391433	0.762094	0.273085
12C	-3.152178	1.242907	-0.800105
13C	-3.662797	2.535820	-0.733494
14C	-3.429118	3.355440	0.385584
15C	-2.662855	2.844313	1.443302
16C	-2.144753	1.548284	1.399926
17C	-3.996495	4.751700	0.432450
18C	-3.346866	-1.782409	2.242467
19H	-3.273019	-3.051196	-1.629860
20H	-5.301895	-3.106214	-3.069007
21H	-7.522580	-1.028330	-0.275866
22H	-5.600512	-0.848832	1.267093
23H	-3.330504	0.622239	-1.672217
24H	-4.250863	2.919063	-1.564225
25H	-2.462172	3.466248	2.312168
26H	-1.541978	1.165375	2.216751
27H	-5.093893	4.725934	0.453194
28H	-3.654635	5.297708	1.317531
29H	-3.706564	5.324610	-0.457188
30H	-3.686199	-0.785409	2.552022
31H	-4.110672	-2.518960	2.500370
32H	-2.426166	-2.032944	2.768861
33P	2.810209	-0.544547	-0.232124
34C	1.913544	-2.069244	-0.630030
35C	1.745630	0.893842	-0.510827
36C	3.329069	-0.592164	1.503766
37C	4.269612	-0.415035	-1.300412
38C	1.819675	2.005470	0.343805
39C	1.052197	3.139235	0.070406
40C	0.216428	3.167636	-1.049608
41C	0.139645	2.058325	-1.896922
42C	0.901929	0.920261	-1.633113
43C	4.668733	-0.375550	1.860264
44C	5.037989	-0.405805	3.207710
45C	4.076854	-0.646651	4.193402
46C	2.740158	-0.859014	3.835860

47C	2.359591	-0.832247	2.494154
48C	4.656899	0.831987	-1.816875
49C	5.802081	0.928179	-2.610432
50C	6.559422	-0.212698	-2.891671
51C	6.174743	-1.455574	-2.376875
52C	5.034621	-1.561135	-1.578967
53H	1.643015	-2.072291	-1.689381
54H	2.555172	-2.928380	-0.413465
55H	1.010972	-2.123750	-0.017567
56H	2.466484	1.989775	1.216160
57H	1.103971	3.996281	0.736201
58H	-0.382232	4.049904	-1.257798
59H	-0.522594	2.071526	-2.757604
60H	0.824411	0.061580	-2.292287
61H	5.420034	-0.187759	1.099176
62H	6.075884	-0.240535	3.483560
63H	4.367782	-0.669652	5.240295
64H	1.992189	-1.044515	4.601895
65H	1.319673	-0.987486	2.222703
66H	4.068901	1.721398	-1.610154
67H	6.097686	1.893890	-3.010959
68H	7.447526	-0.134947	-3.513054
69H	6.761273	-2.343726	-2.595158
70H	4.752752	-2.530950	-1.179234

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1C	4.929943	-2.285001	-0.782572
2C	6.115575	-2.553782	-0.100383
3N	7.008344	-1.612805	0.249783
4C	6.720528	-0.347089	-0.086335
5C	5.557079	0.035131	-0.756980
6C	4.635090	-0.956769	-1.113152
7N	3.425436	-0.647987	-1.816321
8S	1.980368	-0.794358	-0.902948
9O	0.889483	-0.554202	-1.863190
10O	2.052759	-2.065357	-0.174578
11C	2.016850	0.554649	0.265544
12C	2.744221	0.406569	1.449612
13C	2.846440	1.493958	2.317649
14C	2.233663	2.721126	2.021910
15C	1.510369	2.838209	0.822318
16C	1.401792	1.767608	-0.061898
17C	2.328112	3.890490	2.969897
18C	3.447370	0.523698	-2.715522
19H	4.249955	-3.084345	-1.051160
20H	6.365303	-3.577823	0.168307
21H	7.450196	0.406577	0.201870
22H	5.382669	1.081715	-0.980078
23H	3.211628	-0.541230	1.695031
24H	3.405469	1.381444	3.243137
25H	1.021468	3.779022	0.579564
26H	0.837935	1.865531	-0.982642
27H	2.713041	4.782450	2.460361
28H	1.338582	4.151330	3.367750
29H	2.985460	3.671300	3.817261
30H	3.437045	1.480240	-2.177008
31H	4.357743	0.458407	-3.315059
32H	2.584910	0.471590	-3.380440
33P	-2.814137	-0.632865	-0.446544
34C	-2.199385	-1.841499	-1.650942
35C	-1.706042	-0.562875	0.981128
36C	-2.905698	1.001732	-1.225482
37C	-4.469229	-1.134659	0.095599
38C	-1.615581	0.619815	1.733344
39C	-0.820019	0.650636	2.878732
40C	-0.110732	-0.488996	3.270403
41C	-0.193996	-1.663081	2.516814
42C	-0.992319	-1.706323	1.373571
43C	-4.007004	1.840379	-0.993331
44C	-4.042797	3.112627	-1.569526
45C	-2.987402	3.547045	-2.376597
46C	-1.890756	2.709435	-2.609253
47C	-1.842757	1.438075	-2.036000
48C	-4.828334	-1.088230	1.451296
49C	-6.116602	-1.465515	1.838914
50C	-7.042285	-1.888674	0.881121
51C	-6.683784	-1.935614	-0.471082
52C	-5.400585	-1.558842	-0.868224
53H	-2.279427	-2.848504	-1.231653
54H	-2.807647	-1.778724	-2.557661
55H	-1.154926	-1.622888	-1.888385
56H	-2.157127	1.510749	1.427556
57H	-0.745147	1.567620	3.455893
58H	0.518163	-0.457189	4.155715
59H	0.373835	-2.542371	2.806490

60H	-1.043335	-2.621766	0.793057
61H	-4.834060	1.507399	-0.372957
62H	-4.896954	3.759338	-1.388669
63H	-3.019494	4.535862	-2.826340
64H	-1.070971	3.044547	-3.239182
65H	-0.980548	0.802606	-2.211826
66H	-4.113167	-0.765646	2.201778
67H	-6.392160	-1.431385	2.889351
68H	-8.042576	-2.184134	1.186422
69H	-7.402010	-2.266979	-1.215894
70H	-5.132410	-1.595438	-1.920785

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1C	-4.954259	1.656868	0.552710
2C	-5.474321	2.602030	-0.334480
3N	-4.800337	3.680476	-0.758960
4C	-3.557590	3.849540	-0.277584
5C	-2.947769	2.977220	0.621831
6C	-3.655568	1.843696	1.041873
7N	-3.054399	0.932755	1.969409
8S	-1.779598	-0.033588	1.347799
9O	-1.230101	-0.757051	2.502432
10O	-0.916541	0.861123	0.563302
11C	-2.543540	-1.198366	0.235752
12C	-3.014850	-2.416787	0.737345
13C	-3.664949	-3.292433	-0.128849
14C	-3.853966	-2.969273	-1.484585
15C	-3.368630	-1.739625	-1.955288
16C	-2.716114	-0.846124	-1.104809
17C	-4.554779	-3.937871	-2.404195
18C	-3.954331	0.213442	2.893958
19H	-5.555247	0.800757	0.839042
20H	-6.480804	2.476923	-0.727996
21H	-3.026154	4.735449	-0.618415
22H	-1.948804	3.171009	0.993089
23H	-2.859856	-2.678429	1.779026
24H	-4.028685	-4.244703	0.250434
25H	-3.498264	-1.475960	-3.001978
26H	-2.334312	0.097943	-1.479020
27H	-4.677834	-3.523624	-3.409908
28H	-3.989138	-4.875002	-2.489479
29H	-5.548182	-4.197886	-2.017815
30H	-4.633775	0.950235	3.328034
31H	-4.540552	-0.571667	2.399618
32H	-3.357072	-0.227431	3.692335
33P	2.717987	0.217871	0.395862
34C	2.051360	0.766593	1.990484
35C	2.764658	1.620706	-0.750419
36C	4.402429	-0.402398	0.652980
37C	1.693913	-1.103975	-0.294976
38C	3.915610	1.885496	-1.509089
39C	3.922064	2.957781	-2.404688
40C	2.786989	3.761063	-2.546288
41C	1.637668	3.491764	-1.794439
42C	1.619548	2.423782	-0.897029
43C	4.810164	-1.621722	0.090215
44C	6.119435	-2.070174	0.282815
45C	7.019943	-1.307665	1.031797
46C	6.614699	-0.090392	1.591260
47C	5.309936	0.365887	1.403763
48C	1.223897	-2.123759	0.547958
49C	0.476830	-3.172515	0.012006
50C	0.202677	-3.210953	-1.358693
51C	0.671918	-2.196117	-2.197302
52C	1.419177	-1.140670	-1.670608
53H	1.040015	1.150901	1.847412
54H	2.032660	-0.074261	2.689694
55H	2.697840	1.554595	2.388328
56H	4.801805	1.267054	-1.404263
57H	4.814984	3.164031	-2.988420
58H	2.795765	4.594808	-3.243475
59H	0.752132	4.111235	-1.907715
60H	0.718396	2.211877	-0.331201
61H	4.115788	-2.221377	-0.490368
62H	6.431930	-3.015809	-0.151380
63H	8.037156	-1.659931	1.180743
64H	7.313951	0.504455	2.172335
65H	5.008682	1.316908	1.834463
66H	1.423292	-2.098752	1.614669
67H	0.100467	-3.952219	0.667757
68H	-0.386184	-4.025900	-1.770215
69H	0.451113	-2.219231	-3.260827
70H	1.775444	-0.352135	-2.326769

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1C	5.405856	-0.978558	0.431002
2C	6.374590	-1.219270	-0.545213
3N	6.200243	-2.048948	-1.583968
4C	5.019488	-2.685313	-1.661332
5C	3.989083	-2.529754	-0.735546
6C	4.178100	-1.645335	0.334186
7N	3.141165	-1.461612	1.304745
8S	1.740929	-0.639521	0.751260
9O	0.805970	-0.656729	1.889814
10O	1.354488	-1.249538	-0.524938
11C	2.251642	1.044821	0.459744
12C	2.105525	1.993683	1.477378
13C	2.570693	3.288807	1.260747
14C	3.188372	3.647488	0.049567
15C	3.323692	2.670593	-0.948809
16C	2.859496	1.369105	-0.755807
17C	3.679956	5.057392	-0.163154
18C	3.553751	-1.092905	2.674591
19H	5.613566	-0.280094	1.233537
20H	7.334208	-0.709723	-0.490187
21H	4.893130	-3.364613	-2.501484
22H	3.060424	-3.076947	-0.841915
23H	1.623340	1.723489	2.411289
24H	2.453181	4.034946	2.043426
25H	3.794872	2.929408	-1.893627
26H	2.958237	0.625397	-1.539750
27H	4.204681	5.162965	-1.118081
28H	2.843810	5.768969	-0.156010
29H	4.365070	5.360392	0.638318
30H	4.369851	-1.760274	2.959904
31H	3.892953	-0.052206	2.757288
32H	2.714109	-1.256600	3.349962
33P	-2.876684	-0.066902	0.495858
34C	-2.435251	0.104839	2.246885
35C	-4.591740	0.481891	0.284421
36C	-1.786877	0.967852	-0.508843
37C	-2.738468	-1.799525	-0.008805
38C	-4.927822	1.457453	-0.665898
39C	-6.260528	1.854088	-0.807321
40C	-7.252571	1.280458	-0.007520
41C	-6.917138	0.304527	0.938579
42C	-5.590053	-0.097616	1.087047
43C	-1.329651	0.511324	-1.754353
44C	-0.534841	1.343612	-2.544576
45C	-0.193920	2.622058	-2.095371
46C	-0.647386	3.075962	-0.852307
47C	-1.444007	2.253557	-0.056273
48C	-1.682182	-2.585898	0.481529
49C	-1.554636	-3.909539	0.058384
50C	-2.469967	-4.449987	-0.850570
51C	-3.518817	-3.665690	-1.341102
52C	-3.657247	-2.340723	-0.923578
53H	-3.040506	-0.588256	2.838852
54H	-1.372634	-0.112378	2.381675
55H	-2.645587	1.129839	2.566395
56H	-4.161118	1.906817	-1.289806
57H	-6.520181	2.610464	-1.542759
58H	-8.287818	1.591279	-0.120320
59H	-7.688217	-0.144567	1.558393
60H	-5.339110	-0.864781	1.815003
61H	-1.575423	-0.487510	-2.101426
62H	-0.171469	0.984932	-3.503475
63H	0.433187	3.262882	-2.708711
64H	-0.375128	4.066397	-0.499390
65H	-1.794327	2.615684	0.906253
66H	-0.954111	-2.173361	1.171701
67H	-0.735436	-4.514767	0.436696
68H	-2.366268	-5.481537	-1.176617
69H	-4.231509	-4.082988	-2.047109
70H	-4.476753	-1.739736	-1.306579

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1C	-5.278371	-1.213504	-0.448656
2C	-6.210134	-1.694111	0.473798
3N	-5.942094	-2.641556	1.383748
4C	-4.699478	-3.152889	1.380479
5C	-3.697564	-2.756849	0.496425
6C	-3.986529	-1.753772	-0.438092
7N	-2.984001	-1.334055	-1.369811
8S	-1.665993	-0.451924	-0.712428
9O	-0.702732	-0.314831	-1.817788
10O	-1.273832	-1.128380	0.527772

11C	-2.308540	1.162925	-0.312924
12C	-2.209075	2.198128	-1.245249
13C	-2.771539	3.437819	-0.937564
14C	-3.436418	3.651575	0.279929
15C	-3.525219	2.586429	1.193559
16C	-2.967721	1.342417	0.908583
17C	-4.014357	5.001367	0.622682
18C	-3.445163	-0.831074	-2.679757
19H	-5.564241	-0.434526	-1.146304
20H	-7.219245	-1.287641	0.483005
21H	-4.496627	-3.928584	2.115625
22H	-2.715880	-3.213206	0.530587
23H	-1.689963	2.042421	-2.185327
24H	-2.690426	4.250048	-1.655719
25H	-4.036575	2.734603	2.141783
26H	-3.032475	0.529706	1.624688
27H	-4.970391	4.904115	1.149342
28H	-3.334289	5.554392	1.285083
29H	-4.173184	5.611055	-0.272785
30H	-4.178892	-1.542613	-3.064994
31H	-3.902579	0.164807	-2.620046
32H	-2.595691	-0.800324	-3.362618
33P	2.901857	-0.097796	-0.573898
34C	2.600184	-0.055934	-2.363912
35C	4.641697	0.310574	-0.266400
36C	1.850819	1.125485	0.246567
37C	2.566963	-1.758728	0.061510
38C	4.999624	1.248655	0.713491
39C	6.349698	1.523352	0.947699
40C	7.338311	0.865688	0.210792
41C	6.981135	-0.072089	-0.765260
42C	5.636442	-0.353561	-1.005637
43C	1.197216	0.814439	1.447639
44C	0.431256	1.790591	2.088586
45C	0.315401	3.068142	1.536249
46C	0.963129	3.376239	0.334764
47C	1.733002	2.410170	-0.312080
48C	1.519057	-2.519792	-0.481851
49C	1.243503	-3.783787	0.041270
50C	2.000878	-4.286670	1.103482
51C	3.041856	-3.526496	1.647215
52C	3.329371	-2.262951	1.128904
53H	3.170403	-0.854826	-2.846852
54H	1.532032	-0.186475	-2.554237
55H	2.926675	0.911242	-2.757211
56H	4.237118	1.764796	1.289038
57H	6.625448	2.250849	1.706050
58H	8.387188	1.082548	0.394949
59H	7.749078	-0.584505	-1.338108
60H	5.368100	-1.088280	-1.760413
61H	1.269026	-0.180397	1.874624
62H	-0.087136	1.544189	3.010761
63H	-0.288456	3.821692	2.033931
64H	0.864988	4.366479	-0.101164
65H	2.235832	2.658648	-1.242569
66H	0.908152	-2.129904	-1.288345
67H	0.430845	-4.370226	-0.378288
68H	1.780656	-5.270972	1.508213
69H	3.632499	-3.916319	2.471569
70H	4.144626	-1.680832	1.548178

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1C	-5.132341	-1.372233	-1.841462
2C	-6.122781	-0.633592	-2.487202
3N	-6.856367	0.320078	-1.889265
4C	-6.603700	0.557784	-0.594105
5C	-5.626211	-0.111778	0.144607
6C	-4.867032	-1.100321	-0.493758
7N	-3.852874	-1.838466	0.198700
8S	-2.239494	-1.487999	-0.259098
9O	-1.390299	-2.392382	0.528255
10O	-2.181869	-1.514989	-1.726669
11C	-1.941445	0.192590	0.277437
12C	-2.345036	1.248654	-0.546875
13C	-2.174145	2.558627	-0.096996
14C	-1.610495	2.827346	1.160042
15C	-1.219245	1.744342	1.966121
16C	-1.384966	0.427908	1.540100
17C	-1.403842	4.242138	1.637095
18C	-4.035773	-2.040545	1.650792
19H	-4.577461	-2.138912	-2.368575
20H	-6.345165	-0.826047	-3.534432
21H	-7.203973	1.330837	-0.118899
22H	-5.467370	0.147490	1.185305
23H	-2.775026	1.052969	-1.523816

24H	-2.480250	3.382925	-0.736084
25H	-0.768905	1.934304	2.937209
26H	-1.064380	-0.401313	2.161888
27H	-1.954663	4.425942	2.568328
28H	-0.344115	4.433618	1.848186
29H	-1.742147	4.971790	0.894646
30H	-3.871070	-1.127038	2.236750
31H	-5.060341	-2.386834	1.804456
32H	-3.348242	-2.816791	1.986364
33P	2.545895	-0.312551	-0.473901
34C	1.289012	-1.006245	-1.581424
35C	2.625321	1.475854	-0.752245
36C	2.086475	-0.616383	1.250517
37C	4.153289	-1.067800	-0.823509
38C	3.848282	2.125109	-0.976335
39C	3.870825	3.511553	-1.152947
40C	2.682566	4.245994	-1.102723
41C	1.463568	3.597158	-0.873258
42C	1.430209	2.214677	-0.698661
43C	1.506308	-1.842013	1.613770
44C	1.175954	-2.080749	2.948347
45C	1.426592	-1.107142	3.920100
46C	2.010587	0.111825	3.559106
47C	2.341456	0.361559	2.226599
48C	4.990349	-1.472542	0.228029
49C	6.240216	-2.026810	-0.058284
50C	6.655466	-2.174937	-1.384735
51C	5.822397	-1.767423	-2.432959
52C	4.572356	-1.212677	-2.157850
53H	1.594237	-0.838293	-2.618347
54H	1.171663	-2.078113	-1.405483
55H	0.340013	-0.496422	-1.405329
56H	4.775136	1.560450	-1.015264
57H	4.817475	4.014759	-1.329370
58H	2.705104	5.323623	-1.241231
59H	0.538609	4.164828	-0.827580
60H	0.480460	1.722950	-0.512317
61H	1.290672	-2.601466	0.870347
62H	0.712651	-3.024099	3.222967
63H	1.164258	-1.296454	4.957684
64H	2.204129	0.870777	4.312049
65H	2.785150	1.313884	1.952121
66H	4.671366	-1.364820	1.260399
67H	6.885306	-2.344906	0.755989
68H	7.627008	-2.609895	-1.603597
69H	6.144305	-1.881768	-3.464306
70H	3.935774	-0.893615	-2.978710

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1C	-5.299241	0.951255	0.220089
2C	-5.651423	1.604368	1.402705
3N	-5.608743	1.032125	2.614628
4C	-5.214512	-0.251282	2.667561
5C	-4.854254	-1.001234	1.549036
6C	-4.885371	-0.384646	0.292175
7N	-4.513719	-1.123944	-0.877172
8S	-2.847122	-1.487165	-1.020410
9O	-2.706598	-2.285158	-2.245645
10O	-2.408750	-2.029537	0.272323
11C	-2.032989	0.086513	-1.264036
12C	-1.884385	0.591238	-2.560764
13C	-1.322881	1.856832	-2.730634
14C	-0.912919	2.625740	-1.628123
15C	-1.072308	2.089770	-0.340248
16C	-1.636212	0.829266	-0.146961
17C	-0.283347	3.981880	-1.827110
18C	-5.170827	-0.760447	-2.149195
19H	-5.339603	1.485672	-0.722340
20H	-5.973787	2.642928	1.370359
21H	-5.196062	-0.708803	3.654253
22H	-4.552840	-2.037099	1.647063
23H	-2.191554	0.000740	-3.418084
24H	-1.202706	2.252938	-3.736224
25H	-0.747482	2.661149	0.524297
26H	-1.755042	0.425856	0.852994
27H	-0.366376	4.597986	-0.926190
28H	0.785121	3.885191	-2.063489
29H	-0.750066	4.520899	-2.659002
30H	-6.243641	-0.698781	-1.953945
31H	-4.820669	0.196286	-2.557902
32H	-4.990234	-1.553164	-2.875026
33P	2.678307	-0.116779	-0.187996
34C	1.883532	0.124600	-1.801993
35C	4.475523	-0.038739	-0.394048
36C	2.129615	1.201413	0.929575

37C	2.203691	-1.734664	0.464530
38C	5.278941	0.624547	0.546848
39C	6.666456	0.636268	0.386908
40C	7.252785	-0.012134	-0.703806
41C	6.452795	-0.679813	-1.637943
42C	5.065982	-0.698279	-1.486585
43C	1.430975	0.906594	2.109407
44C	0.991556	1.949036	2.929961
45C	1.252189	3.276837	2.580547
46C	1.955257	3.570092	1.405989
47C	2.392918	2.537067	0.578293
48C	0.864935	-2.150537	0.362774
49C	0.483072	-3.388269	0.879322
50C	1.431633	-4.211398	1.495966
51C	2.762990	-3.796081	1.601703
52C	3.155060	-2.557678	1.088791
53H	2.158245	-0.694342	-2.472694
54H	0.799946	0.136232	-1.670295
55H	2.213472	1.075531	-2.228906
56H	4.831753	1.129799	1.397128
57H	7.285908	1.151943	1.115436
58H	8.332347	0.000905	-0.826808
59H	6.907895	-1.187224	-2.483942
60H	4.456703	-1.229852	-2.212772
61H	1.222957	-0.121715	2.388126
62H	0.445979	1.720188	3.841254
63H	0.908386	4.083906	3.221952
64H	2.159478	4.601679	1.133281
65H	2.940787	2.770758	-0.330814
66H	0.116151	-1.518036	-0.102595
67H	-0.554277	-3.696661	0.797875
68H	1.132281	-5.177365	1.893870
69H	3.499394	-4.435896	2.080092
70H	4.191494	-2.243720	1.169507

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1C	3.364978	3.028532	-0.446255
2C	4.458612	3.827402	-0.116369
3N	5.238730	3.625762	0.958755
4C	4.929098	2.584659	1.744245
5C	3.865942	1.713123	1.500441
6C	3.061301	1.934967	0.375788
7N	1.934590	1.102822	0.082111
8S	2.044243	0.130345	-1.330425
9O	0.708724	-0.472342	-1.480928
10O	2.595766	0.973357	-2.396671
11C	3.209970	-1.161382	-0.940161
12C	4.577666	-0.914048	-1.099436
13C	5.485042	-1.906159	-0.730788
14C	5.049238	-3.134371	-0.204948
15C	3.668528	-3.349686	-0.058301
16C	2.742800	-2.370678	-0.417019
17C	6.042296	-4.187867	0.217361
18C	1.286480	0.417606	1.218027
19H	2.765484	3.247508	-1.321360
20H	4.713211	4.679830	-0.742299
21H	5.565596	2.428150	2.612640
22H	3.687054	0.883923	2.174884
23H	4.924204	0.026584	-1.514985
24H	6.549193	-1.725163	-0.860949
25H	3.312327	-4.298660	0.335481
26H	1.677759	-2.545228	-0.307917
27H	6.315388	-4.056048	1.273484
28H	5.628149	-5.196289	0.109559
29H	6.965528	-4.128034	-0.368875
30H	1.896773	-0.392146	1.637213
31H	1.094201	1.165628	1.990077
32H	0.335619	0.011342	0.882811
33P	-3.018559	-0.201741	-0.539224
34C	-2.505672	-0.506939	-2.250970
35C	-4.788481	-0.560925	-0.401312
36C	-2.073332	-1.248541	0.595152
37C	-2.707982	1.528172	-0.099491
38C	-5.286220	-1.398350	0.608141
39C	-6.658726	-1.649971	0.682838
40C	-7.530507	-1.070883	-0.243203
41C	-7.033494	-0.237077	-1.251932
42C	-5.665223	0.019916	-1.335326
43C	-1.983292	-0.877621	1.947826
44C	-1.264444	-1.674795	2.838753
45C	-0.632114	-2.837125	2.384031
46C	-0.720090	-3.204364	1.037791
47C	-1.439830	-2.414305	0.138910
48C	-3.667576	2.277111	0.599137
49C	-3.372492	3.587331	0.984983

50C	-2.127414	4.145941	0.681197
51C	-1.170085	3.395823	-0.011261
52C	-1.454412	2.087868	-0.403201
53H	-3.022975	0.205223	-2.900425
54H	-1.424803	-0.377976	-2.347326
55H	-2.788168	-1.524438	-2.536267
56H	-4.614959	-1.855241	1.328945
57H	-7.042874	-2.300325	1.463768
58H	-8.596997	-1.270537	-0.182471
59H	-7.710438	0.212256	-1.973156
60H	-5.286670	0.671425	-2.119176
61H	-2.457481	0.034863	2.299512
62H	-1.192732	-1.384935	3.883311
63H	-0.067356	-3.453763	3.078175
64H	-0.224591	-4.103798	0.683045
65H	-1.486701	-2.701641	-0.906550
66H	-4.637493	1.850306	0.836905
67H	-4.117010	4.168774	1.521820
68H	-1.902189	5.165272	0.983237
69H	-0.199932	3.825123	-0.244944
70H	-0.699187	1.510227	-0.926158

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1C	2.625247	-1.508146	-2.269863
2C	1.470920	-2.181839	-2.670102
3N	0.902025	-3.175287	-1.971363
4C	1.513230	-3.540116	-0.831437
5C	2.673075	-2.942931	-0.342899
6C	3.242929	-1.888558	-1.069990
7N	4.440552	-1.262773	-0.611865
8S	4.325381	-0.342044	0.835018
9O	5.699376	0.072487	1.144903
10O	3.548352	-1.138613	1.791620
11C	3.372200	1.110974	0.407708
12C	4.024451	2.225344	-0.131676
13C	3.268413	3.339085	-0.495864
14C	1.874070	3.358134	-0.325263
15C	1.251756	2.225951	0.223994
16C	1.985887	1.096342	0.585327
17C	1.065099	4.564769	-0.730698
18C	5.339124	-0.687289	-1.631570
19H	3.022756	-0.708881	-2.885300
20H	0.971616	-1.896314	-3.593815
21H	1.056129	-4.360715	-0.282951
22H	3.128308	-3.286525	0.577608
23H	5.104039	2.230266	-0.241882
24H	3.771151	4.212739	-0.903793
25H	0.178709	2.234885	0.391279
26H	1.495438	0.234637	1.024472
27H	0.109588	4.603477	-0.198523
28H	1.609929	5.494324	-0.531708
29H	0.847888	4.541981	-1.807585
30H	5.475719	-1.438859	-2.412441
31H	4.945840	0.233461	-2.081176
32H	6.305756	-0.482955	-1.171551
33P	-2.436326	-0.149335	-0.301128
34C	-1.484595	-0.573186	-1.784266
35C	-2.954293	1.583873	-0.368257
36C	-3.907276	-1.203740	-0.223081
37C	-1.401173	-0.441721	1.155365
38C	-4.072077	1.992052	0.379785
39C	-4.461547	3.331715	0.369133
40C	-3.746096	4.263539	-0.390567
41C	-2.639268	3.856510	-1.141659
42C	-2.237056	2.519145	-1.132067
43C	-4.330160	-1.754921	0.996368
44C	-5.489314	-2.533686	1.037652
45C	-6.222927	-2.763421	-0.129678
46C	-5.801972	-2.211499	-1.344976
47C	-4.648663	-1.428502	-1.396022
48C	-0.727453	-1.671959	1.262880
49C	0.061608	-1.931079	2.382340
50C	0.180736	-0.972664	3.395023
51C	-0.491645	0.247450	3.289392
52C	-1.284732	0.518091	2.171550
53H	-0.549136	-0.007559	-1.793968
54H	-1.256881	-1.642106	-1.756507
55H	-2.065095	-0.345937	-2.682863
56H	-4.636492	1.269492	0.963504
57H	-5.325334	3.644757	0.948816
58H	-4.054102	5.305520	-0.400697
59H	-2.086704	4.579153	-1.734980
60H	-1.374021	2.219522	-1.718386
61H	-3.760145	-1.588300	1.905699
62H	-5.814454	-2.961874	1.981707

63H	-7.121679	-3.373217	-0.094496
64H	-6.370575	-2.390126	-2.253381
65H	-4.337582	-0.996022	-2.343205
66H	-0.811849	-2.420323	0.479888
67H	0.593209	-2.874645	2.459505
68H	0.807048	-1.175493	4.259106
69H	-0.393265	0.995866	4.070692
70H	-1.797869	1.471637	2.094487

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1C	-4.938075	-2.370101	-0.514299
2C	-6.330915	-2.417411	-0.482400
3N	-7.086188	-1.717008	0.380167
4C	-6.439132	-0.929813	1.251354
5C	-5.050187	-0.795732	1.297955
6C	-4.276124	-1.531673	0.391789
7N	-2.845324	-1.469411	0.399714
8S	-2.118836	-0.720500	-0.962383
9O	-0.668781	-0.846305	-0.742712
10O	-2.734609	-1.298129	-2.162005
11C	-2.555085	1.006174	-0.860517
12C	-3.760879	1.444633	-1.421179
13C	-4.120027	2.781957	-1.272080
14C	-3.300918	3.684580	-0.569499
15C	-2.101253	3.210854	-0.017100
16C	-1.720998	1.875072	-0.153763
17C	-3.713975	5.127573	-0.423802
18C	-2.188943	-1.140312	1.681110
19H	-4.379530	-2.968917	-1.223295
20H	-6.865379	-3.060838	-1.177746
21H	-7.059167	-0.367561	1.946475
22H	-4.599365	-0.127843	2.023285
23H	-4.396492	0.756065	-1.968461
24H	-5.050958	3.133889	-1.710163
25H	-1.449967	3.892308	0.524178
26H	-0.789520	1.518903	0.270098
27H	-4.670833	5.209279	0.107474
28H	-2.967425	5.706640	0.129240
29H	-3.850760	5.597678	-1.405883
30H	-2.278709	-0.080322	1.949611
31H	-2.658852	-1.749714	2.456291
32H	-1.135505	-1.407431	1.611924
33P	2.943936	-0.064454	-0.470762
34C	2.163263	0.225123	-2.082317
35C	4.639116	0.578844	-0.497393
36C	2.017670	0.830155	0.806496
37C	2.978294	-1.838160	-0.103941
38C	5.224764	1.078918	0.677952
39C	6.546961	1.526765	0.656960
40C	7.286223	1.479051	-0.528975
41C	6.705141	0.979199	-1.698812
42C	5.384475	0.527146	-1.687454
43C	1.380751	0.146077	1.850801
44C	0.680252	0.866161	2.822069
45C	0.618073	2.260419	2.755257
46C	1.254237	2.943558	1.711886
47C	1.952584	2.233499	0.735642
48C	4.025571	-2.363457	0.672025
49C	4.040033	-3.722988	0.987080
50C	3.017477	-4.560444	0.529350
51C	1.977243	-4.037910	-0.245310
52C	1.950255	-2.678659	-0.563825
53H	2.656276	-0.373226	-2.853673
54H	1.107255	-0.049506	-2.017593
55H	2.246184	1.288476	-2.326487
56H	4.656857	1.125269	1.602691
57H	6.996329	1.915445	1.566568
58H	8.313870	1.831947	-0.542001
59H	7.276892	0.942584	-2.621917
60H	4.948214	0.138349	-2.602646
61H	1.424050	-0.936984	1.908112
62H	0.183886	0.334734	3.629198
63H	0.073776	2.816192	3.514124
64H	1.208202	4.027642	1.658599
65H	2.450821	2.770643	-0.067481
66H	4.829715	-1.723806	1.023114
67H	4.852891	-4.126860	1.584198
68H	3.033597	-5.619424	0.773009
69H	1.181951	-4.685693	-0.603790
70H	1.126494	-2.287282	-1.149294

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1C	-3.221927	-1.374093	2.133881
2C	-2.430877	-1.401530	3.285029
3N	-1.191599	-1.911655	3.331006
4C	-0.709433	-2.434344	2.190898
5C	-1.413979	-2.467509	0.990872
6C	-2.701830	-1.917715	0.952506
7N	-3.460552	-1.975872	-0.255898
8S	-2.946177	-0.979959	-1.554211
9O	-3.653317	-1.477823	-2.741249
10O	-1.477801	-0.960002	-1.515745
11C	-3.548133	0.660112	-1.181386
12C	-4.794812	1.062686	-1.673306
13C	-5.273905	2.327804	-1.338260
14C	-4.530535	3.192652	-0.516846
15C	-3.285188	2.756385	-0.037850
16C	-2.785660	1.494281	-0.359089
17C	-5.071689	4.553074	-0.155701
18C	-4.925753	-2.105350	-0.136607
19H	-4.214381	-0.938306	2.171515
20H	-2.814965	-0.983673	4.213255
21H	0.290810	-2.859150	2.239948
22H	-0.979255	-2.916156	0.107171
23H	-5.366679	0.404463	-2.319357
24H	-6.236372	2.652549	-1.726535
25H	-2.692461	3.415406	0.590061
26H	-1.815926	1.176454	0.009327
27H	-4.302316	5.185615	0.298975
28H	-5.464265	5.070373	-1.039048
29H	-5.899259	4.464760	0.560985
30H	-5.128520	-2.903745	0.580896
31H	-5.411590	-1.181207	0.200839
32H	-5.332189	-2.397230	-1.105687
33P	3.362017	-0.071433	0.700858
34C	4.212561	-0.623724	2.207893
35C	4.506678	0.917791	-0.293753
36C	2.834737	-1.515295	-0.251378
37C	1.941263	0.946483	1.175377
38C	4.524305	0.788974	-1.691366
39C	5.385785	1.586917	-2.448100
40C	6.225382	2.508766	-1.816341
41C	6.206535	2.637838	-0.422939
42C	5.348290	1.847009	0.341674
43C	1.576258	-1.543526	-0.870376
44C	1.219655	-2.642166	-1.656932
45C	2.109656	-3.706404	-1.821476
46C	3.363917	-3.679904	-1.199378
47C	3.732685	-2.585787	-0.417458
48C	1.122678	0.532430	2.239798
49C	0.043772	1.325278	2.630389
50C	-0.219586	2.526515	1.964530
51C	0.582360	2.929045	0.892523
52C	1.665047	2.142349	0.493686
53H	4.466955	0.245922	2.820651
54H	3.551942	-1.285491	2.775598
55H	5.126115	-1.161312	1.937110
56H	3.877134	0.072365	-2.188431
57H	5.400126	1.484565	-3.529540
58H	6.895965	3.126171	-2.408038
59H	6.859385	3.353484	0.069122
60H	5.337898	1.960085	1.421861
61H	0.870610	-0.729109	-0.744194
62H	0.243886	-2.654855	-2.131128
63H	1.827426	-4.559464	-2.432916
64H	4.056146	-4.507675	-1.325943
65H	4.712969	-2.567502	0.050263
66H	1.315926	-0.398828	2.763328
67H	-0.588422	0.998835	3.450124
68H	-1.054590	3.146127	2.279436
69H	0.370105	3.855408	0.365940
70H	2.290839	2.463010	-0.333986

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1C	3.540736	2.177281	-1.722723
2C	4.097807	3.440352	-1.512218
3N	3.644081	4.317388	-0.605210
4C	2.582139	3.939470	0.125281
5C	1.941462	2.709410	-0.011716
6C	2.434673	1.796415	-0.952531
7N	1.791895	0.527914	-1.127025
8S	1.981063	-0.598075	0.165544
9O	1.186998	-1.768279	-0.231681
10O	1.657551	0.130096	1.399901
11C	3.709846	-1.031609	0.188122
12C	4.151851	-2.120203	-0.568296
13C	5.515979	-2.415653	-0.587099

14C	6.437791	-1.638220	0.130962
15C	5.960042	-0.545805	0.876979
16C	4.603726	-0.232949	0.912428
17C	7.909272	-1.966910	0.125253
18C	1.872790	-0.084309	-2.468574
19H	3.974393	1.517350	-2.465722
20H	4.958663	3.754249	-2.098629
21H	2.215433	4.661562	0.851600
22H	1.080973	2.466065	0.597622
23H	3.443376	-2.733289	-1.115896
24H	5.866030	-3.267914	-1.164058
25H	6.661312	0.064265	1.441436
26H	4.243125	0.606355	1.498106
27H	8.508582	-1.090225	-0.149559
28H	8.239847	-2.282780	1.123388
29H	8.139342	-2.774360	-0.577120
30H	1.595124	0.682287	-3.195856
31H	2.872940	-0.466200	-2.709176
32H	1.154493	-0.901614	-2.524826
33P	-2.812035	-0.079241	-0.286929
34C	-1.671021	0.328131	-1.638905
35C	-4.501415	-0.185794	-0.930014
36C	-2.338355	-1.666077	0.443066
37C	-2.698964	1.231154	0.958693
38C	-5.376654	-1.172031	-0.447488
39C	-6.689250	-1.223726	-0.921365
40C	-7.130099	-0.297548	-1.871337
41C	-6.258997	0.687018	-2.350684
42C	-4.945906	0.747761	-1.882268
43C	-2.319892	-1.836981	1.835641
44C	-1.980922	-3.079772	2.374907
45C	-1.668120	-4.149302	1.531772
46C	-1.695472	-3.981013	0.143148
47C	-2.028896	-2.743300	-0.404575
48C	-1.450005	1.472522	1.557707
49C	-1.323747	2.486582	2.506531
50C	-2.436150	3.259782	2.859287
51C	-3.678211	3.015616	2.266251
52C	-3.816524	1.999954	1.316043
53H	-1.966820	1.281068	-2.087960
54H	-0.661125	0.423785	-1.231102
55H	-1.695550	-0.458373	-2.398605
56H	-5.039047	-1.898230	0.286003
57H	-7.364381	-1.989445	-0.549556
58H	-8.151559	-0.342769	-2.239365
59H	-6.601074	1.407943	-3.087941
60H	-4.280606	1.521654	-2.253357
61H	-2.559169	-1.011739	2.498710
62H	-1.958739	-3.208234	3.453379
63H	-1.400053	-5.113362	1.955672
64H	-1.448522	-4.810663	-0.513342
65H	-2.043102	-2.623403	-1.484295
66H	-0.583420	0.867947	1.305095
67H	-0.358827	2.666602	2.972695
68H	-2.334941	4.049560	3.599012
69H	-4.543062	3.612403	2.542670
70H	-4.785421	1.814206	0.862433

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1C	4.840849	-0.029216	-0.566878
2C	6.078378	-0.171123	0.004511
3N	6.508091	-1.352006	0.527789
4C	5.683845	-2.439222	0.468898
5C	4.436180	-2.364942	-0.084270
6C	3.933795	-1.140424	-0.635626
7N	2.685936	-1.172959	-1.132826
8S	2.000500	0.164456	-1.788748
9O	0.661531	-0.267749	-2.256995
10O	2.862285	0.850932	-2.784771
11C	1.737009	1.325813	-0.432861
12C	1.100936	0.879934	0.730565
13C	0.847227	1.785098	1.757182
14C	1.217706	3.136847	1.643295
15C	1.865235	3.553492	0.471911
16C	2.128092	2.656939	-0.568449
17C	0.894740	4.110758	2.749125
18C	7.873341	-1.478243	1.062190
19H	4.577000	0.937200	-0.974715
20H	6.778731	0.654876	0.062546
21H	6.079185	-3.357662	0.887514
22H	3.810083	-3.250179	-0.107305
23H	0.813309	-0.160221	0.831850
24H	0.347797	1.439855	2.659766
25H	2.165667	4.593395	0.366115
26H	2.627191	2.987872	-1.473965

27H	-0.184758	4.311095	2.783470
28H	1.179941	3.711460	3.729988
29H	1.407596	5.067995	2.607499
30H	8.566027	-1.742020	0.257025
31H	8.174008	-0.528936	1.509344
32H	7.889360	-2.255265	1.829017
33P	-2.806105	-0.612929	-0.623113
34C	-2.490351	-1.062315	-2.349206
35C	-2.619423	1.177219	-0.405522
36C	-4.510046	-1.085233	-0.211576
37C	-1.655393	-1.483826	0.469030
38C	-3.364174	1.846348	0.580083
39C	-3.174098	3.214103	0.783181
40C	-2.247257	3.916315	0.005772
41C	-1.503110	3.248638	-0.970768
42C	-1.678807	1.879423	-1.177415
43C	-4.775516	-2.214508	0.578191
44C	-6.098261	-2.596330	0.817839
45C	-7.152674	-1.859154	0.272114
46C	-6.888468	-0.734262	-0.517721
47C	-5.571547	-0.345475	-0.762687
48C	-1.695716	-1.207785	1.847362
49C	-0.800771	-1.841829	2.706873
50C	0.138430	-2.746744	2.195619
51C	0.178916	-3.018103	0.826239
52C	-0.715778	-2.389036	-0.043734
53H	-1.452228	-0.854090	-2.618457
54H	-2.705637	-2.126816	-2.481688
55H	-3.164882	-0.479266	-2.983232
56H	-4.095909	1.312324	1.178834
57H	-3.753559	3.729179	1.544604
58H	-2.101437	4.981465	0.165272
59H	-0.772780	3.787160	-1.566929
60H	-1.067478	1.369332	-1.914432
61H	-3.963239	-2.793490	1.006887
62H	-6.301480	-3.470356	1.430516
63H	-8.180007	-2.158927	0.461330
64H	-7.706580	-0.158716	-0.941895
65H	-5.374036	0.533413	-1.370464
66H	-2.414301	-0.495193	2.243590
67H	-0.830077	-1.625399	3.771205
68H	0.842136	-3.232612	2.866370
69H	0.916069	-3.706127	0.423945
70H	-0.650573	-2.588362	-1.107153

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1C	4.841268	-0.040963	-0.586716
2C	6.082792	-0.187397	-0.024925
3N	6.515348	-1.372225	0.487012
4C	5.681315	-2.453047	0.447296
5C	4.429835	-2.374008	-0.096304
6C	3.929091	-1.148385	-0.646920
7N	2.679215	-1.177884	-1.139186
8S	1.994615	0.160547	-1.793775
9O	0.651824	-0.268185	-2.254136
10O	2.853220	0.842371	-2.795667
11C	1.742445	1.324920	-0.438296
12C	1.110905	0.883309	0.729606
13C	0.865651	1.791552	1.755243
14C	1.240672	3.141885	1.636878
15C	1.880195	3.554735	0.460160
16C	2.135187	2.654739	-0.579522
17C	0.949830	4.111275	2.755813
18C	7.830765	-1.470019	1.138351
19H	4.580558	0.924337	-0.999257
20H	6.785251	0.637212	0.030854
21H	6.073059	-3.371548	0.869446
22H	3.801454	-3.257663	-0.117577
23H	0.818225	-0.155237	0.833704
24H	0.367439	1.451283	2.660412
25H	2.179628	4.594214	0.348156
26H	2.627590	2.983006	-1.489663
27H	1.239604	5.133443	2.490635
28H	-0.119337	4.114441	3.003308
29H	1.490544	3.833750	3.670053
30H	8.220261	-2.481759	1.012805
31H	8.518040	-0.764150	0.669242
32H	7.738377	-1.241257	2.204748
33P	-2.809057	-0.609215	-0.619312
34C	-2.496076	-1.058824	-2.345815
35C	-2.622617	1.180906	-0.401911
36C	-4.512528	-1.081920	-0.206275
37C	-1.656808	-1.479391	0.471782
38C	-3.368040	1.850349	0.582950
39C	-3.177990	3.218153	0.785779

40C	-2.250653	3.920072	0.008784
41C	-1.505726	3.252037	-0.966950
42C	-1.681351	1.882790	-1.173356
43C	-4.777202	-2.210926	0.584110
44C	-6.099704	-2.593198	0.824431
45C	-7.154634	-1.856699	0.278794
46C	-6.891212	-0.732046	-0.511650
47C	-5.574548	-0.342850	-0.757331
48C	-1.694967	-1.202203	1.849945
49C	-0.799216	-1.836166	2.708681
50C	0.138566	-2.742208	2.196823
51C	0.176977	-3.014596	0.827601
52C	-0.718417	-2.385481	-0.041619
53H	-1.459013	-0.849010	-2.617712
54H	-2.709999	-2.123715	-2.477383
55H	-3.173230	-0.477222	-2.978392
56H	-4.100251	1.316540	1.181306
57H	-3.757896	3.733510	1.546672
58H	-2.104687	4.985182	0.168378
59H	-0.774790	3.790330	-1.562609
60H	-1.069605	1.372221	-1.909691
61H	-3.964497	-2.789394	1.012702
62H	-6.302333	-3.467062	1.437533
63H	-8.181770	-2.156827	0.468516
64H	-7.709731	-0.157045	-0.935779
65H	-5.377607	0.535775	-1.365679
66H	-2.412580	-0.488939	2.246714
67H	-0.826938	-1.618948	3.772896
68H	0.842742	-3.228222	2.866983
69H	0.913029	-3.703486	0.424787
70H	-0.654640	-2.585387	-1.105006

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1C	4.604988	-0.225374	-0.455705
2C	5.708449	-0.701737	0.204903
3N	5.866047	-2.019933	0.500623
4C	4.893379	-2.903008	0.125807
5C	3.769224	-2.494079	-0.534332
6C	3.557609	-1.114585	-0.865868
7N	2.407734	-0.819962	-1.498030
8S	2.076555	0.711649	-1.976516
9O	0.761766	0.641150	-2.663578
10O	3.179583	1.351175	-2.737089
11C	1.829378	1.696048	-0.481883
12C	1.316504	1.103036	0.673965
13C	1.042005	1.900342	1.784377
14C	1.261413	3.286585	1.757837
15C	1.790838	3.854070	0.587938
16C	2.077322	3.069590	-0.531234
17C	0.897866	4.144527	2.944230
18C	7.070434	-2.514302	1.186863
19H	4.559762	0.834162	-0.670208
20H	6.510657	-0.044694	0.520529
21H	5.072971	-3.941512	0.382013
22H	3.021429	-3.224348	-0.822374
23H	1.134614	0.034855	0.708865
24H	0.640076	1.436303	2.681672
25H	1.981022	4.924308	0.549704
26H	2.490890	3.518182	-1.429540
27H	-0.168575	4.408149	2.912955
28H	1.075081	3.619439	3.889804
29H	1.467947	5.079804	2.957419
30H	7.618341	-3.192124	0.526460
31H	7.708234	-1.668056	1.444302
32H	6.782774	-3.041846	2.100254
33P	-2.572262	-0.628262	-0.561096
34C	-2.055485	-0.965405	-2.262306
35C	-2.688165	1.159680	-0.292517
36C	-4.196660	-1.389055	-0.295716
37C	-1.374413	-1.325265	0.604178
38C	-3.681123	1.691260	0.546895
39C	-3.707057	3.063666	0.803201
40C	-2.750448	3.903789	0.223991
41C	-1.765629	3.372848	-0.614829
42C	-1.725543	2.002021	-0.874541
43C	-4.396806	-2.363872	0.692753
44C	-5.658533	-2.945905	0.844370
45C	-6.715183	-2.558470	0.016178
46C	-6.514887	-1.586477	-0.971402
47C	-5.259258	-1.000756	-1.130791
48C	-1.377239	-0.877461	1.936704
49C	-0.463533	-1.405910	2.847390
50C	0.456844	-2.375665	2.433016
51C	0.458935	-2.820697	1.108672
52C	-0.454903	-2.299923	0.189272

53H	-1.034382	-0.608170	-2.429530
54H	-2.116512	-2.041143	-2.449552
55H	-2.741129	-0.445964	-2.939019
56H	-4.432753	1.046382	0.993080
57H	-4.476661	3.474152	1.451252
58H	-2.773906	4.971673	0.425198
59H	-1.018539	4.020651	-1.063455
60H	-0.943757	1.603610	-1.513797
61H	-3.580433	-2.672898	1.338475
62H	-5.811377	-3.701752	1.609788
63H	-7.694681	-3.013376	0.137397
64H	-7.335562	-1.284049	-1.615971
65H	-5.112484	-0.241187	-1.894540
66H	-2.079398	-0.113545	2.259440
67H	-0.464040	-1.055577	3.875742
68H	1.175590	-2.778394	3.141840
69H	1.181627	-3.561954	0.781932
70H	-0.426967	-2.639943	-0.840738

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1C	-2.338225	1.923281	-0.202015
2C	-2.466387	3.170074	0.353679
3N	-1.772567	3.545908	1.461880
4C	-0.916152	2.652438	2.042381
5C	-0.745275	1.393271	1.542905
6C	-1.456621	0.951450	0.376917
7N	-1.214559	-0.304024	-0.027808
8S	-1.982760	-0.969952	-1.313609
9O	-1.373639	-2.314126	-1.462945
10O	-1.985696	-0.104906	-2.522677
11C	-3.697490	-1.197951	-0.813361
12C	-3.976006	-1.970652	0.320473
13C	-5.299906	-2.139432	0.717767
14C	-6.356952	-1.548478	0.000673
15C	-6.047875	-0.781098	-1.130732
16C	-4.723838	-0.599173	-1.542349
17C	-7.786073	-1.761069	0.436040
18C	-1.904913	4.896100	2.029619
19H	-2.905411	1.700433	-1.095630
20H	-3.126895	3.917915	-0.070617
21H	-0.386101	3.007939	2.919162
22H	-0.062190	0.710632	2.034693
23H	-3.168666	-2.430798	0.883058
24H	-5.521350	-2.739959	1.597459
25H	-6.850061	-0.318319	-1.700831
26H	-4.491660	-0.005465	-2.420780
27H	-8.091192	-2.803686	0.275442
28H	-7.912429	-1.550047	1.505064
29H	-8.476321	-1.120685	-0.123107
30H	-0.970331	5.448338	1.893999
31H	-2.713521	5.421930	1.521040
32H	-2.138327	4.824102	3.095029
33P	2.564112	-0.761597	-0.431347
34C	1.946998	-2.042552	-1.550769
35C	2.018451	-1.096931	1.264151
36C	4.379393	-0.806934	-0.455614
37C	2.008814	0.874583	-0.979286
38C	2.642111	-0.420647	2.327892
39C	2.196337	-0.620476	3.633841
40C	1.135345	-1.499713	3.883454
41C	0.520681	-2.175849	2.826599
42C	0.953268	-1.974529	1.513409
43C	5.101768	0.012671	-1.337484
44C	6.492135	-0.100317	-1.408243
45C	7.163645	-1.028337	-0.606723
46C	6.444334	-1.848437	0.269149
47C	5.054924	-1.741836	0.347426
48C	2.511032	2.020894	-0.338461
49C	2.084120	3.285439	-0.741347
50C	1.150288	3.412138	-1.776609
51C	0.643096	2.272910	-2.405965
52C	1.072604	1.002732	-2.014459
53H	0.853065	-2.078275	-1.558944
54H	2.322716	-1.832373	-2.556771
55H	2.344380	-3.006052	-1.216741
56H	3.472273	0.254096	2.138034
57H	2.680420	-0.098376	4.454664
58H	0.791064	-1.657146	4.902321
59H	-0.306580	-2.853790	3.017451
60H	0.440306	-2.476212	0.701578
61H	4.590591	0.737645	-1.963818
62H	7.047733	0.538431	-2.089352
63H	8.245616	-1.112557	-0.663586
64H	6.963060	-2.570335	0.893953
65H	4.505848	-2.378547	1.035576

66H	3.235648	1.929680	0.465963
67H	2.480210	4.169085	-0.248196
68H	0.815497	4.398647	-2.086920
69H	-0.095514	2.361500	-3.196901
70H	0.653379	0.133065	-2.505618

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1C	5.729190	-0.591281	-1.786578
2C	6.828723	-0.943819	-1.056462
3N	6.724186	-1.369002	0.238714
4C	5.491421	-1.453584	0.805884
5C	4.347365	-1.117810	0.128424
6C	4.409877	-0.649854	-1.226560
7N	3.401939	-0.252664	-2.023092
8S	1.853321	-0.256603	-1.490700
9O	1.444716	-1.532890	-0.847802
10O	1.024193	0.191834	-2.635984
11C	1.731095	1.030442	-0.234652
12C	1.285193	0.718019	1.047938
13C	1.151760	1.741863	1.990452
14C	1.462295	3.069802	1.670078
15C	1.917159	3.354468	0.368999
16C	2.051600	2.347920	-0.583412
17C	1.325378	4.173926	2.689489
18C	7.934981	-1.757730	0.978243
19H	5.851954	-0.255214	-2.810641
20H	7.833593	-0.904668	-1.462413
21H	5.463012	-1.805507	1.830806
22H	3.402018	-1.229527	0.641729
23H	1.029793	-0.304525	1.303161
24H	0.794237	1.498735	2.987928
25H	2.159900	4.380073	0.099444
26H	2.391647	2.581600	-1.588422
27H	2.311343	4.539752	3.005995
28H	0.782501	5.031753	2.274239
29H	0.792708	3.832896	3.583558
30H	8.665142	-0.945199	0.938850
31H	7.672118	-1.952679	2.018636
32H	8.365560	-2.661176	0.536752
33P	-2.737371	-0.601256	-0.528543
34C	-2.048348	-1.287288	-2.057603
35C	-1.801464	-1.169016	0.913715
36C	-2.709545	1.208861	-0.593961
37C	-4.456102	-1.163538	-0.382220
38C	-1.047259	-2.350321	0.858322
39C	-0.371182	-2.791220	1.997795
40C	-0.450332	-2.064184	3.188967
41C	-1.203521	-0.885928	3.243911
42C	-1.876281	-0.434095	2.109265
43C	-1.622386	1.861905	-1.199011
44C	-1.566252	3.256617	-1.188509
45C	-2.581471	3.999128	-0.577859
46C	-3.663932	3.347811	0.022482
47C	-3.733173	1.953435	0.016233
48C	-5.354292	-0.856913	-1.419798
49C	-6.676133	-1.295194	-1.343568
50C	-7.105942	-2.038982	-0.238082
51C	-6.213679	-2.342906	0.793289
52C	-4.887133	-1.907573	0.725950
53H	-2.600840	-0.862803	-2.901309
54H	-0.987604	-1.042036	-2.156204
55H	-2.182562	-2.372877	-2.052861
56H	-0.960157	-2.915854	-0.062464
57H	0.223763	-3.698807	1.947695
58H	0.079360	-2.410755	4.072559
59H	-1.260978	-0.314904	4.166486
60H	-2.441446	0.492495	2.153428
61H	-0.822094	1.303263	-1.674180
62H	-0.724283	3.758406	-1.655980
63H	-2.531645	5.084906	-0.572616
64H	-4.456774	3.922623	0.493357
65H	-4.580358	1.455500	0.479026
66H	-5.031360	-0.273600	-2.278150
67H	-7.369112	-1.056112	-2.145448
68H	-8.136440	-2.379530	-0.182385
69H	-6.545591	-2.920085	1.651981
70H	-4.199806	-2.149299	1.530749

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1C	-2.598684	1.921005	-0.367724
2C	-2.880690	3.219780	-0.033563
3N	-2.445308	3.783861	1.125139

4C	-1.702545	3.029123	1.990437
5C	-1.388190	1.728413	1.718966
6C	-1.820647	1.093174	0.507374
7N	-1.448172	-0.184625	0.339589
8S	-1.907865	-1.059425	-0.969697
9O	-1.169513	-2.340373	-0.848689
10O	-1.769588	-0.334247	-2.259596
11C	-3.654860	-1.417751	-0.733559
12C	-4.041672	-2.176871	0.377859
13C	-5.392690	-2.444305	0.579043
14C	-6.371340	-1.967061	-0.313136
15C	-5.954945	-1.209314	-1.415974
16C	-4.601588	-0.929222	-1.632623
17C	-7.828950	-2.280033	-0.078699
18C	-2.731506	5.190961	1.445206
19H	-2.955860	1.548293	-1.317900
20H	-3.461526	3.862059	-0.685369
21H	-1.380097	3.529354	2.896994
22H	-0.793154	1.161121	2.426420
23H	-3.295583	-2.554478	1.070976
24H	-5.696944	-3.037807	1.438570
25H	-6.693889	-0.834869	-2.120523
26H	-4.286703	-0.349953	-2.494832
27H	-8.007171	-3.362817	-0.107408
28H	-8.154837	-1.927208	0.908243
29H	-8.468986	-1.813232	-0.834557
30H	-1.807557	5.775405	1.404395
31H	-3.443122	5.586339	0.719025
32H	-3.164879	5.258507	2.446202
33P	2.710851	-0.665323	-0.418188
34C	2.002005	-1.853907	-1.583948
35C	2.486551	-1.258493	1.280207
36C	4.485063	-0.532450	-0.778026
37C	1.933922	0.958844	-0.600156
38C	3.499527	-1.087953	2.238078
39C	3.281188	-1.496112	3.555599
40C	2.058312	-2.069543	3.918753
41C	1.049522	-2.234273	2.963904
42C	1.254499	-1.829975	1.643637
43C	5.055840	0.666098	-1.230367
44C	6.417822	0.709105	-1.542439
45C	7.207544	-0.435157	-1.403945
46C	6.637998	-1.632108	-0.953513
47C	5.279752	-1.685176	-0.642338
48C	2.201966	1.946459	0.363514
49C	1.656563	3.221575	0.219056
50C	0.834467	3.511040	-0.875672
51C	0.550252	2.522049	-1.820318
52C	1.099641	1.244256	-1.689933
53H	0.931491	-1.991880	-1.407151
54H	2.174818	-1.503348	-2.605596
55H	2.520190	-2.807589	-1.441885
56H	4.453648	-0.647477	1.965015
57H	4.067590	-1.368503	4.294628
58H	1.892717	-2.388377	4.944638
59H	0.097229	-2.677045	3.243028
60H	0.452882	-1.943385	0.920610
61H	4.449878	1.559643	-1.344262
62H	6.857672	1.638017	-1.894843
63H	8.266005	-0.396948	-1.647417
64H	7.249943	-2.523323	-0.844989
65H	4.843432	-2.616799	-0.291014
66H	2.829407	1.719938	1.221604
67H	1.866079	3.983936	0.964396
68H	0.403790	4.503216	-0.982977
69H	-0.108679	2.735212	-2.656752
70H	0.847699	0.483893	-2.420316

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1C	-4.293185	0.982676	-0.699247
2C	-5.468741	0.302090	-0.520567
3N	-5.604164	-0.683762	0.409797
4C	-4.533228	-1.002706	1.197932
5C	-3.332907	-0.364360	1.072590
6C	-3.142714	0.680525	0.105474
7N	-1.929272	1.242020	0.056530
8S	-1.593346	2.417923	-1.045643
9O	-2.359812	3.663909	-0.786395
10O	-1.635166	1.896710	-2.438329
11C	0.125058	2.715348	-0.620950
12C	0.424032	3.492123	0.501935
13C	1.756981	3.691426	0.853406
14C	2.800811	3.130758	0.095833
15C	2.470257	2.363780	-1.030018
16C	1.137380	2.150105	-1.394208

17C	4.237704	3.355011	0.499291
18C	-6.888887	-1.368347	0.615724
19H	-4.257677	1.753675	-1.459125
20H	-6.350255	0.518889	-1.113693
21H	-4.699351	-1.791600	1.923547
22H	-2.504966	-0.645760	1.714278
23H	-0.375338	3.932025	1.090260
24H	1.994913	4.295589	1.726443
25H	3.262270	1.923525	-1.629363
26H	0.887660	1.554637	-2.266573
27H	4.932823	2.964402	-0.250290
28H	4.446119	4.423445	0.635044
29H	4.459504	2.860235	1.453922
30H	-6.728643	-2.449254	0.631150
31H	-7.334908	-1.048039	1.562079
32H	-7.562502	-1.118846	-0.204601
33P	1.637547	-2.226691	0.488022
34C	2.095344	-3.871699	1.110820
35C	0.852821	-1.284236	1.820873
36C	3.150625	-1.380977	-0.042465
37C	0.517380	-2.405101	-0.920918
38C	0.982320	0.112694	1.878874
39C	0.347700	0.822259	2.899685
40C	-0.415887	0.150372	3.856782
41C	-0.552011	-1.240882	3.795693
42C	0.078422	-1.960949	2.780753
43C	3.451990	-1.249582	-1.406224
44C	4.658611	-0.660914	-1.792861
45C	5.557639	-0.202144	-0.826456
46C	5.254382	-0.329653	0.533910
47C	4.054583	-0.920014	0.930333
48C	0.530279	-3.574753	-1.699442
49C	-0.294008	-3.661652	-2.823465
50C	-1.117619	-2.586865	-3.176419
51C	-1.128381	-1.423312	-2.400548
52C	-0.314577	-1.329704	-1.270852
53H	1.201894	-4.469015	1.315727
54H	2.713172	-4.377436	0.363406
55H	2.677679	-3.747195	2.028495
56H	1.561305	0.651919	1.136109
57H	0.444013	1.902392	2.932479
58H	-0.909497	0.709475	4.647139
59H	-1.145757	-1.766382	4.538682
60H	-0.033588	-3.040486	2.747103
61H	2.754283	-1.595168	-2.162930
62H	4.889826	-0.555514	-2.849240
63H	6.492058	0.261287	-1.131496
64H	5.949042	0.035086	1.285344
65H	3.819434	-1.008824	1.987598
66H	1.171486	-4.412282	-1.441731
67H	-0.287700	-4.566913	-3.424395
68H	-1.751428	-2.657088	-4.056535
69H	-1.755328	-0.577827	-2.666837
70H	-0.349375	-0.426017	-0.670165

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1C	-2.731298	1.908998	-0.385868
2C	-3.130501	3.175879	-0.047618
3N	-2.782348	3.758308	1.131783
4C	-2.012303	3.054781	2.016323
5C	-1.580709	1.789279	1.741037
6C	-1.921947	1.134349	0.510289
7N	-1.447429	-0.109721	0.348121
8S	-1.835775	-1.022647	-0.959993
9O	-1.026444	-2.257523	-0.815174
10O	-1.729122	-0.305606	-2.256134
11C	-3.562064	-1.478516	-0.736343
12C	-3.915040	-2.263762	0.367818
13C	-5.251869	-2.600676	0.561113
14C	-6.249929	-2.165092	-0.330812
15C	-5.866705	-1.382542	-1.428535
16C	-4.528526	-1.032901	-1.636859
17C	-7.694489	-2.532642	-0.093816
18C	-3.255867	5.104255	1.489275
19H	-3.019281	1.521785	-1.353857
20H	-3.741036	3.777838	-0.711092
21H	-1.769641	3.566202	2.941502
22H	-0.964369	1.262854	2.461789
23H	-3.153434	-2.609632	1.060639
24H	-5.529038	-3.215526	1.414721
25H	-6.620230	-1.041786	-2.134721
26H	-4.239144	-0.433316	-2.494127
27H	-7.806556	-3.610607	0.075532
28H	-8.085251	-2.024818	0.798155
29H	-8.327161	-2.253639	-0.942990

30H	-2.406171	5.727454	1.779720
31H	-3.749941	5.550576	0.625627
32H	-3.966615	5.040100	2.318629
33P	2.794191	-0.660122	-0.409384
34C	2.156213	-1.951231	-1.504939
35C	2.569738	-1.183766	1.311437
36C	4.563410	-0.442458	-0.748660
37C	1.919372	0.899526	-0.682962
38C	3.599908	-1.035883	2.253509
39C	3.382199	-1.415908	3.580089
40C	2.143920	-1.938765	3.965670
41C	1.118771	-2.084009	3.024419
42C	1.322860	-1.708557	1.695879
43C	5.116412	0.825889	-0.978732
44C	6.485596	0.948718	-1.230798
45C	7.300741	-0.186113	-1.254120
46C	6.749039	-1.452317	-1.026833
47C	5.383585	-1.584363	-0.774950
48C	1.921060	1.873416	0.330426
49C	1.302022	3.102990	0.108072
50C	0.669850	3.358453	-1.113296
51C	0.652425	2.382686	-2.112967
52C	1.280240	1.152988	-1.905456
53H	1.075370	-2.058280	-1.369776
54H	2.385041	-1.699724	-2.544341
55H	2.650447	-2.892849	-1.246178
56H	4.565616	-0.634901	1.960515
57H	4.180893	-1.305206	4.308601
58H	1.978823	-2.235194	4.998354
59H	0.155132	-2.488927	3.321653
60H	0.512737	-1.809395	0.979912
61H	4.490639	1.712852	-0.967512
62H	6.911567	1.931960	-1.410709
63H	8.364691	-0.086547	-1.452086
64H	7.380535	-2.336267	-1.045931
65H	4.962632	-2.569890	-0.594578
66H	2.395859	1.672317	1.287429
67H	1.303614	3.855015	0.892205
68H	0.176423	4.312644	-1.279118
69H	0.138016	2.567994	-3.051445
70H	1.245647	0.399780	-2.685463

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1C	-4.291253	0.979711	-0.695519
2C	-5.463790	0.297228	-0.511265
3N	-5.591892	-0.694807	0.415877
4C	-4.515829	-1.014520	1.194761
5C	-3.316347	-0.374309	1.062695
6C	-3.134210	0.675429	0.101177
7N	-1.922436	1.239380	0.046853
8S	-1.590550	2.421331	-1.049168
9O	-2.360988	3.663955	-0.785262
10O	-1.629069	1.906639	-2.444391
11C	0.126729	2.720450	-0.619780
12C	0.421772	3.492541	0.507405
13C	1.753428	3.690561	0.864436
14C	2.800090	3.133859	0.107834
15C	2.473509	2.371947	-1.022595
16C	1.141928	2.159871	-1.392554
17C	4.235582	3.356609	0.517106
18C	-6.894873	-1.343286	0.628782
19H	-4.260823	1.753727	-1.452678
20H	-6.351314	0.514903	-1.095856
21H	-4.672089	-1.806369	1.918340
22H	-2.483618	-0.660023	1.696113
23H	-0.379721	3.929253	1.095249
24H	1.988140	4.290699	1.741128
25H	3.267578	1.934496	-1.621307
26H	0.895293	1.568293	-2.268450
27H	4.933191	2.963057	-0.228613
28H	4.445214	4.425086	0.650892
29H	4.452370	2.864027	1.473992
30H	-6.742322	-2.304717	1.122656
31H	-7.530923	-0.708779	1.254017
32H	-7.379347	-1.510838	-0.335529
33P	1.632438	-2.229473	0.483395
34C	2.088439	-3.876425	1.102315
35C	0.518896	-2.403387	-0.931399
36C	0.842190	-1.291854	1.816502
37C	3.147489	-1.381076	-0.037578
38C	-0.304610	-1.323305	-1.286822
39C	-1.113007	-1.413097	-2.420684
40C	-1.104941	-2.577320	-3.195592
41C	-0.289720	-3.656680	-2.837269
42C	0.529050	-3.573752	-1.708872

43C	0.966701	0.105469	1.876529
44C	0.328443	0.811533	2.897513
45C	-0.433830	0.135759	3.852902
46C	-0.564751	-1.255892	3.790060
47C	0.069316	-1.972471	2.774912
48C	4.045710	-0.920799	0.940787
49C	5.247087	-0.328598	0.551923
50C	5.557483	-0.198202	-0.806523
51C	4.663979	-0.655940	-1.778553
52C	3.456005	-1.246732	-1.399491
53H	2.709638	-4.379012	0.355579
54H	2.666905	-3.754959	2.022813
55H	1.194523	-4.475023	1.301302
56H	-0.337478	-0.419014	-0.686961
57H	-1.733904	-0.564290	-2.690598
58H	-1.734387	-2.644501	-4.079075
59H	-0.285473	-4.562441	-3.437462
60H	1.163833	-4.414915	-1.447125
61H	1.544833	0.647622	1.135188
62H	0.420507	1.891993	2.931525
63H	-0.930464	0.692098	4.643314
64H	-1.157442	-1.784454	4.531718
65H	-0.038694	-3.052380	2.740104
66H	3.805124	-1.011576	1.996663
67H	5.937311	0.035306	1.307836
68H	6.493037	0.266769	-1.105674
69H	4.900624	-0.548177	-2.833483
70H	2.762870	-1.591773	-2.160633

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1C	4.026819	-1.145961	0.851169
2C	4.770601	-2.275932	0.637223
3N	4.857627	-2.869699	-0.585998
4C	4.200772	-2.304957	-1.643405
5C	3.444079	-1.177174	-1.498929
6C	3.304341	-0.528102	-0.226785
7N	2.514484	0.553726	-0.182279
8S	2.284886	1.347755	1.240618
9O	3.563436	1.766644	1.872597
10O	1.345982	0.606302	2.132809
11C	1.438616	2.819241	0.664912
12C	2.082122	3.668234	-0.241923
13C	1.442944	4.837103	-0.645099
14C	0.171396	5.180097	-0.150571
15C	-0.444048	4.313706	0.761476
16C	0.180585	3.133087	1.173455
17C	-0.505430	6.448692	-0.607996
18C	5.726080	-4.037961	-0.793943
19H	4.001200	-0.732417	1.851213
20H	5.323163	-2.754968	1.438054
21H	4.315581	-2.809361	-2.596219
22H	2.930274	-0.765838	-2.361162
23H	3.063836	3.415119	-0.630796
24H	1.937291	5.498077	-1.353693
25H	-1.428786	4.557956	1.151960
26H	-0.305986	2.465785	1.876896
27H	-1.475973	6.585771	-0.119856
28H	0.112753	7.327972	-0.386525
29H	-0.670481	6.438129	-1.693369
30H	5.276671	-4.694709	-1.541518
31H	6.713996	-3.714032	-1.136288
32H	5.826186	-4.583533	0.145790
33P	-2.169917	-0.815235	0.516415
34C	-1.830231	-0.251935	2.206320
35C	-1.889638	0.557740	-0.634262
36C	-1.081134	-2.213249	0.124270
37C	-3.903390	-1.329483	0.383908
38C	-0.702961	0.638661	-1.376190
39C	-0.489384	1.729515	-2.221396
40C	-1.455993	2.730378	-2.334499
41C	-2.638921	2.652879	-1.590117
42C	-2.858312	1.573040	-0.736372
43C	-1.556111	-3.275044	-0.664465
44C	-0.711233	-4.342636	-0.972292
45C	0.602520	-4.357588	-0.493773
46C	1.074163	-3.301040	0.290080
47C	0.241193	-2.224527	0.601915
48C	-4.597039	-1.769998	1.523345
49C	-5.922117	-2.195343	1.407609
50C	-6.556311	-2.187190	0.161628
51C	-5.866043	-1.751799	-0.974360
52C	-4.542727	-1.321458	-0.868038
53H	-2.543195	0.535251	2.468654
54H	-1.915699	-1.086143	2.908856
55H	-0.811826	0.145747	2.242514

56H	0.064178	-0.122504	-1.286578
57H	0.440825	1.797716	-2.777262
58H	-1.284295	3.577408	-2.992802
59H	-3.388111	3.435846	-1.670234
60H	-3.780369	1.518369	-0.163763
61H	-2.578143	-3.281111	-1.030386
62H	-1.083874	-5.163508	-1.578835
63H	1.255866	-5.193719	-0.729745
64H	2.094562	-3.305166	0.659518
65H	0.630808	-1.403591	1.196537
66H	-4.118920	-1.782062	2.497892
67H	-6.457687	-2.529176	2.292035
68H	-7.588477	-2.516407	0.076489
69H	-6.357637	-1.741443	-1.943142
70H	-4.018506	-0.972727	-1.753027

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1C	4.177716	-1.229518	-0.920252
2C	5.090385	-2.136206	-0.448040
3N	4.732040	-3.382335	-0.033799
4C	3.418839	-3.750504	-0.107669
5C	2.458126	-2.892827	-0.565297
6C	2.783659	-1.563589	-0.995867
7N	1.760086	-0.794038	-1.400306
8S	2.011283	0.742886	-1.926646
9O	0.666738	1.246786	-2.299420
10O	3.073530	0.846021	-2.957611
11C	2.563806	1.699105	-0.500604
12C	1.825675	1.643352	0.685550
13C	2.248340	2.387171	1.785050
14C	3.397285	3.195072	1.719397
15C	4.117192	3.232525	0.516180
16C	3.710362	2.488329	-0.594627
17C	3.829065	4.014389	2.910943
18C	5.747888	-4.353133	0.402799
19H	4.542529	-0.264747	-1.245547
20H	6.147232	-1.901327	-0.387694
21H	3.189228	-4.759657	0.216047
22H	1.426548	-3.223851	-0.607852
23H	0.942255	1.018230	0.755172
24H	1.678736	2.335744	2.709837
25H	5.011847	3.846842	0.444733
26H	4.276171	2.516533	-1.520550
27H	3.262169	4.954115	2.962494
28H	3.653264	3.477114	3.850200
29H	4.891877	4.273809	2.856854
30H	6.048212	-4.983656	-0.439866
31H	6.616970	-3.816696	0.786845
32H	5.331067	-4.975227	1.197347
33P	-2.595394	-0.369734	-0.344181
34C	-1.760882	-0.969293	-1.835233
35C	-1.461132	-0.411195	1.068276
36C	-3.148373	1.334546	-0.603574
37C	-4.025767	-1.427208	0.007189
38C	-1.560499	0.567754	2.070856
39C	-0.713431	0.511974	3.179210
40C	0.231351	-0.512807	3.289032
41C	0.330939	-1.486618	2.290360
42C	-0.514271	-1.442195	1.181082
43C	-4.448367	1.732345	-0.255387
44C	-4.831634	3.064471	-0.430093
45C	-3.923011	3.993960	-0.945020
46C	-2.626729	3.594271	-1.289635
47C	-2.231739	2.266516	-1.121460
48C	-4.277203	-1.882786	1.310119
49C	-5.402962	-2.670501	1.563990
50C	-6.274380	-3.004829	0.523711
51C	-6.023898	-2.550989	-0.776345
52C	-4.903428	-1.762207	-1.038830
53H	-1.493754	-2.021769	-1.708592
54H	-2.443978	-0.867335	-2.683989
55H	-0.859557	-0.376644	-2.015289
56H	-2.284127	1.373404	1.986577
57H	-0.787981	1.273738	3.950342
58H	0.897669	-0.545808	4.146944
59H	1.075838	-2.273798	2.366161
60H	-0.419727	-2.196556	0.406788
61H	-5.158318	1.014811	0.145151
62H	-5.839204	3.372209	-0.163839
63H	-4.224584	5.029473	-1.079919
64H	-1.919584	4.314202	-1.692439
65H	-1.222471	1.967648	-1.392306
66H	-3.603349	-1.629645	2.122940
67H	-5.595253	-3.022036	2.573900
68H	-7.149163	-3.617624	0.724565

69H	-6.700716	-2.809464	-1.585979
70H	-4.724028	-1.406313	-2.049877

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1C	-2.087773	-2.508577	1.013934
2C	-2.953410	-3.112066	1.881594
3N	-4.300833	-2.889939	1.823138
4C	-4.788611	-2.054897	0.866000
5C	-3.975982	-1.420277	-0.037248
6C	-2.554276	-1.611947	-0.005882
7N	-1.617723	-1.054264	-0.788395
8S	-2.022906	-0.038887	-2.012838
9O	-3.089184	-0.575754	-2.895051
10O	-0.736649	0.318101	-2.660203
11C	-2.668436	1.462405	-1.250881
12C	-3.899644	1.977381	-1.653608
13C	-4.372086	3.153773	-1.062983
14C	-3.633208	3.815834	-0.072629
15C	-2.395954	3.270147	0.316068
16C	-1.908390	2.103368	-0.266525
17C	-4.145930	5.077707	0.577206
18C	-5.195905	-3.597044	2.752934
19H	-1.025804	-2.713753	1.090527
20H	-2.620123	-3.794661	2.655587
21H	-5.863713	-1.918021	0.855795
22H	-4.439717	-0.783599	-0.778475
23H	-4.478282	1.469050	-2.418512
24H	-5.329894	3.559517	-1.380694
25H	-1.808080	3.766246	1.085127
26H	-0.955985	1.690084	0.046810
27H	-4.377168	4.907112	1.637149
28H	-3.395303	5.876713	0.536260
29H	-5.056378	5.441099	0.089676
30H	-4.835669	-3.466299	3.776391
31H	-6.201425	-3.182360	2.670655
32H	-5.220902	-4.662378	2.505320
33P	2.731502	0.303017	-0.407810
34C	2.332386	1.250555	-1.899968
35C	1.600541	0.793507	0.922273
36C	2.574023	-1.469014	-0.739736
37C	4.427634	0.674894	0.112672
38C	1.578557	2.138765	1.332325
39C	0.714336	2.536595	2.351763
40C	-0.128957	1.599387	2.960886
41C	-0.109159	0.264804	2.549970
42C	0.754615	-0.143628	1.530588
43C	1.547823	-1.926487	-1.583117
44C	1.403771	-3.297540	-1.805514
45C	2.272789	-4.207123	-1.195558
46C	3.293407	-3.748980	-0.354681
47C	3.448133	-2.381322	-0.123780
48C	5.422389	0.880975	-0.857962
49C	6.740704	1.108892	-0.459928
50C	7.071024	1.127878	0.899413
51C	6.081694	0.921567	1.865729
52C	4.759898	0.694062	1.477034
53H	2.947080	0.908198	-2.736988
54H	1.275031	1.105562	-2.142335
55H	2.524294	2.310608	-1.708615
56H	2.233700	2.869984	0.865528
57H	0.698265	3.575618	2.668620
58H	-0.805779	1.913981	3.750744
59H	-0.775058	-0.459616	3.009941
60H	0.755986	-1.177449	1.203579
61H	0.850262	-1.236194	-2.045128
62H	0.605870	-3.649034	-2.453806
63H	2.157148	-5.272751	-1.376435
64H	3.972612	-4.453914	0.116981
65H	4.246363	-2.032739	0.525242
66H	5.179557	0.863128	-1.916678
67H	7.508342	1.270442	-1.211592
68H	8.098841	1.305876	1.204446
69H	6.335703	0.938086	2.922018
70H	3.994717	0.537493	2.231913

6bc-PhNCO2-001

1C	1.073094	2.186712	0.432791
2C	0.578861	3.359093	1.002014
3N	0.858667	4.587761	0.537708
4C	1.660015	4.666457	-0.537808
5C	2.198782	3.554733	-1.187705
6C	1.897903	2.285879	-0.691163

7N	2.408088	1.102696	-1.319011
8S	4.034126	0.690123	-0.993150
9O	4.696989	1.973475	-0.693940
10O	4.536927	-0.132326	-2.098359
11C	4.054437	-0.269994	0.520573
12C	4.115913	-1.664493	0.465880
13C	4.137298	-2.384014	1.659377
14C	4.084840	-1.733597	2.904777
15C	4.020068	-0.332908	2.925338
16C	4.008354	0.406885	1.741036
17C	4.075800	-2.532992	4.185124
18C	1.421429	0.108803	-1.765943
19O	0.365235	0.614568	-2.224759
20N	1.787689	-1.136295	-1.572979
21C	1.073400	-2.187162	-2.135746
22C	1.053919	-3.415509	-1.434087
23C	0.390822	-4.534813	-1.941382
24C	-0.267614	-4.472372	-3.175724
25C	-0.240085	-3.268814	-3.893931
26C	0.413738	-2.144493	-3.388736
27H	0.819528	1.217370	0.845152
28H	-0.073647	3.308233	1.870885
29H	1.877910	5.668139	-0.902527
30H	2.834567	3.668329	-2.058725
31H	4.142681	-2.166271	-0.493625
32H	4.193333	-3.470115	1.623861
33H	3.986725	0.190869	3.877799
34H	3.975786	1.491072	1.769044
35H	4.866218	-3.293320	4.184843
36H	4.219546	-1.891978	5.061435
37H	3.121736	-3.063347	4.309954
38H	1.573908	-3.470249	-0.480428
39H	0.393886	-5.462616	-1.372024
40H	-0.780411	-5.343993	-3.575392
41H	-0.734561	-3.204840	-4.861739
42H	0.416953	-1.218723	-3.953826
43P	-2.835036	-0.165917	-0.045322
44C	-2.301743	-0.972833	-1.571752
45C	-3.133342	1.596819	-0.343707
46C	-4.367995	-0.955733	0.519932
47C	-1.555942	-0.323458	1.224861
48C	-4.243245	2.247100	0.219654
49C	-4.406937	3.621213	0.029917
50C	-3.468200	4.342862	-0.714499
51C	-2.361819	3.692698	-1.270642
52C	-2.184090	2.320274	-1.087668
53C	-4.436562	-1.621685	1.752221
54C	-5.623535	-2.254191	2.133176
55C	-6.737813	-2.223624	1.290646
56C	-6.669751	-1.560026	0.059869
57C	-5.489143	-0.927011	-0.328483
58C	-0.515674	-1.253162	1.082489
59C	0.464654	-1.347677	2.072913
60C	0.405466	-0.527015	3.201363
61C	-0.633243	0.400866	3.343884
62C	-1.611240	0.510471	2.355838
63H	-1.362117	-0.526798	-1.918647
64H	-2.167425	-2.042271	-1.387402
65H	-3.082917	-0.836016	-2.325660
66H	-4.976424	1.693163	0.798642
67H	-5.265976	4.124856	0.465060
68H	-3.595856	5.412815	-0.857264
69H	-1.625394	4.252982	-1.839461
70H	-1.305984	1.831358	-1.504211
71H	-3.574519	-1.653203	2.411622
72H	-5.673030	-2.770839	3.087782
73H	-7.658526	-2.717572	1.589796
74H	-7.534577	-1.535421	-0.597485
75H	-5.446504	-0.410551	-1.284187
76H	-0.441176	-1.882739	0.202889
77H	1.289386	-2.040847	1.942153
78H	1.180841	-0.594714	3.959182
79H	-0.671534	1.050166	4.214340
80H	-2.402131	1.249260	2.456629

6bc-PhNCO2-002

1C	1.021084	2.130618	0.427799
2C	0.490670	3.279351	1.012365
3N	0.709336	4.520066	0.547539
4C	1.480628	4.635812	-0.546289
5C	2.052318	3.549857	-1.211629
6C	1.818901	2.268267	-0.711476
7N	2.376601	1.110832	-1.346989
8S	4.020750	0.771672	-1.016464
9O	4.635615	2.088557	-0.763887

10O	4.547066	-0.066094	-2.098808
11C	4.077820	-0.135443	0.528700
12C	4.171395	-1.529589	0.521084
13C	4.183228	-2.208485	1.737635
14C	4.090759	-1.518938	2.959393
15C	4.000904	-0.119975	2.933375
16C	3.998398	0.580461	1.725024
17C	4.081891	-2.278693	4.263849
18C	1.430728	0.059098	-1.751736
19O	0.350992	0.502536	-2.219781
20N	1.852715	-1.160247	-1.518222
21C	1.185988	-2.262205	-2.038843
22C	1.225983	-3.463690	-1.292895
23C	0.621463	-4.632340	-1.759550
24C	-0.036058	-4.647847	-2.996065
25C	-0.068774	-3.470819	-3.756591
26C	0.524396	-2.296560	-3.290755
27H	0.819340	1.149802	0.841790
28H	-0.139480	3.198346	1.895182
29H	1.646720	5.646924	-0.912326
30H	2.664393	3.692671	-2.095228
31H	4.220274	-2.061913	-0.420652
32H	4.257656	-3.294085	1.739834
33H	3.934633	0.433178	3.867319
34H	3.938548	1.663742	1.715420
35H	5.028059	-2.814522	4.414672
36H	3.934078	-1.610951	5.119092
37H	3.283387	-3.031746	4.276968
38H	1.745503	-3.456509	-0.337358
39H	0.669961	-5.537694	-1.157116
40H	-0.501870	-5.558531	-3.364918
41H	-0.563525	-3.466647	-4.726369
42H	0.482013	-1.392222	-3.888329
43P	-2.857561	-0.205849	-0.094234
44C	-2.357120	-1.032844	-1.621619
45C	-3.116885	1.562126	-0.400584
46C	-4.409083	-0.946427	0.487929
47C	-1.576411	-0.395165	1.169446
48C	-4.214726	2.236973	0.157798
49C	-4.355425	3.611692	-0.045534
50C	-3.406830	4.309422	-0.800112
51C	-2.313158	3.634673	-1.351718
52C	-2.157176	2.261710	-1.153730
53C	-4.513845	-1.522091	1.762492
54C	-5.723197	-2.094349	2.167615
55C	-6.824054	-2.093866	1.307126
56C	-6.719664	-1.521437	0.033871
57C	-5.516380	-0.949542	-0.379034
58C	-0.559446	-1.348571	1.017825
59C	0.423578	-1.470529	2.002405
60C	0.388767	-0.654273	3.135173
61C	-0.628312	0.295918	3.288046
62C	-1.607983	0.433566	2.305152
63H	-1.392826	-0.633358	-1.958488
64H	-2.280563	-2.108697	-1.441307
65H	-3.123939	-0.849853	-2.380341
66H	-4.957170	1.701644	0.742405
67H	-5.204919	4.134131	0.386170
68H	-3.516718	5.379788	-0.953990
69H	-1.568018	4.176355	-1.927151
70H	-1.287861	1.753820	-1.565892
71H	-3.663599	-1.528706	2.437724
72H	-5.800645	-2.540368	3.155402
73H	-7.762689	-2.539516	1.625711
74H	-7.573624	-1.520868	-0.638006
75H	-5.446148	-0.503270	-1.367826
76H	-0.505798	-1.975996	0.135224
77H	1.231703	-2.182162	1.864761
78H	1.166638	-0.743360	3.888189
79H	-0.647557	0.941191	4.162111
80H	-2.380743	1.190614	2.412098

6bc-PhNCO2-003

1C	1.091157	2.181090	0.426283
2C	0.599479	3.355500	0.993519
3N	0.879745	4.582680	0.525595
4C	1.678988	4.657746	-0.551768
5C	2.215102	3.543758	-1.199964
6C	1.913788	2.276500	-0.699549
7N	2.421235	1.091092	-1.325472
8S	4.047788	0.678495	-1.000577
9O	4.712950	1.962839	-0.710934
10O	4.547110	-0.151443	-2.101752
11C	4.068642	-0.272077	0.518927
12C	4.126142	-1.667068	0.472496

13C	4.144106	-2.379490	1.670190
14C	4.092624	-1.721559	2.911666
15C	4.032320	-0.320547	2.923979
16C	4.023776	0.412267	1.735276
17C	4.080682	-2.513712	4.196464
18C	1.431454	0.094855	-1.760567
19O	0.373280	0.598604	-2.217238
20N	1.796796	-1.149360	-1.561463
21C	1.076642	-2.201700	-2.114099
22C	1.045905	-3.421988	-1.399236
23C	0.374519	-4.541174	-1.895818
24C	-0.280587	-4.486701	-3.132333
25C	-0.241153	-3.291463	-3.863816
26C	0.421071	-2.167308	-3.369373
27H	0.837104	1.212971	0.841316
28H	-0.051492	3.307504	1.863646
29H	1.897135	5.658246	-0.919560
30H	2.849063	3.654405	-2.072677
31H	4.151928	-2.174664	-0.483948
32H	4.196857	-3.465951	1.641180
33H	4.000040	0.208970	3.873311
34H	3.994140	1.496697	1.756750
35H	4.871057	-3.274092	4.201886
36H	4.222795	-1.867873	5.069454
37H	3.126301	-3.043243	4.322176
38H	1.562915	-3.470419	-0.443647
39H	0.368357	-5.462658	-1.316325
40H	-0.799898	-5.358313	-3.523534
41H	-0.732746	-3.234037	-4.833499
42H	0.433260	-1.247535	-3.944180
43P	-2.841833	-0.177803	-0.046488
44C	-2.296564	-0.994616	-1.562650
45C	-3.137106	1.581418	-0.367640
46C	-4.379911	-0.955017	0.522101
47C	-1.563582	-0.317123	1.227615
48C	-4.281701	2.223609	0.130561
49C	-4.450883	3.594105	-0.080577
50C	-3.483177	4.319405	-0.782882
51C	-2.343470	3.676301	-1.277162
52C	-2.160009	2.307917	-1.071767
53C	-4.528112	-1.407299	1.841325
54C	-5.729450	-1.999659	2.240562
55C	-6.778932	-2.142659	1.329098
56C	-6.630826	-1.693888	0.011504
57C	-5.435411	-1.101205	-0.395544
58C	-0.531919	-1.259291	1.102748
59C	0.451179	-1.340897	2.091343
60C	0.402958	-0.496194	3.202575
61C	-0.626994	0.443500	3.328390
62C	-1.606424	0.541896	2.340281
63H	-1.347062	-0.555620	-1.891883
64H	-2.176673	-2.065791	-1.379485
65H	-3.057990	-0.844484	-2.333700
66H	-5.037552	1.665079	0.675143
67H	-5.336651	4.091841	0.304966
68H	-3.614987	5.386436	-0.942757
69H	-1.586642	4.239153	-1.815887
70H	-1.260482	1.823259	-1.445685
71H	-3.715554	-1.306347	2.554293
72H	-5.840188	-2.350828	3.262868
73H	-7.711184	-2.605185	1.642395
74H	-7.444676	-1.805596	-0.699670
75H	-5.331387	-0.752441	-1.419921
76H	-0.465818	-1.909180	0.237100
77H	1.269754	-2.043661	1.972757
78H	1.180535	-0.554403	3.958958
79H	-0.656395	1.112281	4.184329
80H	-2.388082	1.292329	2.426206

6bc-PhNCO2-004

1C	-1.344176	-1.488725	-1.400601
2C	-0.645665	-2.521373	-2.026154
3N	-0.221450	-2.468586	-3.298917
4C	-0.510475	-1.353193	-3.994086
5C	-1.217483	-0.272707	-3.466226
6C	-1.642244	-0.340450	-2.138616
7N	-2.385258	0.732879	-1.548635
8S	-4.062187	0.523806	-1.402453
9O	-4.388602	-0.551741	-2.357939
10O	-4.713544	1.831411	-1.541897
11C	-4.408763	-0.114196	0.240525
12C	-4.608471	0.767988	1.306419
13C	-4.884516	0.246180	2.568717
14C	-4.965521	-1.140788	2.784718
15C	-4.764839	-1.999249	1.694381

16C	-4.489892	-1.496278	0.420788
17C	-5.259775	-1.680787	4.163033
18C	-1.713756	1.853636	-0.858446
19O	-2.336869	2.364139	0.091293
20N	-0.533195	2.109004	-1.400650
21C	0.327371	3.063694	-0.861882
22C	0.236932	3.675794	0.415944
23C	1.232108	4.550298	0.863493
24C	2.338506	4.861687	0.067549
25C	2.435064	4.279890	-1.203772
26C	1.453041	3.401551	-1.655705
27H	-1.651291	-1.575872	-0.364840
28H	-0.407521	-3.428817	-1.474680
29H	-0.162375	-1.326511	-5.024421
30H	-1.432274	0.606019	-4.064577
31H	-4.532349	1.836149	1.144264
32H	-5.041075	0.927689	3.402158
33H	-4.826801	-3.075492	1.837639
34H	-4.348203	-2.166313	-0.420528
35H	-6.252886	-1.362783	4.506333
36H	-5.232274	-2.775405	4.182329
37H	-4.534038	-1.307999	4.897230
38H	-0.617550	3.462020	1.044839
39H	1.135029	4.995766	1.852323
40H	3.107620	5.541150	0.426762
41H	3.284800	4.509082	-1.844303
42H	1.534977	2.947614	-2.640750
43P	2.509698	-0.646693	0.015460
44C	1.983836	-0.092457	-1.624261
45C	1.049855	-0.971969	1.036080
46C	3.485229	-2.169068	-0.142681
47C	3.535442	0.627337	0.799730
48C	0.791653	-2.251883	1.548561
49C	-0.369641	-2.474197	2.293112
50C	-1.268488	-1.427971	2.522737
51C	-1.009571	-0.151617	2.011794
52C	0.149424	0.080299	1.272638
53C	4.568584	-2.401717	0.720037
54C	5.284325	-3.597466	0.629620
55C	4.922717	-4.562197	-0.315808
56C	3.843062	-4.332320	-1.174797
57C	3.121475	-3.140152	-1.092028
58C	3.310718	1.024122	2.126106
59C	4.147014	1.974366	2.716983
60C	5.208220	2.523101	1.993341
61C	5.436843	2.123933	0.671906
62C	4.604509	1.179489	0.072656
63H	1.180846	0.645969	-1.522784
64H	2.835950	0.339710	-2.155622
65H	1.603032	-0.944457	-2.188516
66H	1.480825	-3.070717	1.366038
67H	-0.572557	-3.466673	2.686679
68H	-2.178180	-1.607852	3.086961
69H	-1.717936	0.657747	2.155807
70H	0.344331	1.071288	0.878955
71H	4.858969	-1.655292	1.453520
72H	6.124986	-3.771773	1.295639
73H	5.482904	-5.490938	-0.385622
74H	3.559637	-5.078782	-1.911667
75H	2.283212	-2.982516	-1.763930
76H	2.488018	0.605287	2.696569
77H	3.962900	2.285853	3.741453
78H	5.853870	3.265640	2.454732
79H	6.257567	2.553785	0.104473
80H	4.792864	0.877747	-0.954197

6bc-PhNCO2-005

1C	4.486639	0.495796	1.405880
2C	5.540112	1.033694	2.142867
3N	6.557555	1.719172	1.594838
4C	6.540188	1.880869	0.262347
5C	5.534547	1.377276	-0.565116
6C	4.484363	0.673197	0.021209
7N	3.431503	0.143628	-0.798022
8S	3.510957	-1.503363	-1.224566
9O	4.801797	-1.963636	-0.679489
10O	3.254435	-1.669718	-2.660544
11C	2.208838	-2.327455	-0.306879
12C	0.987923	-2.603594	-0.922977
13C	-0.000793	-3.261639	-0.192758
14C	0.205199	-3.628722	1.146493
15C	1.445571	-3.341032	1.736802
16C	2.453179	-2.697014	1.018426
17C	-0.896605	-4.284240	1.942029
18C	2.205555	0.901694	-1.022964

19O	1.307108	0.323738	-1.683527
20N	2.226142	2.072958	-0.420449
21C	1.203485	2.984861	-0.672987
22C	0.800867	3.361481	-1.976175
23C	-0.185006	4.328749	-2.173506
24C	-0.807922	4.951759	-1.082744
25C	-0.413639	4.595458	0.213183
26C	0.578290	3.632103	0.415041
27H	3.684575	-0.047439	1.894626
28H	5.570247	0.910836	3.223738
29H	7.371918	2.436299	-0.166022
30H	5.561262	1.530255	-1.639436
31H	0.822303	-2.302085	-1.950179
32H	-0.948768	-3.488749	-0.669992
33H	1.628982	-3.627356	2.769890
34H	3.416866	-2.496335	1.475321
35H	-1.547355	-4.890662	1.302779
36H	-0.494658	-4.926308	2.733745
37H	-1.525478	-3.523450	2.424271
38H	1.269909	2.880163	-2.829629
39H	-0.472212	4.598311	-3.188335
40H	-1.576239	5.705005	-1.240206
41H	-0.878529	5.072743	1.074177
42H	0.883592	3.358709	1.422327
43P	-2.695200	0.242801	-0.222888
44C	-1.781113	1.301877	-1.361173
45C	-1.779953	0.070252	1.330788
46C	-4.287122	1.036594	0.140604
47C	-2.986522	-1.384322	-0.963070
48C	-2.466250	-0.170500	2.533381
49C	-1.747725	-0.324685	3.719540
50C	-0.351186	-0.230510	3.710170
51C	0.327893	0.010460	2.513257
52C	-0.379128	0.154798	1.318436
53C	-5.494211	0.531801	-0.364152
54C	-6.688041	1.215020	-0.115633
55C	-6.678562	2.397968	0.628344
56C	-5.472992	2.904465	1.128112
57C	-4.277132	2.228667	0.886371
58C	-3.619126	-2.382388	-0.201966
59C	-3.852784	-3.638189	-0.760895
60C	-3.450081	-3.906710	-2.074642
61C	-2.813440	-2.917555	-2.828929
62C	-2.581245	-1.653848	-2.278708
63H	-0.788116	0.896933	-1.587345
64H	-2.367005	1.422483	-2.277296
65H	-1.670008	2.277954	-0.882385
66H	-3.551222	-0.222982	2.549761
67H	-2.278361	-0.507836	4.650089
68H	0.205445	-0.341915	4.637152
69H	1.410055	0.091925	2.501196
70H	0.160146	0.327318	0.394082
71H	-5.509666	-0.384925	-0.945447
72H	-7.622546	0.821356	-0.505994
73H	-7.608757	2.926944	0.818798
74H	-5.462965	3.825169	1.704944
75H	-3.343980	2.625682	1.277738
76H	-3.921911	-2.184661	0.822704
77H	-4.340275	-4.408457	-0.169668
78H	-3.625501	-4.888673	-2.505790
79H	-2.489329	-3.126663	-3.844482
80H	-2.075250	-0.899787	-2.872880

6bc-PhNCO2-006

1C	4.277490	0.414144	1.444898
2C	5.312765	0.868136	2.260551
3N	6.375881	1.550757	1.803336
4C	6.425727	1.795576	0.484127
5C	5.444886	1.378866	-0.417540
6C	4.346653	0.676970	0.075381
7N	3.317590	0.230904	-0.821810
8S	3.393218	-1.386838	-1.351427
9O	4.726606	-1.851065	-0.926790
10O	3.037119	-1.463950	-2.773099
11C	2.177052	-2.298688	-0.399803
12C	0.888954	-2.476796	-0.904404
13C	-0.039118	-3.190052	-0.145805
14C	0.297715	-3.716968	1.109911
15C	1.600541	-3.515372	1.593981
16C	2.546592	-2.814917	0.846320
17C	-0.708577	-4.505225	1.911174
18C	2.102394	1.020001	-1.007922
19O	1.184824	0.490136	-1.677969
20N	2.162389	2.173941	-0.370526
21C	1.186273	3.138790	-0.603864

22C	0.748824	3.514668	-1.896593
23C	-0.199890	4.522234	-2.070463
24C	-0.749162	5.190477	-0.967100
25C	-0.313237	4.841976	0.317426
26C	0.642770	3.838769	0.496063
27H	3.435671	-0.129243	1.861161
28H	5.289327	0.676634	3.331656
29H	7.293326	2.348299	0.129783
30H	5.525830	1.596785	-1.477764
31H	0.623026	-2.051656	-1.863799
32H	-1.042756	-3.333823	-0.534954
33H	1.880773	-3.915497	2.565863
34H	3.556690	-2.678124	1.218194
35H	-0.591694	-5.582292	1.727202
36H	-0.579978	-4.342821	2.986944
37H	-1.735292	-4.235972	1.641323
38H	1.157453	2.997224	-2.759574
39H	-0.516100	4.787971	-3.077747
40H	-1.490692	5.973440	-1.106634
41H	-0.717640	5.356319	1.187395
42H	0.980980	3.572561	1.495060
43P	-2.658085	0.289315	-0.154697
44C	-1.804862	1.539210	-1.134175
45C	-1.697453	-0.107815	1.328577
46C	-4.279931	0.934061	0.347160
47C	-2.913327	-1.201823	-1.154013
48C	-2.261785	-0.931105	2.318821
49C	-1.524551	-1.248415	3.458310
50C	-0.226408	-0.747504	3.615298
51C	0.333505	0.068690	2.630410
52C	-0.395347	0.388209	1.482598
53C	-5.364677	0.844328	-0.541255
54C	-6.589543	1.421474	-0.202402
55C	-6.736968	2.088620	1.018284
56C	-5.657037	2.181302	1.901564
57C	-4.427405	1.607864	1.570160
58C	-3.803869	-2.193197	-0.707415
59C	-3.953414	-3.371741	-1.437508
60C	-3.220197	-3.565379	-2.614301
61C	-2.338707	-2.577733	-3.061615
62C	-2.179330	-1.395180	-2.334428
63H	-0.801885	1.198969	-1.418910
64H	-2.404355	1.747736	-2.025220
65H	-1.723546	2.451877	-0.537658
66H	-3.271029	-1.317893	2.204140
67H	-1.961776	-1.885566	4.222113
68H	0.346711	-0.996756	4.504599
69H	1.340404	0.459991	2.741571
70H	0.063546	1.010081	0.724399
71H	-5.259085	0.324777	-1.489609
72H	-7.426527	1.348786	-0.891569
73H	-7.692223	2.535880	1.280455
74H	-5.768757	2.700196	2.849681
75H	-3.594389	1.686617	2.262509
76H	-4.383453	-2.045553	0.199468
77H	-4.641878	-4.136915	-1.089166
78H	-3.336344	-4.486221	-3.179668
79H	-1.763698	-2.727327	-3.971160
80H	-1.474338	-0.647719	-2.683391

6bc-PhNCO2-007

1C	-1.410680	-0.918746	-2.740489
2C	-0.432771	-1.619428	-3.435170
3N	-0.151345	-2.922160	-3.251299
4C	-0.923107	-3.558690	-2.354693
5C	-1.931944	-2.960456	-1.603454
6C	-2.176545	-1.580603	-1.757441
7N	-3.085900	-0.834449	-0.995047
8S	-3.859578	-1.410184	0.405881
9O	-4.348634	-2.770299	0.125271
10O	-4.810448	-0.354240	0.771654
11C	-2.634154	-1.532226	1.712942
12C	-2.330993	-0.394638	2.465351
13C	-1.369939	-0.487580	3.471988
14C	-0.707485	-1.696010	3.739152
15C	-1.042863	-2.825934	2.974603
16C	-2.002340	-2.753809	1.964591
17C	0.348118	-1.789158	4.813825
18C	-3.026359	0.688896	-1.124109
19O	-3.712736	1.162091	-2.040050
20N	-2.188727	1.183488	-0.238521
21C	-1.976847	2.556623	-0.099011
22C	-1.018353	2.928121	0.875296
23C	-0.688402	4.261800	1.107236
24C	-1.313420	5.281704	0.377581

25C	-2.270044	4.934503	-0.582734
26C	-2.602158	3.598248	-0.827611
27H	-1.553551	0.133756	-2.947120
28H	0.172031	-1.094478	-4.171796
29H	-0.722618	-4.619789	-2.216276
30H	-2.505128	-3.566070	-0.917100
31H	-2.831967	0.542969	2.260373
32H	-1.133248	0.396738	4.058721
33H	-0.552149	-3.775905	3.174995
34H	-2.268015	-3.638724	1.397807
35H	0.424214	-0.859076	5.386469
36H	0.125449	-2.602409	5.515546
37H	1.334453	-2.002986	4.380740
38H	-0.530702	2.140174	1.442784
39H	0.059485	4.504575	1.859340
40H	-1.061306	6.324414	0.555612
41H	-2.768962	5.714468	-1.155114
42H	-3.341741	3.349491	-1.578136
43P	2.010281	-0.033684	-0.109155
44C	0.417711	-0.812688	0.224491
45C	1.988738	0.746481	-1.743328
46C	2.362496	1.220763	1.150694
47C	3.283458	-1.325145	-0.067191
48C	0.900582	1.570243	-2.076227
49C	0.863766	2.199658	-3.319796
50C	1.907339	2.010878	-4.232604
51C	2.993944	1.196361	-3.898347
52C	3.041009	0.563435	-2.653581
53C	3.037053	2.399804	0.797785
54C	3.314453	3.359097	1.773770
55C	2.920225	3.147415	3.098120
56C	2.250288	1.971129	3.451328
57C	1.972485	1.005127	2.483598
58C	3.136678	-2.441860	-0.910789
59C	4.088627	-3.460775	-0.879288
60C	5.183304	-3.373325	-0.010886
61C	5.329592	-2.262925	0.825128
62C	4.383394	-1.234379	0.798535
63H	0.287956	-1.626860	-0.490774
64H	0.427072	-1.233567	1.231929
65H	-0.406439	-0.093417	0.122683
66H	0.082973	1.718039	-1.380220
67H	0.015081	2.829269	-3.572359
68H	1.872984	2.497757	-5.203656
69H	3.805210	1.049184	-4.605987
70H	3.888282	-0.067617	-2.403345
71H	3.330789	2.579325	-0.232021
72H	3.829051	4.274618	1.495655
73H	3.128518	3.900349	3.853548
74H	1.938063	1.807180	4.479072
75H	1.446756	0.101365	2.773872
76H	2.293842	-2.517261	-1.594296
77H	3.974630	-4.320451	-1.533888
78H	5.921975	-4.170376	0.011374
79H	6.179540	-2.193097	1.498554
80H	4.503737	-0.373418	1.449715

6bc-PhNCO2-008

1C	-0.955474	-2.263143	-0.569179
2C	-0.281272	-3.483742	-0.565869
3N	-0.003301	-4.183297	-1.678252
4C	-0.416506	-3.664770	-2.847289
5C	-1.108067	-2.456860	-2.957230
6C	-1.381657	-1.740370	-1.792892
7N	-2.078243	-0.484882	-1.849261
8S	-3.777105	-0.566424	-1.731953
9O	-4.124401	-1.887194	-2.292307
10O	-4.344794	0.640920	-2.341841
11C	-4.211088	-0.608538	0.007124
12C	-4.582646	0.567426	0.663879
13C	-4.886563	0.512444	2.022462
14C	-4.815369	-0.695804	2.738145
15C	-4.446476	-1.860587	2.049309
16C	-4.147500	-1.827699	0.685280
17C	-5.141530	-0.728629	4.211548
18C	-1.295154	0.708754	-1.470977
19O	-0.105689	0.672645	-1.871185
20N	-1.960288	1.572568	-0.741496
21C	-1.416695	2.802890	-0.386372
22C	-2.027880	3.467014	0.705800
23C	-1.581818	4.710634	1.150859
24C	-0.508937	5.349957	0.514962
25C	0.101623	4.714220	-0.572139
26C	-0.332314	3.463278	-1.018183
27H	-1.143150	-1.729187	0.355151

28H	0.058191	-3.914946	0.373418
29H	-0.183555	-4.243148	-3.738828
30H	-1.427285	-2.076886	-3.921976
31H	-4.621732	1.500683	0.115968
32H	-5.181390	1.423569	2.538997
33H	-4.398272	-2.808291	2.580616
34H	-3.878535	-2.736766	0.157760
35H	-6.167749	-0.385394	4.395351
36H	-5.045108	-1.738888	4.622955
37H	-4.475627	-0.065587	4.779062
38H	-2.864408	2.976994	1.197543
39H	-2.076147	5.185778	1.996460
40H	-0.160025	6.321395	0.857664
41H	0.937860	5.191788	-1.078972
42H	0.169201	2.982853	-1.848954
43P	2.858049	-0.420608	-0.125817
44C	2.296799	-1.250590	-1.630821
45C	4.362643	-1.242316	0.481721
46C	3.222768	1.319585	-0.476734
47C	1.587917	-0.530617	1.165951
48C	5.102716	-0.641406	1.514151
49C	6.241386	-1.272152	2.014082
50C	6.648995	-2.503752	1.488477
51C	5.915724	-3.102912	0.461150
52C	4.772120	-2.477393	-0.044503
53C	3.227647	2.266210	0.561469
54C	3.556980	3.593912	0.289238
55C	3.881991	3.983519	-1.013350
56C	3.874166	3.043955	-2.048182
57C	3.546737	1.712613	-1.784892
58C	0.565296	0.428520	1.229987
59C	-0.455509	0.290853	2.171309
60C	-0.462932	-0.801107	3.043970
61C	0.557410	-1.757276	2.981700
62C	1.585770	-1.625402	2.046908
63H	2.038605	-2.284460	-1.392086
64H	1.403917	-0.721419	-1.981385
65H	3.083306	-1.237470	-2.390648
66H	4.796756	0.315768	1.926094
67H	6.810156	-0.801349	2.811276
68H	7.537489	-2.992905	1.879023
69H	6.230127	-4.058328	0.049963
70H	4.214823	-2.958183	-0.842382
71H	2.954075	1.980514	1.572586
72H	3.541526	4.325516	1.092218
73H	4.127862	5.021012	-1.224023
74H	4.113063	3.345813	-3.064193
75H	3.534422	0.997889	-2.601448
76H	0.550036	1.265600	0.543119
77H	-1.249513	1.030511	2.200332
78H	-1.264397	-0.909815	3.769927
79H	0.555039	-2.605915	3.660665
80H	2.375473	-2.370851	2.007752

6bc-PhNCO2-009

1C	0.904282	2.388475	-0.745741
2C	0.140534	3.548674	-0.876153
3N	-0.216421	4.076054	-2.058241
4C	0.209506	3.442982	-3.164859
5C	0.994782	2.289218	-3.142044
6C	1.347169	1.749050	-1.906086
7N	2.130724	0.545960	-1.834879
8S	3.797386	0.735034	-1.563128
9O	4.093564	2.103385	-2.031923
10O	4.503008	-0.398739	-2.170500
11C	4.088407	0.715124	0.206854
12C	4.440723	-0.479217	0.839859
13C	4.632975	-0.479662	2.220052
14C	4.475900	0.693334	2.978479
15C	4.137437	1.880161	2.311956
16C	3.946091	1.901859	0.928937
17C	4.677248	0.666436	4.473912
18C	1.390022	-0.710554	-1.612180
19O	0.239880	-0.707826	-2.114614
20N	2.041118	-1.585280	-0.881349
21C	1.514486	-2.842308	-0.598650
22C	2.170378	-3.575072	0.422705
23C	1.741325	-4.842891	0.810818
24C	0.637709	-5.441483	0.187876
25C	-0.018742	-4.739592	-0.828813
26C	0.398999	-3.464145	-1.219040
27H	1.141642	1.989471	0.233621
28H	-0.210373	4.071807	0.011320
29H	-0.089939	3.881526	-4.114318
30H	1.321157	1.812174	-4.060253

31H	4.549523	-1.383819	0.255398
32H	4.904811	-1.407345	2.719397
33H	4.022407	2.801557	2.878316
34H	3.694649	2.827029	0.420863
35H	5.732097	0.491862	4.724756
36H	4.374679	1.610692	4.939072
37H	4.099692	-0.143501	4.936793
38H	3.030153	-3.118631	0.905947
39H	2.273073	-5.369179	1.601653
40H	0.301321	-6.431692	0.486488
41H	-0.877959	-5.185879	-1.326085
42H	-0.134361	-2.937497	-1.999653
43P	-2.833627	0.348950	-0.097927
44C	-2.322348	1.025159	-1.696273
45C	-4.303462	1.255083	0.472975
46C	-3.218580	-1.412434	-0.262780
47C	-1.494482	0.533980	1.114213
48C	-5.334687	0.586094	1.151093
49C	-6.447246	1.299069	1.602953
50C	-6.536894	2.676716	1.382041
51C	-5.511508	3.345415	0.705731
52C	-4.396231	2.640419	0.249311
53C	-3.188601	-2.241156	0.871655
54C	-3.514559	-3.592162	0.752908
55C	-3.866845	-4.121028	-0.492780
56C	-3.891230	-3.298942	-1.622984
57C	-3.568451	-1.945065	-1.513307
58C	-0.418901	-0.368056	1.068790
59C	0.655793	-0.211003	1.943480
60C	0.660271	0.840178	2.865303
61C	-0.413077	1.735945	2.915431
62C	-1.493255	1.587668	2.042325
63H	-2.042340	2.072326	-1.563760
64H	-1.450370	0.460100	-2.045159
65H	-3.149801	0.962674	-2.409355
66H	-5.279659	-0.484859	1.320844
67H	-7.244805	0.775363	2.122847
68H	-7.405582	3.227837	1.732510
69H	-5.577789	4.415462	0.528952
70H	-3.608240	3.175598	-0.272202
71H	-2.895806	-1.840605	1.837801
72H	-3.478220	-4.232598	1.629641
73H	-4.109522	-5.176386	-0.584436
74H	-4.149564	-3.710988	-2.594509
75H	-3.576238	-1.323059	-2.402410
76H	-0.410471	-1.179754	0.351070
77H	1.493863	-0.897567	1.880238
78H	1.503825	0.964841	3.538020
79H	-0.412592	2.551601	3.633794
80H	-2.322247	2.287314	2.091545

6bc-PhNCO2-010

1C	-0.904215	-2.392479	-0.757448
2C	-0.143995	-3.553800	-0.898461
3N	0.204717	-4.075674	-2.085474
4C	-0.226056	-3.435611	-3.186177
5C	-1.008304	-2.280100	-3.152635
6C	-1.352148	-1.745764	-1.911697
7N	-2.132681	-0.541468	-1.829291
8S	-3.798826	-0.728425	-1.552446
9O	-4.098862	-2.095265	-2.023169
10O	-4.505176	0.407609	-2.154754
11C	-4.082938	-0.711805	0.218643
12C	-4.432952	0.481366	0.855069
13C	-4.620087	0.479221	2.235941
14C	-4.460036	-0.695176	2.991611
15C	-4.124053	-1.880768	2.321668
16C	-3.937834	-1.899882	0.937886
17C	-4.654556	-0.670675	4.488018
18C	-1.389055	0.712585	-1.604969
19O	-0.239347	0.708638	-2.108377
20N	-2.037515	1.587535	-0.871952
21C	-1.508989	2.844132	-0.591188
22C	-2.158786	3.576531	0.434319
23C	-1.727960	4.844677	0.819450
24C	-0.628627	5.443840	0.189470
25C	0.021878	4.742113	-0.831185
26C	-0.397643	3.466397	-1.218506
27H	-1.134815	-1.998048	0.225370
28H	0.211086	-4.082444	-0.015980
29H	0.066632	-3.869924	-4.139689
30H	-1.338947	-1.797494	-4.066400
31H	-4.543994	1.387018	0.272637
32H	-4.890131	1.405967	2.738006
33H	-4.006860	-2.803186	2.885903

34H	-3.688119	-2.824021	0.427077
35H	-5.706414	-0.486536	4.744349
36H	-4.358772	-1.619067	4.949066
37H	-4.066919	0.132302	4.950441
38H	-3.015543	3.119860	0.922729
39H	-2.255196	5.370897	1.613348
40H	-0.291168	6.434421	0.485633
41H	0.877874	5.188530	-1.333860
42H	0.131300	2.939795	-2.002168
43P	2.832041	-0.344782	-0.116889
44C	2.320086	-1.025574	-1.712308
45C	4.297784	-1.246307	0.469449
46C	3.215654	1.417050	-0.284328
47C	1.497281	-0.537988	1.096718
48C	5.210316	-0.624545	1.337618
49C	6.305207	-1.340582	1.824069
50C	6.495559	-2.674804	1.449440
51C	5.590252	-3.294732	0.583064
52C	4.491779	-2.585773	0.091552
53C	3.157343	2.256440	0.840991
54C	3.488515	3.605934	0.717753
55C	3.874604	4.122390	-0.522938
56C	3.926890	3.289586	-1.644419
57C	3.599111	1.937431	-1.530369
58C	0.420429	0.362809	1.072762
59C	-0.647767	0.189551	1.952454
60C	-0.643746	-0.876660	2.856984
61C	0.430471	-1.772649	2.883806
62C	1.503947	-1.608520	2.005395
63H	2.015828	-2.064990	-1.572413
64H	1.458678	-0.447143	-2.065441
65H	3.147977	-0.982211	-2.426142
66H	5.077656	0.413165	1.628936
67H	7.010893	-0.854014	2.491858
68H	7.350223	-3.228623	1.828873
69H	5.736074	-4.329920	0.286777
70H	3.797640	-3.080800	-0.580681
71H	2.837958	1.866150	1.802790
72H	3.429216	4.255026	1.586803
73H	4.121586	5.176428	-0.618164
74H	4.212011	3.691744	-2.612603
75H	3.629686	1.306747	-2.413055
76H	0.406172	1.185827	0.368205
77H	-1.487532	0.875487	1.906529
78H	-1.481971	-1.013325	3.533980
79H	0.435358	-2.600667	3.587861
80H	2.334407	-2.308189	2.034295

6bc-PhNCO2-011

1C	1.252749	2.398406	-0.902013
2C	0.776102	3.697261	-1.067564
3N	1.081077	4.474215	-2.120411
4C	1.895286	3.948848	-3.050686
5C	2.422503	2.657671	-2.981464
6C	2.091422	1.862887	-1.884262
7N	2.586362	0.522791	-1.765486
8S	4.187228	0.335232	-1.197734
9O	4.845693	1.621843	-1.496941
10O	4.746931	-0.899015	-1.759038
11C	4.115842	0.190411	0.588626
12C	4.238702	-1.061681	1.194983
13C	4.165238	-1.146374	2.583881
14C	3.956435	-0.002344	3.374296
15C	3.846199	1.240804	2.735742
16C	3.929021	1.348076	1.345782
17C	3.833366	-0.124687	4.873425
18C	1.581053	-0.551379	-1.669870
19O	0.524636	-0.317120	-2.305036
20N	1.947457	-1.545018	-0.893474
21C	1.185519	-2.704274	-0.788890
22C	1.373938	-3.482250	0.378916
23C	0.685623	-4.678196	0.581235
24C	-0.213742	-5.151890	-0.382727
25C	-0.407396	-4.400498	-1.547785
26C	0.268744	-3.195702	-1.752465
27H	0.976647	1.810066	-0.034587
28H	0.121615	4.137584	-0.317288
29H	2.134703	4.589252	-3.896989
30H	3.071463	2.275298	-3.761722
31H	4.374787	-1.945309	0.583455
32H	4.260138	-2.118320	3.063487
33H	3.692372	2.139235	3.328609
34H	3.852672	2.316622	0.862535
35H	4.707945	-0.627866	5.304587
36H	3.736979	0.855592	5.352180

37H	2.954040	-0.723145	5.146472
38H	2.077752	-3.120979	1.124482
39H	0.855983	-5.245866	1.494482
40H	-0.752432	-6.083986	-0.228606
41H	-1.103484	-4.750679	-2.307756
42H	0.093512	-2.624054	-2.655941
43P	-2.873842	0.511484	-0.159964
44C	-2.151983	1.227772	-1.655490
45C	-4.348349	1.451409	0.322906
46C	-3.342003	-1.212201	-0.459718
47C	-1.652186	0.585762	1.174947
48C	-5.390845	0.810496	1.011885
49C	-6.503667	1.545475	1.424602
50C	-6.580943	2.915406	1.152306
51C	-5.544002	3.554178	0.464873
52C	-4.426409	2.826913	0.049937
53C	-3.148795	-2.189606	0.528541
54C	-3.563274	-3.501852	0.294273
55C	-4.171785	-3.840242	-0.916973
56C	-4.365011	-2.866358	-1.902427
57C	-3.953507	-1.552462	-1.678076
58C	-0.473977	-0.167425	1.041964
59C	0.514485	-0.085257	2.021356
60C	0.327143	0.738893	3.136033
61C	-0.849954	1.481294	3.274105
62C	-1.844414	1.409969	2.294615
63H	-1.828606	2.250950	-1.445248
64H	-1.275755	0.631211	-1.940156
65H	-2.888587	1.234616	-2.463987
66H	-5.340268	-0.254559	1.219489
67H	-7.310947	1.046645	1.953802
68H	-7.450598	3.483808	1.471504
69H	-5.603256	4.617282	0.248207
70H	-3.628269	3.333210	-0.484622
71H	-2.663411	-1.939710	1.466783
72H	-3.397269	-4.259570	1.054429
73H	-4.484215	-4.865135	-1.098957
74H	-4.830713	-3.129205	-2.848262
75H	-4.109430	-0.804364	-2.450035
76H	-0.320564	-0.803041	0.177530
77H	1.432516	-0.649841	1.895615
78H	1.103270	0.804691	3.893180
79H	-0.996653	2.119438	4.141434
80H	-2.755072	1.991064	2.405892

6bc-PhNCO2-012

1C	-2.100205	2.381862	-0.713763
2C	-1.961625	3.670587	-1.230384
3N	-2.202609	4.783894	-0.520971
4C	-2.601154	4.626106	0.752473
5C	-2.774486	3.381915	1.360928
6C	-2.517248	2.235365	0.610857
7N	-2.674238	0.932053	1.193959
8S	-4.153424	0.136718	0.917430
9O	-5.086341	1.216010	0.539096
10O	-4.466806	-0.703367	2.078948
11C	-3.958520	-0.914313	-0.524628
12C	-3.600679	-2.253514	-0.370346
13C	-3.445538	-3.045436	-1.509464
14C	-3.638280	-2.519141	-2.794970
15C	-4.006339	-1.168237	-2.917798
16C	-4.171395	-0.361783	-1.792469
17C	-3.454115	-3.371981	-4.026225
18C	-1.471186	0.258453	1.694796
19O	-0.562551	1.042210	2.076880
20N	-1.517272	-1.047554	1.612730
21C	-0.535343	-1.814385	2.233098
22C	0.011870	-2.907765	1.528431
23C	0.971137	-3.738598	2.111238
24C	1.407365	-3.512496	3.422841
25C	0.858536	-2.440868	4.141750
26C	-0.094635	-1.603888	3.560893
27H	-1.892868	1.511078	-1.327057
28H	-1.636234	3.815054	-2.258627
29H	-2.792503	5.538885	1.312749
30H	-3.098485	3.299541	2.393194
31H	-3.433289	-2.657524	0.620100
32H	-3.160136	-4.088223	-1.393002
33H	-4.169972	-0.744494	-3.906436
34H	-4.468625	0.676822	-1.894394
35H	-3.074323	-4.367572	-3.774338
36H	-4.404430	-3.501546	-4.560676
37H	-2.753180	-2.905708	-4.730169
38H	-0.315029	-3.075938	0.506321
39H	1.381830	-4.566502	1.535723

40H	2.150197	-4.162384	3.879514
41H	1.176618	-2.255850	5.166308
42H	-0.505391	-0.771282	4.124184
43P	2.888528	0.220301	0.095459
44C	2.509952	-0.058909	1.840667
45C	4.605430	-0.242182	-0.259420
46C	1.795438	-0.807519	-0.928077
47C	2.629327	1.978014	-0.283655
48C	5.007108	-0.478864	-1.585985
49C	6.336120	-0.798432	-1.865388
50C	7.269025	-0.888103	-0.826761
51C	6.871577	-0.657952	0.493364
52C	5.543551	-0.333870	0.781447
53C	0.558914	-0.301003	-1.353815
54C	-0.317299	-1.118079	-2.068251
55C	0.041803	-2.432869	-2.374996
56C	1.276201	-2.938506	-1.955385
57C	2.150810	-2.134188	-1.223726
58C	1.550521	2.655719	0.312310
59C	1.331688	4.000956	0.006363
60C	2.174975	4.670638	-0.884354
61C	3.248205	3.995044	-1.475098
62C	3.479567	2.650767	-1.177924
63H	3.133482	0.587123	2.466318
64H	1.454565	0.184529	2.009639
65H	2.680182	-1.111004	2.084909
66H	4.286308	-0.425402	-2.396983
67H	6.639869	-0.981580	-2.892476
68H	8.303019	-1.140843	-1.046276
69H	7.592987	-0.731833	1.302523
70H	5.253046	-0.160933	1.812958
71H	0.272908	0.718945	-1.122346
72H	-1.286913	-0.734420	-2.369473
73H	-0.647120	-3.065127	-2.927706
74H	1.554606	-3.963871	-2.183524
75H	3.098096	-2.542688	-0.884571
76H	0.867406	2.148510	0.990193
77H	0.491317	4.518041	0.459445
78H	1.995485	5.716783	-1.118603
79H	3.909452	4.513467	-2.164375
80H	4.321983	2.141098	-1.634664

6bc-PhNCO-001

1C	-2.964322	-2.887654	-1.506943
2C	-1.718295	-3.444292	-1.426915
3N	-0.907861	-3.238457	-0.347784
4C	-1.393122	-2.529082	0.708818
5C	-2.630588	-1.945753	0.692609
6C	-3.464470	-2.031486	-0.472610
7N	-4.622266	-1.392726	-0.718984
8S	-5.226538	-0.288161	0.338193
9O	-5.292291	-0.778770	1.740215
10O	-6.483227	0.202909	-0.266917
11C	-4.060222	1.095397	0.323979
12C	-3.326121	1.413250	1.466025
13C	-2.428751	2.484703	1.428056
14C	-2.250441	3.241003	0.262432
15C	-2.998721	2.896444	-0.877605
16C	-3.900617	1.834370	-0.854062
17C	-1.267653	4.385228	0.217362
18C	0.527848	-3.708933	-0.410816
19O	0.791250	-4.446662	-1.375312
20N	1.227397	-3.209204	0.581587
21C	2.611667	-3.348901	0.651966
22C	3.212361	-3.035011	1.894955
23C	4.597295	-3.025157	2.054470
24C	5.438235	-3.326451	0.975124
25C	4.861393	-3.651386	-0.257975
26C	3.473998	-3.671595	-0.425407
27H	-3.566944	-3.049493	-2.394639
28H	-1.287070	-4.047727	-2.214880
29H	-0.726385	-2.456037	1.555026
30H	-2.957882	-1.413364	1.574396
31H	-3.462106	0.839566	2.377002
32H	-1.858419	2.730313	2.319472
33H	-2.876393	3.471194	-1.793333
34H	-4.479055	1.583725	-1.738490
35H	-1.693837	5.256044	-0.295099
36H	-0.965275	4.696091	1.222724
37H	-0.359760	4.103084	-0.331144
38H	2.562366	-2.784227	2.729701
39H	5.022937	-2.777250	3.024814
40H	6.518727	-3.317772	1.095843
41H	5.498613	-3.897065	-1.105673
42H	3.047571	-3.929364	-1.387000

43P	2.341490	1.075218	-0.175296
44C	3.863662	0.099739	-0.023567
45C	1.247264	0.320608	-1.398097
46C	1.505420	1.116405	1.431355
47C	2.778665	2.757761	-0.692843
48C	1.797385	-0.370747	-2.489957
49C	0.952447	-0.907629	-3.462415
50C	-0.432851	-0.756361	-3.348298
51C	-0.979789	-0.070792	-2.259726
52C	-0.145048	0.468535	-1.281005
53C	1.008750	-0.095103	1.941681
54C	0.383146	-0.108352	3.188469
55C	0.257289	1.073603	3.926860
56C	0.753748	2.276656	3.416326
57C	1.375893	2.304856	2.165675
58C	3.879033	3.398223	-0.096632
59C	4.209291	4.701606	-0.469874
60C	3.449198	5.368388	-1.437141
61C	2.358689	4.730169	-2.034891
62C	2.019483	3.426262	-1.666070
63H	4.444427	0.479164	0.821745
64H	3.602756	-0.945485	0.158753
65H	4.453599	0.183898	-0.940245
66H	2.870740	-0.508531	-2.579358
67H	1.376641	-1.456505	-4.298371
68H	-1.089045	-1.187224	-4.099458
69H	-2.055150	0.032014	-2.159786
70H	-0.580776	0.987293	-0.432559
71H	1.098025	-1.020025	1.374637
72H	-0.005095	-1.043730	3.582724
73H	-0.232629	1.057320	4.896879
74H	0.648507	3.197052	3.984228
75H	1.748739	3.244781	1.770697
76H	4.475936	2.889512	0.655058
77H	5.059874	5.193934	-0.006537
78H	3.710311	6.382851	-1.726568
79H	1.770496	5.243964	-2.790269
80H	1.174175	2.936069	-2.139455

6bc-PhNCO-002

1C	-2.576700	-3.304647	-1.055674
2C	-1.239976	-3.581838	-0.974772
3N	-0.456233	-3.052636	0.008598
4C	-1.044325	-2.299606	0.978323
5C	-2.373095	-1.976372	0.951539
6C	-3.210290	-2.414345	-0.128648
7N	-4.489196	-2.081738	-0.381962
8S	-5.279562	-0.967092	0.530265
9O	-5.139008	-1.178577	1.995443
10O	-6.652828	-0.901574	-0.014606
11C	-4.497057	0.621216	0.156921
12C	-3.708545	1.265319	1.110089
13C	-3.126398	2.498565	0.799999
14C	-3.324922	3.098025	-0.450736
15C	-4.107320	2.418652	-1.401797
16C	-4.694181	1.189856	-1.107042
17C	-2.750438	4.457160	-0.769774
18C	1.043980	-3.242057	-0.058208
19O	1.426065	-4.054688	-0.917981
20N	1.648373	-2.476742	0.819394
21C	3.038501	-2.414023	0.907188
22C	3.571720	-1.901820	2.113725
23C	4.945630	-1.755675	2.299682
24C	5.840033	-2.098388	1.277817
25C	5.329649	-2.590721	0.071888
26C	3.954510	-2.753649	-0.118175
27H	-3.162129	-3.724912	-1.866789
28H	-0.719347	-4.206100	-1.688936
29H	-0.380177	-1.977600	1.765998
30H	-2.774441	-1.389459	1.765185
31H	-3.565399	0.821396	2.089592
32H	-2.516389	2.998508	1.548308
33H	-4.268671	2.866800	-2.380025
34H	-5.309264	0.682161	-1.844024
35H	-3.531420	5.227910	-0.716749
36H	-1.962781	4.740338	-0.063464
37H	-2.339006	4.492758	-1.785836
38H	2.878324	-1.629940	2.906361
39H	5.319910	-1.368965	3.245730
40H	6.912009	-1.982213	1.418454
41H	6.009963	-2.859140	-0.734353
42H	3.579942	-3.153621	-1.052311
43P	1.530939	2.072060	-0.628411
44C	1.090975	3.658416	-1.395802
45C	0.784430	0.745834	-1.607063

46C	3.334630	1.923309	-0.640232
47C	0.882746	2.019122	1.058637
48C	-0.597722	0.797582	-1.865396
49C	-1.189096	-0.192115	-2.647778
50C	-0.409823	-1.231084	-3.169843
51C	0.957910	-1.292914	-2.895334
52C	1.561122	-0.307943	-2.109429
53C	4.030222	2.200171	-1.831437
54C	5.419467	2.084824	-1.863147
55C	6.117247	1.698014	-0.713126
56C	5.425706	1.422250	0.468557
57C	4.033874	1.531239	0.510504
58C	0.617000	3.204334	1.764460
59C	0.106620	3.133850	3.061729
60C	-0.133306	1.889631	3.654944
61C	0.143390	0.711959	2.953891
62C	0.652344	0.769147	1.655610
63H	1.616463	4.475979	-0.893866
64H	1.390692	3.630478	-2.447360
65H	0.011790	3.815701	-1.333058
66H	-1.215273	1.591320	-1.453599
67H	-2.258428	-0.159992	-2.835403
68H	-0.875738	-2.003412	-3.774919
69H	1.555273	-2.117341	-3.271661
70H	2.621170	-0.372285	-1.885185
71H	3.495706	2.494387	-2.730843
72H	5.955897	2.294402	-2.784594
73H	7.199738	1.606004	-0.741698
74H	5.963490	1.109195	1.357750
75H	3.504857	1.301479	1.429714
76H	0.794911	4.176309	1.314168
77H	-0.107583	4.049574	3.605982
78H	-0.536938	1.838931	4.662683
79H	-0.038024	-0.254441	3.416301
80H	0.874273	-0.152787	1.122792

6bc-PhNCO-003

1C	-2.634334	-3.286055	-1.060029
2C	-1.298755	-3.570040	-0.981728
3N	-0.507013	-3.034669	-0.007712
4C	-1.086386	-2.264620	0.953736
5C	-2.413934	-1.936304	0.930484
6C	-3.259483	-2.383545	-0.139028
7N	-4.538593	-2.047794	-0.387454
8S	-5.318028	-0.924872	0.524425
9O	-5.180363	-1.139196	1.989406
10O	-6.690297	-0.845257	-0.021113
11C	-4.519195	0.656119	0.153271
12C	-3.742003	1.301872	1.114395
13C	-3.146277	2.528900	0.804868
14C	-3.321038	3.120881	-0.452886
15C	-4.092981	2.439811	-1.411465
16C	-4.692372	1.216973	-1.117703
17C	-2.729872	4.472228	-0.774452
18C	0.990879	-3.241931	-0.074687
19O	1.363369	-4.054458	-0.938695
20N	1.605438	-2.490123	0.807670
21C	2.996087	-2.437490	0.890807
22C	3.535436	-1.919614	2.092312
23C	4.910585	-1.779534	2.273907
24C	5.800482	-2.135260	1.252605
25C	5.284219	-2.634473	0.051951
26C	3.907758	-2.790670	-0.133929
27H	-3.225673	-3.712663	-1.863528
28H	-0.785324	-4.205928	-1.690839
29H	-0.418864	-1.930396	1.732857
30H	-2.806719	-1.337223	1.739351
31H	-3.617112	0.863144	2.098790
32H	-2.544413	3.030194	1.559171
33H	-4.235306	2.881749	-2.395479
34H	-5.298424	0.707917	-1.861263
35H	-3.509562	5.245975	-0.765877
36H	-1.969144	4.766332	-0.043382
37H	-2.278993	4.488159	-1.774073
38H	2.845716	-1.636527	2.884007
39H	5.289248	-1.387186	3.215875
40H	6.873450	-2.024060	1.389528
41H	5.961059	-2.913356	-0.753666
42H	3.528606	-3.194972	-1.064337
43P	1.568233	2.062887	-0.595841
44C	1.119993	3.666718	-1.321302
45C	0.789646	0.759861	-1.581676
46C	3.369637	1.900559	-0.659493
47C	0.964559	1.981682	1.106345
48C	-0.594511	0.834664	-1.821832

49C	-1.212360	-0.140992	-2.601494
50C	-0.456823	-1.189029	-3.139746
51C	0.913583	-1.273402	-2.884602
52C	1.542819	-0.302901	-2.101217
53C	4.024742	2.163722	-1.876158
54C	5.411434	2.041930	-1.955016
55C	6.146375	1.661581	-0.825927
56C	5.494597	1.398886	0.381067
57C	4.105431	1.514935	0.470117
58C	0.690930	3.153580	1.830789
59C	0.227803	3.059024	3.144424
60C	0.045460	1.804400	3.736264
61C	0.329678	0.640185	3.015869
62C	0.786280	0.721228	1.699465
63H	1.661742	4.471023	-0.815167
64H	1.394498	3.659076	-2.380198
65H	0.043460	3.828461	-1.229773
66H	-1.194078	1.634923	-1.396813
67H	-2.283489	-0.089743	-2.774179
68H	-0.942855	-1.950613	-3.742546
69H	1.492801	-2.104519	-3.274234
70H	2.604826	-0.385618	-1.892847
71H	3.457616	2.451041	-2.757635
72H	5.917295	2.240835	-2.895864
73H	7.226869	1.564230	-0.890753
74H	6.061323	1.091021	1.254120
75H	3.607150	1.294523	1.408527
76H	0.827609	4.133616	1.383829
77H	0.007159	3.964557	3.703004
78H	-0.318071	1.735280	4.758096
79H	0.195792	-0.335386	3.475696
80H	1.007731	-0.193095	1.152252

6bc-PhNCO-004

1C	-2.572906	-3.324703	-1.109538
2C	-1.235269	-3.599620	-1.036606
3N	-0.441755	-3.050240	-0.072365
4C	-1.020382	-2.276161	0.885986
5C	-2.349741	-1.953916	0.866278
6C	-3.197107	-2.415335	-0.195311
7N	-4.477005	-2.083198	-0.445993
8S	-5.269063	-0.981500	0.479382
9O	-5.132719	-1.219386	1.940734
10O	-6.640545	-0.907130	-0.069142
11C	-4.492748	0.619160	0.140653
12C	-3.797037	1.295083	1.142838
13C	-3.244601	2.550306	0.868407
14C	-3.381752	3.140875	-0.395133
15C	-4.062775	2.426024	-1.396710
16C	-4.620631	1.175645	-1.137341
17C	-2.854130	4.528012	-0.672195
18C	1.058321	-3.250740	-0.144790
19O	1.431142	-4.047102	-1.023373
20N	1.669996	-2.515147	0.752978
21C	3.059813	-2.477945	0.856552
22C	3.582342	-1.931439	2.053346
23C	4.955242	-1.812677	2.263905
24C	5.861417	-2.221232	1.276691
25C	5.362556	-2.749155	0.080940
26C	3.987758	-2.882928	-0.133893
27H	-3.166560	-3.761598	-1.905791
28H	-0.721626	-4.237839	-1.743474
29H	-0.348940	-1.933653	1.658013
30H	-2.740658	-1.344956	1.669197
31H	-3.702369	0.855329	2.130191
32H	-2.710746	3.077865	1.655364
33H	-4.169884	2.862950	-2.387260
34H	-5.160842	0.642855	-1.914376
35H	-3.667194	5.265030	-0.619697
36H	-2.095917	4.827881	0.059337
37H	-2.421897	4.603342	-1.676928
38H	2.880463	-1.609246	2.818918
39H	5.319774	-1.398478	3.202082
40H	6.933081	-2.130365	1.437239
41H	6.051918	-3.069685	-0.698127
42H	3.621717	-3.306883	-1.060716
43P	1.474085	2.111135	-0.543336
44C	0.867152	3.685921	-1.213825
45C	0.751784	0.774764	-1.525920
46C	3.280071	2.064748	-0.666824
47C	0.932478	1.951484	1.175139
48C	-0.649436	0.661287	-1.578922
49C	-1.229692	-0.321932	-2.377136
50C	-0.420173	-1.194190	-3.113819
51C	0.970840	-1.095084	-3.042719

52C	1.564040	-0.110623	-2.248581
53C	3.912727	2.661341	-1.771914
54C	5.300137	2.583458	-1.900083
55C	6.056939	1.908447	-0.936305
56C	5.426961	1.310000	0.158225
57C	4.040168	1.386136	0.298567
58C	0.614531	3.089273	1.935872
59C	0.196071	2.939668	3.259149
60C	0.099610	1.663701	3.824868
61C	0.426137	0.534387	3.068330
62C	0.841023	0.670329	1.742471
63H	1.356410	4.531032	-0.721717
64H	1.070769	3.719452	-2.287427
65H	-0.213354	3.737146	-1.059339
66H	-1.287380	1.320083	-0.995673
67H	-2.310618	-0.418841	-2.405273
68H	-0.877022	-1.965905	-3.726475
69H	1.598205	-1.793416	-3.588687
70H	2.646059	-0.044532	-2.189500
71H	3.336182	3.178137	-2.533572
72H	5.787256	3.046252	-2.753976
73H	7.136753	1.844872	-1.041909
74H	6.006949	0.770018	0.899798
75H	3.563310	0.906137	1.146998
76H	0.683717	4.085494	1.509421
77H	-0.057569	3.818829	3.845171
78H	-0.231087	1.550764	4.853944
79H	0.355373	-0.457685	3.505880
80H	1.089354	-0.218567	1.166295

6bc-PhNCO-005

1C	-2.014224	-3.305823	-1.414636
2C	-0.660703	-3.478390	-1.329507
3N	0.028350	-3.193316	-0.185496
4C	-0.669632	-2.814765	0.922653
5C	-2.024850	-2.621810	0.903094
6C	-2.773602	-2.793781	-0.310911
7N	-4.067553	-2.517524	-0.544957
8S	-5.021681	-1.812803	0.595872
9O	-4.891411	-2.422700	1.945301
10O	-6.375491	-1.755072	0.004740
11C	-4.436787	-0.107789	0.731100
12C	-3.735558	0.313309	1.861178
13C	-3.279846	1.633679	1.932042
14C	-3.515329	2.540276	0.888489
15C	-4.229663	2.090857	-0.235685
16C	-4.688293	0.778379	-0.322069
17C	-3.006345	3.959727	0.953416
18C	1.543670	-3.251747	-0.206298
19O	2.024368	-3.834429	-1.193638
20N	2.037359	-2.630016	0.837051
21C	3.409267	-2.534999	1.072822
22C	3.781815	-1.850267	2.254463
23C	5.118152	-1.671260	2.606717
24C	6.138017	-2.172077	1.786865
25C	5.787920	-2.852543	0.616017
26C	4.450398	-3.035082	0.254066
27H	-2.523279	-3.519459	-2.348614
28H	-0.053420	-3.821869	-2.157153
29H	-0.072356	-2.665730	1.811635
30H	-2.517055	-2.346939	1.825148
31H	-3.568910	-0.372534	2.685331
32H	-2.749513	1.964199	2.822833
33H	-4.428698	2.780003	-1.053024
34H	-5.241922	0.444772	-1.194368
35H	-3.741749	4.664875	0.548662
36H	-2.778320	4.259529	1.981909
37H	-2.088593	4.073898	0.361879
38H	2.989480	-1.467423	2.893994
39H	5.365342	-1.142453	3.525324
40H	7.182524	-2.038269	2.058307
41H	6.567289	-3.247594	-0.033181
42H	4.201162	-3.557388	-0.660464
43P	1.178064	1.493837	-0.105228
44C	0.770729	0.472879	1.337264
45C	2.724868	0.900546	-0.834729
46C	-0.155993	1.401676	-1.326716
47C	1.394238	3.214217	0.422416
48C	3.905659	0.985102	-0.076223
49C	5.100348	0.499704	-0.604056
50C	5.120521	-0.077360	-1.878385
51C	3.946161	-0.166605	-2.629203
52C	2.744173	0.322902	-2.112303
53C	-0.875046	0.205373	-1.479227
54C	-1.877914	0.118159	-2.445117

55C	-2.160945	1.215945	-3.262523
56C	-1.444812	2.407475	-3.112503
57C	-0.443382	2.506621	-2.144917
58C	0.610458	3.718227	1.473342
59C	0.741079	5.054237	1.855456
60C	1.646447	5.888525	1.191381
61C	2.425698	5.387788	0.143585
62C	2.303156	4.051852	-0.243617
63H	-0.283002	0.593138	1.603035
64H	0.994810	-0.575686	1.107004
65H	1.403048	0.785840	2.173359
66H	3.895427	1.424582	0.917445
67H	6.009404	0.552095	-0.013139
68H	6.051243	-0.470027	-2.278641
69H	3.958419	-0.625379	-3.613850
70H	1.833569	0.244935	-2.698256
71H	-0.663620	-0.650675	-0.849145
72H	-2.443992	-0.801886	-2.545553
73H	-2.947855	1.145226	-4.008770
74H	-1.670176	3.264535	-3.741326
75H	0.100068	3.439862	-2.030417
76H	-0.100411	3.080215	1.989778
77H	0.135478	5.442366	2.669722
78H	1.746359	6.927946	1.492586
79H	3.132261	6.033659	-0.370392
80H	2.916981	3.663556	-1.051058

6bc-PhNCO-006

1C	2.111124	1.290306	-2.655752
2C	0.813227	1.639956	-2.412349
3N	0.430053	2.210869	-1.231816
4C	1.381222	2.469392	-0.290569
5C	2.699634	2.148601	-0.474841
6C	3.138810	1.499364	-1.677644
7N	4.366094	1.051604	-1.994614
8S	5.625319	1.160286	-0.943692
9O	5.740628	2.486209	-0.281932
10O	6.807799	0.665656	-1.681406
11C	5.268676	-0.047153	0.351586
12C	5.027340	0.370034	1.660315
13C	4.729499	-0.583468	2.637976
14C	4.662625	-1.948299	2.324970
15C	4.921335	-2.342608	1.000249
16C	5.223776	-1.404595	0.014526
17C	4.276659	-2.965457	3.370369
18C	-1.027929	2.526725	-1.013755
19O	-1.774206	2.191516	-1.961534
20N	-1.244327	3.058506	0.158340
21C	-2.520726	3.489730	0.528841
22C	-2.823358	3.493330	1.908502
23C	-4.053120	3.952612	2.381403
24C	-5.016853	4.443918	1.491917
25C	-4.724741	4.463453	0.123014
26C	-3.503023	3.987671	-0.359197
27H	2.374402	0.835587	-3.605027
28H	0.017562	1.489812	-3.129224
29H	1.011732	2.935465	0.612505
30H	3.399814	2.397524	0.310336
31H	5.081215	1.424210	1.912383
32H	4.546532	-0.257453	3.659446
33H	4.885382	-3.398172	0.739259
34H	5.424206	-1.720868	-1.004966
35H	4.762191	-3.931381	3.191020
36H	4.543328	-2.628977	4.378363
37H	3.190902	-3.136914	3.357077
38H	-2.068368	3.129810	2.601573
39H	-4.256626	3.935543	3.450309
40H	-5.972589	4.810532	1.858737
41H	-5.458010	4.850311	-0.582289
42H	-3.298722	4.003166	-1.423497
43P	-2.189420	-1.614693	-0.756201
44C	-1.850454	-1.012789	-2.430552
45C	-0.907809	-1.014596	0.370992
46C	-3.814638	-1.031249	-0.214466
47C	-2.170319	-3.428971	-0.760772
48C	0.443328	-1.210756	0.031118
49C	1.442449	-0.794680	0.908275
50C	1.100166	-0.186159	2.121335
51C	-0.240019	0.014295	2.455613
52C	-1.250229	-0.397680	1.582348
53C	-4.166610	0.314183	-0.422076
54C	-5.399507	0.778298	0.038429
55C	-6.278621	-0.087292	0.697004
56C	-5.927039	-1.425413	0.901338
57C	-4.694460	-1.901753	0.449812

58C	-2.774263	-4.124435	-1.822323
59C	-2.796637	-5.519737	-1.812845
60C	-2.222751	-6.224287	-0.748796
61C	-1.625695	-5.533120	0.309417
62C	-1.598248	-4.136528	0.308064
63H	-2.632634	-1.365611	-3.109013
64H	-1.842405	0.083043	-2.417408
65H	-0.879502	-1.392926	-2.760734
66H	0.716158	-1.682299	-0.909885
67H	2.485039	-0.934131	0.644715
68H	1.886120	0.141937	2.795521
69H	-0.505199	0.503158	3.388816
70H	-2.290088	-0.223759	1.840496
71H	-3.489148	1.004429	-0.918934
72H	-5.658323	1.822544	-0.106710
73H	-7.236219	0.282446	1.054540
74H	-6.608688	-2.099741	1.412708
75H	-4.425876	-2.941206	0.614168
76H	-3.230502	-3.589536	-2.650504
77H	-3.261647	-6.054904	-2.636160
78H	-2.240089	-7.310992	-0.746405
79H	-1.178103	-6.077628	1.136271
80H	-1.129079	-3.606152	1.131363

6bc-PhNCO-007

1C	-1.765339	-2.314186	-2.721276
2C	-0.422030	-2.458077	-2.517714
3N	0.099070	-2.649153	-1.269229
4C	-0.751316	-2.769070	-0.212904
5C	-2.107076	-2.625770	-0.347915
6C	-2.687985	-2.315857	-1.623545
7N	-3.963065	-1.994326	-1.905607
8S	-5.068288	-1.807623	-0.705158
9O	-5.163028	-2.980379	0.203218
10O	-6.315195	-1.364221	-1.365700
11C	-4.468962	-0.423484	0.299383
12C	-4.319701	-0.578536	1.678794
13C	-3.863413	0.496911	2.442589
14C	-3.545445	1.728137	1.849066
15C	-3.702060	1.857904	0.459188
16C	-4.165953	0.793972	-0.317466
17C	-3.019119	2.864681	2.690097
18C	1.597878	-2.590862	-1.079107
19O	2.204023	-2.062371	-2.037803
20N	1.951117	-3.086241	0.075318
21C	3.263879	-3.032247	0.545130
22C	3.504146	-3.685937	1.776422
23C	4.759506	-3.667120	2.381210
24C	5.826748	-2.986979	1.778487
25C	5.608565	-2.338415	0.558448
26C	4.354148	-2.360291	-0.058669
27H	-2.141945	-2.151513	-3.725736
28H	0.304937	-2.401398	-3.317274
29H	-0.271211	-2.959834	0.736789
30H	-2.723390	-2.736706	0.533920
31H	-4.556594	-1.529871	2.144706
32H	-3.751007	0.376598	3.517917
33H	-3.464386	2.804519	-0.021065
34H	-4.290485	0.911004	-1.390346
35H	-3.041050	3.813841	2.146212
36H	-3.604327	2.979668	3.610300
37H	-1.979377	2.676399	2.988700
38H	2.672369	-4.202208	2.249904
39H	4.906681	-4.183201	3.327936
40H	6.807321	-2.968546	2.248088
41H	6.426267	-1.808628	0.072640
42H	4.209165	-1.857797	-1.005330
43P	1.057741	1.712465	-0.597826
44C	0.213802	0.854749	-1.949567
45C	1.012820	0.674444	0.883147
46C	2.771239	2.028386	-1.094301
47C	0.211109	3.274936	-0.241712
48C	-0.237986	0.250483	1.365050
49C	-0.301158	-0.533202	2.515894
50C	0.873497	-0.897970	3.183344
51C	2.115612	-0.478414	2.701442
52C	2.190842	0.310162	1.551575
53C	3.497561	1.001390	-1.724169
54C	4.824530	1.227281	-2.092894
55C	5.428087	2.463052	-1.837509
56C	4.704858	3.481032	-1.208051
57C	3.376073	3.268639	-0.834261
58C	-0.468210	3.958751	-1.263601
59C	-1.084771	5.180824	-0.988386
60C	-1.019711	5.726262	0.297919

61C	-0.340452	5.047719	1.314409
62C	0.273500	3.822223	1.050424
63H	0.250761	1.459151	-2.860170
64H	0.737686	-0.086861	-2.131032
65H	-0.824877	0.656668	-1.673602
66H	-1.156725	0.526546	0.855562
67H	-1.268549	-0.863776	2.882228
68H	0.819852	-1.520036	4.072827
69H	3.029720	-0.777534	3.204964
70H	3.160371	0.620187	1.175283
71H	3.049117	0.029270	-1.912506
72H	5.385311	0.432929	-2.577873
73H	6.461645	2.632082	-2.128210
74H	5.171992	4.441666	-1.009105
75H	2.820537	4.065886	-0.349506
76H	-0.526236	3.547939	-2.266797
77H	-1.616893	5.703223	-1.778531
78H	-1.504375	6.675848	0.509019
79H	-0.296474	5.465061	2.316428
80H	0.788116	3.295102	1.848669

6bc-PhNCO-008

1C	-2.644062	-3.306985	-1.118144
2C	-1.311628	-3.606169	-1.045201
3N	-0.507656	-3.069291	-0.082513
4C	-1.070625	-2.280339	0.872890
5C	-2.394220	-1.935090	0.853997
6C	-3.252112	-2.387060	-0.203308
7N	-4.528827	-2.039226	-0.448178
8S	-5.299891	-0.922362	0.476965
9O	-5.161102	-1.157197	1.938591
10O	-6.672403	-0.828474	-0.065825
11C	-4.499674	0.664357	0.129356
12C	-3.793751	1.334947	1.127891
13C	-3.225862	2.582015	0.847857
14C	-3.357224	3.169297	-0.417914
15C	-4.046191	2.457930	-1.416621
16C	-4.620075	1.215957	-1.151474
17C	-2.820787	4.552205	-0.698157
18C	0.987862	-3.299017	-0.153817
19O	1.345089	-4.112420	-1.023293
20N	1.614108	-2.564442	0.734897
21C	3.003885	-2.555657	0.840867
22C	3.535384	-1.993791	2.026570
23C	4.910044	-1.899901	2.238433
24C	5.809647	-2.352029	1.264065
25C	5.302213	-2.895616	0.078920
26C	3.925368	-3.002685	-0.137747
27H	-3.246341	-3.735949	-1.912235
28H	-0.810465	-4.256408	-1.750100
29H	-0.391716	-1.946413	1.642238
30H	-2.773000	-1.316856	1.655582
31H	-3.704343	0.898196	2.117129
32H	-2.686298	3.106799	1.632760
33H	-4.149404	2.892423	-2.408671
34H	-5.168080	0.686985	-1.925676
35H	-3.628721	5.294532	-0.640842
36H	-2.056562	4.846772	0.029150
37H	-2.393945	4.624953	-1.705388
38H	2.838763	-1.638418	2.782132
39H	5.281211	-1.471349	3.167428
40H	6.882609	-2.282208	1.426392
41H	5.986473	-3.248796	-0.690451
42H	3.552403	-3.437429	-1.056669
43P	1.506672	2.115453	-0.546464
44C	0.866870	3.668106	-1.234382
45C	0.833429	0.754104	-1.528918
46C	3.314859	2.114301	-0.634174
47C	0.940581	1.946893	1.164865
48C	-0.564386	0.614223	-1.610509
49C	-1.108362	-0.391267	-2.406565
50C	-0.266819	-1.261008	-3.109612
51C	1.120137	-1.134313	-3.010970
52C	1.677332	-0.125000	-2.222082
53C	3.982049	2.950682	-1.545269
54C	5.374743	2.902983	-1.635720
55C	6.101469	2.021706	-0.829029
56C	5.436493	1.186469	0.073772
57C	4.045797	1.230516	0.176739
58C	0.631353	3.083667	1.930824
59C	0.201777	2.930898	3.250062
60C	0.086297	1.652667	3.807295
61C	0.404622	0.524398	3.045982
62C	0.829941	0.663649	1.723696
63H	1.307908	4.532157	-0.730297

64H	1.093637	3.706913	-2.303237
65H	-0.217613	3.678881	-1.105038
66H	-1.226518	1.269821	-1.050489
67H	-2.186240	-0.508527	-2.459955
68H	-0.695641	-2.052304	-3.717625
69H	1.771797	-1.829454	-3.531870
70H	2.756346	-0.037178	-2.141379
71H	3.433209	3.636678	-2.182949
72H	5.888759	3.553325	-2.338236
73H	7.184931	1.984337	-0.905503
74H	5.991099	0.490123	0.694749
75H	3.546084	0.569675	0.878403
76H	0.715415	4.081844	1.511099
77H	-0.045762	3.809393	3.839705
78H	-0.252716	1.537326	4.833385
79H	0.318595	-0.469577	3.476413
80H	1.068022	-0.225076	1.143533

6bc-PhNCO-009

1C	-2.130414	-0.657699	-2.581410
2C	-0.872374	-1.138325	-2.356793
3N	-0.600334	-1.988804	-1.323213
4C	-1.626270	-2.394372	-0.522328
5C	-2.909928	-1.950759	-0.695070
6C	-3.230476	-1.012581	-1.733643
7N	-4.405798	-0.415655	-1.997857
8S	-5.736196	-0.654367	-1.061180
9O	-5.965833	-2.075841	-0.692533
10O	-6.838866	0.055230	-1.745050
11C	-5.409380	0.242258	0.472418
12C	-5.156886	-0.449463	1.656357
13C	-4.871940	0.269146	2.822847
14C	-4.834872	1.669743	2.820748
15C	-5.101488	2.342955	1.614007
16C	-5.387617	1.642304	0.444855
17C	-4.506162	2.449170	4.070617
18C	0.814110	-2.461533	-1.117454
19O	1.620110	-2.085371	-1.997464
20N	0.940349	-3.154934	-0.016588
21C	2.133478	-3.806642	0.301805
22C	2.357460	-4.101406	1.665421
23C	3.485101	-4.809887	2.080519
24C	4.425448	-5.259937	1.144824
25C	4.214476	-4.981769	-0.211113
26C	3.094787	-4.260159	-0.632513
27H	-2.301452	0.030050	-3.402864
28H	-0.021206	-0.873190	-2.969025
29H	-1.345561	-3.084781	0.261352
30H	-3.675192	-2.328540	-0.031824
31H	-5.193521	-1.533821	1.671382
32H	-4.677335	-0.272098	3.745988
33H	-5.084750	3.430826	1.593909
34H	-5.595365	2.172939	-0.479692
35H	-3.568275	3.007191	3.948588
36H	-5.289674	3.182854	4.297911
37H	-4.395269	1.790814	4.938574
38H	1.620736	-3.765295	2.391541
39H	3.627460	-5.017755	3.139138
40H	5.301015	-5.819526	1.464849
41H	4.931441	-5.327628	-0.953373
42H	2.952221	-4.048859	-1.685754
43P	2.665327	1.586709	-0.722267
44C	2.727609	0.972981	-2.427030
45C	0.983362	1.372120	-0.089412
46C	3.846746	0.663140	0.291954
47C	3.079478	3.351590	-0.686194
48C	-0.054880	2.108252	-0.687825
49C	-1.364638	1.942226	-0.241841
50C	-1.642270	1.045953	0.795882
51C	-0.610665	0.316730	1.390164
52C	0.706023	0.474616	0.952088
53C	3.950336	-0.729609	0.130961
54C	4.828541	-1.451469	0.940889
55C	5.603437	-0.792715	1.900281
56C	5.501889	0.593452	2.057145
57C	4.623137	1.325979	1.257078
58C	4.001236	3.876005	-1.607581
59C	4.351360	5.226155	-1.545683
60C	3.792094	6.052767	-0.565778
61C	2.879307	5.530244	0.355941
62C	2.520786	4.182136	0.299667
63H	3.751334	1.025417	-2.808276
64H	2.385643	-0.068158	-2.429493
65H	2.065284	1.580893	-3.050943
66H	0.156127	2.804458	-1.495821

67H	-2.171714	2.496429	-0.712250
68H	-2.665134	0.906412	1.127140
69H	-0.829743	-0.391751	2.183887
70H	1.498726	-0.108392	1.409765
71H	3.344988	-1.257681	-0.600793
72H	4.893943	-2.528139	0.824173
73H	6.285062	-1.361005	2.527967
74H	6.104830	1.106649	2.801470
75H	4.549132	2.401800	1.384309
76H	4.449043	3.244492	-2.369438
77H	5.059957	5.630362	-2.263353
78H	4.065943	7.103583	-0.522202
79H	2.442581	6.170506	1.117434
80H	1.805507	3.784197	1.013770

6bc-PhNCO-010

1C	-2.362597	-3.551058	-1.110160
2C	-1.025370	-3.833510	-1.123258
3N	-0.160857	-3.257350	-0.238000
4C	-0.655206	-2.390511	0.687534
5C	-1.981623	-2.057377	0.750623
6C	-2.922500	-2.616263	-0.178685
7N	-4.238654	-2.364977	-0.297265
8S	-4.999117	-1.249858	0.638093
9O	-4.634172	-1.317370	2.078435
10O	-6.435319	-1.352046	0.300632
11C	-4.427659	0.350712	0.027556
12C	-3.648334	1.176662	0.835098
13C	-3.189215	2.395140	0.326011
14C	-3.492976	2.796434	-0.981027
15C	-4.290237	1.948821	-1.772016
16C	-4.758523	0.733433	-1.278007
17C	-2.955361	4.089222	-1.545018
18C	1.317042	-3.558950	-0.353852
19O	1.625284	-4.249747	-1.340290
20N	1.995931	-3.021339	0.632124
21C	3.390414	-3.068500	0.653615
22C	4.014154	-2.904020	1.911921
23C	5.401312	-2.835033	2.035523
24C	6.220027	-2.918894	0.901474
25C	5.619779	-3.084684	-0.351923
26C	4.230070	-3.164560	-0.482126
27H	-3.016546	-4.028184	-1.832518
28H	-0.569955	-4.512200	-1.832285
29H	0.084040	-1.987997	1.364874
30H	-2.302898	-1.371391	1.522064
31H	-3.405774	0.877007	1.849079
32H	-2.579538	3.035378	0.957051
33H	-4.545571	2.246462	-2.786946
34H	-5.373129	0.086664	-1.897193
35H	-3.744221	4.668207	-2.040280
36H	-2.512525	4.715592	-0.763044
37H	-2.179211	3.894142	-2.297805
38H	3.379779	-2.827369	2.792317
39H	5.846314	-2.713839	3.021213
40H	7.302005	-2.864994	0.994333
41H	6.239461	-3.159172	-1.243769
42H	3.786387	-3.307541	-1.459891
43P	1.927501	1.407699	0.286645
44C	3.074947	0.291906	1.135775
45C	1.030623	0.495126	-0.988297
46C	0.756427	2.063757	1.505768
47C	2.848236	2.773527	-0.466666
48C	1.686648	-0.509006	-1.720413
49C	0.995042	-1.193578	-2.719612
50C	-0.343260	-0.885905	-2.985350
51C	-0.995264	0.111975	-2.255783
52C	-0.310549	0.807296	-1.258246
53C	0.126719	1.168776	2.388363
54C	-0.783839	1.648847	3.329551
55C	-1.064186	3.018268	3.398961
56C	-0.437695	3.908406	2.522170
57C	0.469920	3.435627	1.570534
58C	3.828990	3.443385	0.285745
59C	4.530359	4.506411	-0.283704
60C	4.257357	4.904291	-1.597757
61C	3.281666	4.238685	-2.345078
62C	2.574316	3.172748	-1.783715
63H	3.551970	0.821255	1.965256
64H	2.514844	-0.567219	1.511441
65H	3.838295	-0.057683	0.436515
66H	2.717437	-0.775211	-1.507471
67H	1.493034	-1.989038	-3.264761
68H	-0.883421	-1.438376	-3.749190
69H	-2.040251	0.338782	-2.442430

70H	-0.829649	1.567380	-0.683753
71H	0.340148	0.104470	2.344871
72H	-1.273406	0.954146	4.006303
73H	-1.774422	3.388597	4.133218
74H	-0.657874	4.971208	2.572329
75H	0.951995	4.133063	0.891954
76H	4.045480	3.142411	1.307467
77H	5.290589	5.021679	0.296839
78H	4.807798	5.731103	-2.038789
79H	3.071300	4.543194	-3.366619
80H	1.821666	2.655057	-2.370938

6bc-PhNCO-011

1C	1.565530	-0.663542	-0.584155
2C	0.367644	-1.317611	-0.689109
3N	-0.409700	-1.241933	-1.803143
4C	0.043478	-0.527486	-2.873631
5C	1.237454	0.140112	-2.838570
6C	2.061944	0.134725	-1.666898
7N	3.188550	0.870813	-1.711469
8S	4.129712	1.057560	-0.381058
9O	3.344517	1.452441	0.820857
10O	5.228165	1.961617	-0.788635
11C	4.863991	-0.551748	-0.020899
12C	4.757266	-1.101566	1.255541
13C	5.332952	-2.350131	1.511809
14C	6.008276	-3.057022	0.507457
15C	6.098847	-2.478700	-0.771947
16C	5.535152	-1.233912	-1.042054
17C	6.628060	-4.406951	0.776594
18C	-1.792636	-1.868576	-1.861918
19O	-2.334852	-1.805871	-2.980676
20N	-2.152312	-2.306662	-0.681849
21C	-3.404386	-2.873555	-0.448972
22C	-3.748986	-3.070677	0.909387
23C	-4.980873	-3.604813	1.281658
24C	-5.914411	-3.979448	0.305838
25C	-5.583804	-3.809357	-1.042829
26C	-4.354372	-3.263706	-1.424417
27H	2.107006	-0.750553	0.347543
28H	-0.042503	-1.918088	0.108662
29H	-0.615280	-0.521297	-3.732475
30H	1.556971	0.710320	-3.704517
31H	4.226258	-0.563454	2.034377
32H	5.250545	-2.779766	2.507608
33H	6.617249	-3.013587	-1.564992
34H	5.607049	-0.799792	-2.035217
35H	7.716193	-4.375986	0.634137
36H	6.431373	-4.744385	1.799725
37H	6.234886	-5.165370	0.087622
38H	-3.025056	-2.781824	1.667950
39H	-5.214250	-3.731939	2.337083
40H	-6.875904	-4.399129	0.592044
41H	-6.293306	-4.102008	-1.814895
42H	-4.123068	-3.129051	-2.473399
43P	-1.761895	2.352469	1.283073
44C	-2.296469	3.602330	2.489981
45C	-0.837101	3.198557	-0.024387
46C	-0.736614	1.134340	2.143696
47C	-3.209954	1.548039	0.560245
48C	0.500631	2.890305	-0.307802
49C	1.164331	3.579503	-1.327467
50C	0.499991	4.566145	-2.058092
51C	-0.837242	4.872925	-1.775540
52C	-1.508859	4.192135	-0.761873
53C	-1.086177	-0.224228	2.123252
54C	-0.302004	-1.147492	2.818260
55C	0.827563	-0.722486	3.522439
56C	1.179328	0.632173	3.536537
57C	0.398991	1.563866	2.853376
58C	-3.137825	1.041026	-0.747717
59C	-4.234443	0.374253	-1.293488
60C	-5.398960	0.208483	-0.539691
61C	-5.473028	0.711896	0.763034
62C	-4.380522	1.378319	1.319810
63H	-2.975395	4.312333	2.008723
64H	-2.795979	3.121487	3.335561
65H	-1.411203	4.134590	2.850906
66H	1.037194	2.128408	0.247538
67H	2.194295	3.322837	-1.553545
68H	1.021021	5.094715	-2.852136
69H	-1.357063	5.637733	-2.346338
70H	-2.550902	4.423780	-0.556795
71H	-1.942544	-0.570854	1.554036
72H	-0.569534	-2.200390	2.791732

73H	1.440329	-1.446538	4.053220
74H	2.067480	0.962969	4.067073
75H	0.687511	2.611430	2.858006
76H	-2.231617	1.154628	-1.335494
77H	-4.158832	-0.046461	-2.290843
78H	-6.243027	-0.329208	-0.961820
79H	-6.376455	0.574926	1.350935
80H	-4.445395	1.753757	2.336952

6bc-PhNCO-012

1C	-1.565227	0.676388	-0.582979
2C	-0.367471	1.330689	-0.688526
3N	0.412288	1.249962	-1.800575
4C	-0.039063	0.531655	-2.869250
5C	-1.232620	-0.136601	-2.833466
6C	-2.058067	-0.128400	-1.662503
7N	-3.182040	-0.868612	-1.704581
8S	-4.119420	-1.058714	-0.372001
9O	-3.328511	-1.436023	0.831766
10O	-5.206527	-1.979339	-0.772933
11C	-4.875219	0.542499	-0.021197
12C	-4.772228	1.103556	1.250874
13C	-5.374866	2.340090	1.502753
14C	-6.073294	3.024301	0.498267
15C	-6.157770	2.436179	-0.776823
16C	-5.566950	1.202912	-1.042668
17C	-6.710344	4.367534	0.760031
18C	1.796219	1.874187	-1.858749
19O	2.338062	1.812188	-2.977739
20N	2.157238	2.309489	-0.677979
21C	3.410559	2.873774	-0.445130
22C	3.756779	3.067645	0.913283
23C	4.990145	3.598522	1.285402
24C	5.923555	3.973111	0.309465
25C	5.591293	3.806410	-1.039227
26C	4.360406	3.264010	-1.420696
27H	-2.109417	0.767854	0.346745
28H	0.040617	1.935156	0.107311
29H	0.621069	0.522564	-3.727011
30H	-1.550303	-0.710653	-3.697542
31H	-4.226877	0.581257	2.030620
32H	-5.297961	2.777033	2.495844
33H	-6.695705	2.952409	-1.569131
34H	-5.637852	0.759183	-2.031654
35H	-7.743928	4.394163	0.393827
36H	-6.721418	4.607587	1.828576
37H	-6.163957	5.167381	0.242195
38H	3.033107	2.778894	1.672128
39H	5.224775	3.723037	2.340861
40H	6.886223	4.390138	0.595600
41H	6.300659	4.099080	-1.811414
42H	4.127869	3.131862	-2.469720
43P	1.770129	-2.345946	1.280086
44C	2.305050	-3.594807	2.487887
45C	0.842047	-3.192763	-0.024527
46C	0.748299	-1.125002	2.140809
47C	3.218042	-1.544437	0.553786
48C	-0.496634	-2.885205	-0.304077
49C	-1.163401	-3.575906	-1.320745
50C	-0.501039	-4.563160	-2.052323
51C	0.837270	-4.869012	-1.773838
52C	1.511885	-4.186843	-0.763095
53C	1.098035	0.233400	2.114670
54C	0.317376	1.158792	2.810813
55C	-0.808972	0.736153	3.521508
56C	-1.161282	-0.618303	3.540730
57C	-0.384352	-1.552147	2.856632
58C	3.143500	-1.036902	-0.753853
59C	4.239985	-0.372102	-1.302249
60C	5.406832	-0.208877	-0.551463
61C	5.483217	-0.712603	0.750979
62C	4.390773	-1.376899	1.310445
63H	2.981829	-4.306668	2.006324
64H	2.807070	-3.113493	3.331719
65H	1.419741	-4.125191	2.851429
66H	-1.031474	-2.122579	0.251991
67H	-2.194138	-3.319824	-1.543960
68H	-1.024443	-5.092895	-2.844032
69H	1.355557	-5.634206	-2.345513
70H	2.554674	-4.417862	-0.561057
71H	1.951216	0.578553	1.539804
72H	0.585086	2.211543	2.779817
73H	-1.418864	1.461850	4.053363
74H	-2.047218	-0.947302	4.076055
75H	-0.673368	-2.599545	2.865244

76H	2.235508	-1.148500	-1.339289
77H	4.162498	0.049177	-2.299207
78H	6.250934	0.327055	-0.975752
79H	6.388376	-0.577492	1.336634
80H	4.457492	-1.752463	2.327412

6bc-PhNCO-013

1C	-3.174737	0.003430	-0.664888
2C	-2.270662	0.958677	-1.049554
3N	-1.236567	1.348344	-0.256523
4C	-1.110844	0.785053	0.983296
5C	-1.979061	-0.170362	1.427842
6C	-3.064879	-0.637717	0.613970
7N	-3.844313	-1.595954	1.144568
8S	-5.114087	-2.225034	0.310353
9O	-5.679627	-3.281910	1.177834
10O	-4.764978	-2.608700	-1.083946
11C	-6.344205	-0.907773	0.201639
12C	-6.856366	-0.359729	1.383876
13C	-7.788839	0.671857	1.307037
14C	-8.228039	1.167084	0.065145
15C	-7.704789	0.595039	-1.101959
16C	-6.764358	-0.438679	-1.041743
17C	-9.227605	2.296690	0.007547
18C	-0.206744	2.307120	-0.812369
19O	-0.425290	2.677930	-1.980732
20N	0.748970	2.525761	0.057292
21C	1.879391	3.277131	-0.253500
22C	2.196588	3.863722	-1.505506
23C	3.405644	4.544075	-1.687673
24C	4.331945	4.668922	-0.647189
25C	4.027822	4.100232	0.597589
26C	2.828240	3.419244	0.788958
27H	-3.952358	-0.271280	-1.363777
28H	-2.315260	1.447440	-2.013989
29H	-0.275929	1.150287	1.564151
30H	-1.845792	-0.595209	2.417446
31H	-6.525534	-0.732412	2.348965
32H	-8.186491	1.101565	2.224157
33H	-8.032564	0.958746	-2.073149
34H	-6.362316	-0.875780	-1.950404
35H	-9.501082	2.541472	-1.024269
36H	-10.146256	2.041255	0.550996
37H	-8.820415	3.203980	0.472738
38H	1.490232	3.784197	-2.321720
39H	3.620934	4.984551	-2.659664
40H	5.267378	5.202022	-0.799457
41H	4.733465	4.182583	1.422001
42H	2.604770	2.958949	1.747658
43P	3.866612	-0.529114	-0.321093
44C	4.606503	0.839855	-1.250250
45C	5.030939	-1.920921	-0.310634
46C	3.563418	0.008739	1.379887
47C	2.325858	-1.057761	-1.102898
48C	5.303421	-2.627838	0.870194
49C	6.182049	-3.714080	0.839911
50C	6.785654	-4.095398	-0.361403
51C	6.510116	-3.393066	-1.540590
52C	5.633148	-2.308575	-1.520331
53C	2.304145	-0.161852	1.969918
54C	2.088608	0.279448	3.277499
55C	3.124188	0.885424	3.993070
56C	4.383754	1.051826	3.404079
57C	4.607332	0.616138	2.099101
58C	1.589622	-0.170453	-1.904149
59C	0.378244	-0.588136	-2.458061
60C	-0.110106	-1.871801	-2.200037
61C	0.622276	-2.754616	-1.398749
62C	1.843093	-2.354942	-0.855173
63H	4.772909	0.537918	-2.288056
64H	3.944656	1.708301	-1.217609
65H	5.562740	1.098944	-0.787287
66H	4.839303	-2.336632	1.807709
67H	6.392075	-4.259328	1.756052
68H	7.470205	-4.939347	-0.380966
69H	6.976682	-3.690053	-2.475834
70H	5.417502	-1.775131	-2.442449
71H	1.491509	-0.615992	1.413225
72H	1.108759	0.156574	3.730504
73H	2.951045	1.233337	5.007956
74H	5.188185	1.527960	3.957809
75H	5.583758	0.758780	1.643758
76H	1.934483	0.842197	-2.087215
77H	-0.190802	0.107286	-3.066535
78H	-1.065250	-2.183001	-2.613915

79H	0.242169	-3.751738	-1.194984
80H	2.411462	-3.046834	-0.239104

6bc-PhNCO-014

1C	-1.644965	1.166348	0.075461
2C	-0.500558	1.483836	-0.603302
3N	0.432407	2.338854	-0.107607
4C	0.169488	2.986125	1.068173
5C	-0.970488	2.737457	1.779420
6C	-1.909705	1.739208	1.361095
7N	-2.912173	1.448531	2.211745
8S	-3.884565	0.154773	1.941775
9O	-4.809911	0.091746	3.095129
10O	-3.111934	-1.079083	1.630330
11C	-4.878704	0.523346	0.477499
12C	-5.504509	1.770089	0.368577
13C	-6.270237	2.050848	-0.761218
14C	-6.429398	1.102337	-1.787934
15C	-5.793522	-0.139272	-1.650703
16C	-5.017308	-0.434512	-0.525953
17C	-7.262955	1.428085	-3.003591
18C	1.759543	2.443514	-0.821473
19O	1.822704	1.784040	-1.882566
20N	2.605403	3.175694	-0.147703
21C	3.917466	3.384991	-0.573986
22C	4.470238	3.032714	-1.830456
23C	5.807831	3.315935	-2.124659
24C	6.637184	3.947539	-1.192098
25C	6.103176	4.304131	0.053583
26C	4.769837	4.030539	0.353571
27H	-2.308781	0.438175	-0.369120
28H	-0.254249	1.050144	-1.560053
29H	0.938596	3.671235	1.396485
30H	-1.134529	3.251992	2.720497
31H	-5.385543	2.513795	1.151537
32H	-6.753241	3.021767	-0.850093
33H	-5.902344	-0.887107	-2.433251
34H	-4.513615	-1.391184	-0.433239
35H	-7.269885	0.600657	-3.721158
36H	-8.302630	1.641330	-2.723310
37H	-6.879600	2.318971	-3.517429
38H	3.844671	2.546185	-2.567904
39H	6.203153	3.039071	-3.100518
40H	7.675727	4.163217	-1.431356
41H	6.728076	4.801547	0.792717
42H	4.353685	4.313327	1.317894
43P	1.884689	-1.934253	-0.479185
44C	3.079470	-1.227870	-1.644936
45C	2.452472	-3.586994	0.013705
46C	1.763355	-0.885608	0.991058
47C	0.280897	-2.116927	-1.303346
48C	2.736456	-3.890550	1.352593
49C	3.184019	-5.170937	1.691175
50C	3.347049	-6.142717	0.700627
51C	3.061934	-5.839464	-0.636363
52C	2.613952	-4.565162	-0.982920
53C	0.590060	-0.881653	1.764958
54C	0.544980	-0.137601	2.943807
55C	1.658079	0.604697	3.350217
56C	2.818716	0.614997	2.572036
57C	2.877792	-0.129962	1.393319
58C	-0.014735	-1.368406	-2.454124
59C	-1.265040	-1.500237	-3.061729
60C	-2.218709	-2.371175	-2.526124
61C	-1.922550	-3.121460	-1.383668
62C	-0.673648	-3.002235	-0.773795
63H	3.058586	-1.808924	-2.571507
64H	2.823638	-0.180718	-1.843906
65H	4.081873	-1.289925	-1.212367
66H	2.609915	-3.140396	2.127344
67H	3.401327	-5.405578	2.729604
68H	3.693236	-7.137534	0.968490
69H	3.184237	-6.595545	-1.407164
70H	2.382055	-4.338022	-2.020587
71H	-0.293882	-1.429524	1.453801
72H	-0.371376	-0.119780	3.526218
73H	1.611212	1.193517	4.262373
74H	3.674906	1.214405	2.867820
75H	3.783058	-0.103622	0.795003
76H	0.710458	-0.676910	-2.871017
77H	-1.493262	-0.916553	-3.949329
78H	-3.191516	-2.466951	-3.000754
79H	-2.662135	-3.796613	-0.962901
80H	-0.447233	-3.596164	0.107399

6bc-PhNCO-015

1C	1.586207	1.474660	-0.856119
2C	2.652016	0.629660	-1.033870
3N	2.946366	-0.366609	-0.159003
4C	2.173382	-0.513543	0.955921
5C	1.101972	0.300406	1.196643
6C	0.729786	1.336903	0.281215
7N	-0.372341	2.050122	0.595598
8S	-0.892457	3.296209	-0.330713
9O	-2.162534	3.737357	0.296682
10O	-0.946431	2.984275	-1.784191
11C	0.306889	4.623478	-0.113701
12C	0.473638	5.181601	1.159595
13C	1.422230	6.184197	1.343032
14C	2.214229	6.642594	0.273719
15C	2.022284	6.070129	-0.990567
16C	1.073809	5.061950	-1.191866
17C	3.240640	7.725720	0.499638
18C	4.107196	-1.299779	-0.475444
19O	4.764034	-0.970846	-1.480194
20N	4.157847	-2.285878	0.383102
21C	5.134158	-3.281740	0.317422
22C	6.232589	-3.340003	-0.576031
23C	7.140273	-4.402530	-0.518693
24C	6.992866	-5.434323	0.414042
25C	5.911280	-5.389421	1.304180
26C	5.003860	-4.332921	1.256807
27H	1.390496	2.217643	-1.616513
28H	3.311222	0.693196	-1.889972
29H	2.468304	-1.319361	1.613398
30H	0.509229	0.146647	2.091474
31H	-0.130404	4.834601	1.992890
32H	1.554344	6.620681	2.330892
33H	2.620655	6.411799	-1.831973
34H	0.928241	4.626185	-2.175130
35H	3.783773	7.965258	-0.420605
36H	2.767614	8.646871	0.863880
37H	3.974444	7.419895	1.256337
38H	6.363906	-2.553849	-1.308456
39H	7.975202	-4.420229	-1.217067
40H	7.704862	-6.255566	0.448578
41H	5.776830	-6.179587	2.040353
42H	4.167040	-4.295728	1.950882
43P	-3.356396	-0.748619	-0.117218
44C	-3.974484	0.935223	-0.367992
45C	-3.061259	-1.017995	1.650852
46C	-4.630495	-1.907697	-0.691917
47C	-1.825666	-1.034431	-1.035753
48C	-3.460094	-2.210441	2.275322
49C	-3.180654	-2.408101	3.629568
50C	-2.507197	-1.422569	4.357995
51C	-2.105664	-0.237614	3.731715
52C	-2.376252	-0.029498	2.378420
53C	-4.331895	-2.910345	-1.626306
54C	-5.338723	-3.780065	-2.054989
55C	-6.637192	-3.653057	-1.554766
56C	-6.935541	-2.653777	-0.620804
57C	-5.937318	-1.781044	-0.188232
58C	-1.556415	-0.326346	-2.217907
59C	-0.404321	-0.620385	-2.947817
60C	0.474722	-1.614835	-2.507720
61C	0.209804	-2.315044	-1.327142
62C	-0.937717	-2.026570	-0.587611
63H	-3.256305	1.673739	-0.003035
64H	-4.166853	1.104198	-1.431309
65H	-4.912341	1.039026	0.186357
66H	-3.984724	-2.979631	1.716268
67H	-3.489579	-3.331152	4.112522
68H	-2.292037	-1.579041	5.411868
69H	-1.575105	0.526895	4.293034
70H	-2.025449	0.877713	1.893181
71H	-3.326529	-3.015766	-2.022089
72H	-5.104553	-4.554607	-2.780140
73H	-7.417502	-4.330541	-1.891368
74H	-7.944323	-2.553563	-0.229749
75H	-6.175914	-1.011228	0.541045
76H	-2.217449	0.461945	-2.560738
77H	-0.185276	-0.056466	-3.850111
78H	1.378234	-1.830214	-3.071790
79H	0.904816	-3.070015	-0.971136
80H	-1.130927	-2.564210	0.336585

6bc-PhNCO-016

1C	2.820236	0.266728	-0.014024
2C	1.857176	1.238621	-0.043451
3N	1.045948	1.488584	1.021545
4C	1.234590	0.782871	2.174500
5C	2.171487	-0.208801	2.264218
6C	2.988696	-0.565009	1.142387
7N	3.798985	-1.628360	1.297687
8S	4.716782	-2.187558	0.056320
9O	3.962952	-2.301184	-1.222580
10O	5.368963	-3.416864	0.559204
11C	6.016539	-0.962010	-0.204934
12C	6.203518	-0.387649	-1.460986
13C	7.222359	0.554825	-1.637375
14C	8.051695	0.933302	-0.573178
15C	7.839521	0.338158	0.684112
16C	6.833016	-0.605005	0.875001
17C	9.151873	1.950662	-0.755700
18C	-0.111692	2.454698	0.940167
19O	-0.616918	2.751870	2.040319
20N	-0.389662	2.744920	-0.306977
21C	-1.471510	3.546857	-0.662449
22C	-1.729979	3.643423	-2.051990
23C	-2.819035	4.357534	-2.545809
24C	-3.694179	5.012854	-1.667998
25C	-3.443178	4.947302	-0.293710
26C	-2.352915	4.231683	0.212216
27H	3.406916	0.108768	-0.908121
28H	1.663915	1.843699	-0.918416
29H	0.577016	1.053260	2.990399
30H	2.274799	-0.765810	3.189614
31H	5.563014	-0.674019	-2.289367
32H	7.369545	1.000400	-2.618604
33H	8.474471	0.618269	1.522080
34H	6.680089	-1.057376	1.850570
35H	10.126385	1.531971	-0.473771
36H	9.217444	2.292180	-1.794125
37H	8.983916	2.830515	-0.121009
38H	-1.056912	3.124577	-2.730804
39H	-2.989059	4.402560	-3.619791
40H	-4.546201	5.570414	-2.049498
41H	-4.104946	5.459916	0.402195
42H	-2.179963	4.190131	1.279919
43P	-3.649492	-0.510778	-0.295598
44C	-4.137136	1.093254	-0.984322
45C	-4.789723	-1.786456	-0.895913
46C	-1.964481	-0.924627	-0.799873
47C	-3.736478	-0.421057	1.510178
48C	-4.303606	-3.033367	-1.317800
49C	-5.198206	-4.014151	-1.753572
50C	-6.571527	-3.755059	-1.769149
51C	-7.057056	-2.511991	-1.347246
52C	-6.171341	-1.526763	-0.909620
53C	-1.126924	-1.635080	0.076660
54C	0.148634	-2.014955	-0.341646
55C	0.592703	-1.689747	-1.626828
56C	-0.240308	-0.979039	-2.496930
57C	-1.518557	-0.593606	-2.089877
58C	-4.391213	-1.412047	2.257510
59C	-4.406644	-1.325059	3.651960
60C	-3.770237	-0.259393	4.296443
61C	-3.114938	0.725225	3.548561
62C	-3.096291	0.649676	2.156149
63H	-5.135825	1.347314	-0.618136
64H	-3.429504	1.858922	-0.659269
65H	-4.150438	1.042979	-2.076146
66H	-3.237623	-3.240790	-1.312181
67H	-4.819046	-4.977776	-2.082499
68H	-7.264140	-4.519495	-2.111236
69H	-8.124331	-2.308504	-1.358714
70H	-6.559324	-0.567713	-0.577324
71H	-1.460083	-1.879315	1.081366
72H	0.805932	-2.546548	0.340062
73H	1.597295	-1.972046	-1.928814
74H	0.108592	-0.711474	-3.490672
75H	-2.152874	-0.035468	-2.772379
76H	-4.884297	-2.242958	1.761905
77H	-4.913487	-2.091556	4.231956
78H	-3.782299	-0.197592	5.381547
79H	-2.610810	1.551814	4.040849
80H	-2.570515	1.415946	1.595871

6bc-PhNCO-017

1C	-2.503835	0.319362	0.025107
2C	-1.407803	1.119595	-0.158160

3N	-0.561533	0.962969	-1.213762
4C	-0.835410	-0.004902	-2.137082
5C	-1.908972	-0.840446	-2.009146
6C	-2.800150	-0.744205	-0.891899
7N	-3.791089	-1.651745	-0.832561
8S	-4.847984	-1.684157	0.423281
9O	-4.174751	-1.622912	1.749471
10O	-5.731172	-2.845589	0.176250
11C	-5.861840	-0.198402	0.274326
12C	-5.941549	0.710246	1.328312
13C	-6.728232	1.857855	1.183951
14C	-7.431534	2.110324	-0.001493
15C	-7.334227	1.175239	-1.048417
16C	-6.559691	0.025334	-0.918610
17C	-8.264311	3.357632	-0.171255
18C	0.683566	1.808177	-1.392418
19O	1.250160	1.653077	-2.490754
20N	0.922580	2.531285	-0.327122
21C	2.032100	3.372597	-0.239322
22C	2.050091	4.263028	0.860438
23C	3.116659	5.132496	1.080501
24C	4.217833	5.138179	0.213357
25C	4.221206	4.259423	-0.875636
26C	3.151324	3.389691	-1.108388
27H	-3.115216	0.489915	0.900406
28H	-1.138949	1.912067	0.526862
29H	-0.139692	-0.059082	-2.963754
30H	-2.080737	-1.609155	-2.755242
31H	-5.395754	0.524301	2.248142
32H	-6.790466	2.566214	2.007017
33H	-7.874637	1.352405	-1.975990
34H	-6.492626	-0.688269	-1.734707
35H	-9.287072	3.111700	-0.483284
36H	-8.322133	3.933266	0.758625
37H	-7.838658	4.010066	-0.945243
38H	1.201610	4.251497	1.540713
39H	3.091305	5.806572	1.934456
40H	5.052462	5.814260	0.382548
41H	5.068077	4.248586	-1.559615
42H	3.171276	2.722092	-1.960201
43P	3.376495	-2.117810	0.586550
44C	4.257521	-3.607295	1.140838
45C	3.813629	-1.778926	-1.134779
46C	1.599426	-2.427857	0.728881
47C	3.854241	-0.721829	1.634767
48C	2.913906	-1.068548	-1.943415
49C	3.269995	-0.732441	-3.250040
50C	4.514001	-1.118898	-3.756300
51C	5.410826	-1.832383	-2.952549
52C	5.069388	-2.158757	-1.639283
53C	0.785453	-1.622628	1.540147
54C	-0.571160	-1.928915	1.672844
55C	-1.116502	-3.023185	0.997764
56C	-0.307026	-3.815722	0.176144
57C	1.049711	-3.524409	0.039625
58C	4.025558	0.553767	1.075522
59C	4.353054	1.633142	1.897986
60C	4.512130	1.442035	3.272927
61C	4.341742	0.170310	3.832527
62C	4.010747	-0.914243	3.019432
63H	5.334065	-3.419963	1.178842
64H	3.900424	-3.883183	2.136944
65H	4.046800	-4.427092	0.447909
66H	1.947334	-0.763890	-1.558656
67H	2.577447	-0.152915	-3.851666
68H	4.789300	-0.858690	-4.775020
69H	6.379288	-2.130843	-3.344872
70H	5.780543	-2.700615	-1.022938
71H	1.198742	-0.762708	2.058668
72H	-1.208591	-1.304888	2.290733
73H	-2.175210	-3.238187	1.097482
74H	-0.735582	-4.656526	-0.362318
75H	1.671728	-4.142768	-0.603211
76H	3.901628	0.717572	0.009939
77H	4.471194	2.618480	1.459499
78H	4.764625	2.285518	3.910127
79H	4.462315	0.021921	4.902215
80H	3.870700	-1.894786	3.466016

6bc-PhNCO-018

1C	0.738346	1.926825	-0.624196
2C	2.086670	1.808805	-0.846902
3N	2.895468	1.067260	-0.045955
4C	2.355935	0.449978	1.045314
5C	1.022781	0.539028	1.331415

6C	0.123262	1.261304	0.483511
7N	-1.180676	1.225425	0.825790
8S	-2.333970	1.944905	-0.087143
9O	-3.621658	1.591170	0.555516
10O	-2.206267	1.647981	-1.538622
11C	-2.101886	3.723291	0.107733
12C	-2.130391	4.275246	1.394059
13C	-1.929671	5.644371	1.551405
14C	-1.702654	6.479889	0.441913
15C	-1.684913	5.901344	-0.834201
16C	-1.880354	4.527514	-1.008929
17C	-1.489040	7.961716	0.635814
18C	4.354850	0.894426	-0.439602
19O	4.694659	1.559592	-1.435552
20N	4.955029	0.046790	0.356378
21C	6.293410	-0.311830	0.189657
22C	7.170344	0.123462	-0.835188
23C	8.492085	-0.331274	-0.881985
24C	8.987860	-1.222144	0.075371
25C	8.132387	-1.660192	1.095558
26C	6.813194	-1.214245	1.149078
27H	0.153070	2.503524	-1.327262
28H	2.583714	2.279094	-1.685568
29H	3.056297	-0.117144	1.641935
30H	0.631564	0.029806	2.205566
31H	-2.302058	3.641116	2.259177
32H	-1.947255	6.075035	2.550357
33H	-1.511262	6.527401	-1.706366
34H	-1.858321	4.085429	-1.999975
35H	-1.238043	8.459975	-0.306658
36H	-2.391221	8.439918	1.039559
37H	-0.676807	8.154332	1.348027
38H	6.808258	0.815354	-1.584685
39H	9.141999	0.020869	-1.681219
40H	10.018202	-1.566855	0.030325
41H	8.495961	-2.351898	1.853034
42H	6.150455	-1.554515	1.941838
43P	-2.032453	-3.308766	-0.184791
44C	-1.974944	-5.108244	-0.435927
45C	-3.354127	-2.603543	-1.202869
46C	-2.319759	-2.967162	1.569653
47C	-0.432414	-2.628095	-0.695972
48C	-3.967348	-1.399321	-0.822678
49C	-4.939376	-0.827946	-1.645243
50C	-5.308348	-1.454875	-2.837967
51C	-4.698141	-2.655408	-3.218284
52C	-3.717866	-3.230472	-2.408604
53C	-2.025556	-1.688460	2.069032
54C	-2.278481	-1.396162	3.409805
55C	-2.810637	-2.374005	4.255481
56C	-3.100023	-3.649292	3.758103
57C	-2.860393	-3.950499	2.415776
58C	0.736332	-3.119798	-0.085985
59C	1.982715	-2.667206	-0.515382
60C	2.069609	-1.726657	-1.548721
61C	0.908317	-1.226696	-2.140875
62C	-0.347099	-1.671850	-1.717847
63H	-1.641738	-5.312676	-1.456977
64H	-1.255189	-5.543663	0.262875
65H	-2.962287	-5.550466	-0.276638
66H	-3.691861	-0.884778	0.091349
67H	-5.390777	0.114368	-1.350861
68H	-6.065711	-1.006279	-3.475487
69H	-4.979659	-3.143197	-4.147552
70H	-3.244479	-4.155129	-2.725043
71H	-1.623740	-0.905833	1.430625
72H	-2.061662	-0.399114	3.783377
73H	-3.003088	-2.143317	5.300051
74H	-3.513954	-4.410958	4.413377
75H	-3.095977	-4.943093	2.043411
76H	0.675681	-3.845696	0.721211
77H	2.887156	-3.036038	-0.039932
78H	3.043482	-1.372552	-1.874103
79H	0.972170	-0.480422	-2.926867
80H	-1.243258	-1.266818	-2.176912

6bc-PhNCO-019

1C	0.925783	1.844726	-0.609653
2C	2.265068	1.665413	-0.845834
3N	3.048026	0.889954	-0.050989
4C	2.491832	0.300501	1.047361
5C	1.167454	0.452711	1.348068
6C	0.292705	1.213297	0.507836
7N	-1.007524	1.240395	0.864979
8S	-2.136586	2.008738	-0.038154

9O	-3.429977	1.727672	0.628631
10O	-2.047232	1.689884	-1.487802
11C	-1.818277	3.775953	0.133848
12C	-1.817478	4.343118	1.413821
13C	-1.560576	5.704671	1.553889
14C	-1.304235	6.516787	0.433558
15C	-1.312765	5.922897	-0.835539
16C	-1.566505	4.556461	-0.993139
17C	-1.039084	7.992296	0.609327
18C	4.499383	0.661431	-0.451266
19O	4.858669	1.310653	-1.450676
20N	5.071616	-0.203647	0.346369
21C	6.395597	-0.611681	0.175677
22C	7.276997	-0.226859	-0.865427
23C	8.581618	-0.728322	-0.915519
24C	9.055433	-1.617260	0.054622
25C	8.195175	-2.006072	1.090599
26C	6.892740	-1.513499	1.147451
27H	0.360103	2.444686	-1.309288
28H	2.773947	2.111549	-1.690628
29H	3.171812	-0.296169	1.638935
30H	0.762156	-0.036700	2.227199
31H	-2.012115	3.726478	2.286678
32H	-1.557605	6.148062	2.547414
33H	-1.116248	6.531370	-1.715258
34H	-1.568661	4.102479	-1.979048
35H	-0.762406	8.468445	-0.337354
36H	-1.928447	8.506179	0.997548
37H	-0.227608	8.166569	1.327039
38H	6.932069	0.463365	-1.624573
39H	9.235559	-0.414315	-1.727253
40H	10.072731	-1.998474	0.007073
41H	8.541960	-2.695634	1.857835
42H	6.226141	-1.815814	1.952231
43P	-2.327877	-3.188573	-0.213511
44C	-2.368633	-4.984201	-0.491097
45C	-3.661412	-2.399810	-1.150126
46C	-2.511402	-2.860713	1.557185
47C	-0.728079	-2.564423	-0.788899
48C	-4.160198	-1.155657	-0.733733
49C	-5.141263	-0.516046	-1.492224
50C	-5.631878	-1.113906	-2.655980
51C	-5.132703	-2.352908	-3.073555
52C	-4.143554	-2.996663	-2.328461
53C	-2.075921	-1.628777	2.070674
54C	-2.255898	-1.345005	3.425202
55C	-2.856174	-2.284901	4.268239
56C	-3.286648	-3.513770	3.755843
57C	-3.120671	-3.805347	2.400602
58C	0.447997	-3.098563	-0.231290
59C	1.689909	-2.673641	-0.700689
60C	1.764084	-1.718905	-1.721668
61C	0.596302	-1.176480	-2.261187
62C	-0.654210	-1.594053	-1.798519
63H	-2.115027	-5.191036	-1.534448
64H	-1.623229	-5.458934	0.153445
65H	-3.361420	-5.385172	-0.269045
66H	-3.785907	-0.663282	0.157099
67H	-5.506089	0.454844	-1.171183
68H	-6.397687	-0.612558	-3.242104
69H	-5.508753	-2.816785	-3.981453
70H	-3.753622	-3.950028	-2.672051
71H	-1.618909	-0.876461	1.433068
72H	-1.929104	-0.383721	3.812140
73H	-2.991356	-2.060674	5.323170
74H	-3.753211	-4.245862	4.409412
75H	-3.464735	-4.760796	2.015877
76H	0.397743	-3.832362	0.569347
77H	2.600511	-3.075325	-0.265257
78H	2.733909	-1.387037	-2.080301
79H	0.651486	-0.415874	-3.034052
80H	-1.554056	-1.151631	-2.212794

6bc-PhNCO-020

1C	-3.310620	1.710903	0.673267
2C	-1.979058	1.966530	0.868797
3N	-1.218657	2.630217	-0.045698
4C	-1.812016	3.076662	-1.195830
5C	-3.132585	2.845996	-1.454785
6C	-3.966078	2.125950	-0.534433
7N	-5.237835	1.917138	-0.913758
8S	-6.286697	1.074905	0.030333
9O	-7.578443	1.091821	-0.690411
10O	-6.296828	1.519349	1.449142
11C	-5.700694	-0.635671	0.023116

12C	-5.504873	-1.280998	-1.203873
13C	-5.079681	-2.607114	-1.216206
14C	-4.852348	-3.309371	-0.018641
15C	-5.055023	-2.639635	1.195198
16C	-5.475420	-1.305427	1.224423
17C	-4.407710	-4.751464	-0.056110
18C	0.250788	2.816213	0.227754
19O	0.667068	2.208787	1.238802
20N	0.833373	3.541995	-0.691559
21C	2.199600	3.830199	-0.628063
22C	2.999601	3.821823	0.539933
23C	4.359234	4.139159	0.474515
24C	4.968885	4.463794	-0.742491
25C	4.186009	4.485309	-1.904765
26C	2.826140	4.181287	-1.846017
27H	-3.855216	1.202041	1.457227
28H	-1.452374	1.658778	1.762438
29H	-1.157560	3.610476	-1.871080
30H	-3.566307	3.207809	-2.381218
31H	-5.682818	-0.750561	-2.134958
32H	-4.926403	-3.110636	-2.168581
33H	-4.885782	-3.163460	2.133455
34H	-5.631586	-0.792704	2.168397
35H	-4.224058	-5.143894	0.949727
36H	-5.170964	-5.384236	-0.527530
37H	-3.487916	-4.868233	-0.643110
38H	2.553104	3.558287	1.490523
39H	4.947830	4.126964	1.390147
40H	6.028111	4.706257	-0.784294
41H	4.636191	4.745245	-2.860792
42H	2.218028	4.204614	-2.747574
43P	2.878110	-1.089722	-0.156618
44C	2.596578	0.458072	-1.050491
45C	3.870026	-2.205769	-1.183461
46C	3.755938	-0.725422	1.383051
47C	1.281737	-1.862227	0.211526
48C	4.930275	-2.941885	-0.633323
49C	5.664407	-3.810337	-1.445202
50C	5.343671	-3.944986	-2.799099
51C	4.285675	-3.210996	-3.347669
52C	3.546756	-2.341645	-2.544586
53C	3.461414	-1.438937	2.554967
54C	4.163932	-1.158817	3.729046
55C	5.152549	-0.170074	3.736499
56C	5.443647	0.542443	2.568151
57C	4.750459	0.267124	1.389196
58C	0.234910	-1.057341	0.696194
59C	-0.997624	-1.641448	0.990133
60C	-1.184957	-3.016926	0.817483
61C	-0.140490	-3.815818	0.343479
62C	1.095348	-3.242171	0.034820
63H	1.916939	0.284252	-1.889135
64H	2.152759	1.171595	-0.355361
65H	3.546226	0.850164	-1.422474
66H	5.186919	-2.838073	0.416953
67H	6.487019	-4.377420	-1.018191
68H	5.918261	-4.619491	-3.428357
69H	4.036287	-3.313286	-4.400252
70H	2.725809	-1.777180	-2.978647
71H	2.684995	-2.198617	2.559011
72H	3.931811	-1.707536	4.637726
73H	5.691596	0.050545	4.654132
74H	6.204493	1.318160	2.574131
75H	4.979764	0.831284	0.490190
76H	0.375754	0.009787	0.852910
77H	-1.813494	-1.020060	1.347526
78H	-2.148161	-3.461532	1.046448
79H	-0.286967	-4.883849	0.206597
80H	1.900260	-3.865154	-0.344248

6bc-PhNCO-021

1C	2.368811	1.234722	-0.660409
2C	3.475617	0.477882	-0.377548
3N	4.736932	0.898418	-0.664878
4C	4.903435	2.117988	-1.252293
5C	3.840114	2.926602	-1.551762
6C	2.494928	2.527288	-1.268897
7N	1.520285	3.402964	-1.590419
8S	-0.058855	3.052819	-1.347156
9O	-0.434103	1.687768	-1.808565
10O	-0.826063	4.180999	-1.921430
11C	-0.339458	3.095497	0.436282
12C	-0.589761	1.923313	1.147119
13C	-0.804158	1.988334	2.526635
14C	-0.770253	3.211828	3.208103

15C	-0.512368	4.380443	2.468130
16C	-0.296473	4.330975	1.092870
17C	-0.994989	3.288648	4.698577
18C	5.964788	0.047296	-0.368344
19O	7.037390	0.557343	-0.738886
20N	5.626730	-1.062566	0.237577
21C	6.566333	-2.026530	0.604495
22C	6.075178	-3.105075	1.379315
23C	6.905722	-4.142168	1.800123
24C	8.264840	-4.145557	1.457808
25C	8.767573	-3.089896	0.690107
26C	7.943034	-2.042017	0.268402
27H	1.400059	0.821742	-0.422130
28H	3.417420	-0.497254	0.086556
29H	5.930418	2.390226	-1.458762
30H	4.016738	3.890953	-2.016395
31H	-0.640231	0.970919	0.631359
32H	-1.007056	1.071959	3.076180
33H	-0.482949	5.341069	2.978222
34H	-0.104520	5.240498	0.531285
35H	-1.806532	3.986513	4.941217
36H	-1.251050	2.310240	5.118946
37H	-0.095265	3.651199	5.212628
38H	5.019943	-3.104541	1.644110
39H	6.491516	-4.952137	2.397605
40H	8.916012	-4.953415	1.783249
41H	9.820488	-3.075321	0.413910
42H	8.354170	-1.231447	-0.319528
43P	-4.103461	-1.436648	-1.026094
44C	-4.872735	-1.405873	-2.671791
45C	-5.059697	-2.500812	0.082876
46C	-2.430397	-2.115013	-1.198306
47C	-4.072933	0.252849	-0.371325
48C	-4.437245	-3.063255	1.210663
49C	-5.183995	-3.834327	2.102286
50C	-6.547923	-4.046341	1.874645
51C	-7.168282	-3.486344	0.753585
52C	-6.429617	-2.711345	-0.142991
53C	-1.325620	-1.256119	-1.289563
54C	-0.052430	-1.789693	-1.505857
55C	0.121468	-3.171012	-1.622086
56C	-0.982585	-4.027436	-1.532442
57C	-2.259816	-3.505508	-1.325525
58C	-4.438707	0.505457	0.962308
59C	-4.414229	1.813210	1.449491
60C	-4.022027	2.866322	0.618088
61C	-3.653498	2.616087	-0.706117
62C	-3.681893	1.314139	-1.206251
63H	-5.852731	-0.922571	-2.628101
64H	-4.221608	-0.840024	-3.345148
65H	-4.970205	-2.429524	-3.045103
66H	-3.377699	-2.904445	1.390397
67H	-4.699531	-4.270116	2.971614
68H	-7.126185	-4.649523	2.569482
69H	-8.226930	-3.652105	0.574063
70H	-6.924879	-2.279031	-1.007078
71H	-1.435584	-0.180506	-1.214177
72H	0.796254	-1.117891	-1.589780
73H	1.114542	-3.581203	-1.785463
74H	-0.849809	-5.102009	-1.623534
75H	-3.110247	-4.178318	-1.255684
76H	-4.744285	-0.304753	1.616859
77H	-4.693415	2.006033	2.481653
78H	-3.984944	3.880307	1.006408
79H	-3.309676	3.424522	-1.343226
80H	-3.378586	1.136624	-2.233081

6bc-001

1C	0.699427	1.066736	2.022644
2C	0.873812	2.120632	2.905915
3N	1.724947	3.149885	2.710371
4C	2.428844	3.106377	1.564426
5C	2.328800	2.104990	0.603295
6C	1.436651	1.020866	0.810369
7N	1.200635	-0.053789	-0.013263
8S	2.017005	-0.283764	-1.372638
9O	1.480659	-1.547183	-1.962490
10O	2.043793	0.877078	-2.312646
11C	3.743993	-0.606995	-0.933094
12C	4.772065	-0.134730	-1.748779
13C	6.099449	-0.418802	-1.413822
14C	6.415201	-1.166215	-0.270196
15C	5.360586	-1.623346	0.539330
16C	4.032126	-1.351590	0.215287
17C	7.847347	-1.484851	0.086907

18H	-0.003558	0.269936	2.246177
19H	0.298301	2.148153	3.830788
20H	3.117169	3.934627	1.397792
21H	2.921968	2.174823	-0.301509
22H	4.536567	0.456586	-2.628293
23H	6.900046	-0.046675	-2.049587
24H	5.584897	-2.194816	1.437900
25H	3.225786	-1.697609	0.855851
26H	8.067269	-2.547176	-0.086242
27H	8.551138	-0.897428	-0.512653
28H	8.048646	-1.281320	1.145826
29P	-2.430305	-0.485234	-0.615590
30C	-1.769181	-1.200230	-2.140112
31C	-1.970807	1.259589	-0.480074
32C	-4.245810	-0.593664	-0.683258
33C	-1.872586	-1.443013	0.816748
34C	-2.541526	2.039946	0.540088
35C	-2.174397	3.377498	0.678227
36C	-1.236801	3.938692	-0.195846
37C	-0.668094	3.161717	-1.207967
38C	-1.033335	1.822129	-1.356709
39C	-4.882936	-1.791713	-0.318602
40C	-6.268678	-1.908345	-0.439834
41C	-7.024139	-0.834854	-0.923350
42C	-6.391636	0.356592	-1.290578
43C	-5.005145	0.480716	-1.173652
44C	-0.768698	-2.302671	0.715795
45C	-0.336689	-3.000238	1.846567
46C	-0.987038	-2.832336	3.071651
47C	-2.082890	-1.966747	3.173317
48C	-2.528990	-1.274160	2.048345
49H	-0.674206	-1.212054	-2.136536
50H	-2.144850	-2.224877	-2.222866
51H	-2.139146	-0.615237	-2.987500
52H	-3.266579	1.606102	1.223344
53H	-2.609984	3.976518	1.473156
54H	-0.939031	4.977028	-0.076564
55H	0.077728	3.585524	-1.873772
56H	-0.557304	1.230190	-2.128803
57H	-4.305733	-2.628382	0.064823
58H	-6.756929	-2.835739	-0.152825
59H	-8.103483	-0.926896	-1.012242
60H	-6.975121	1.192952	-1.665860
61H	-4.524378	1.411983	-1.457447
62H	-0.222895	-2.406614	-0.214764
63H	0.521792	-3.661563	1.767794
64H	-0.639679	-3.371911	3.949019
65H	-2.589802	-1.832195	4.125012
66H	-3.384374	-0.608891	2.129122

6bc-002

1C	1.430515	3.011697	-0.160355
2C	0.727370	3.739479	0.787092
3N	0.934997	3.662897	2.118843
4C	1.924457	2.832381	2.497517
5C	2.691718	2.052310	1.637955
6C	2.439422	2.089534	0.238450
7N	2.994437	1.327105	-0.757952
8S	4.045511	0.132521	-0.463020
9O	4.524120	-0.338652	-1.786224
10O	5.089439	0.453103	0.551443
11C	3.093677	-1.252674	0.228222
12C	3.075182	-1.494114	1.605131
13C	2.301947	-2.541397	2.111341
14C	1.542823	-3.363205	1.262123
15C	1.584866	-3.108154	-0.117680
16C	2.355247	-2.065053	-0.636135
17C	0.718924	-4.496794	1.825781
18H	1.196137	3.117306	-1.216189
19H	-0.061672	4.417506	0.465688
20H	2.117139	2.782045	3.568985
21H	3.475719	1.427197	2.045024
22H	3.673370	-0.882839	2.271848
23H	2.293385	-2.726485	3.183719
24H	1.013704	-3.736152	-0.798350
25H	2.386085	-1.886180	-1.705086
26H	0.087612	-4.957142	1.058149
27H	1.364196	-5.283137	2.239288
28H	0.071255	-4.154270	2.642680
29P	-1.645451	0.010795	-0.000626
30C	-0.277341	0.005449	1.182778
31C	-2.883884	-1.194474	0.548360
32C	-2.371597	1.668421	-0.046776
33C	-1.061080	-0.450085	-1.648934
34C	-4.248572	-0.872738	0.575231

35C	-5.177419	-1.831891	0.988445
36C	-4.747866	-3.105517	1.371761
37C	-3.385840	-3.427732	1.340510
38C	-2.451809	-2.477661	0.928167
39C	-2.623424	2.309676	-1.268980
40C	-3.171381	3.594663	-1.273617
41C	-3.465744	4.236874	-0.067335
42C	-3.216897	3.595042	1.151156
43C	-2.670281	2.312402	1.165741
44C	0.181918	0.018245	-2.103700
45C	0.608912	-0.305034	-3.392698
46C	-0.195291	-1.088943	-4.225548
47C	-1.433683	-1.555960	-3.770651
48C	-1.871680	-1.238099	-2.483940
49H	0.200407	-0.975705	1.190771
50H	0.447693	0.765814	0.895993
51H	-0.665758	0.235568	2.178874
52H	-4.587404	0.116898	0.282972
53H	-6.234237	-1.580488	1.012041
54H	-5.472316	-3.847571	1.696744
55H	-3.050929	-4.417790	1.637952
56H	-1.397293	-2.737706	0.901007
57H	-2.385894	1.820196	-2.208737
58H	-3.358853	4.095099	-2.219690
59H	-3.883034	5.240301	-0.074965
60H	-3.434753	4.097532	2.089321
61H	-2.469260	1.824040	2.115398
62H	0.841327	0.607435	-1.474196
63H	1.579698	0.047533	-3.729755
64H	0.144744	-1.342445	-5.226350
65H	-2.058155	-2.169460	-4.414485
66H	-2.832968	-1.604856	-2.135416

6bc-003

1C	0.927297	0.242091	2.239096
2C	0.963211	1.211278	3.229403
3N	1.639189	2.376135	3.136325
4C	2.309864	2.560377	1.984914
5C	2.337552	1.662025	0.922352
6C	1.621746	0.439763	1.017027
7N	1.516272	-0.561767	0.078012
8S	2.263953	-0.466778	-1.344372
9O	1.896326	-1.702413	-2.088792
10O	2.026501	0.811890	-2.082889
11C	4.047021	-0.546823	-1.044571
12C	4.909443	0.360942	-1.657355
13C	6.285419	0.266426	-1.423168
14C	6.811421	-0.722272	-0.580625
15C	5.919327	-1.624554	0.026498
16C	4.546931	-1.544038	-0.199567
17C	8.293434	-0.815858	-0.307349
18H	0.359937	-0.671394	2.384523
19H	0.416490	1.049768	4.158038
20H	2.860066	3.497354	1.900420
21H	2.889538	1.920684	0.026653
22H	4.508662	1.133423	-2.306138
23H	6.956554	0.975347	-1.903354
24H	6.307603	-2.398068	0.686127
25H	3.867112	-2.241611	0.281653
26H	8.663240	-1.836282	-0.467945
27H	8.865856	-0.141202	-0.953036
28H	8.517401	-0.552433	0.735111
29P	-2.516887	-0.355116	-0.561729
30C	-1.559512	-1.068249	-1.921690
31C	-2.147028	1.406341	-0.373382
32C	-4.280365	-0.523939	-0.965738
33C	-2.172685	-1.246201	0.976626
34C	-3.089889	2.252588	0.237106
35C	-2.782054	3.597315	0.441789
36C	-1.541824	4.102294	0.034405
37C	-0.610036	3.262027	-0.579550
38C	-0.903777	1.911995	-0.783123
39C	-5.094917	-1.447751	-0.294777
40C	-6.434773	-1.588247	-0.667266
41C	-6.960189	-0.812927	-1.704427
42C	-6.146764	0.107675	-2.375695
43C	-4.808728	0.255339	-2.009726
44C	-1.460600	-2.454287	0.958666
45C	-1.219432	-3.130916	2.157016
46C	-1.684952	-2.607673	3.366218
47C	-2.391748	-1.399722	3.383602
48C	-2.636047	-0.717042	2.192848
49H	-0.497608	-1.127199	-1.669775
50H	-1.942653	-2.071595	-2.130416
51H	-1.695463	-0.443383	-2.809312

52H	-4.059932	1.870408	0.543492
53H	-3.510247	4.249515	0.916372
54H	-1.303244	5.150037	0.197745
55H	0.355954	3.645713	-0.893662
56H	-0.156515	1.276865	-1.245931
57H	-4.693452	-2.052195	0.512996
58H	-7.064875	-2.302731	-0.144548
59H	-8.003077	-0.923347	-1.989926
60H	-6.554206	0.712728	-3.181031
61H	-4.184477	0.979699	-2.527305
62H	-1.068880	-2.859896	0.032137
63H	-0.654811	-4.058858	2.142314
64H	-1.487402	-3.133599	4.296634
65H	-2.744065	-0.984266	4.323659
66H	-3.172359	0.227460	2.216167

6bc-004

1C	1.022782	1.479334	1.603070
2C	0.837727	2.852741	1.593209
3N	1.239784	3.673316	0.598727
4C	1.860015	3.067057	-0.429794
5C	2.091403	1.697879	-0.531752
6C	1.669865	0.831809	0.515053
7N	1.796348	-0.532511	0.597428
8S	2.527633	-1.389465	-0.556208
9O	2.418840	-2.816617	-0.153107
10O	2.069461	-1.079237	-1.944795
11C	4.288757	-0.969421	-0.507064
12C	4.973432	-0.650781	-1.678573
13C	6.338603	-0.350407	-1.616660
14C	7.029282	-0.362498	-0.397510
15C	6.313514	-0.680640	0.771219
16C	4.954650	-0.984420	0.724028
17C	8.505365	-0.052082	-0.327176
18H	0.665004	0.882186	2.436372
19H	0.330407	3.331645	2.429962
20H	2.190408	3.720412	-1.237081
21H	2.581941	1.309746	-1.416275
22H	4.444115	-0.634815	-2.626088
23H	6.871148	-0.102902	-2.532472
24H	6.829782	-0.689707	1.729190
25H	4.411114	-1.223133	1.633889
26H	9.074959	-0.927764	0.011274
27H	8.900442	0.248592	-1.303515
28H	8.707871	0.758346	0.384627
29P	-2.462917	-0.328712	-0.343180
30C	-1.118382	-0.878271	-1.421808
31C	-2.854909	1.403373	-0.706505
32C	-3.930430	-1.349069	-0.654441
33C	-1.981836	-0.473839	1.394122
34C	-1.802616	2.331043	-0.798336
35C	-2.087380	3.677659	-1.024721
36C	-3.413868	4.101857	-1.160533
37C	-4.460352	3.179032	-1.068894
38C	-4.186164	1.828324	-0.840283
39C	-4.314047	-1.607400	-1.981798
40C	-5.455903	-2.366657	-2.238725
41C	-6.218358	-2.867761	-1.177461
42C	-5.836599	-2.612432	0.142554
43C	-4.693430	-1.854293	0.408950
44C	-1.114590	-1.499291	1.799681
45C	-0.779013	-1.623172	3.148877
46C	-1.303353	-0.731374	4.088542
47C	-2.164918	0.294328	3.682464
48C	-2.505750	0.427351	2.336427
49H	-0.932519	-1.944903	-1.273044
50H	-1.402956	-0.701332	-2.463167
51H	-0.207980	-0.321108	-1.198165
52H	-0.770240	2.016015	-0.682521
53H	-1.271004	4.391583	-1.082640
54H	-3.631111	5.152466	-1.335014
55H	-5.490998	3.507299	-1.173832
56H	-5.003619	1.116704	-0.770994
57H	-3.731877	-1.217477	-2.812349
58H	-5.748773	-2.566285	-3.265858
59H	-7.107124	-3.459354	-1.380969
60H	-6.424430	-3.004869	0.967872
61H	-4.400244	-1.664569	1.437097
62H	-0.678055	-2.180949	1.079082
63H	-0.090626	-2.404813	3.456821
64H	-1.031209	-0.826840	5.136547
65H	-2.563066	0.995988	4.410379
66H	-3.160046	1.235267	2.021068

6bc-005

1C	2.066859	3.341718	-0.461898
2C	2.853974	4.305365	0.150377
3N	4.174769	4.172380	0.391793
4C	4.720499	3.013332	-0.019883
5C	4.029257	1.980483	-0.646079
6C	2.634806	2.109250	-0.882251
7N	1.773863	1.189433	-1.435417
8S	2.291830	-0.236326	-1.992121
9O	1.091919	-0.908319	-2.556994
10O	3.486340	-0.160972	-2.879131
11C	2.797980	-1.225654	-0.559003
12C	4.112192	-1.671680	-0.429427
13C	4.479268	-2.416136	0.697457
14C	3.550176	-2.718924	1.701372
15C	2.229667	-2.259935	1.545694
16C	1.851452	-1.520422	0.428428
17C	3.940979	-3.515059	2.923435
18H	1.006962	3.520253	-0.620364
19H	2.402891	5.243668	0.471817
20H	5.788982	2.900814	0.161724
21H	4.570510	1.095171	-0.955513
22H	4.838885	-1.442203	-1.202283
23H	5.506024	-2.762390	0.793700
24H	1.487948	-2.490366	2.307734
25H	0.826284	-1.184802	0.321097
26H	3.311856	-4.408062	3.032231
27H	4.985099	-3.842236	2.875089
28H	3.816931	-2.920381	3.838086
29P	-2.336302	0.238845	-0.370782
30C	-1.621318	0.994867	-1.851364
31C	-4.145974	0.339789	-0.470872
32C	-1.834065	-1.493391	-0.224505
33C	-1.760238	1.118735	1.105001
34C	-4.942919	-0.808708	-0.353447
35C	-6.333150	-0.701214	-0.449633
36C	-6.928242	0.545183	-0.661075
37C	-6.133921	1.691939	-0.777345
38C	-4.745713	1.593532	-0.683423
39C	-1.847269	-2.102773	1.043028
40C	-1.477802	-3.441183	1.170774
41C	-1.088521	-4.171033	0.041645
42C	-1.070833	-3.563057	-1.215839
43C	-1.445164	-2.224913	-1.355901
44C	-0.394726	1.437645	1.201583
45C	0.088133	2.042046	2.363382
46C	-0.779552	2.325156	3.423474
47C	-2.138023	2.006841	3.324667
48C	-2.633763	1.401644	2.167379
49H	-1.919860	2.047455	-1.878507
50H	-0.528015	0.925247	-1.829247
51H	-2.007598	0.487580	-2.739897
52H	-4.488688	-1.781740	-0.193852
53H	-6.947010	-1.593408	-0.361094
54H	-8.009465	0.625136	-0.736880
55H	-6.594712	2.662170	-0.941588
56H	-4.137817	2.489784	-0.770886
57H	-2.128409	-1.534613	1.925478
58H	-1.480999	-3.909222	2.151372
59H	-0.785380	-5.209522	0.145897
60H	-0.746632	-4.120299	-2.089977
61H	-1.394737	-1.758799	-2.332689
62H	0.289504	1.222587	0.383860
63H	1.142132	2.294830	2.432291
64H	-0.396916	2.796894	4.324837
65H	-2.813727	2.229615	4.146082
66H	-3.689600	1.156370	2.097012

6bc-006

1C	2.060382	2.650913	1.554965
2C	2.850968	3.087529	2.607014
3N	4.179207	2.869720	2.706464
4C	4.728684	2.188770	1.684104
5C	4.034545	1.708307	0.577605
6C	2.633640	1.920169	0.480229
7N	1.773878	1.490505	-0.502134
8S	2.292775	0.672787	-1.783745
9O	1.074649	0.353784	-2.586915
10O	3.403188	1.314629	-2.542911
11C	2.944855	-0.919655	-1.209659
12C	4.111339	-1.441932	-1.767437
13C	4.583143	-2.685239	-1.334201
14C	3.906976	-3.413696	-0.345509

15C	2.737049	-2.861212	0.204578
16C	2.254724	-1.624217	-0.218606
17C	4.422985	-4.747411	0.139714
18H	0.994861	2.862990	1.542114
19H	2.397329	3.646135	3.425382
20H	5.802367	2.015574	1.751320
21H	4.577910	1.185523	-0.200909
22H	4.646272	-0.879262	-2.526153
23H	5.493788	-3.089843	-1.770759
24H	2.200178	-3.403521	0.979660
25H	1.360837	-1.201919	0.227918
26H	3.629684	-5.505472	0.139018
27H	5.242924	-5.114329	-0.487058
28H	4.797026	-4.672976	1.169764
29P	-2.453848	-0.312545	-0.438852
30C	-1.790314	-1.006678	-1.973471
31C	-2.528173	1.490799	-0.567135
32C	-4.117943	-0.969054	-0.137372
33C	-1.386139	-0.809717	0.938063
34C	-3.624938	2.197094	-0.044084
35C	-3.647407	3.590556	-0.122050
36C	-2.582134	4.277523	-0.715113
37C	-1.491737	3.571854	-1.232433
38C	-1.457609	2.177659	-1.164644
39C	-4.570830	-1.155680	1.179010
40C	-5.870607	-1.611811	1.407745
41C	-6.718599	-1.883363	0.329491
42C	-6.268957	-1.696700	-0.981900
43C	-4.972049	-1.237874	-1.219821
44C	-1.212769	-2.181711	1.194584
45C	-0.381248	-2.590221	2.236306
46C	0.282302	-1.637078	3.018460
47C	0.111083	-0.275078	2.761802
48C	-0.724826	0.143940	1.723485
49H	-0.759460	-0.658046	-2.105084
50H	-1.806017	-2.098964	-1.911074
51H	-2.393361	-0.673884	-2.823471
52H	-4.456260	1.670529	0.415561
53H	-4.496569	4.137241	0.279186
54H	-2.602266	5.362872	-0.771884
55H	-0.656767	4.099642	-1.684662
56H	-0.591296	1.648825	-1.549308
57H	-3.914872	-0.951803	2.020487
58H	-6.217030	-1.756699	2.427372
59H	-7.728785	-2.241272	0.510170
60H	-6.925713	-1.909041	-1.821022
61H	-4.636913	-1.091364	-2.242646
62H	-1.723599	-2.926523	0.589513
63H	-0.245922	-3.650310	2.432672
64H	0.940623	-1.958167	3.821220
65H	0.641089	0.465269	3.353312
66H	-0.839415	1.202796	1.518043

6bc-007

1C	-1.968879	-2.668398	1.554236
2C	-2.736354	-3.112998	2.620003
3N	-4.061669	-2.894639	2.751244
4C	-4.633188	-2.205631	1.746468
5C	-3.963170	-1.715965	0.629321
6C	-2.564409	-1.926058	0.499601
7N	-1.725875	-1.483052	-0.494814
8S	-2.278742	-0.690231	-1.778234
9O	-1.077733	-0.356023	-2.600879
10O	-3.385536	-1.365193	-2.513333
11C	-2.956708	0.895936	-1.216580
12C	-4.145380	1.384314	-1.759252
13C	-4.639518	2.619466	-1.329177
14C	-3.965511	3.373158	-0.357413
15C	-2.771331	2.856992	0.174405
16C	-2.266125	1.628049	-0.246901
17C	-4.521351	4.687356	0.136268
18H	-0.904868	-2.884760	1.515600
19H	-2.265316	-3.679594	3.422898
20H	-5.705146	-2.032998	1.838393
21H	-4.523760	-1.186218	-0.132113
22H	-4.679682	0.801417	-2.503013
23H	-5.567105	2.998376	-1.753125
24H	-2.233502	3.419749	0.934089
25H	-1.353997	1.232031	0.185861
26H	-3.729350	5.434780	0.266044
27H	-5.265202	5.094976	-0.557068
28H	-5.011861	4.561293	1.111383
29P	2.441445	0.332662	-0.446515
30C	1.788448	1.023157	-1.987740
31C	2.528653	-1.469920	-0.575566

32C	4.099962	0.997059	-0.130638
33C	1.358586	0.825665	0.920302
34C	3.614714	-2.169949	-0.022602
35C	3.648769	-3.562930	-0.102136
36C	2.605657	-4.255683	-0.727203
37C	1.526248	-3.556283	-1.274937
38C	1.480655	-2.162356	-1.205452
39C	4.537196	1.200282	1.188544
40C	5.834156	1.659651	1.426881
41C	6.695243	1.917131	0.355661
42C	6.261123	1.714228	-0.958568
43C	4.967004	1.252745	-1.206046
44C	1.201722	2.196385	1.194712
45C	0.357681	2.602135	2.227452
46C	-0.334571	1.647598	2.982753
47C	-0.181516	0.287319	2.706664
48C	0.665799	-0.129168	1.676600
49H	0.759568	0.671891	-2.127310
50H	1.800659	2.115547	-1.925475
51H	2.399424	0.691817	-2.832611
52H	4.428789	-1.638264	0.461351
53H	4.489434	-4.104751	0.322826
54H	2.634487	-5.340783	-0.785033
55H	0.708211	-4.089056	-1.751579
56H	0.621698	-1.638122	-1.611989
57H	3.871667	1.006603	2.024828
58H	6.168327	1.817387	2.448707
59H	7.703399	2.276825	0.543969
60H	6.928025	1.915592	-1.792381
61H	4.644152	1.093421	-2.230940
62H	1.735675	2.942234	0.611224
63H	0.235895	3.661103	2.438282
64H	-1.001745	1.966676	3.778974
65H	-0.735602	-0.453750	3.274620
66H	0.763261	-1.185823	1.453814

6bc-008

1C	-1.995535	-3.141200	-0.677399
2C	-2.658953	-4.211479	-0.097006
3N	-3.982590	-4.240152	0.160721
4C	-4.660716	-3.135556	-0.201324
5C	-4.100206	-2.005307	-0.789073
6C	-2.703126	-1.963424	-1.043226
7N	-1.951001	-0.945575	-1.582476
8S	-2.537093	0.525201	-1.914081
9O	-1.498423	1.211641	-2.723283
10O	-3.925890	0.544221	-2.454098
11C	-2.591461	1.408201	-0.333807
12C	-3.693033	1.273985	0.514452
13C	-3.676160	1.892081	1.768586
14C	-2.576052	2.652759	2.189542
15C	-1.488481	2.788288	1.310681
16C	-1.487888	2.171683	0.060922
17C	-2.545596	3.309279	3.548927
18H	-0.924783	-3.193697	-0.849907
19H	-2.098688	-5.102971	0.183567
20H	-5.733394	-3.153896	-0.010043
21H	-4.741221	-1.180202	-1.071462
22H	-4.563060	0.708142	0.200832
23H	-4.537235	1.784378	2.424606
24H	-0.628443	3.384450	1.608366
25H	-0.645183	2.286359	-0.610741
26H	-2.320668	4.380393	3.468883
27H	-3.502936	3.202367	4.070438
28H	-1.767365	2.862551	4.182342
29P	2.117583	-0.409455	-0.368968
30C	1.333131	-1.388083	-1.671601
31C	3.865250	-0.886860	-0.260791
32C	1.985289	1.353970	-0.746677
33C	1.313921	-0.743175	1.219707
34C	4.181974	-2.236123	-0.020369
35C	5.517291	-2.632832	0.047579
36C	6.538686	-1.690396	-0.122812
37C	6.224202	-0.350033	-0.360829
38C	4.888540	0.056532	-0.430620
39C	1.726696	1.784540	-2.056385
40C	1.618262	3.150899	-2.324030
41C	1.770834	4.082995	-1.294387
42C	2.031672	3.652768	0.012050
43C	2.135787	2.290719	0.290545
44C	-0.085466	-0.862507	1.259706
45C	-0.721529	-1.079594	2.482867
46C	0.026708	-1.164412	3.660842
47C	1.419557	-1.037058	3.620155
48C	2.068450	-0.827725	2.401551

49H	0.272751	-1.120806	-1.774834
50H	1.860325	-1.220918	-2.615614
51H	1.420212	-2.444805	-1.400976
52H	3.394177	-2.972466	0.119212
53H	5.760193	-3.675467	0.233495
54H	7.578300	-2.002938	-0.070359
55H	7.015402	0.382805	-0.493764
56H	4.651217	1.099232	-0.618423
57H	1.581107	1.070207	-2.859208
58H	1.393327	3.480851	-3.334049
59H	1.673792	5.144538	-1.506101
60H	2.139623	4.376778	0.815050
61H	2.313442	1.960471	1.310513
62H	-0.679039	-0.784866	0.353190
63H	-1.802796	-1.179153	2.508622
64H	-0.475024	-1.333111	4.610262
65H	2.002406	-1.105354	4.534831
66H	3.150647	-0.738705	2.375781

6bc-009

1C	1.783991	3.545624	1.367078
2C	1.408158	4.880497	1.338245
3N	1.360568	5.638961	0.222834
4C	1.722531	5.013863	-0.913738
5C	2.114932	3.682576	-1.004090
6C	2.151100	2.878299	0.167269
7N	2.463172	1.546192	0.265187
8S	2.832761	0.678065	-1.049211
9O	1.739050	0.655319	-2.072517
10O	4.186745	0.967996	-1.605579
11C	2.879862	-0.961493	-0.305809
12C	3.805391	-1.237094	0.706873
13C	3.820923	-2.501796	1.290037
14C	2.928259	-3.507255	0.873565
15C	2.022280	-3.207796	-0.151060
16C	1.992049	-1.940924	-0.744080
17C	2.956524	-4.868555	1.525695
18H	1.797891	2.997668	2.305835
19H	1.125910	5.379290	2.265030
20H	1.695101	5.620468	-1.818547
21H	2.385157	3.272594	-1.971349
22H	4.493060	-0.466492	1.042472
23H	4.534943	-2.715591	2.082958
24H	1.323531	-3.968038	-0.491948
25H	1.280370	-1.714096	-1.530162
26H	2.207483	-5.539241	1.090790
27H	3.940202	-5.342511	1.411723
28H	2.758456	-4.794639	2.603072
29P	-1.855489	0.154596	-0.125611
30C	-1.051482	1.711481	-0.579707
31C	-1.238289	-0.418475	1.478049
32C	-3.646036	0.420343	0.005071
33C	-1.512675	-1.088914	-1.396213
34C	-2.064955	-1.176141	2.325714
35C	-1.555199	-1.665823	3.529285
36C	-0.229221	-1.399710	3.889360
37C	0.588215	-0.641670	3.046087
38C	0.091758	-0.148366	1.837674
39C	-4.543836	-0.222943	-0.858993
40C	-5.914437	0.027569	-0.744921
41C	-6.387874	0.914317	0.225755
42C	-5.491537	1.556793	1.088234
43C	-4.122576	1.312876	0.981496
44C	-1.642670	-2.453333	-1.087752
45C	-1.374332	-3.412346	-2.064102
46C	-0.970560	-3.015476	-3.344064
47C	-0.840327	-1.657988	-3.650017
48C	-1.111024	-0.690379	-2.680047
49H	-0.018190	1.518470	-0.878225
50H	-1.595075	2.162816	-1.414838
51H	-1.078117	2.393388	0.274399
52H	-3.098118	-1.377841	2.056481
53H	-2.194536	-2.250063	4.185731
54H	0.163999	-1.781321	4.828219
55H	1.618595	-0.431611	3.318675
56H	0.752570	0.434651	1.198718
57H	-4.182763	-0.913420	-1.615236
58H	-6.608793	-0.471723	-1.415232
59H	-7.454083	1.106908	0.311495
60H	-5.857723	2.246284	1.843905
61H	-3.432711	1.808235	1.660040
62H	-1.931736	-2.769457	-0.089460
63H	-1.466452	-4.467514	-1.821444
64H	-0.748079	-3.764938	-4.098969
65H	-0.510378	-1.347522	-4.637272

66H -0.978529 0.358115 -2.922066

6bc-010

1C -2.712594 -2.583447 1.631066
2C -2.902813 -3.946128 1.802023
3N -3.293049 -4.793371 0.826415
4C -3.510308 -4.225324 -0.375200
5C -3.345544 -2.874527 -0.662795
6C -2.918328 -1.983599 0.359891
7N -2.671571 -0.637629 0.257957
8S -2.771023 0.109433 -1.166338
9O -1.627501 -0.213335 -2.084975
10O -4.107681 0.017448 -1.826862
11C -2.551971 1.821041 -0.652701
12C -3.455460 2.388072 0.252303
13C -3.319748 3.729046 0.602843
14C -2.294191 4.523884 0.059532
15C -1.406422 3.932235 -0.847043
16C -1.530150 2.586702 -1.207871
17C -2.157439 5.972354 0.461845
18H -2.389393 -1.964747 2.464457
19H -2.727207 -4.394861 2.779183
20H -3.834806 -4.899414 -1.167474
21H -3.548628 -2.516522 -1.666231
22H -4.248960 1.783482 0.681135
23H -4.020197 4.169586 1.309628
24H -0.602253 4.525800 -1.275889
25H -0.837449 2.136857 -1.910900
26H -1.350801 6.468974 -0.088147
27H -3.086233 6.525767 0.273427
28H -1.941112 6.065820 1.534488
29P 2.163120 -0.100828 -0.510099
30C 1.599296 0.270233 -2.192606
31C 1.745581 -1.819156 -0.113488
32C 3.956403 0.141444 -0.398771
33C 1.359055 1.040590 0.646921
34C 2.638135 -2.609904 0.630254
35C 2.295920 -3.924224 0.952162
36C 1.069735 -4.451553 0.535142
37C 0.183405 -3.664733 -0.205086
38C 0.512827 -2.348579 -0.535296
39C 4.559696 0.357674 0.852440
40C 5.944905 0.502047 0.939772
41C 6.732042 0.434996 -0.214905
42C 6.133723 0.221565 -1.460228
43C 4.748115 0.073156 -1.556227
44C 0.208875 0.647385 1.344631
45C -0.435482 1.559607 2.183138
46C 0.066350 2.853254 2.332361
47C 1.212027 3.248240 1.631258
48C 1.858710 2.348709 0.785274
49H 0.507604 0.183280 -2.217031
50H 1.893388 1.291479 -2.452714
51H 2.031871 -0.440733 -2.902803
52H 3.596000 -2.213758 0.952618
53H 2.988891 -4.533849 1.525890
54H 0.800663 -5.473154 0.790416
55H -0.775158 -4.065660 -0.516932
56H -0.199016 -1.746461 -1.093485
57H 3.953778 0.419967 1.751950
58H 6.407528 0.669810 1.908512
59H 7.810242 0.551491 -0.143702
60H 6.742168 0.172659 -2.359088
61H 4.295734 -0.090395 -2.529309
62H -0.212703 -0.343372 1.219875
63H -1.340632 1.256026 2.699822
64H -0.441159 3.560103 2.983197
65H 1.597748 4.258563 1.737681
66H 2.747342 2.662476 0.244589

6bc-011

1C -1.399944 3.709384 -1.360292
2C -0.775073 4.947953 -1.348937
3N -0.494161 5.652954 -0.233041
4C -0.878205 5.078297 0.922895
5C -1.508845 3.843659 1.031447
6C -1.788787 3.090774 -0.141457
7N -2.348735 1.842191 -0.228986
8S -2.769782 1.026585 1.099530
9O -1.628667 0.794973 2.047600
10O -4.005648 1.540155 1.758958
11C -3.161633 -0.571094 0.369536

12C	-4.219496	-0.676594	-0.539086
13C	-4.513815	-1.917032	-1.101514
14C	-3.767575	-3.062793	-0.771025
15C	-2.721875	-2.930676	0.151294
16C	-2.415425	-1.692690	0.724132
17C	-4.074299	-4.389670	-1.422756
18H	-1.595324	3.199266	-2.300308
19H	-0.477435	5.408357	-2.290584
20H	-0.664682	5.645196	1.828671
21H	-1.773644	3.466991	2.013634
22H	-4.799166	0.201720	-0.807002
23H	-5.334708	-1.999338	-1.811210
24H	-2.130749	-3.802426	0.422763
25H	-1.599839	-1.599515	1.432815
26H	-3.546212	-5.212313	-0.928518
27H	-5.148536	-4.609636	-1.397254
28H	-3.771999	-4.385300	-2.478911
29P	1.902102	-0.094914	0.079349
30C	1.198795	1.501996	0.549887
31C	0.853604	-0.921705	-1.141176
32C	3.552917	0.193736	-0.618406
33C	2.062055	-1.151825	1.544755
34C	1.157439	-2.242403	-1.518911
35C	0.364931	-2.889826	-2.464909
36C	-0.733756	-2.228792	-3.029101
37C	-1.043072	-0.924421	-2.640698
38C	-0.253020	-0.263854	-1.696066
39C	4.556349	0.702287	0.225296
40C	5.818553	0.989884	-0.293264
41C	6.084920	0.774592	-1.650645
42C	5.087202	0.272232	-2.490088
43C	3.819363	-0.019350	-1.978716
44C	3.115773	-2.075605	1.640159
45C	3.188405	-2.933333	2.739446
46C	2.216107	-2.870700	3.742997
47C	1.166791	-1.951237	3.646563
48C	1.081606	-1.090092	2.550437
49H	0.201755	1.372365	0.978705
50H	1.859959	1.959122	1.292364
51H	1.149933	2.148587	-0.330365
52H	2.002872	-2.762317	-1.076167
53H	0.598748	-3.910528	-2.755376
54H	-1.356215	-2.739647	-3.759010
55H	-1.913361	-0.419394	-3.048800
56H	-0.543250	0.730469	-1.374587
57H	4.357570	0.867443	1.281240
58H	6.592282	1.381887	0.361164
59H	7.069272	1.000760	-2.052085
60H	5.291065	0.106921	-3.544488
61H	3.048961	-0.405283	-2.639150
62H	3.880544	-2.122514	0.870285
63H	4.005968	-3.645603	2.812146
64H	2.276196	-3.537807	4.599044
65H	0.408864	-1.899906	4.423637
66H	0.250965	-0.392861	2.485588

6bc-012

1C	1.257572	3.655173	1.311816
2C	0.650368	4.901811	1.279001
3N	0.465027	5.633625	0.160033
4C	0.931502	5.078635	-0.974903
5C	1.554855	3.838240	-1.061014
6C	1.733010	3.057733	0.113277
7N	2.265478	1.798588	0.216004
8S	2.765708	0.988637	-1.091871
9O	1.689559	0.789863	-2.115208
10O	4.060423	1.478615	-1.648126
11C	3.062475	-0.616532	-0.331173
12C	4.073807	-0.748923	0.626454
13C	4.280487	-1.985452	1.233572
14C	3.493927	-3.102812	0.897161
15C	2.495918	-2.943985	-0.072523
16C	2.275641	-1.708436	-0.690356
17C	3.719626	-4.428310	1.583971
18H	1.369348	3.120725	2.251729
19H	0.284496	5.345939	2.204344
20H	0.794122	5.666603	-1.882002
21H	1.889908	3.477207	-2.027581
22H	4.684247	0.107247	0.897944
23H	5.065615	-2.088770	1.980045
24H	1.876184	-3.792570	-0.352476
25H	1.496703	-1.594317	-1.436096
26H	3.153030	-5.232885	1.102814
27H	4.780819	-4.705854	1.573228
28H	3.408882	-4.382389	2.636631

29P	-1.867191	-0.052366	-0.148298
30C	-1.212843	1.539440	-0.708583
31C	-1.234701	-0.443130	1.503167
32C	-3.677635	0.040918	-0.079487
33C	-1.357154	-1.353413	-1.300298
34C	-2.034594	-1.148846	2.417575
35C	-1.507490	-1.512590	3.658214
36C	-0.189566	-1.175525	3.986021
37C	0.601167	-0.467236	3.075867
38C	0.086440	-0.096672	1.832147
39C	-4.482802	-0.873706	-0.773334
40C	-5.874560	-0.763963	-0.701586
41C	-6.460392	0.252714	0.057280
42C	-5.656228	1.167381	0.747862
43C	-4.266827	1.065249	0.682807
44C	-1.283860	-2.685290	-0.859361
45C	-0.879896	-3.685371	-1.744108
46C	-0.543444	-3.360732	-3.062966
47C	-0.615990	-2.035091	-3.500825
48C	-1.024127	-1.028077	-2.624255
49H	-0.173166	1.414295	-1.020606
50H	-1.806519	1.892974	-1.556482
51H	-1.277157	2.264504	0.106555
52H	-3.060039	-1.408817	2.169803
53H	-2.126778	-2.055842	4.367017
54H	0.217851	-1.461292	4.952509
55H	1.623800	-0.198129	3.325590
56H	0.723407	0.461031	1.147344
57H	-4.033809	-1.663925	-1.367554
58H	-6.497242	-1.473219	-1.240092
59H	-7.542746	0.335813	0.110036
60H	-6.110349	1.959961	1.336242
61H	-3.648939	1.777023	1.224679
62H	-1.519840	-2.939210	0.170224
63H	-0.814820	-4.713934	-1.400059
64H	-0.213483	-4.139455	-3.745512
65H	-0.338216	-1.777850	-4.518954
66H	-1.050262	-0.000106	-2.969017

6b-Me2-001

1C	2.867260	0.197019	0.624743
2C	3.467423	1.432143	0.861755
3N	3.227116	2.536496	0.134317
4C	2.351983	2.416783	-0.874426
5C	1.682809	1.232936	-1.190465
6C	1.940642	0.090383	-0.421479
7N	1.312360	-1.163436	-0.698428
8S	0.195367	-1.728836	0.482891
9O	-0.209984	-3.067158	0.032114
10O	0.825703	-1.542595	1.795309
11C	-1.208613	-0.628525	0.363324
12C	-1.172529	0.591062	1.046363
13C	-2.240519	1.476326	0.899165
14C	-3.338894	1.161741	0.082802
15C	-3.344965	-0.072310	-0.588980
16C	-2.286360	-0.970550	-0.459895
17C	-4.483104	2.129876	-0.088561
18C	0.886514	-1.416404	-2.089149
19H	3.110902	-0.663742	1.235243
20H	4.187388	1.536044	1.670623
21H	2.163642	3.315237	-1.458644
22H	0.977689	1.218392	-2.013627
23H	-0.333360	0.838019	1.688349
24H	-2.222345	2.422254	1.434479
25H	-4.193209	-0.336461	-1.216205
26H	-2.302120	-1.926278	-0.973887
27H	-4.401782	2.659254	-1.047779
28H	-5.447735	1.609348	-0.086219
29H	-4.495089	2.883284	0.705950
30H	0.000658	-0.837317	-2.381288
31H	1.721546	-1.153039	-2.742382
32H	0.675974	-2.479895	-2.202651

6b-Me2-002

1C	1.686397	1.230848	1.190986
2C	2.357081	2.414157	0.876175
3N	3.232337	2.533794	-0.132481
4C	3.471176	1.429947	-0.861160
5C	2.869337	0.195377	-0.625513
6C	1.942667	0.088829	0.420673
7N	1.312782	-1.164493	0.696175
8S	0.194190	-1.726393	-0.485422

9O	-0.211946	-3.065324	-0.037099
10O	0.823610	-1.537978	-1.797955
11C	-1.209075	-0.625521	-0.362731
12C	-2.284361	-0.966704	0.465009
13C	-3.340432	-0.067240	0.599033
14C	-3.336333	1.166962	-0.073849
15C	-2.240157	1.481554	-0.892071
16C	-1.173616	0.594348	-1.044172
17C	-4.497952	2.117036	0.078655
18C	0.887294	-1.418806	2.086724
19H	0.981265	1.216276	2.014152
20H	2.169945	3.312243	1.461342
21H	4.191234	1.533818	-1.669948
22H	3.111693	-0.665075	-1.236966
23H	-2.297801	-1.921521	0.980734
24H	-4.185446	-0.328976	1.231914
25H	-2.220549	2.429296	-1.424083
26H	-0.334979	0.842254	-1.686493
27H	-4.320512	3.060862	-0.447160
28H	-5.418386	1.673804	-0.323244
29H	-4.685544	2.344361	1.135576
30H	1.723036	-1.157579	2.739925
31H	0.002516	-0.838739	2.380156
32H	0.675197	-2.482139	2.198856

6b-Me2-003

1C	0.948329	1.472411	-0.855631
2C	1.309520	2.786751	-0.555433
3N	2.426737	3.118896	0.109851
4C	3.226532	2.114286	0.501450
5C	2.954815	0.766558	0.261246
6C	1.787315	0.436004	-0.435123
7N	1.433653	-0.923597	-0.743828
8S	0.404695	-1.668781	0.424560
9O	0.212968	-3.047552	-0.056587
10O	0.921528	-1.454359	1.789704
11C	-1.118805	-0.756348	0.248456
12C	-1.503246	0.143340	1.243087
13C	-2.693784	0.853916	1.081209
14C	-3.497354	0.676618	-0.055436
15C	-3.077608	-0.235559	-1.040824
16C	-1.894863	-0.956465	-0.897391
17C	-4.800515	1.420511	-0.204714
18C	2.542419	-1.804131	-1.178550
19H	0.040017	1.258057	-1.408259
20H	0.673890	3.610750	-0.872438
21H	4.126607	2.398188	1.042528
22H	3.634637	0.001147	0.619322
23H	-0.881467	0.290007	2.120218
24H	-3.000138	1.558009	1.850965
25H	-3.687021	-0.384746	-1.929049
26H	-1.577676	-1.657990	-1.662973
27H	-5.012885	1.652132	-1.254502
28H	-5.634110	0.810650	0.170020
29H	-4.796588	2.357196	0.363143
30H	3.096476	-1.262424	-1.948664
31H	3.227205	-2.080366	-0.367202
32H	2.120713	-2.709261	-1.617245

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1C	-1.669718	0.114285	0.799421
2C	-2.661419	1.043147	0.976789
3N	-3.645455	1.244845	0.058116
4C	-3.654107	0.482338	-1.077545
5C	-2.696448	-0.461229	-1.315707
6C	-1.629496	-0.700380	-0.383687
7N	-0.730543	-1.631104	-0.733332
8S	0.576357	-1.967690	0.212588
9O	1.268244	-3.093525	-0.449611
10O	0.236374	-2.127674	1.650839
11C	1.649198	-0.522245	0.079801
12C	2.130987	-0.150139	-1.181365
13C	2.949654	0.970697	-1.293237
14C	3.303803	1.730657	-0.162705
15C	2.811610	1.332763	1.087282
16C	1.983562	0.212587	1.216115
17C	4.203422	2.934109	-0.306081
18C	-4.725310	2.213278	0.297661
19H	-0.932925	-0.000690	1.582259
20H	-2.707266	1.661619	1.866418
21H	-4.462628	0.677617	-1.773283
22H	-2.732317	-1.040608	-2.232007

23H	1.868337	-0.730112	-2.061375
24H	3.324882	1.261752	-2.272195
25H	3.075989	1.902576	1.975270
26H	1.609581	-0.091170	2.188821
27H	5.201282	2.637837	-0.655380
28H	3.803035	3.643494	-1.041506
29H	4.324328	3.462810	0.645366
30H	-5.639325	1.689169	0.593998
31H	-4.424669	2.896889	1.092759
32H	-4.909408	2.786053	-0.614318

6b-Me-002

1C	-2.689879	-0.812556	-0.020271
2C	-4.052814	-0.691186	-0.041373
3N	-4.678175	0.520710	-0.039925
4C	-3.915841	1.655252	0.000377
5C	-2.551409	1.605423	0.022140
6C	-1.847199	0.353354	0.010398
7N	-0.509931	0.404642	0.026120
8S	0.355390	-1.003648	0.016223
9O	0.156201	-1.766342	-1.245298
10O	0.172870	-1.768358	1.278876
11C	2.026376	-0.350073	0.005135
12C	2.661199	-0.109649	-1.214742
13C	3.960766	0.398879	-1.214532
14C	4.633785	0.671818	-0.012672
15C	3.971434	0.413571	1.198392
16C	2.671963	-0.094827	1.216357
17C	6.027160	1.251576	-0.022590
18C	-6.144599	0.610037	0.012978
19H	-2.265874	-1.808638	-0.032279
20H	-4.701890	-1.559506	-0.063745
21H	-4.460625	2.592821	0.010000
22H	-1.983081	2.529181	0.044606
23H	2.150380	-0.327449	-2.147575
24H	4.462337	0.581113	-2.162457
25H	4.481384	0.607459	2.139499
26H	2.169450	-0.301026	2.156317
27H	6.593815	0.949843	0.865479
28H	6.586213	0.937148	-0.911057
29H	5.990463	2.349951	-0.030266
30H	-6.469258	1.513343	-0.507594
31H	-6.578425	-0.259943	-0.483832
32H	-6.482617	0.644487	1.053755

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1C	-2.688879	-0.814308	0.016698
2C	-4.052323	-0.699379	0.040216
3N	-4.683400	0.509446	0.041957
4C	-3.926390	1.647633	0.001641
5C	-2.561769	1.604256	-0.022747
6C	-1.851652	0.355480	-0.013074
7N	-0.514542	0.412654	-0.029458
8S	0.355638	-0.992573	-0.019738
9O	0.178201	-1.756104	-1.283895
10O	0.156157	-1.757767	1.240241
11C	2.025507	-0.336515	-0.004355
12C	2.671671	-0.073531	-1.214754
13C	3.970352	0.433780	-1.193499
14C	4.634876	0.680911	0.019986
15C	3.959540	0.407504	1.219221
16C	2.658790	-0.100901	1.216106
17C	6.054091	1.194967	0.023314
18C	-6.150410	0.592518	-0.006408
19H	-2.260365	-1.808461	0.026437
20H	-4.697096	-1.570845	0.062216
21H	-4.475674	2.582612	-0.005648
22H	-1.997778	2.530665	-0.045081
23H	2.167337	-0.269850	-2.155856
24H	4.478926	0.637544	-2.133426
25H	4.457633	0.589198	2.168807
26H	2.145786	-0.317912	2.147917
27H	6.344120	1.572563	1.009772
28H	6.756831	0.394670	-0.246061
29H	6.188431	2.002652	-0.706177
30H	-6.478376	1.486577	0.527972
31H	-6.490966	0.640362	-1.045841
32H	-6.578713	-0.286830	0.478443

6b-PhNCO2-001

1C	0.113076	-1.769450	1.410781
2C	0.228871	-2.880648	2.243481
3N	0.384929	-4.137963	1.792932
4C	0.434143	-4.306452	0.461790
5C	0.332741	-3.261023	-0.457457
6C	0.168542	-1.962530	0.026358
7N	0.042917	-0.855851	-0.872966
8S	-1.480177	-0.619045	-1.594914
9O	-2.145419	-1.935103	-1.537507
10O	-1.296070	0.024701	-2.901129
11C	-2.407465	0.479439	-0.521300
12C	-2.418973	1.853433	-0.765103
13C	-3.139706	2.684343	0.093247
14C	-3.837086	2.164948	1.195881
15C	-3.808528	0.777625	1.412743
16C	-3.101680	-0.071219	0.560689
17C	-4.576956	3.076053	2.145111
18C	0.981243	0.289478	-0.769016
19O	0.529495	1.405190	-1.094844
20N	2.158716	-0.126341	-0.339653
21C	3.201726	0.751343	-0.070771
22C	3.206592	2.163198	-0.232789
23C	4.336946	2.918749	0.095396
24C	5.498438	2.316604	0.591212
25C	5.512556	0.923486	0.753830
26C	4.391846	0.161718	0.430650
27H	-0.006040	-0.773180	1.824335
28H	0.191803	-2.758459	3.324223
29H	0.563217	-5.328725	0.111545
30H	0.380318	-3.447823	-1.524784
31H	-1.863536	2.256982	-1.602822
32H	-3.154886	3.755476	-0.095320
33H	-4.352052	0.353401	2.254268
34H	-3.098235	-1.143631	0.726345
35H	-4.865378	4.014815	1.659439
36H	-5.482895	2.598152	2.535525
37H	-3.945082	3.331541	3.007181
38H	2.321595	2.650985	-0.620199
39H	4.304826	3.998840	-0.042047
40H	6.372077	2.914485	0.841077
41H	6.403527	0.428562	1.136922
42H	4.405633	-0.918473	0.560183

6b-PhNCO2-002

1C	2.528661	-0.810758	-1.524269
2C	3.769303	-0.980126	-2.136433
3N	4.895982	-1.286779	-1.470774
4C	4.791215	-1.446188	-0.141475
5C	3.595730	-1.312831	0.565518
6C	2.435844	-0.979009	-0.137993
7N	1.182582	-0.822731	0.530266
8S	0.993194	0.521049	1.566382
9O	2.361076	1.023112	1.813338
10O	0.176731	0.131903	2.723492
11C	0.137641	1.799607	0.642571
12C	-1.154593	2.176041	1.006630
13C	-1.789180	3.188232	0.288449
14C	-1.157442	3.816376	-0.798141
15C	0.144344	3.416322	-1.137101
16C	0.801427	2.414687	-0.419710
17C	-1.879181	4.875188	-1.596482
18C	0.016811	-1.585870	0.013305
19O	0.316370	-2.669538	-0.530283
20N	-1.120697	-0.955479	0.215194
21C	-2.351454	-1.545373	-0.042527
22C	-3.478744	-0.685453	0.005762
23C	-4.773486	-1.156954	-0.202584
24C	-5.003933	-2.515283	-0.462861
25C	-3.905889	-3.381851	-0.511265
26C	-2.602563	-2.916761	-0.312372
27H	1.650584	-0.561435	-2.110932
28H	3.865174	-0.857716	-3.213615
29H	5.708570	-1.698648	0.386779
30H	3.564742	-1.459692	1.639188
31H	-1.652519	1.672741	1.827457
32H	-2.797368	3.486512	0.568205
33H	0.654648	3.895537	-1.969424
34H	1.813008	2.121857	-0.683797
35H	-2.471170	5.531851	-0.948033
36H	-1.180557	5.496254	-2.167934
37H	-2.573642	4.413938	-2.312127
38H	-3.304961	0.367340	0.212984
39H	-5.609554	-0.460717	-0.158809
40H	-6.013285	-2.886765	-0.624902

41H	-4.061551	-4.441069	-0.711183
42H	-1.768784	-3.605637	-0.365273

6b-PhNCO2-003

1C	1.300489	1.491949	1.167407
2C	1.578769	2.857798	1.126517
3N	1.286778	3.654450	0.084786
4C	0.685595	3.076551	-0.968812
5C	0.346637	1.725963	-1.024841
6C	0.660003	0.907653	0.068394
7N	0.368940	-0.486215	0.027099
8S	-0.775438	-1.103641	1.107348
9O	-0.538502	-0.445297	2.406625
10O	-0.692541	-2.567671	1.016990
11C	-2.391130	-0.567029	0.544023
12C	-2.868351	0.677903	0.959046
13C	-4.112948	1.113631	0.498058
14C	-4.884527	0.320534	-0.363584
15C	-4.376571	-0.929349	-0.759657
16C	-3.132953	-1.377616	-0.319464
17C	-6.227030	0.791789	-0.867855
18C	0.555736	-1.186018	-1.316076
19O	-0.474343	-1.611543	-1.866178
20N	1.784919	-1.178361	-1.772610
21C	2.897285	-0.888283	-0.984671
22C	3.850432	0.038954	-1.457872
23C	5.004117	0.327705	-0.725915
24C	5.249159	-0.308542	0.497347
25C	4.321036	-1.245660	0.970769
26C	3.166225	-1.536806	0.243211
27H	1.581509	0.891527	2.023194
28H	2.077193	3.332524	1.969359
29H	0.455120	3.728218	-1.809419
30H	-0.145444	1.314952	-1.900641
31H	-2.284079	1.291674	1.637028
32H	-4.488542	2.082274	0.819950
33H	-4.961814	-1.557459	-1.428133
34H	-2.732469	-2.330361	-0.644881
35H	-6.193366	0.986007	-1.948237
36H	-7.002014	0.033096	-0.701562
37H	-6.542370	1.715391	-0.370728
38H	3.656433	0.541039	-2.402961
39H	5.713213	1.058235	-1.111224
40H	6.147678	-0.084158	1.067660
41H	4.498702	-1.757551	1.915122
42H	2.454046	-2.266921	0.617337

6b-PhNCO2-004

1C	0.703081	1.619463	-0.732710
2C	1.102350	2.910059	-0.385787
3N	1.037141	3.399597	0.863570
4C	0.546065	2.586334	1.814071
5C	0.117948	1.281403	1.571014
6C	0.203347	0.785265	0.267627
7N	-0.180786	-0.564954	-0.049281
8S	0.920660	-1.776344	0.465486
9O	0.740179	-2.966225	-0.380497
10O	0.914507	-1.929852	1.935623
11C	2.483969	-1.015908	0.008427
12C	3.252155	-0.365658	0.976749
13C	4.440553	0.252682	0.592855
14C	4.874124	0.227866	-0.743798
15C	4.089283	-0.449397	-1.690083
16C	2.895032	-1.072152	-1.323750
17C	6.156323	0.918515	-1.140262
18C	-1.636511	-0.895019	0.000153
19O	-1.934769	-2.056952	0.329337
20N	-2.341943	0.167317	-0.346025
21C	-3.731004	0.155649	-0.374530
22C	-4.590947	-0.948034	-0.125681
23C	-5.980432	-0.803482	-0.194196
24C	-6.572191	0.425143	-0.506952
25C	-5.738148	1.524936	-0.756703
26C	-4.352935	1.391437	-0.692266
27H	0.778094	1.263665	-1.754803
28H	1.498114	3.581285	-1.145474
29H	0.496251	2.998641	2.819885
30H	-0.270198	0.660274	2.371673
31H	2.915888	-0.334932	2.007780
32H	5.037326	0.769775	1.341118
33H	4.411755	-0.486577	-2.727899
34H	2.287635	-1.585766	-2.062613

35H	6.341713	0.839034	-2.216637
36H	6.124197	1.984102	-0.879280
37H	7.016976	0.484029	-0.615360
38H	-4.157732	-1.909556	0.118002
39H	-6.608366	-1.671605	0.001784
40H	-7.654211	0.524887	-0.556719
41H	-6.171415	2.493084	-1.002833
42H	-3.709172	2.247072	-0.885024

6b-PhNCO2-005

1C	2.145111	-0.723817	-1.375089
2C	3.478359	-0.967057	-1.702223
3N	4.369512	-1.514378	-0.859269
4C	3.923050	-1.846056	0.363425
5C	2.607412	-1.660175	0.786146
6C	1.694065	-1.078900	-0.100188
7N	0.350287	-0.817674	0.313255
8S	-0.875201	-1.780424	-0.386563
9O	-1.150671	-3.010157	0.375808
10O	-0.498409	-1.940050	-1.807219
11C	-2.301156	-0.700391	-0.307180
12C	-3.275620	-0.900737	0.669269
13C	-4.391473	-0.063105	0.687080
14C	-4.540855	0.970810	-0.250509
15C	-3.539780	1.146631	-1.220796
16C	-2.420286	0.316650	-1.257893
17C	-5.735022	1.892193	-0.203362
18C	0.107760	-0.227674	1.677756
19O	-0.745204	-0.799083	2.379099
20N	0.852364	0.809960	1.996961
21C	1.459924	1.643046	1.066575
22C	2.795452	2.057839	1.268984
23C	3.420675	2.941352	0.387568
24C	2.733076	3.453165	-0.720674
25C	1.401456	3.067438	-0.924326
26C	0.772276	2.183356	-0.047624
27H	1.474386	-0.259743	-2.086702
28H	3.852133	-0.694563	-2.687249
29H	4.652291	-2.289158	1.038798
30H	2.302596	-1.946352	1.787473
31H	-3.149430	-1.686901	1.404180
32H	-5.155507	-0.213867	1.446125
33H	-3.639923	1.938891	-1.959335
34H	-1.655186	0.452665	-2.015624
35H	-5.504799	2.794362	0.380164
36H	-6.029510	2.219052	-1.207222
37H	-6.597540	1.408201	0.267991
38H	3.336479	1.656422	2.122768
39H	4.455413	3.229229	0.564897
40H	3.221818	4.141502	-1.406218
41H	0.845029	3.462860	-1.772841
42H	-0.262442	1.895757	-0.211942

6b-PhNCO-001

1C	0.785066	-0.729254	0.916441
2C	-0.483832	-0.263060	1.149595
3N	-1.531319	-0.553171	0.332880
4C	-1.314847	-1.355730	-0.752444
5C	-0.074943	-1.853603	-1.040135
6C	1.064744	-1.549947	-0.224887
7N	2.246561	-2.053933	-0.629911
8S	3.636532	-1.725577	0.174864
9O	4.706590	-2.440025	-0.558428
10O	3.551174	-1.965891	1.640736
11C	3.931121	0.044207	-0.044954
12C	3.981548	0.567109	-1.342506
13C	4.206260	1.930248	-1.519393
14C	4.385191	2.788048	-0.418566
15C	4.333965	2.237528	0.869017
16C	4.104559	0.871312	1.063205
17C	4.613619	4.265094	-0.632517
18C	-2.895766	0.033109	0.655541
19O	-2.924760	0.715924	1.696495
20N	-3.778678	-0.305719	-0.250023
21C	-5.106692	0.116014	-0.190553
22C	-5.693899	0.951616	0.792863
23C	-7.046832	1.298187	0.718255
24C	-7.859619	0.834731	-0.321428
25C	-7.293243	0.006716	-1.300551
26C	-5.946139	-0.343298	-1.234964
27H	1.562097	-0.470294	1.622712
28H	-0.728068	0.362966	1.998217

29H	-2.190403	-1.554888	-1.354613
30H	0.057640	-2.483413	-1.913738
31H	3.841689	-0.083997	-2.200652
32H	4.242879	2.338582	-2.527276
33H	4.470989	2.881322	1.734940
34H	4.061398	0.451924	2.063456
35H	4.862141	4.774552	0.304772
36H	5.431029	4.442154	-1.342718
37H	3.717020	4.744968	-1.047090
38H	-5.083417	1.320431	1.607086
39H	-7.468283	1.941655	1.488834
40H	-8.910488	1.110723	-0.369173
41H	-7.904870	-0.367257	-2.119596
42H	-5.507420	-0.984672	-1.996155

6b-PhNCO-002

1C	0.410116	-2.436043	1.169525
2C	-0.923266	-2.149008	1.274340
3N	-1.528776	-1.233625	0.463694
4C	-0.779838	-0.601273	-0.481946
5C	0.559569	-0.845121	-0.641170
6C	1.242223	-1.783631	0.202924
7N	2.548509	-2.113505	0.209473
8S	3.621686	-1.394895	-0.801679
9O	3.172858	-1.348942	-2.219433
10O	4.925855	-2.042609	-0.533116
11C	3.754277	0.317267	-0.239410
12C	3.409921	1.368663	-1.087691
13C	3.501889	2.683836	-0.620848
14C	3.928038	2.961180	0.685039
15C	4.272793	1.881922	1.518774
16C	4.189566	0.566647	1.067370
17C	3.993569	4.377961	1.201953
18C	-3.012433	-0.958791	0.647882
19O	-3.547860	-1.634095	1.546647
20N	-3.429171	-0.046448	-0.193452
21C	-4.752435	0.392272	-0.225460
22C	-5.049855	1.379073	-1.197213
23C	-6.331513	1.907705	-1.336546
24C	-7.373281	1.470781	-0.506549
25C	-7.099565	0.496678	0.459204
26C	-5.816425	-0.040347	0.606106
27H	0.852881	-3.167490	1.837450
28H	-1.574628	-2.620457	1.998592
29H	-1.323706	0.104022	-1.095474
30H	1.082103	-0.322308	-1.430472
31H	3.078506	1.161819	-2.100334
32H	3.234664	3.503509	-1.284108
33H	4.609265	2.077282	2.534879
34H	4.454616	-0.258552	1.721992
35H	4.907198	4.549020	1.783886
36H	3.967046	5.106700	0.384440
37H	3.143179	4.590342	1.864365
38H	-4.242782	1.719547	-1.842157
39H	-6.519321	2.664500	-2.095916
40H	-8.374930	1.881119	-0.611787
41H	-7.895617	0.144491	1.113193
42H	-5.626306	-0.793612	1.359802

6b-PhNCO-003

1C	-0.552374	-0.865727	0.646626
2C	0.787028	-0.621261	0.488388
3N	1.530082	-1.229203	-0.477677
4C	0.919291	-2.122346	-1.308854
5C	-0.413615	-2.411427	-1.203835
6C	-1.240530	-1.780803	-0.218551
7N	-2.547878	-2.106283	-0.229322
8S	-3.618479	-1.399118	0.792575
9O	-3.167473	-1.367471	2.210055
10O	-4.923414	-2.043532	0.519958
11C	-3.751962	0.318163	0.246548
12C	-3.389241	1.361559	1.096305
13C	-3.482138	2.681211	0.640296
14C	-3.929160	2.969837	-0.655544
15C	-4.288547	1.897454	-1.492892
16C	-4.204559	0.579123	-1.052679
17C	-4.032924	4.390753	-1.155181
18C	3.010114	-0.941083	-0.670914
19O	3.526881	-1.548293	-1.627235
20N	3.445943	-0.097497	0.230316
21C	4.762309	0.362016	0.246951
22C	5.124374	1.157447	1.361403

23C	6.403040	1.695634	1.492649
24C	7.374451	1.465698	0.508507
25C	7.034471	0.685372	-0.601618
26C	5.755674	0.135900	-0.738965
27H	-1.071021	-0.361683	1.450523
28H	1.335278	0.066451	1.117812
29H	1.565867	-2.573828	-2.049902
30H	-0.860753	-3.125316	-1.887693
31H	-3.042365	1.146326	2.101949
32H	-3.198954	3.494052	1.305278
33H	-4.637262	2.102149	-2.503142
34H	-4.481195	-0.240114	-1.709899
35H	-5.068499	4.639669	-1.421693
36H	-3.696748	5.109586	-0.400431
37H	-3.424463	4.537706	-2.056827
38H	4.370028	1.340490	2.123515
39H	6.642801	2.299452	2.365888
40H	8.372928	1.885431	0.606389
41H	7.775121	0.495474	-1.376673
42H	5.515710	-0.469827	-1.603561

6b-PhNCO-004

1C	-0.011842	-1.433193	-0.034094
2C	-1.378445	-1.536535	-0.033043
3N	-2.193999	-0.446871	-0.013933
4C	-1.627104	0.797521	0.002434
5C	-0.271489	0.969834	0.000993
6C	0.626447	-0.148665	-0.016168
7N	1.943297	0.123193	-0.013059
8S	3.032916	-1.108469	-0.026348
9O	3.001625	-1.874528	-1.303329
10O	2.986383	-1.923966	1.218570
11C	4.562329	-0.164806	0.000431
12C	5.069094	0.352950	-1.195024
13C	6.254004	1.086253	-1.169684
14C	6.944195	1.312047	0.034452
15C	6.413291	0.778414	1.217321
16C	5.225681	0.040757	1.208833
17C	8.234831	2.095416	0.036819
18C	-3.696751	-0.657436	-0.010762
19O	-4.045864	-1.852743	-0.032476
20N	-4.333303	0.487333	0.017017
21C	-5.725406	0.566485	0.021115
22C	-6.642945	-0.514290	-0.017666
23C	-8.021668	-0.279558	-0.012525
24C	-8.537768	1.019685	0.031121
25C	-7.643283	2.098298	0.070738
26C	-6.268018	1.874368	0.065231
27H	0.571151	-2.345647	-0.049272
28H	-1.891424	-2.489553	-0.047006
29H	-2.331823	1.617341	0.016595
30H	0.139110	1.974246	0.014485
31H	4.544234	0.180244	-2.129687
32H	6.652042	1.490025	-2.098473
33H	6.933009	0.938347	2.159324
34H	4.822434	-0.373028	2.127832
35H	8.597647	2.271329	1.055190
36H	9.020467	1.558570	-0.511486
37H	8.109106	3.069693	-0.452154
38H	-6.265129	-1.527987	-0.051026
39H	-8.700472	-1.130236	-0.043665
40H	-9.611901	1.189917	0.034806
41H	-8.019947	3.118864	0.105327
42H	-5.575202	2.712422	0.095345

6b-PhNCO-005

1C	-0.010780	1.445064	-0.034036
2C	-1.377723	1.544988	-0.030345
3N	-2.190525	0.453217	-0.012302
4C	-1.620601	-0.789841	0.000242
5C	-0.264666	-0.958772	-0.003645
6C	0.630479	0.161993	-0.019682
7N	1.947673	-0.107363	-0.018827
8S	3.036915	1.124519	-0.031763
9O	2.990575	1.940074	1.213127
10O	3.006028	1.890440	-1.308781
11C	4.563886	0.176769	-0.003917
12C	5.225869	-0.030570	1.205707
13C	6.405925	-0.778756	1.216644
14C	6.930551	-1.324384	0.035507
15C	6.246480	-1.090609	-1.169769
16C	5.068005	-0.345588	-1.197608

17C	8.183425	-2.167012	0.055549
18C	-3.693957	0.659392	-0.006637
19O	-4.046666	1.853724	-0.022124
20N	-4.326889	-0.487485	0.015496
21C	-5.718664	-0.571451	0.020888
22C	-6.256541	-1.881584	0.055517
23C	-7.630959	-2.110502	0.061710
24C	-8.529310	-1.034756	0.032590
25C	-8.017925	0.266621	-0.001602
26C	-6.640027	0.506357	-0.007553
27H	0.570262	2.358859	-0.048373
28H	-1.893148	2.496738	-0.041228
29H	-2.323380	-1.611315	0.013444
30H	0.148537	-1.962152	0.006979
31H	4.827024	0.391385	2.122916
32H	6.925747	-0.938342	2.158750
33H	6.642708	-1.497228	-2.097914
34H	4.547554	-0.167303	-2.133695
35H	8.807262	-1.978137	-0.825923
36H	8.785678	-1.972575	0.949869
37H	7.932171	-3.236677	0.052625
38H	-5.560653	-2.717348	0.077570
39H	-8.003911	-3.132670	0.088730
40H	-9.602814	-1.208911	0.036955
41H	-8.699858	1.115054	-0.024458
42H	-6.265931	1.521680	-0.033743

6b-PhNCO-006

1C	0.526100	-2.702324	-1.224807
2C	1.867157	-2.449646	-1.127817
3N	2.380695	-1.693742	-0.117394
4C	1.549631	-1.243746	0.858204
5C	0.198711	-1.476634	0.833898
6C	-0.399873	-2.183599	-0.260858
7N	-1.706928	-2.406994	-0.499418
8S	-2.871618	-1.727027	0.436316
9O	-2.667937	-1.929745	1.896292
10O	-4.162495	-2.181769	-0.128155
11C	-2.749133	0.049608	0.128731
12C	-2.378570	0.921885	1.150468
13C	-2.239715	2.285484	0.870973
14C	-2.463452	2.787232	-0.417147
15C	-2.843117	1.886313	-1.429003
16C	-2.986410	0.526155	-1.166413
17C	-2.298350	4.255155	-0.728657
18C	3.880905	-1.367977	-0.123600
19O	4.588470	-2.351927	-0.390443
20N	4.233844	-0.145998	0.179634
21C	3.389981	0.962265	0.131182
22C	2.480294	1.209126	-0.924369
23C	1.676426	2.350012	-0.929645
24C	1.764112	3.291992	0.101760
25C	2.685299	3.078576	1.135461
26C	3.490057	1.937986	1.147830
27H	0.147231	-3.284809	-2.058113
28H	2.589505	-2.817611	-1.846385
29H	2.016898	-0.688971	1.661945
30H	-0.398665	-1.116917	1.659696
31H	-2.200530	0.541862	2.151249
32H	-1.941951	2.963013	1.667859
33H	-3.023105	2.257768	-2.436028
34H	-3.272623	-0.160788	-1.957588
35H	-1.968133	4.818680	0.150233
36H	-1.560096	4.408456	-1.526206
37H	-3.242332	4.694929	-1.076301
38H	2.400845	0.491497	-1.736574
39H	0.974360	2.500407	-1.747097
40H	1.130520	4.175494	0.097807
41H	2.775572	3.804489	1.941413
42H	4.200488	1.772435	1.954591

6b-001

1C	-3.045697	-0.478503	-1.163767
2C	-3.717728	-1.642293	-0.824059
3N	-3.500718	-2.350764	0.305362
4C	-2.562795	-1.844129	1.126802
5C	-1.831549	-0.684062	0.891151
6C	-2.048762	0.057486	-0.303159
7N	-1.415708	1.200042	-0.727352
8S	-0.198997	1.849240	0.110776
9O	0.243861	3.052392	-0.641855
10O	-0.472310	2.055734	1.563925

11C	1.179460	0.671141	0.030931
12C	1.752895	0.162393	1.194925
13C	2.808819	-0.751328	1.101565
14C	3.296963	-1.170168	-0.143022
15C	2.703760	-0.640510	-1.303504
16C	1.652490	0.270347	-1.224262
17C	4.418528	-2.175933	-0.249799
18H	-3.269420	0.034497	-2.095533
19H	-4.477585	-2.039979	-1.496341
20H	-2.382817	-2.404582	2.044322
21H	-1.114866	-0.352470	1.632631
22H	1.377802	0.479151	2.162972
23H	3.253314	-1.145586	2.013138
24H	3.069819	-0.950581	-2.280445
25H	1.199137	0.666555	-2.128532
26H	5.187753	-1.841160	-0.956874
27H	4.899533	-2.346907	0.719561
28H	4.045560	-3.143382	-0.612758

6b-002

1C	-2.933934	1.726066	-0.004736
2C	-4.317650	1.809589	0.005564
3N	-5.151098	0.746970	0.016821
4C	-4.544812	-0.455987	0.017506
5C	-3.169537	-0.659696	0.007951
6C	-2.288862	0.458355	-0.003705
7N	-0.918180	0.450120	-0.013065
8S	-0.116002	-0.956040	-0.013781
9O	-0.296722	-1.755863	1.237244
10O	-0.282460	-1.744185	-1.274269
11C	1.580244	-0.346181	-0.002000
12C	2.233590	-0.096888	-1.211629
13C	3.546055	0.374807	-1.195392
14C	4.221418	0.603932	0.015758
15C	3.543100	0.343056	1.215364
16C	2.227986	-0.130514	1.213762
17C	5.648634	1.098547	0.012133
18H	-2.327380	2.628251	-0.013597
19H	-4.796102	2.788910	0.004827
20H	-5.207953	-1.320880	0.026697
21H	-2.783654	-1.673523	0.010689
22H	1.719215	-0.276667	-2.150796
23H	4.056615	0.567281	-2.137180
24H	4.048231	0.509057	2.164501
25H	1.711396	-0.335575	2.146495
26H	6.002026	1.316010	1.025983
27H	6.323667	0.350667	-0.425163
28H	5.750981	2.013339	-0.585504

6cg-Me2-001

1C	4.905445	-0.336390	-1.457337
2C	4.860720	-0.872569	-2.746048
3N	4.518636	-2.140538	-3.017451
4C	4.221349	-2.927959	-1.970088
5C	4.243623	-2.499018	-0.644590
6C	4.582235	-1.166849	-0.377166
7N	4.605637	-0.700471	0.976034
8S	3.070564	-0.483529	1.708970
9O	3.334016	-0.197095	3.126344
10O	2.248368	-1.638993	1.327351
11C	2.374216	0.975817	0.958263
12C	2.468381	2.213504	1.611662
13C	1.961332	3.348501	0.993592
14C	1.376614	3.257786	-0.283603
15C	1.302233	2.016642	-0.937070
16C	1.799751	0.874793	-0.311931
17O	0.902307	4.417106	-0.797752
18C	0.306340	4.403634	-2.101185
19C	5.581576	0.353977	1.318310
20H	5.174665	0.704282	-1.315069
21H	5.104225	-0.245503	-3.601215
22H	3.959200	-3.957961	-2.201752
23H	4.001074	-3.177179	0.164628
24H	2.919874	2.278621	2.596357
25H	2.006432	4.316447	1.483381
26H	0.851715	1.922126	-1.916096
27H	1.722080	-0.085972	-0.808541
28H	-0.006102	5.431886	-2.290018
29H	1.034848	4.096076	-2.861044
30H	-0.569815	3.746277	-2.129017
31H	6.546666	0.055019	0.903478
32H	5.306470	1.340659	0.923323

33H	5.667614	0.410180	2.403862
34P	-2.510796	-0.387633	0.012504
35C	-2.096070	-0.879352	1.707347
36C	-4.101739	-1.107895	-0.473813
37C	-2.642517	1.423163	-0.086849
38C	-1.206012	-0.970925	-1.107752
39C	-5.296621	-0.556041	0.022743
40C	-6.517594	-1.145166	-0.305827
41C	-6.552153	-2.276753	-1.128761
42C	-5.364743	-2.820851	-1.626759
43C	-4.136478	-2.240771	-1.301609
44C	-1.946405	2.235570	0.823023
45C	-2.027676	3.624817	0.713631
46C	-2.799317	4.207221	-0.295539
47C	-3.491635	3.399547	-1.203762
48C	-3.417258	2.009332	-1.103457
49C	-0.479517	-2.133399	-0.801682
50C	0.512155	-2.579931	-1.676397
51C	0.779054	-1.878631	-2.855361
52C	0.043311	-0.730503	-3.168768
53C	-0.946939	-0.273347	-2.299398
54C	-3.082485	-1.362960	2.582246
55C	-2.738579	-1.684091	3.897144
56C	-1.420782	-1.529694	4.339776
57C	-0.436369	-1.059400	3.465001
58C	-0.771220	-0.732709	2.151546
59H	-5.276401	0.326339	0.656771
60H	-7.440093	-0.719195	0.078581
61H	-7.505499	-2.731855	-1.383677
62H	-5.390953	-3.695728	-2.270405
63H	-3.217912	-2.667772	-1.692832
64H	-1.345064	1.797236	1.612730
65H	-1.484731	4.249285	1.416669
66H	-2.858903	5.289175	-0.376110
67H	-4.093911	3.849102	-1.988493
68H	-3.965309	1.390215	-1.807935
69H	-0.663501	-2.678036	0.118690
70H	1.086480	-3.465690	-1.423593
71H	1.567581	-2.216767	-3.521460
72H	0.249490	-0.183106	-4.084517
73H	-1.499570	0.628026	-2.545506
74H	-4.106440	-1.497480	2.249017
75H	-3.501078	-2.061763	4.572759
76H	-1.158782	-1.786132	5.362801
77H	0.593144	-0.955862	3.795002
78H	0.000632	-0.389650	1.473345

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1C	4.936214	-0.307763	-1.451524
2C	4.891146	-0.847737	-2.738598
3N	4.557139	-2.118812	-3.005477
4C	4.269843	-2.905594	-1.954858
5C	4.293340	-2.472952	-0.630600
6C	4.621971	-1.137294	-0.367805
7N	4.643315	-0.665924	0.983782
8S	3.106777	-0.462998	1.719455
9O	3.369842	-0.155734	3.132572
10O	2.300078	-1.634026	1.353105
11C	2.387572	0.977535	0.952749
12C	2.427286	2.218709	1.604661
13C	1.885559	3.333002	0.977684
14C	1.321560	3.218860	-0.307058
15C	1.301714	1.974550	-0.958597
16C	1.832658	0.853602	-0.324002
17O	0.811498	4.358834	-0.830124
18C	0.225433	4.319728	-2.137793
19C	5.605780	0.403230	1.318462
20H	5.198136	0.735339	-1.313381
21H	5.127146	-0.221174	-3.596254
22H	4.014092	-3.938003	-2.183032
23H	4.058149	-3.150713	0.181087
24H	2.861087	2.302197	2.595822
25H	1.887969	4.302839	1.465867
26H	0.866577	1.861075	-1.942619
27H	1.791622	-0.111319	-0.816263
28H	-0.132039	5.332993	-2.327463
29H	0.972713	4.046215	-2.892438
30H	-0.619380	3.623290	-2.171679
31H	6.572468	0.118398	0.897473
32H	5.312818	1.385099	0.924145
33H	5.698257	0.462082	2.403291
34P	-2.517100	-0.387633	0.008408
35C	-2.075073	-0.718202	1.735966
36C	-4.069174	-1.230335	-0.403999
37C	-2.737317	1.401165	-0.231015

38C	-1.185294	-0.991196	-1.070105
39C	-5.294851	-0.661725	-0.014094
40C	-6.486172	-1.337875	-0.278731
41C	-6.460645	-2.576803	-0.928459
42C	-5.242066	-3.141290	-1.316946
43C	-4.043765	-2.472735	-1.057637
44C	-2.111833	2.308752	0.639493
45C	-2.253400	3.681767	0.429976
46C	-3.016617	4.154000	-0.640974
47C	-3.640222	3.251875	-1.509627
48C	-3.504348	1.877210	-1.309595
49C	-0.435732	-2.120038	-0.699787
50C	0.567253	-2.592928	-1.547291
51C	0.824519	-1.950203	-2.761396
52C	0.070438	-0.832797	-3.135192
53C	-0.932359	-0.350438	-2.294213
54C	-3.042818	-1.154474	2.655217
55C	-2.683417	-1.354875	3.989775
56C	-1.368692	-1.125536	4.408203
57C	-0.403577	-0.698062	3.490917
58C	-0.753905	-0.493762	2.156927
59H	-5.322501	0.301786	0.487526
60H	-7.432173	-0.895809	0.021342
61H	-7.390615	-3.099988	-1.134611
62H	-5.220992	-4.100764	-1.826023
63H	-3.103181	-2.917438	-1.368155
64H	-1.519727	1.956383	1.477993
65H	-1.763017	4.378532	1.103118
66H	-3.124748	5.223464	-0.800243
67H	-4.237474	3.615681	-2.341189
68H	-4.001015	1.185962	-1.984081
69H	-0.613617	-2.617663	0.248298
70H	1.158490	-3.451847	-1.246347
71H	1.620549	-2.308471	-3.407716
72H	0.270754	-0.327796	-4.076251
73H	-1.499331	0.526440	-2.589030
74H	-4.063773	-1.346816	2.340854
75H	-3.430725	-1.698719	4.699460
76H	-1.093530	-1.289404	5.446701
77H	0.623257	-0.535343	3.805856
78H	0.001256	-0.179700	1.447161

6cg-Me2-003

1C	-3.626825	2.372959	1.485068
2C	-3.091597	2.900054	2.662170
3N	-1.939749	3.584067	2.721678
4C	-1.290628	3.779504	1.561276
5C	-1.740731	3.309689	0.330028
6C	-2.932408	2.572195	0.284697
7N	-3.417953	2.079353	-0.964829
8S	-2.499564	0.821148	-1.695284
9O	-1.086599	1.160716	-1.489611
10O	-3.038835	0.671162	-3.052895
11C	-2.871678	-0.649459	-0.764881
12C	-2.245354	-0.847760	0.474576
13C	-2.549968	-1.978981	1.214973
14C	-3.478673	-2.918770	0.726454
15C	-4.108252	-2.708079	-0.511833
16C	-3.804676	-1.564428	-1.253306
17O	-3.693097	-3.994042	1.521916
18C	-4.612697	-5.007496	1.091454
19C	-4.876433	1.903522	-1.109690
20H	-4.557800	1.818286	1.520209
21H	-3.613294	2.751321	3.605271
22H	-0.365348	4.348984	1.617311
23H	-1.184695	3.510361	-0.577066
24H	-1.515531	-0.137322	0.844970
25H	-2.067996	-2.159241	2.170277
26H	-4.825584	-3.417622	-0.906898
27H	-4.280747	-1.398911	-2.214543
28H	-4.285388	-5.459016	0.147311
29H	-4.604564	-5.761615	1.880304
30H	-5.624513	-4.598748	0.983837
31H	-5.357245	2.813567	-0.744369
32H	-5.110136	1.784239	-2.168182
33H	-5.261986	1.039565	-0.552848
34P	2.452720	-0.205746	-0.030049
35C	1.491656	-0.341439	1.506145
36C	3.964053	-1.188544	0.168555
37C	1.494004	-0.839069	-1.433263
38C	2.880397	1.530491	-0.340870
39C	4.461005	-1.941746	-0.906463
40C	5.649727	-2.659527	-0.756077
41C	6.340511	-2.628536	0.458908
42C	5.844385	-1.878583	1.531122

43C	4.657572	-1.158711	1.391600
44C	0.536832	-1.844975	-1.234556
45C	-0.181913	-2.341365	-2.321995
46C	0.050097	-1.839026	-3.605286
47C	1.010473	-0.842549	-3.805204
48C	1.735269	-0.340552	-2.724221
49C	1.893543	2.408095	-0.826699
50C	2.205084	3.753837	-1.022548
51C	3.490822	4.228432	-0.741406
52C	4.472451	3.353498	-0.267444
53C	4.172689	2.004238	-0.065703
54C	0.808202	0.769858	2.022976
55C	0.039570	0.635743	3.181309
56C	-0.046664	-0.601251	3.826601
57C	0.640528	-1.708462	3.317263
58C	1.411430	-1.583622	2.160987
59H	3.926243	-1.976999	-1.850923
60H	6.030809	-3.246213	-1.587352
61H	7.263455	-3.190847	0.572872
62H	6.377931	-1.856107	2.477285
63H	4.273751	-0.584844	2.230444
64H	0.329524	-2.228318	-0.241540
65H	-0.935117	-3.107153	-2.160709
66H	-0.523933	-2.215436	-4.447675
67H	1.188419	-0.445980	-4.800845
68H	2.469793	0.442136	-2.887556
69H	0.898818	2.046251	-1.064308
70H	1.443703	4.429532	-1.402787
71H	3.729006	5.276992	-0.899090
72H	5.475071	3.716109	-0.058230
73H	4.946410	1.334364	0.295080
74H	0.869293	1.736395	1.535790
75H	-0.488528	1.500498	3.571977
76H	-0.644902	-0.702257	4.728172
77H	0.579037	-2.669888	3.819520
78H	1.949597	-2.446031	1.778075

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1C	-4.414652	-1.381120	1.495398
2C	-4.116087	-1.789616	2.797149
3N	-3.199072	-2.720056	3.097766
4C	-2.551145	-3.288956	2.067349
5C	-2.778109	-2.965895	0.731664
6C	-3.728206	-1.980864	0.432062
7N	-3.988175	-1.631563	-0.931156
8S	-2.741464	-0.750141	-1.719266
9O	-3.160410	-0.624140	-3.121738
10O	-1.476415	-1.418573	-1.382247
11C	-2.737912	0.864358	-0.973331
12C	-3.449405	1.916958	-1.564747
13C	-3.444109	3.163051	-0.953346
14C	-2.739867	3.360392	0.249183
15C	-2.047223	2.292861	0.845483
16C	-2.048300	1.045102	0.226951
17O	-2.778381	4.618538	0.750434
18C	-2.110386	4.894356	1.988072
19C	-5.347132	-1.155134	-1.260149
20H	-5.160045	-0.611170	1.330508
21H	-4.637093	-1.335809	3.637738
22H	-1.816576	-4.049052	2.321635
23H	-2.234317	-3.464544	-0.061294
24H	-3.979000	1.764942	-2.499710
25H	-3.970977	4.003006	-1.395910
26H	-1.496594	2.426196	1.769160
27H	-1.497119	0.223324	0.668409
28H	-2.280136	5.954875	2.181250
29H	-2.537275	4.300925	2.805285
30H	-1.033382	4.704284	1.907656
31H	-6.057360	-1.853407	-0.811615
32H	-5.549441	-0.142612	-0.887063
33H	-5.471801	-1.174235	-2.342981
34P	2.507396	-0.114557	-0.037282
35C	2.750387	-1.472382	-1.215629
36C	4.114064	0.491356	0.547710
37C	1.632816	1.273352	-0.818400
38C	1.548416	-0.735837	1.372640
39C	4.885771	1.317192	-0.289477
40C	6.138644	1.757152	0.138194
41C	6.623682	1.379547	1.395518
42C	5.854883	0.561700	2.228544
43C	4.599563	0.114682	1.809392
44C	0.797870	1.063967	-1.926947
45C	0.102587	2.139476	-2.482560
46C	0.232587	3.419227	-1.938425
47C	1.065969	3.630084	-0.834748

48C	1.766127	2.563114	-0.271826
49C	1.680046	-2.074778	1.778351
50C	0.984294	-2.528885	2.899802
51C	0.159511	-1.657086	3.617114
52C	0.031357	-0.324362	3.214799
53C	0.723537	0.140209	2.095882
54C	4.008019	-1.702559	-1.796166
55C	4.160440	-2.734306	-2.725153
56C	3.067301	-3.532030	-3.076577
57C	1.816099	-3.305381	-2.493263
58C	1.652759	-2.281094	-1.560743
59H	4.510498	1.620211	-1.263146
60H	6.733424	2.395719	-0.509000
61H	7.598975	1.726444	1.726431
62H	6.227577	0.271846	3.207100
63H	4.007252	-0.517043	2.464490
64H	0.676122	0.075690	-2.355576
65H	-0.546860	1.969619	-3.336134
66H	-0.315341	4.251486	-2.371383
67H	1.172053	4.625238	-0.411583
68H	2.417408	2.739295	0.579006
69H	2.314253	-2.760569	1.224915
70H	1.081388	-3.566397	3.206981
71H	-0.394696	-2.018477	4.478176
72H	-0.618656	0.350366	3.765056
73H	0.606163	1.172447	1.781682
74H	4.865177	-1.094309	-1.525868
75H	5.134741	-2.913551	-3.171362
76H	3.190593	-4.332219	-3.801537
77H	0.963496	-3.922538	-2.762817
78H	0.677257	-2.111747	-1.117462

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1C	4.728045	-1.891608	-0.659914
2C	4.977007	-2.233256	-1.990558
3N	4.112078	-2.903616	-2.765922
4C	2.949186	-3.268474	-2.200886
5C	2.602799	-2.990099	-0.880522
6C	3.508349	-2.274617	-0.086376
7N	3.184781	-1.974372	1.274979
8S	1.933107	-0.816562	1.497652
9O	1.726733	-0.728047	2.950334
10O	0.827364	-1.218075	0.618215
11C	2.581541	0.729758	0.906199
12C	3.300300	1.561745	1.777044
13C	3.840352	2.743885	1.292678
14C	3.671079	3.099391	-0.059242
15C	2.957776	2.255001	-0.926485
16C	2.416734	1.066134	-0.438859
17O	4.226658	4.278682	-0.428120
18C	4.105888	4.708039	-1.791015
19C	4.309974	-1.832119	2.220524
20H	5.472407	-1.335423	-0.101295
21H	5.917086	-1.943660	-2.455364
22H	2.258046	-3.819404	-2.833767
23H	1.650763	-3.313372	-0.478419
24H	3.414094	1.294869	2.822717
25H	4.390050	3.414305	1.946434
26H	2.813106	2.513611	-1.968697
27H	1.854441	0.415519	-1.099450
28H	4.638899	5.658605	-1.845520
29H	4.571340	3.987559	-2.473909
30H	3.054349	4.860503	-2.062776
31H	4.966573	-2.693198	2.077846
32H	4.885796	-0.910463	2.068723
33H	3.918478	-1.853180	3.237495
34P	-2.566550	0.055236	-0.084965
35C	-3.063823	-0.988319	1.313833
36C	-4.044457	0.764935	-0.867914
37C	-1.530487	1.434508	0.481724
38C	-1.685602	-0.963941	-1.301028
39C	-4.646529	1.903476	-0.303995
40C	-5.809147	2.425570	-0.871765
41C	-6.373489	1.818476	-1.998871
42C	-5.775079	0.686363	-2.559943
43C	-4.611394	0.155834	-1.998350
44C	-0.910477	1.396135	1.739323
45C	-0.103330	2.460072	2.145201
46C	0.090513	3.558509	1.304559
47C	-0.530108	3.600119	0.051776
48C	-1.343634	2.545186	-0.361790
49C	-2.016860	-2.320456	-1.445465
50C	-1.387291	-3.086311	-2.429296
51C	-0.432787	-2.504743	-3.268140
52C	-0.101355	-1.153945	-3.121923

53C	-0.724433	-0.382206	-2.141828
54C	-4.363021	-0.899210	1.839374
55C	-4.721740	-1.690827	2.932802
56C	-3.792758	-2.567545	3.500843
57C	-2.499567	-2.657433	2.974626
58C	-2.129596	-1.873268	1.881842
59H	-4.211035	2.383876	0.567494
60H	-6.270492	3.306910	-0.434801
61H	-7.276589	2.230593	-2.441164
62H	-6.209362	0.216702	-3.438187
63H	-4.149806	-0.719284	-2.445296
64H	-1.041337	0.546502	2.399955
65H	0.380984	2.420640	3.116103
66H	0.725405	4.380570	1.623212
67H	-0.384773	4.454687	-0.603300
68H	-1.838254	2.596172	-1.327585
69H	-2.754501	-2.782839	-0.796830
70H	-1.643361	-4.136892	-2.535604
71H	0.056962	-3.102934	-4.031311
72H	0.650591	-0.704020	-3.764342
73H	-0.451539	0.661624	-2.029585
74H	-5.095580	-0.227935	1.403102
75H	-5.728478	-1.622931	3.335632
76H	-4.076263	-3.181908	4.351317
77H	-1.774672	-3.337674	3.413206
78H	-1.124312	-1.944795	1.480103

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1C	3.513097	2.619623	-1.348688
2C	3.019405	3.268909	-2.482338
3N	1.870232	3.959444	-2.510048
4C	1.176870	4.029931	-1.360542
5C	1.584947	3.433931	-0.170140
6C	2.777204	2.696763	-0.159650
7N	3.230572	2.094922	1.052431
8S	2.317794	0.767536	1.650795
9O	0.914442	1.046083	1.323541
10O	2.736705	0.591093	3.047464
11C	2.854975	-0.650700	0.717106
12C	2.353912	-0.850319	-0.578420
13C	2.800955	-1.934989	-1.316983
14C	3.746404	-2.825639	-0.772514
15C	4.247020	-2.615231	0.523295
16C	3.801605	-1.518718	1.263447
17O	4.106780	-3.855928	-1.574688
18C	5.064801	-4.808929	-1.093363
19C	4.686395	1.946285	1.240658
20H	4.445491	2.069204	-1.406318
21H	3.574341	3.219377	-3.416837
22H	0.251722	4.601758	-1.390208
23H	0.997037	3.539733	0.733054
24H	1.614292	-0.177175	-0.996586
25H	2.423139	-2.115948	-2.317819
26H	4.974179	-3.289187	0.961014
27H	4.178551	-1.353090	2.267496
28H	4.695659	-5.316333	-0.194128
29H	5.185130	-5.534163	-1.899584
30H	6.027541	-4.326277	-0.886425
31H	5.151929	2.902330	0.991203
32H	4.882011	1.726048	2.290996
33H	5.121640	1.156055	0.615802
34P	-2.432711	-0.279177	0.015277
35C	-1.356671	-0.254540	-1.447244
36C	-3.867972	-1.319219	-0.378755
37C	-1.560748	-0.966991	1.448065
38C	-2.979644	1.406559	0.406262
39C	-4.405673	-2.181882	0.589118
40C	-5.533509	-2.947088	0.283461
41C	-6.123837	-2.855228	-0.980359
42C	-5.586187	-1.997575	-1.946620
43C	-4.458945	-1.230368	-1.651690
44C	-0.506149	-1.872633	1.262626
45C	0.146038	-2.412016	2.371038
46C	-0.247951	-2.049669	3.662277
47C	-1.303205	-1.151154	3.847875
48C	-1.963577	-0.607748	2.745266
49C	-2.094633	2.280926	1.062717
50C	-2.491167	3.592671	1.324988
51C	-3.761074	4.035416	0.939350
52C	-4.641117	3.163618	0.291469
53C	-4.256134	1.848027	0.023234
54C	-0.763962	0.939991	-1.883033
55C	0.065342	0.931610	-3.006700
56C	0.309487	-0.262479	-3.690886
57C	-0.280646	-1.454346	-3.257091

58C	-1.116243	-1.454702	-2.140230
59H	-3.948824	-2.266713	1.570187
60H	-5.945082	-3.618277	1.032168
61H	-6.999819	-3.454122	-1.215043
62H	-6.040559	-1.927913	-2.931040
63H	-4.039661	-0.574921	-2.409765
64H	-0.171736	-2.140487	0.266488
65H	0.973996	-3.099309	2.222766
66H	0.272862	-2.459356	4.523499
67H	-1.607546	-0.864097	4.850534
68H	-2.773588	0.099028	2.898860
69H	-1.109569	1.942082	1.365543
70H	-1.808093	4.266591	1.834888
71H	-4.065597	5.057544	1.148415
72H	-5.630846	3.502525	-0.001986
73H	-4.951077	1.177312	-0.471777
74H	-0.938434	1.872462	-1.357799
75H	0.521045	1.858604	-3.339520
76H	0.958428	-0.264232	-4.562656
77H	-0.094279	-2.383951	-3.787779
78H	-1.583839	-2.381125	-1.818750

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1C	-1.194358	-1.930552	-0.683749
2C	-1.397335	-3.306145	-0.765949
3N	-2.086328	-4.020757	0.140184
4C	-2.612154	-3.341486	1.169828
5C	-2.483282	-1.961987	1.341224
6C	-1.752955	-1.232247	0.394962
7N	-1.535004	0.175035	0.532539
8S	-2.292809	1.171292	-0.660728
9O	-1.944479	0.600683	-1.967023
10O	-1.884543	2.542289	-0.319523
11C	-4.041825	1.002941	-0.398814
12C	-4.693994	1.873021	0.488208
13C	-6.047875	1.698878	0.734512
14C	-6.755581	0.657425	0.103598
15C	-6.093468	-0.210187	-0.782711
16C	-4.732150	-0.035986	-1.029309
17O	-8.070874	0.575499	0.412863
18C	-8.875030	-0.433644	-0.213639
19C	-1.607631	0.729346	1.899943
20H	-0.611154	-1.414726	-1.434332
21H	-0.969346	-3.865189	-1.595092
22H	-3.171629	-3.925032	1.897988
23H	-2.945547	-1.483609	2.196746
24H	-4.149346	2.683212	0.961965
25H	-6.581856	2.364247	1.406308
26H	-6.621996	-1.012654	-1.283464
27H	-4.218407	-0.698839	-1.717963
28H	-9.880303	-0.294481	0.187391
29H	-8.891811	-0.300995	-1.302003
30H	-8.515208	-1.437885	0.040134
31H	-2.630197	0.762093	2.298204
32H	-0.987886	0.100439	2.542074
33H	-1.193683	1.737004	1.892038
34P	2.950071	0.131253	-0.005941
35C	2.697296	1.924514	-0.021005
36C	2.268409	-0.620244	-1.510407
37C	4.723879	-0.246988	0.048464
38C	2.140390	-0.528305	1.480726
39C	2.587940	-1.959726	-1.802462
40C	2.064240	-2.561954	-2.945678
41C	1.233254	-1.833415	-3.805325
42C	0.929176	-0.499688	-3.523359
43C	1.443864	0.111737	-2.377762
44C	5.354594	-0.574257	1.258986
45C	6.730547	-0.814793	1.278017
46C	7.475601	-0.730901	0.098183
47C	6.846306	-0.406958	-1.108932
48C	5.472888	-0.165212	-1.139188
49C	1.537752	-1.794730	1.476093
50C	0.989643	-2.305551	2.654247
51C	1.042216	-1.560029	3.835293
52C	1.636181	-0.293170	3.839370
53C	2.183157	0.227481	2.666082
54C	3.769829	2.814159	-0.185027
55C	3.524997	4.189863	-0.200636
56C	2.221107	4.675007	-0.060719
57C	1.152308	3.786152	0.101166
58C	1.387719	2.413084	0.130183
59H	3.248838	-2.525819	-1.151590
60H	2.309047	-3.597023	-3.167269
61H	0.826642	-2.306268	-4.695242
62H	0.282193	0.068607	-4.184676

63H	1.193915	1.146052	-2.170735
64H	4.784887	-0.648848	2.180172
65H	7.217059	-1.071754	2.214909
66H	8.545124	-0.922575	0.117326
67H	7.422349	-0.345074	-2.028012
68H	4.990458	0.080535	-2.081086
69H	1.473559	-2.377045	0.564333
70H	0.514204	-3.281901	2.642180
71H	0.613402	-1.961404	4.749625
72H	1.670499	0.292854	4.753573
73H	2.636739	1.214579	2.675703
74H	4.785340	2.446269	-0.293419
75H	4.354937	4.880420	-0.321978
76H	2.036469	5.745806	-0.078490
77H	0.134308	4.150528	0.197645
78H	0.556850	1.728589	0.261704

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1C	-4.127245	-1.623339	1.643524
2C	-3.640853	-2.102971	2.861677
3N	-2.636658	-2.983524	2.973481
4C	-2.089769	-3.426746	1.829029
5C	-2.506883	-3.028165	0.561197
6C	-3.547442	-2.094251	0.458441
7N	-4.009058	-1.674749	-0.828034
8S	-2.928369	-0.693805	-1.734429
9O	-3.545762	-0.531575	-3.057331
10O	-1.598009	-1.305279	-1.608301
11C	-2.898454	0.888103	-0.920312
12C	-3.682891	1.943420	-1.405617
13C	-3.645298	3.170050	-0.756647
14C	-2.837257	3.344279	0.382454
15C	-2.077109	2.271329	0.878408
16C	-2.106579	1.044530	0.219597
17O	-2.851147	4.584640	0.927198
18C	-2.041905	4.848573	2.080430
19C	-5.419911	-1.252249	-0.939207
20H	-4.935276	-0.900358	1.634508
21H	-4.079608	-1.750605	3.792999
22H	-1.281905	-4.147958	1.929573
23H	-2.042506	-3.434857	-0.328769
24H	-4.294303	1.808358	-2.291802
25H	-4.227717	4.011020	-1.120871
26H	-1.454170	2.383211	1.757246
27H	-1.500751	0.223180	0.585471
28H	-2.212374	5.899058	2.321537
29H	-2.348592	4.223833	2.928096
30H	-0.979039	4.689835	1.860156
31H	-6.028924	-2.001727	-0.429396
32H	-5.609508	-0.266427	-0.494911
33H	-5.697087	-1.233588	-1.993370
34P	2.511545	-0.062238	-0.058933
35C	2.584722	-1.515198	-1.140605
36C	4.193214	0.477493	0.351658
37C	1.650632	1.311905	-0.877966
38C	1.614508	-0.521190	1.451584
39C	4.928753	1.209717	-0.597347
40C	6.244739	1.578682	-0.316712
41C	6.828622	1.223147	0.904237
42C	6.095638	0.498970	1.848964
43C	4.778119	0.122925	1.577553
44C	0.733167	1.061375	-1.909721
45C	0.030036	2.122980	-2.482588
46C	0.233343	3.428425	-2.030097
47C	1.151552	3.680341	-1.004408
48C	1.863029	2.628696	-0.426981
49C	1.732671	-1.822022	1.970943
50C	1.061207	-2.161316	3.145942
51C	0.272928	-1.213105	3.805247
52C	0.160259	0.082080	3.292387
53C	0.828482	0.432040	2.118365
54C	3.769986	-1.855144	-1.812292
55C	3.783902	-2.957964	-2.669038
56C	2.624764	-3.716445	-2.859763
57C	1.446043	-3.379491	-2.185946
58C	1.422184	-2.283937	-1.323496
59H	4.480826	1.494243	-1.545251
60H	6.811609	2.144296	-1.050951
61H	7.853249	1.513851	1.119864
62H	6.545735	0.227642	2.799807
63H	4.216662	-0.436352	2.319857
64H	0.547633	0.052972	-2.261647
65H	-0.683063	1.922194	-3.276645
66H	-0.322037	4.249655	-2.474787
67H	1.315415	4.695830	-0.654164

68H	2.578008	2.834382	0.364483
69H	2.333803	-2.569445	1.461841
70H	1.143364	-3.170297	3.539533
71H	-0.264513	-1.489228	4.707476
72H	-0.458251	0.818225	3.798563
73H	0.725158	1.435430	1.719832
74H	4.677011	-1.276603	-1.669602
75H	4.701919	-3.222505	-3.186489
76H	2.640285	-4.570842	-3.531223
77H	0.541304	-3.962378	-2.334052
78H	0.502309	-2.027121	-0.810081

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1C	-4.193813	-1.517794	1.627158
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4C	-2.206682	-3.358412	1.947528
5C	-2.582829	-3.009585	0.652480
6C	-3.596848	-2.057773	0.480927
7N	-4.009161	-1.683699	-0.836842
8S	-2.884140	-0.736823	-1.726171
9O	-3.453504	-0.594594	-3.072823
10O	-1.567544	-1.363352	-1.541111
11C	-2.860637	0.859217	-0.941258
12C	-3.639971	1.906895	-1.450892
13C	-3.612992	3.141485	-0.816719
14C	-2.820349	3.331261	0.330798
15C	-2.065305	2.266080	0.850475
16C	-2.084675	1.031009	0.207013
17O	-2.842872	4.578367	0.859672
18C	-2.042194	4.858767	2.014965
19C	-5.410969	-1.252066	-1.011323
20H	-4.981360	-0.775056	1.563658
21H	-4.201171	-1.544909	3.781189
22H	-1.418760	-4.091832	2.101741
23H	-2.106119	-3.466050	-0.206399
24H	-4.238871	1.759917	-2.343741
25H	-4.191151	3.977181	-1.199446
26H	-1.455019	2.389705	1.736658
27H	-1.482939	0.214569	0.589826
28H	-2.215213	5.912261	2.240759
29H	-2.353807	4.245355	2.869025
30H	-0.977740	4.698124	1.804014
31H	-6.044860	-1.980454	-0.500961
32H	-5.606937	-0.251987	-0.603744
33H	-5.650138	-1.262024	-2.074877
34P	2.505338	-0.074743	-0.064854
35C	2.641736	-1.510404	-1.162687
36C	4.162739	0.487460	0.412790
37C	1.646159	1.294512	-0.893755
38C	1.581984	-0.559567	1.421301
39C	4.915809	1.266489	-0.483297
40C	6.213881	1.650412	-0.144488
41C	6.763519	1.261715	1.082085
42C	6.013548	0.489860	1.974337
43C	4.713621	0.099995	1.644709
44C	0.745321	1.036837	-1.938744
45C	0.041868	2.092345	-2.521980
46C	0.228571	3.399605	-2.067347
47C	1.129374	3.658792	-1.028396
48C	1.840303	2.612815	-0.439799
49C	1.686247	-1.868563	1.921863
50C	1.011161	-2.217072	3.092441
51C	0.234305	-1.269683	3.766037
52C	0.136567	0.034220	3.271957
53C	0.808488	0.393382	2.103052
54C	3.853856	-1.805851	-1.806929
55C	3.920932	-2.889966	-2.684594
56C	2.787839	-3.673798	-2.923576
57C	1.582491	-3.381915	-2.276302
58C	1.505556	-2.305231	-1.393270
59H	4.494514	1.576913	-1.435292
60H	6.793486	2.253315	-0.838003
61H	7.774397	1.563318	1.343040
62H	6.436330	0.191602	2.929705
63H	4.138735	-0.497143	2.346196
64H	0.572742	0.026756	-2.292795
65H	-0.658406	1.885467	-3.325874
66H	-0.326767	4.216285	-2.520345
67H	1.279594	4.675508	-0.675637
68H	2.540918	2.824721	0.362640
69H	2.282109	-2.614234	1.404240
70H	1.084648	-3.231795	3.472820
71H	-0.306070	-1.552214	4.664364
72H	-0.472369	0.770230	3.789774

73H	0.718984	1.404392	1.720411
74H	4.740394	-1.206463	-1.626040
75H	4.859688	-3.120016	-3.180922
76H	2.844557	-4.513446	-3.611207
77H	0.698445	-3.986044	-2.460163
78H	0.566126	-2.083130	-0.899973

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1C	-2.415631	-1.855317	-1.400162
2C	-2.480846	-3.227171	-1.150108
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4C	-1.322731	-3.019423	0.807433
5C	-1.184333	-1.643085	0.647847
6C	-1.744920	-1.035004	-0.483608
7N	-1.589686	0.369302	-0.704005
8S	-2.353584	1.405327	0.455031
9O	-2.086455	2.769312	-0.024220
10O	-1.874531	0.983933	1.777205
11C	-4.092609	1.064064	0.328844
12C	-4.875238	1.791056	-0.581296
13C	-6.215814	1.467335	-0.730174
14C	-6.779623	0.416590	0.019129
15C	-5.987537	-0.306186	0.928445
16C	-4.640321	0.019297	1.078835
17O	-8.093443	0.180337	-0.204984
18C	-8.748820	-0.868177	0.522419
19C	-1.717326	0.845808	-2.096036
20H	-2.879477	-1.454956	-2.294081
21H	-2.991481	-3.878971	-1.855935
22H	-0.888389	-3.504926	1.678749
23H	-0.646170	-1.059892	1.381483
24H	-4.440335	2.606801	-1.149239
25H	-6.849453	2.019143	-1.417800
26H	-6.404842	-1.112909	1.519307
27H	-4.025405	-0.533507	1.781356
28H	-9.781487	-0.864930	0.170341
29H	-8.290373	-1.840987	0.307994
30H	-8.728081	-0.669695	1.600717
31H	-1.093857	0.204627	-2.722244
32H	-2.750615	0.823066	-2.465300
33H	-1.337794	1.865266	-2.155481
34P	2.966604	0.094027	0.018970
35C	2.669455	1.872900	-0.140549
36C	4.745046	-0.253356	-0.037572
37C	2.336498	-0.501456	1.613908
38C	2.134161	-0.753375	-1.354957
39C	5.522276	-0.005330	1.107979
40C	6.899075	-0.226254	1.069889
41C	7.501701	-0.697640	-0.101892
42C	6.727813	-0.947819	-1.238887
43C	5.348865	-0.726206	-1.212822
44C	1.432872	0.266691	2.363510
45C	0.935082	-0.232501	3.569371
46C	1.334881	-1.489967	4.028409
47C	2.244480	-2.252705	3.286447
48C	2.750786	-1.761852	2.083268
49C	2.041065	-0.114732	-2.603896
50C	1.462511	-0.784965	-3.683007
51C	0.977245	-2.087068	-3.523096
52C	1.068125	-2.721764	-2.280983
53C	1.644216	-2.059510	-1.196013
54C	3.718336	2.796818	-0.014597
55C	3.444649	4.164046	-0.101940
56C	2.134624	4.608237	-0.305327
57C	1.089592	3.686122	-0.430613
58C	1.353452	2.319200	-0.355808
59H	5.059270	0.352429	2.023717
60H	7.498276	-0.034134	1.955595
61H	8.573686	-0.874437	-0.126142
62H	7.193946	-1.320744	-2.146637
63H	4.755342	-0.929828	-2.099057
64H	1.104960	1.240333	2.017759
65H	0.228101	0.362468	4.139796
66H	0.943250	-1.875061	4.966109
67H	2.564737	-3.226821	3.645696
68H	3.469998	-2.351294	1.522040
69H	2.411535	0.897362	-2.736133
70H	1.388691	-0.286891	-4.645780
71H	0.521344	-2.603468	-4.363610
72H	0.678644	-3.726743	-2.147993
73H	1.693778	-2.559852	-0.235268
74H	4.739102	2.463105	0.143123
75H	4.256758	4.880021	-0.010322
76H	1.926544	5.673236	-0.365768
77H	0.066956	4.020216	-0.574964

78H 0.540616 1.607602 -0.463840

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1C -3.593492 2.778252 0.905102
2C -3.257829 3.400967 2.109470
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8S -2.047419 0.617887 -1.649371
9O -0.701776 0.789295 -1.090263
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23H -0.615197 3.313315 -0.633738
24H -2.006787 0.010229 1.173228
25H -3.215471 -1.697993 2.514022
26H -5.133852 -3.144282 -1.073517
27H -3.936504 -1.443856 -2.398462
28H -5.253909 -5.029376 0.347041
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30H -6.612181 -3.881573 0.609105
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40C 6.583150 -0.400956 0.075448
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43C 4.491399 -2.231886 0.417625
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48C 2.677136 2.437126 -0.134334
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62H 6.030630 -3.701390 0.728929
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74H -0.046916 -1.684968 0.716510
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76H -0.530980 -4.352656 -2.613153
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1C	-4.970613	-0.718951	-1.315899
2C	-5.009635	-1.404894	-2.531359
3N	-4.618949	-2.678723	-2.685330
4C	-4.184235	-3.317603	-1.585887
5C	-4.111819	-2.731558	-0.323674
6C	-4.501322	-1.393676	-0.181643
7N	-4.432836	-0.766206	1.101672
8S	-2.857262	-0.413941	1.690992
9O	-2.008219	-1.554519	1.326408
10O	-3.032149	-0.028988	3.097522
11C	-2.319601	1.021918	0.778551
12C	-1.945396	0.877629	-0.566348
13C	-1.566022	1.997822	-1.290058
14C	-1.538536	3.264681	-0.675541
15C	-1.923713	3.403062	0.668110
16C	-2.325009	2.276401	1.389257
17O	-1.108957	4.283309	-1.460140
18C	-1.004974	5.599823	-0.900748
19C	-5.424027	0.286624	1.397398
20H	-5.287604	0.317031	-1.271931
21H	-5.364755	-0.897594	-3.425984
22H	-3.883954	-4.354725	-1.719318
23H	-3.759148	-3.295040	0.531813
24H	-1.932119	-0.097933	-1.037335
25H	-1.265773	1.910179	-2.329917
26H	-1.916228	4.369299	1.158726
27H	-2.623006	2.374223	2.427982
28H	-0.308414	5.613523	-0.054050
29H	-0.617687	6.228121	-1.704392
30H	-1.986880	5.972707	-0.586012
31H	-6.408005	-0.099268	1.121893
32H	-5.412662	0.486583	2.469424
33H	-5.235017	1.219898	0.850785
34P	2.530799	-0.353754	-0.024113
35C	1.754763	-0.358865	1.616685
36C	3.988653	-1.432212	0.012807
37C	1.351234	-0.973592	-1.255744
38C	3.014974	1.338161	-0.480547
39C	4.222299	-2.350316	-1.022851
40C	5.364558	-3.153602	-0.989626
41C	6.270617	-3.043749	0.068982
42C	6.036628	-2.130304	1.103096
43C	4.897496	-1.325735	1.080489
44C	0.335008	-1.856517	-0.860119
45C	-0.540371	-2.375201	-1.815897
46C	-0.414224	-2.009008	-3.158510
47C	0.598013	-1.126018	-3.553076
48C	1.484830	-0.609096	-2.607736
49C	2.028322	2.232279	-0.930826
50C	2.368239	3.549308	-1.239992
51C	3.692376	3.979933	-1.106371
52C	4.676808	3.090224	-0.665642
53C	4.344710	1.769953	-0.352349
54C	1.033216	0.762612	2.056793
55C	0.363813	0.718086	3.279304
56C	0.409487	-0.436218	4.065540
57C	1.133038	-1.550808	3.632467
58C	1.804443	-1.518916	2.409458
59H	3.521658	-2.447182	-1.846368
60H	5.540922	-3.867182	-1.789539
61H	7.156788	-3.672281	0.091931
62H	6.737120	-2.047392	1.929425
63H	4.712793	-0.627161	1.891461
64H	0.198183	-2.118591	0.182894
65H	-1.335270	-3.044269	-1.502731
66H	-1.109089	-2.404128	-3.894869
67H	0.697345	-0.837876	-4.596014
68H	2.267733	0.074862	-2.922217
69H	1.000553	1.906727	-1.046241
70H	1.595273	4.228101	-1.589104
71H	3.957978	5.004943	-1.351165
72H	5.707944	3.418939	-0.569970
73H	5.121772	1.088645	-0.021614
74H	0.983933	1.664253	1.455707
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76H	-0.126054	-0.469141	5.010000
77H	1.168360	-2.450915	4.239687
78H	2.357106	-2.393010	2.078862

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1C	-3.391077	2.845500	0.904565
2C	-2.988082	3.475068	2.084555
3N	-1.756899	3.966702	2.288433
4C	-0.883001	3.855302	1.273254

5C	-1.182803	3.258919	0.050647
6C	-2.464413	2.724270	-0.138376
7N	-2.791595	2.095044	-1.379876
8S	-2.055465	0.566035	-1.656969
9O	-0.697342	0.661741	-1.111070
10O	-2.268438	0.267216	-3.079393
11C	-2.977535	-0.605914	-0.684682
12C	-2.714620	-0.707298	0.690233
13C	-3.452415	-1.592039	1.461088
14C	-4.462412	-2.376357	0.869004
15C	-4.723891	-2.264609	-0.507172
16C	-3.980220	-1.371637	-1.280963
17O	-5.122881	-3.207186	1.709205
18C	-6.176404	-4.032716	1.192456
19C	-4.192061	2.170284	-1.838835
20H	-4.399052	2.454812	0.819988
21H	-3.690630	3.575710	2.909195
22H	0.109254	4.266329	1.443968
23H	-0.439060	3.203122	-0.735274
24H	-1.931221	-0.113412	1.146370
25H	-3.261677	-1.695393	2.525285
26H	-5.492927	-2.861263	-0.983167
27H	-4.171996	-1.285991	-2.345791
28H	-5.793452	-4.735958	0.443126
29H	-6.558520	-4.586481	2.051438
30H	-6.978914	-3.421631	0.762250
31H	-4.515187	3.209719	-1.749642
32H	-4.231179	1.880809	-2.889897
33H	-4.868521	1.528792	-1.259191
34P	2.489354	-0.371458	0.052349
35C	1.604811	-1.602558	-0.940740
36C	4.226904	-0.896771	0.158089
37C	2.391554	1.284019	-0.684605
38C	1.768441	-0.280964	1.716951
39C	5.260339	0.052981	0.194843
40C	6.585972	-0.368453	0.317530
41C	6.885939	-1.731387	0.402161
42C	5.857855	-2.678872	0.361518
43C	4.529855	-2.267852	0.238575
44C	2.035082	1.455777	-2.029256
45C	1.986586	2.740454	-2.572710
46C	2.288786	3.851956	-1.780734
47C	2.641810	3.681876	-0.437666
48C	2.692039	2.401534	0.114403
49C	0.649818	0.541631	1.935204
50C	0.071130	0.601233	3.203216
51C	0.597357	-0.161563	4.251145
52C	1.708559	-0.982275	4.032978
53C	2.300156	-1.042972	2.769119
54C	0.383692	-2.126300	-0.494990
55C	-0.301738	-3.052506	-1.281635
56C	0.225767	-3.453649	-2.511781
57C	1.448925	-2.937128	-2.955225
58C	2.144379	-2.015894	-2.171886
59H	5.042309	1.113289	0.119656
60H	7.382541	0.370278	0.339791
61H	7.919364	-2.055130	0.493158
62H	6.087656	-3.739242	0.420055
63H	3.740508	-3.012891	0.198077
64H	1.767098	0.604399	-2.644196
65H	1.696360	2.870466	-3.611544
66H	2.241348	4.850738	-2.206323
67H	2.871645	4.544060	0.182254
68H	2.949996	2.277095	1.162281
69H	0.234890	1.130045	1.124428
70H	-0.784293	1.249852	3.371075
71H	0.146463	-0.110666	5.238651
72H	2.123214	-1.569210	4.847860
73H	3.171852	-1.671345	2.613474
74H	-0.041115	-1.807670	0.449535
75H	-1.251306	-3.449602	-0.934250
76H	-0.313214	-4.170659	-3.125393
77H	1.862714	-3.253002	-3.908846
78H	3.100419	-1.627578	-2.513631

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1C	-4.290450	1.093561	-0.600330
2C	-4.415979	2.151123	-1.461178
3N	-3.774822	3.336234	-1.263874
4C	-3.003584	3.489587	-0.146034
5C	-2.839657	2.478423	0.755432
6C	-3.459965	1.194339	0.569472
7N	-3.171045	0.267980	1.490959
8S	-3.726254	-1.283323	1.429586
9O	-5.073891	-1.414284	0.816859

10O	-3.538584	-1.824422	2.791561
11C	-2.569339	-2.153786	0.360734
12C	-2.788439	-2.217549	-1.021991
13C	-1.863995	-2.860090	-1.837707
14C	-0.716492	-3.450858	-1.278307
15C	-0.506636	-3.394732	0.108425
16C	-1.436441	-2.743871	0.921344
17O	0.133830	-4.047632	-2.156968
18C	1.229589	-4.811223	-1.637762
19C	-3.950681	4.460942	-2.192428
20H	-4.838239	0.186531	-0.814431
21H	-5.031848	2.090087	-2.351911
22H	-2.529492	4.457574	-0.026987
23H	-2.217111	2.638068	1.629049
24H	-3.682962	-1.784130	-1.456396
25H	-2.019682	-2.926912	-2.910581
26H	0.362901	-3.852289	0.564974
27H	-1.278629	-2.701226	1.992401
28H	1.737515	-5.227874	-2.509060
29H	1.927411	-4.178881	-1.077579
30H	0.866391	-5.626468	-0.999846
31H	-4.668254	5.178505	-1.781996
32H	-2.989916	4.956533	-2.349674
33H	-4.321668	4.085478	-3.147215
34P	2.147652	0.527191	0.145175
35C	3.144473	-0.668152	-0.794430
36C	0.848099	1.194827	-0.929048
37C	1.384631	-0.259647	1.589047
38C	3.240586	1.865758	0.700471
39C	-0.251295	0.382537	-1.255462
40C	-1.204837	0.840992	-2.162478
41C	-1.076144	2.109756	-2.734996
42C	0.006661	2.926167	-2.396452
43C	0.973380	2.472956	-1.496036
44C	2.041451	-1.309807	2.252634
45C	1.483528	-1.846431	3.413516
46C	0.275140	-1.344741	3.910457
47C	-0.385023	-0.310797	3.241695
48C	0.167430	0.236286	2.083112
49C	4.242979	2.348785	-0.159187
50C	5.054757	3.406990	0.250214
51C	4.872270	3.984000	1.511869
52C	3.876662	3.502701	2.367300
53C	3.058601	2.443693	1.967080
54C	2.646902	-1.252452	-1.970306
55C	3.421114	-2.186326	-2.661648
56C	4.686676	-2.541064	-2.187201
57C	5.186171	-1.956487	-1.018184
58C	4.422446	-1.018627	-0.322580
59H	-0.365456	-0.598098	-0.806308
60H	-2.050371	0.207993	-2.407933
61H	-1.823943	2.465828	-3.437945
62H	0.104677	3.916263	-2.833481
63H	1.813767	3.112231	-1.245172
64H	2.973968	-1.713436	1.871065
65H	1.988474	-2.662293	3.923526
66H	-0.164579	-1.776402	4.805490
67H	-1.349307	0.045232	3.587065
68H	-0.364473	1.023637	1.559972
69H	4.393620	1.901058	-1.137382
70H	5.830719	3.776660	-0.414351
71H	5.509435	4.805094	1.829269
72H	3.738491	3.945518	3.349782
73H	2.293411	2.071044	2.641198
74H	1.669880	-0.984671	-2.357453
75H	3.028238	-2.635973	-3.569049
76H	5.285384	-3.268725	-2.728518
77H	6.172904	-2.224052	-0.650492
78H	4.826723	-0.556096	0.573430

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1C	2.760858	-3.025464	-0.176456
2C	3.601942	-3.570295	-1.104475
3N	4.786949	-2.975904	-1.435620
4C	5.137057	-1.815042	-0.818306
5C	4.339002	-1.215446	0.121946
6C	3.079512	-1.795926	0.489447
7N	2.161996	-1.327356	1.352730
8S	2.408460	0.070468	2.180241
9O	3.728157	0.131978	2.860053
10O	1.216043	0.240708	3.041487
11C	2.394291	1.387488	0.949858
12C	3.000155	2.604961	1.258064
13C	2.935393	3.669400	0.355237
14C	2.263971	3.502967	-0.866590

15C	1.669235	2.267650	-1.175755
16C	1.725958	1.218891	-0.268861
17O	2.134254	4.471805	-1.812101
18C	2.740914	5.748812	-1.581353
19C	5.637817	-3.579050	-2.473490
20H	1.828344	-3.525935	0.059934
21H	3.374776	-4.494910	-1.623893
22H	6.089887	-1.389098	-1.111257
23H	4.692252	-0.302560	0.583267
24H	3.526734	2.730182	2.199717
25H	3.409804	4.609199	0.612849
26H	1.156164	2.152359	-2.125503
27H	1.253328	0.273437	-0.509592
28H	2.512399	6.346335	-2.465745
29H	2.317144	6.232792	-0.692775
30H	3.828547	5.655408	-1.473400
31H	6.598391	-3.063543	-2.494056
32H	5.801589	-4.634939	-2.244719
33H	5.154049	-3.483810	-3.450083
34P	-2.468806	-0.276391	-0.092339
35C	-2.397880	-1.276997	1.414643
36C	-4.161144	-0.250028	-0.743205
37C	-1.965082	1.433451	0.243052
38C	-1.366323	-1.015075	-1.333835
39C	-4.530821	-1.086688	-1.807653
40C	-5.850721	-1.080782	-2.264834
41C	-6.798781	-0.246944	-1.664581
42C	-6.429891	0.587281	-0.603296
43C	-5.113972	0.589683	-0.140109
44C	-2.349906	2.453495	-0.647057
45C	-1.919504	3.761327	-0.426455
46C	-1.114508	4.057898	0.679776
47C	-0.738241	3.045600	1.564584
48C	-1.156833	1.730767	1.350454
49C	-1.161924	-2.404815	-1.350616
50C	-0.356175	-2.973992	-2.338466
51C	0.244085	-2.165229	-3.308206
52C	0.035658	-0.782561	-3.295214
53C	-0.768878	-0.204366	-2.312223
54C	-1.144884	-1.676763	1.909103
55C	-1.074003	-2.403858	3.097151
56C	-2.242505	-2.739503	3.787490
57C	-3.490066	-2.346215	3.290759
58C	-3.574285	-1.613641	2.105445
59H	-3.799758	-1.733222	-2.283660
60H	-6.134530	-1.724691	-3.092638
61H	-7.823965	-0.243740	-2.024903
62H	-7.164434	1.238168	-0.137252
63H	-4.831218	1.243122	0.680597
64H	-2.987080	2.233364	-1.499080
65H	-2.215228	4.547555	-1.115598
66H	-0.779514	5.078076	0.847252
67H	-0.105746	3.267290	2.418746
68H	-0.830378	0.958826	2.038135
69H	-1.619297	-3.039331	-0.597689
70H	-0.195003	-4.048462	-2.345155
71H	0.875238	-2.611200	-4.072375
72H	0.503491	-0.151180	-4.045580
73H	-0.916607	0.870458	-2.305424
74H	-0.221705	-1.428914	1.394169
75H	-0.100131	-2.694014	3.480189
76H	-2.182153	-3.305082	4.713630
77H	-4.399485	-2.608184	3.824611
78H	-4.546542	-1.314429	1.727393

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1C	-2.794627	2.329218	-0.868344
2C	-2.163845	3.021083	-1.867839
3N	-0.979583	3.667113	-1.674800
4C	-0.400212	3.626303	-0.436974
5C	-0.974921	2.952931	0.602247
6C	-2.214747	2.242337	0.445030
7N	-2.652448	1.572071	1.515837
8S	-4.060446	0.710453	1.506773
9O	-5.183170	1.448269	0.873944
10O	-4.230700	0.248857	2.900428
11C	-3.755375	-0.751007	0.503028
12C	-4.358812	-0.893749	-0.752148
13C	-4.091668	-2.022168	-1.518592
14C	-3.215442	-3.011035	-1.040857
15C	-2.624075	-2.872697	0.225572
16C	-2.903295	-1.742257	0.993843
17O	-2.999948	-4.059934	-1.878217
18C	-2.147769	-5.126328	-1.448276
19C	-0.301469	4.340159	-2.791833

20H	-3.747288	1.868373	-1.088577
21H	-2.581815	3.091552	-2.866383
22H	0.540546	4.153123	-0.334027
23H	-0.484968	2.946335	1.569282
24H	-5.047472	-0.137517	-1.114854
25H	-4.554291	-2.156707	-2.492098
26H	-1.958577	-3.630888	0.621730
27H	-2.460248	-1.640999	1.978868
28H	-2.129172	-5.838198	-2.275893
29H	-1.130973	-4.766144	-1.250900
30H	-2.551186	-5.617167	-0.554177
31H	0.237592	5.211810	-2.415832
32H	0.402161	3.653135	-3.271385
33H	-1.045861	4.669869	-3.518446
34P	2.240947	-0.278061	0.156496
35C	3.781830	-1.234970	0.117126
36C	2.609267	1.455041	-0.245305
37C	1.086445	-0.920403	-1.091453
38C	1.539016	-0.368253	1.827036
39C	2.734539	1.851537	-1.588193
40C	3.099989	3.164399	-1.889629
41C	3.341024	4.081399	-0.860714
42C	3.212816	3.687389	0.474749
43C	2.847248	2.376214	0.786971
44C	1.278596	-2.185692	-1.669300
45C	0.374823	-2.654033	-2.625998
46C	-0.720667	-1.873440	-3.003070
47C	-0.912446	-0.613633	-2.428007
48C	-0.010659	-0.132328	-1.481217
49C	2.389229	-0.544905	2.934336
50C	1.854530	-0.525106	4.223425
51C	0.483484	-0.320094	4.414345
52C	-0.358981	-0.132593	3.314769
53C	0.164555	-0.159493	2.021520
54C	4.940857	-0.699949	-0.467084
55C	6.109237	-1.464379	-0.511267
56C	6.126113	-2.755590	0.023265
57C	4.972242	-3.288432	0.608844
58C	3.801164	-2.532698	0.660086
59H	2.552706	1.145053	-2.392852
60H	3.199595	3.468940	-2.927680
61H	3.625328	5.102614	-1.100134
62H	3.392541	4.399021	1.275623
63H	2.743688	2.081326	1.826639
64H	2.127533	-2.802340	-1.393239
65H	0.529047	-3.630761	-3.075605
66H	-1.427232	-2.248780	-3.736973
67H	-1.768548	-0.006880	-2.705620
68H	-0.158513	0.852435	-1.053147
69H	3.455424	-0.696824	2.797830
70H	2.510927	-0.667762	5.077407
71H	0.072268	-0.302204	5.420031
72H	-1.421117	0.048550	3.448232
73H	-0.508103	-0.010805	1.185367
74H	4.943595	0.305112	-0.876613
75H	7.006145	-1.045722	-0.959103
76H	7.038511	-3.344854	-0.010564
77H	4.983763	-4.289404	1.030926
78H	2.913723	-2.948105	1.129319

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1C	5.577605	-1.818122	-1.185544
2C	6.746153	-1.274677	-1.638403
3N	7.285513	-0.154714	-1.068795
4C	6.639715	0.425965	-0.022048
5C	5.464543	-0.068932	0.481894
6C	4.856556	-1.237139	-0.088728
7N	3.707828	-1.839375	0.260558
8S	2.765773	-1.229441	1.460893
9O	3.507396	-0.925311	2.713166
10O	1.618058	-2.156733	1.580250
11C	2.135545	0.339208	0.838686
12C	2.159268	1.473740	1.646393
13C	1.603875	2.673038	1.189668
14C	1.031487	2.724849	-0.089513
15C	1.032490	1.580724	-0.907699
16C	1.569619	0.389220	-0.441667
17O	0.438474	3.826542	-0.627633
18C	0.365257	5.022843	0.156268
19C	8.541311	0.399095	-1.598915
20H	5.180934	-2.707506	-1.663322
21H	7.302351	-1.699714	-2.466806
22H	7.111987	1.306277	0.398523
23H	5.022884	0.435172	1.330769
24H	2.601818	1.424254	2.636068

25H	1.617255	3.542847	1.836135
26H	0.590061	1.641107	-1.896723
27H	1.544491	-0.497586	-1.066438
28H	-0.140229	5.757641	-0.472947
29H	-0.217202	4.858516	1.071165
30H	1.366401	5.391368	0.410907
31H	8.838227	1.257528	-0.994673
32H	9.325681	-0.361435	-1.556114
33H	8.395374	0.719112	-2.634590
34P	-2.824212	-0.318564	-0.157912
35C	-3.425997	1.139425	-1.055293
36C	-4.186830	-1.483594	0.130438
37C	-1.581187	-1.171991	-1.169341
38C	-2.150625	0.249511	1.429240
39C	-4.886292	-1.483527	1.347419
40C	-5.956432	-2.361947	1.529636
41C	-6.331229	-3.236070	0.504916
42C	-5.632585	-3.238244	-0.707219
43C	-4.559720	-2.366742	-0.898184
44C	-1.055465	-2.396503	-0.720992
45C	-0.090991	-3.056983	-1.480339
46C	0.334633	-2.515895	-2.697407
47C	-0.207234	-1.312115	-3.157972
48C	-1.161173	-0.634359	-2.396299
49C	-2.813723	1.291856	2.104350
50C	-2.356400	1.707556	3.354589
51C	-1.243146	1.089279	3.935542
52C	-0.582339	0.060410	3.260535
53C	-1.028800	-0.362130	2.006547
54C	-2.616712	2.288680	-1.095420
55C	-3.028806	3.401152	-1.827574
56C	-4.248363	3.376312	-2.513775
57C	-5.056044	2.235998	-2.468457
58C	-4.649038	1.114108	-1.741316
59H	-4.598479	-0.815902	2.153438
60H	-6.491687	-2.365771	2.475061
61H	-7.162242	-3.920624	0.652515
62H	-5.917445	-3.920988	-1.502856
63H	-4.014040	-2.381217	-1.837375
64H	-1.392461	-2.835954	0.212751
65H	0.332535	-3.987185	-1.114061
66H	1.088814	-3.032724	-3.284677
67H	0.116697	-0.893635	-4.106995
68H	-1.568670	0.303047	-2.759847
69H	-3.676342	1.778623	1.658568
70H	-2.869545	2.513376	3.872468
71H	-0.887992	1.416281	4.909373
72H	0.292306	-0.413609	3.695779
73H	-0.475312	-1.141845	1.497851
74H	-1.671257	2.319802	-0.564456
75H	-2.394898	4.282886	-1.858125
76H	-4.568951	4.245712	-3.081709
77H	-6.005416	2.216943	-2.996339
78H	-5.283222	0.233356	-1.711609

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1C	-2.858189	2.324323	-0.826209
2C	-2.276876	3.053613	-1.829200
3N	-1.088300	3.699664	-1.667281
4C	-0.463207	3.637413	-0.452359
5C	-0.989198	2.929405	0.589456
6C	-2.229832	2.213414	0.462037
7N	-2.621980	1.515184	1.532582
8S	-4.020013	0.637310	1.553637
9O	-5.169843	1.368340	0.963246
10O	-4.143697	0.156257	2.945570
11C	-3.722912	-0.805883	0.522600
12C	-4.345312	-0.934672	-0.724994
13C	-4.078430	-2.047632	-1.513995
14C	-3.185160	-3.035183	-1.065986
15C	-2.576124	-2.911501	0.193483
16C	-2.853832	-1.796541	0.984168
17O	-2.971331	-4.068203	-1.923377
18C	-2.114880	-5.139946	-1.515220
19C	-0.528325	4.540540	-2.735645
20H	-3.810294	1.852629	-1.023678
21H	-2.740820	3.151720	-2.804659
22H	0.474851	4.173742	-0.374949
23H	-0.459776	2.897659	1.534937
24H	-5.048809	-0.181016	-1.064176
25H	-4.555196	-2.171507	-2.482071
26H	-1.897506	-3.669135	0.567429
27H	-2.395878	-1.706497	1.963508
28H	-2.100824	-5.839805	-2.353081
29H	-1.097191	-4.781357	-1.319355

30H	-2.511910	-5.643616	-0.625364
31H	-0.755187	5.593328	-2.540235
32H	0.553660	4.399431	-2.775394
33H	-0.964551	4.245625	-3.691163
34P	2.251324	-0.261550	0.142181
35C	3.798115	-1.206371	0.072205
36C	2.599904	1.482859	-0.223849
37C	1.090731	-0.887730	-1.108785
38C	1.564020	-0.392216	1.816231
39C	2.714217	1.910148	-1.558065
40C	3.065336	3.233103	-1.831643
41C	3.300601	4.129957	-0.783692
42C	3.181408	3.705444	0.543333
43C	2.832674	2.383357	0.827790
44C	1.284504	-2.143330	-1.706969
45C	0.374904	-2.603508	-2.661979
46C	-0.728356	-1.823960	-3.017936
47C	-0.920995	-0.573118	-2.424139
48C	-0.013798	-0.100004	-1.478157
49C	2.419807	-0.614250	2.910535
50C	1.894629	-0.628867	4.203777
51C	0.527725	-0.413161	4.411799
52C	-0.320196	-0.178979	3.325249
53C	0.194040	-0.171873	2.028203
54C	4.952619	-0.647021	-0.497774
55C	6.125783	-1.402380	-0.565213
56C	6.151336	-2.708447	-0.068423
57C	5.001850	-3.265370	0.503426
58C	3.826056	-2.519022	0.577905
59H	2.535286	1.219939	-2.377364
60H	3.158369	3.560746	-2.863403
61H	3.573307	5.159157	-1.001470
62H	3.356984	4.401219	1.358931
63H	2.738731	2.063398	1.861037
64H	2.139222	-2.759028	-1.447759
65H	0.530556	-3.573021	-3.126513
66H	-1.440024	-2.193386	-3.749933
67H	-1.782223	0.033246	-2.686513
68H	-0.163973	0.878500	-1.036394
69H	3.482790	-0.774515	2.760718
70H	2.555285	-0.807343	5.047712
71H	0.124182	-0.422534	5.420718
72H	-1.379228	0.010845	3.471887
73H	-0.482283	0.014872	1.203143
74H	4.947584	0.369331	-0.878570
75H	7.019389	-0.965510	-1.002114
76H	7.067301	-3.290776	-0.120846
77H	5.020529	-4.278132	0.896071
78H	2.941089	-2.952666	1.035605

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1C	5.409597	-0.341501	0.736957
2C	6.643854	0.241091	0.865278
3N	7.612662	0.111018	-0.080850
4C	7.353557	-0.640840	-1.192836
5C	6.144460	-1.247495	-1.382774
6C	5.085977	-1.125620	-0.421137
7N	3.929560	-1.738351	-0.722700
8S	2.636288	-1.658156	0.286923
9O	2.968845	-1.974240	1.701634
10O	1.580393	-2.477089	-0.348433
11C	2.080806	0.056618	0.259958
12C	1.921576	0.764276	1.456838
13C	1.472369	2.079545	1.425372
14C	1.190379	2.698665	0.195507
15C	1.352221	1.985823	-1.002872
16C	1.791318	0.661595	-0.963406
17O	0.751605	3.985583	0.267994
18C	0.488370	4.693475	-0.948176
19C	8.944015	0.707828	0.107421
20H	4.696800	-0.204603	1.538455
21H	6.906170	0.834663	1.733965
22H	8.163677	-0.721881	-1.909355
23H	5.973747	-1.830695	-2.281321
24H	2.140950	0.281467	2.402886
25H	1.332511	2.642927	2.343415
26H	1.132348	2.442701	-1.960175
27H	1.896360	0.105195	-1.889594
28H	0.174388	5.694025	-0.645506
29H	1.393441	4.767576	-1.563455
30H	-0.315316	4.215721	-1.520578
31H	9.657684	-0.062247	0.415822
32H	9.274941	1.161008	-0.829906
33H	8.886731	1.479835	0.876577
34P	-2.904097	-0.242886	-0.006946

35C	-3.363662	1.512905	-0.009059
36C	-4.393917	-1.279085	-0.091961
37C	-1.907448	-0.612799	-1.475168
38C	-2.006131	-0.577315	1.532032
39C	-5.019508	-1.476224	-1.336033
40C	-6.186238	-2.237488	-1.411394
41C	-6.729366	-2.806460	-0.254181
42C	-6.102553	-2.618087	0.980936
43C	-4.935467	-1.855826	1.067025
44C	-1.483867	0.412278	-2.333820
45C	-0.746140	0.095358	-3.476213
46C	-0.423315	-1.234394	-3.758262
47C	-0.846532	-2.256803	-2.902472
48C	-1.595874	-1.952578	-1.767815
49C	-2.478304	-0.000849	2.726865
50C	-1.831435	-0.280328	3.930120
51C	-0.718498	-1.129503	3.947655
52C	-0.246454	-1.693581	2.760326
53C	-0.885728	-1.419868	1.548566
54C	-4.630887	1.933544	-0.439936
55C	-4.936331	3.296818	-0.458154
56C	-3.985560	4.236450	-0.048457
57C	-2.722223	3.815828	0.382111
58C	-2.407958	2.457339	0.404098
59H	-4.596853	-1.047427	-2.240327
60H	-6.667263	-2.389622	-2.373670
61H	-7.636067	-3.402146	-0.317220
62H	-6.515829	-3.068848	1.878928
63H	-4.449230	-1.726982	2.028875
64H	-1.727771	1.447915	-2.121943
65H	-0.420894	0.890238	-4.141967
66H	0.158939	-1.476096	-4.643440
67H	-0.589685	-3.290530	-3.113757
68H	-1.936172	-2.753905	-1.117641
69H	-3.336909	0.664913	2.719689
70H	-2.195091	0.167394	4.851004
71H	-0.212760	-1.340509	4.886414
72H	0.637380	-2.323790	2.760262
73H	-0.482025	-1.845415	0.636926
74H	-5.378557	1.212105	-0.754192
75H	-5.919774	3.620994	-0.787268
76H	-4.229743	5.295430	-0.060127
77H	-1.979563	4.538908	0.705103
78H	-1.428654	2.136027	0.744211

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1C	5.482074	-0.270028	0.709073
2C	6.715024	0.318830	0.800152
3N	7.661002	0.185633	-0.170579
4C	7.374306	-0.568915	-1.271994
5C	6.162192	-1.182931	-1.425560
6C	5.131927	-1.065546	-0.435286
7N	3.973223	-1.693357	-0.694147
8S	2.715715	-1.631655	0.361137
9O	3.107514	-1.911540	1.768424
10O	1.662586	-2.492721	-0.221238
11C	2.100471	0.061720	0.325611
12C	2.037869	0.815028	1.503405
13C	1.519228	2.104612	1.470936
14C	1.072873	2.652909	0.256790
15C	1.145964	1.897215	-0.923809
16C	1.652680	0.597816	-0.881912
17O	0.569773	3.916923	0.326166
18C	0.210593	4.583919	-0.888912
19C	8.977902	0.819173	0.001407
20H	4.789785	-0.133701	1.528281
21H	6.999132	0.919982	1.657246
22H	8.161010	-0.649446	-2.013703
23H	5.971034	-1.771014	-2.316713
24H	2.378526	0.384805	2.439069
25H	1.449301	2.700756	2.376169
26H	0.795134	2.295038	-1.867831
27H	1.678360	0.005472	-1.791425
28H	-0.108676	5.584638	-0.592475
29H	1.072388	4.660688	-1.563380
30H	-0.616408	4.072761	-1.395838
31H	9.521686	0.331418	0.815614
32H	9.545476	0.717785	-0.923963
33H	8.847607	1.880449	0.228378
34P	-2.890236	-0.245286	-0.030449
35C	-3.533810	1.451533	-0.057136
36C	-4.261899	-1.435093	-0.075688
37C	-1.879061	-0.531074	-1.509785
38C	-1.951691	-0.462747	1.507157
39C	-4.852208	-1.759760	-1.310004

40C	-5.936631	-2.636795	-1.349080
41C	-6.432815	-3.193197	-0.165238
42C	-5.841233	-2.876045	1.061062
43C	-4.756588	-1.997854	1.111088
44C	-1.596107	0.515772	-2.400444
45C	-0.833847	0.264595	-3.542718
46C	-0.348605	-1.021545	-3.794943
47C	-0.637959	-2.067370	-2.912230
48C	-1.410585	-1.829762	-1.776858
49C	-2.428887	0.146463	2.683414
50C	-1.771712	-0.078789	3.892856
51C	-0.645767	-0.908992	3.936165
52C	-0.169821	-1.507216	2.767307
53C	-0.818006	-1.286644	1.550004
54C	-4.853783	1.717378	-0.451719
55C	-5.310319	3.037230	-0.492395
56C	-4.457276	4.087395	-0.140632
57C	-3.141579	3.821366	0.254763
58C	-2.676132	2.507409	0.299149
59H	-4.467395	-1.339795	-2.234884
60H	-6.389886	-2.887461	-2.304176
61H	-7.274421	-3.879946	-0.200048
62H	-6.218247	-3.315450	1.980358
63H	-4.298763	-1.765422	2.067474
64H	-1.966948	1.517678	-2.212216
65H	-0.617250	1.076146	-4.232115
66H	0.252269	-1.211834	-4.680250
67H	-0.258812	-3.067048	-3.101657
68H	-1.647032	-2.651493	-1.106588
69H	-3.302047	0.792009	2.660285
70H	-2.140016	0.394766	4.798875
71H	-0.133940	-1.080121	4.879676
72H	0.722706	-2.125033	2.786197
73H	-0.412214	-1.742115	0.654630
74H	-5.525955	0.907783	-0.718482
75H	-6.334336	3.241149	-0.792584
76H	-4.817909	5.112103	-0.169628
77H	-2.475058	4.632968	0.531688
78H	-1.656260	2.309680	0.614856

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1C	-4.394634	-0.051231	-0.805494
2C	-5.402155	-0.966629	-0.656327
3N	-5.601877	-1.648153	0.506975
4C	-4.779991	-1.394539	1.570272
5C	-3.758880	-0.491800	1.490192
6C	-3.498886	0.239315	0.281318
7N	-2.457431	1.080412	0.296172
8S	-2.066213	1.930087	-1.061826
9O	-3.212163	2.726299	-1.578639
10O	-1.375675	1.065589	-2.056921
11C	-0.855565	3.063247	-0.391852
12C	-1.221773	3.934635	0.643296
13C	-0.289062	4.830864	1.142965
14C	1.013728	4.868919	0.608951
15C	1.369331	4.005292	-0.436740
16C	0.424400	3.101822	-0.934733
17O	1.852657	5.774829	1.178864
18C	3.182153	5.903648	0.664845
19C	-6.736813	-2.570428	0.660688
20H	-4.295807	0.449995	-1.759784
21H	-6.089426	-1.195458	-1.463487
22H	-4.990269	-1.955426	2.474540
23H	-3.121777	-0.323098	2.350696
24H	-2.223117	3.901871	1.061704
25H	-0.545146	5.511816	1.949389
26H	2.362914	4.022206	-0.869510
27H	0.694141	2.423925	-1.736920
28H	3.745429	4.969503	0.784898
29H	3.169860	6.199842	-0.391289
30H	3.651619	6.690023	1.258578
31H	-6.418401	-3.447411	1.228821
32H	-7.557292	-2.070311	1.184699
33H	-7.076276	-2.890109	-0.325544
34P	1.607918	-1.514947	0.005379
35C	2.230847	-0.435995	-1.314860
36C	3.004778	-2.504883	0.616170
37C	0.914531	-0.529319	1.359503
38C	0.304898	-2.608365	-0.628386
39C	3.168616	-2.748722	1.988696
40C	4.230897	-3.542081	2.428591
41C	5.127832	-4.090917	1.507658
42C	4.967706	-3.845067	0.139590
43C	3.911185	-3.052523	-0.309629
44C	1.263700	0.820373	1.509166

45C	0.752771	1.553889	2.580428
46C	-0.098470	0.944706	3.504818
47C	-0.444867	-0.402872	3.358323
48C	0.052346	-1.142073	2.285738
49C	-0.986583	-2.083483	-0.807720
50C	-1.997651	-2.901242	-1.313454
51C	-1.728607	-4.235186	-1.636611
52C	-0.443998	-4.756850	-1.454242
53C	0.576711	-3.947772	-0.950743
54C	1.473435	-0.215318	-2.474095
55C	1.962764	0.637506	-3.466460
56C	3.197756	1.270430	-3.305002
57C	3.954290	1.050286	-2.147721
58C	3.477432	0.197340	-1.153017
59H	2.483859	-2.320891	2.714128
60H	4.358291	-3.725292	3.491989
61H	5.954323	-4.705177	1.855027
62H	5.666623	-4.265130	-0.578412
63H	3.799937	-2.858059	-1.372681
64H	1.908472	1.310777	0.789036
65H	1.004182	2.605828	2.672986
66H	-0.502159	1.521640	4.332539
67H	-1.111469	-0.876689	4.073714
68H	-0.235568	-2.183110	2.169731
69H	-1.200207	-1.048551	-0.563796
70H	-2.992111	-2.488524	-1.454475
71H	-2.519694	-4.869045	-2.028966
72H	-0.233783	-5.794074	-1.700197
73H	1.568032	-4.365018	-0.807015
74H	0.503979	-0.681078	-2.603362
75H	1.368848	0.812377	-4.358918
76H	3.572435	1.934773	-4.079254
77H	4.916599	1.538713	-2.020708
78H	4.075152	0.022580	-0.262782

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1C	-5.083856	-0.225098	-0.408798
2C	-5.938038	-1.292397	-0.330512
3N	-5.593629	-2.457894	0.286841
4C	-4.355419	-2.562914	0.856311
5C	-3.454024	-1.537790	0.813733
6C	-3.771958	-0.291148	0.174461
7N	-2.824430	0.653178	0.182729
8S	-3.104206	2.121874	-0.512343
9O	-4.189082	2.863986	0.181018
10O	-3.217889	2.018240	-1.992188
11C	-1.550766	2.926127	-0.134935
12C	-1.362399	3.492448	1.132229
13C	-0.144506	4.079525	1.445944
14C	0.889197	4.116136	0.491701
15C	0.691139	3.557029	-0.780274
16C	-0.534948	2.960268	-1.087291
17O	2.039358	4.717580	0.895111
18C	3.064315	4.960880	-0.075393
19C	-6.565280	-3.552454	0.428290
20H	-5.423961	0.667409	-0.919281
21H	-6.933234	-1.259941	-0.759536
22H	-4.137237	-3.506536	1.344367
23H	-2.482127	-1.660862	1.279120
24H	-2.166540	3.477501	1.861382
25H	0.024521	4.530824	2.419241
26H	1.467653	3.588089	-1.535828
27H	-0.694073	2.525440	-2.068217
28H	3.441932	4.025920	-0.500334
29H	2.694378	5.614896	-0.875044
30H	3.868105	5.462937	0.466269
31H	-6.045581	-4.509868	0.349504
32H	-7.067721	-3.484479	1.398398
33H	-7.306078	-3.482690	-0.370291
34P	1.923917	-1.149945	-0.037098
35C	0.981725	-1.075609	-1.584413
36C	2.759955	-2.759639	0.035030
37C	3.170799	0.169250	0.008275
38C	0.834886	-0.963609	1.400176
39C	4.071552	-2.864086	0.523628
40C	4.679271	-4.118871	0.609927
41C	3.984035	-5.265363	0.214735
42C	2.676787	-5.161305	-0.273632
43C	2.062137	-3.912392	-0.366724
44C	3.735851	0.648373	-1.184554
45C	4.770915	1.583256	-1.132055
46C	5.238360	2.047174	0.101923
47C	4.665855	1.581592	1.289170
48C	3.635295	0.640771	1.247582
49C	0.318829	0.303970	1.719421

50C	-0.520936	0.447889	2.823143
51C	-0.849493	-0.660217	3.608478
52C	-0.338254	-1.922166	3.290125
53C	0.505129	-2.079029	2.188820
54C	-0.282095	-0.468542	-1.616474
55C	-0.971535	-0.371611	-2.828022
56C	-0.407667	-0.882379	-3.999827
57C	0.849951	-1.497216	-3.966538
58C	1.547962	-1.597070	-2.763151
59H	4.622060	-1.979579	0.828882
60H	5.696893	-4.196916	0.982393
61H	4.461725	-6.239149	0.281548
62H	2.136524	-6.050686	-0.586109
63H	1.050978	-3.836311	-0.756252
64H	3.377358	0.300783	-2.148112
65H	5.206118	1.953746	-2.056061
66H	6.040218	2.779809	0.137336
67H	5.018294	1.949105	2.248702
68H	3.199174	0.279036	2.173899
69H	0.558938	1.173512	1.114724
70H	-0.927517	1.425900	3.056678
71H	-1.507027	-0.540541	4.465359
72H	-0.588883	-2.785480	3.900614
73H	0.907131	-3.060596	1.959485
74H	-0.748898	-0.075538	-0.718867
75H	-1.941961	0.115501	-2.842887
76H	-0.947599	-0.804346	-4.939909
77H	1.287132	-1.901648	-4.875354
78H	2.518541	-2.084203	-2.743440

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1C	-5.076354	0.149500	0.277015
2C	-5.917253	1.230443	0.238495
3N	-5.511590	2.452307	-0.208197
4C	-4.220613	2.606173	-0.633204
5C	-3.330475	1.571521	-0.620183
6C	-3.712032	0.266656	-0.155479
7N	-2.765084	-0.677339	-0.171211
8S	-3.082589	-2.196422	0.379140
9O	-4.104613	-2.886901	-0.450187
10O	-3.305636	-2.208670	1.850034
11C	-1.495745	-2.959523	0.059027
12C	-1.186457	-3.392595	-1.236809
13C	0.057750	-3.953198	-1.492661
14C	0.996371	-4.096179	-0.453440
15C	0.680831	-3.660353	0.842342
16C	-0.570429	-3.090127	1.092376
17O	2.177931	-4.671066	-0.801468
18C	3.090371	-5.047357	0.236649
19C	-6.419808	3.609484	-0.223325
20H	-5.468210	-0.793191	0.638629
21H	-6.949601	1.159585	0.561958
22H	-3.952637	3.598519	-0.979530
23H	-2.317874	1.729363	-0.973479
24H	-1.917094	-3.297245	-2.033928
25H	0.318777	-4.304115	-2.486797
26H	1.389409	-3.762210	1.656108
27H	-0.820730	-2.748608	2.091023
28H	3.449133	-4.173400	0.789915
29H	2.621105	-5.761461	0.924918
30H	3.930590	-5.524788	-0.270781
31H	-6.061409	4.371060	0.475394
32H	-6.465438	4.027163	-1.232661
33H	-7.418087	3.288568	0.075889
34P	1.872012	1.187969	0.043856
35C	0.981341	0.987221	1.612153
36C	2.742177	2.779405	0.074515
37C	3.080545	-0.152532	-0.160105
38C	0.733548	1.152339	-1.366799
39C	4.003810	2.909401	-0.527471
40C	4.636416	4.154277	-0.545319
41C	4.016800	5.265930	0.033711
42C	2.759100	5.136661	0.632861
43C	2.118454	3.897272	0.655148
44C	3.698647	-0.716162	0.968034
45C	4.687782	-1.686106	0.802006
46C	5.057474	-2.102408	-0.481193
47C	4.437738	-1.547076	-1.603846
48C	3.451598	-0.570930	-1.448953
49C	0.160582	-0.069051	-1.757017
50C	-0.713787	-0.108075	-2.842169
51C	-1.012877	1.061598	-3.545711
52C	-0.441319	2.278785	-3.159667
53C	0.431318	2.330738	-2.071147
54C	-0.279253	0.373047	1.632770

55C	-0.925171	0.158406	2.852795
56C	-0.319894	0.556427	4.047363
57C	0.935920	1.175898	4.027264
58C	1.590600	1.393287	2.814746
59H	4.495503	2.051094	-0.975572
60H	5.614541	4.252196	-1.007998
61H	4.514581	6.231821	0.021355
62H	2.276966	5.998616	1.085658
63H	1.143498	3.803195	1.124484
64H	3.412999	-0.409439	1.969380
65H	5.162187	-2.122919	1.676487
66H	5.820591	-2.866097	-0.604353
67H	4.715828	-1.874321	-2.601729
68H	2.976251	-0.145009	-2.327047
69H	0.387964	-0.986858	-1.224038
70H	-1.166675	-1.052958	-3.125061
71H	-1.695235	1.025979	-4.390807
72H	-0.669375	3.189150	-3.707471
73H	0.877952	3.278274	-1.786453
74H	-0.780520	0.060711	0.722178
75H	-1.895266	-0.330702	2.854863
76H	-0.825735	0.387363	4.994485
77H	1.405981	1.492636	4.954335
78H	2.560293	1.882785	2.806747

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1C	-0.391399	3.422831	0.745461
2C	0.763234	4.145000	0.622488
3N	1.445472	4.237642	-0.555573
4C	0.956855	3.590195	-1.653691
5C	-0.189124	2.848013	-1.599191
6C	-0.939839	2.717396	-0.382744
7N	-2.032913	1.947286	-0.424183
8S	-2.993437	1.795015	0.909227
9O	-3.757734	3.046325	1.152895
10O	-2.262922	1.246271	2.084704
11C	-4.120102	0.530548	0.336302
12C	-4.878032	0.747898	-0.823244
13C	-5.745678	-0.239072	-1.266902
14C	-5.873961	-1.444144	-0.548851
15C	-5.128566	-1.647235	0.621327
16C	-4.246734	-0.653250	1.057700
17O	-6.742321	-2.347785	-1.075189
18C	-6.942353	-3.591444	-0.395125
19C	2.671003	5.046904	-0.625422
20H	-0.876365	3.389691	1.712279
21H	1.195939	4.680856	1.460280
22H	1.532608	3.694272	-2.564347
23H	-0.542346	2.349567	-2.495387
24H	-4.779618	1.675363	-1.378881
25H	-6.338001	-0.098632	-2.166411
26H	-5.214852	-2.565094	1.191295
27H	-3.654171	-0.809838	1.953231
28H	-6.009315	-4.166493	-0.339210
29H	-7.343132	-3.429860	0.613133
30H	-7.672245	-4.139132	-0.993937
31H	3.094319	4.968174	-1.627131
32H	2.436241	6.094417	-0.415549
33H	3.398146	4.681364	0.104755
34P	2.133217	-1.092177	0.024402
35C	0.548901	-1.831166	-0.450780
36C	2.661664	0.053032	-1.284639
37C	1.988841	-0.210747	1.604857
38C	3.395821	-2.382043	0.213774
39C	3.497666	1.137016	-0.971503
40C	3.989601	1.949879	-1.993188
41C	3.644556	1.693259	-3.323819
42C	2.805443	0.619105	-3.635737
43C	2.316631	-0.206793	-2.621552
44C	0.741555	0.238999	2.062938
45C	0.661336	0.946362	3.264862
46C	1.815721	1.208212	4.006497
47C	3.061162	0.760119	3.549975
48C	3.152624	0.049166	2.353671
49C	3.400857	-3.170721	1.378109
50C	4.348817	-4.183576	1.524316
51C	5.293969	-4.410132	0.517494
52C	5.291280	-3.623703	-0.638199
53C	4.344217	-2.608946	-0.795631
54C	0.331398	-3.212444	-0.321781
55C	-0.910953	-3.749108	-0.667592
56C	-1.932446	-2.916634	-1.134741
57C	-1.715482	-1.541137	-1.263321
58C	-0.476759	-0.997024	-0.928311
59H	3.762280	1.353246	0.058643

60H	4.636852	2.786616	-1.746877
61H	4.027062	2.330372	-4.116932
62H	2.532823	0.418804	-4.668162
63H	1.672438	-1.043219	-2.874525
64H	-0.172409	0.053817	1.510228
65H	-0.310904	1.289474	3.602679
66H	1.746823	1.755720	4.942953
67H	3.960721	0.956160	4.127206
68H	4.120678	-0.308576	2.014705
69H	2.675283	-2.992722	2.166748
70H	4.351153	-4.790533	2.425345
71H	6.034498	-5.196589	0.636242
72H	6.028291	-3.794246	-1.417931
73H	4.355955	-1.999260	-1.693696
74H	1.117400	-3.869376	0.036561
75H	-1.077271	-4.818526	-0.571699
76H	-2.898797	-3.338034	-1.397594
77H	-2.507829	-0.885698	-1.609517
78H	-0.319986	0.069672	-1.036001

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1C	-5.621754	-0.944588	0.763463
2C	-6.779007	-1.672031	0.670781
3N	-7.596813	-1.604657	-0.415768
4C	-7.248528	-0.786563	-1.454561
5C	-6.107517	-0.036616	-1.428018
6C	-5.217401	-0.069695	-0.301687
7N	-4.126800	0.707155	-0.364012
8S	-3.058721	0.706549	0.887587
9O	-2.389965	-0.618712	1.023251
10O	-3.630479	1.256822	2.145102
11C	-1.851395	1.880179	0.278404
12C	-1.243896	1.678638	-0.968927
13C	-0.240438	2.538974	-1.389413
14C	0.170619	3.604620	-0.565520
15C	-0.445138	3.806140	0.678495
16C	-1.461001	2.939042	1.093660
17O	1.162866	4.383945	-1.067795
18C	1.682206	5.445335	-0.262342
19C	-8.827829	-2.405084	-0.500599
20H	-5.025355	-1.047869	1.661407
21H	-7.098403	-2.336115	1.465481
22H	-7.934713	-0.770703	-2.294305
23H	-5.869195	0.603790	-2.270589
24H	-1.555102	0.856260	-1.604005
25H	0.245131	2.402480	-2.350728
26H	-0.153902	4.625535	1.325232
27H	-1.946434	3.091676	2.052076
28H	0.911097	6.196587	-0.052111
29H	2.095431	5.062327	0.678896
30H	2.478871	5.900533	-0.852965
31H	-9.677745	-1.749913	-0.709135
32H	-8.734004	-3.149508	-1.296943
33H	-8.991871	-2.912534	0.451035
34P	2.666371	-0.869532	-0.010860
35C	1.400395	-1.572948	-1.103560
36C	4.044855	-2.046968	0.081076
37C	3.271098	0.714338	-0.660552
38C	1.981718	-0.587466	1.643235
39C	5.374110	-1.596969	0.085689
40C	6.416039	-2.520234	0.201423
41C	6.136761	-3.885597	0.311938
42C	4.811592	-4.334467	0.305039
43C	3.764020	-3.420620	0.188436
44C	3.193446	1.000716	-2.032350
45C	3.728412	2.193164	-2.522260
46C	4.339301	3.099514	-1.651414
47C	4.413921	2.817319	-0.284053
48C	3.880521	1.628874	0.216428
49C	1.099929	0.489379	1.842688
50C	0.523556	0.685718	3.096633
51C	0.830610	-0.175715	4.154486
52C	1.716893	-1.238937	3.959366
53C	2.293461	-1.451236	2.705188
54C	0.042994	-1.498440	-0.761409
55C	-0.919347	-2.012627	-1.633733
56C	-0.532385	-2.602003	-2.839489
57C	0.824426	-2.685928	-3.177265
58C	1.793245	-2.177489	-2.312721
59H	5.601905	-0.539478	-0.006353
60H	7.444762	-2.170806	0.199818
61H	6.950399	-4.600915	0.398330
62H	4.591655	-5.395408	0.385886
63H	2.738222	-3.777230	0.177807
64H	2.712205	0.309245	-2.716786

65H	3.657256	2.416994	-3.582995
66H	4.748189	4.029567	-2.036725
67H	4.881458	3.523374	0.396591
68H	3.938079	1.420080	1.280770
69H	0.854477	1.164954	1.029087
70H	-0.173166	1.505416	3.240305
71H	0.375889	-0.019542	5.129071
72H	1.960985	-1.906456	4.781099
73H	2.979120	-2.280679	2.564376
74H	-0.290167	-1.050837	0.167532
75H	-1.966649	-1.942375	-1.354778
76H	-1.283580	-3.001847	-3.515762
77H	1.129264	-3.152456	-4.110041
78H	2.844817	-2.258261	-2.574403

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1C	0.548384	3.365946	0.752161
2C	-0.544783	4.167357	0.571866
3N	-1.129641	4.342106	-0.648228
4C	-0.603894	3.695659	-1.729918
5C	0.482652	2.874111	-1.618829
6C	1.133386	2.658848	-0.357114
7N	2.172904	1.816874	-0.342870
8S	2.997048	1.552728	1.063995
9O	2.130318	0.990644	2.135827
10O	3.793687	2.749680	1.441440
11C	4.113605	0.257006	0.542690
12C	4.090512	-0.978011	1.198591
13C	4.974556	-1.977168	0.808245
14C	5.880955	-1.748691	-0.240613
15C	5.901987	-0.503910	-0.894051
16C	5.018781	0.498489	-0.491686
17O	6.695555	-2.791005	-0.553978
18C	7.681613	-2.612656	-1.576976
19C	-2.279492	5.247976	-0.781687
20H	0.954749	3.272011	1.750875
21H	-1.002532	4.704312	1.395651
22H	-1.100357	3.870061	-2.676509
23H	0.866567	2.376904	-2.503135
24H	3.383112	-1.154395	2.001931
25H	4.975237	-2.944272	1.302542
26H	6.596628	-0.307022	-1.702598
27H	5.033830	1.461139	-0.993800
28H	7.212947	-2.401111	-2.546159
29H	8.380207	-1.808814	-1.315354
30H	8.220878	-3.559948	-1.633609
31H	-2.689247	5.160070	-1.788215
32H	-3.048177	4.975369	-0.054165
33H	-1.961990	6.280669	-0.609318
34P	-2.269152	-1.036707	-0.002477
35C	-2.154000	-0.192400	1.598520
36C	-3.553754	-2.311022	0.126403
37C	-2.722682	0.151951	-1.299171
38C	-0.683917	-1.787309	-0.455803
39C	-4.499385	-2.487868	-0.895063
40C	-5.462252	-3.493377	-0.777828
41C	-5.482122	-4.320337	0.348950
42C	-4.540177	-4.142536	1.368641
43C	-3.577280	-3.138942	1.263273
44C	-3.415760	1.328382	-0.974962
45C	-3.828417	2.190552	-1.992183
46C	-3.545669	1.889513	-3.327746
47C	-2.845138	0.722600	-3.650756
48C	-2.434183	-0.149265	-2.641515
49C	0.354488	-0.954552	-0.907448
50C	1.593540	-1.504125	-1.231160
51C	1.798070	-2.882962	-1.118077
52C	0.764023	-3.713341	-0.675647
53C	-0.478853	-3.171393	-0.340142
54C	-0.911655	0.239261	2.085781
55C	-0.846748	0.922387	3.302480
56C	-2.012276	1.176579	4.029670
57C	-3.252775	0.745858	3.543375
58C	-3.329393	0.060741	2.330788
59H	-4.497725	-1.845967	-1.770554
60H	-6.198170	-3.625497	-1.566116
61H	-6.234037	-5.100170	0.436103
62H	-4.556063	-4.781012	2.247535
63H	-2.855009	-2.997573	2.062762
64H	-3.633005	1.576399	0.059381
65H	-4.369998	3.097104	-1.738682
66H	-3.868763	2.563716	-4.116664
67H	-2.619628	0.488095	-4.687348
68H	-1.892620	-1.054528	-2.899699
69H	0.205386	0.115095	-1.002359

70H	2.396344	-0.849191	-1.552710
71H	2.765733	-3.308247	-1.369225
72H	0.921795	-4.784897	-0.590008
73H	-1.274587	-3.826328	-0.000295
74H	0.010585	0.057368	1.545856
75H	0.122404	1.248657	3.666106
76H	-1.956258	1.703912	4.978491
77H	-4.160356	0.936935	4.109595
78H	-4.294373	-0.279413	1.965966

6cg-001

1C	-2.709513	-2.251761	-1.437088
2C	-2.103242	-2.594710	-2.641129
3N	-0.887156	-3.158911	-2.765372
4C	-0.250475	-3.414007	-1.601435
5C	-0.756442	-3.111697	-0.347283
6C	-2.026688	-2.484097	-0.211507
7N	-2.412417	-2.154809	1.060267
8S	-3.803533	-1.399714	1.380971
9O	-3.860499	-1.266421	2.860575
10O	-4.999851	-1.993794	0.717369
11C	-3.680407	0.291730	0.747443
12C	-4.436085	0.702887	-0.347556
13C	-4.318895	2.008445	-0.839321
14C	-3.431450	2.900772	-0.224886
15C	-2.677196	2.486355	0.887268
16C	-2.802516	1.191263	1.370256
17O	-3.224867	4.186581	-0.630975
18C	-3.978906	4.686007	-1.737099
19H	-3.701602	-1.818426	-1.448610
20H	-2.632736	-2.399387	-3.573676
21H	0.731774	-3.874145	-1.686679
22H	-0.179588	-3.334221	0.545843
23H	-5.131799	0.012075	-0.812498
24H	-4.918678	2.307598	-1.691214
25H	-2.000088	3.194870	1.355849
26H	-2.228667	0.879144	2.236274
27H	-5.055279	4.669592	-1.523949
28H	-3.651199	5.718410	-1.875058
29H	-3.774565	4.114257	-2.651587
30P	2.275693	0.247551	0.100811
31C	1.652446	-0.175513	1.751072
32C	3.729625	1.320896	0.291515
33C	2.755843	-1.274197	-0.763879
34C	1.015478	1.099230	-0.892185
35C	4.895154	1.079323	-0.451554
36C	5.992487	1.933704	-0.317747
37C	5.932530	3.024526	0.553626
38C	4.772097	3.264989	1.297900
39C	3.672164	2.416304	1.172745
40C	3.076766	-2.427311	-0.030689
41C	3.492313	-3.578709	-0.701872
42C	3.585106	-3.583901	-2.097082
43C	3.259015	-2.436590	-2.827379
44C	2.844682	-1.280157	-2.166017
45C	-0.014033	0.351871	-1.491386
46C	-0.995001	1.002302	-2.239180
47C	-0.951916	2.389177	-2.400893
48C	0.074028	3.132649	-1.812174
49C	1.058832	2.493743	-1.057457
50C	0.307626	-0.540163	1.913838
51C	-0.155042	-0.954374	3.164076
52C	0.720239	-1.001373	4.252476
53C	2.064366	-0.644575	4.091368
54C	2.536913	-0.234943	2.843862
55H	4.955789	0.231960	-1.127124
56H	6.894521	1.740174	-0.891788
57H	6.789169	3.685370	0.656350
58H	4.723766	4.108726	1.980832
59H	2.779806	2.604574	1.763368
60H	2.990034	-2.437711	1.051453
61H	3.728787	-4.474416	-0.134193
62H	3.896336	-4.486139	-2.616781
63H	3.313159	-2.443831	-3.912291
64H	2.581394	-0.396856	-2.740403
65H	-0.055460	-0.726435	-1.383411
66H	-1.794205	0.418077	-2.683268
67H	-1.722250	2.892292	-2.978039
68H	0.107288	4.211692	-1.933902
69H	1.853318	3.083207	-0.612906
70H	-0.389575	-0.521328	1.085063
71H	-1.196607	-1.245553	3.262672
72H	0.357199	-1.322258	5.225420
73H	2.747934	-0.686456	4.935201
74H	3.582493	0.033858	2.727456

6cg-002

1C	-2.831814	-2.264720	-1.349383
2C	-2.206423	-2.770523	-2.484412
3N	-1.028054	-3.421416	-2.497132
4C	-0.453183	-3.593523	-1.286904
5C	-0.984353	-3.132179	-0.092894
6C	-2.214143	-2.415254	-0.077230
7N	-2.624399	-1.933259	1.136766
8S	-3.968815	-1.058107	1.320931
9O	-4.073991	-0.780237	2.777650
10O	-5.177741	-1.628175	0.659667
11C	-3.694651	0.552454	0.540364
12C	-2.798134	1.446090	1.128920
13C	-2.544263	2.686433	0.541080
14C	-3.201415	3.033407	-0.649053
15C	-4.114866	2.140861	-1.230837
16C	-4.358446	0.904619	-0.639726
17O	-3.011961	4.207505	-1.317358
18C	-2.126963	5.180278	-0.758527
19H	-3.789078	-1.768704	-1.449065
20H	-2.685961	-2.639297	-3.454408
21H	0.499577	-4.119396	-1.282140
22H	-0.456822	-3.297068	0.842418
23H	-2.299589	1.182229	2.055546
24H	-1.841791	3.363650	1.013153
25H	-4.622260	2.430536	-2.146763
26H	-5.073373	0.218914	-1.082422
27H	-2.123186	6.013828	-1.463896
28H	-2.487498	5.529620	0.217550
29H	-1.109697	4.783558	-0.657196
30P	2.222596	0.124794	0.114606
31C	2.654293	-1.499412	-0.570679
32C	1.525091	-0.099976	1.773931
33C	3.713480	1.153226	0.249129
34C	1.044196	0.921602	-1.013158
35C	2.371510	-0.096148	2.898173
36C	1.839856	-0.353964	4.162275
37C	0.474138	-0.624060	4.309480
38C	-0.363811	-0.641000	3.191251
39C	0.158138	-0.377395	1.923368
40C	4.879633	0.815507	-0.454730
41C	5.999363	1.647569	-0.379427
42C	5.960090	2.811219	0.393817
43C	4.799014	3.146699	1.099475
44C	3.675973	2.322232	1.030461
45C	-0.043268	0.178503	-1.506036
46C	-0.951838	0.777467	-2.376852
47C	-0.777113	2.106839	-2.770747
48C	0.308713	2.843340	-2.290151
49C	1.220437	2.257702	-1.409483
50C	2.954542	-2.564235	0.293829
51C	3.328036	-3.800164	-0.236172
52C	3.400978	-3.977345	-1.621462
53C	3.098230	-2.917729	-2.482157
54C	2.724308	-1.678016	-1.962415
55H	3.432958	0.107453	2.793703
56H	2.494058	-0.346342	5.030021
57H	0.064432	-0.827823	5.295382
58H	-1.421344	-0.870879	3.282000
59H	-0.511877	-0.405096	1.072613
60H	4.921989	-0.088559	-1.054231
61H	6.901644	1.381962	-0.923356
62H	6.834142	3.454542	0.450897
63H	4.767621	4.047854	1.705681
64H	2.779914	2.584553	1.586243
65H	-0.178468	-0.860930	-1.227260
66H	-1.796150	0.199908	-2.737607
67H	-1.490163	2.570242	-3.446110
68H	0.447726	3.875716	-2.598847
69H	2.063643	2.838147	-1.049994
70H	2.885700	-2.439327	1.370206
71H	3.549250	-4.626277	0.433847
72H	3.680019	-4.944692	-2.030421
73H	3.136350	-3.058504	-3.558471
74H	2.475039	-0.864466	-2.636875

6cg-003

1C	-4.213633	-1.561103	-1.055076
2C	-4.226876	-2.318347	-2.221930
3N	-3.461923	-3.400685	-2.455250
4C	-2.646896	-3.755542	-1.439155

5C	-2.553166	-3.078445	-0.233821
6C	-3.336273	-1.914857	0.007056
7N	-3.144532	-1.292118	1.213600
8S	-3.820562	0.121074	1.604305
9O	-3.566823	0.324428	3.052831
10O	-5.230304	0.298015	1.147798
11C	-2.868294	1.412742	0.761596
12C	-3.236265	1.847339	-0.511809
13C	-2.460492	2.793012	-1.191533
14C	-1.311842	3.313977	-0.580026
15C	-0.954303	2.891514	0.712266
16C	-1.724916	1.943754	1.375792
17O	-0.478754	4.229678	-1.154425
18C	-0.748150	4.660340	-2.490082
19H	-4.891078	-0.722733	-0.956597
20H	-4.901913	-2.032628	-3.028824
21H	-2.027321	-4.635204	-1.611035
22H	-1.872673	-3.427968	0.538297
23H	-4.137297	1.465397	-0.978679
24H	-2.766122	3.113155	-2.181134
25H	-0.066127	3.311291	1.175543
26H	-1.444660	1.614010	2.369713
27H	-1.717758	5.169178	-2.558396
28H	0.045466	5.367965	-2.738680
29H	-0.721461	3.817588	-3.193053
30P	2.140736	-0.324755	0.058089
31C	2.905542	1.281916	-0.316587
32C	3.461368	-1.562418	0.208877
33C	1.246456	-0.212867	1.629243
34C	1.010489	-0.805867	-1.273996
35C	3.368832	-2.563388	1.188322
36C	4.360387	-3.543398	1.272684
37C	5.440589	-3.527800	0.385683
38C	5.533192	-2.530628	-0.591759
39C	4.546484	-1.548500	-0.685539
40C	1.728341	0.635937	2.641668
41C	1.085490	0.665150	3.879105
42C	-0.035445	-0.141405	4.108520
43C	-0.521962	-0.972843	3.097592
44C	0.117400	-1.014449	1.857769
45C	-0.250515	-0.193328	-1.372582
46C	-1.093768	-0.514590	-2.435272
47C	-0.695334	-1.451867	-3.392097
48C	0.553017	-2.072368	-3.286925
49C	1.409650	-1.753036	-2.232330
50C	2.223594	2.221459	-1.105201
51C	2.784745	3.480650	-1.324551
52C	4.022336	3.807301	-0.763840
53C	4.703751	2.872522	0.022919
54C	4.150212	1.611812	0.249760
55H	2.536384	-2.579745	1.885368
56H	4.287649	-4.314811	2.034415
57H	6.211663	-4.290533	0.456612
58H	6.372325	-2.516913	-1.281995
59H	4.624982	-0.776024	-1.445627
60H	2.587461	1.276793	2.469112
61H	1.452089	1.328088	4.658313
62H	-0.547886	-0.099613	5.065784
63H	-1.428261	-1.549259	3.239949
64H	-0.290401	-1.642397	1.073543
65H	-0.583624	0.511307	-0.619212
66H	-2.072634	-0.052027	-2.493639
67H	-1.366375	-1.715806	-4.203983
68H	0.858492	-2.815173	-4.018697
69H	2.372717	-2.247574	-2.158222
70H	1.260286	1.987304	-1.544397
71H	2.245170	4.204708	-1.926811
72H	4.455725	4.788723	-0.937432
73H	5.665997	3.122416	0.461336
74H	4.686900	0.893002	0.861689

6cg-004

1C	-1.828716	1.985634	-0.724051
2C	-1.738218	2.914144	-1.754639
3N	-1.947476	4.237353	-1.627228
4C	-2.279182	4.648849	-0.384718
5C	-2.398230	3.812945	0.714990
6C	-2.162262	2.418006	0.587725
7N	-2.277656	1.660399	1.728068
8S	-2.070338	0.063148	1.686469
9O	-2.214884	-0.428860	3.082117
10O	-0.832581	-0.387182	0.978718
11C	-3.435788	-0.638543	0.730886
12C	-4.745647	-0.258191	1.025305
13C	-5.813662	-0.791492	0.300079

14C	-5.560380	-1.711980	-0.729741
15C	-4.239835	-2.091058	-1.022079
16C	-3.181701	-1.554646	-0.295405
17O	-6.526357	-2.286598	-1.502157
18C	-7.892705	-1.933076	-1.269779
19H	-1.617026	0.944764	-0.929241
20H	-1.471660	2.570916	-2.754646
21H	-2.456787	5.717688	-0.269382
22H	-2.663417	4.217665	1.688365
23H	-4.938872	0.462871	1.814572
24H	-6.824206	-0.482321	0.540763
25H	-4.062432	-2.800323	-1.825861
26H	-2.159456	-1.834129	-0.525715
27H	-8.471960	-2.502219	-1.999633
28H	-8.208447	-2.212000	-0.256459
29H	-8.057927	-0.860100	-1.429926
30P	2.532283	-0.334453	-0.105142
31C	4.089816	-0.210699	-1.035476
32C	1.312141	-1.195623	-1.136806
33C	2.825405	-1.302446	1.403452
34C	2.003650	1.355748	0.278219
35C	1.215548	-2.594443	-1.081344
36C	0.314218	-3.258957	-1.916090
37C	-0.485393	-2.533146	-2.804037
38C	-0.387942	-1.138952	-2.856431
39C	0.508112	-0.467259	-2.025088
40C	4.133912	-1.633243	1.792692
41C	4.342602	-2.368491	2.961654
42C	3.254723	-2.772830	3.741337
43C	1.952103	-2.447616	3.348843
44C	1.728637	-1.717413	2.180753
45C	2.129224	2.345986	-0.713607
46C	1.688569	3.643480	-0.456433
47C	1.136229	3.960354	0.788690
48C	1.023657	2.980006	1.777043
49C	1.449991	1.675743	1.526224
50C	4.334336	-1.039935	-2.140262
51C	5.557682	-0.958954	-2.810666
52C	6.535027	-0.056128	-2.382307
53C	6.290856	0.773204	-1.281849
54C	5.071513	0.700522	-0.608018
55H	1.826633	-3.164272	-0.387903
56H	0.233170	-4.341249	-1.864507
57H	-1.193406	-3.051419	-3.445480
58H	-1.023406	-0.571127	-3.530443
59H	0.556322	0.615609	-2.053262
60H	4.987373	-1.331805	1.194471
61H	5.355886	-2.625249	3.258761
62H	3.421817	-3.342889	4.651695
63H	1.102288	-2.759211	3.950111
64H	0.715042	-1.465162	1.880815
65H	2.569472	2.110263	-1.678420
66H	1.767951	4.402446	-1.229503
67H	0.784205	4.969135	0.983381
68H	0.575292	3.218073	2.736743
69H	1.334790	0.920506	2.294114
70H	3.578201	-1.739244	-2.483879
71H	5.742233	-1.597932	-3.669958
72H	7.484350	0.006115	-2.907828
73H	7.046883	1.479193	-0.949221
74H	4.885006	1.351699	0.241417

6cg-005

1C	-4.130460	1.930388	0.523483
2C	-4.786709	2.560826	1.576214
3N	-4.280540	3.568197	2.312134
4C	-3.043325	3.975703	1.958988
5C	-2.297399	3.418933	0.931199
6C	-2.818698	2.341257	0.166351
7N	-1.987636	1.803849	-0.786395
8S	-2.485253	0.695465	-1.840649
9O	-1.343149	0.452201	-2.764532
10O	-3.788566	0.995362	-2.503166
11C	-2.745647	-0.865262	-0.957216
12C	-2.344326	-1.018881	0.365367
13C	-2.506294	-2.245293	1.019803
14C	-3.068170	-3.326261	0.328439
15C	-3.481532	-3.166308	-1.006828
16C	-3.323453	-1.942256	-1.644294
17O	-3.255612	-4.568953	0.860989
18C	-2.908354	-4.785256	2.230640
19H	-4.631156	1.132070	-0.012388
20H	-5.789574	2.232515	1.847949
21H	-2.628734	4.798805	2.540384
22H	-1.305718	3.799524	0.701216

23H	-1.902980	-0.185349	0.897538
24H	-2.193314	-2.336805	2.053426
25H	-3.924338	-4.012832	-1.524245
26H	-3.647369	-1.821679	-2.673990
27H	-3.148838	-5.830768	2.433666
28H	-1.837038	-4.618131	2.402523
29H	-3.496999	-4.139385	2.894601
30P	2.296700	0.032355	0.041878
31C	1.614631	-1.105188	-1.193666
32C	1.267430	0.030611	1.538098
33C	3.965842	-0.499312	0.530090
34C	2.356221	1.692402	-0.680254
35C	1.383158	-1.033277	2.451071
36C	0.568909	-1.065376	3.583076
37C	-0.356663	-0.039874	3.810329
38C	-0.468408	1.018370	2.904974
39C	0.340153	1.057719	1.766215
40C	4.716103	-1.349605	-0.297082
41C	6.009994	-1.718360	0.078785
42C	6.557036	-1.243334	1.274302
43C	5.809143	-0.397954	2.100947
44C	4.515461	-0.025273	1.734283
45C	1.272691	2.119389	-1.466885
46C	1.271014	3.416378	-1.983272
47C	2.341720	4.278243	-1.728900
48C	3.423147	3.846888	-0.951760
49C	3.435242	2.555169	-0.423182
50C	0.708733	-2.106926	-0.816159
51C	0.191828	-2.972531	-1.780545
52C	0.577051	-2.844361	-3.116956
53C	1.483256	-1.848061	-3.494477
54C	2.001522	-0.974649	-2.539276
55H	2.104608	-1.827780	2.281383
56H	0.659174	-1.888194	4.287121
57H	-0.991578	-0.067218	4.691945
58H	-1.195357	1.808646	3.066536
59H	0.225133	1.870584	1.057983
60H	4.297414	-1.730440	-1.223482
61H	6.585976	-2.380497	-0.561892
62H	7.563117	-1.534504	1.564591
63H	6.229321	-0.030519	3.033229
64H	3.938552	0.624028	2.386424
65H	0.430574	1.467153	-1.676210
66H	0.424874	3.743988	-2.580537
67H	2.335799	5.286029	-2.136198
68H	4.259015	4.513723	-0.757954
69H	4.280949	2.228753	0.174394
70H	0.380557	-2.200628	0.212598
71H	-0.531932	-3.726471	-1.486530
72H	0.158720	-3.509289	-3.867830
73H	1.771818	-1.736384	-4.535892
74H	2.683630	-0.186981	-2.846053

6cg-006

1C	4.001524	-2.211920	0.363872
2C	4.662161	-2.960698	1.333096
3N	4.135213	-4.007715	1.994979
4C	2.869681	-4.328664	1.652916
5C	2.116423	-3.650478	0.706891
6C	2.661308	-2.532896	0.019892
7N	1.827626	-1.881443	-0.856056
8S	2.347929	-0.697338	-1.811974
9O	1.181153	-0.288521	-2.641961
10O	3.595496	-1.002842	-2.572181
11C	2.759446	0.736161	-0.781649
12C	3.545683	1.754062	-1.321507
13C	3.824826	2.903889	-0.577074
14C	3.313981	3.025082	0.724919
15C	2.536521	1.990743	1.269876
16C	2.257181	0.854888	0.517563
17O	3.517735	4.102677	1.537295
18C	4.348563	5.169213	1.071361
19H	4.523069	-1.393407	-0.118933
20H	5.686950	-2.699864	1.596218
21H	2.437183	-5.182588	2.173841
22H	1.100753	-3.965242	0.481672
23H	3.948155	1.653641	-2.325282
24H	4.437208	3.683370	-1.016152
25H	2.160074	2.091567	2.283588
26H	1.654964	0.060118	0.941248
27H	3.925878	5.642750	0.175996
28H	4.376947	5.896663	1.885326
29H	5.365918	4.816542	0.860002
30P	-2.323915	0.087164	0.056657
31C	-1.283235	-0.138664	1.526594

32C	-3.934795	0.708956	0.627468
33C	-1.580012	1.276686	-1.090672
34C	-2.540356	-1.494433	-0.798806
35C	-4.645141	1.652760	-0.130244
36C	-5.900061	2.087380	0.302831
37C	-6.447617	1.585278	1.487112
38C	-5.739012	0.646922	2.245032
39C	-4.484256	0.207907	1.820574
40C	-0.642107	2.215696	-0.638432
41C	-0.100197	3.138513	-1.533984
42C	-0.492732	3.129849	-2.874552
43C	-1.430442	2.195102	-3.325650
44C	-1.974219	1.265541	-2.439890
45C	-1.506865	-1.959710	-1.630299
46C	-1.634796	-3.206303	-2.245824
47C	-2.781153	-3.980332	-2.042650
48C	-3.810896	-3.510406	-1.219579
49C	-3.695567	-2.268000	-0.593727
50C	-0.518616	-1.302976	1.691549
51C	0.288204	-1.444456	2.823430
52C	0.340663	-0.429817	3.782147
53C	-0.424294	0.731059	3.619845
54C	-1.241000	0.877440	2.499197
55H	-4.225460	2.055265	-1.047003
56H	-6.444634	2.822366	-0.283586
57H	-7.422954	1.928063	1.822546
58H	-6.159256	0.258263	3.168638
59H	-3.936351	-0.514049	2.419097
60H	-0.308460	2.218443	0.392492
61H	0.645916	3.845802	-1.183827
62H	-0.057060	3.840081	-3.572308
63H	-1.725733	2.176208	-4.370979
64H	-2.685116	0.528648	-2.802734
65H	-0.608924	-1.372550	-1.800008
66H	-0.829683	-3.566030	-2.880369
67H	-2.874634	-4.948938	-2.527161
68H	-4.705619	-4.107602	-1.065267
69H	-4.502003	-1.910135	0.039084
70H	-0.528864	-2.086082	0.942317
71H	0.890131	-2.340440	2.938485
72H	0.978804	-0.542169	4.654563
73H	-0.388177	1.520815	4.365351
74H	-1.844876	1.773805	2.387427

6cg-007

1C	-2.573925	1.933923	-1.123882
2C	-2.774450	3.268865	-1.458935
3N	-2.400554	4.320549	-0.706853
4C	-1.794771	4.008912	0.458287
5C	-1.551453	2.716649	0.896272
6C	-1.936630	1.603998	0.102442
7N	-1.657029	0.357368	0.608963
8S	-2.161159	-0.983543	-0.132250
9O	-1.733030	-2.119602	0.728545
10O	-1.781812	-1.088813	-1.572014
11C	-3.969724	-0.956311	-0.100364
12C	-4.624671	-0.631401	1.087973
13C	-6.020181	-0.617248	1.143654
14C	-6.760947	-0.935260	-0.006064
15C	-6.097110	-1.261555	-1.200268
16C	-4.706594	-1.270098	-1.247420
17O	-8.123321	-0.950066	-0.063645
18C	-8.864928	-0.598879	1.107540
19H	-2.889195	1.161530	-1.815443
20H	-3.264033	3.509741	-2.402410
21H	-1.486083	4.852756	1.074750
22H	-1.055930	2.542978	1.847865
23H	-4.048691	-0.376785	1.973123
24H	-6.510870	-0.356741	2.074423
25H	-6.687455	-1.498545	-2.081004
26H	-4.189190	-1.510192	-2.170856
27H	-9.916603	-0.671365	0.823048
28H	-8.661023	-1.294245	1.931750
29H	-8.642421	0.428151	1.423435
30P	2.927118	-0.198658	0.069596
31C	2.106523	1.221980	-0.695303
32C	2.377220	-1.731649	-0.727379
33C	4.728169	-0.088818	-0.154141
34C	2.523300	-0.188223	1.840097
35C	3.031227	-2.171094	-1.893963
36C	2.572032	-3.309854	-2.554947
37C	1.461020	-4.006779	-2.064480
38C	0.806233	-3.561436	-0.914514
39C	1.261748	-2.427038	-0.240073
40C	5.337196	1.080921	-0.631737

41C	6.725583	1.126311	-0.785989
42C	7.506033	0.012193	-0.466111
43C	6.899365	-1.157064	0.006875
44C	5.514337	-1.212632	0.160079
45C	1.181590	0.002840	2.214751
46C	0.839270	-0.009498	3.567523
47C	1.822834	-0.193345	4.544448
48C	3.158910	-0.367495	4.169115
49C	3.514573	-0.367734	2.818619
50C	1.351579	1.069039	-1.866768
51C	0.743793	2.186178	-2.443978
52C	0.889267	3.446927	-1.861468
53C	1.632213	3.595993	-0.685352
54C	2.234893	2.487165	-0.094247
55H	3.889421	-1.632888	-2.285407
56H	3.079086	-3.649301	-3.454191
57H	1.101113	-4.889476	-2.586766
58H	-0.075343	-4.073255	-0.542369
59H	0.718641	-2.091012	0.634963
60H	4.741186	1.949437	-0.892405
61H	7.192799	2.032213	-1.162386
62H	8.585044	0.051216	-0.590311
63H	7.501938	-2.027902	0.250310
64H	5.047576	-2.128570	0.512599
65H	0.393210	0.153198	1.477867
66H	-0.201726	0.125623	3.848415
67H	1.550489	-0.197394	5.596827
68H	3.927724	-0.500386	4.925638
69H	4.555484	-0.497350	2.541049
70H	1.213395	0.090634	-2.315194
71H	0.138999	2.062135	-3.337249
72H	0.399511	4.308981	-2.304565
73H	1.722769	4.571749	-0.216395
74H	2.789211	2.603155	0.833347

6cg-008

1C	-1.787206	1.982254	-0.850241
2C	-1.676480	2.825694	-1.949455
3N	-1.852373	4.159552	-1.925147
4C	-2.170873	4.673868	-0.717921
5C	-2.308318	3.928911	0.443286
6C	-2.106792	2.522716	0.424618
7N	-2.232762	1.860974	1.621410
8S	-2.065086	0.260851	1.714463
9O	-2.174122	-0.100969	3.151948
10O	-0.866476	-0.282994	1.005499
11C	-3.485347	-0.482061	0.881954
12C	-3.303853	-1.324163	-0.211709
13C	-4.408852	-1.883272	-0.864712
14C	-5.700966	-1.586245	-0.410410
15C	-5.879088	-0.734804	0.696136
16C	-4.777975	-0.183792	1.337229
17O	-6.847071	-2.067518	-0.970695
18C	-6.748921	-2.914978	-2.117354
19H	-1.597620	0.924841	-0.973905
20H	-1.419785	2.400107	-2.919970
21H	-2.320880	5.752644	-0.685357
22H	-2.558869	4.414990	1.382638
23H	-2.300284	-1.545973	-0.557768
24H	-4.246459	-2.535511	-1.715650
25H	-6.888983	-0.516864	1.031943
26H	-4.918582	0.478797	2.186412
27H	-6.201259	-3.837129	-1.884655
28H	-7.776924	-3.162526	-2.389593
29H	-6.264554	-2.395128	-2.953870
30P	2.486126	-0.358279	-0.085288
31C	1.228613	-1.249349	-1.047912
32C	2.770462	-1.228226	1.484182
33C	4.035462	-0.355964	-1.040704
34C	2.008089	1.367505	0.194716
35C	4.078170	-1.527567	1.901481
36C	4.282233	-2.185946	3.116107
37C	3.190925	-2.545286	3.913119
38C	1.889714	-2.247533	3.495310
39C	1.671001	-1.592268	2.282697
40C	4.273679	-1.348871	-2.003596
41C	5.489871	-1.372305	-2.689976
42C	6.467001	-0.409293	-2.421300
43C	6.231217	0.580473	-1.460824
44C	5.019385	0.610486	-0.769179
45C	2.142034	2.294584	-0.855242
46C	1.737572	3.615821	-0.669708
47C	1.212082	4.020039	0.561598
48C	1.090181	3.102466	1.607416
49C	1.480992	1.775493	1.428928

50C	0.473277	-0.562667	-2.009478
51C	-0.449917	-1.257940	-2.790408
52C	-0.624857	-2.634326	-2.613774
53C	0.126008	-3.318286	-1.653645
54C	1.055617	-2.630205	-0.870607
55H	4.933922	-1.259832	1.290025
56H	5.294577	-2.418958	3.435155
57H	3.354495	-3.058141	4.857497
58H	1.037495	-2.521055	4.111477
59H	0.659215	-1.357181	1.963783
60H	3.518458	-2.097158	-2.223789
61H	5.668339	-2.140128	-3.437803
62H	7.410277	-0.427970	-2.960761
63H	6.987968	1.331318	-1.251007
64H	4.841809	1.382443	-0.025976
65H	2.559555	1.991730	-1.811137
66H	1.823829	4.324904	-1.487974
67H	0.888107	5.047228	0.700677
68H	0.662355	3.407862	2.557383
69H	1.358357	1.071034	2.242579
70H	0.580629	0.509080	-2.135525
71H	-1.044435	-0.720628	-3.524169
72H	-1.353710	-3.169980	-3.216520
73H	-0.013929	-4.385580	-1.505639
74H	1.628834	-3.168269	-0.122181

6cg-009

1C	2.444193	2.780512	-1.120945
2C	2.065172	3.443600	-2.283619
3N	0.848259	3.970230	-2.515641
4C	-0.038347	3.830145	-1.507803
5C	0.229118	3.183554	-0.312132
6C	1.505443	2.608351	-0.069522
7N	1.659936	1.947667	1.124247
8S	3.089286	1.428777	1.666444
9O	2.861858	1.012606	3.075927
10O	4.212977	2.376944	1.419517
11C	3.551172	-0.101099	0.808123
12C	4.495421	-0.090392	-0.216589
13C	4.863927	-1.279835	-0.856632
14C	4.284147	-2.490014	-0.452353
15C	3.338996	-2.499810	0.588640
16C	2.974254	-1.313481	1.211015
17O	4.565984	-3.705788	-1.003454
18C	5.553228	-3.781017	-2.035626
19H	3.457640	2.411998	-1.031516
20H	2.792714	3.558493	-3.086966
21H	-1.025601	4.260374	-1.675230
22H	-0.537788	3.111751	0.452295
23H	4.972553	0.840361	-0.504568
24H	5.604731	-1.246633	-1.647706
25H	2.908391	-3.448305	0.897869
26H	2.256314	-1.328017	2.022908
27H	6.528941	-3.428500	-1.678257
28H	5.622418	-4.838123	-2.299812
29H	5.249125	-3.203884	-2.918337
30P	-2.268587	-0.458534	0.034964
31C	-3.490555	-1.665535	-0.560654
32C	-3.100110	1.150237	0.185172
33C	-1.627653	-0.980798	1.647626
34C	-0.903358	-0.361215	-1.154687
35C	-2.873650	1.973125	1.298962
36C	-3.482998	3.227897	1.369560
37C	-4.315881	3.664928	0.336361
38C	-4.552227	2.841093	-0.769608
39C	-3.951436	1.584699	-0.847024
40C	-2.282174	-1.982113	2.384570
41C	-1.800438	-2.334896	3.646656
42C	-0.675161	-1.692429	4.174292
43C	-0.022493	-0.699132	3.437347
44C	-0.489448	-0.342223	2.170664
45C	0.185328	-1.241423	-1.037385
46C	1.205122	-1.207781	-1.988583
47C	1.146066	-0.304734	-3.052658
48C	0.065254	0.573289	-3.168303
49C	-0.958898	0.549694	-2.222275
50C	-3.094040	-2.692964	-1.430946
51C	-4.024893	-3.647247	-1.846907
52C	-5.347906	-3.579397	-1.400037
53C	-5.744711	-2.554233	-0.534605
54C	-4.821031	-1.597020	-0.112277
55H	-2.223312	1.651944	2.105507
56H	-3.297691	3.862454	2.231634
57H	-4.783665	4.644193	0.393081
58H	-5.204899	3.174232	-1.571863

59H	-4.151738	0.946480	-1.703133
60H	-3.154074	-2.488607	1.982630
61H	-2.304019	-3.113258	4.213679
62H	-0.304139	-1.970398	5.157584
63H	0.860752	-0.198756	3.824324
64H	0.047773	0.425590	1.615324
65H	0.253249	-1.936769	-0.206659
66H	2.053987	-1.874323	-1.882606
67H	1.952947	-0.270186	-3.779858
68H	0.029552	1.298639	-3.975194
69H	-1.776802	1.255540	-2.311001
70H	-2.071124	-2.748464	-1.790365
71H	-3.715161	-4.438923	-2.523585
72H	-6.070616	-4.321260	-1.729373
73H	-6.773174	-2.496982	-0.188797
74H	-5.137572	-0.802484	0.557342

6cg-010

1C	-2.527654	2.012232	-0.927345
2C	-2.696393	3.342440	-1.296405
3N	-2.338699	4.405165	-0.552008
4C	-1.780789	4.109744	0.641039
5C	-1.570447	2.823593	1.113080
6C	-1.944404	1.698680	0.329819
7N	-1.695373	0.460924	0.871428
8S	-2.161280	-0.899532	0.136957
9O	-1.711572	-2.013676	1.014550
10O	-1.767656	-1.004315	-1.298561
11C	-3.967704	-0.925187	0.163779
12C	-4.700601	-0.957362	-1.019518
13C	-6.100256	-0.956724	-0.984976
14C	-6.759732	-0.920810	0.251112
15C	-6.014901	-0.888041	1.444810
16C	-4.627585	-0.889567	1.401182
17O	-8.114704	-0.913504	0.403246
18C	-8.935920	-0.926588	-0.766962
19H	-2.822060	1.230487	-1.616727
20H	-3.143768	3.570117	-2.263927
21H	-1.485315	4.962120	1.252267
22H	-1.114536	2.663374	2.086506
23H	-4.182782	-0.984875	-1.972927
24H	-6.652694	-0.982174	-1.917605
25H	-6.544549	-0.859815	2.392907
26H	-4.054788	-0.858713	2.323492
27H	-8.772291	-1.837658	-1.356334
28H	-9.965787	-0.908692	-0.404959
29H	-8.752426	-0.041926	-1.389669
30P	2.922702	-0.228592	-0.011835
31C	4.711203	-0.110210	-0.310243
32C	2.350692	-1.808325	-0.695684
33C	2.590706	-0.126427	1.769770
34C	2.064909	1.140488	-0.827548
35C	1.234462	-2.448860	-0.139462
36C	0.750351	-3.622146	-0.719673
37C	1.377697	-4.160612	-1.845208
38C	2.489632	-3.519192	-2.404290
39C	2.977604	-2.341826	-1.836879
40C	3.618141	-0.297259	2.712396
41C	3.321111	-0.238480	4.075531
42C	2.007175	-0.014845	4.500090
43C	0.987700	0.158373	3.559068
44C	1.271859	0.111943	2.193632
45C	2.079244	2.412064	-0.228645
46C	1.449073	3.480844	-0.864901
47C	0.801071	3.284683	-2.088584
48C	0.780686	2.018096	-2.678389
49C	1.411457	0.941456	-2.053200
50C	5.281830	1.060530	-0.831408
51C	6.663556	1.128803	-1.029562
52C	7.474804	0.036634	-0.709770
53C	6.906243	-1.132752	-0.191988
54C	5.527842	-1.211052	0.006154
55H	0.712956	-2.041765	0.718522
56H	-0.129852	-4.093330	-0.293812
57H	0.996041	-5.074001	-2.294307
58H	2.975286	-3.932635	-3.284260
59H	3.837856	-1.847386	-2.278592
60H	4.642541	-0.466271	2.397322
61H	4.117968	-0.365162	4.803559
62H	1.779758	0.026377	5.562296
63H	-0.037150	0.329229	3.876899
64H	0.454477	0.255499	1.489068
65H	2.562886	2.563505	0.732237
66H	1.444100	4.460305	-0.395847
67H	0.290710	4.115130	-2.567599

68H	0.252549	1.858841	-3.614148
69H	1.370709	-0.044307	-2.505348
70H	4.660154	1.912362	-1.088948
71H	7.101881	2.034892	-1.438774
72H	8.548562	0.093110	-0.868201
73H	7.533418	-1.985660	0.052767
74H	5.090090	-2.126262	0.395581

6cg-011

1C	-3.962850	2.300463	0.428766
2C	-4.551808	3.056896	1.437320
3N	-3.950317	4.058993	2.105270
4C	-2.682654	4.325592	1.726545
5C	-1.997133	3.635670	0.738128
6C	-2.620388	2.562993	0.045915
7N	-1.849506	1.891185	-0.871827
8S	-2.454435	0.738846	-1.817120
9O	-1.343758	0.297954	-2.706223
10O	-3.723383	1.096476	-2.516257
11C	-2.866207	-0.690702	-0.780783
12C	-3.659360	-1.706429	-1.314799
13C	-3.941951	-2.851914	-0.565300
14C	-3.427083	-2.972013	0.735361
15C	-2.642479	-1.940222	1.274553
16C	-2.360808	-0.808328	0.517071
17O	-3.632045	-4.047542	1.550101
18C	-4.466357	-5.112855	1.087406
19H	-4.540892	1.520850	-0.054035
20H	-5.579186	2.841055	1.729392
21H	-2.190005	5.142788	2.252810
22H	-0.975119	3.905870	0.485076
23H	-4.064042	-1.609008	-2.318124
24H	-4.559121	-3.629994	-1.000067
25H	-2.261131	-2.041068	2.286914
26H	-1.751028	-0.016692	0.935554
27H	-4.047162	-5.587820	0.191153
28H	-4.493829	-5.839594	1.902010
29H	-5.483593	-4.758272	0.878727
30P	2.387172	-0.120966	0.049487
31C	1.455728	0.133258	1.586533
32C	4.052827	-0.697954	0.496608
33C	1.543515	-1.353385	-0.975649
34C	2.501519	1.427926	-0.884244
35C	4.682965	-1.713434	-0.239332
36C	5.979708	-2.110620	0.095877
37C	6.649427	-1.500152	1.160121
38C	6.021066	-0.490675	1.897320
39C	4.725577	-0.088391	1.571170
40C	0.566750	-2.190630	-0.417605
41C	-0.083603	-3.128141	-1.220976
42C	0.243920	-3.238824	-2.573813
43C	1.221241	-2.406996	-3.131076
44C	1.867429	-1.458556	-2.339674
45C	1.409126	1.820787	-1.675494
46C	1.455289	3.043598	-2.347632
47C	2.582003	3.863953	-2.244136
48C	3.673398	3.464562	-1.463564
49C	3.638180	2.248184	-0.780640
50C	0.534593	1.186688	1.689959
51C	-0.217899	1.333197	2.857679
52C	-0.058523	0.433422	3.915069
53C	0.857451	-0.619524	3.810567
54C	1.616767	-0.772927	2.650340
55H	4.170121	-2.200945	-1.062397
56H	6.462019	-2.900622	-0.473233
57H	7.657581	-1.812868	1.419010
58H	6.536133	-0.017423	2.728785
59H	4.242379	0.689195	2.155901
60H	0.287281	-2.100707	0.625697
61H	-0.864208	-3.747975	-0.790025
62H	-0.274507	-3.959656	-3.200407
63H	1.464157	-2.478944	-4.187525
64H	2.601677	-0.794361	-2.786416
65H	0.523466	1.200980	-1.774776
66H	0.601564	3.346007	-2.947278
67H	2.612564	4.813531	-2.772280
68H	4.553692	4.097235	-1.387991
69H	4.491783	1.944410	-0.182942
70H	0.378072	1.873901	0.865483
71H	-0.939183	2.142027	2.925557
72H	-0.650079	0.550345	4.819289
73H	0.981605	-1.322145	4.630145
74H	2.328356	-1.590583	2.576981

6cg-012

1C	1.840857	1.313276	0.466012
2C	1.543364	2.577355	0.964683
3N	1.179379	3.636832	0.219661
4C	1.108542	3.408938	-1.109263
5C	1.376583	2.191222	-1.714278
6C	1.766686	1.070891	-0.932363
7N	2.021152	-0.098349	-1.608673
8S	2.607316	-1.396658	-0.849684
9O	2.819587	-2.433431	-1.894077
10O	1.813515	-1.840986	0.336596
11C	4.234435	-0.947098	-0.199442
12C	5.137598	-0.275726	-1.024373
13C	6.401456	0.077597	-0.546055
14C	6.758184	-0.248487	0.772164
15C	5.846495	-0.926560	1.598205
16C	4.588796	-1.272364	1.114584
17O	7.960101	0.053081	1.340727
18C	8.928322	0.765903	0.566292
19H	2.103099	0.521472	1.156046
20H	1.595079	2.746504	2.040022
21H	0.812621	4.258678	-1.722448
22H	1.295130	2.081753	-2.792643
23H	4.856192	-0.015246	-2.040733
24H	7.087698	0.603016	-1.200101
25H	6.139542	-1.168358	2.616111
26H	3.877454	-1.787196	1.752475
27H	9.787594	0.904668	1.225381
28H	9.234617	0.189444	-0.315994
29H	8.544840	1.746240	0.256197
30P	-2.854224	-0.151194	0.121831
31C	-2.642852	1.333956	-0.899923
32C	-1.933127	0.004644	1.676077
33C	-4.612161	-0.330295	0.550592
34C	-2.296262	-1.594485	-0.818946
35C	-2.474804	0.782554	2.716431
36C	-1.761633	0.941578	3.903628
37C	-0.516623	0.319902	4.061766
38C	0.014718	-0.456553	3.030069
39C	-0.686112	-0.616346	1.831966
40C	-5.601358	0.344040	-0.180980
41C	-6.947602	0.168773	0.148650
42C	-7.309080	-0.674128	1.203451
43C	-6.322966	-1.345411	1.935112
44C	-4.976005	-1.175092	1.614086
45C	-1.072107	-1.524247	-1.505129
46C	-0.600929	-2.641104	-2.194950
47C	-1.351256	-3.820429	-2.213171
48C	-2.574747	-3.888187	-1.537950
49C	-3.050768	-2.779789	-0.835626
50C	-2.350993	2.568349	-0.300071
51C	-2.278292	3.719069	-1.086135
52C	-2.489987	3.642949	-2.465296
53C	-2.767211	2.410580	-3.065978
54C	-2.845531	1.254353	-2.288896
55H	-3.446418	1.255307	2.604090
56H	-2.179170	1.545747	4.704539
57H	0.035769	0.443530	4.989771
58H	0.982086	-0.937372	3.142290
59H	-0.236729	-1.207132	1.041242
60H	-5.330261	1.006976	-0.996692
61H	-7.711001	0.696011	-0.416946
62H	-8.357362	-0.804892	1.458955
63H	-6.600368	-1.997887	2.758450
64H	-4.214007	-1.691892	2.190783
65H	-0.471993	-0.620350	-1.498111
66H	0.364297	-2.587874	-2.688562
67H	-0.978755	-4.689580	-2.749135
68H	-3.159322	-4.804163	-1.553565
69H	-4.000147	-2.842889	-0.313621
70H	-2.157519	2.638434	0.765119
71H	-2.032878	4.668386	-0.619312
72H	-2.422662	4.540558	-3.074448
73H	-2.916607	2.345484	-4.140254
74H	-3.055640	0.300580	-2.763964

6cg-PhNCO2-001

1C	-4.482623	0.196134	-1.986532
2C	-5.435122	0.761468	-2.833450
3N	-6.554344	1.362751	-2.397650
4C	-6.749101	1.405337	-1.069413
5C	-5.859017	0.866974	-0.138925
6C	-4.696427	0.256103	-0.609405

7N	-3.741853	-0.295971	0.306237
8S	-3.866943	-1.945287	0.685149
9O	-4.725565	-2.506262	-0.378373
10O	-4.279390	-2.161392	2.081304
11C	-2.214696	-2.594468	0.463959
12C	-1.588896	-2.458420	-0.780264
13C	-0.325159	-3.000612	-0.967500
14C	0.316957	-3.675473	0.084868
15C	-0.325678	-3.825959	1.320757
16C	-1.595636	-3.275504	1.507207
17O	1.570786	-4.137294	-0.192665
18C	2.311685	-4.781794	0.849785
19C	-2.784117	0.545247	1.028444
20O	-2.094854	-0.043572	1.889401
21N	-2.793874	1.784597	0.570995
22C	-1.893923	2.742609	1.018776
23C	-0.973702	2.627443	2.095433
24C	-0.081082	3.662651	2.389032
25C	-0.065489	4.845280	1.642114
26C	-0.981002	4.984707	0.589534
27C	-1.875052	3.959374	0.288929
28H	-3.592679	-0.278884	-2.384250
29H	-5.294379	0.731298	-3.912233
30H	-7.661999	1.891994	-0.732433
31H	-6.055747	0.929669	0.926690
32H	-2.073820	-1.921707	-1.589182
33H	0.186362	-2.897097	-1.918268
34H	0.154283	-4.335861	2.147439
35H	-2.089856	-3.357186	2.469188
36H	1.803071	-5.690823	1.192607
37H	3.271493	-5.052356	0.405614
38H	2.477350	-4.100802	1.692800
39H	-0.959276	1.717936	2.680664
40H	0.618863	3.535481	3.213455
41H	0.640024	5.639546	1.873505
42H	-0.995242	5.897660	-0.003220
43H	-2.580725	4.068397	-0.531820
44P	2.693553	0.330074	-0.353811
45C	2.297188	-0.486674	1.218232
46C	1.298071	0.328477	-1.512115
47C	3.140520	2.059361	-0.025957
48C	4.094274	-0.551121	-1.096366
49C	0.168449	1.108812	-1.212151
50C	-0.916505	1.125093	-2.087665
51C	-0.868357	0.385520	-3.273533
52C	0.263636	-0.373762	-3.584298
53C	1.348366	-0.408894	-2.706018
54C	3.628980	2.437676	1.234297
55C	4.003682	3.763028	1.461362
56C	3.888743	4.710403	0.439933
57C	3.395823	4.335029	-0.813845
58C	3.020073	3.012533	-1.051593
59C	4.029051	-1.952424	-1.204781
60C	5.080732	-2.646306	-1.803139
61C	6.196824	-1.952824	-2.286084
62C	6.261884	-0.561272	-2.127235
63C	5.211805	0.144630	-1.579409
64C	0.987212	-0.485626	1.716548
65C	0.728958	-1.009044	2.984596
66C	1.768176	-1.537988	3.752785
67C	3.074961	-1.554613	3.249978
68C	3.345317	-1.028851	1.986370
69H	0.129893	1.709119	-0.308826
70H	-1.796156	1.702233	-1.821776
71H	-1.712524	0.403795	-3.958095
72H	0.304695	-0.942613	-4.509294
73H	2.219781	-1.003803	-2.957871
74H	3.702007	1.714245	2.040412
75H	4.370494	4.056195	2.441172
76H	4.170941	5.743678	0.623985
77H	3.293158	5.072519	-1.605070
78H	2.625605	2.731260	-2.023747
79H	3.165723	-2.497601	-0.831250
80H	5.027953	-3.727989	-1.892117
81H	7.015089	-2.497834	-2.749286
82H	7.129207	-0.021870	-2.543292
83H	5.270437	1.225260	-1.493648
84H	0.151843	-0.096459	1.148958
85H	-0.293900	-1.000800	3.345669
86H	1.561605	-1.944998	4.739415
87H	3.885267	-1.973221	3.841033
88H	4.362919	-1.039908	1.606892

6cg-PhNCO2-002

1C	-1.964334	-1.287133	3.358282
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2C	-1.263383	-0.494649	4.269009
3N	-0.674332	0.669207	3.948182
4C	-0.768330	1.066004	2.669078
5C	-1.440177	0.346886	1.681893
6C	-2.059911	-0.855169	2.035060
7N	-2.824115	-1.596226	1.075384
8S	-4.489258	-1.225009	1.015233
9O	-4.818342	-0.755181	2.374454
10O	-5.206246	-2.381357	0.466409
11C	-4.695715	0.172824	-0.083167
12C	-4.971610	-0.030827	-1.441499
13C	-5.119091	1.068258	-2.276457
14C	-4.982037	2.371804	-1.764775
15C	-4.705864	2.568780	-0.403237
16C	-4.565930	1.461513	0.436823
17O	-5.125657	3.377118	-2.670706
18C	-5.015548	4.731334	-2.221390
19C	-2.171186	-2.152743	-0.131132
20O	-2.830252	-2.111653	-1.187731
21N	-0.965603	-2.616795	0.162665
22C	-0.136418	-3.157059	-0.817441
23C	-0.367171	-3.198930	-2.219268
24C	0.602544	-3.699810	-3.093363
25C	1.825933	-4.188654	-2.623175
26C	2.058043	-4.185783	-1.241508
27C	1.099067	-3.686600	-0.362805
28H	-2.435194	-2.214216	3.667508
29H	-1.174394	-0.807750	5.307188
30H	-0.287549	2.009846	2.419866
31H	-1.487367	0.712451	0.663842
32H	-5.056094	-1.038670	-1.828648
33H	-5.337499	0.939359	-3.332543
34H	-4.604826	3.564345	0.012840
35H	-4.366160	1.607505	1.493025
36H	-5.786021	4.965250	-1.476281
37H	-4.020205	4.930491	-1.804265
38H	-5.168249	5.348526	-3.108607
39H	-1.307335	-2.832909	-2.608591
40H	0.392110	-3.706621	-4.161844
41H	2.576239	-4.568907	-3.312230
42H	2.995230	-4.571780	-0.844879
43H	1.291010	-3.686487	0.705856
44P	2.836733	0.776857	-0.031211
45C	2.702973	-0.148332	1.522032
46C	3.767758	-0.218207	-1.231647
47C	1.208995	1.149522	-0.744711
48C	3.712817	2.335180	0.293800
49C	3.619352	0.020584	-2.608459
50C	4.357658	-0.729154	-3.524593
51C	5.243726	-1.712996	-3.074358
52C	5.391435	-1.950256	-1.704797
53C	4.653979	-1.208703	-0.780308
54C	0.644568	2.430761	-0.622045
55C	-0.606903	2.689755	-1.184238
56C	-1.296372	1.679478	-1.862507
57C	-0.736859	0.404480	-1.979886
58C	0.515688	0.136912	-1.428200
59C	4.675253	2.811891	-0.609643
60C	5.304776	4.035530	-0.369634
61C	4.977695	4.783662	0.765058
62C	4.018443	4.309162	1.666403
63C	3.384641	3.087707	1.435793
64C	1.650161	-1.057385	1.704382
65C	1.610286	-1.840358	2.859304
66C	2.605196	-1.715544	3.831338
67C	3.654575	-0.807691	3.650162
68C	3.711685	-0.026780	2.495772
69H	2.925575	0.774928	-2.967095
70H	4.232717	-0.549409	-4.588811
71H	5.810077	-2.301376	-3.791423
72H	6.068633	-2.723627	-1.353125
73H	4.760071	-1.415426	0.280110
74H	1.171732	3.224351	-0.102384
75H	-1.043728	3.680123	-1.087939
76H	-2.276014	1.877963	-2.285978
77H	-1.284238	-0.392730	-2.470990
78H	0.939992	-0.855923	-1.531673
79H	4.940425	2.235299	-1.490643
80H	6.053171	4.399482	-1.068185
81H	5.473406	5.733008	0.950319
82H	3.765702	4.885636	2.552093
83H	2.649074	2.721205	2.146194
84H	0.857947	-1.175875	0.973076
85H	0.791179	-2.539941	2.990236
86H	2.562866	-2.321904	4.732458
87H	4.430413	-0.707812	4.404518
88H	4.534337	0.668570	2.358746

6cg-PhNCO2-003

1C	-2.981939	-2.647326	2.530647
2C	-2.424579	-2.570040	3.808135
3N	-1.629517	-1.567477	4.215750
4C	-1.363817	-0.597504	3.326016
5C	-1.868333	-0.581698	2.027179
6C	-2.699881	-1.629265	1.620656
7N	-3.277928	-1.637890	0.309351
8S	-4.796286	-0.890696	0.136549
9O	-5.356557	-0.859961	1.501004
10O	-5.540494	-1.572861	-0.928822
11C	-4.504321	0.802935	-0.355277
12C	-4.561085	1.161000	-1.707381
13C	-4.299880	2.474098	-2.072911
14C	-3.960659	3.427273	-1.095871
15C	-3.913417	3.063827	0.258292
16C	-4.192794	1.745424	0.625245
17O	-3.678469	4.673019	-1.565599
18C	-3.298623	5.692752	-0.636009
19C	-2.421383	-1.830872	-0.877391
20O	-2.766904	-1.233886	-1.917270
21N	-1.423530	-2.651956	-0.599625
22C	-0.419288	-2.915067	-1.524382
23C	-0.021074	-2.079973	-2.600048
24C	1.086397	-2.404140	-3.388460
25C	1.828678	-3.567374	-3.155370
26C	1.436490	-4.414984	-2.110623
27C	0.338065	-4.094594	-1.314758
28H	-3.624260	-3.473974	2.245790
29H	-2.629643	-3.348691	4.540055
30H	-0.712079	0.203697	3.667831
31H	-1.628667	0.228315	1.347198
32H	-4.789016	0.410404	-2.454228
33H	-4.334141	2.778786	-3.114831
34H	-3.667088	3.785933	1.027831
35H	-4.169397	1.460134	1.671921
36H	-4.105413	5.898593	0.078191
37H	-2.383881	5.416196	-0.096654
38H	-3.111473	6.583553	-1.238751
39H	-0.582641	-1.177760	-2.804633
40H	1.373155	-1.733171	-4.196328
41H	2.690866	-3.808222	-3.772251
42H	1.992554	-5.329524	-1.911966
43H	0.041577	-4.749482	-0.498687
44P	2.857923	0.608586	0.241154
45C	2.317799	-0.617272	1.461428
46C	1.456714	1.472333	-0.525405
47C	3.907299	1.850003	1.050641
48C	3.810990	-0.245844	-1.045002
49C	1.633497	2.785947	-0.997894
50C	0.586633	3.429845	-1.658560
51C	-0.630352	2.769400	-1.856096
52C	-0.805564	1.462542	-1.392869
53C	0.235179	0.809972	-0.728466
54C	5.297717	1.843796	0.864632
55C	6.088360	2.791464	1.519854
56C	5.497876	3.741747	2.357255
57C	4.110405	3.750010	2.541771
58C	3.312902	2.809492	1.890389
59C	3.770386	0.211943	-2.370975
60C	4.551728	-0.415272	-3.342828
61C	5.367315	-1.496865	-2.997479
62C	5.401281	-1.958168	-1.677555
63C	4.625547	-1.336973	-0.698196
64C	2.503477	-0.404855	2.838392
65C	2.088827	-1.378876	3.747564
66C	1.486424	-2.555630	3.293062
67C	1.302737	-2.766348	1.924299
68C	1.723758	-1.806336	1.005435
69H	2.576126	3.305677	-0.853653
70H	0.723830	4.445724	-2.019587
71H	-1.443136	3.274495	-2.369354
72H	-1.740775	0.936532	-1.557542
73H	0.083731	-0.206675	-0.382488
74H	5.765284	1.113852	0.211095
75H	7.164485	2.786737	1.370092
76H	6.116174	4.478398	2.863361
77H	3.648393	4.489411	3.190162
78H	2.235624	2.825075	2.031955
79H	3.126553	1.040034	-2.650965
80H	4.511270	-0.066289	-4.370884
81H	5.966808	-1.988547	-3.759057
82H	6.023607	-2.807601	-1.410024
83H	4.649731	-1.706421	0.322702
84H	2.973937	0.501221	3.205390

85H	2.228423	-1.212544	4.812146
86H	1.148260	-3.301372	4.006465
87H	0.819162	-3.668009	1.563493
88H	1.593026	-1.994520	-0.055251

6cg-PhNCO2-004

1C	-2.613359	-1.468525	2.135502
2C	-2.350450	-2.352691	3.180022
3N	-1.562383	-3.436791	3.061731
4C	-1.007630	-3.657447	1.860582
5C	-1.205295	-2.831720	0.752820
6C	-2.026889	-1.712883	0.889220
7N	-2.277484	-0.856188	-0.229812
8S	-3.445310	-1.396596	-1.358208
9O	-3.581952	-2.841366	-1.089978
10O	-3.056603	-0.973416	-2.709108
11C	-4.991612	-0.621037	-0.920064
12C	-5.780542	-1.202025	0.083428
13C	-6.974940	-0.593801	0.445917
14C	-7.387871	0.589883	-0.192519
15C	-6.594802	1.159873	-1.201652
16C	-5.390138	0.552530	-1.558299
17O	-8.571414	1.104742	0.235086
18C	-9.053854	2.314176	-0.360204
19C	-1.942717	0.579863	-0.177139
20O	-2.533794	1.314251	-0.991855
21N	-1.049237	0.822328	0.767622
22C	-0.537739	2.099120	0.966178
23C	-0.416751	3.113080	-0.018016
24C	0.182351	4.338103	0.284371
25C	0.676651	4.607251	1.566478
26C	0.572123	3.613973	2.548579
27C	-0.015542	2.384408	2.252193
28H	-3.249371	-0.602520	2.284743
29H	-2.794998	-2.186549	4.159288
30H	-0.367526	-4.533685	1.779201
31H	-0.733876	-3.052650	-0.197792
32H	-5.467754	-2.122096	0.566198
33H	-7.607136	-1.023120	1.217589
34H	-6.896079	2.070372	-1.706059
35H	-4.757582	0.993659	-2.318833
36H	-9.236385	2.180424	-1.433817
37H	-9.996778	2.534029	0.143877
38H	-8.351788	3.141658	-0.199473
39H	-0.797346	2.924859	-1.013933
40H	0.261829	5.094372	-0.495266
41H	1.138387	5.565449	1.792873
42H	0.953985	3.796130	3.551859
43H	-0.087532	1.611721	3.014379
44P	3.514561	-0.143168	-0.303080
45C	4.886053	-1.072632	-1.056504
46C	2.104218	-0.080100	-1.431441
47C	2.999122	-0.950649	1.236744
48C	4.110230	1.537095	0.034905
49C	1.286661	-1.215831	-1.574760
50C	0.200310	-1.177657	-2.445356
51C	-0.077859	-0.014610	-3.170497
52C	0.735549	1.111251	-3.029583
53C	1.825204	1.087702	-2.157444
54C	3.908036	-1.730189	1.973771
55C	3.505846	-2.298780	3.183090
56C	2.205369	-2.093671	3.658599
57C	1.304148	-1.322319	2.921057
58C	1.690997	-0.749633	1.708401
59C	4.935390	2.179748	-0.905714
60C	5.357726	3.488826	-0.674938
61C	4.963596	4.157693	0.489444
62C	4.141811	3.519053	1.421519
63C	3.709947	2.209901	1.198482
64C	4.642041	-1.992014	-2.088666
65C	5.699462	-2.729409	-2.626410
66C	6.998353	-2.553070	-2.140912
67C	7.244051	-1.634497	-1.114774
68C	6.193918	-0.893161	-0.571697
69H	1.481349	-2.110995	-0.990907
70H	-0.452812	-2.038759	-2.537650
71H	-0.952717	0.017899	-3.810510
72H	0.504938	2.023012	-3.573432
73H	2.429049	1.979889	-2.028508
74H	4.916113	-1.904948	1.610544
75H	4.205983	-2.908139	3.748387
76H	1.890981	-2.546713	4.595215
77H	0.287492	-1.174391	3.271168
78H	0.954958	-0.179899	1.145823
79H	5.249854	1.663987	-1.808526

80H	5.994395	3.983914	-1.403135
81H	5.294343	5.177701	0.666914
82H	3.826544	4.038764	2.320915
83H	3.059155	1.729672	1.921845
84H	3.639576	-2.131215	-2.480881
85H	5.505759	-3.436222	-3.428613
86H	7.819088	-3.126103	-2.564270
87H	8.253198	-1.490774	-0.738362
88H	6.396054	-0.175860	0.218458

6cg-PhNCO2-005

1C	5.963032	-1.014461	0.034128
2C	6.942477	-1.415715	-0.875750
3N	6.810892	-1.306099	-2.207598
4C	5.665740	-0.775789	-2.668355
5C	4.629765	-0.340182	-1.843417
6C	4.780568	-0.465533	-0.461882
7N	3.742712	-0.032190	0.425735
8S	3.925239	1.479510	1.184863
9O	5.061684	2.107168	0.481516
10O	3.999962	1.339941	2.646984
11C	2.458285	2.422051	0.774301
12C	1.402355	2.524153	1.686819
13C	0.285021	3.278088	1.354800
14C	0.209735	3.922310	0.106334
15C	1.273169	3.816407	-0.804151
16C	2.401145	3.067572	-0.460308
17O	-0.933626	4.619964	-0.128476
18C	-1.102141	5.262207	-1.395904
19C	2.640849	-0.907903	0.826311
20O	1.831146	-0.401546	1.634115
21N	2.691943	-2.074655	0.209933
22C	1.699830	-3.033317	0.376495
23C	0.629514	-3.011924	1.309538
24C	-0.315029	-4.041231	1.345708
25C	-0.241399	-5.129208	0.468334
26C	0.820287	-5.177251	-0.446667
27C	1.766240	-4.154891	-0.489500
28H	6.112146	-1.126518	1.103570
29H	7.875976	-1.845184	-0.518117
30H	5.575571	-0.693914	-3.749914
31H	3.720589	0.078055	-2.260680
32H	1.458404	2.003807	2.634568
33H	-0.548770	3.369927	2.044532
34H	1.242273	4.312395	-1.767037
35H	3.233606	2.998573	-1.153592
36H	-0.334638	6.029523	-1.556486
37H	-1.078730	4.531326	-2.213205
38H	-2.084722	5.734141	-1.357458
39H	0.548313	-2.183076	1.997717
40H	-1.119947	-3.987612	2.078110
41H	-0.981630	-5.925460	0.503924
42H	0.909751	-6.016808	-1.134098
43H	2.583565	-4.194634	-1.206347
44P	-2.847533	-0.189334	-0.176532
45C	-2.468919	-0.202723	1.595273
46C	-3.479929	1.445568	-0.656478
47C	-1.378006	-0.532657	-1.177423
48C	-4.115731	-1.453157	-0.473067
49C	-3.500889	1.800117	-2.017229
50C	-4.025927	3.033252	-2.404193
51C	-4.525323	3.916675	-1.440950
52C	-4.495381	3.568940	-0.088072
53C	-3.973615	2.335751	0.308945
54C	-1.214564	-1.769230	-1.820081
55C	-0.062446	-2.009696	-2.570494
56C	0.924011	-1.027354	-2.678432
57C	0.756382	0.207586	-2.045187
58C	-0.390959	0.462159	-1.297349
59C	-5.257824	-1.174664	-1.237958
60C	-6.208312	-2.176715	-1.450229
61C	-6.020560	-3.450206	-0.905430
62C	-4.880120	-3.727829	-0.143060
63C	-3.928137	-2.733073	0.079286
64C	-1.152857	-0.020172	2.037123
65C	-0.880163	-0.009674	3.406957
66C	-1.914073	-0.170924	4.331491
67C	-3.230699	-0.355808	3.888940
68C	-3.513028	-0.377764	2.523644
69H	-3.108148	1.122028	-2.769824
70H	-4.039842	3.304478	-3.456323
71H	-4.928148	4.879139	-1.745179
72H	-4.867936	4.259799	0.663146
73H	-3.945848	2.081483	1.363746
74H	-1.965974	-2.546808	-1.735610

75H	0.069009	-2.972762	-3.053585
76H	1.829946	-1.231274	-3.241606
77H	1.523173	0.972273	-2.114377
78H	-0.506846	1.422916	-0.805915
79H	-5.414130	-0.187184	-1.660658
80H	-7.095462	-1.958013	-2.038284
81H	-6.763026	-4.226271	-1.071718
82H	-4.731211	-4.716790	0.281456
83H	-3.045844	-2.953151	0.673977
84H	-0.323220	0.072294	1.347225
85H	0.149634	0.102222	3.731992
86H	-1.696224	-0.166613	5.396442
87H	-4.035433	-0.492324	4.606366
88H	-4.533448	-0.538469	2.186660

6cg-PhNCO2-006

1C	4.870601	-0.302010	-1.851775
2C	5.945707	-0.905007	-2.505498
3N	6.907380	-1.595883	-1.873180
4C	6.812253	-1.695595	-0.536466
5C	5.779949	-1.127957	0.210128
6C	4.783087	-0.421670	-0.465086
7N	3.690444	0.174115	0.248845
8S	3.885774	1.781821	0.760363
9O	4.918145	2.339191	-0.137928
10O	4.120091	1.884779	2.210637
11C	2.326958	2.567783	0.370587
12C	1.781765	2.431559	-0.910791
13C	0.601930	3.092425	-1.223892
14C	-0.028571	3.906140	-0.264408
15C	0.534769	4.050422	1.012581
16C	1.713524	3.370125	1.327536
17O	-1.186032	4.497905	-0.664729
18C	-1.908485	5.302230	0.271844
19C	2.624065	-0.642312	0.849871
20O	1.818039	-0.019421	1.574089
21N	2.681595	-1.889754	0.424985
22C	1.712099	-2.828913	0.754266
23C	0.639884	-2.678707	1.673305
24C	-0.272434	-3.717520	1.881689
25C	-0.168052	-4.932001	1.195156
26C	0.886045	-5.096998	0.284873
27C	1.804982	-4.071178	0.075357
28H	4.120289	0.250768	-2.407764
29H	6.039691	-0.828838	-3.587046
30H	7.601296	-2.255527	-0.038898
31H	5.741144	-1.240457	1.288799
32H	2.261330	1.796656	-1.648679
33H	0.146168	2.984359	-2.203628
34H	0.063879	4.667461	1.768683
35H	2.140667	3.451348	2.321401
36H	-1.315391	6.169389	0.588672
37H	-2.797295	5.643900	-0.260041
38H	-2.209775	4.714845	1.147773
39H	0.525270	-1.744441	2.206781
40H	-1.082374	-3.567065	2.592907
41H	-0.885773	-5.731281	1.366367
42H	0.993338	-6.032169	-0.262024
43H	2.620914	-4.200238	-0.632436
44P	-2.741384	-0.317220	-0.239351
45C	-1.460430	-0.756983	-1.442753
46C	-2.093453	-0.109907	1.438336
47C	-3.527910	1.253950	-0.708930
48C	-3.967240	-1.655775	-0.254151
49C	-1.230537	0.965875	1.703553
50C	-0.736164	1.154444	2.991838
51C	-1.108212	0.284665	4.020342
52C	-1.976563	-0.779662	3.760077
53C	-2.470514	-0.983365	2.470885
54C	-3.443072	1.747468	-2.019407
55C	-4.095623	2.935551	-2.355701
56C	-4.830322	3.631648	-1.392257
57C	-4.908558	3.145188	-0.082995
58C	-4.256830	1.961467	0.263469
59C	-3.502978	-2.982821	-0.214604
60C	-4.420034	-4.033411	-0.187837
61C	-5.794053	-3.766971	-0.206499
62C	-6.253585	-2.447434	-0.250312
63C	-5.343586	-1.387316	-0.272894
64C	-0.099118	-0.593858	-1.156099
65C	0.850028	-0.926356	-2.127085
66C	0.447169	-1.413404	-3.371101
67C	-0.913909	-1.583734	-3.653926
68C	-1.869710	-1.263162	-2.692131
69H	-0.931501	1.645161	0.912632

70H	-0.040811	1.965229	3.180749
71H	-0.712242	0.429356	5.021914
72H	-2.263696	-1.459685	4.557381
73H	-3.138573	-1.815948	2.278433
74H	-2.866702	1.222536	-2.774246
75H	-4.019687	3.319859	-3.369043
76H	-5.333953	4.557366	-1.657944
77H	-5.469697	3.689442	0.671745
78H	-4.311217	1.595819	1.285034
79H	-2.437326	-3.195899	-0.199849
80H	-4.059360	-5.057796	-0.155451
81H	-6.505983	-4.588158	-0.190294
82H	-7.319899	-2.239314	-0.270325
83H	-5.708054	-0.365554	-0.311793
84H	0.233638	-0.241687	-0.185946
85H	1.902996	-0.836834	-1.885494
86H	1.193347	-1.679201	-4.115482
87H	-1.230176	-1.976289	-4.616592
88H	-2.923196	-1.418392	-2.907511

6cg-PhNCO2-007

1C	-1.183333	-1.191846	2.659042
2C	-0.574772	-2.024591	3.598574
3N	-0.880010	-3.322079	3.756016
4C	-1.845241	-3.819638	2.962730
5C	-2.527447	-3.068506	2.007099
6C	-2.183789	-1.723425	1.841278
7N	-2.843202	-0.925847	0.856780
8S	-3.886806	0.321778	1.384572
9O	-3.624767	0.444254	2.832118
10O	-5.268313	0.071572	0.951313
11C	-3.278678	1.808010	0.602099
12C	-2.166268	2.446547	1.164083
13C	-1.664115	3.593253	0.566113
14C	-2.268520	4.103818	-0.596011
15C	-3.395064	3.469238	-1.141158
16C	-3.894592	2.312233	-0.540594
17O	-1.682066	5.212495	-1.122065
18C	-2.219295	5.771357	-2.325020
19C	-2.775718	-1.226473	-0.580475
20O	-3.511131	-0.529633	-1.309584
21N	-1.870279	-2.151951	-0.848932
22C	-1.694175	-2.634729	-2.141142
23C	-2.618956	-2.546386	-3.214949
24C	-2.328967	-3.113241	-4.459182
25C	-1.116883	-3.773847	-4.694120
26C	-0.192953	-3.869515	-3.644724
27C	-0.478001	-3.316464	-2.397471
28H	-0.882927	-0.153904	2.569155
29H	0.205451	-1.630438	4.245331
30H	-2.087934	-4.871095	3.102157
31H	-3.297675	-3.517992	1.389908
32H	-1.700714	2.048141	2.058816
33H	-0.798772	4.106322	0.975046
34H	-3.875605	3.849112	-2.035201
35H	-4.743853	1.793376	-0.968572
36H	-3.250050	6.116049	-2.176550
37H	-1.581210	6.624926	-2.562501
38H	-2.183640	5.047595	-3.148461
39H	-3.559985	-2.033064	-3.061512
40H	-3.064738	-3.033789	-5.258117
41H	-0.899517	-4.206698	-5.667900
42H	0.755339	-4.382688	-3.796872
43H	0.237627	-3.402234	-1.585508
44P	2.656270	0.264528	0.079021
45C	2.181294	0.732813	1.767582
46C	1.467365	0.963823	-1.093227
47C	4.302323	0.926553	-0.311367
48C	2.692932	-1.547878	-0.012016
49C	1.635001	2.283164	-1.554125
50C	0.681586	2.838182	-2.407013
51C	-0.432923	2.086433	-2.796129
52C	-0.601032	0.779629	-2.333152
53C	0.347394	0.213109	-1.479014
54C	5.172647	1.334246	0.711150
55C	6.447834	1.804816	0.389208
56C	6.856854	1.869479	-0.945821
57C	5.988864	1.465662	-1.966236
58C	4.712411	0.996358	-1.655050
59C	1.718986	-2.286718	0.679105
60C	1.733388	-3.680221	0.620574
61C	2.710163	-4.339698	-0.130929
62C	3.675344	-3.604553	-0.827199
63C	3.674161	-2.209816	-0.768438
64C	1.305581	1.809717	1.972644

65C	0.953430	2.178675	3.272351
66C	1.470435	1.478152	4.365658
67C	2.342499	0.403001	4.161480
68C	2.698685	0.025107	2.866615
69H	2.499036	2.869714	-1.254698
70H	0.802464	3.859582	-2.757104
71H	-1.178132	2.523276	-3.454973
72H	-1.477167	0.202986	-2.610078
73H	0.191740	-0.798032	-1.117316
74H	4.862429	1.296060	1.750636
75H	7.116969	2.124781	1.183238
76H	7.849033	2.237981	-1.192550
77H	6.301639	1.519711	-3.005324
78H	4.040600	0.695857	-2.454413
79H	0.949463	-1.788420	1.257196
80H	0.971151	-4.241501	1.152513
81H	2.716287	-5.425400	-0.178256
82H	4.435574	-4.115065	-1.412087
83H	4.437731	-1.651739	-1.300514
84H	0.882621	2.344125	1.128826
85H	0.264460	3.004237	3.428212
86H	1.184879	1.760555	5.375339
87H	2.735790	-0.151076	5.009215
88H	3.360403	-0.822948	2.716235

6cg-PhNCO2-008

1C	-4.323520	-1.830288	-0.940196
2C	-5.308623	-2.617123	-1.533268
3N	-5.229094	-3.094341	-2.788034
4C	-4.125958	-2.785552	-3.487358
5C	-3.077990	-2.013352	-2.983958
6C	-3.176719	-1.523279	-1.680564
7N	-2.137717	-0.716788	-1.119982
8S	-2.005006	0.895005	-1.672518
9O	-2.750923	0.927572	-2.944921
10O	-0.591650	1.282127	-1.670850
11C	-2.897105	1.916146	-0.510672
12C	-4.284576	2.054063	-0.655543
13C	-4.988881	2.832296	0.253940
14C	-4.311818	3.477391	1.304764
15C	-2.920567	3.337773	1.437869
16C	-2.216549	2.546869	0.529097
17O	-5.091176	4.216842	2.138735
18C	-4.477218	4.884930	3.245324
19C	-1.545475	-1.081664	0.173834
20O	-1.058124	-0.153378	0.854557
21N	-1.589765	-2.388009	0.367511
22C	-1.370251	-2.927727	1.626681
23C	-1.674692	-2.282572	2.853116
24C	-1.515585	-2.943680	4.072475
25C	-1.032557	-4.258208	4.125347
26C	-0.724091	-4.908004	2.922620
27C	-0.894764	-4.258980	1.699777
28H	-4.435203	-1.474260	0.078702
29H	-6.208103	-2.873308	-0.977088
30H	-4.074401	-3.176722	-4.501655
31H	-2.208059	-1.790281	-3.590395
32H	-4.802467	1.565503	-1.474408
33H	-6.063825	2.958764	0.164920
34H	-2.380249	3.824907	2.241228
35H	-1.147718	2.413656	0.632163
36H	-3.745663	5.627439	2.902516
37H	-5.289782	5.391227	3.769823
38H	-3.995593	4.168040	3.921723
39H	-2.035436	-1.259857	2.836102
40H	-1.766785	-2.421400	4.994352
41H	-0.906058	-4.765239	5.078960
42H	-0.351409	-5.930641	2.936811
43H	-0.666764	-4.772675	0.768121
44P	3.014951	0.291275	-0.167376
45C	2.212601	1.795057	0.460943
46C	2.162369	-0.376568	-1.622194
47C	4.708502	0.731216	-0.662875
48C	3.079365	-0.948576	1.152719
49C	2.358575	0.228991	-2.875918
50C	1.678786	-0.255939	-3.992145
51C	0.806397	-1.342330	-3.865105
52C	0.617332	-1.946894	-2.620819
53C	1.293180	-1.469139	-1.498023
54C	5.324675	1.871553	-0.124749
55C	6.644396	2.174097	-0.467849
56C	7.349749	1.344499	-1.344659
57C	6.736258	0.207557	-1.882175
58C	5.418073	-0.102320	-1.544609
59C	1.900550	-1.277378	1.846816

60C	1.943283	-2.258101	2.838829
61C	3.145517	-2.903660	3.143786
62C	4.316497	-2.571958	2.455658
63C	4.288602	-1.595018	1.458352
64C	1.703027	2.736651	-0.445808
65C	1.174926	3.937596	0.027195
66C	1.147700	4.201546	1.400142
67C	1.649712	3.261272	2.304692
68C	2.186889	2.058975	1.839787
69H	3.042030	1.065864	-2.986382
70H	1.827815	0.217823	-4.958649
71H	0.272445	-1.712798	-4.736470
72H	-0.068640	-2.780284	-2.507044
73H	1.119690	-1.947068	-0.541377
74H	4.781287	2.522905	0.553019
75H	7.117272	3.059734	-0.052232
76H	8.375476	1.584898	-1.611903
77H	7.281286	-0.437478	-2.565993
78H	4.946046	-0.984300	-1.967810
79H	0.954597	-0.789701	1.614821
80H	1.030975	-2.521091	3.362799
81H	3.166322	-3.668453	3.916125
82H	5.252599	-3.071413	2.691000
83H	5.202979	-1.342320	0.930843
84H	1.692053	2.532062	-1.509894
85H	0.765908	4.655902	-0.677682
86H	0.726333	5.134936	1.764635
87H	1.623229	3.458389	3.372977
88H	2.574515	1.335719	2.549972

6cg-PhNCO2-009

1C	4.534380	-0.312198	-1.747223
2C	5.439893	-0.744763	-2.714544
3N	6.526839	-1.484180	-2.437488
4C	6.734446	-1.809745	-1.151208
5C	5.889520	-1.424902	-0.108705
6C	4.762567	-0.663871	-0.415521
7N	3.861948	-0.248892	0.620056
8S	4.116804	1.277394	1.326207
9O	5.396540	1.740774	0.756384
10O	3.985925	1.184322	2.786321
11C	2.835084	2.359243	0.702337
12C	3.034140	3.002528	-0.526591
13C	2.028877	3.808329	-1.046215
14C	0.823836	3.975463	-0.340822
15C	0.643079	3.349403	0.903019
16C	1.652631	2.535426	1.418975
17O	-0.110883	4.754853	-0.947865
18C	-1.380024	4.928027	-0.307784
19C	2.621580	-0.982816	0.896687
20O	1.803915	-0.396111	1.637221
21N	2.597187	-2.145316	0.270431
22C	1.532548	-3.027056	0.407364
23C	0.481572	-2.958199	1.359601
24C	-0.527932	-3.923944	1.389379
25C	-0.542299	-4.990662	0.483342
26C	0.495909	-5.082846	-0.455005
27C	1.508729	-4.126102	-0.488994
28H	3.667148	0.279811	-2.017700
29H	5.288237	-0.486329	-3.760951
30H	7.620459	-2.406248	-0.943682
31H	6.094573	-1.713497	0.917243
32H	3.966472	2.874674	-1.066966
33H	2.156678	4.316694	-1.997426
34H	-0.272913	3.476389	1.468309
35H	1.514723	2.023186	2.362638
36H	-1.268462	5.427208	0.662819
37H	-1.962163	5.562451	-0.977239
38H	-1.889587	3.967151	-0.178533
39H	0.466065	-2.142669	2.068625
40H	-1.313104	-3.837596	2.139691
41H	-1.332402	-5.737738	0.513627
42H	0.516021	-5.907499	-1.165665
43H	2.310649	-4.202949	-1.220073
44P	-2.917045	-0.097565	-0.181570
45C	-3.594895	1.537770	-0.597152
46C	-2.506955	-0.151159	1.583379
47C	-4.169111	-1.368601	-0.505843
48C	-1.449565	-0.383321	-1.200704
49C	-3.526068	-0.397232	2.522609
50C	-3.223057	-0.395930	3.883987
51C	-1.909875	-0.160631	4.311337
52C	-0.898302	0.067592	3.375547
53C	-1.191874	0.077297	2.010159
54C	-5.311369	-1.079695	-1.267515

55C	-6.249486	-2.085553	-1.512707
56C	-6.049272	-3.372340	-1.004222
57C	-4.909077	-3.659547	-0.245210
58C	-3.968831	-2.661377	0.009718
59C	-0.483779	0.633779	-1.299963
60C	0.684413	0.409929	-2.024799
61C	0.890981	-0.818008	-2.660309
62C	-0.077044	-1.821306	-2.578784
63C	-1.247147	-1.612289	-1.847113
64C	-4.228083	2.315391	0.385701
65C	-4.805184	3.538288	0.036964
66C	-4.751860	3.988491	-1.285585
67C	-4.113985	3.218770	-2.263590
68C	-3.535307	1.994625	-1.924955
69H	-4.542492	-0.600109	2.196577
70H	-4.008955	-0.588944	4.609240
71H	-1.675013	-0.173321	5.372553
72H	0.131613	0.209700	3.688329
73H	-0.377211	0.213257	1.309350
74H	-5.475717	-0.081844	-1.662280
75H	-7.136370	-1.860390	-2.098694
76H	-6.781973	-4.151549	-1.196887
77H	-4.750043	-4.659026	0.149995
78H	-3.085385	-2.888521	0.599361
79H	-0.632243	1.590406	-0.809660
80H	1.433213	1.193348	-2.076703
81H	1.811379	-0.999595	-3.207190
82H	0.084702	-2.777843	-3.065609
83H	-1.980807	-2.408068	-1.777289
84H	-4.268780	1.979141	1.417022
85H	-5.290262	4.139322	0.801191
86H	-5.198473	4.942632	-1.552400
87H	-4.062002	3.570608	-3.290116
88H	-3.039395	1.403362	-2.689003

6cg-PhNCO2-010

1C	0.468159	-2.964504	1.107683
2C	0.562287	-4.012524	2.022816
3N	1.414411	-4.029948	3.059476
4C	2.220152	-2.962830	3.196930
5C	2.217683	-1.872376	2.329615
6C	1.319519	-1.865965	1.254184
7N	1.276057	-0.753852	0.350406
8S	1.873318	-1.042068	-1.235807
9O	1.362239	0.014420	-2.118049
10O	1.496434	-2.438595	-1.538662
11C	3.653796	-0.980989	-1.173224
12C	4.330356	0.165701	-1.583836
13C	5.721613	0.217852	-1.498010
14C	6.426119	-0.882228	-0.981964
15C	5.733436	-2.036374	-0.573265
16C	4.349154	-2.089637	-0.669695
17O	7.777614	-0.928380	-0.842484
18C	8.549426	0.220265	-1.210014
19C	1.393837	0.597686	0.990953
20O	0.680099	0.720413	2.007608
21N	2.216262	1.399968	0.355816
22C	2.413048	2.716448	0.759774
23C	3.057614	3.567634	-0.172294
24C	3.319103	4.906915	0.112346
25C	2.955561	5.454573	1.350578
26C	2.327543	4.628269	2.289345
27C	2.053783	3.286736	2.008000
28H	-0.254342	-3.007951	0.303590
29H	-0.092417	-4.875809	1.923098
30H	2.909086	-2.984693	4.038995
31H	2.899070	-1.043550	2.489203
32H	3.771327	1.013312	-1.958382
33H	6.237490	1.114773	-1.820075
34H	6.297702	-2.879121	-0.185012
35H	3.815093	-2.982853	-0.362967
36H	8.264491	1.095617	-0.613418
37H	9.586994	-0.043214	-0.995901
38H	8.442273	0.443036	-2.278898
39H	3.337702	3.151293	-1.136585
40H	3.809402	5.527760	-0.635590
41H	3.160128	6.498269	1.577724
42H	2.038230	5.033112	3.258035
43H	1.550669	2.669988	2.741458
44P	-3.331377	0.101761	-0.275237
45C	-2.964274	-0.985373	1.127542
46C	-3.023281	-0.846817	-1.789809
47C	-5.072155	0.621334	-0.228746
48C	-2.314717	1.597564	-0.231264
49C	-3.973119	-0.931653	-2.818957

50C	-3.680350	-1.676114	-3.964774
51C	-2.448453	-2.327139	-4.087225
52C	-1.501457	-2.240312	-3.061004
53C	-1.789953	-1.508656	-1.910658
54C	-6.009143	-0.022090	0.593115
55C	-7.344115	0.390388	0.576549
56C	-7.746015	1.439260	-0.255097
57C	-6.810796	2.084909	-1.071789
58C	-5.475434	1.681930	-1.059631
59C	-2.648785	2.612541	0.685075
60C	-1.861715	3.760290	0.759618
61C	-0.747401	3.903129	-0.075322
62C	-0.423296	2.898271	-0.988206
63C	-1.200208	1.742241	-1.070036
64C	-2.188392	-0.536452	2.204777
65C	-1.950886	-1.392418	3.283544
66C	-2.482112	-2.683076	3.289894
67C	-3.242890	-3.136762	2.204839
68C	-3.479710	-2.295539	1.119246
69H	-4.932913	-0.432044	-2.732593
70H	-4.417635	-1.746397	-4.760102
71H	-2.225299	-2.901243	-4.982763
72H	-0.535723	-2.729188	-3.144314
73H	-1.053515	-1.443489	-1.117800
74H	-5.707415	-0.831696	1.249724
75H	-8.066053	-0.106142	1.219205
76H	-8.784952	1.758137	-0.263305
77H	-7.118208	2.905510	-1.714167
78H	-4.751468	2.195099	-1.686584
79H	-3.512813	2.506747	1.335444
80H	-2.111593	4.537987	1.476081
81H	-0.121255	4.787491	-0.000879
82H	0.454220	2.992863	-1.618284
83H	-0.909965	0.965787	-1.767421
84H	-1.724848	0.442977	2.191811
85H	-1.321955	-1.053334	4.101405
86H	-2.282082	-3.347153	4.126497
87H	-3.638192	-4.148933	2.197757
88H	-4.053061	-2.656958	0.269669

6cg-PhNCO2-011

1C	-1.982174	3.974727	0.625922
2C	-2.671856	5.169891	0.831836
3N	-3.945326	5.233451	1.252541
4C	-4.571868	4.066489	1.479298
5C	-3.977090	2.819175	1.292719
6C	-2.649902	2.770410	0.856094
7N	-1.990735	1.514890	0.665613
8S	-1.700838	1.012462	-0.943857
9O	-0.431550	0.274107	-0.979988
10O	-1.822905	2.239221	-1.756475
11C	-3.015950	-0.084895	-1.441971
12C	-2.793797	-1.459648	-1.483293
13C	-3.819489	-2.314204	-1.888707
14C	-5.073726	-1.780358	-2.227846
15C	-5.288558	-0.391150	-2.173681
16C	-4.260432	0.458588	-1.786724
17O	-6.140769	-2.523986	-2.624873
18C	-5.997831	-3.945299	-2.712937
19C	-1.978580	0.566471	1.804011
20O	-2.003679	1.114796	2.927315
21N	-1.946353	-0.690103	1.422245
22C	-1.693428	-1.709014	2.331342
23C	-2.272022	-2.974168	2.078161
24C	-1.993696	-4.078311	2.884488
25C	-1.118234	-3.963825	3.972329
26C	-0.536158	-2.716751	4.238137
27C	-0.819367	-1.606128	3.441365
28H	-0.950181	3.976719	0.293913
29H	-2.174693	6.121993	0.656552
30H	-5.602578	4.132223	1.821728
31H	-4.527444	1.905072	1.490956
32H	-1.829245	-1.857428	-1.191869
33H	-3.635506	-3.381849	-1.922149
34H	-6.263736	0.001284	-2.446511
35H	-4.420635	1.531813	-1.760457
36H	-5.756314	-4.379951	-1.735109
37H	-6.968143	-4.317472	-3.047047
38H	-5.228666	-4.220526	-3.445326
39H	-2.939995	-3.069284	1.225321
40H	-2.461085	-5.035897	2.660921
41H	-0.898827	-4.823572	4.601082
42H	0.146404	-2.606277	5.079392
43H	-0.359018	-0.649203	3.661581
44P	3.093134	-0.038244	-0.371211

45C	2.054091	-1.522714	-0.352615
46C	2.779960	0.939991	1.123624
47C	4.842639	-0.536668	-0.411289
48C	2.774547	0.957567	-1.854405
49C	3.838163	1.576026	1.794562
50C	3.568188	2.364088	2.914966
51C	2.252619	2.519532	3.364840
52C	1.199804	1.883356	2.699623
53C	1.459175	1.090960	1.579747
54C	5.229413	-1.806554	0.044440
55C	6.580960	-2.159022	0.051645
56C	7.546942	-1.251723	-0.393439
57C	7.162557	0.013597	-0.850130
58C	5.814412	0.373846	-0.861602
59C	3.313580	0.552231	-3.088681
60C	3.024736	1.280409	-4.242943
61C	2.203282	2.411071	-4.171394
62C	1.674495	2.817719	-2.943665
63C	1.956071	2.093941	-1.783950
64C	1.570049	-2.055379	-1.556692
65C	0.812483	-3.226610	-1.537605
66C	0.528382	-3.859740	-0.323742
67C	1.002002	-3.323438	0.876411
68C	1.767668	-2.157789	0.866833
69H	4.863357	1.456792	1.458104
70H	4.387152	2.851589	3.437100
71H	2.047286	3.131790	4.239312
72H	0.174667	1.984998	3.044435
73H	0.642482	0.596898	1.065574
74H	4.487157	-2.521454	0.386019
75H	6.875632	-3.144789	0.401106
76H	8.597347	-1.530718	-0.388526
77H	7.909874	0.720101	-1.201016
78H	5.522539	1.355563	-1.223382
79H	3.957245	-0.320985	-3.151195
80H	3.440155	0.963792	-5.195775
81H	1.976526	2.974212	-5.072939
82H	1.029242	3.689404	-2.885380
83H	1.528555	2.409061	-0.839186
84H	1.754873	-1.552495	-2.499915
85H	0.427132	-3.629908	-2.470244
86H	-0.081625	-4.759099	-0.308776
87H	0.750117	-3.790199	1.823287
88H	2.112126	-1.738887	1.807182

6cg-PhNCO2-012

1C	-1.061120	3.978714	0.224790
2C	-1.281683	5.347111	0.379533
3N	-2.395582	5.868492	0.918090
4C	-3.341030	5.000969	1.317649
5C	-3.226960	3.616910	1.193026
6C	-2.058605	3.089202	0.634842
7N	-1.891791	1.678303	0.513213
8S	-1.672345	1.011189	-1.044160
9O	-0.457169	0.184081	-1.047124
10O	-1.738453	2.158259	-1.971824
11C	-3.076038	-0.032928	-1.393109
12C	-2.905131	-1.411251	-1.485405
13C	-3.996180	-2.224173	-1.794296
14C	-5.260034	-1.643251	-1.989366
15C	-5.419711	-0.249016	-1.888142
16C	-4.328026	0.558228	-1.596223
17O	-6.389445	-2.342696	-2.281076
18C	-6.313220	-3.767597	-2.388832
19C	-1.965476	0.829374	1.723104
20O	-1.890151	1.446427	2.806355
21N	-2.110355	-0.441854	1.422428
22C	-1.974177	-1.438894	2.376876
23C	-2.709084	-2.633624	2.185639
24C	-2.560357	-3.725844	3.041315
25C	-1.664176	-3.672063	4.117049
26C	-0.928302	-2.497243	4.320967
27C	-1.078266	-1.397599	3.473707
28H	-0.138588	3.613901	-0.213429
29H	-0.522715	6.058798	0.060091
30H	-4.238172	5.435103	1.754343
31H	-4.021699	2.960619	1.531429
32H	-1.930056	-1.846775	-1.298969
33H	-3.851879	-3.296128	-1.862591
34H	-6.404833	0.180114	-2.045342
35H	-4.449277	1.634974	-1.526645
36H	-5.983864	-4.219256	-1.444927
37H	-7.328311	-4.098727	-2.615915
38H	-5.640682	-4.067220	-3.202418
39H	-3.397186	-2.680574	1.344730

40H	-3.146156	-4.626697	2.865859
41H	-1.545296	-4.523255	4.783290
42H	-0.226242	-2.434517	5.151014
43H	-0.501705	-0.496623	3.647744
44P	2.980672	-0.300993	-0.362388
45C	2.014222	-1.815991	-0.613435
46C	4.730919	-0.721651	-0.614164
47C	2.506183	0.996756	-1.539361
48C	2.753324	0.345697	1.315874
49C	5.586696	0.163197	-1.287348
50C	6.938532	-0.157422	-1.433987
51C	7.437242	-1.354588	-0.912365
52C	6.583573	-2.238611	-0.242805
53C	5.231622	-1.927725	-0.093282
54C	1.984330	0.658011	-2.795846
55C	1.639930	1.665536	-3.696486
56C	1.805509	3.008635	-3.345685
57C	2.325533	3.347122	-2.092916
58C	2.679822	2.345187	-1.187546
59C	1.529343	0.953205	1.646203
60C	1.338363	1.474627	2.925707
61C	2.362424	1.390521	3.874788
62C	3.578910	0.783513	3.547989
63C	3.780811	0.260015	2.268939
64C	0.948205	-2.140939	0.237518
65C	0.210986	-3.304104	0.008168
66C	0.525805	-4.135957	-1.069147
67C	1.588210	-3.812131	-1.920935
68C	2.337276	-2.657830	-1.693653
69H	5.206951	1.092517	-1.700702
70H	7.598300	0.527792	-1.959207
71H	8.489077	-1.601620	-1.030427
72H	6.967953	-3.171650	0.160070
73H	4.571504	-2.620399	0.421441
74H	1.812867	-0.379171	-3.062751
75H	1.215895	1.400317	-4.660884
76H	1.514760	3.791080	-4.041518
77H	2.446859	4.390104	-1.813260
78H	3.070835	2.618025	-0.211886
79H	0.731791	1.010123	0.912559
80H	0.379253	1.918855	3.173492
81H	2.208994	1.795785	4.871661
82H	4.374834	0.719244	4.285215
83H	4.732189	-0.200093	2.021541
84H	0.674412	-1.500295	1.066811
85H	-0.614212	-3.543341	0.671991
86H	-0.053213	-5.039162	-1.245002
87H	1.839263	-4.458671	-2.757524
88H	3.170449	-2.423066	-2.350346

6cg-PhNCO-001

1C	2.722589	-2.356404	0.597219
2C	1.410549	-2.744718	0.620042
3N	0.825380	-3.391811	-0.425256
4C	1.593903	-3.732652	-1.499423
5C	2.908860	-3.366984	-1.588080
6C	3.534510	-2.584113	-0.564416
7N	4.777121	-2.131728	-0.813488
8S	5.557479	-1.162597	0.260296
9O	5.579678	-1.714162	1.641396
10O	6.860589	-0.842648	-0.362247
11C	4.621136	0.380063	0.340090
12C	4.031592	0.783696	1.535799
13C	3.313852	1.982177	1.599497
14C	3.191408	2.775802	0.450510
15C	3.785510	2.362047	-0.756724
16C	4.498744	1.171474	-0.811333
17O	2.515946	3.956902	0.404118
18C	1.992525	4.490696	1.624044
19C	-0.661807	-3.686568	-0.450105
20O	-1.041016	-4.355101	-1.428499
21N	-1.252564	-3.138556	0.582487
22C	-2.624453	-3.219110	0.796867
23C	-3.592514	-3.780346	-0.073306
24C	-4.949197	-3.759691	0.265530
25C	-5.390357	-3.187365	1.463356
26C	-4.443775	-2.626007	2.331653
27C	-3.090155	-2.641856	2.003621
28H	3.128595	-1.872873	1.474371
29H	0.753463	-2.552969	1.456489
30H	1.077122	-4.280796	-2.276213
31H	3.479596	-3.630791	-2.472335
32H	4.137676	0.170487	2.424993
33H	2.865179	2.280220	2.539791
34H	3.680684	2.991703	-1.635665

35H	4.964917	0.859252	-1.741193
36H	1.212791	3.841468	2.039675
37H	2.790798	4.637733	2.362499
38H	1.557541	5.454677	1.359384
39H	-3.270505	-4.229479	-1.004320
40H	-5.670469	-4.198299	-0.421886
41H	-6.448045	-3.177041	1.715823
42H	-4.763257	-2.169468	3.266566
43H	-2.357193	-2.192030	2.668263
44P	-1.735459	1.367157	-0.319951
45C	-1.270211	3.116575	-0.488788
46C	-1.452830	0.830225	1.391889
47C	-3.499451	1.205016	-0.711785
48C	-0.743729	0.395863	-1.484122
49C	-2.443308	1.050686	2.364388
50C	-2.199263	0.699077	3.692566
51C	-0.974051	0.130066	4.054867
52C	0.008395	-0.093482	3.085844
53C	-0.227587	0.250251	1.754599
54C	-4.159647	2.223862	-1.419018
55C	-5.505575	2.070998	-1.756779
56C	-6.192945	0.908670	-1.393520
57C	-5.535653	-0.104206	-0.688240
58C	-4.190785	0.038103	-0.343502
59C	0.636219	0.646126	-1.598786
60C	1.400383	-0.089973	-2.501967
61C	0.796159	-1.070952	-3.294742
62C	-0.571597	-1.327015	-3.174886
63C	-1.346217	-0.598011	-2.270877
64C	-1.473517	3.997000	0.586174
65C	-1.216864	5.358985	0.424187
66C	-0.749583	5.845632	-0.800588
67C	-0.542455	4.969166	-1.869787
68C	-0.806673	3.606600	-1.721057
69H	-3.401985	1.480382	2.089513
70H	-2.970824	0.860261	4.440354
71H	-0.789935	-0.149486	5.088778
72H	0.955716	-0.548111	3.361692
73H	0.534763	0.049809	1.010153
74H	-3.636233	3.131434	-1.702535
75H	-6.014660	2.861876	-2.300828
76H	-7.240947	0.793459	-1.657767
77H	-6.060989	-1.009449	-0.400714
78H	-3.693712	-0.753417	0.207609
79H	1.115209	1.413249	-0.998761
80H	2.466441	0.100621	-2.578280
81H	1.395929	-1.642857	-3.996607
82H	-1.039357	-2.103249	-3.772656
83H	-2.406315	-0.812137	-2.185480
84H	-1.826748	3.628647	1.544715
85H	-1.371696	6.036941	1.258972
86H	-0.541299	6.905589	-0.919794
87H	-0.174492	5.342752	-2.821263
88H	-0.649451	2.934406	-2.558641

6cg-PhNCO-002

1C	2.225833	-2.406783	0.816680
2C	0.914270	-2.767861	0.670067
3N	0.508001	-3.677777	-0.258555
4C	1.451994	-4.292602	-1.031011
5C	2.779788	-3.979481	-0.931033
6C	3.243587	-2.975729	-0.018348
7N	4.554357	-2.675265	-0.055896
8S	5.171643	-1.445630	0.842399
9O	4.744755	-1.459839	2.268469
10O	6.627745	-1.448668	0.581065
11C	4.502178	0.064992	0.117815
12C	3.796588	0.975660	0.899518
13C	3.297130	2.153930	0.331089
14C	3.509625	2.407184	-1.030773
15C	4.224549	1.483084	-1.814806
16C	4.720013	0.319758	-1.244725
17O	3.059549	3.511341	-1.687276
18C	2.321822	4.491303	-0.951481
19C	-0.958942	-3.971222	-0.512631
20O	-1.168796	-4.883873	-1.330930
21N	-1.721266	-3.171370	0.192363
22C	-3.112057	-3.187299	0.083388
23C	-3.864392	-3.723261	-0.990004
24C	-5.258323	-3.612683	-1.006005
25C	-5.947360	-2.979331	0.034084
26C	-5.214920	-2.447155	1.102920
27C	-3.825431	-2.546565	1.123378
28H	2.476917	-1.687274	1.581998
29H	0.121937	-2.345263	1.270739

30H	1.066495	-5.022314	-1.731435
31H	3.497463	-4.479523	-1.572989
32H	3.639777	0.773345	1.954279
33H	2.755628	2.855973	0.955140
34H	4.378260	1.697984	-2.868008
35H	5.271035	-0.391325	-1.853022
36H	1.419384	4.057141	-0.511910
37H	2.938804	4.940893	-0.163394
38H	2.043912	5.257228	-1.677438
39H	-3.350827	-4.226425	-1.800139
40H	-5.811069	-4.033248	-1.844265
41H	-7.031779	-2.901658	0.012827
42H	-5.729106	-1.946515	1.921180
43H	-3.254915	-2.127256	1.947264
44P	-1.502816	1.633797	0.083635
45C	-1.098961	0.739225	1.607156
46C	-3.263008	1.445752	-0.314739
47C	-1.179297	3.403264	0.336963
48C	-0.476874	0.986102	-1.262779
49C	-4.202155	2.280823	0.316414
50C	-5.562881	2.109295	0.059739
51C	-5.989865	1.110766	-0.822211
52C	-5.056133	0.282755	-1.450782
53C	-3.692586	0.445634	-1.201298
54C	-0.499691	3.858686	1.477373
55C	-0.231406	5.221799	1.625855
56C	-0.637384	6.129000	0.643696
57C	-1.330917	5.678198	-0.485325
58C	-1.608244	4.320174	-0.639261
59C	-0.336813	-0.408272	-1.377348
60C	0.421530	-0.940381	-2.419938
61C	1.044059	-0.093247	-3.341128
62C	0.904369	1.292181	-3.225302
63C	0.144093	1.837690	-2.190294
64C	-2.110319	0.379291	2.509763
65C	-1.771875	-0.243066	3.713118
66C	-0.432360	-0.497152	4.020555
67C	0.575739	-0.137722	3.119502
68C	0.248371	0.472099	1.908677
69H	-3.877201	3.062209	0.997871
70H	-6.286879	2.756245	0.547681
71H	-7.050570	0.976402	-1.017233
72H	-5.383791	-0.501509	-2.125894
73H	-2.980775	-0.208105	-1.693613
74H	-0.179586	3.163659	2.246790
75H	0.296226	5.570770	2.509189
76H	-0.421462	7.187701	0.760276
77H	-1.658783	6.382728	-1.244572
78H	-2.158810	3.976976	-1.511214
79H	-0.814677	-1.077570	-0.666774
80H	0.532846	-2.016537	-2.504750
81H	1.647125	-0.513304	-4.141613
82H	1.401045	1.954443	-3.928060
83H	0.057720	2.914979	-2.107127
84H	-3.153237	0.563962	2.273556
85H	-2.557347	-0.538259	4.403138
86H	-0.172957	-0.985992	4.955708
87H	1.615780	-0.347464	3.352562
88H	1.035627	0.726194	1.205176

6cg-PhNCO-003

1C	1.570822	-2.807618	0.537385
2C	0.201137	-2.809382	0.524679
3N	-0.517614	-3.232400	-0.551574
4C	0.152842	-3.714909	-1.638410
5C	1.518399	-3.741756	-1.688163
6C	2.317120	-3.247605	-0.606205
7N	3.649538	-3.231702	-0.797237
8S	4.679555	-2.665347	0.348404
9O	4.395237	-3.185031	1.712727
10O	6.039364	-2.887116	-0.190650
11C	4.435036	-0.879113	0.418227
12C	3.997839	-0.271737	1.592436
13C	3.814826	1.114172	1.643721
14C	4.069384	1.887358	0.503061
15C	4.520554	1.269555	-0.678906
16C	4.704453	-0.105571	-0.720642
17O	3.901468	3.237067	0.436257
18C	3.559849	3.943868	1.632914
19C	-2.032334	-3.167041	-0.589818
20O	-2.537719	-3.593577	-1.644001
21N	-2.508400	-2.643847	0.514313
22C	-3.876385	-2.512219	0.749384
23C	-4.933375	-2.932666	-0.095879
24C	-6.266311	-2.725845	0.274813

25C	-6.596029	-2.092999	1.477843
26C	-5.560447	-1.670082	2.322919
27C	-4.230283	-1.878564	1.965950
28H	2.072767	-2.467493	1.432555
29H	-0.392947	-2.466363	1.359442
30H	-0.475936	-4.054096	-2.450755
31H	2.013213	-4.119411	-2.576717
32H	3.804901	-0.875669	2.473085
33H	3.470211	1.568776	2.564955
34H	4.722113	1.886888	-1.549724
35H	5.059135	-0.579870	-1.630876
36H	2.583786	3.626605	2.017152
37H	4.329554	3.805882	2.402801
38H	3.511968	4.995966	1.348561
39H	-4.700022	-3.418375	-1.034665
40H	-7.056794	-3.064350	-0.392720
41H	-7.635786	-1.935219	1.754273
42H	-5.791679	-1.175909	3.264623
43H	-3.426461	-1.547972	2.619717
44P	-1.021313	1.794403	-0.333970
45C	-0.244534	3.433609	-0.409681
46C	-0.771946	1.096132	1.324001
47C	-2.801948	1.939691	-0.622373
48C	-0.273184	0.752613	-1.617587
49C	-1.713288	1.353190	2.336506
50C	-1.501849	0.853331	3.621694
51C	-0.356289	0.101549	3.903462
52C	0.582654	-0.144735	2.898666
53C	0.380157	0.349932	1.609845
54C	-3.363352	3.112444	-1.150575
55C	-4.739514	3.166828	-1.385313
56C	-5.548168	2.062620	-1.095014
57C	-4.986474	0.895685	-0.565477
58C	-3.614192	0.831621	-0.327938
59C	1.124336	0.749247	-1.775777
60C	1.707718	-0.035361	-2.768847
61C	0.906547	-0.812514	-3.610782
62C	-0.481405	-0.811015	-3.454740
63C	-1.076349	-0.032810	-2.460265
64C	-0.078948	4.185197	0.764252
65C	0.471940	5.465848	0.693808
66C	0.863161	5.995351	-0.539275
67C	0.700059	5.246126	-1.709106
68C	0.145446	3.966907	-1.650150
69H	-2.611696	1.924905	2.126408
70H	-2.237814	1.042674	4.398151
71H	-0.200260	-0.297685	4.902060
72H	1.468838	-0.735581	3.109164
73H	1.110551	0.131466	0.839780
74H	-2.742411	3.975104	-1.373276
75H	-5.178411	4.073643	-1.792480
76H	-6.618210	2.112367	-1.279251
77H	-5.605818	0.034505	-0.333062
78H	-3.181675	-0.073083	0.085645
79H	1.758609	1.357922	-1.139000
80H	2.787646	-0.045125	-2.875750
81H	1.366723	-1.426978	-4.379568
82H	-1.107793	-1.423227	-4.096941
83H	-2.155343	-0.044887	-2.352933
84H	-0.369988	3.777143	1.727765
85H	0.605877	6.042687	1.604712
86H	1.299979	6.989252	-0.588658
87H	1.008030	5.653661	-2.667942
88H	0.024442	3.390253	-2.562461

6cg-PhNCO-004

1C	1.570148	-2.807938	0.537501
2C	0.200466	-2.809439	0.524738
3N	-0.518327	-3.232419	-0.551477
4C	0.152067	-3.715022	-1.638303
5C	1.517628	-3.742106	-1.688023
6C	2.316414	-3.248067	-0.606054
7N	3.648842	-3.232401	-0.797085
8S	4.678995	-2.666075	0.348482
9O	4.394762	-3.185671	1.712851
10O	6.038737	-2.888041	-0.190660
11C	4.434674	-0.879828	0.418221
12C	3.997602	-0.272342	1.592435
13C	3.814727	1.113584	1.643653
14C	4.069373	1.886682	0.502947
15C	4.520457	1.268768	-0.678994
16C	4.704151	-0.106379	-0.720693
17O	3.901716	3.236424	0.436092
18C	3.560106	3.943332	1.632674
19C	-2.033076	-3.166857	-0.589727

20O	-2.538460	-3.593270	-1.643950
21N	-2.509080	-2.643662	0.514427
22C	-3.877047	-2.511724	0.749408
23C	-4.934038	-2.931980	-0.095952
24C	-6.266966	-2.725010	0.274665
25C	-6.596669	-2.092145	1.477697
26C	-5.561088	-1.669352	2.322825
27C	-4.230922	-1.878007	1.965940
28H	2.072081	-2.467646	1.432601
29H	-0.393536	-2.466214	1.359463
30H	-0.476753	-4.054134	-2.450650
31H	2.012401	-4.119784	-2.576592
32H	3.804592	-0.876245	2.473090
33H	3.470157	1.568287	2.564857
34H	4.722059	1.886045	-1.549841
35H	5.058710	-0.580763	-1.630932
36H	2.584002	3.626139	2.016863
37H	4.329740	3.805367	2.402636
38H	3.512308	4.995408	1.348240
39H	-4.700668	-3.417711	-1.034723
40H	-7.057455	-3.063397	-0.392920
41H	-7.636420	-1.934235	1.754075
42H	-5.792305	-1.175161	3.264524
43H	-3.427099	-1.547553	2.619777
44P	-1.020677	1.794781	-0.334011
45C	-0.243958	3.434037	-0.409565
46C	-0.771360	1.096416	1.323928
47C	-2.801320	1.939925	-0.622288
48C	-0.272726	0.752998	-1.617734
49C	-1.712568	1.353770	2.336488
50C	-1.501259	0.853813	3.621648
51C	-0.355963	0.101600	3.903382
52C	0.582856	-0.144967	2.898556
53C	0.380495	0.349830	1.609739
54C	-3.362703	3.112428	-1.151074
55C	-4.738852	3.166667	-1.385926
56C	-5.547475	2.062516	-1.095289
57C	-4.985786	0.895814	-0.565238
58C	-3.613535	0.831918	-0.327517
59C	1.124821	0.749173	-1.775784
60C	1.708047	-0.035581	-2.768813
61C	0.906707	-0.812402	-3.610913
62C	-0.481258	-0.810357	-3.455090
63C	-1.076049	-0.032085	-2.460563
64C	-0.078870	4.185665	0.764421
65C	0.472141	5.466264	0.694193
66C	0.863962	5.995711	-0.538722
67C	0.701369	5.246457	-1.708602
68C	0.146670	3.967251	-1.649877
69H	-2.610727	1.925899	2.126456
70H	-2.237121	1.043439	4.398135
71H	-0.200053	-0.297665	4.901983
72H	1.468868	-0.736117	3.108949
73H	1.110806	0.131041	0.839700
74H	-2.741770	3.975035	-1.374025
75H	-5.177770	4.073276	-1.793529
76H	-6.617499	2.112138	-1.279660
77H	-5.605107	0.034669	-0.332609
78H	-3.181013	-0.072634	0.086378
79H	1.759234	1.357550	-1.138874
80H	2.787984	-0.045673	-2.875578
81H	1.366766	-1.427033	-4.379634
82H	-1.107791	-1.422261	-4.097444
83H	-2.155067	-0.043788	-2.353414
84H	-0.370319	3.777670	1.727841
85H	0.605748	6.043076	1.605159
86H	1.300889	6.989574	-0.587922
87H	1.009851	5.653938	-2.667295
88H	0.026074	3.390602	-2.562235

6cg-PhNCO-005

1C	1.400873	-2.699363	0.567419
2C	0.041805	-2.657007	0.407858
3N	-0.586511	-3.240712	-0.648869
4C	0.166097	-3.905538	-1.573152
5C	1.526681	-3.992234	-1.467228
6C	2.235088	-3.375377	-0.383993
7N	3.575637	-3.490293	-0.393646
8S	4.518423	-2.789163	0.755117
9O	3.984132	-2.920196	2.137904
10O	5.888159	-3.290486	0.510620
11C	4.529940	-1.029154	0.367667
12C	3.892999	-0.115104	1.202899
13C	3.872377	1.244897	0.875300
14C	4.497241	1.679837	-0.301365

15C	5.157777	0.754787	-1.131293
16C	5.172387	-0.592905	-0.800674
17O	4.509073	2.971481	-0.732687
18C	3.773881	3.947479	0.012089
19C	-2.088194	-3.166401	-0.834197
20O	-2.492006	-3.603769	-1.927126
21N	-2.667588	-2.646124	0.221521
22C	-4.052205	-2.514061	0.324546
23C	-5.013348	-2.780606	-0.682258
24C	-6.376865	-2.592097	-0.433130
25C	-6.831655	-2.132141	0.807112
26C	-5.891586	-1.859419	1.810831
27C	-4.531702	-2.044690	1.572213
28H	1.827389	-2.227012	1.439878
29H	-0.614030	-2.161172	1.109150
30H	-0.392946	-4.346777	-2.387787
31H	2.087913	-4.530995	-2.223429
32H	3.419121	-0.456077	2.116923
33H	3.374074	1.942258	1.539263
34H	5.644817	1.114077	-2.033246
35H	5.676967	-1.306507	-1.444976
36H	2.714703	3.676081	0.078632
37H	4.189717	4.075706	1.019294
38H	3.876964	4.879725	-0.544644
39H	-4.683102	-3.139140	-1.648742
40H	-7.091459	-2.808977	-1.225076
41H	-7.894108	-1.991445	0.990874
42H	-6.221264	-1.500929	2.784069
43H	-3.802620	-1.831936	2.350957
44P	-1.021059	1.910187	-0.068735
45C	-0.232273	3.546356	-0.064106
46C	-0.810249	1.147103	1.565272
47C	-2.793246	2.068733	-0.405218
48C	-0.229200	0.901852	-1.352467
49C	-1.774101	1.348564	2.568106
50C	-1.580886	0.791652	3.833273
51C	-0.431290	0.042506	4.103657
52C	0.531008	-0.149674	3.107806
53C	0.345760	0.400210	1.839004
54C	-3.335156	3.254920	-0.924887
55C	-4.700826	3.318183	-1.210872
56C	-5.520708	2.208222	-0.982133
57C	-4.980315	1.028613	-0.459683
58C	-3.618871	0.956518	-0.167379
59C	1.148134	1.050519	-1.589478
60C	1.782113	0.243387	-2.532688
61C	1.046554	-0.706612	-3.247598
62C	-0.325069	-0.848946	-3.020242
63C	-0.967908	-0.050620	-2.073524
64C	0.062426	4.185368	1.150469
65C	0.626364	5.463424	1.142469
66C	0.895590	6.104405	-0.069894
67C	0.609509	5.465332	-1.281174
68C	0.047413	4.188756	-1.283592
69H	-2.673249	1.922373	2.366456
70H	-2.332952	0.937615	4.603676
71H	-0.289000	-0.398910	5.086356
72H	1.417303	-0.742974	3.313739
73H	1.087070	0.225589	1.067312
74H	-2.708186	4.123090	-1.102494
75H	-5.122239	4.236501	-1.610610
76H	-6.582370	2.263044	-1.208413
77H	-5.608494	0.162913	-0.275855
78H	-3.208642	0.038925	0.241419
79H	1.725067	1.790544	-1.045704
80H	2.849473	0.352421	-2.696552
81H	1.544403	-1.341547	-3.975240
82H	-0.899360	-1.592481	-3.564212
83H	-2.031014	-0.181240	-1.905964
84H	-0.137600	3.692353	2.096890
85H	0.856713	5.954170	2.084088
86H	1.336734	7.097536	-0.072208
87H	0.827239	5.957896	-2.224778
88H	-0.165719	3.694723	-2.227217

6cg-PhNCO-006

1C	1.714127	-3.140066	-0.071988
2C	0.348145	-3.179186	0.030446
3N	-0.469805	-2.825319	-0.998633
4C	0.092148	-2.502754	-2.200972
5C	1.446516	-2.474945	-2.377140
6C	2.345843	-2.714407	-1.287997
7N	3.651414	-2.487473	-1.527304
8S	4.759670	-2.440877	-0.315539
9O	4.639840	-3.546678	0.672175

10O	6.071618	-2.264582	-0.975454
11C	4.397608	-0.908094	0.562102
12C	3.700099	-0.928848	1.768509
13C	3.338955	0.268849	2.394251
14C	3.672597	1.491229	1.795161
15C	4.395703	1.506915	0.587575
16C	4.755216	0.314413	-0.025398
17O	3.339153	2.711222	2.299636
18C	2.622152	2.768778	3.536480
19C	-1.965243	-2.676502	-0.823971
20O	-2.535094	-2.112103	-1.781677
21N	-2.359625	-3.153595	0.326913
22C	-3.675945	-3.042848	0.771301
23C	-4.747311	-2.390787	0.111904
24C	-6.011079	-2.316369	0.705898
25C	-6.258804	-2.887933	1.958349
26C	-5.211649	-3.547439	2.616940
27C	-3.948014	-3.620712	2.034543
28H	2.304926	-3.431642	0.785418
29H	-0.165005	-3.466885	0.936925
30H	-0.610401	-2.249108	-2.982708
31H	1.853877	-2.199722	-3.342432
32H	3.445191	-1.876125	2.231279
33H	2.794195	0.232785	3.329857
34H	4.660679	2.463674	0.146398
35H	5.314247	0.326116	-0.955748
36H	1.645121	2.278690	3.450772
37H	3.199771	2.311005	4.349169
38H	2.479263	3.830019	3.744420
39H	-4.579466	-1.948955	-0.861338
40H	-6.813649	-1.805978	0.176005
41H	-7.246218	-2.828018	2.409833
42H	-5.381566	-4.006253	3.589128
43H	-3.133254	-4.125111	2.548838
44P	-1.006256	1.788879	-0.445054
45C	-0.315696	3.318445	0.253600
46C	-1.126277	0.575977	0.900680
47C	-2.669546	2.112430	-1.087786
48C	0.088331	1.262005	-1.795045
49C	-2.331535	0.439469	1.612022
50C	-2.383776	-0.390193	2.732281
51C	-1.240195	-1.074040	3.153326
52C	-0.042710	-0.936223	2.446804
53C	0.018791	-0.118230	1.319117
54C	-3.146251	3.427612	-1.203106
55C	-4.428742	3.653759	-1.708506
56C	-5.231168	2.576203	-2.096066
57C	-4.752807	1.266394	-1.980885
58C	-3.474107	1.026298	-1.477472
59C	1.480108	1.246428	-1.590204
60C	2.331830	0.907315	-2.639388
61C	1.808021	0.597103	-3.898174
62C	0.426818	0.610000	-4.103221
63C	-0.436725	0.938353	-3.056147
64C	-0.502826	3.610370	1.614087
65C	-0.022534	4.812187	2.136929
66C	0.647131	5.719778	1.311111
67C	0.835091	5.428989	-0.044036
68C	0.353616	4.232640	-0.577503
69H	-3.227120	0.963368	1.294650
70H	-3.323205	-0.514109	3.262405
71H	-1.287854	-1.728058	4.019725
72H	0.845041	-1.478172	2.758405
73H	0.954120	-0.036600	0.778020
74H	-2.531377	4.269430	-0.900047
75H	-4.799109	4.671573	-1.795073
76H	-6.229705	2.756330	-2.485764
77H	-5.373091	0.426105	-2.280375
78H	-3.113286	0.003265	-1.398123
79H	1.906577	1.512700	-0.627798
80H	3.403101	0.880712	-2.470223
81H	2.477624	0.334271	-4.712570
82H	0.014010	0.361120	-5.076966
83H	-1.506388	0.944918	-3.233133
84H	-1.014406	2.907193	2.264467
85H	-0.166451	5.034263	3.190668
86H	1.026863	6.650849	1.723477
87H	1.358273	6.131083	-0.687321
88H	0.504341	4.013800	-1.630539

6cg-PhNCO-007

1C	1.851472	-2.884571	-0.160534
2C	0.525864	-3.122387	0.092541
3N	-0.419789	-3.078403	-0.885263
4C	-0.031200	-2.834064	-2.169706

5C	1.271552	-2.565734	-2.485195
6C	2.292560	-2.534765	-1.479845
7N	3.519263	-2.153173	-1.880138
8S	4.789810	-2.093490	-0.839940
9O	4.953853	-3.346813	-0.057323
10O	5.940792	-1.639909	-1.652014
11C	4.455117	-0.783348	0.355560
12C	4.379111	-1.078251	1.715037
13C	4.169488	-0.057323	2.647035
14C	4.027305	1.264728	2.203559
15C	4.094089	1.555902	0.828749
16C	4.315385	0.538931	-0.090046
17O	3.823628	2.332372	3.023663
18C	3.868323	2.126972	4.438205
19C	-1.896745	-3.253720	-0.590209
20O	-2.583167	-3.577977	-1.574788
21N	-2.146543	-2.964812	0.664029
22C	-3.436627	-3.016339	1.192049
23C	-4.578966	-3.591823	0.584858
24C	-5.820465	-3.554361	1.225879
25C	-5.973407	-2.945660	2.476798
26C	-4.848837	-2.379980	3.093231
27C	-3.605513	-2.420776	2.464422
28H	2.551098	-2.965072	0.659784
29H	0.152844	-3.352294	1.081200
30H	-0.827818	-2.852031	-2.902578
31H	1.539029	-2.346923	-3.513033
32H	4.496224	-2.102889	2.053006
33H	4.121635	-0.306263	3.700648
34H	3.985950	2.586665	0.503525
35H	4.389742	0.772735	-1.146893
36H	3.074637	1.446983	4.769199
37H	4.845222	1.734827	4.747702
38H	3.713613	3.111127	4.884784
39H	-4.485996	-4.051548	-0.390839
40H	-6.681301	-4.005538	0.735424
41H	-6.944762	-2.918948	2.964919
42H	-4.941696	-1.906222	4.068727
43H	-2.734068	-1.976829	2.940014
44P	-1.197690	1.945451	-0.515964
45C	-2.659132	0.951806	-0.915377
46C	0.026354	1.802191	-1.845283
47C	-1.653560	3.698934	-0.368667
48C	-0.518321	1.358307	1.060875
49C	-0.133793	2.577486	-3.009220
50C	0.761494	2.428981	-4.067808
51C	1.812341	1.509183	-3.972593
52C	1.972656	0.741096	-2.817220
53C	1.083163	0.885261	-1.749339
54C	-2.985967	4.074972	-0.139482
55C	-3.309087	5.426054	0.008163
56C	-2.310525	6.400861	-0.073303
57C	-0.981920	6.026978	-0.303086
58C	-0.649460	4.680297	-0.452665
59C	-0.537303	-0.016868	1.348245
60C	-0.002844	-0.475811	2.552096
61C	0.543289	0.425059	3.470225
62C	0.554940	1.793914	3.186597
63C	0.027981	2.265288	1.984387
64C	-2.903379	0.547044	-2.237337
65C	-4.050035	-0.192989	-2.531320
66C	-4.944899	-0.536024	-1.514478
67C	-4.697710	-0.140590	-0.196519
68C	-3.558996	0.603789	0.107664
69H	-0.946561	3.293866	-3.088574
70H	0.636824	3.029190	-4.965048
71H	2.508321	1.391360	-4.799078
72H	2.778651	0.017275	-2.742342
73H	1.222440	0.286750	-0.854412
74H	-3.770957	3.327145	-0.085266
75H	-4.342649	5.713764	0.180265
76H	-2.566746	7.451207	0.037827
77H	-0.203728	6.782420	-0.369918
78H	0.383388	4.399165	-0.637611
79H	-0.989345	-0.734654	0.670803
80H	-0.027832	-1.539305	2.769870
81H	0.954406	0.060577	4.407799
82H	0.975796	2.498418	3.897097
83H	0.037847	3.330895	1.779847
84H	-2.204037	0.789725	-3.030940
85H	-4.229418	-0.520397	-3.551461
86H	-5.821809	-1.135199	-1.742547
87H	-5.371559	-0.439970	0.600308
88H	-3.363139	0.885495	1.137927

1C	-1.716906	0.540345	-0.485843
2C	-0.839256	1.589885	-0.421677
3N	-0.372066	2.220158	-1.532062
4C	-0.806736	1.803225	-2.755935
5C	-1.678485	0.757127	-2.891830
6C	-2.184793	0.051493	-1.751310
7N	-3.016744	-0.978296	-1.995768
8S	-3.725753	-1.823211	-0.777047
9O	-4.462099	-2.924433	-1.436568
10O	-2.779846	-2.201932	0.307858
11C	-4.942008	-0.717583	-0.048550
12C	-4.775792	-0.240455	1.249592
13C	-5.708371	0.647073	1.796861
14C	-6.806625	1.056227	1.027080
15C	-6.968284	0.569649	-0.284207
16C	-6.041588	-0.312820	-0.820218
17O	-7.769363	1.916435	1.455918
18C	-7.663103	2.472182	2.770353
19C	0.662301	3.330656	-1.452877
20O	0.873092	3.909517	-2.533390
21N	1.144525	3.426133	-0.239049
22C	2.159770	4.319798	0.092855
23C	2.795602	5.246695	-0.770262
24C	3.835064	6.057430	-0.303422
25C	4.275627	5.982553	1.022254
26C	3.649845	5.076813	1.889949
27C	2.613746	4.264813	1.432992
28H	-2.016552	0.070975	0.440632
29H	-0.450686	1.970233	0.511180
30H	-0.408000	2.355678	-3.596809
31H	-1.995244	0.449929	-3.883112
32H	-3.925173	-0.564225	1.840569
33H	-5.567471	1.005465	2.810012
34H	-7.828000	0.896307	-0.862054
35H	-6.167875	-0.687801	-1.831451
36H	-8.533494	3.120586	2.886093
37H	-7.688376	1.686420	3.535875
38H	-6.746823	3.066642	2.875147
39H	2.471933	5.319135	-1.800570
40H	4.304996	6.758994	-0.990627
41H	5.084392	6.618443	1.374291
42H	3.971519	5.004117	2.927197
43H	2.132904	3.557629	2.105376
44P	2.235522	-1.705812	0.303720
45C	1.039025	-1.140768	1.547089
46C	2.862579	-0.300242	-0.651790
47C	3.642627	-2.505252	1.132250
48C	1.432300	-2.886336	-0.812676
49C	2.359536	-0.043517	-1.937236
50C	2.822095	1.063305	-2.650023
51C	3.772007	1.916969	-2.084545
52C	4.272791	1.662759	-0.804209
53C	3.825745	0.554667	-0.086024
54C	4.879759	-2.597869	0.470548
55C	5.948283	-3.251624	1.085859
56C	5.789835	-3.813148	2.357195
57C	4.560162	-3.720753	3.015874
58C	3.485064	-3.068795	2.408089
59C	0.086971	-2.699252	-1.168322
60C	-0.510981	-3.555879	-2.093462
61C	0.227348	-4.597330	-2.662186
62C	1.566383	-4.788846	-2.302807
63C	2.173792	-3.936608	-1.379587
64C	0.096127	-2.041078	2.071418
65C	-0.801158	-1.611530	3.049575
66C	-0.760210	-0.291668	3.508815
67C	0.178243	0.604401	2.986756
68C	1.077376	0.186199	2.005156
69H	1.614050	-0.694351	-2.382689
70H	2.425149	1.268149	-3.639566
71H	4.108141	2.791600	-2.633097
72H	4.997781	2.336978	-0.358027
73H	4.220612	0.362825	0.907919
74H	5.014379	-2.156000	-0.512535
75H	6.903647	-3.317954	0.572586
76H	6.625136	-4.317784	2.835439
77H	4.435692	-4.151076	4.005804
78H	2.537484	-2.997997	2.932896
79H	-0.503425	-1.909844	-0.719858
80H	-1.552236	-3.403559	-2.360474
81H	-0.242452	-5.264403	-3.380159
82H	2.138562	-5.603794	-2.737776
83H	3.211898	-4.095652	-1.104809
84H	0.041288	-3.062223	1.707770
85H	-1.542157	-2.305528	3.435144
86H	-1.466716	0.042124	4.264337
87H	0.201166	1.635991	3.327075

88H 1.774650 0.902405 1.583469

6cg-PhNCO-009

1C -1.718341 0.551228 -0.447374
2C -0.838388 1.599235 -0.388536
3N -0.379348 2.230923 -1.501379
4C -0.827998 1.820370 -2.722169
5C -1.701818 0.775455 -2.853179
6C -2.195055 0.064238 -1.710276
7N -3.024968 -0.968160 -1.951058
8S -3.737879 -1.807781 -0.731071
9O -4.457373 -2.922132 -1.387323
10O -2.802084 -2.168489 0.368685
11C -4.970328 -0.702629 -0.030263
12C -4.808150 -0.185857 1.253211
13C -5.751033 0.705310 1.776280
14C -6.855282 1.078860 0.996871
15C -7.012866 0.552150 -0.299350
16C -6.076142 -0.334080 -0.811195
17O -7.827455 1.940011 1.402052
18C -7.732695 2.524083 2.705104
19C 0.671453 3.326064 -1.429591
20O 0.871399 3.913103 -2.507587
21N 1.175557 3.402093 -0.223010
22C 2.219122 4.267105 0.097021
23C 2.879966 5.165843 -0.777246
24C 3.948936 5.944818 -0.323526
25C 4.395596 5.865483 0.999901
26C 3.745670 4.987979 1.878641
27C 2.679864 4.207566 1.434830
28H -2.010978 0.080226 0.480569
29H -0.439877 1.975481 0.541599
30H -0.436851 2.375646 -3.564690
31H -2.029034 0.472387 -3.842330
32H -3.952962 -0.481573 1.852247
33H -5.612697 1.094071 2.778530
34H -7.877647 0.850770 -0.884787
35H -6.199277 -0.740456 -1.810585
36H -8.610267 3.165594 2.803745
37H -7.753349 1.753836 3.486357
38H -6.823134 3.130172 2.801481
39H 2.551546 5.241899 -1.805768
40H 4.437292 6.625147 -1.019201
41H 5.227359 6.476802 1.341675
42H 4.071194 4.912864 2.914506
43H 2.179308 3.523511 2.116821
44P 2.236650 -1.702099 0.285851
45C 1.088142 -1.076937 1.544977
46C 2.810433 -0.347437 -0.775473
47C 3.683942 -2.438170 1.102775
48C 1.394666 -2.951672 -0.723514
49C 2.222289 -0.140778 -2.033620
50C 2.636640 0.934091 -2.820657
51C 3.624619 1.806137 -2.357163
52C 4.212549 1.600349 -1.105754
53C 3.812675 0.524410 -0.313988
54C 4.885363 -2.589249 0.388093
55C 5.984728 -3.193021 0.999818
56C 5.893046 -3.644857 2.320624
57C 4.699444 -3.492996 3.032366
58C 3.593421 -2.891083 2.428438
59C 0.050224 -2.756901 -1.081559
60C -0.583463 -3.672415 -1.922216
61C 0.117715 -4.780915 -2.405033
62C 1.454385 -4.980521 -2.042517
63C 2.097662 -4.069915 -1.202781
64C 0.122352 -1.932327 2.101126
65C -0.737533 -1.453706 3.090369
66C -0.634647 -0.130477 3.529881
67C 0.329520 0.719655 2.978227
68C 1.190686 0.252781 1.984823
69H 1.445944 -0.804590 -2.399910
70H 2.171704 1.099767 -3.787853
71H 3.923363 2.656186 -2.963055
72H 4.968816 2.287154 -0.737416
73H 4.275634 0.370512 0.656467
74H 4.967107 -2.232893 -0.634677
75H 6.912338 -3.306019 0.445442
76H 6.752533 -4.110562 2.795510
77H 4.627362 -3.837135 4.060452
78H 2.673807 -2.772897 2.993058
79H -0.511638 -1.914519 -0.696742
80H -1.624055 -3.515814 -2.189300
81H -0.380036 -5.493852 -3.057075
82H 1.997238 -5.847631 -2.408808

83H	3.133289	-4.237706	-0.924236
84H	0.023101	-2.956275	1.755721
85H	-1.497233	-2.112549	3.500620
86H	-1.312572	0.241682	4.293643
87H	0.400172	1.754210	3.302654
88H	1.906023	0.935006	1.537842

6cg-PhNCO-010

1C	-1.833178	-0.822510	0.717429
2C	-0.807141	-1.715476	0.565989
3N	-0.247990	-2.370715	1.620620
4C	-0.770716	-2.176287	2.866053
5C	-1.803090	-1.306300	3.083283
6C	-2.363004	-0.530433	2.017529
7N	-3.291578	0.382827	2.357574
8S	-3.933154	1.402362	1.242446
9O	-4.794184	2.336184	2.001339
10O	-2.905163	2.009052	0.350954
11C	-5.010583	0.408178	0.199163
12C	-4.775095	0.306558	-1.169351
13C	-5.611395	-0.476859	-1.971754
14C	-6.684365	-1.163378	-1.385406
15C	-6.915833	-1.057431	-0.000596
16C	-6.085049	-0.275022	0.788417
17O	-7.556236	-1.955382	-2.066256
18C	-7.392541	-2.105915	-3.479337
19C	0.972301	-3.256845	1.462135
20O	1.335488	-3.824849	2.507563
21N	1.414387	-3.222985	0.228113
22C	2.560613	-3.906890	-0.173250
23C	3.476067	-4.595849	0.660998
24C	4.625988	-5.182865	0.123165
25C	4.903805	-5.114590	-1.246268
26C	4.000404	-4.447898	-2.085028
27C	2.854554	-3.857387	-1.557190
28H	-2.191159	-0.312290	-0.165452
29H	-0.364599	-1.937819	-0.393184
30H	-0.296420	-2.742916	3.656760
31H	-2.177455	-1.162127	4.091260
32H	-3.940827	0.838324	-1.613580
33H	-5.416498	-0.540871	-3.036307
34H	-7.753793	-1.595234	0.433412
35H	-6.266782	-0.194238	1.856066
36H	-8.197573	-2.770423	-3.798755
37H	-7.489453	-1.141695	-3.994029
38H	-6.424819	-2.563880	-3.719812
39H	3.280156	-4.658901	1.723736
40H	5.313166	-5.701546	0.789306
41H	5.800683	-5.575245	-1.653479
42H	4.193452	-4.384122	-3.154108
43H	2.159354	-3.332141	-2.207878
44P	2.104077	1.679130	-0.313614
45C	1.577199	1.549226	1.417057
46C	0.845466	1.033891	-1.455516
47C	2.343122	3.433280	-0.717995
48C	3.667374	0.783156	-0.515026
49C	1.002992	-0.211571	-2.083840
50C	0.012074	-0.679802	-2.948478
51C	-1.130082	0.088485	-3.192469
52C	-1.282468	1.333004	-2.573479
53C	-0.299943	1.809778	-1.706866
54C	2.404193	3.829448	-2.065463
55C	2.615688	5.170972	-2.383570
56C	2.764197	6.118834	-1.364563
57C	2.700797	5.725039	-0.024940
58C	2.490363	4.383513	0.303457
59C	3.748962	-0.556512	-0.093584
60C	4.943195	-1.259127	-0.254513
61C	6.055998	-0.631315	-0.823468
62C	5.977471	0.702436	-1.235047
63C	4.785446	1.414487	-1.083375
64C	2.545956	1.365943	2.419560
65C	2.159998	1.364547	3.760787
66C	0.817521	1.552089	4.104122
67C	-0.144011	1.735156	3.106433
68C	0.227712	1.731922	1.761088
69H	1.879198	-0.823257	-1.901602
70H	0.134043	-1.648319	-3.425471
71H	-1.899712	-0.282021	-3.864667
72H	-2.165591	1.936463	-2.758710
73H	-0.429921	2.778757	-1.235567
74H	2.281487	3.099503	-2.860605
75H	2.658985	5.475463	-3.425721
76H	2.922632	7.164265	-1.616025
77H	2.806577	6.460728	0.767578

78H	2.432334	4.087644	1.346403
79H	2.890565	-1.057805	0.344957
80H	4.995701	-2.297624	0.056542
81H	6.983396	-1.184455	-0.947110
82H	6.842241	1.192950	-1.673671
83H	4.735751	2.450802	-1.401696
84H	3.590314	1.219252	2.162622
85H	2.908790	1.213808	4.533625
86H	0.518319	1.545259	5.148958
87H	-1.191230	1.857990	3.365610
88H	-0.540739	1.858971	1.004976

6cg-PhNCO-011

1C	1.803339	0.636723	0.626716
2C	0.841697	1.608853	0.562914
3N	0.206895	2.082968	1.669402
4C	0.577343	1.605442	2.893546
5C	1.552057	0.655110	3.028914
6C	2.211054	0.090194	1.888135
7N	3.116047	-0.875863	2.128220
8S	3.845943	-1.692643	0.905959
9O	4.663756	-2.737550	1.561298
10O	2.884936	-2.146171	-0.137862
11C	4.982673	-0.551765	0.105073
12C	4.801083	-0.187624	-1.227150
13C	5.685802	0.707409	-1.838013
14C	6.752493	1.237371	-1.097628
15C	6.927517	0.867638	0.249461
16C	6.048650	-0.023389	0.848341
17O	7.670857	2.112739	-1.588957
18C	7.564176	2.529596	-2.953330
19C	-0.947655	3.065027	1.573464
20O	-1.456332	3.364198	2.669949
21N	-1.209197	3.359358	0.324981
22C	-2.266924	4.193841	-0.033574
23C	-3.021446	5.025061	0.830315
24C	-4.069831	5.804609	0.332578
25C	-4.406914	5.784977	-1.025082
26C	-3.663391	4.973859	-1.892888
27C	-2.611763	4.199852	-1.406039
28H	2.221486	0.280191	-0.303755
29H	0.510570	2.044227	-0.367235
30H	0.038583	2.026274	3.732578
31H	1.815208	0.296354	4.018306
32H	3.972991	-0.602951	-1.792828
33H	5.532860	0.978019	-2.876524
34H	7.760841	1.288627	0.804375
35H	6.187954	-0.310203	1.886490
36H	8.403128	3.207831	-3.119999
37H	7.644320	1.674580	-3.636176
38H	6.622127	3.063434	-3.130625
39H	-2.784181	5.046825	1.886376
40H	-4.631145	6.434507	1.020525
41H	-5.226727	6.392465	-1.401054
42H	-3.903981	4.946300	-2.953922
43H	-2.035268	3.570492	-2.080408
44P	-2.163143	-1.696636	-0.322994
45C	-1.438038	-2.186362	1.265062
46C	-0.921718	-1.049136	-1.475094
47C	-2.927724	-3.139698	-1.123127
48C	-3.407073	-0.419327	-0.002081
49C	-0.968341	0.290715	-1.888271
50C	-0.018341	0.765680	-2.794787
51C	0.977093	-0.086391	-3.281121
52C	1.019839	-1.423843	-2.871846
53C	0.068785	-1.911295	-1.977159
54C	-3.188838	-3.092541	-2.503914
55C	-3.805218	-4.175977	-3.130883
56C	-4.155432	-5.309490	-2.389395
57C	-3.886826	-5.360736	-1.018546
58C	-3.274301	-4.279144	-0.381431
59C	-3.146390	0.546686	0.984555
60C	-4.049900	1.588490	1.190266
61C	-5.210819	1.670463	0.416015
62C	-5.475428	0.704863	-0.560868
63C	-4.576251	-0.341462	-0.775440
64C	-2.299839	-2.369355	2.364279
65C	-1.782033	-2.795171	3.586385
66C	-0.409740	-3.037389	3.719642
67C	0.444625	-2.847853	2.631786
68C	-0.061812	-2.420086	1.401542
69H	-1.722235	0.967846	-1.500274
70H	-0.051777	1.806273	-3.105518
71H	1.720355	0.290704	-3.978902
72H	1.796034	-2.087718	-3.240597

73H	0.102925	-2.953121	-1.672288
74H	-2.905229	-2.222079	-3.089030
75H	-4.005257	-4.136045	-4.198156
76H	-4.629883	-6.154365	-2.881541
77H	-4.146249	-6.244697	-0.442378
78H	-3.059474	-4.336258	0.680716
79H	-2.243008	0.493922	1.583673
80H	-3.825465	2.345130	1.935050
81H	-5.902995	2.494155	0.567516
82H	-6.379526	0.766342	-1.160423
83H	-4.788399	-1.085748	-1.536974
84H	-3.364344	-2.172557	2.272528
85H	-2.448949	-2.930463	4.433497
86H	-0.006453	-3.362739	4.675006
87H	1.513305	-3.002906	2.737465
88H	0.630507	-2.258346	0.582472

6cg-PhNCO-012

1C	1.810855	0.640210	0.621023
2C	0.852687	1.615773	0.556429
3N	0.217233	2.090554	1.662351
4C	0.583826	1.610560	2.886707
5C	1.554729	0.656497	3.022860
6C	2.213499	0.090206	1.882627
7N	3.113672	-0.880128	2.123455
8S	3.842403	-1.699330	0.902220
9O	4.651651	-2.750283	1.558540
10O	2.882081	-2.145324	-0.145476
11C	4.988757	-0.564195	0.107068
12C	4.813586	-0.196492	-1.225020
13C	5.706015	0.693794	-1.831556
14C	6.773843	1.215478	-1.086968
15C	6.942393	0.842157	0.259958
16C	6.055921	-0.044217	0.854536
17O	7.699267	2.085805	-1.574019
18C	7.599197	2.505809	-2.937939
19C	-0.936278	3.073887	1.565300
20O	-1.444858	3.374505	2.661460
21N	-1.197506	3.366980	0.316492
22C	-2.254389	4.201927	-0.043698
23C	-3.014284	5.028864	0.819693
24C	-4.060675	5.809564	0.319589
25C	-4.390322	5.795691	-1.039954
26C	-3.641573	4.988861	-1.907225
27C	-2.591972	4.213525	-1.418038
28H	2.230205	0.283550	-0.308874
29H	0.524262	2.053197	-0.373764
30H	0.044832	2.032295	3.725131
31H	1.814733	0.295687	4.012334
32H	3.984623	-0.605552	-1.793991
33H	5.558231	0.967109	-2.870073
34H	7.776768	1.256630	0.818193
35H	6.190170	-0.333899	1.892550
36H	8.442838	3.179128	-3.100799
37H	7.676094	1.651607	-3.622176
38H	6.661020	3.045836	-3.117094
39H	-2.782385	5.046774	1.876999
40H	-4.626147	6.436134	1.007168
41H	-5.208519	6.404238	-1.417721
42H	-3.876264	4.965843	-2.969688
43H	-2.011113	3.587966	-2.092150
44P	-2.170856	-1.692400	-0.324191
45C	-1.441491	-2.190108	1.259788
46C	-0.933841	-1.030198	-1.472542
47C	-2.931895	-3.129541	-1.137133
48C	-3.422039	-0.427644	0.016001
49C	-0.990999	0.309484	-1.884786
50C	-0.044681	0.792128	-2.791247
51C	0.957478	-0.051670	-3.277981
52C	1.010690	-1.388983	-2.869564
53C	0.063323	-1.884399	-1.975448
54C	-3.196551	-3.068571	-2.516830
55C	-3.812847	-4.146826	-3.152797
56C	-4.159344	-5.288251	-2.421667
57C	-3.887412	-5.352801	-1.052032
58C	-3.275004	-4.276586	-0.405757
59C	-3.138617	0.556148	0.978629
60C	-4.049753	1.586430	1.205955
61C	-5.243972	1.635784	0.480657
62C	-5.532865	0.650065	-0.468797
63C	-4.624630	-0.383700	-0.706702
64C	-2.301722	-2.377342	2.359535
65C	-1.782123	-2.807051	3.579524
66C	-0.409466	-3.048348	3.710395
67C	0.443489	-2.853829	2.622288

68C	-0.064785	-2.422331	1.394103
69H	-1.750119	0.980627	-1.496568
70H	-0.085772	1.832591	-3.101329
71H	1.697795	0.331720	-3.975468
72H	1.791835	-2.046735	-3.238852
73H	0.105308	-2.926445	-1.672362
74H	-2.916857	-2.191386	-3.093668
75H	-4.016002	-4.096669	-4.219041
76H	-4.633839	-6.128887	-2.920974
77H	-4.144232	-6.242784	-0.484028
78H	-3.057677	-4.343445	0.655347
79H	-2.212773	0.523498	1.543945
80H	-3.808170	2.356948	1.930943
81H	-5.944604	2.448766	0.650314
82H	-6.463610	0.685321	-1.028377
83H	-4.855693	-1.145045	-1.445480
84H	-3.366534	-2.181093	2.270000
85H	-2.447920	-2.945842	4.426959
86H	-0.004725	-3.376594	4.664154
87H	1.512456	-3.007828	2.726430
88H	0.626698	-2.255982	0.575308

6c-Me2-001

1C	1.634671	1.418331	1.251062
2C	1.951087	2.750257	0.977906
3N	2.698427	3.144913	-0.062999
4C	3.170559	2.178485	-0.869087
5C	2.929208	0.819008	-0.681204
6C	2.130489	0.421247	0.400155
7N	1.864535	-0.964546	0.627310
8S	0.865586	-1.741996	-0.544995
9O	0.806485	-3.151472	-0.133407
10O	1.390243	-1.373217	-1.865648
11C	-0.747730	-1.013850	-0.347546
12C	-1.670845	-1.598774	0.531998
13C	-2.896996	-0.982065	0.737655
14C	-3.205098	0.221686	0.075928
15C	-2.273745	0.801743	-0.802206
16C	-1.042330	0.180666	-1.010026
17O	-4.426149	0.743058	0.349605
18C	-4.816290	1.973267	-0.274703
19C	1.576890	-1.376043	2.015282
20H	1.009889	1.179914	2.103972
21H	1.573737	3.537803	1.627084
22H	3.785387	2.506886	-1.704326
23H	3.348626	0.083806	-1.356664
24H	-1.433621	-2.530393	1.035323
25H	-3.634605	-1.417887	1.404856
26H	-2.493209	1.723883	-1.327046
27H	-0.322072	0.623117	-1.690482
28H	-5.817277	2.186283	0.103985
29H	-4.137646	2.788970	0.002829
30H	-4.851665	1.867733	-1.365608
31H	2.346983	-0.938561	2.654634
32H	0.588250	-1.050945	2.366234
33H	1.643261	-2.461946	2.079267

6c-Me2-002

1C	1.814395	1.386898	-1.200105
2C	2.361002	2.630511	-0.878264
3N	3.242016	2.828274	0.112907
4C	3.613539	1.745189	0.816800
5C	3.143036	0.456721	0.571700
6C	2.209405	0.266546	-0.456604
7N	1.716375	-1.043124	-0.746933
8S	0.706863	-1.761193	0.450242
9O	1.362654	-1.547774	1.746216
10O	0.436721	-3.122209	-0.034166
11C	-0.810193	-0.827493	0.420474
12C	-0.906119	0.349832	1.179234
13C	-2.064779	1.108751	1.109392
14C	-3.130693	0.702565	0.283874
15C	-3.025563	-0.474586	-0.475559
16C	-1.858377	-1.237153	-0.406434
17O	-4.217152	1.513280	0.291601
18C	-5.356519	1.157889	-0.501805
19C	1.277879	-1.308215	-2.130569
20H	1.095707	1.310949	-2.008346
21H	2.065868	3.511722	-1.444287
22H	4.336613	1.913112	1.612024
23H	3.491388	-0.381490	1.162386
24H	-0.088925	0.658290	1.822880

25H	-2.169687	2.019078	1.691960
26H	-3.836740	-0.806503	-1.112879
27H	-1.774998	-2.152867	-0.982797
28H	-5.766731	0.189930	-0.189899
29H	-6.093380	1.942344	-0.321170
30H	-5.102034	1.133509	-1.568500
31H	2.057723	-0.938924	-2.800541
32H	1.181113	-2.385169	-2.267525
33H	0.325669	-0.822045	-2.381012

6c-Me2-003

1C	-2.924344	1.290038	0.359951
2C	-2.867540	2.670217	0.560719
3N	-1.909945	3.460357	0.050014
4C	-0.965364	2.870677	-0.699356
5C	-0.933727	1.501483	-0.968330
6C	-1.933988	0.690093	-0.424923
7N	-1.915937	-0.722448	-0.700201
8S	-1.018046	-1.649718	0.447177
9O	-1.126518	-3.042651	-0.020055
10O	-1.440769	-1.326303	1.824103
11C	0.640664	-1.057163	0.211067
12C	1.213413	-0.212868	1.161060
13C	2.502177	0.282790	0.958189
14C	3.205168	-0.071728	-0.204649
15C	2.617027	-0.932258	-1.153937
16C	1.337993	-1.424687	-0.949451
17O	4.453522	0.360204	-0.504624
18C	5.118242	1.251430	0.400649
19C	-3.221819	-1.334756	-1.036997
20H	-3.715448	0.704231	0.814988
21H	-3.624308	3.162170	1.168000
22H	-0.198880	3.523629	-1.111271
23H	-0.153027	1.073926	-1.588249
24H	0.658326	0.063489	2.051394
25H	2.939165	0.938203	1.702012
26H	3.183181	-1.198937	-2.041292
27H	0.881487	-2.084181	-1.681061
28H	4.559153	2.188477	0.510870
29H	5.263276	0.781921	1.380923
30H	6.089427	1.456277	-0.052811
31H	-3.047443	-2.331973	-1.443099
32H	-3.906329	-1.405355	-0.182397
33H	-3.675974	-0.711357	-1.810857

6c-Me2-004

1C	3.152624	1.000002	0.170952
2C	3.295460	2.363728	0.432357
3N	2.381826	3.288386	0.097382
4C	1.277320	2.857264	-0.531343
5C	1.039996	1.519148	-0.848911
6C	1.996254	0.565792	-0.486392
7N	1.766093	-0.816198	-0.812354
8S	0.885398	-1.684716	0.394309
9O	1.476656	-1.462414	1.728156
10O	0.788663	-3.060773	-0.122675
11C	-0.714035	-0.910568	0.352976
12C	-1.571414	-1.183817	-0.714803
13C	-2.818703	-0.564985	-0.774818
14C	-3.198797	0.328191	0.243546
15C	-2.325564	0.592710	1.314804
16C	-1.083225	-0.023123	1.371667
17O	-4.385038	0.981685	0.280670
18C	-5.338941	0.756346	-0.765540
19C	2.935560	-1.567105	-1.323280
20H	3.921731	0.301580	0.482557
21H	4.183857	2.728556	0.943450
22H	0.548244	3.617869	-0.802131
23H	0.135368	1.223004	-1.368936
24H	-1.271999	-1.873961	-1.497616
25H	-3.480528	-0.785527	-1.604020
26H	-2.640205	1.284280	2.090395
27H	-0.403064	0.182877	2.191396
28H	-5.643081	-0.296659	-0.800811
29H	-6.200257	1.377301	-0.513581
30H	-4.936704	1.065295	-1.737886
31H	3.382074	-0.960483	-2.114847
32H	3.692482	-1.775202	-0.556912
33H	2.588829	-2.508269	-1.751686

6c-Me-001

1C	3.095159	0.208498	1.202297
2C	3.849248	-0.908843	0.986475
3N	3.630562	-1.728369	-0.086545
4C	2.633817	-1.415227	-0.959448
5C	1.841444	-0.308316	-0.803578
6C	2.025735	0.574774	0.315580
7N	1.330620	1.673335	0.640722
8S	0.049810	2.179100	-0.266160
9O	0.343477	2.217833	-1.723306
10O	-0.410010	3.434311	0.364889
11C	-1.236688	0.943333	-0.022152
12C	-1.803197	0.289367	-1.113719
13C	-2.810702	-0.661660	-0.917800
14C	-3.241127	-0.953665	0.384410
15C	-2.661215	-0.291279	1.483191
16C	-1.667530	0.655995	1.281867
17O	-4.209002	-1.859511	0.690471
18C	-4.873660	-2.546139	-0.374763
19C	4.415763	-2.962491	-0.236590
20H	3.301122	0.834686	2.063762
21H	4.654336	-1.203132	1.650670
22H	2.504528	-2.094317	-1.794561
23H	1.089597	-0.108378	-1.554420
24H	-1.465133	0.521776	-2.118678
25H	-3.244630	-1.157776	-1.778278
26H	-3.010697	-0.530580	2.483332
27H	-1.225682	1.169282	2.130807
28H	-5.609307	-3.193061	0.107093
29H	-5.386720	-1.840885	-1.040439
30H	-4.170071	-3.159992	-0.951350
31H	4.327883	-3.325396	-1.261931
32H	5.466242	-2.752915	-0.021708
33H	4.045307	-3.726829	0.453970

6c-Me-002

1C	1.843284	-0.323499	-0.787056
2C	2.641727	-1.426702	-0.933488
3N	3.630875	-1.735686	-0.049399
4C	3.848634	-0.903496	1.013395
5C	3.088501	0.212169	1.219224
6C	2.022059	0.569263	0.325983
7N	1.321495	1.667169	0.641213
8S	0.046007	2.167026	-0.275891
9O	0.346885	2.193350	-1.731900
10O	-0.414923	3.428099	0.342630
11C	-1.243937	0.935767	-0.028101
12C	-1.809484	0.277066	-1.117329
13C	-2.821018	-0.669059	-0.918484
14C	-3.256390	-0.951403	0.384202
15C	-2.677451	-0.284236	1.480591
16C	-1.679882	0.658301	1.276359
17O	-4.228354	-1.851965	0.692861
18C	-4.892655	-2.542183	-0.370282
19C	4.511320	-2.889871	-0.283752
20H	1.088249	-0.135444	-1.537802
21H	2.522861	-2.109918	-1.767311
22H	4.654715	-1.186112	1.681314
23H	3.285394	0.841607	2.080439
24H	-1.467558	0.501970	-2.122696
25H	-3.254317	-1.168824	-1.777151
26H	-3.030794	-0.516022	2.481145
27H	-1.238922	1.175533	2.123362
28H	-5.631831	-3.183855	0.113191
29H	-5.401458	-1.838766	-1.041157
30H	-4.189732	-3.161588	-0.941725
31H	5.372180	-2.588964	-0.889481
32H	4.857742	-3.278896	0.675612
33H	3.953653	-3.672092	-0.802478

6c-Me-003

1C	-2.000429	-0.181728	0.779672
2C	-2.868895	-1.221139	0.983256
3N	-3.743948	-1.640703	0.027815
4C	-3.769175	-0.988805	-1.174141
5C	-2.930036	0.054274	-1.442925
6C	-1.978229	0.522783	-0.473739
7N	-1.188496	1.535290	-0.855029
8S	-0.017152	2.147258	0.133003
9O	-0.476262	2.351505	1.532265
10O	0.525385	3.321110	-0.582839

11C	1.278897	0.900138	0.179901
12C	1.557959	0.205907	1.362848
13C	2.554932	-0.763768	1.373615
14C	3.275436	-1.049630	0.201716
15C	2.992833	-0.350747	-0.984245
16C	1.994132	0.623912	-0.987497
17O	4.227160	-2.015314	0.315396
18C	5.007662	-2.354810	-0.835359
19C	-4.715617	-2.706340	0.313005
20H	-1.348055	0.104742	1.592434
21H	-2.900400	-1.760913	1.923253
22H	-4.490776	-1.353435	-1.896558
23H	-2.974656	0.540066	-2.411678
24H	1.007764	0.435129	2.269698
25H	2.793246	-1.308300	2.282797
26H	3.541052	-0.549190	-1.897855
27H	1.779716	1.170026	-1.901358
28H	5.698481	-3.131889	-0.503021
29H	4.374974	-2.748447	-1.640691
30H	5.578007	-1.490186	-1.196590
31H	-5.649356	-2.272885	0.685426
32H	-4.913446	-3.268626	-0.601905
33H	-4.302091	-3.383029	1.063270

6c-Me-004

1C	3.076456	-0.766568	-0.100860
2C	4.433505	-0.592811	-0.116967
3N	5.013269	0.638874	-0.035889
4C	4.210151	1.739352	0.080536
5C	2.848583	1.636871	0.102772
6C	2.190954	0.362729	0.011479
7N	0.853237	0.363705	0.037118
8S	0.038550	-1.071659	-0.078011
9O	0.315547	-1.956940	1.085289
10O	0.205538	-1.685243	-1.422770
11C	-1.650437	-0.498260	0.059466
12C	-2.233475	-0.362831	1.325583
13C	-3.542360	0.089407	1.430721
14C	-4.274911	0.409239	0.273138
15C	-3.686166	0.268336	-0.993212
16C	-2.368985	-0.187057	-1.093170
17O	-5.547218	0.842735	0.484035
18C	-6.349968	1.200296	-0.645319
19C	6.475856	0.770701	0.018539
20H	2.689419	-1.774920	-0.175247
21H	5.116437	-1.431686	-0.196520
22H	4.720181	2.693455	0.151898
23H	2.246581	2.535291	0.188062
24H	-1.668004	-0.616091	2.216886
25H	-4.019231	0.199140	2.400350
26H	-4.235006	0.502411	-1.897954
27H	-1.908782	-0.303481	-2.069401
28H	-5.896432	2.026328	-1.207072
29H	-6.507492	0.339666	-1.307501
30H	-7.308326	1.522655	-0.233816
31H	6.763588	1.750661	-0.366947
32H	6.825767	0.666734	1.050839
33H	6.932776	-0.002496	-0.602654

6c-001

1C	1.968019	-0.936180	0.854578
2C	2.508482	-2.207383	1.022384
3N	3.394500	-2.789775	0.193787
4C	3.761349	-2.042803	-0.870463
5C	3.285531	-0.769237	-1.139492
6C	2.343954	-0.151257	-0.270599
7N	1.910660	1.102495	-0.622512
8S	0.780760	1.880073	0.228722
9O	0.578733	3.193775	-0.436577
10O	1.023645	1.926239	1.701717
11C	-0.765623	0.964063	0.012646
12C	-1.419560	0.395259	1.101904
13C	-2.603452	-0.329760	0.918008
14C	-3.125005	-0.483247	-0.372985
15C	-2.462240	0.093518	-1.472020
16C	-1.289631	0.811980	-1.279735
17O	-4.266439	-1.171756	-0.667577
18C	-4.973963	-1.811148	0.396641
19H	1.278640	-0.553499	1.596903
20H	2.209246	-2.798450	1.888118
21H	4.481059	-2.502086	-1.547714
22H	3.624223	-0.229561	-2.020142

23H	-1.009763	0.518343	2.099227
24H	-3.096912	-0.763954	1.779996
25H	-2.882491	-0.035949	-2.465471
26H	-0.776827	1.252644	-2.129821
27H	-5.338093	-1.079152	1.129071
28H	-5.825577	-2.308497	-0.072446
29H	-4.346463	-2.558945	0.898076

6c-002

1C	2.106772	-0.780544	0.882786
2C	2.706890	-2.003757	1.164881
3N	3.504063	-2.689846	0.325235
4C	3.712095	-2.104609	-0.874372
5C	3.164187	-0.892777	-1.264436
6C	2.316562	-0.166178	-0.383077
7N	1.802450	1.015593	-0.855590
8S	0.756530	1.889218	0.010769
9O	0.439136	3.093963	-0.799928
10O	1.169253	2.143979	1.423225
11C	-0.777619	0.931672	0.113125
12C	-1.450155	0.606004	-1.066068
13C	-2.626823	-0.145301	-1.025130
14C	-3.129986	-0.575065	0.213481
15C	-2.451419	-0.246099	1.397358
16C	-1.279134	0.503292	1.346481
17O	-4.267378	-1.314465	0.367634
18C	-5.008986	-1.684827	-0.796496
19H	1.501002	-0.301525	1.641803
20H	2.535607	-2.464022	2.138050
21H	4.358713	-2.648166	-1.562938
22H	3.373952	-0.485498	-2.250245
23H	-1.057389	0.936116	-2.023427
24H	-3.134040	-0.386677	-1.952182
25H	-2.854633	-0.587996	2.346546
26H	-0.754170	0.762552	2.260089
27H	-5.865610	-2.254887	-0.430750
28H	-5.365673	-0.800282	-1.339747
29H	-4.410220	-2.316012	-1.465672

6c-003

1C	3.210315	1.784407	-0.128267
2C	4.587578	1.934858	-0.082819
3N	5.467403	0.919286	0.054826
4C	4.915521	-0.305903	0.149548
5C	3.551988	-0.575581	0.116868
6C	2.622389	0.492871	-0.026970
7N	1.254819	0.420098	-0.075423
8S	0.512716	-1.013916	0.058092
9O	0.673619	-1.649535	1.402645
10O	0.771699	-1.935807	-1.091504
11C	-1.203380	-0.491485	-0.069505
12C	-1.797780	-0.354243	-1.329470
13C	-3.121090	0.060654	-1.426061
14C	-3.858988	0.342406	-0.263192
15C	-3.262525	0.199738	0.998003
16C	-1.930741	-0.218592	1.086212
17O	-5.148486	0.743185	-0.464494
18C	-5.950761	1.065704	0.673426
19H	2.565377	2.652544	-0.239858
20H	5.021590	2.931644	-0.159296
21H	5.615609	-1.133991	0.260069
22H	3.213086	-1.602667	0.201675
23H	-1.226760	-0.574895	-2.226005
24H	-3.603082	0.172138	-2.393288
25H	-3.814026	0.405960	1.908129
26H	-1.461928	-0.334529	2.058449
27H	-6.920903	1.368532	0.273922
28H	-6.081858	0.194070	1.327455
29H	-5.515903	1.896415	1.243640

6c-PhNCO2-001

1C	0.501733	-1.649665	1.505270
2C	0.713808	-2.623843	2.478965
3N	1.082040	-3.887436	2.203436
4C	1.254865	-4.202934	0.909616
5C	1.073064	-3.301667	-0.140330
6C	0.686919	-1.995306	0.162151
7N	0.464701	-1.037262	-0.878637
8S	-1.036293	-1.124621	-1.682083

9O	-1.452925	-2.535763	-1.568357
10O	-0.888692	-0.533653	-3.017538
11C	-2.204661	-0.159643	-0.731995
12C	-2.876019	-0.770503	0.336918
13C	-3.760563	-0.022274	1.103239
14C	-3.981458	1.333796	0.804035
15C	-3.311594	1.935777	-0.273192
16C	-2.416089	1.184464	-1.036291
17O	-4.864930	1.977829	1.614512
18C	-5.134476	3.363324	1.378811
19C	1.188728	0.258918	-0.828813
20O	0.576095	1.259205	-1.252212
21N	2.398630	0.076143	-0.331707
22C	3.262434	1.133586	-0.075767
23C	2.994824	2.521503	-0.223219
24C	3.963942	3.476909	0.099087
25C	5.227652	3.103758	0.569743
26C	5.509851	1.737871	0.718494
27C	4.549766	0.778250	0.405207
28H	0.209079	-0.641658	1.781403
29H	0.578985	-2.380567	3.531081
30H	1.556026	-5.227674	0.700739
31H	1.225527	-3.603009	-1.170825
32H	-2.712344	-1.819577	0.559414
33H	-4.293991	-0.471568	1.935866
34H	-3.468755	2.979128	-0.520826
35H	-1.872750	1.642935	-1.853317
36H	-5.576854	3.517207	0.386579
37H	-5.852981	3.656662	2.146639
38H	-4.224027	3.966675	1.480575
39H	2.027133	2.833531	-0.594242
40H	3.723025	4.531940	-0.024843
41H	5.975263	3.855548	0.812775
42H	6.485524	1.419368	1.081945
43H	4.771509	-0.279978	0.525893

6c-PhNCO2-002

1C	0.974633	-3.307596	-0.165116
2C	1.116444	-4.229059	0.873477
3N	0.940994	-3.926287	2.169956
4C	0.610676	-2.655371	2.459808
5C	0.439701	-1.661362	1.498221
6C	0.628642	-1.993515	0.152237
7N	0.454053	-1.013640	-0.875927
8S	-1.023063	-1.043434	-1.725142
9O	-1.526629	-2.422339	-1.570909
10O	-0.798976	-0.516834	-3.077148
11C	-2.163483	0.030002	-0.861902
12C	-2.324760	1.360299	-1.268846
13C	-3.202524	2.180796	-0.574083
14C	-3.909931	1.684636	0.536142
15C	-3.742576	0.350907	0.939640
16C	-2.867264	-0.476485	0.231705
17O	-4.736069	2.573886	1.151845
18C	-5.475258	2.148565	2.300368
19C	1.225488	0.252415	-0.812477
20O	0.658055	1.271267	-1.254740
21N	2.416071	0.028503	-0.286854
22C	3.309787	1.054511	-0.007984
23C	3.088591	2.451871	-0.141549
24C	4.081148	3.371641	0.211682
25C	5.324232	2.952397	0.698476
26C	5.561165	1.576419	0.831894
27C	4.577185	0.652075	0.488202
28H	1.129418	-3.599327	-1.198143
29H	1.386854	-5.259847	0.652690
30H	0.473746	-2.422626	3.514066
31H	0.178091	-0.648044	1.785675
32H	-1.755366	1.739751	-2.108160
33H	-3.347768	3.216115	-0.868705
34H	-4.283759	-0.054386	1.786673
35H	-2.744029	-1.512133	0.531493
36H	-6.163585	1.331946	2.048871
37H	-4.803812	1.835727	3.109862
38H	-6.047883	3.021252	2.620426
39H	2.137898	2.799536	-0.524830
40H	3.875586	4.435367	0.099113
41H	6.090147	3.676808	0.966309
42H	6.519847	1.222288	1.207485
43H	4.763380	-0.414231	0.597457

6c-PhNCO2-003

1C	3.877790	0.871010	0.260486
2C	4.955617	0.683295	-0.605397
3N	4.827497	0.423524	-1.917024
4C	3.576120	0.344631	-2.400794
5C	2.432249	0.504349	-1.620716
6C	2.582395	0.772556	-0.254741
7N	1.432124	0.950374	0.574883
8S	1.083313	-0.274708	1.712183
9O	0.271039	0.317030	2.783196
10O	2.388916	-0.871948	2.059789
11C	0.137952	-1.553547	0.895574
12C	-1.236549	-1.645524	1.102007
13C	-1.969981	-2.642108	0.456316
14C	-1.317468	-3.531170	-0.412469
15C	0.069793	-3.426975	-0.617583
16C	0.799488	-2.443688	0.038862
17O	-1.940547	-4.528742	-1.098665
18C	-3.355931	-4.682844	-0.956200
19C	0.366586	1.850727	0.046297
20O	0.805738	2.908165	-0.450517
21N	-0.840539	1.341875	0.164135
22C	-1.977625	2.092311	-0.110319
23C	-3.165199	1.367733	-0.379603
24C	-4.378709	2.011909	-0.618735
25C	-4.460023	3.410660	-0.588556
26C	-3.297839	4.144187	-0.318870
27C	-2.075487	3.507134	-0.090493
28H	4.037202	1.086840	1.310294
29H	5.973536	0.752273	-0.226754
30H	3.483807	0.135634	-3.464817
31H	1.444182	0.423269	-2.063097
32H	-1.732068	-0.935218	1.753073
33H	-3.037999	-2.705775	0.628439
34H	0.557260	-4.127878	-1.288989
35H	1.872155	-2.371542	-0.109465
36H	-3.888023	-3.782565	-1.288056
37H	-3.625347	-5.522577	-1.599940
38H	-3.626299	-4.916549	0.081182
39H	-3.105624	0.281884	-0.397041
40H	-5.268104	1.418890	-0.826215
41H	-5.405398	3.916553	-0.771263
42H	-3.339753	5.232046	-0.289879
43H	-1.186357	4.095722	0.102821

6c-PhNCO2-004

1C	-1.643523	1.506202	1.140173
2C	-1.919411	2.871494	1.074392
3N	-1.563717	3.662248	0.048010
4C	-0.898698	3.078686	-0.963286
5C	-0.558122	1.727509	-0.991406
6C	-0.937631	0.915677	0.085477
7N	-0.644409	-0.478373	0.073174
8S	0.449145	-1.077343	1.217728
9O	0.366559	-2.542684	1.144984
10O	0.145426	-0.399495	2.492986
11C	2.086916	-0.551785	0.731365
12C	2.851594	-1.353752	-0.114930
13C	4.116788	-0.925053	-0.518862
14C	4.602167	0.317577	-0.080622
15C	3.820150	1.121623	0.767167
16C	2.564503	0.689241	1.175056
17O	5.817566	0.828470	-0.419757
18C	6.663385	0.073884	-1.293259
19C	-0.755899	-1.189046	-1.270529
20O	0.302574	-1.619515	-1.760954
21N	-1.958218	-1.186740	-1.794612
22C	-3.113050	-0.901705	-1.068586
23C	-3.439881	-1.545871	0.147654
24C	-4.634744	-1.264424	0.811034
25C	-5.546379	-0.339706	0.283942
26C	-5.242785	0.293918	-0.927410
27C	-4.048768	0.014180	-1.595873
28H	-1.976202	0.910269	1.980566
29H	-2.468887	3.350897	1.882174
30H	-0.615812	3.726268	-1.790948
31H	-0.013088	1.311311	-1.832771
32H	2.455088	-2.297927	-0.468203
33H	4.703061	-1.558316	-1.174368
34H	4.214414	2.078223	1.097587
35H	1.962669	1.302707	1.837567
36H	6.187311	-0.080299	-2.269601
37H	6.928822	-0.893890	-0.849478
38H	7.565774	0.675497	-1.418978
39H	-2.740547	-2.265580	0.563661
40H	-4.856419	-1.773837	1.747340

41H	-6.476281	-0.122569	0.804577
42H	-5.937950	1.015027	-1.353670
43H	-3.810551	0.513659	-2.532147

6c-PhNCO2-005

1C	0.457565	1.735398	-1.015248
2C	0.672440	3.110067	-0.935760
3N	1.214034	3.723645	0.129939
4C	1.573124	2.939618	1.160422
5C	1.418571	1.553991	1.178981
6C	0.837057	0.930868	0.067784
7N	0.671872	-0.480918	0.005022
8S	-0.397760	-1.221568	1.085630
9O	-0.186679	-0.585595	2.400535
10O	-0.190821	-2.669614	0.944455
11C	-2.060432	-0.813259	0.570633
12C	-2.733140	-1.639970	-0.338740
13C	-4.008941	-1.290386	-0.758324
14C	-4.612635	-0.110153	-0.287174
15C	-3.931935	0.715215	0.620692
16C	-2.651631	0.356481	1.049516
17O	-5.859695	0.145411	-0.769049
18C	-6.526848	1.342655	-0.358685
19C	0.901063	-1.135251	-1.354554
20O	-0.104242	-1.588650	-1.928278
21N	2.132414	-1.061184	-1.798692
22C	3.225307	-0.740807	-0.995630
23C	4.152716	0.219593	-1.454191
24C	5.292078	0.537507	-0.711689
25C	5.548616	-0.101442	0.507697
26C	4.646461	-1.070617	0.966797
27C	3.506179	-1.390947	0.228919
28H	0.007714	1.296412	-1.900187
29H	0.387256	3.751537	-1.767423
30H	2.024350	3.443446	2.012972
31H	1.750750	0.967813	2.026212
32H	-2.249815	-2.532238	-0.717978
33H	-4.553714	-1.914072	-1.461093
34H	-4.380833	1.625338	1.000627
35H	-2.125283	0.985963	1.759603
36H	-6.706611	1.345059	0.723855
37H	-5.954760	2.234005	-0.645517
38H	-7.482867	1.340665	-0.885818
39H	3.951184	0.721642	-2.397785
40H	5.981418	1.292064	-1.086477
41H	6.436437	0.144811	1.085697
42H	4.833636	-1.585585	1.907629
43H	2.814867	-2.146365	0.591763

6c-PhNCO2-006

1C	-2.940041	-1.509701	0.895799
2C	-4.282739	-1.618805	0.536307
3N	-4.763227	-1.280825	-0.671777
4C	-3.878857	-0.807125	-1.565027
5C	-2.519322	-0.644085	-1.303111
6C	-2.033071	-1.004404	-0.042527
7N	-0.658404	-0.822935	0.304977
8S	0.468265	-1.879797	-0.425552
9O	0.034140	-2.022519	-1.831814
10O	0.668275	-3.121185	0.342501
11C	1.968413	-0.915393	-0.400728
12C	2.944601	-1.163243	0.560846
13C	4.117988	-0.407079	0.565500
14C	4.295727	0.603686	-0.392183
15C	3.301666	0.845684	-1.358414
16C	2.139527	0.087016	-1.365040
17O	5.394472	1.401299	-0.468799
18C	6.436581	1.235034	0.498333
19C	-0.321138	-0.226364	1.647982
20O	0.508075	-0.848715	2.335347
21N	-0.971725	0.872928	1.964795
22C	-1.556569	1.719574	1.031086
23C	-2.859731	2.215088	1.258264
24C	-3.458087	3.111509	0.371017
25C	-2.773344	3.554831	-0.768001
26C	-1.471893	3.088643	-0.996781
27C	-0.869950	2.191578	-0.114068
28H	-2.607125	-1.798275	1.887499
29H	-5.006817	-2.002170	1.252586
30H	-4.279769	-0.528819	-2.537687
31H	-1.854140	-0.236565	-2.053469
32H	2.780580	-1.927982	1.310422

33H	4.870002	-0.605138	1.319975
34H	3.459998	1.631437	-2.091124
35H	1.370879	0.269067	-2.109325
36H	6.065442	1.415459	1.514699
37H	6.880411	0.233689	0.433608
38H	7.190498	1.983472	0.247047
39H	-3.398948	1.865120	2.135507
40H	-4.469879	3.461757	0.567446
41H	-3.241152	4.252654	-1.458556
42H	-0.917991	3.429912	-1.870040
43H	0.140990	1.839253	-0.299113

6c-PhNCO2-007

1C	-3.016500	-1.494763	0.685446
2C	-4.337300	-1.525787	0.239941
3N	-4.729834	-1.086927	-0.967465
4C	-3.775560	-0.588185	-1.770437
5C	-2.429915	-0.496947	-1.416970
6C	-2.036069	-0.961151	-0.158246
7N	-0.680136	-0.856332	0.283950
8S	0.449799	-1.906952	-0.451151
9O	0.101975	-1.926027	-1.888496
10O	0.549205	-3.210017	0.229473
11C	1.986343	-1.021545	-0.260193
12C	2.236808	0.070932	-1.090466
13C	3.439172	0.769945	-0.973657
14C	4.387786	0.356206	-0.024136
15C	4.125718	-0.751332	0.801842
16C	2.924165	-1.437399	0.690608
17O	5.589725	0.962359	0.169666
18C	5.915905	2.113584	-0.614649
19C	-0.408653	-0.362115	1.681765
20O	0.362867	-1.051861	2.371443
21N	-1.052685	0.729976	2.037079
22C	-1.551797	1.658800	1.133158
23C	-2.853089	2.179449	1.310529
24C	-3.366979	3.151111	0.450026
25C	-2.597272	3.647516	-0.610181
26C	-1.295508	3.159093	-0.785055
27C	-0.777770	2.187385	0.071425
28H	-2.756619	-1.862685	1.672665
29H	-5.117325	-1.928644	0.883065
30H	-4.104946	-0.228759	-2.743322
31H	-1.705623	-0.065488	-2.095765
32H	1.502106	0.379820	-1.827447
33H	3.623196	1.620013	-1.620128
34H	4.871689	-1.049233	1.532630
35H	2.702469	-2.278257	1.336898
36H	5.948238	1.869383	-1.683853
37H	5.201446	2.927348	-0.438121
38H	6.908770	2.423553	-0.282714
39H	-3.458507	1.788743	2.125161
40H	-4.379882	3.518725	0.604486
41H	-2.999748	4.403809	-1.280023
42H	-0.675991	3.541334	-1.595106
43H	0.235447	1.820150	-0.066155

6c-PhNCO2-008

1C	-0.261736	2.140841	1.179103
2C	-1.084023	3.254029	1.360392
3N	-1.961000	3.689778	0.441493
4C	-2.028728	3.006675	-0.713150
5C	-1.253284	1.880719	-0.991488
6C	-0.354781	1.434200	-0.022405
7N	0.448814	0.265193	-0.270315
8S	-0.034470	-1.146077	0.584203
9O	0.216550	-1.039786	2.036658
10O	0.461322	-2.322426	-0.148628
11C	-1.811102	-1.074401	0.349377
12C	-2.636256	-0.593007	1.372423
13C	-4.007616	-0.520061	1.166567
14C	-4.560097	-0.926127	-0.061187
15C	-3.727292	-1.414046	-1.081801
16C	-2.349852	-1.485667	-0.869476
17O	-5.911178	-0.810894	-0.163948
18C	-6.547601	-1.188412	-1.389136
19C	1.891981	0.537904	-0.529521
20O	2.082617	1.534533	-1.259673
21N	2.684266	-0.329843	0.059313
22C	4.061170	-0.331231	-0.130261
23C	4.831354	0.605892	-0.869244
24C	6.221034	0.475980	-0.961519

25C	6.897956	-0.573857	-0.331078
26C	6.152193	-1.506932	0.404335
27C	4.767810	-1.387005	0.501488
28H	0.429265	1.823032	1.953206
29H	-1.037543	3.821226	2.287868
30H	-2.740080	3.375529	-1.449412
31H	-1.343911	1.355141	-1.936275
32H	-2.203317	-0.272511	2.314103
33H	-4.669126	-0.146597	1.942743
34H	-4.133736	-1.737646	-2.032861
35H	-1.699606	-1.858152	-1.655068
36H	-7.610881	-0.992082	-1.239055
37H	-6.179061	-0.585994	-2.228724
38H	-6.398327	-2.254792	-1.599998
39H	4.327721	1.427858	-1.361986
40H	6.781436	1.211873	-1.536694
41H	7.979278	-0.664032	-0.408626
42H	6.653995	-2.333798	0.904257
43H	4.189590	-2.112094	1.070060

6c-PhNCO-001

1C	-0.536577	-0.896021	0.916869
2C	0.699459	-0.340965	1.130838
3N	1.766794	-0.601183	0.329898
4C	1.604917	-1.461355	-0.720431
5C	0.399959	-2.048329	-0.987724
6C	-0.759489	-1.784503	-0.186114
7N	-1.904080	-2.384137	-0.566086
8S	-3.312684	-2.120135	0.233289
9O	-4.327736	-2.949900	-0.455296
10O	-3.200098	-2.283515	1.708260
11C	-3.741397	-0.395067	-0.065383
12C	-3.917202	0.483267	1.000771
13C	-4.240402	1.823489	0.762519
14C	-4.379706	2.276082	-0.556801
15C	-4.202040	1.383078	-1.630253
16C	-3.885649	0.053849	-1.386674
17O	-4.682488	3.558400	-0.902373
18C	-4.852864	4.527608	0.135677
19C	3.094328	0.070031	0.638304
20O	3.079202	0.788540	1.655339
21N	4.000023	-0.248738	-0.251989
22C	5.304693	0.240626	-0.197616
23C	5.851430	1.109499	0.780377
24C	7.186703	1.518559	0.703747
25C	8.020481	1.087462	-0.333271
26C	7.493902	0.227956	-1.307439
27C	6.165082	-0.185487	-1.239031
28H	-1.330352	-0.657118	1.611139
29H	0.900603	0.335357	1.951752
30H	2.494125	-1.631877	-1.311343
31H	0.311230	-2.722344	-1.833389
32H	-3.802790	0.126311	2.019445
33H	-4.374240	2.492829	1.604312
34H	-4.314334	1.753957	-2.645037
35H	-3.743831	-0.632783	-2.216140
36H	-5.060845	5.470664	-0.373614
37H	-5.699032	4.269520	0.785246
38H	-3.939765	4.630212	0.735529
39H	5.223321	1.455196	1.591412
40H	7.577495	2.185607	1.470410
41H	9.057355	1.411848	-0.382673
42H	8.122609	-0.121471	-2.124373
43H	5.757421	-0.852205	-1.995685

6c-PhNCO-002

1C	0.327727	-1.090710	-0.644395
2C	-0.992544	-0.755284	-0.489546
3N	-1.780791	-1.319873	0.467247
4C	-1.237597	-2.260873	1.292864
5C	0.072160	-2.640557	1.190856
6C	0.945453	-2.060376	0.214996
7N	2.226086	-2.477138	0.229956
8S	3.348637	-1.836476	-0.779341
9O	4.606794	-2.564603	-0.495179
10O	2.915183	-1.778092	-2.201913
11C	3.584552	-0.133522	-0.237221
12C	3.417193	0.922514	-1.129205
13C	3.612869	2.241241	-0.703276
14C	3.973321	2.490062	0.628313
15C	4.135504	1.418392	1.526355
16C	3.945908	0.112856	1.095763

17O	4.187448	3.729767	1.150528
18C	4.078397	4.867758	0.291114
19C	-3.237658	-0.933774	0.659503
20O	-3.796001	-1.511890	1.610595
21N	-3.616333	-0.057261	-0.236478
22C	-4.902803	0.481063	-0.251432
23C	-5.912741	0.301962	0.727489
24C	-7.155794	0.928580	0.592435
25C	-7.444355	1.741155	-0.508923
26C	-6.456716	1.924929	-1.486634
27C	-5.213291	1.309067	-1.357856
28H	0.885367	-0.615778	-1.440249
29H	-1.489217	-0.025779	-1.114805
30H	-1.917970	-2.672369	2.026821
31H	0.466504	-3.390456	1.868557
32H	3.135579	0.721345	-2.157958
33H	3.479827	3.050615	-1.411860
34H	4.413482	1.632986	2.554247
35H	4.072900	-0.712757	1.789881
36H	4.303945	5.732160	0.918821
37H	4.803762	4.813725	-0.530668
38H	3.062706	4.966090	-0.112132
39H	-5.714098	-0.327581	1.585449
40H	-7.909673	0.773538	1.362516
41H	-8.415360	2.221511	-0.604446
42H	-6.656689	2.552065	-2.353455
43H	-4.446898	1.455849	-2.115775

6c-PhNCO-003

1C	0.543676	-1.017271	0.862888
2C	-0.693873	-0.485545	1.123424
3N	-1.741441	-0.617565	0.266774
4C	-1.556317	-1.313900	-0.895211
5C	-0.346550	-1.861657	-1.217865
6C	0.790421	-1.734734	-0.353643
7N	1.942225	-2.280360	-0.789352
8S	3.331326	-2.132908	0.071125
9O	3.195716	-2.535385	1.497436
10O	4.372119	-2.827922	-0.721256
11C	3.734128	-0.374453	0.067458
12C	3.996361	0.295380	1.267454
13C	4.305776	1.651347	1.246186
14C	4.347454	2.347092	0.026572
15C	4.084801	1.671809	-1.176674
16C	3.781095	0.309474	-1.148487
17O	4.648446	3.672786	0.113345
18C	4.656646	4.458267	-1.081942
19C	-3.072903	0.015480	0.633426
20O	-3.059216	0.650781	1.704319
21N	-3.981977	-0.245372	-0.272213
22C	-5.289517	0.229865	-0.175839
23C	-5.824833	1.057507	0.843453
24C	-7.163397	1.461032	0.803884
25C	-8.011994	1.062943	-0.234374
26C	-7.496955	0.244026	-1.248770
27C	-6.164373	-0.161871	-1.218649
28H	1.320427	-0.891653	1.605031
29H	-0.911594	0.068598	2.027554
30H	-2.431066	-1.388523	-1.526254
31H	-0.237326	-2.401001	-2.153035
32H	3.950410	-0.242740	2.208919
33H	4.509249	2.191635	2.166354
34H	4.112294	2.188542	-2.129044
35H	3.573258	-0.213317	-2.077672
36H	4.897424	5.474879	-0.764738
37H	5.422088	4.105257	-1.784662
38H	3.673020	4.450102	-1.568024
39H	-5.185617	1.374757	1.657402
40H	-7.545381	2.096648	1.601074
41H	-9.051617	1.381695	-0.253951
42H	-8.137456	-0.079319	-2.067248
43H	-5.765386	-0.796782	-2.006671

6c-PhNCO-004

1C	0.351779	-1.131068	0.664055
2C	-0.970492	-0.806097	0.506363
3N	-1.738919	-1.337445	-0.484767
4C	-1.172816	-2.235341	-1.342613
5C	0.141053	-2.601079	-1.240690
6C	0.995422	-2.050597	-0.230884
7N	2.282714	-2.445369	-0.249435
8S	3.392107	-1.811282	0.780462

9O	2.947875	-1.778736	2.200467
10O	4.659086	-2.521586	0.492506
11C	3.609845	-0.099622	0.261503
12C	3.268836	0.949383	1.111556
13C	3.412008	2.275168	0.686842
14C	3.895827	2.538327	-0.602031
15C	4.240211	1.473733	-1.456175
16C	4.098024	0.161661	-1.027715
17O	4.070114	3.785797	-1.120221
18C	3.720607	4.918461	-0.320006
19C	-3.197633	-0.959861	-0.678305
20O	-3.745527	-1.522251	-1.644700
21N	-3.587987	-0.103851	0.232514
22C	-4.877923	0.425735	0.251548
23C	-5.885584	0.251205	-0.730627
24C	-7.132878	0.868114	-0.589810
25C	-7.428027	1.666038	0.520497
26C	-6.442756	1.845065	1.501458
27C	-5.195252	1.238764	1.367159
28H	0.890934	-0.688205	1.490062
29H	-1.484857	-0.111364	1.156365
30H	-1.838205	-2.624203	-2.102284
31H	0.553958	-3.314224	-1.946474
32H	2.895954	0.738280	2.108676
33H	3.141893	3.078803	1.362118
34H	4.614197	1.699437	-2.450708
35H	4.360139	-0.658443	-1.689444
36H	2.654507	4.906218	-0.060655
37H	4.326642	4.962669	0.593773
38H	3.933548	5.792180	-0.939067
39H	-5.681400	-0.366813	-1.595661
40H	-7.884892	0.717166	-1.362520
41H	-8.402177	2.139117	0.620237
42H	-6.647738	2.461005	2.375123
43H	-4.430763	1.381828	2.127708

6c-PhNCO-005

1C	0.271645	-1.111525	-0.549419
2C	-1.038026	-0.736841	-0.395984
3N	-1.789661	-1.132155	0.668711
4C	-1.218415	-1.935643	1.612264
5C	0.081182	-2.350478	1.515206
6C	0.915275	-1.950474	0.421237
7N	2.188157	-2.390528	0.440716
8S	3.269717	-1.938027	-0.708011
9O	4.525249	-2.652445	-0.381642
10O	2.761974	-2.076498	-2.100007
11C	3.569438	-0.180976	-0.436048
12C	3.322539	0.750067	-1.450634
13C	3.554816	2.102010	-1.217726
14C	4.029748	2.531195	0.032431
15C	4.274951	1.594229	1.049989
16C	4.044562	0.239139	0.807833
17O	4.220763	3.873689	0.163850
18C	4.710219	4.381478	1.408336
19C	-3.237513	-0.709031	0.846791
20O	-3.738128	-1.051029	1.934528
21N	-3.674726	-0.070115	-0.209087
22C	-4.966575	0.450363	-0.280871
23C	-5.910077	0.534487	0.773952
24C	-7.165961	1.112372	0.562408
25C	-7.532632	1.614704	-0.690549
26C	-6.611517	1.534661	-1.744102
27C	-5.355063	0.967179	-1.540863
28H	0.798878	-0.771769	-1.430379
29H	-1.555216	-0.109518	-1.109262
30H	-1.867757	-2.211149	2.433030
31H	0.497135	-2.989851	2.286848
32H	2.954430	0.414421	-2.414750
33H	3.371249	2.840949	-1.992428
34H	4.639780	1.903626	2.022514
35H	4.232897	-0.485784	1.594402
36H	4.781030	5.462892	1.276204
37H	4.016393	4.159462	2.228896
38H	5.703314	3.975619	1.639474
39H	-5.650065	0.145177	1.750103
40H	-7.867956	1.165592	1.393001
41H	-8.513473	2.058533	-0.844646
42H	-6.873734	1.917763	-2.728581
43H	-4.639216	0.910825	-2.357976

6c-PhNCO-006

1C	-0.462806	-0.964461	0.848664
2C	0.773414	-0.428755	1.108007
3N	1.812628	-0.531805	0.237280
4C	1.618680	-1.197694	-0.941085
5C	0.410292	-1.748502	-1.262818
6C	-0.715578	-1.660211	-0.379262
7N	-1.861194	-2.222047	-0.809508
8S	-3.236997	-2.154807	0.081524
9O	-4.251836	-2.907154	-0.691427
10O	-3.046443	-2.549808	1.503430
11C	-3.749936	-0.425945	0.089292
12C	-3.914439	0.260625	1.297187
13C	-4.319493	1.591331	1.284286
14C	-4.559494	2.244345	0.064136
15C	-4.389928	1.553710	-1.147372
16C	-3.987441	0.217291	-1.126990
17O	-4.952318	3.545563	0.157121
18C	-5.222865	4.270374	-1.045982
19C	3.149377	0.085861	0.612560
20O	3.151225	0.672432	1.710949
21N	4.042488	-0.128089	-0.320526
22C	5.361370	0.309162	-0.206660
23C	5.965291	0.912507	0.925276
24C	7.314544	1.280042	0.902074
25C	8.105503	1.069421	-0.232267
26C	7.521507	0.475601	-1.359785
27C	6.179329	0.101457	-1.344188
28H	-1.231960	-0.863379	1.602267
29H	0.997267	0.104366	2.023249
30H	2.486395	-1.249045	-1.583992
31H	0.294708	-2.266440	-2.209270
32H	-3.729071	-0.247818	2.237902
33H	-4.455138	2.142100	2.210720
34H	-4.567593	2.039123	-2.099998
35H	-3.857739	-0.318437	-2.062973
36H	-5.527881	5.268529	-0.725280
37H	-4.325506	4.347599	-1.672757
38H	-6.037575	3.805052	-1.614784
39H	5.370705	1.087703	1.812788
40H	7.750544	1.738790	1.788017
41H	9.153334	1.360647	-0.239388
42H	8.116168	0.300634	-2.254500
43H	5.728843	-0.364129	-2.218130

6c-PhNCO-007

1C	0.614460	-0.697929	0.039430
2C	1.966561	-0.478657	0.045487
3N	2.502605	0.773153	-0.029149
4C	1.659225	1.842939	-0.115822
5C	0.300472	1.692963	-0.130672
6C	-0.309233	0.398354	-0.051721
7N	-1.652531	0.352045	-0.068810
8S	-2.424736	-1.097582	0.035196
9O	-2.159835	-1.967472	-1.144434
10O	-2.237653	-1.737498	1.366787
11C	-4.129442	-0.553065	-0.068098
12C	-4.736815	-0.412236	-1.321612
13C	-6.053707	0.023626	-1.400223
14C	-6.769847	0.322593	-0.227520
15C	-6.157942	0.175814	1.026625
16C	-4.832983	-0.263308	1.098881
17O	-8.052656	0.743500	-0.412056
18C	-8.836726	1.082077	0.735132
19C	3.999102	1.022633	-0.016743
20O	4.315690	2.227530	-0.041841
21N	4.666081	-0.104054	0.017373
22C	6.059680	-0.146176	0.030784
23C	6.637584	-1.439290	0.061637
24C	8.018453	-1.624996	0.075643
25C	8.883235	-0.521723	0.059597
26C	8.331894	0.763375	0.029341
27C	6.947301	0.959767	0.014490
28H	0.261584	-1.720072	0.103108
29H	2.690884	-1.279254	0.109568
30H	2.148501	2.806517	-0.170437
31H	-0.333636	2.570582	-0.202615
32H	-4.182154	-0.646817	-2.224725
33H	-6.548005	0.138182	-2.360630
34H	-6.693403	0.395064	1.943115
35H	-4.353117	-0.381704	2.065395
36H	-9.806351	1.398547	0.345534
37H	-8.973027	0.213986	1.392457
38H	-8.381635	1.907514	1.296764
39H	5.967999	-2.296322	0.073681
40H	8.423136	-2.635058	0.098642

41H	9.961597	-0.662385	0.070296
42H	8.987060	1.632832	0.016045
43H	6.541254	1.962628	-0.010694

6c-PhNCO-008

1C	-0.404394	1.528972	-0.077541
2C	-1.773875	1.587279	-0.085546
3N	-2.553912	0.472539	-0.039986
4C	-1.946914	-0.751862	0.011931
5C	-0.586814	-0.879847	0.019797
6C	0.275023	0.266185	-0.023309
7N	1.599057	0.034879	-0.007156
8S	2.651888	1.298390	-0.057645
9O	2.630253	1.987611	-1.378029
10O	2.540397	2.182354	1.135568
11C	4.207198	0.416320	0.069579
12C	4.773198	-0.149883	-1.071542
13C	5.978149	-0.850974	-0.981043
14C	6.612165	-0.977773	0.265216
15C	6.036983	-0.399185	1.409713
16C	4.836646	0.295065	1.313355
17O	7.787323	-1.637591	0.466614
18C	8.430926	-2.254995	-0.651434
19C	-4.062752	0.631443	-0.046496
20O	-4.454142	1.811723	-0.114826
21N	-4.658520	-0.533058	0.027705
22C	-6.046300	-0.663834	0.028284
23C	-7.004099	0.373575	-0.105287
24C	-8.372757	0.085100	-0.097586
25C	-8.838959	-1.226048	0.044145
26C	-7.904032	-2.261824	0.179583
27C	-6.538665	-1.984740	0.170262
28H	0.148499	2.459763	-0.113062
29H	-2.317631	2.522182	-0.127573
30H	-2.624994	-1.593094	0.045816
31H	-0.144215	-1.869847	0.061111
32H	4.279911	-0.045094	-2.033124
33H	6.406289	-1.285090	-1.877130
34H	6.546329	-0.503954	2.363375
35H	4.389710	0.745403	2.193962
36H	9.336933	-2.715391	-0.252281
37H	7.794635	-3.029371	-1.097960
38H	8.703517	-1.511970	-1.411398
39H	-6.665962	1.396468	-0.212380
40H	-9.083473	0.903150	-0.203363
41H	-9.905662	-1.438033	0.049931
42H	-8.241045	-3.290696	0.291981
43H	-5.814423	-2.789806	0.273378

8a-001

1C	1.614074	0.521710	0.816528
2C	2.885662	1.030422	0.881423
3N	3.869484	0.562321	0.071794
4C	3.628673	-0.426230	-0.831499
5C	2.378490	-0.970584	-0.942479
6C	1.299081	-0.516496	-0.118971
7N	0.109174	-1.125770	-0.335674
8S	-1.241439	-0.777777	0.469756
9O	-1.081752	-0.291663	1.856667
10O	-2.230418	-1.829880	0.202651
11C	-1.920868	0.729324	-0.453772
12F	-3.067644	1.144251	0.109274
13F	-2.157215	0.441232	-1.743356
14F	-1.030132	1.742686	-0.403791
15H	0.861950	0.917856	1.484318
16H	3.165701	1.819115	1.569932
17H	4.801448	0.959747	0.139237
18H	4.469904	-0.741014	-1.437805
19H	2.195018	-1.757175	-1.665678

8a-002

1C	-2.070533	-0.982683	0.023102
2C	-3.435950	-1.084489	0.033864
3N	-4.219263	0.025341	0.015850
4C	-3.674124	1.274251	-0.011892
5C	-2.317535	1.438695	-0.023365
6C	-1.439030	0.305843	-0.008790
7N	-0.120216	0.562789	-0.026308
8S	0.967301	-0.634996	-0.028151

9O	1.064279	-1.371880	-1.304759
10O	1.017975	-1.427537	1.217711
11C	2.493640	0.463641	0.022663
12F	3.581414	-0.326647	0.003610
13F	2.524582	1.202786	1.141759
14F	2.542503	1.281414	-1.039333
15H	-1.486251	-1.895144	0.041410
16H	-3.952358	-2.037014	0.056996
17H	-5.228951	-0.078096	0.023693
18H	-4.372671	2.102782	-0.023936
19H	-1.893571	2.436314	-0.045974

8a-003

1C	-2.149427	0.572097	-1.193011
2C	-3.406161	0.877088	-0.672047
3N	-3.889370	0.356136	0.465995
4C	-3.103736	-0.517573	1.114006
5C	-1.839266	-0.914161	0.676710
6C	-1.349450	-0.345169	-0.502848
7N	-0.087025	-0.697223	-1.060804
8S	1.339124	-0.859035	-0.224336
9O	2.360648	-1.196882	-1.210271
10O	1.123108	-1.625303	0.996284
11C	1.745216	0.900779	0.347542
12F	1.768377	1.715574	-0.716382
13F	2.941034	0.912706	0.941584
14F	0.813200	1.327675	1.207024
15H	-1.805417	1.040671	-2.110848
16H	-4.048787	1.583453	-1.192840
17H	-3.507375	-0.938674	2.031937
18H	-1.267655	-1.641796	1.239107
19H	0.081411	-0.375975	-2.014573

8a-004

1C	2.352573	-0.690942	-1.129026
2C	3.606608	-0.115524	-0.938587
3N	3.946821	0.599422	0.145030
4C	3.003779	0.745020	1.087553
5C	1.719027	0.206090	1.012628
6C	1.383681	-0.527547	-0.130518
7N	0.126083	-1.149062	-0.336385
8S	-1.325631	-0.808684	0.382650
9O	-1.149246	-0.575627	1.810789
10O	-2.286108	-1.764712	-0.158402
11C	-1.814744	0.867402	-0.349020
12F	-0.975633	1.816064	0.082440
13F	-3.060386	1.166094	0.029584
14F	-1.757750	0.802096	-1.685328
15H	2.137529	-1.251594	-2.034694
16H	4.372579	-0.232570	-1.702056
17H	3.285174	1.322978	1.965017
18H	1.020582	0.359349	1.825112
19H	0.005115	-1.654320	-1.213836

8a-005

1C	1.752328	0.131450	1.052503
2C	3.033789	-0.389173	1.238238
3N	3.939522	-0.547514	0.261494
4C	3.563764	-0.178429	-0.972870
5C	2.307668	0.339126	-1.280756
6C	1.379658	0.500404	-0.244166
7N	0.122440	1.072042	-0.574362
8S	-1.328926	0.869696	0.199146
9O	-2.299155	1.675554	-0.534991
10O	-1.150597	0.954059	1.643239
11C	-1.803329	-0.932849	-0.146512
12F	-0.968786	-1.757848	0.495274
13F	-1.728899	-1.166814	-1.463557
14F	-3.053173	-1.145802	0.273289
15H	1.083439	0.242747	1.896172
16H	3.345260	-0.687640	2.236666
17H	4.300428	-0.307024	-1.762783
18H	2.060527	0.611295	-2.303388
19H	-0.008103	1.327898	-1.552585

10h-Me-001

1C	2.525835	-1.720893	0.569376
2C	3.256695	-2.876292	0.622068
3N	3.328416	-3.740032	-0.431574
4C	2.637175	-3.445400	-1.574711
5C	1.890859	-2.307255	-1.692148
6C	1.789198	-1.355904	-0.615706
7N	1.045731	-0.266168	-0.790441
8P	0.892603	0.931231	0.352036
9C	2.504260	1.795780	0.470275
10O	0.389387	0.564187	1.739915
11C	-0.252821	2.101014	-0.458471
12C	-0.317372	2.239872	-1.853495
13C	-1.217159	3.139202	-2.430783
14C	-2.058523	3.909848	-1.619514
15C	-1.992952	3.781905	-0.227912
16C	-1.091925	2.882172	0.349951
17C	2.965892	2.214527	1.726206
18C	4.189814	2.881973	1.839667
19C	4.956163	3.138113	0.698193
20C	4.499766	2.721627	-0.558340
21C	3.278459	2.053581	-0.672506
22C	4.061884	-5.008800	-0.321648
23H	2.505333	-1.083727	1.445728
24H	3.817351	-3.160296	1.506007
25H	2.724057	-4.169775	-2.377456
26H	1.365545	-2.106881	-2.620501
27H	0.320392	1.628985	-2.485205
28H	-1.263853	3.237318	-3.512716
29H	-2.758749	4.609017	-2.070171
30H	-2.641533	4.381204	0.406603
31H	-1.046131	2.774366	1.430156
32H	2.367242	2.008752	2.609448
33H	4.542483	3.202640	2.816991
34H	5.906419	3.659155	0.786207
35H	5.094130	2.918208	-1.447326
36H	2.929345	1.728921	-1.649527
37H	4.579848	-5.211804	-1.261928
38H	4.798950	-4.931085	0.479275
39H	3.368632	-5.826840	-0.100645
40P	-3.297577	-1.090043	0.368962
41C	-2.559687	-0.450965	-1.169799
42C	-2.925210	-1.247197	-2.428326
43C	-2.681409	-2.775819	0.708226
44C	-2.851159	0.022339	1.740975
45C	-5.118448	-1.170820	0.209179
46C	-3.303412	-0.477707	3.119818
47C	-5.769636	0.181915	-0.112472
48C	-1.151813	-2.862330	0.802533
49H	-1.475282	-0.446015	-1.016393
50H	-2.871086	0.595553	-1.259065
51H	-2.426534	-0.794071	-3.292251
52H	-2.591661	-2.288896	-2.362428
53H	-4.003289	-1.241378	-2.623600
54H	-3.068665	-3.425946	-0.085021
55H	-3.156263	-3.096895	1.642940
56H	-3.302446	0.992984	1.505829
57H	-1.762716	0.157884	1.711137
58H	-5.499276	-1.577009	1.154006
59H	-5.340973	-1.909911	-0.569270
60H	-3.047093	0.273783	3.874398
61H	-4.385312	-0.646131	3.167744
62H	-2.796114	-1.408456	3.395977
63H	-6.854947	0.054928	-0.187976
64H	-5.573264	0.922508	0.670548
65H	-5.412076	0.587350	-1.065353
66H	-0.862687	-3.879921	1.087654
67H	-0.678505	-2.632797	-0.156001
68H	-0.747632	-2.170575	1.548179

10h-Me-002

1C	-1.775275	2.379713	1.644914
2C	-2.476148	3.543201	1.498189
3N	-3.135091	3.847015	0.338534
4C	-3.092222	2.957783	-0.695501
5C	-2.407188	1.776486	-0.613354
6C	-1.702018	1.403946	0.588382
7N	-1.005209	0.289064	0.792060
8P	-0.889312	-0.939754	-0.319780
9C	0.218443	-2.131283	0.511040
10O	-0.379916	-0.621347	-1.717549
11C	-2.524728	-1.760771	-0.413739
12C	-3.290797	-1.988381	0.740761
13C	-4.528872	-2.628144	0.647969
14C	-5.009922	-3.046416	-0.598825
15C	-4.251611	-2.820151	-1.751862

16C	-3.010923	-2.180600	-1.659862
17C	0.410921	-2.147536	1.900831
18C	1.263697	-3.090290	2.483025
19C	1.926934	-4.026905	1.682594
20C	1.734665	-4.019414	0.296300
21C	0.884841	-3.075510	-0.286024
22C	-3.944973	5.070862	0.251592
23H	-1.262868	2.179305	2.580442
24H	-2.548349	4.282618	2.288823
25H	-3.631242	3.247623	-1.590902
26H	-2.392390	1.126855	-1.480662
27H	-2.921122	-1.663709	1.710266
28H	-5.116735	-2.802141	1.545938
29H	-5.972927	-3.546189	-0.670021
30H	-4.623329	-3.142670	-2.721471
31H	-2.417585	-1.998749	-2.551895
32H	-0.094871	-1.413778	2.520782
33H	1.410282	-3.093321	3.560524
34H	2.587974	-4.761066	2.136827
35H	2.246354	-4.746237	-0.329958
36H	0.746474	-3.060831	-1.363953
37H	-4.138416	5.299876	-0.797477
38H	-4.896438	4.928849	0.774083
39H	-3.399287	5.902089	0.704338
40P	3.253200	1.049534	-0.412128
41C	5.053323	1.261405	-0.177469
42C	5.747656	0.046763	0.452817
43C	2.437525	0.825500	1.200595
44C	2.629008	2.553146	-1.242260
45C	2.921688	-0.413091	-1.445134
46C	1.098373	2.635309	-1.327646
47C	3.643962	-0.401177	-2.798758
48C	2.634073	1.998638	2.169675
49H	5.188675	2.157604	0.439674
50H	5.475296	1.488078	-1.164051
51H	6.817663	0.254488	0.561805
52H	5.347961	-0.177875	1.447757
53H	5.642354	-0.848904	-0.169175
54H	2.826030	-0.108095	1.623194
55H	1.372508	0.662230	0.999118
56H	3.081845	2.554741	-2.241050
57H	3.044224	3.412943	-0.703153
58H	1.834062	-0.462120	-1.579110
59H	3.208334	-1.287791	-0.850704
60H	0.816806	3.510850	-1.923456
61H	0.660804	1.747374	-1.794842
62H	0.649561	2.747715	-0.336322
63H	3.378206	-1.307848	-3.353484
64H	3.346671	0.458114	-3.410403
65H	4.733839	-0.384888	-2.686483
66H	2.080034	1.798004	3.093267
67H	3.687062	2.142906	2.436002
68H	2.253048	2.937002	1.751076

10h-Me-003

1C	-2.423025	-1.779013	-0.595863
2C	-3.097352	-2.966668	-0.675111
3N	-3.115510	-3.862345	0.354119
4C	-2.427471	-3.566718	1.498904
5C	-1.736693	-2.396836	1.642402
6C	-1.692563	-1.412291	0.592400
7N	-0.999869	-0.293885	0.790660
8P	-0.900713	0.937255	-0.320435
9C	-2.542520	1.746092	-0.408194
10O	-0.394082	0.623096	-1.720159
11C	0.200681	2.137387	0.506425
12C	0.400013	2.153609	1.895228
13C	1.247296	3.103234	2.474344
14C	1.898086	4.046696	1.671771
15C	1.698920	4.039189	0.286437
16C	0.854566	3.088531	-0.292810
17C	-3.035265	2.164587	-1.652218
18C	-4.280807	2.795281	-1.739540
19C	-5.037543	3.013756	-0.583949
20C	-4.550000	2.596654	0.660698
21C	-3.306966	1.965858	0.748830
22C	-3.794988	-5.158524	0.218433
23H	-2.440420	-1.117608	-1.454143
24H	-3.651247	-3.253848	-1.562245
25H	-2.470410	-4.316839	2.281431
26H	-1.211254	-2.197465	2.570893
27H	-0.096224	1.414712	2.516817
28H	1.399206	3.106301	3.551108
29H	2.554791	4.786215	2.123595
30H	2.200957	4.771314	-0.341448

31H	0.710894	3.074067	-1.370044
32H	-2.443191	1.988629	-2.546283
33H	-4.657563	3.116932	-2.707492
34H	-6.004424	3.506493	-0.651504
35H	-5.136682	2.764530	1.560597
36H	-2.932156	1.642188	1.716710
37H	-4.316822	-5.395776	1.148632
38H	-4.524220	-5.098837	-0.591047
39H	-3.066754	-5.944905	-0.004665
40P	3.254027	-1.027321	-0.414706
41C	2.438448	-0.814384	1.199709
42C	2.643978	-1.989666	2.164419
43C	2.638529	-2.531778	-1.249989
44C	2.911408	0.436849	-1.442098
45C	5.055612	-1.228223	-0.181828
46C	3.635835	0.437130	-2.794596
47C	5.740534	-0.014055	0.459294
48C	1.108393	-2.623301	-1.333737
49H	1.372100	-0.656702	1.000116
50H	2.821963	0.120017	1.625111
51H	2.090251	-1.795800	3.089636
52H	2.268409	-2.929102	1.743317
53H	3.698315	-2.127987	2.428598
54H	3.059714	-3.390871	-0.714390
55H	3.090068	-2.527027	-2.249317
56H	3.188835	1.311832	-0.843688
57H	1.823567	0.476016	-1.577655
58H	5.479398	-1.442900	-1.170263
59H	5.197597	-2.128902	0.427194
60H	3.360239	1.342133	-3.347217
61H	4.725626	0.433428	-2.680635
62H	3.349698	-0.423914	-3.409122
63H	6.812685	-0.213162	0.563154
64H	5.625262	0.887047	-0.153024
65H	5.341674	0.196500	1.457598
66H	0.831693	-3.498411	-1.932473
67H	0.662037	-2.742302	-0.342046
68H	0.664338	-1.736531	-1.797017

10h-Me-004

1C	0.653317	2.545530	-1.985906
2C	0.730655	3.905662	-1.886595
3N	1.073149	4.526259	-0.716059
4C	1.345877	3.758953	0.379197
5C	1.279869	2.392807	0.347606
6C	0.935549	1.686857	-0.863692
7N	0.840445	0.370472	-1.022377
8P	1.140030	-0.717702	0.197848
9C	0.848440	-2.331288	-0.604609
10O	0.333259	-0.600781	1.483312
11C	2.932693	-0.658944	0.579908
12C	3.893870	-0.508300	-0.432592
13C	5.252413	-0.461208	-0.110591
14C	5.661065	-0.564777	1.224624
15C	4.707824	-0.716051	2.236641
16C	3.347473	-0.763188	1.915462
17C	0.827141	-2.494491	-1.997573
18C	0.596225	-3.756359	-2.554669
19C	0.390401	-4.864084	-1.725788
20C	0.414726	-4.708128	-0.335052
21C	0.641360	-3.447523	0.222456
22C	1.231173	5.987270	-0.677589
23H	0.377261	2.095483	-2.934123
24H	0.527993	4.561614	-2.726490
25H	1.614430	4.298369	1.280824
26H	1.485529	1.846778	1.260721
27H	3.582149	-0.424141	-1.470936
28H	5.991823	-0.343779	-0.899138
29H	6.718855	-0.528454	1.473730
30H	5.021611	-0.796110	3.274748
31H	2.601215	-0.873394	2.697698
32H	0.977502	-1.632958	-2.640649
33H	0.577134	-3.873720	-3.635457
34H	0.213129	-5.844513	-2.161123
35H	0.254031	-5.565906	0.313371
36H	0.648361	-3.325993	1.302677
37H	1.182706	6.328243	0.357649
38H	2.195562	6.271997	-1.110250
39H	0.423489	6.456111	-1.244289
40P	-3.396942	0.034012	0.505543
41C	-2.535377	-1.460575	-0.075027
42C	-3.425058	-2.702704	-0.202480
43C	-4.069253	-0.235911	2.182635
44C	-2.202756	1.410050	0.504632
45C	-4.793387	0.422178	-0.606618

46C	-2.751806	2.731829	1.053544
47C	-4.373724	0.629052	-2.068467
48C	-3.002441	-0.542863	3.242608
49H	-1.712356	-1.618906	0.627970
50H	-2.075386	-1.202009	-1.035442
51H	-2.818723	-3.537907	-0.568916
52H	-3.851549	-3.001021	0.761593
53H	-4.246562	-2.549899	-0.911752
54H	-4.791474	-1.057549	2.099845
55H	-4.640333	0.663368	2.443867
56H	-1.873000	1.520589	-0.534175
57H	-1.332527	1.058916	1.069713
58H	-5.281678	1.318627	-0.206415
59H	-5.512201	-0.401197	-0.517466
60H	-1.973176	3.499781	0.983848
61H	-3.621834	3.085601	0.488643
62H	-3.037318	2.647107	2.107667
63H	-5.256481	0.871532	-2.670035
64H	-3.659606	1.453443	-2.172646
65H	-3.918225	-0.273317	-2.490538
66H	-3.490673	-0.696272	4.211268
67H	-2.436408	-1.448572	3.002037
68H	-2.288440	0.279759	3.351270

10h-Me-005

1C	-2.334541	1.838607	0.612591
2C	-2.955037	3.054189	0.698397
3N	-2.953597	3.946875	-0.334291
4C	-2.302105	3.617056	-1.490490
5C	-1.664627	2.417649	-1.640946
6C	-1.640877	1.436766	-0.587028
7N	-0.996022	0.291318	-0.790629
8P	-0.935072	-0.946868	0.314987
9C	-2.592405	-1.727404	0.364419
10O	-0.451881	-0.649252	1.726935
11C	0.166198	-2.158886	-0.495226
12C	0.497851	-2.098414	-1.856650
13C	1.357538	-3.049846	-2.415591
14C	1.886438	-4.071860	-1.620387
15C	1.552844	-4.141956	-0.262460
16C	0.698114	-3.189655	0.296807
17C	-3.141969	-2.094644	1.600723
18C	-4.404122	-2.695231	1.659086
19C	-5.120766	-2.934169	0.482343
20C	-4.575728	-2.569665	-0.755023
21C	-3.316594	-1.968421	-0.814348
22C	-3.564128	5.274578	-0.175212
23H	-2.363699	1.182022	1.474060
24H	-3.480153	3.369184	1.593544
25H	-2.329210	4.363068	-2.277564
26H	-1.168696	2.192062	-2.579459
27H	0.092644	-1.299607	-2.469784
28H	1.612018	-2.993486	-3.471373
29H	2.552378	-4.812722	-2.056176
30H	1.959548	-4.935764	0.359360
31H	0.451886	-3.237077	1.354548
32H	-2.579994	-1.904044	2.511128
33H	-4.825376	-2.976729	2.621220
34H	-6.100894	-3.402702	0.527341
35H	-5.131211	-2.754370	-1.671318
36H	-2.897630	-1.685064	-1.776838
37H	-3.953062	5.611996	-1.137874
38H	-4.387377	5.208808	0.538484
39H	-2.820647	5.990564	0.190380
40P	3.235374	0.975692	0.432728
41C	2.396930	0.943193	-1.185917
42C	2.531317	2.249736	-1.979764
43C	2.639729	2.394224	1.416788
44C	2.893492	-0.580593	1.314935
45C	5.034517	1.173671	0.182580
46C	3.696338	-0.749913	2.611390
47C	5.679318	0.008093	-0.580826
48C	1.109501	2.503702	1.470846
49H	1.343076	0.703643	-1.002317
50H	2.824030	0.097701	-1.737331
51H	2.009979	2.143720	-2.937337
52H	2.080031	3.093835	-1.446707
53H	3.576952	2.495591	-2.195802
54H	3.087169	3.296164	0.982487
55H	3.065964	2.275471	2.420399
56H	3.097953	-1.396266	0.612595
57H	1.815559	-0.593317	1.515445
58H	5.484348	1.296760	1.174913
59H	5.177164	2.120502	-0.351615
60H	3.390644	-1.680819	3.101135

61H	4.774392	-0.807271	2.424944
62H	3.509787	0.069523	3.314470
63H	6.750803	0.199661	-0.703298
64H	5.567675	-0.940384	-0.043862
65H	5.244304	-0.110437	-1.579684
66H	0.829261	3.337296	2.124605
67H	0.692827	2.699882	0.478151
68H	0.642060	1.592074	1.856144

10h-Me-006

1C	-0.579646	2.606350	1.850394
2C	-0.651485	3.966435	1.746111
3N	-1.037014	4.582547	0.586887
4C	-1.361978	3.810724	-0.491205
5C	-1.307120	2.444312	-0.453882
6C	-0.917548	1.743306	0.746957
7N	-0.831456	0.427354	0.912380
8P	-1.218504	-0.672723	-0.272176
9C	-0.764421	-2.267449	0.491215
10O	-0.568006	-0.535515	-1.641148
11C	-3.043205	-0.681857	-0.443128
12C	-3.885382	-0.441961	0.654517
13C	-5.273043	-0.460197	0.493688
14C	-5.829767	-0.720217	-0.764074
15C	-4.995530	-0.959506	-1.861052
16C	-3.606534	-0.940061	-1.701780
17C	-0.751608	-2.462002	1.881122
18C	-0.394999	-3.703821	2.413707
19C	-0.048772	-4.760204	1.563418
20C	-0.063235	-4.573060	0.177107
21C	-0.420758	-3.331841	-0.356915
22C	-1.190106	6.044089	0.544610
23H	-0.268703	2.159910	2.789495
24H	-0.411641	4.625343	2.573647
25H	-1.664926	4.348097	-1.383159
26H	-1.557432	1.892822	-1.352570
27H	-3.456569	-0.234847	1.631553
28H	-5.918994	-0.270177	1.347404
29H	-6.909736	-0.734557	-0.888528
30H	-5.425311	-1.158641	-2.839817
31H	-2.954797	-1.116019	-2.553448
32H	-1.004423	-1.638264	2.541657
33H	-0.384492	-3.846763	3.491520
34H	0.230203	-5.725004	1.979996
35H	0.205705	-5.390700	-0.487243
36H	-0.419187	-3.179533	-1.432600
37H	-1.142950	6.381969	-0.491821
38H	-2.152168	6.333877	0.979289
39H	-0.379143	6.511075	1.107873
40P	3.362869	-0.004358	-0.502678
41C	2.673310	-0.970962	0.880508
42C	3.613736	-2.051242	1.429385
43C	3.710789	-1.099808	-1.922071
44C	2.143964	1.265546	-0.972577
45C	4.931275	0.782348	0.005254
46C	2.610353	2.211395	-2.085684
47C	4.788323	1.718665	1.212443
48C	2.539113	-2.020868	-2.292989
49H	1.743672	-1.414188	0.512016
50H	2.387850	-0.256006	1.660328
51H	3.099467	-2.604074	2.222683
52H	3.900302	-2.771950	0.655319
53H	4.526328	-1.621283	1.856741
54H	4.608094	-1.677719	-1.670723
55H	3.978983	-0.440607	-2.756774
56H	1.905928	1.817749	-0.056596
57H	1.236357	0.724527	-1.266388
58H	5.314161	1.320831	-0.869608
59H	5.638627	-0.028085	0.216487
60H	1.813810	2.933713	-2.295986
61H	3.507544	2.774585	-1.804730
62H	2.818235	1.671466	-3.016183
63H	5.761056	2.165697	1.444672
64H	4.084503	2.534431	1.012565
65H	4.447043	1.181485	2.104442
66H	2.784900	-2.566659	-3.210755
67H	2.348990	-2.757264	-1.505759
68H	1.612211	-1.462894	-2.458360

10h-Me-007

1C	0.553374	2.256937	1.913630
2C	1.091129	3.512176	1.874712

3N	1.035125	4.286624	0.748196
4C	0.418188	3.788995	-0.363056
5C	-0.135810	2.538379	-0.391143
6C	-0.115017	1.684515	0.772437
7N	-0.622292	0.460075	0.873299
8P	-1.475519	-0.284987	-0.343968
9C	-1.828058	-1.933894	0.351972
10O	-0.830884	-0.396213	-1.718028
11C	-3.094020	0.564941	-0.477929
12C	-3.825612	0.922458	0.666257
13C	-5.056743	1.569448	0.539265
14C	-5.566134	1.863817	-0.731606
15C	-4.841226	1.509974	-1.873870
16C	-3.608802	0.860322	-1.747905
17C	-1.716568	-2.221799	1.720373
18C	-1.995104	-3.508312	2.193333
19C	-2.391867	-4.512787	1.304620
20C	-2.510634	-4.228931	-0.060911
21C	-2.229086	-2.946065	-0.534786
22C	1.552488	5.662345	0.773929
23H	0.618825	1.677852	2.828978
24H	1.583805	3.960188	2.731005
25H	0.397855	4.445963	-1.225604
26H	-0.588280	2.192169	-1.312897
27H	-3.432732	0.696024	1.654636
28H	-5.619076	1.842515	1.428904
29H	-6.525037	2.366923	-0.829680
30H	-5.234320	1.737443	-2.861877
31H	-3.038802	0.582547	-2.630481
32H	-1.400111	-1.443345	2.407776
33H	-1.902939	-3.725226	3.254923
34H	-2.609413	-5.512399	1.673132
35H	-2.818093	-5.006872	-0.755414
36H	-2.306651	-2.731513	-1.597529
37H	1.721915	6.001884	-0.249156
38H	0.831233	6.325628	1.262009
39H	2.498548	5.686386	1.319690
40P	3.187465	-1.064911	-0.428047
41C	5.006688	-0.905643	-0.473796
42C	5.518975	0.502849	-0.147339
43C	2.430808	0.132421	-1.573228
44C	2.778678	-2.773498	-0.919750
45C	2.592271	-0.720091	1.259934
46C	1.286070	-3.111201	-0.809638
47C	3.057206	-1.744135	2.302468
48C	2.936815	0.009317	-3.016352
49H	5.324719	-1.218600	-1.475670
50H	5.404505	-1.643223	0.233396
51H	6.612605	0.517021	-0.208337
52H	5.135070	1.247592	-0.853060
53H	5.238652	0.811372	0.866164
54H	2.636841	1.128943	-1.165561
55H	1.345163	-0.021740	-1.528992
56H	3.388036	-3.434804	-0.291555
57H	3.137652	-2.890365	-1.949277
58H	1.498696	-0.661515	1.212906
59H	2.949756	0.286730	1.506843
60H	1.118489	-4.137104	-1.155088
61H	0.931889	-3.046212	0.223914
62H	0.670893	-2.441401	-1.416735
63H	2.700303	-1.440144	3.292643
64H	2.652023	-2.740471	2.095997
65H	4.149857	-1.818748	2.349035
66H	2.432221	0.757301	-3.637636
67H	4.016719	0.180749	-3.094367
68H	2.709178	-0.975511	-3.438778

10h-Me-008

1C	3.054332	1.948427	1.843872
2C	3.961638	2.949225	1.641898
3N	4.358306	3.321079	0.386038
4C	3.813336	2.684798	-0.691200
5C	2.901321	1.673932	-0.557798
6C	2.467289	1.226305	0.744245
7N	1.610132	0.244426	1.004779
8P	0.957704	-0.745966	-0.151651
9C	2.272231	-1.913713	-0.672368
10O	0.297847	-0.134151	-1.380008
11C	-0.244272	-1.751180	0.789940
12C	-0.409685	-1.640358	2.178476
13C	-1.368167	-2.417321	2.838326
14C	-2.160610	-3.316686	2.118758
15C	-1.994707	-3.438281	0.733852
16C	-1.044727	-2.657493	0.072966
17C	3.099490	-2.545469	0.270815

18C	4.100674	-3.423889	-0.148736
19C	4.284231	-3.677809	-1.513804
20C	3.463799	-3.051431	-2.456905
21C	2.459345	-2.172538	-2.037386
22C	5.290828	4.442587	0.204600
23H	2.777796	1.676125	2.857330
24H	4.418807	3.492284	2.461931
25H	4.151409	3.029316	-1.662482
26H	2.501737	1.213248	-1.453684
27H	0.210393	-0.944111	2.734247
28H	-1.492233	-2.321073	3.914287
29H	-2.901912	-3.923188	2.633419
30H	-2.605964	-4.139411	0.170742
31H	-0.924789	-2.751581	-1.003651
32H	2.962037	-2.348993	1.331425
33H	4.737622	-3.909614	0.586601
34H	5.064623	-4.361395	-1.839287
35H	3.604414	-3.246109	-3.517515
36H	1.819959	-1.679296	-2.764756
37H	5.792565	4.341751	-0.759352
38H	4.749092	5.393609	0.237512
39H	6.041518	4.421519	0.997666
40P	-3.646817	1.151291	-0.407200
41C	-3.684892	-0.144979	0.874531
42C	-4.217151	0.325206	2.233802
43C	-2.731410	2.610812	0.200780
44C	-2.855358	0.459244	-1.892867
45C	-5.346374	1.697014	-0.794842
46C	-2.860286	1.402499	-3.102928
47C	-6.246287	0.586975	-1.352620
48C	-1.284140	2.309360	0.612597
49H	-2.663610	-0.527085	0.963233
50H	-4.294129	-0.961442	0.470336
51H	-4.244570	-0.525019	2.923487
52H	-3.569433	1.089851	2.676027
53H	-5.232493	0.730979	2.161062
54H	-3.312179	3.013931	1.039367
55H	-2.766465	3.359727	-0.599539
56H	-3.384959	-0.474331	-2.119134
57H	-1.826649	0.191688	-1.616253
58H	-5.252095	2.524006	-1.508797
59H	-5.763445	2.119241	0.127077
60H	-2.354217	0.909217	-3.939888
61H	-3.875575	1.657289	-3.426985
62H	-2.318191	2.331515	-2.893746
63H	-7.238200	0.996914	-1.571481
64H	-5.844997	0.168777	-2.282519
65H	-6.374256	-0.230386	-0.634091
66H	-0.802857	3.232482	0.954249
67H	-1.235460	1.585633	1.432513
68H	-0.701122	1.907300	-0.220262

10h-Me-009

1C	-1.994119	-2.087127	-0.492072
2C	-2.469074	-3.366048	-0.596454
3N	-2.734782	-4.137131	0.497263
4C	-2.523605	-3.609724	1.742831
5C	-2.051743	-2.340451	1.917445
6C	-1.761455	-1.479431	0.797568
7N	-1.309292	-0.253981	1.034361
8P	-1.000092	0.882867	-0.131497
9C	-2.586097	1.716506	-0.509162
10O	-0.313992	0.456028	-1.423069
11C	0.018685	2.117267	0.750710
12C	0.487987	1.921563	2.057147
13C	1.361081	2.847908	2.638825
14C	1.763691	3.979421	1.922973
15C	1.284695	4.188957	0.623711
16C	0.418805	3.262176	0.041247
17C	-2.958799	1.907587	-1.846968
18C	-4.166755	2.541705	-2.157488
19C	-5.006313	2.988138	-1.132591
20C	-4.638291	2.799151	0.205637
21C	-3.433784	2.165266	0.517031
22C	-3.304967	-5.484988	0.363109
23H	-1.786606	-1.532884	-1.399687
24H	-2.657219	-3.830354	-1.558229
25H	-2.758663	-4.263007	2.576440
26H	-1.899924	-1.961712	2.923072
27H	0.168791	1.045180	2.612674
28H	1.721358	2.687440	3.652237
29H	2.440627	4.699662	2.375876
30H	1.587411	5.071603	0.065733
31H	0.060583	3.424780	-0.972833
32H	-2.300713	1.558724	-2.638297

33H	-4.449664	2.686995	-3.197352
34H	-5.943566	3.484087	-1.373224
35H	-5.289412	3.146531	1.004139
36H	-3.151135	2.021287	1.557157
37H	-4.352711	-5.480870	0.679145
38H	-3.244726	-5.798920	-0.679880
39H	-2.739390	-6.187197	0.981121
40P	3.250257	-0.851770	-0.528794
41C	1.746060	-1.658731	0.107563
42C	1.883415	-3.171338	0.320273
43C	3.709665	-1.583081	-2.138491
44C	2.930338	0.930930	-0.720585
45C	4.642573	-1.116830	0.623852
46C	4.080953	1.710424	-1.369181
47C	4.386191	-0.568687	2.034686
48C	2.629372	-1.432359	-3.218558
49H	0.951666	-1.416992	-0.605606
50H	1.481750	-1.149071	1.040153
51H	0.941459	-3.563353	0.718728
52H	2.091529	-3.697375	-0.618124
53H	2.676204	-3.417161	1.035748
54H	3.938248	-2.639479	-1.952732
55H	4.646166	-1.102939	-2.446523
56H	2.708901	1.317105	0.280376
57H	2.002083	1.014291	-1.295612
58H	5.520742	-0.642489	0.169746
59H	4.837704	-2.195418	0.647174
60H	3.806546	2.769388	-1.424279
61H	5.008133	1.637501	-0.789360
62H	4.283878	1.365540	-2.389032
63H	5.266425	-0.749037	2.661119
64H	4.198527	0.510456	2.021745
65H	3.530609	-1.059646	2.511715
66H	2.982458	-1.889591	-4.149395
67H	1.696055	-1.928362	-2.931557
68H	2.402810	-0.380831	-3.423190

10h-Me-010

1C	1.005777	2.571594	1.587825
2C	1.453126	3.860029	1.507182
3N	2.162136	4.310969	0.428163
4C	2.426161	3.445856	-0.594371
5C	2.004073	2.144681	-0.576212
6C	1.270249	1.612962	0.546002
7N	0.819155	0.370365	0.692856
8P	1.083163	-0.848035	-0.405870
9C	2.874532	-1.235856	-0.381147
10O	0.600804	-0.658089	-1.835445
11C	0.251795	-2.277543	0.369320
12C	-0.144332	-3.339610	-0.459513
13C	-0.773957	-4.462252	0.083152
14C	-1.013255	-4.533748	1.460638
15C	-0.617939	-3.480340	2.291751
16C	0.013481	-2.356890	1.749221
17C	3.596608	-1.251971	0.823252
18C	4.960652	-1.551378	0.821182
19C	5.613859	-1.836209	-0.384228
20C	4.899368	-1.821063	-1.586351
21C	3.532736	-1.522442	-1.585385
22C	2.708078	5.676325	0.422262
23H	0.446873	2.255691	2.462826
24H	1.274349	4.586548	2.292344
25H	2.988245	3.854975	-1.426944
26H	2.225886	1.519611	-1.433247
27H	0.029420	-3.277867	-1.530604
28H	-1.079602	-5.278365	-0.567085
29H	-1.503510	-5.407125	1.883886
30H	-0.804141	-3.530290	3.361929
31H	0.307872	-1.534283	2.393393
32H	3.093444	-1.029123	1.761032
33H	5.513907	-1.562290	1.757178
34H	6.675758	-2.069879	-0.384938
35H	5.404759	-2.040706	-2.523793
36H	2.972380	-1.504101	-2.516373
37H	2.914870	5.975477	-0.606356
38H	1.976250	6.363625	0.852344
39H	3.633977	5.713465	1.005101
40P	-3.375346	0.522710	-0.411332
41C	-2.515177	0.834626	1.164612
42C	-2.903268	-0.141011	2.282872
43C	-3.058124	1.905730	-1.560482
44C	-2.752883	-1.024821	-1.140564
45C	-5.175232	0.380466	-0.126561
46C	-3.501701	-1.474179	-2.402117
47C	-5.781552	1.570232	0.629694

48C	-1.567555	2.240746	-1.721855
49H	-2.729471	1.871877	1.449586
50H	-1.441352	0.762596	0.949133
51H	-3.960755	-0.052689	2.555626
52H	-2.699866	-1.179213	2.001474
53H	-2.306251	0.079191	3.174663
54H	-3.621876	2.769407	-1.187801
55H	-3.504888	1.616799	-2.519647
56H	-2.803633	-1.788987	-0.356876
57H	-1.692889	-0.858107	-1.362837
58H	-5.334020	-0.556911	0.420417
59H	-5.643115	0.259940	-1.110746
60H	-3.027930	-2.382228	-2.791065
61H	-4.552807	-1.705471	-2.198582
62H	-3.458785	-0.715535	-3.191571
63H	-5.652833	2.508698	0.079137
64H	-6.856576	1.407394	0.762998
65H	-5.335860	1.687592	1.623605
66H	-1.453247	3.016177	-2.487611
67H	-1.141814	2.626008	-0.790151
68H	-0.978619	1.369759	-2.027062

10h-Me-011

1C	0.798654	2.502753	-2.148294
2C	0.781247	3.867044	-2.086442
3N	0.903091	4.538358	-0.899876
4C	1.032329	3.817953	0.252272
5C	1.055823	2.450415	0.258991
6C	0.943461	1.692688	-0.965317
7N	0.949880	0.369926	-1.090054
8P	1.165213	-0.673504	0.184859
9C	1.042858	-2.314390	-0.602014
10O	0.224233	-0.579181	1.377637
11C	2.904721	-0.504023	0.739504
12C	3.193945	-0.521184	2.111254
13C	4.514557	-0.390333	2.553677
14C	5.552167	-0.243858	1.627483
15C	5.268409	-0.227443	0.256355
16C	3.950136	-0.356795	-0.186163
17C	1.360941	-2.526249	-1.951872
18C	1.271664	-3.807928	-2.501978
19C	0.864799	-4.886478	-1.708442
20C	0.547572	-4.680862	-0.361239
21C	0.638680	-3.999699	0.190356
22C	0.803352	6.004657	-0.867029
23H	0.709948	2.011746	-3.111961
24H	0.677054	4.486650	-2.970601
25H	1.117174	4.397258	1.165485
26H	1.154866	1.941210	1.210543
27H	2.382372	-0.631243	2.825721
28H	4.732189	-0.402829	3.619043
29H	6.578899	-0.143654	1.971098
30H	6.073130	-0.114068	-0.466044
31H	3.733123	-0.340802	-1.251243
32H	1.659423	-1.686164	-2.571541
33H	1.516483	-3.964170	-3.549794
34H	0.795801	-5.882822	-2.138151
35H	0.230815	-5.516188	0.258593
36H	0.387547	-3.236822	1.235135
37H	1.286349	6.378822	0.037177
38H	1.312431	6.422256	-1.738279
39H	-0.247395	6.312481	-0.874740
40P	-3.432892	-0.086002	0.468099
41C	-2.630916	-1.558263	-0.247728
42C	-2.259872	-1.416467	-1.729815
43C	-3.919984	-0.451390	2.190836
44C	-2.266455	1.313490	0.429906
45C	-4.926810	0.359438	-0.487618
46C	-2.792460	2.595037	1.088892
47C	-5.976175	-0.756556	-0.581808
48C	-2.760043	-0.925749	3.078816
49H	-3.309061	-2.404829	-0.085639
50H	-1.737324	-1.725724	0.361555
51H	-3.142265	-1.250377	-2.358505
52H	-1.551294	-0.598216	-1.890884
53H	-1.773722	-2.338044	-2.065292
54H	-4.711465	-1.208813	2.142192
55H	-4.375607	0.464139	2.586917
56H	-2.019255	1.482549	-0.624213
57H	-1.354404	0.950837	0.916007
58H	-4.579961	0.659487	-1.483851
59H	-5.346531	1.254717	-0.013469
60H	-2.020517	3.370330	1.027614
61H	-3.691837	2.977966	0.593601
62H	-3.022258	2.440794	2.149094

63H	-6.356921	-1.039505	0.405419
64H	-6.825490	-0.409018	-1.179904
65H	-5.571257	-1.652641	-1.065004
66H	-3.121109	-1.049455	4.105794
67H	-2.364251	-1.888468	2.740006
68H	-1.930754	-0.212570	3.086670

10h-Me-012

1C	2.212593	2.370962	-1.707073
2C	3.026119	3.455580	-1.542593
3N	3.692685	3.686850	-0.370126
4C	3.542031	2.801970	0.657151
5C	2.740804	1.697278	0.557686
6C	2.022315	1.401433	-0.658338
7N	1.228473	0.358098	-0.883843
8P	0.961954	-0.845632	0.227329
9C	-0.218218	-1.943735	-0.630938
10O	0.431905	-0.465371	1.602509
11C	2.510008	-1.812835	0.397687
12C	3.290564	-2.144049	-0.721842
13C	4.466739	-2.880718	-0.565121
14C	4.871928	-3.292564	0.710535
15C	4.098407	-2.964772	1.828515
16C	2.919796	-2.227992	1.672558
17C	-0.474028	-1.861621	-2.007735
18C	-1.405280	-2.718668	-2.602983
19C	-2.082645	-3.667303	-1.830253
20C	-1.824797	-3.761026	-0.457489
21C	-0.897123	-2.903937	0.138711
22C	4.606147	4.833039	-0.257499
23H	1.702269	2.226894	-2.653982
24H	3.187457	4.185843	-2.328223
25H	4.094271	3.029826	1.562420
26H	2.651307	1.046740	1.419711
27H	2.981220	-1.824348	-1.714146
28H	5.066800	-3.133605	-1.435930
29H	5.787746	-3.866009	0.831487
30H	4.410852	-3.282092	2.820575
31H	2.315538	-1.965534	2.536901
32H	0.045980	-1.119050	-2.604728
33H	-1.601850	-2.644668	-3.669935
34H	-2.806625	-4.332386	-2.294644
35H	-2.347364	-4.498064	0.147330
36H	-0.708148	-2.969157	1.207057
37H	4.815128	5.023808	0.796437
38H	5.543312	4.620059	-0.781720
39H	4.136482	5.718258	-0.692753
40P	-3.492548	1.037915	0.516697
41C	-3.629057	-0.361294	-0.647225
42C	-4.963413	-1.112761	-0.553896
43C	-3.766879	0.455493	2.226437
44C	-1.830270	1.771439	0.380307
45C	-4.771886	2.280601	0.121416
46C	-1.666883	3.098322	1.134567
47C	-4.637139	2.881666	-1.284580
48C	-2.920063	-0.769994	2.601675
49H	-2.787756	-1.028841	-0.440816
50H	-3.472287	0.049663	-1.650991
51H	-4.973690	-1.919816	-1.294003
52H	-5.101319	-1.564822	0.434561
53H	-5.819508	-0.460057	-0.758825
54H	-4.838492	0.244575	2.324782
55H	-3.545159	1.306228	2.882455
56H	-1.611338	1.887394	-0.687128
57H	-1.133508	1.021304	0.770776
58H	-4.707708	3.058304	0.891821
59H	-5.742432	1.786552	0.247508
60H	-0.626243	3.429569	1.049206
61H	-2.307188	3.888394	0.726748
62H	-1.890942	2.986263	2.201371
63H	-5.420798	3.631542	-1.437539
64H	-3.669117	3.375321	-1.422898
65H	-4.747307	2.119249	-2.063453
66H	-3.089453	-1.013664	3.656496
67H	-3.204050	-1.643924	2.005814
68H	-1.849137	-0.592748	2.457510

10h-Me-013

1C	2.230105	2.373607	-1.696676
2C	3.026114	3.468554	-1.516497
3N	3.674725	3.703418	-0.334649
4C	3.524445	2.810888	0.686116

5C	2.739943	1.695655	0.571197
6C	2.037084	1.398198	-0.653677
7N	1.252345	0.350710	-0.890818
8P	0.972298	-0.852649	0.217245
9C	-0.224334	-1.933099	-0.641226
10O	0.447700	-0.470993	1.594355
11C	2.511406	-1.834283	0.382790
12C	3.290764	-2.163622	-0.738143
13C	4.463595	-2.906254	-0.584594
14C	4.866723	-3.325716	0.689226
15C	4.094234	-3.000067	1.808543
16C	2.918889	-2.257435	1.655810
17C	-0.494970	-1.833200	-2.013976
18C	-1.437743	-2.677748	-2.609121
19C	-2.112127	-3.631613	-1.840311
20C	-1.840239	-3.742514	-0.471497
21C	-0.901070	-2.897974	0.124607
22C	4.566272	4.865233	-0.206102
23H	1.732598	2.228172	-2.650163
24H	3.186691	4.205431	-2.296161
25H	4.062821	3.040933	1.599115
26H	2.648490	1.039405	1.428682
27H	2.983574	-1.836845	-1.728794
28H	5.063067	-3.157195	-1.456367
29H	5.780390	-3.903081	0.807765
30H	4.405325	-3.323014	2.799208
31H	2.316027	-1.995750	2.521373
32H	0.024467	-1.087874	-2.608069
33H	-1.644774	-2.590355	-3.673086
34H	-2.844438	-4.287531	-2.304674
35H	-2.360429	-4.483642	0.130343
36H	-0.701196	-2.977386	1.190034
37H	4.786158	5.034741	0.849125
38H	5.500222	4.683909	-0.747471
39H	4.073050	5.751276	-0.613277
40P	-3.484286	1.039019	0.534601
41C	-3.687000	-0.376980	-0.599506
42C	-5.024723	-1.111646	-0.454494
43C	-3.701654	0.496957	2.264991
44C	-1.808997	1.714640	0.301321
45C	-4.743670	2.309777	0.163877
46C	-1.579138	3.090707	0.938635
47C	-4.657883	2.860126	-1.266807
48C	-2.903032	-0.765613	2.622107
49H	-2.844993	-1.050300	-0.412721
50H	-3.558639	0.019015	-1.613340
51H	-5.060627	-1.940134	-1.169825
52H	-5.145650	-1.531998	0.549845
53H	-5.877795	-0.455229	-0.660385
54H	-4.776523	0.345535	2.419923
55H	-3.403979	1.344991	2.893894
56H	-1.618811	1.740010	-0.777522
57H	-1.123224	0.975588	0.730147
58H	-4.613941	3.109055	0.903809
59H	-5.722879	1.854770	0.354223
60H	-0.535604	3.384508	0.782738
61H	-2.216677	3.862812	0.494040
62H	-1.758308	3.073478	2.019890
63H	-5.418664	3.635835	-1.405878
64H	-3.679937	3.309635	-1.470160
65H	-4.837432	2.077748	-2.012199
66H	-3.033025	-0.981704	3.688509
67H	-3.262349	-1.633017	2.058475
68H	-1.832198	-0.647769	2.425144

10h-Me-014

1C	2.250061	2.356632	-1.700332
2C	3.098961	3.414439	-1.542452
3N	3.786379	3.621247	-0.377122
4C	3.605337	2.750027	0.656463
5C	2.768966	1.670717	0.562790
6C	2.040729	1.391443	-0.650945
7N	1.225505	0.364418	-0.875859
8P	0.948948	-0.840910	0.231200
9C	-0.235601	-1.930077	-0.632353
10O	0.418818	-0.461623	1.606574
11C	2.491576	-1.816934	0.401268
12C	3.271369	-2.149919	-0.718261
13C	4.444335	-2.891755	-0.561944
14C	4.847098	-3.307021	0.713365
15C	4.074243	-2.977638	1.831344
16C	2.898850	-2.235651	1.675747
17C	-0.488714	-1.842408	-2.009306
18C	-1.422452	-2.693636	-2.608998
19C	-2.104930	-3.642102	-1.840588

20C	-1.849785	-3.741455	-0.467699
21C	-0.919688	-2.890119	0.132960
22C	4.680792	4.781540	-0.257019
23H	1.732011	2.225999	-2.644978
24H	3.276707	4.141020	-2.328224
25H	4.165316	2.962403	1.560700
26H	2.664176	1.024559	1.426400
27H	2.964042	-1.827472	-1.710311
28H	5.043841	-3.145886	-1.432778
29H	5.760501	-3.884363	0.834040
30H	4.384815	-3.297640	2.823130
31H	2.295306	-1.971672	2.540136
32H	0.035592	-1.100264	-2.603073
33H	-1.616863	-2.615276	-3.676034
34H	-2.830780	-4.302702	-2.308455
35H	-2.376255	-4.478504	0.133712
36H	-0.732523	-2.959963	1.201324
37H	5.203271	4.734795	0.698895
38H	5.416064	4.765235	-1.066385
39H	4.100715	5.707888	-0.306769
40P	-3.502895	1.055352	0.514804
41C	-3.647410	-0.342636	-0.649700
42C	-4.984772	-1.088479	-0.555884
43C	-3.780859	0.474154	2.224297
44C	-1.835533	1.776699	0.378215
45C	-4.774273	2.306750	0.121006
46C	-1.660409	3.099198	1.137253
47C	-4.642431	2.901790	-1.287854
48C	-2.938532	-0.753949	2.601109
49H	-2.808774	-1.013899	-0.444416
50H	-3.489650	0.068253	-1.653325
51H	-4.999194	-1.894826	-1.296708
52H	-5.123742	-1.540830	0.432297
53H	-5.838187	-0.431809	-0.759414
54H	-4.853212	0.266409	2.321390
55H	-3.557563	1.324317	2.880553
56H	-1.617044	1.894489	-0.689100
57H	-1.144184	1.020056	0.765500
58H	-4.699579	3.086670	0.888284
59H	-5.748218	1.821223	0.254045
60H	-0.617989	3.424036	1.048943
61H	-2.297342	3.895270	0.735863
62H	-1.880566	2.983705	2.204458
63H	-5.419780	3.658687	-1.438430
64H	-3.670633	3.385704	-1.434092
65H	-4.764772	2.137758	-2.063298
66H	-3.110644	-0.997043	3.655621
67H	-3.224181	-1.627037	2.004807
68H	-1.866760	-0.580230	2.459005

10h-Me-015

1C	2.252411	2.171999	-2.089606
2C	2.777899	3.428702	-1.991729
3N	2.997524	4.028002	-0.780842
4C	2.683194	3.344380	0.357269
5C	2.151144	2.084104	0.327862
6C	1.910169	1.402856	-0.920928
7N	1.407732	0.181865	-1.080834
8P	1.032775	-0.830703	0.179483
9C	0.360970	-2.306484	-0.661886
10O	0.070081	-0.345763	1.255120
11C	2.608847	-1.367838	0.948624
12C	3.748243	-1.629169	0.170620
13C	4.934835	-2.045446	0.778863
14C	4.992488	-2.203608	2.169002
15C	3.861187	-1.942664	2.948709
16C	2.672544	-1.526442	2.340397
17C	0.547072	-2.552476	-2.030075
18C	0.004035	-3.698572	-2.619632
19C	-0.724300	-4.608809	-1.847234
20C	-0.908293	-4.371777	-0.479843
21C	-0.368315	-3.226517	0.109193
22C	3.632792	5.352551	-0.725314
23H	2.092323	1.735086	-3.069945
24H	3.048107	4.014632	-2.863545
25H	2.876731	3.862850	1.290023
26H	1.903442	1.606092	1.268424
27H	3.708227	-1.503489	-0.908523
28H	5.813677	-2.246118	0.170810
29H	5.916343	-2.528649	2.641324
30H	3.903287	-2.062690	4.028669
31H	1.791581	-1.316190	2.941021
32H	1.103206	-1.840112	-2.631369
33H	0.148707	-3.878842	-3.682188
34H	-1.145824	-5.499338	-2.307232

35H	-1.472732	-5.077178	0.125318
36H	-0.522422	-3.038841	1.168786
37H	3.499680	5.776821	0.271289
38H	4.702362	5.265082	-0.941328
39H	3.164749	6.013528	-1.458955
40P	-3.743030	0.809224	0.274893
41C	-5.511840	0.759860	-0.181670
42C	-6.315754	-0.326724	0.545187
43C	-2.944107	-0.776987	-0.122602
44C	-2.973561	2.173444	-0.663904
45C	-3.554714	1.099644	2.066936
46C	-1.502102	2.424066	-0.307243
47C	-4.198402	2.401010	2.562495
48C	-2.897806	-1.111427	-1.618730
49H	-5.543899	0.611544	-1.267885
50H	-5.922952	1.756565	0.016600
51H	-7.356501	-0.299484	0.205031
52H	-5.922616	-1.328348	0.338625
53H	-6.314064	-0.173475	1.629881
54H	-3.493775	-1.544940	0.435398
55H	-1.938230	-0.722308	0.310342
56H	-3.585967	3.066030	-0.487843
57H	-3.083979	1.915897	-1.723948
58H	-2.476632	1.084774	2.264957
59H	-3.982072	0.227051	2.575151
60H	-1.098033	3.199566	-0.967103
61H	-1.390413	2.769131	0.726029
62H	-0.896180	1.523471	-0.425638
63H	-4.022876	2.506795	3.638509
64H	-3.770024	3.279760	2.067580
65H	-5.281643	2.407177	2.398614
66H	-2.435041	-2.094286	-1.749706
67H	-3.898750	-1.146567	-2.065047
68H	-2.293246	-0.387823	-2.175551

10h-Me-016

1C	-2.697901	1.718713	0.611601
2C	-3.460224	2.843708	0.762546
3N	-3.673720	3.722750	-0.260698
4C	-3.092065	3.475478	-1.473060
5C	-2.320825	2.368531	-1.690731
6C	-2.074913	1.400948	-0.652763
7N	-1.322711	0.338766	-0.926265
8P	-0.999909	-0.858312	0.176266
9C	-2.516210	-1.870367	0.358667
10O	-0.469012	-0.463961	1.547316
11C	0.213603	-1.912807	-0.693072
12C	0.546340	-1.740642	-2.044598
13C	1.503331	-2.565649	-2.645277
14C	2.129397	-3.572338	-1.903746
15C	1.795677	-3.754984	-0.556400
16C	0.844505	-2.928639	0.045935
17C	-2.896974	-2.305596	1.635997
18C	-4.055439	-3.071289	1.803028
19C	-4.837539	-3.407968	0.693754
20C	-4.461203	-2.976249	-0.584182
21C	-3.305517	-2.210245	-0.752132
22C	-4.448534	4.949959	-0.028158
23H	-2.560325	1.067723	1.466951
24H	-3.936933	3.093046	1.704708
25H	-3.286941	4.207007	-2.249515
26H	-1.888795	2.207847	-2.673192
27H	0.059354	-0.958065	-2.617957
28H	1.756295	-2.423098	-3.693288
29H	2.870400	-4.214804	-2.373147
30H	2.277934	-4.537553	0.024162
31H	0.598242	-3.065799	1.095998
32H	-2.287129	-2.035089	2.493955
33H	-4.346097	-3.402968	2.797010
34H	-5.738229	-4.003077	0.823390
35H	-5.068772	-3.235283	-1.447942
36H	-3.019766	-1.872776	-1.745548
37H	-4.787178	5.348135	-0.986061
38H	-5.320754	4.719243	0.587508
39H	-3.829109	5.697447	0.478163
40P	3.491031	1.038673	0.524815
41C	1.849195	1.548207	-0.075999
42C	1.482208	3.008646	0.213059
43C	3.483380	0.986858	2.349871
44C	3.846021	-0.615603	-0.156132
45C	4.769377	2.227050	-0.011473
46C	5.158855	-1.236454	0.336508
47C	4.825554	2.424765	-1.532500
48C	2.663417	-0.175051	2.930565
49H	1.138170	0.873824	0.410869

50H	1.814569	1.335020	-1.149899
51H	0.469286	3.198006	-0.158041
52H	1.486254	3.222594	1.287812
53H	2.161345	3.710902	-0.282847
54H	3.084763	1.954095	2.679681
55H	4.528572	0.942385	2.677868
56H	3.843010	-0.513712	-1.247078
57H	2.988667	-1.244751	0.104908
58H	5.727797	1.862702	0.376483
59H	4.556876	3.171906	0.503452
60H	5.273205	-2.232234	-0.105659
61H	6.030413	-0.640438	0.043504
62H	5.170635	-1.352924	1.425787
63H	5.607840	3.151111	-1.777964
64H	5.061793	1.491188	-2.054829
65H	3.877651	2.807694	-1.926088
66H	2.658331	-0.098950	4.023747
67H	1.625426	-0.165202	2.582803
68H	3.102388	-1.143391	2.666427

10h-Me-017

1C	-0.918066	2.562623	-0.379446
2C	-0.764339	3.921295	-0.421715
3N	-0.933651	4.709364	0.679707
4C	-1.289892	4.120093	1.863050
5C	-1.461491	2.770552	1.973590
6C	-1.281877	1.888577	0.846181
7N	-1.442416	0.584621	1.025192
8P	-1.285342	-0.570109	-0.151222
9C	-1.045803	-2.110489	0.801295
10O	-0.194270	-0.431705	-1.205416
11C	-2.922176	-0.723690	-0.959630
12C	-4.112663	-0.658232	-0.217352
13C	-5.347363	-0.783420	-0.858003
14C	-5.402581	-0.973553	-2.244350
15C	-4.220108	-1.037069	-2.988036
16C	-2.982799	-0.914063	-2.347511
17C	-0.531412	-3.228756	0.124518
18C	-0.313731	-4.428711	0.806019
19C	-0.610168	-4.522290	2.170666
20C	-1.128249	-3.413745	2.848471
21C	-1.346576	-2.212207	2.167668
22C	-0.815979	6.171571	0.597777
23H	-0.754915	1.991107	-1.285217
24H	-0.498273	4.438821	-1.337244
25H	-1.424623	4.794716	2.701698
26H	-1.737940	2.344433	2.932565
27H	-4.073825	-0.504903	0.858084
28H	-6.265757	-0.731522	-0.278188
29H	-6.364546	-1.070920	-2.741760
30H	-4.259921	-1.182590	-4.064935
31H	-2.060078	-0.958622	-2.919734
32H	-0.293858	-3.155926	-0.933772
33H	0.088254	-5.287905	0.274499
34H	-0.440334	-5.455618	2.702027
35H	-1.361045	-3.482607	3.908464
36H	-1.735738	-1.347355	2.695589
37H	-0.264271	6.542603	1.465113
38H	-0.272850	6.439088	-0.309855
39H	-1.810013	6.629481	0.573658
40P	3.506597	-0.162794	-0.354504
41C	3.350578	-0.024276	1.459490
42C	1.904400	-0.068740	1.965200
43C	2.613967	1.196867	-1.178112
44C	5.290318	-0.074206	-0.744525
45C	2.810425	-1.741971	-0.937580
46C	5.621263	-0.216424	-2.235988
47C	3.375591	-2.979421	-0.230259
48C	2.966337	2.594147	-0.654400
49H	3.843818	0.913303	1.743320
50H	3.946659	-0.839384	1.887091
51H	1.896134	0.016009	3.057482
52H	1.303865	0.749996	1.560717
53H	1.410276	-1.007266	1.700281
54H	1.547914	0.968986	-1.065407
55H	2.841676	1.106058	-2.247159
56H	5.779271	-0.860961	-0.157382
57H	5.649682	0.884225	-0.351067
58H	2.998696	-1.779065	-2.017648
59H	1.725369	-1.655438	-0.814278
60H	6.705387	-0.144414	-2.375535
61H	5.298453	-1.185089	-2.633334
62H	5.155150	0.573667	-2.835077
63H	2.932812	-3.879879	-0.669091
64H	4.463576	-3.056834	-0.339703

65H	3.134435	-2.978891	0.838024
66H	2.433456	3.346132	-1.246147
67H	2.666782	2.720940	0.391426
68H	4.038485	2.808125	-0.734710

10h-Me-018

1C	-2.013718	2.176652	-0.420553
2C	-2.467555	3.466206	-0.477962
3N	-2.878850	4.144934	0.632439
4C	-2.819858	3.516888	1.847560
5C	-2.379202	2.231185	1.974528
6C	-1.953096	1.460562	0.832768
7N	-1.545278	0.212415	1.020925
8P	-1.088307	-0.830341	-0.180820
9C	-0.200951	-2.149125	0.721836
10O	-0.245344	-0.324563	-1.343980
11C	-2.620853	-1.607509	-0.817192
12C	-3.630666	-2.046549	0.054760
13C	-4.793152	-2.629406	-0.453988
14C	-4.956403	-2.778254	-1.837087
15C	-3.954104	-2.342785	-2.709201
16C	-2.788496	-1.759712	-2.200667
17C	0.345366	-3.202865	-0.031355
18C	1.075185	-4.215308	0.593835
19C	1.271689	-4.182871	1.979973
20C	0.731146	-3.138086	2.735261
21C	-0.006581	-2.126378	2.110413
22C	-3.322033	5.543752	0.553661
23H	-1.695452	1.693947	-1.337097
24H	-2.526162	4.010680	-1.414113
25H	-3.149503	4.104669	2.697611
26H	-2.358553	1.768888	2.956041
27H	-3.507806	-1.929794	1.128750
28H	-5.571485	-2.967249	0.225946
29H	-5.862068	-3.232268	-2.231897
30H	-4.078302	-2.455901	-3.783587
31H	-2.006574	-1.415939	-2.872493
32H	0.204606	-3.227515	-1.109404
33H	1.490734	-5.027476	0.002331
34H	1.840790	-4.970596	2.467640
35H	0.879485	-3.110805	3.812164
36H	-0.433967	-1.317198	2.694220
37H	-2.542279	6.208826	0.938700
38H	-3.532994	5.797149	-0.486503
39H	-4.234347	5.671901	1.141483
40P	3.550982	0.806626	-0.377483
41C	3.049477	1.797427	1.071715
42C	1.571003	1.632219	1.443417
43C	2.542161	1.254724	-1.826411
44C	5.315345	1.160717	-0.698121
45C	3.307496	-0.967189	-0.033580
46C	5.910341	0.376739	-1.875703
47C	4.063030	-1.483117	1.197751
48C	2.486520	2.762046	-2.109621
49H	3.285550	2.841183	0.830909
50H	3.706905	1.503201	1.898462
51H	1.336591	2.262543	2.308248
52H	0.913246	1.929642	0.621794
53H	1.330153	0.598656	1.707040
54H	1.542549	0.838029	-1.646587
55H	2.964600	0.706778	-2.677690
56H	5.856796	0.948588	0.231654
57H	5.387223	2.241424	-0.869162
58H	3.605369	-1.508118	-0.939588
59H	2.228182	-1.111552	0.073180
60H	6.958303	0.664387	-2.013209
61H	5.881580	-0.703902	-1.698720
62H	5.380603	0.586735	-2.811594
63H	3.866823	-2.553358	1.316153
64H	5.146091	-1.346537	1.101301
65H	3.730875	-0.983458	2.114205
66H	1.896109	2.934629	-3.016090
67H	2.003868	3.307610	-1.290992
68H	3.481435	3.193206	-2.272500

10h-Me-019

1C	2.713515	2.035878	-2.015619
2C	3.196864	3.306803	-1.892320
3N	3.103886	4.005082	-0.718565
4C	2.520393	3.403726	0.358718
5C	2.014092	2.133922	0.302235
6C	2.087722	1.352750	-0.911237

7N	1.639277	0.117063	-1.094487
8P	0.977827	-0.833117	0.088783
9C	0.228262	-2.213843	-0.844828
10O	-0.034778	-0.234404	1.057481
11C	2.371327	-1.566183	1.027216
12C	3.477988	-2.124893	0.366741
13C	4.531823	-2.672104	1.101415
14C	4.489878	-2.663938	2.501395
15C	3.391261	-2.108040	3.163606
16C	2.333728	-1.561701	2.428477
17C	0.238925	-2.282696	-2.245339
18C	-0.390504	-3.345102	-2.903340
19C	-1.027275	-4.349559	-2.168551
20C	-1.036100	-4.290035	-0.769810
21C	-0.414490	-3.226930	-0.112447
22C	3.709398	5.339112	-0.602076
23H	2.805537	1.520855	-2.966285
24H	3.678167	3.827335	-2.713100
25H	2.480858	3.996888	1.266112
26H	1.546777	1.720163	1.188107
27H	3.514646	-2.132083	-0.720037
28H	5.385100	-3.104643	0.584713
29H	5.311128	-3.090688	3.072093
30H	3.355908	-2.099877	4.250484
31H	1.476662	-1.127697	2.936315
32H	0.740665	-1.505688	-2.813332
33H	-0.377924	-3.389007	-3.989830
34H	-1.511797	-5.176982	-2.681115
35H	-1.527036	-5.070203	-0.193148
36H	-0.429121	-3.184877	0.974324
37H	3.218011	5.890224	0.201828
38H	4.778432	5.250706	-0.382394
39H	3.573601	5.882307	-1.539819
40P	-3.531402	0.915332	0.330166
41C	-5.301076	1.286323	0.604271
42C	-5.817781	0.888969	1.993065
43C	-3.239699	-0.880157	0.448006
44C	-3.105433	1.522266	-1.338672
45C	-2.507859	1.747937	1.588579
46C	-1.663249	1.218792	-1.765494
47C	-2.643165	3.275584	1.602616
48C	-3.876375	-1.696710	-0.682994
49H	-5.855159	0.765027	-0.185701
50H	-5.431199	2.360862	0.428007
51H	-6.877788	1.152080	2.076631
52H	-5.727341	-0.189089	2.166460
53H	-5.279688	1.411130	2.791669
54H	-3.623975	-1.191691	1.427095
55H	-2.152150	-1.003408	0.480614
56H	-3.299195	2.601391	-1.335736
57H	-3.828651	1.070630	-2.028455
58H	-1.479046	1.422436	1.396024
59H	-2.795987	1.316213	2.555143
60H	-1.486418	1.625717	-2.767206
61H	-0.935649	1.666121	-1.083195
62H	-1.467936	0.143599	-1.799045
63H	-1.989557	3.688633	2.378893
64H	-2.343463	3.718789	0.646146
65H	-3.667356	3.596920	1.824696
66H	-3.675499	-2.759531	-0.515440
67H	-4.963307	-1.563305	-0.727950
68H	-3.453569	-1.433300	-1.657961

10h-Me-020

1C	2.012758	2.422506	-1.786243
2C	2.689682	3.600494	-1.648400
3N	3.281446	3.959326	-0.467745
4C	3.176211	3.119937	0.602341
5C	2.511341	1.925912	0.531137
6C	1.884938	1.490806	-0.694141
7N	1.220227	0.356705	-0.894147
8P	1.035527	-0.818815	0.261728
9C	-0.055765	-2.030590	-0.560592
10O	0.471105	-0.433178	1.621591
11C	2.651174	-1.658779	0.468968
12C	3.073450	-2.020927	1.755952
13C	4.298172	-2.671471	1.938276
14C	5.105233	-2.966009	0.834878
15C	4.688904	-2.604432	-0.452384
16C	3.467002	-1.953027	-0.635515
17C	-0.292057	-2.027997	-1.943439
18C	-1.145446	-2.978067	-2.513040
19C	-1.765638	-3.939018	-1.708219
20C	-1.528034	-3.951393	-0.328710
21C	-0.677637	-3.001874	0.241919

22C	3.961597	5.257643	-0.357165
23H	1.566597	2.172091	-2.743372
24H	2.797226	4.309424	-2.462553
25H	3.654868	3.454790	1.516036
26H	2.459284	1.311489	1.422374
27H	2.442258	-1.786094	2.608788
28H	4.619619	-2.948512	2.939492
29H	6.055784	-3.474662	0.976172
30H	5.315587	-2.830712	-1.311647
31H	3.148515	-1.671684	-1.636418
32H	0.180860	-1.274212	-2.564996
33H	-1.327732	-2.965445	-3.584879
34H	-2.428591	-4.677151	-2.153077
35H	-2.006044	-4.697624	0.301311
36H	-0.504869	-3.004470	1.314829
37H	4.537470	5.284987	0.568868
38H	4.641359	5.388547	-1.202760
39H	3.224614	6.067114	-0.350442
40P	-3.491642	0.858720	0.487186
41C	-3.534866	-0.519253	-0.709477
42C	-3.518038	-0.069888	-2.176765
43C	-3.761079	0.215689	2.175220
44C	-1.871956	1.688388	0.396180
45C	-4.821529	2.052027	0.097650
46C	-1.786934	3.003204	1.182702
47C	-6.207799	1.411309	-0.055636
48C	-2.851129	-0.963820	2.549641
49H	-4.433391	-1.107752	-0.487809
50H	-2.671112	-1.153751	-0.485988
51H	-4.395187	0.535489	-2.430576
52H	-2.616850	0.505639	-2.413300
53H	-3.523050	-0.954306	-2.821840
54H	-4.819736	-0.061725	2.242205
55H	-3.605184	1.064682	2.852139
56H	-1.653256	1.848282	-0.665856
57H	-1.138231	0.967239	0.773856
58H	-4.525106	2.569224	-0.822725
59H	-4.819875	2.798989	0.900297
60H	-0.763898	3.389372	1.117818
61H	-2.461162	3.768384	0.782891
62H	-2.017022	2.858507	2.244391
63H	-6.527461	0.907224	0.862942
64H	-6.944749	2.189098	-0.283287
65H	-6.226924	0.682129	-0.872694
66H	-3.030158	-1.234830	3.596251
67H	-3.068584	-1.843545	1.934867
68H	-1.790018	-0.719821	2.434658

10h-PhNCO-001

1C	0.673773	-2.501334	1.368832
2C	-0.683946	-2.654568	1.376358
3N	-1.457233	-2.304035	0.302702
4C	-0.837791	-1.863279	-0.834619
5C	0.515330	-1.693306	-0.907225
6C	1.364342	-1.946294	0.233709
7N	2.669630	-1.707479	0.321703
8P	3.535895	-0.887988	-0.831562
9C	3.121408	0.890531	-0.578620
10O	3.391018	-1.234035	-2.302498
11C	5.262571	-1.056310	-0.264105
12C	6.283318	-0.709409	-1.164422
13C	7.623339	-0.792559	-0.779110
14C	7.955726	-1.226042	0.509553
15C	6.944040	-1.577982	1.408844
16C	5.601745	-1.491848	1.025634
17C	2.563986	1.620779	-1.637704
18C	2.211808	2.963815	-1.463117
19C	2.422291	3.588431	-0.229822
20C	2.982838	2.866035	0.830684
21C	3.327500	1.523845	0.657862
22C	-2.960025	-2.346190	0.438109
23O	-3.375737	-2.924523	1.458351
24N	-3.533695	-1.704304	-0.553596
25C	-4.915178	-1.539836	-0.643025
26C	-5.892040	-2.004473	0.272679
27C	-7.248021	-1.730938	0.065567
28C	-7.679360	-0.992589	-1.041446
29C	-6.724617	-0.529047	-1.956953
30C	-5.371581	-0.798595	-1.760448
31H	1.245994	-2.771213	2.250850
32H	-1.232847	-3.037073	2.227511
33H	-1.502304	-1.647031	-1.659359
34H	0.950651	-1.357951	-1.841230
35H	6.026536	-0.384058	-2.169388
36H	8.406791	-0.525465	-1.484274

37H	8.999005	-1.294006	0.808776
38H	7.198686	-1.922339	2.408484
39H	4.814777	-1.772737	1.718425
40H	2.415915	1.133801	-2.597682
41H	1.782731	3.521576	-2.292297
42H	2.157884	4.634614	-0.095543
43H	3.151821	3.349041	1.790066
44H	3.761937	0.968264	1.485309
45H	-5.577813	-2.575851	1.136569
46H	-7.976059	-2.103694	0.783882
47H	-8.736356	-0.786709	-1.192319
48H	-7.037016	0.041817	-2.829324
49H	-4.631480	-0.443608	-2.474126
50P	-1.807939	2.141250	0.619062
51C	-1.293000	3.876269	0.367474
52C	-2.410646	4.804726	-0.126338
53C	-0.361700	1.189433	1.194961
54C	-3.125088	2.085599	1.883911
55C	-2.434710	1.439874	-0.938938
56C	-3.553405	0.663500	2.274162
57C	-1.434729	1.493949	-2.102030
58C	0.114244	1.565030	2.603807
59H	-0.460696	3.846472	-0.344416
60H	-0.882542	4.227114	1.321625
61H	-2.821992	4.471856	-1.085536
62H	-3.231905	4.872914	0.595279
63H	-2.007905	5.813690	-0.268342
64H	0.435243	1.342278	0.459477
65H	-0.641152	0.133273	1.152657
66H	-3.975576	2.649819	1.484030
67H	-2.747504	2.640176	2.751644
68H	-3.352374	1.988669	-1.182234
69H	-2.730286	0.402692	-0.727371
70H	-4.330143	0.717758	3.044522
71H	-3.967969	0.116781	1.423484
72H	-2.720253	0.082856	2.683217
73H	-0.505748	0.967176	-1.864942
74H	-1.878314	1.006010	-2.976855
75H	-1.186951	2.522952	-2.384384
76H	1.003815	0.975051	2.846452
77H	0.385184	2.623309	2.677665
78H	-0.648819	1.348740	3.359364

10h-PhNCO-002

1C	-1.101017	-2.552131	-1.498394
2C	0.251415	-2.744996	-1.509988
3N	1.035379	-2.439420	-0.430983
4C	0.429757	-2.002459	0.715165
5C	-0.915430	-1.779745	0.787090
6C	-1.769459	-1.979305	-0.359963
7N	-3.062547	-1.674780	-0.446692
8P	-3.859092	-0.810782	0.725321
9C	-3.207868	0.912074	0.615786
10O	-3.843100	-1.263705	2.174311
11C	-5.567517	-0.708117	0.088067
12C	-6.605760	-0.533227	1.015794
13C	-7.928336	-0.409780	0.580944
14C	-8.222960	-0.457755	-0.785738
15C	-7.191731	-0.633232	-1.715578
16C	-5.868651	-0.756648	-1.282003
17C	-3.060937	1.663646	1.790568
18C	-2.593485	2.980697	1.735513
19C	-2.269531	3.558335	0.503970
20C	-2.407864	2.812409	-0.672809
21C	-2.874961	1.496501	-0.617069
22C	2.533696	-2.488437	-0.577187
23O	2.939102	-2.953460	-1.659466
24N	3.125269	-1.987140	0.482855
25C	4.510301	-1.876203	0.588836
26C	5.462046	-2.084519	-0.440410
27C	6.825665	-1.890013	-0.199042
28C	7.291064	-1.488765	1.057526
29C	6.361705	-1.282223	2.085936
30C	5.000330	-1.468677	1.853673
31H	-1.681980	-2.790509	-2.383767
32H	0.788621	-3.121851	-2.370727
33H	1.098139	-1.837375	1.548263
34H	-1.338702	-1.442197	1.726142
35H	-6.374015	-0.506637	2.077217
36H	-8.726900	-0.281905	1.307887
37H	-9.252073	-0.364565	-1.124774
38H	-7.418317	-0.678907	-2.778317
39H	-5.071068	-0.906810	-2.003527
40H	-3.308850	1.208447	2.745716
41H	-2.481077	3.552908	2.653443

42H	-1.910866	4.584266	0.459964
43H	-2.158500	3.256840	-1.633675
44H	-2.979984	0.921737	-1.533452
45H	5.123321	-2.402746	-1.418201
46H	7.533288	-2.058670	-1.008896
47H	8.354234	-1.345566	1.234987
48H	6.699909	-0.974991	3.073712
49H	4.279677	-1.309458	2.652929
50P	2.595840	2.121739	-0.442715
51C	2.907133	3.878978	-0.046664
52C	3.307659	4.737719	-1.253963
53C	2.154528	1.245076	1.093691
54C	1.230148	2.041510	-1.653026
55C	4.090383	1.371187	-1.173581
56C	0.741447	0.618516	-1.951764
57C	5.368125	1.596771	-0.355277
58C	0.777463	1.628932	1.653201
59H	3.687856	3.894065	0.723114
60H	1.990349	4.259608	0.419531
61H	4.225189	4.370356	-1.726918
62H	2.517298	4.765713	-2.011863
63H	3.490771	5.766433	-0.924791
64H	2.950269	1.472695	1.813353
65H	2.228318	0.171777	0.878739
66H	1.592889	2.536735	-2.561680
67H	0.415286	2.654827	-1.250436
68H	4.188561	1.783679	-2.184711
69H	3.885662	0.299896	-1.277586
70H	-0.040787	0.654353	-2.716893
71H	1.545902	-0.021953	-2.327750
72H	0.312565	0.151720	-1.062462
73H	5.290245	1.162054	0.645397
74H	6.205638	1.104359	-0.858199
75H	5.608752	2.661777	-0.261885
76H	0.587362	1.062638	2.571001
77H	0.722637	2.693903	1.902930
78H	-0.029703	1.398981	0.952234

10h-PhNCO-003

1C	-0.834986	-1.424306	-1.500201
2C	0.506936	-1.580098	-1.713923
3N	1.342167	-2.095288	-0.764454
4C	0.804063	-2.554066	0.408340
5C	-0.531083	-2.452006	0.672785
6C	-1.437058	-1.807872	-0.244863
7N	-2.698571	-1.617356	0.126404
8P	-3.801077	-0.703153	-0.703788
9C	-5.381346	-1.093171	0.128970
10O	-3.943376	-0.802206	-2.212323
11C	-3.445449	1.044696	-0.237453
12C	-2.868617	1.383071	0.997212
13C	-2.652785	2.722768	1.332966
14C	-3.013736	3.737773	0.439669
15C	-3.582822	3.407686	-0.794699
16C	-3.796739	2.067746	-1.131320
17C	-6.571902	-0.882862	-0.584051
18C	-7.809305	-1.126616	0.018648
19C	-7.866993	-1.583437	1.339603
20C	-6.683240	-1.799988	2.053825
21C	-5.445328	-1.554303	1.453000
22C	2.828001	-2.005482	-0.989257
23O	3.170675	-1.901027	-2.182045
24N	3.469500	-1.985981	0.157367
25C	4.849448	-1.795126	0.235434
26C	5.731394	-1.508137	-0.837145
27C	7.088722	-1.267849	-0.597942
28C	7.616380	-1.308380	0.696470
29C	6.758055	-1.600824	1.765609
30C	5.404006	-1.836727	1.537999
31H	-1.448761	-1.002349	-2.287837
32H	0.992051	-1.287709	-2.636898
33H	1.515516	-2.975151	1.105627
34H	-0.919823	-2.830128	1.613147
35H	-2.587271	0.598079	1.693813
36H	-2.210772	2.974332	2.294239
37H	-2.851244	4.780093	0.704194
38H	-3.859050	4.192219	-1.495331
39H	-4.230902	1.807298	-2.092875
40H	-6.524951	-0.539948	-1.614332
41H	-8.725787	-0.964639	-0.543836
42H	-8.829076	-1.775104	1.809023
43H	-6.723269	-2.162932	3.078214
44H	-4.527392	-1.732490	2.005011
45H	5.344027	-1.476371	-1.847236
46H	7.740748	-1.048747	-1.441687

47H	8.673498	-1.122541	0.870272
48H	7.146417	-1.642185	2.781290
49H	4.737462	-2.055569	2.369373
50P	2.241034	2.041637	0.199492
51C	1.031299	3.274912	-0.392972
52C	0.050491	2.720445	-1.435553
53C	3.130732	1.314882	-1.214273
54C	3.418135	2.880244	1.316971
55C	1.382799	0.703907	1.089274
56C	4.510806	1.954375	1.869959
57C	0.774251	1.129390	2.430821
58C	3.820168	2.336023	-2.125851
59H	1.609019	4.113930	-0.798735
60H	0.494941	3.650318	0.487067
61H	-0.625019	3.518238	-1.758096
62H	0.571446	2.341693	-2.321661
63H	-0.565069	1.914101	-1.025900
64H	2.404361	0.714122	-1.770891
65H	3.855994	0.611513	-0.794224
66H	2.823020	3.318348	2.127395
67H	3.853614	3.714346	0.754197
68H	2.107110	-0.109486	1.212520
69H	0.608646	0.334864	0.408572
70H	5.155657	2.520729	2.550816
71H	4.087302	1.113739	2.429066
72H	5.140456	1.546940	1.072763
73H	0.218642	0.286293	2.854999
74H	1.546904	1.417444	3.151596
75H	0.076059	1.965427	2.317314
76H	4.322060	1.801300	-2.939486
77H	3.106200	3.035206	-2.575158
78H	4.582049	2.913743	-1.590462

10h-PhNCO-004

1C	0.361686	-1.366356	-2.465625
2C	-0.979043	-1.634043	-2.463782
3N	-1.689930	-1.747307	-1.300798
4C	-1.015314	-1.706505	-0.112956
5C	0.322261	-1.438743	-0.049344
6C	1.079959	-1.136796	-1.240296
7N	2.319020	-0.650329	-1.294623
8P	3.124779	-0.100245	0.047556
9C	3.640676	-1.551685	1.049120
10O	2.428077	0.918847	0.939065
11C	4.671285	0.581264	-0.642638
12C	5.392815	1.503479	0.132193
13C	6.600379	2.027695	-0.336616
14C	7.096624	1.634618	-1.584594
15C	6.380785	0.717878	-2.362013
16C	5.173011	0.191952	-1.893695
17C	3.983461	-2.770130	0.441579
18C	4.364505	-3.864534	1.221891
19C	4.408231	-3.750111	2.616354
20C	4.069766	-2.538256	3.227590
21C	3.686683	-1.443020	2.446715
22C	-3.196978	-1.779323	-1.366542
23O	-3.663656	-2.075340	-2.481940
24N	-3.715720	-1.434290	-0.210351
25C	-5.092115	-1.324959	-0.012106
26C	-6.110553	-1.487134	-0.984462
27C	-7.454792	-1.305328	-0.643664
28C	-7.834954	-0.960914	0.657673
29C	-6.838879	-0.800206	1.630529
30C	-5.496898	-0.978369	1.300182
31H	0.880888	-1.242947	-3.410818
32H	-1.564705	-1.737162	-3.368659
33H	-1.623692	-1.873980	0.764794
34H	0.791701	-1.399982	0.926546
35H	5.003786	1.814698	1.098505
36H	7.151157	2.743415	0.269091
37H	8.035939	2.042461	-1.950610
38H	6.760076	0.413622	-3.334762
39H	4.611375	-0.511515	-2.500753
40H	3.943086	-2.866292	-0.640582
41H	4.622512	-4.806129	0.743038
42H	4.702390	-4.603109	3.223240
43H	4.099567	-2.446789	4.310874
44H	3.412770	-0.502567	2.917746
45H	-5.838287	-1.753704	-1.997568
46H	-8.214795	-1.436829	-1.411910
47H	-8.883637	-0.824503	0.910796
48H	-7.109925	-0.536215	2.651030
49H	-4.725417	-0.852962	2.056185
50P	-1.631086	2.513308	0.457874
51C	-3.097839	3.161406	-0.418210

52C	-3.769597	2.137275	-1.344592
53C	-0.426961	1.858603	-0.737431
54C	-0.872301	3.885037	1.396872
55C	-2.117645	1.173604	1.596465
56C	0.300232	3.446830	2.287868
57C	-3.047939	1.621944	2.731592
58C	0.055706	2.874947	-1.779455
59H	-2.762906	4.042658	-0.978495
60H	-3.797221	3.519587	0.346667
61H	-4.641869	2.597101	-1.821950
62H	-3.092185	1.803962	-2.138170
63H	-4.114231	1.253762	-0.798761
64H	-0.906746	1.003808	-1.223007
65H	0.416159	1.473182	-0.152412
66H	-1.669444	4.351223	1.988115
67H	-0.548808	4.626819	0.656947
68H	-1.184742	0.754886	1.991032
69H	-2.593010	0.392635	0.990251
70H	0.732466	4.328109	2.775077
71H	-0.029433	2.758927	3.074195
72H	1.091052	2.949024	1.716753
73H	-3.275506	0.761869	3.370276
74H	-2.588562	2.391419	3.361993
75H	-3.998239	2.007701	2.348435
76H	0.775410	2.381997	-2.441787
77H	-0.765177	3.255654	-2.397671
78H	0.566309	3.724934	-1.313322

10h-PhNCO-005

1C	-0.584857	-2.206813	-1.674231
2C	0.772648	-2.355659	-1.701652
3N	1.536694	-2.243159	-0.572098
4C	0.906943	-2.051943	0.627182
5C	-0.447357	-1.895019	0.722329
6C	-1.285595	-1.895888	-0.454957
7N	-2.586261	-1.626042	-0.508691
8P	-3.477550	-1.021416	0.751878
9C	-3.171900	0.797370	0.723846
10O	-3.289737	-1.542405	2.165233
11C	-5.203086	-1.217357	0.187451
12C	-6.221617	-1.101043	1.147503
13C	-7.562389	-1.211587	0.771391
14C	-7.897609	-1.441544	-0.567820
15C	-6.887519	-1.564780	-1.527541
16C	-5.544790	-1.451783	-1.152949
17C	-2.622960	1.415575	1.856055
18C	-2.355895	2.789732	1.853350
19C	-2.644036	3.557210	0.720400
20C	-3.196793	2.946685	-0.412751
21C	-3.456821	1.574406	-0.411045
22C	3.040332	-2.246443	-0.705072
23O	3.462733	-2.585489	-1.826551
24N	3.606934	-1.827986	0.402758
25C	4.986156	-1.657175	0.520909
26C	5.962626	-1.872460	-0.483762
27C	7.313916	-1.615835	-0.229917
28C	7.742067	-1.143134	1.014957
29C	6.788392	-0.932291	2.020361
30C	5.439669	-1.183869	1.776568
31H	-1.148039	-2.281621	-2.599060
32H	1.329402	-2.546661	-2.610142
33H	1.564265	-2.015745	1.484577
34H	-0.892566	-1.755929	1.700549
35H	-5.961088	-0.934424	2.189609
36H	-8.343666	-1.124595	1.522717
37H	-8.941295	-1.530203	-0.860259
38H	-7.143505	-1.752619	-2.567718
39H	-4.758951	-1.557198	-1.894488
40H	-2.413366	0.817426	2.738738
41H	-1.931831	3.259331	2.738114
42H	-2.444250	4.625913	0.719932
43H	-3.425280	3.539467	-1.295431
44H	-3.887578	1.106965	-1.293264
45H	5.651971	-2.238351	-1.453889
46H	8.040834	-1.791068	-1.021101
47H	8.795590	-0.949245	1.201827
48H	7.098661	-0.572304	2.999475
49H	4.700600	-1.020485	2.557885
50P	1.760578	2.301542	-0.479469
51C	1.775170	3.949656	-1.268898
52C	0.586409	4.839849	-0.880342
53C	3.140136	1.297228	-1.117439
54C	1.927674	2.506707	1.327098
55C	0.190301	1.454185	-0.846253
56C	1.850509	1.189240	2.110706

57C	-0.173460	1.426080	-2.335043
58C	4.524359	1.946058	-0.987396
59H	1.802415	3.777330	-2.351212
60H	2.725360	4.422564	-0.995766
61H	-0.370752	4.378776	-1.143873
62H	0.578513	5.057426	0.193016
63H	0.659118	5.793854	-1.413990
64H	2.909110	1.063273	-2.163531
65H	3.107140	0.354008	-0.561262
66H	1.133969	3.195251	1.639260
67H	2.884401	3.015151	1.498332
68H	-0.589806	1.951112	-0.261137
69H	0.288533	0.441122	-0.447033
70H	2.001349	1.395285	3.176141
71H	0.872636	0.710952	1.997253
72H	2.618053	0.477223	1.792319
73H	0.609137	0.954853	-2.939308
74H	-1.090511	0.843468	-2.465366
75H	-0.355236	2.433569	-2.725306
76H	5.277729	1.255164	-1.378869
77H	4.594790	2.881461	-1.553691
78H	4.779446	2.148928	0.058353

10h-PhNCO-006

1C	0.594895	-0.820087	-2.393809
2C	-0.720279	-1.186411	-2.446038
3N	-1.437198	-1.471432	-1.316335
4C	-0.791392	-1.459731	-0.111595
5C	0.521171	-1.100432	0.007699
6C	1.295467	-0.695156	-1.142036
7N	2.540395	-0.224759	-1.139283
8P	3.424288	0.000357	0.248229
9C	3.991278	-1.659405	0.797915
10O	2.811098	0.748724	1.420587
11C	4.925123	0.852405	-0.352426
12C	5.628028	1.668982	0.546956
13C	6.800003	2.316702	0.145884
14C	7.279888	2.151546	-1.157818
15C	6.582980	1.338975	-2.059316
16C	5.411136	0.690652	-1.659222
17C	4.230561	-2.695528	-0.118843
18C	4.667445	-3.945450	0.327676
19C	4.870495	-4.170336	1.694205
20C	4.633597	-3.142308	2.612953
21C	4.194841	-1.891894	2.166322
22C	-2.930088	-1.666730	-1.428796
23O	-3.347185	-1.835606	-2.589677
24N	-3.500801	-1.569897	-0.250299
25C	-4.881805	-1.642255	-0.075031
26C	-5.867666	-1.732923	-1.088609
27C	-7.226830	-1.742005	-0.759412
28C	-7.653241	-1.664801	0.570695
29C	-6.689033	-1.580163	1.584147
30C	-5.332378	-1.569746	1.265669
31H	1.119481	-0.581994	-3.313844
32H	-1.281680	-1.250686	-3.369444
33H	-1.402324	-1.736834	0.735735
34H	0.966554	-1.093839	0.995727
35H	5.248545	1.802447	1.556591
36H	7.335050	2.951113	0.848652
37H	8.190887	2.656098	-1.470977
38H	6.949872	1.212519	-3.075209
39H	4.864764	0.069301	-2.362518
40H	4.067055	-2.527261	-1.180063
41H	4.845147	-4.743841	-0.388871
42H	5.209383	-5.143754	2.040845
43H	4.786150	-3.314717	3.675873
44H	3.999475	-1.092879	2.876686
45H	-5.558893	-1.792117	-2.124570
46H	-7.962087	-1.811485	-1.559213
47H	-8.712983	-1.674398	0.814082
48H	-6.995737	-1.524726	2.626935
49H	-4.585111	-1.503663	2.053238
50P	-2.319237	2.468416	0.536519
51C	-2.436463	1.041473	1.663586
52C	-3.238534	1.315680	2.942294
53C	-1.359672	3.816075	1.311589
54C	-1.494584	1.927658	-0.997302
55C	-3.991428	3.095822	0.154152
56C	-1.229145	3.048178	-2.010336
57C	-4.903647	2.060584	-0.519895
58C	0.088169	3.429914	1.647677
59H	-1.405808	0.752554	1.897827
60H	-2.873861	0.217243	1.084306
61H	-3.220115	0.422445	3.576099

62H	-2.817391	2.143079	3.524885
63H	-4.286937	1.542804	2.722914
64H	-1.907284	4.124024	2.210307
65H	-1.390315	4.662314	0.614699
66H	-2.133757	1.151065	-1.428002
67H	-0.561853	1.440678	-0.697383
68H	-3.865129	3.983677	-0.476423
69H	-4.421177	3.439557	1.102726
70H	-0.755574	2.617960	-2.899347
71H	-2.153835	3.541555	-2.330688
72H	-0.550129	3.808023	-1.608811
73H	-5.885458	2.509956	-0.704823
74H	-4.502485	1.727888	-1.482979
75H	-5.054366	1.176908	0.107178
76H	0.600606	4.292617	2.087247
77H	0.134908	2.610108	2.371720
78H	0.649222	3.126633	0.758198

10h-PhNCO-007

1C	-0.771324	-1.046120	-2.299469
2C	-2.136330	-0.960162	-2.302480
3N	-2.861344	-0.931044	-1.145626
4C	-2.199870	-1.030577	0.044816
5C	-0.836518	-1.117834	0.114572
6C	-0.022421	-1.095594	-1.074689
7N	1.311847	-1.093094	-1.130572
8P	2.286143	-1.120200	0.205716
9C	2.223199	-2.810050	0.919188
10O	2.061105	-0.090339	1.306402
11C	3.964974	-0.939088	-0.491351
12C	4.990654	-0.523115	0.372847
13C	6.293525	-0.357295	-0.103295
14C	6.583091	-0.606730	-1.449746
15C	5.566011	-1.024197	-2.314908
16C	4.261971	-1.191787	-1.838610
17C	2.199987	-3.947698	0.096433
18C	2.148746	-5.224008	0.661655
19C	2.118879	-5.374147	2.053447
20C	2.138898	-4.244521	2.877701
21C	2.191030	-2.966276	2.312062
22C	-4.365543	-0.752577	-1.228244
23O	-4.815737	-0.739787	-2.389717
24N	-4.891226	-0.635629	-0.034264
25C	-6.259072	-0.446920	0.164739
26C	-7.254412	-0.295138	-0.833484
27C	-8.594020	-0.102811	-0.480041
28C	-8.992836	-0.056454	0.859758
29C	-8.019757	-0.205393	1.857682
30C	-6.682381	-0.394540	1.515353
31H	-0.235202	-1.054820	-3.243353
32H	-2.724097	-0.898898	-3.209283
33H	-2.836039	-1.021462	0.919412
34H	-0.372967	-1.175772	1.092686
35H	4.763755	-0.318751	1.416221
36H	7.080262	-0.032127	0.573412
37H	7.596520	-0.477121	-1.822195
38H	5.786723	-1.217308	-3.362121
39H	3.468790	-1.500411	-2.512660
40H	2.214626	-3.835601	-0.984876
41H	2.127478	-6.100179	0.018039
42H	2.076693	-6.368098	2.492269
43H	2.110336	-4.357342	3.958908
44H	2.197603	-2.083276	2.945508
45H	-6.968841	-0.331153	-1.877014
46H	-9.335661	0.009680	-1.269127
47H	-10.037776	0.090769	1.122533
48H	-8.305135	-0.174520	2.907556
49H	-5.928029	-0.509524	2.290735
50P	1.287494	3.549977	0.307671
51C	2.453588	3.117885	1.640685
52C	3.747955	3.940412	1.635528
53C	2.143357	3.538264	-1.306068
54C	-0.071914	2.339288	0.328670
55C	0.636472	5.241126	0.558960
56C	-1.068403	2.480015	-0.828032
57C	-0.128844	5.436341	1.874806
58C	2.812095	2.202097	-1.653469
59H	2.648194	2.043543	1.533090
60H	1.906375	3.243662	2.583128
61H	4.370280	3.639106	2.485584
62H	4.329515	3.770610	0.722822
63H	3.557569	5.016148	1.728060
64H	2.879009	4.351144	-1.272210
65H	1.395522	3.816710	-2.058100
66H	-0.571020	2.451725	1.298771

67H	0.406461	1.355293	0.341922
68H	-0.001872	5.464813	-0.303998
69H	1.496661	5.919100	0.501591
70H	-1.872832	1.749663	-0.700239
71H	-1.525967	3.475582	-0.860512
72H	-0.593371	2.285656	-1.795000
73H	-0.487528	6.469541	1.937104
74H	-1.000633	4.776104	1.941462
75H	0.509196	5.251334	2.745934
76H	3.304877	2.285688	-2.628538
77H	3.573144	1.925861	-0.917734
78H	2.090224	1.382980	-1.710906

10h-PhNCO-008

1C	0.788225	-1.058259	2.283029
2C	2.152661	-0.966178	2.283342
3N	2.873865	-0.918476	1.124845
4C	2.209710	-1.005283	-0.065086
5C	0.846427	-1.099242	-0.132233
6C	0.036177	-1.098591	1.059830
7N	-1.297600	-1.109240	1.121808
8P	-2.283151	-1.122725	-0.205008
9C	-2.219202	-2.800880	-0.946332
10O	-2.080721	-0.073414	-1.291765
11C	-3.957233	-0.963270	0.510881
12C	-4.988207	-0.503392	-0.323998
13C	-6.287375	-0.358291	0.169344
14C	-6.568001	-0.673175	1.503749
15C	-5.545463	-1.134490	2.339920
16C	-4.245606	-1.281799	1.846065
17C	-1.973817	-3.939886	-0.163077
18C	-1.938044	-5.206011	-0.753378
19C	-2.148357	-5.344838	-2.130170
20C	-2.391855	-4.213372	-2.915953
21C	-2.425152	-2.946025	-2.326417
22C	4.378465	-0.745475	1.206932
23O	4.834116	-0.779946	2.365854
24N	4.898285	-0.573260	0.016970
25C	6.270307	-0.412483	-0.179838
26C	7.289667	-0.521295	0.799390
27C	8.633683	-0.354348	0.450361
28C	9.012941	-0.071933	-0.865941
29C	8.015860	0.040426	-1.844669
30C	6.674373	-0.129164	-1.507252
31H	0.254580	-1.081271	3.228064
32H	2.743003	-0.914775	3.189085
33H	2.843328	-0.981244	-0.941369
34H	0.380176	-1.148422	-1.109728
35H	-4.768528	-0.247752	-1.357412
36H	-7.078173	0.000900	-0.485114
37H	-7.578301	-0.559994	1.889718
38H	-5.758865	-1.378377	3.378011
39H	-3.449522	-1.627390	2.498531
40H	-1.803065	-3.836576	0.905443
41H	-1.740791	-6.082568	-0.140893
42H	-2.118528	-6.330375	-2.588601
43H	-2.549909	-4.316574	-3.986961
44H	-2.600322	-2.062865	-2.935064
45H	7.018440	-0.737293	1.824785
46H	9.393914	-0.446857	1.224211
47H	10.061122	0.056941	-1.125408
48H	8.286056	0.257781	-2.876355
49H	5.902653	-0.048632	-2.269791
50P	-1.308308	3.554666	-0.283483
51C	-0.667307	5.250902	-0.526891
52C	0.091867	5.458153	-1.844481
53C	0.058403	2.352582	-0.315288
54C	-2.155813	3.529395	1.334570
55C	-2.476612	3.125163	-1.615453
56C	-2.785610	2.178452	1.696815
57C	-3.773635	3.943393	-1.604167
58C	1.055876	2.494439	0.840602
59H	-0.026474	5.472202	0.334787
60H	-1.530372	5.924490	-0.461793
61H	0.445937	6.493247	-1.901327
62H	0.966076	4.802007	-1.918860
63H	-0.548728	5.276086	-2.714369
64H	0.554987	2.472721	-1.285792
65H	-0.414093	1.365838	-0.332044
66H	-2.913525	4.321816	1.298511
67H	-1.412086	3.834734	2.080251
68H	-2.667243	2.049764	-1.512237
69H	-1.931429	3.257150	-2.558220
70H	-3.282155	2.259599	2.670196
71H	-3.536944	1.870588	0.963909

72H	-2.040976	1.380915	1.764949
73H	-4.394894	3.646245	-2.456492
74H	-4.354722	3.764806	-0.692829
75H	-3.587046	5.020454	-1.688669
76H	1.865453	1.770640	0.708027
77H	1.506031	3.493246	0.877519
78H	0.583718	2.292025	1.807391

10h-PhNCO-009

1C	0.231315	-1.093870	-2.442525
2C	-1.108141	-1.368122	-2.467809
3N	-1.829150	-1.549793	-1.321171
4C	-1.172107	-1.536602	-0.124478
5C	0.162910	-1.261481	-0.031432
6C	0.948041	-0.954133	-1.202437
7N	2.217669	-0.551319	-1.228212
8P	3.089093	-0.206618	0.139489
9C	3.480234	-1.787034	0.991086
10O	2.510899	0.782241	1.142314
11C	4.681197	0.391100	-0.525068
12C	5.465271	1.229194	0.282961
13C	6.708236	1.683076	-0.167136
14C	7.177797	1.301093	-1.428581
15C	6.399442	0.467317	-2.239180
16C	5.155985	0.013279	-1.790288
17C	3.516613	-1.818072	2.392815
18C	3.809853	-3.008603	3.065294
19C	4.068469	-4.176577	2.340378
20C	4.031612	-4.152126	0.941113
21C	3.739227	-2.962647	0.268941
22C	-3.334212	-1.648731	-1.408683
23O	-3.773849	-1.856856	-2.555146
24N	-3.879524	-1.452235	-0.231477
25C	-5.260211	-1.475241	-0.033145
26C	-6.261325	-1.644638	-1.022380
27C	-7.615748	-1.631634	-0.673847
28C	-8.023223	-1.453287	0.652276
29C	-7.044434	-1.284757	1.641371
30C	-5.692454	-1.294262	1.303586
31H	0.761096	-0.932032	-3.376017
32H	-1.683202	-1.433260	-3.382782
33H	-1.792299	-1.737739	0.737429
34H	0.617001	-1.253753	0.952462
35H	5.095623	1.530785	1.259742
36H	7.307475	2.334953	0.464130
37H	8.144806	1.653509	-1.779762
38H	6.758320	0.172550	-3.222543
39H	4.545705	-0.623328	-2.423793
40H	3.305487	-0.909612	2.950848
41H	3.833086	-3.024543	4.152543
42H	4.293800	-5.103269	2.862851
43H	4.226662	-5.059708	0.374760
44H	3.704336	-2.949854	-0.817558
45H	-5.967277	-1.787126	-2.054394
46H	-8.361800	-1.765543	-1.455269
47H	-9.079276	-1.448156	0.911508
48H	-7.336806	-1.147901	2.680794
49H	-4.933849	-1.167067	2.073068
50P	-1.303389	2.852113	0.454484
51C	-2.657592	3.866143	1.147078
52C	-2.226304	4.795992	2.289561
53C	-1.981999	1.767936	-0.845779
54C	-0.039211	3.964563	-0.256675
55C	-0.548235	1.850128	1.776266
56C	1.086346	3.239350	-1.008772
57C	-1.545591	0.964237	2.537105
58C	-2.677551	2.513466	-1.993377
59H	-3.433925	3.166087	1.478706
60H	-3.080447	4.440247	0.314557
61H	-1.813805	4.237095	3.136812
62H	-1.475976	5.523290	1.960152
63H	-3.097155	5.354458	2.650098
64H	-2.672347	1.069843	-0.359521
65H	-1.139558	1.178294	-1.219316
66H	0.364093	4.543896	0.582105
67H	-0.568958	4.669215	-0.909447
68H	-0.055530	2.556130	2.455883
69H	0.254803	1.260288	1.319638
70H	1.801333	3.979750	-1.385073
71H	1.628852	2.546905	-0.358131
72H	0.704840	2.678962	-1.869219
73H	-2.114409	0.311347	1.868307
74H	-0.995549	0.326416	3.237894
75H	-2.258893	1.560729	3.116847
76H	-3.017247	1.785188	-2.737461

77H	-3.557178	3.065776	-1.645521
78H	-2.002012	3.214767	-2.495684

10h-PhNCO-010

1C	0.942629	1.356034	-0.811012
2C	2.292799	1.281780	-1.030738
3N	3.142887	0.684282	-0.148846
4C	2.630904	0.156599	1.003456
5C	1.293525	0.201746	1.281864
6C	0.351791	0.797213	0.374370
7N	-0.947007	0.756260	0.685230
8P	-2.158576	1.364421	-0.259871
9C	-3.659526	0.925778	0.691787
10O	-2.297094	0.880385	-1.697267
11C	-2.057154	3.195491	-0.226247
12C	-1.703698	3.884222	0.945189
13C	-1.630296	5.279085	0.946070
14C	-1.908456	5.996646	-0.223668
15C	-2.257769	5.315362	-1.394036
16C	-2.333241	3.918859	-1.395204
17C	-4.893778	0.950080	0.022137
18C	-6.070597	0.607932	0.692492
19C	-6.024926	0.234007	2.040849
20C	-4.799414	0.209660	2.714827
21C	-3.621443	0.556102	2.044543
22C	4.621629	0.615089	-0.487556
23O	4.920169	1.136941	-1.578071
24N	5.292087	0.005810	0.458225
25C	6.670158	-0.198159	0.382609
26C	7.522861	0.134370	-0.699995
27C	8.892855	-0.139956	-0.638197
28C	9.462766	-0.743643	0.487381
29C	8.632269	-1.077256	1.566207
30C	7.265478	-0.810763	1.512324
31H	0.321390	1.827024	-1.564395
32H	2.766349	1.683055	-1.917632
33H	3.362770	-0.292997	1.660324
34H	0.927786	-0.229893	2.208161
35H	-1.478665	3.330486	1.853403
36H	-1.353267	5.805961	1.856066
37H	-1.848562	7.082396	-0.222618
38H	-2.468053	5.869492	-2.305857
39H	-2.594423	3.381909	-2.303140
40H	-4.928303	1.223414	-1.029443
41H	-7.020560	0.628827	0.163690
42H	-6.940099	-0.033328	2.563894
43H	-4.759126	-0.078596	3.762773
44H	-2.668626	0.528039	2.564154
45H	7.102896	0.606130	-1.578922
46H	9.521855	0.126529	-1.485919
47H	10.529730	-0.950463	0.524992
48H	9.052778	-1.546848	2.453474
49H	6.621938	-1.070312	2.350161
50P	-2.094675	-3.236040	-0.564773
51C	-1.428285	-2.612491	1.012975
52C	-0.178995	-3.364401	1.491950
53C	-2.648624	-4.965754	-0.354788
54C	-3.496744	-2.193325	-1.082014
55C	-0.792979	-3.213765	-1.847108
56C	-4.279505	-2.745427	-2.280562
57C	-0.044031	-1.876423	-1.943046
58C	-3.778789	-5.133649	0.669256
59H	-2.240073	-2.687110	1.746500
60H	-1.224495	-1.542616	0.875483
61H	0.159996	-2.935022	2.440842
62H	-0.378131	-4.428843	1.661414
63H	0.645093	-3.277858	0.776440
64H	-1.766433	-5.549363	-0.066481
65H	-2.957504	-5.323015	-1.344373
66H	-3.081317	-1.205453	-1.313858
67H	-4.145062	-2.072984	-0.206970
68H	-1.287255	-3.463206	-2.793841
69H	-0.106301	-4.037278	-1.617405
70H	-5.076856	-2.039613	-2.538246
71H	-3.642523	-2.858519	-3.164795
72H	-4.745598	-3.712626	-2.062591
73H	0.666138	-1.917741	-2.776313
74H	-0.721476	-1.032956	-2.110824
75H	0.526670	-1.675064	-1.032171
76H	-4.059582	-6.190712	0.732637
77H	-3.471018	-4.809092	1.669455
78H	-4.672180	-4.566808	0.385333

10h-PhNCO-011

1C	0.949260	1.391274	-0.776307
2C	2.299921	1.326539	-0.995040
3N	3.154402	0.740778	-0.109565
4C	2.646890	0.223739	1.049612
5C	1.309501	0.263891	1.329321
6C	0.362024	0.835897	0.412609
7N	-0.937885	0.779228	0.717221
8P	-2.147551	1.360157	-0.248519
9C	-3.654506	0.910425	0.688180
10O	-2.260608	0.860342	-1.682612
11C	-2.072579	3.192795	-0.232399
12C	-1.727643	3.897966	0.931709
13C	-1.674048	5.293687	0.918730
14C	-1.963564	5.995647	-0.257640
15C	-2.304865	5.297998	-1.420766
16C	-2.360449	3.900667	-1.408093
17C	-4.878218	0.892518	-0.000667
18C	-6.059087	0.547388	0.661461
19C	-6.027800	0.212789	2.020395
20C	-4.812654	0.229874	2.713283
21C	-3.631160	0.579550	2.051403
22C	4.631519	0.669073	-0.454602
23O	4.934817	1.237422	-1.520172
24N	5.293993	-0.001608	0.454585
25C	6.669964	-0.215655	0.368518
26C	7.550571	0.279086	-0.626394
27C	8.916468	-0.018558	-0.580759
28C	9.453974	-0.810537	0.439027
29C	8.595543	-1.306367	1.429994
30C	7.233680	-1.013253	1.394148
31H	0.324564	1.849215	-1.534778
32H	2.770201	1.724887	-1.884996
33H	3.381472	-0.215111	1.710698
34H	0.948173	-0.157899	2.261945
35H	-1.493439	3.356177	1.844751
36H	-1.403251	5.833422	1.823053
37H	-1.918815	7.082091	-0.267426
38H	-2.523793	5.840171	-2.337730
39H	-2.614620	3.351333	-2.310669
40H	-4.901007	1.136570	-1.059717
41H	-7.000949	0.536011	0.118071
42H	-6.946068	-0.056421	2.537029
43H	-4.783404	-0.028290	3.769386
44H	-2.686397	0.583049	2.586277
45H	7.156388	0.892019	-1.426843
46H	9.567428	0.376768	-1.358728
47H	10.517352	-1.036829	0.463224
48H	8.990220	-1.923742	2.234768
49H	6.569002	-1.396765	2.165216
50P	-2.075448	-3.256558	-0.555120
51C	-1.611538	-2.573570	1.068726
52C	-0.458457	-3.311275	1.762211
53C	-2.641645	-4.984101	-0.362032
54C	-3.419719	-2.236743	-1.239716
55C	-0.649784	-3.257183	-1.694357
56C	-3.979168	-2.744040	-2.575153
57C	0.072291	-1.904843	-1.778768
58C	-3.932050	-5.126803	0.456532
59H	-2.520974	-2.600182	1.681151
60H	-1.367975	-1.514976	0.911842
61H	-0.249771	-2.827303	2.722445
62H	-0.702642	-4.360313	1.965963
63H	0.461898	-3.279272	1.168810
64H	-1.815612	-5.535368	0.102808
65H	-2.768578	-5.393436	-1.371231
66H	-3.019205	-1.221989	-1.352152
67H	-4.200273	-2.194550	-0.471210
68H	-1.042793	-3.562630	-2.671728
69H	0.030310	-4.050822	-1.362542
70H	-4.791227	-2.082038	-2.895442
71H	-3.216307	-2.731978	-3.361141
72H	-4.384199	-3.759610	-2.498964
73H	0.843775	-1.952243	-2.555093
74H	-0.610106	-1.084221	-2.023568
75H	0.566711	-1.661685	-0.834303
76H	-4.189554	-6.187511	0.550417
77H	-3.819968	-4.719596	1.467555
78H	-4.774841	-4.619081	-0.024987

10h-PhNCO-012

1C	-0.718836	-1.108850	-0.821382
2C	-2.059486	-1.006287	-1.080688
3N	-2.984217	-0.856624	-0.090863

4C	-2.557882	-0.839845	1.208915
5C	-1.234301	-0.941737	1.533378
6C	-0.214604	-1.056777	0.526210
7N	1.065840	-1.077188	0.905310
8P	2.337114	-1.164138	-0.148699
9C	3.792338	-0.957523	0.936469
10O	2.408946	-0.177114	-1.307435
11C	2.426634	-2.879760	-0.792772
12C	2.081880	-3.979383	0.009177
13C	2.152668	-5.276058	-0.505901
14C	2.569413	-5.484160	-1.826103
15C	2.913446	-4.392298	-2.629792
16C	2.842351	-3.093992	-2.114973
17C	4.980632	-0.479447	0.362188
18C	6.119354	-0.286772	1.149152
19C	6.080260	-0.574193	2.518129
20C	4.900232	-1.056926	3.094804
21C	3.760705	-1.248829	2.308069
22C	-4.442235	-0.687926	-0.472796
23O	-4.655284	-0.719228	-1.700061
24N	-5.192428	-0.526081	0.588431
25C	-6.573311	-0.345102	0.503532
26C	-7.367592	-0.384477	-0.670145
27C	-8.751365	-0.193324	-0.601156
28C	-9.391546	0.045957	0.619112
29C	-8.619018	0.088260	1.788026
30C	-7.239951	-0.103751	1.729565
31H	-0.036347	-1.204432	-1.658070
32H	-2.466483	-1.026177	-2.083542
33H	-3.344502	-0.732343	1.943102
34H	-0.938880	-0.917207	2.577784
35H	1.749112	-3.820631	1.031758
36H	1.878670	-6.122367	0.119410
37H	2.621338	-6.493543	-2.227103
38H	3.231523	-4.550278	-3.657679
39H	3.096235	-2.240420	-2.737959
40H	5.006631	-0.245104	-0.698915
41H	7.033461	0.089636	0.695994
42H	6.964948	-0.422672	3.132097
43H	4.865076	-1.279812	4.158642
44H	2.839199	-1.603685	2.759368
45H	-6.892025	-0.566993	-1.625071
46H	-9.334420	-0.232462	-1.519788
47H	-10.468121	0.193792	0.660830
48H	-9.094970	0.270719	2.749686
49H	-6.642446	-0.073467	2.638109
50P	1.543263	3.512836	-0.399887
51C	1.074836	5.233004	-0.810781
52C	0.736386	5.463332	-2.289413
53C	3.023349	3.006429	-1.335078
54C	1.881340	3.477961	1.395916
55C	0.189154	2.373930	-0.835808
56C	2.412559	2.136450	1.916415
57C	-1.081329	2.541846	0.005421
58C	4.313595	3.729310	-0.930189
59H	1.909788	5.869745	-0.494827
60H	0.222430	5.486406	-0.168851
61H	0.479625	6.517048	-2.444443
62H	1.583524	5.227636	-2.942869
63H	-0.121646	4.861498	-2.607717
64H	2.792334	3.172487	-2.394429
65H	3.101499	1.920082	-1.202738
66H	0.945587	3.756797	1.895172
67H	2.596301	4.287472	1.587734
68H	0.605375	1.365111	-0.754807
69H	-0.018308	2.536378	-1.900402
70H	2.591957	2.210012	2.994910
71H	1.706294	1.318340	1.749431
72H	3.358073	1.863946	1.439105
73H	-1.850026	1.855811	-0.363032
74H	-0.902522	2.304169	1.058636
75H	-1.486009	3.558671	-0.056743
76H	5.137855	3.368642	-1.555574
77H	4.243828	4.814882	-1.066720
78H	4.578672	3.527459	0.113108

10h-001

1C	0.288888	2.427011	-2.027975
2C	0.609817	3.775944	-2.064655
3N	0.363887	4.651660	-1.066222
4C	-0.243589	4.128104	0.017704
5C	-0.601723	2.794229	0.164598
6C	-0.339187	1.859141	-0.880964
7N	-0.603999	0.524304	-0.869036
8P	-1.340509	-0.246878	0.370017

9C	-1.538449	-1.956791	-0.261358
10O	-0.690182	-0.282075	1.751735
11C	-3.064775	0.380685	0.541214
12C	-3.667326	0.427879	1.806573
13C	-4.980171	0.888884	1.949334
14C	-5.700800	1.308876	0.826261
15C	-5.102957	1.271860	-0.439171
16C	-3.791562	0.810356	-0.580262
17C	-1.761105	-2.985512	0.667298
18C	-1.913602	-4.307365	0.241098
19C	-1.843937	-4.615450	-1.122502
20C	-1.626558	-3.595227	-2.055096
21C	-1.477206	-2.271892	-1.627051
22H	0.517619	1.785517	-2.876038
23H	1.094586	4.189834	-2.949079
24H	-0.448523	4.826442	0.829133
25H	-1.064397	2.468317	1.091420
26H	-3.098235	0.110700	2.676483
27H	-5.438700	0.922367	2.935169
28H	-6.721401	1.668245	0.936122
29H	-5.656304	1.606546	-1.313654
30H	-3.325569	0.792136	-1.562355
31H	-1.797843	-2.748638	1.727521
32H	-2.080500	-5.096086	0.971210
33H	-1.959483	-5.644334	-1.455728
34H	-1.572425	-3.829280	-3.116049
35H	-1.297996	-1.479623	-2.347881
36P	3.367251	-0.365839	0.337732
37C	5.152012	0.029083	0.252432
38C	5.890712	-0.081116	1.593147
39C	2.641991	-0.152484	-1.318119
40C	3.187646	-2.098760	0.889692
41C	2.544037	0.741859	1.527605
42C	1.747435	-2.624555	0.828589
43C	2.757516	2.234180	1.235897
44C	3.154688	-1.150061	-2.365158
45H	5.227839	1.044389	-0.154309
46H	5.588303	-0.647073	-0.492476
47H	5.472638	0.598361	2.343960
48H	5.856214	-1.100339	1.994106
49H	6.943989	0.185620	1.452158
50H	2.859431	0.878715	-1.619295
51H	1.551592	-0.216980	-1.198965
52H	3.578568	-2.139798	1.913052
53H	3.859695	-2.698950	0.264070
54H	2.934104	0.475153	2.517756
55H	1.477364	0.480588	1.523376
56H	1.720386	-3.654335	1.202326
57H	1.066841	-2.021369	1.435393
58H	1.361954	-2.631058	-0.195594
59H	2.364182	2.518074	0.255501
60H	2.219571	2.824012	1.984723
61H	3.816206	2.514649	1.284530
62H	2.670472	-0.939201	-3.325203
63H	4.238140	-1.076699	-2.514741
64H	2.912023	-2.183557	-2.094742

10h-002

1C	-0.914382	2.919912	-1.639773
2C	-1.230003	4.265188	-1.516293
3N	-1.834088	4.816386	-0.441938
4C	-2.134782	3.955091	0.551309
5C	-1.862222	2.592972	0.535445
6C	-1.219839	2.002575	-0.593199
7N	-0.861884	0.697692	-0.738657
8P	-1.205030	-0.487222	0.330409
9C	-0.493949	-1.976250	-0.475324
10O	-0.701630	-0.416734	1.771215
11C	-3.023081	-0.777480	0.353957
12C	-3.669457	-1.070106	1.563379
13C	-5.051493	-1.285562	1.593813
14C	-5.797922	-1.212364	0.413140
15C	-5.159284	-0.919238	-0.797959
16C	-3.779579	-0.701519	-0.826421
17C	-0.129655	-2.006801	-1.829596
18C	0.441312	-3.157136	-2.384805
19C	0.647974	-4.291901	-1.592970
20C	0.278544	-4.272965	-0.242679
21C	-0.286430	-3.121173	0.311165
22H	-0.429964	2.550260	-2.540605
23H	-0.986002	4.951604	-2.327262
24H	-2.622991	4.389942	1.423531
25H	-2.123487	1.986493	1.397599
26H	-3.084566	-1.117401	2.478175
27H	-5.544809	-1.506810	2.537715

28H	-6.872450	-1.378779	0.435876
29H	-5.736535	-0.854544	-1.717476
30H	-3.288803	-0.463408	-1.767042
31H	-0.282650	-1.121767	-2.439366
32H	0.723651	-3.166864	-3.435295
33H	1.090446	-5.186438	-2.025341
34H	0.435254	-5.152197	0.378139
35H	-0.554027	-3.101619	1.364666
36P	3.255594	0.423638	0.430487
37C	2.473961	0.714886	-1.188366
38C	2.973618	1.979837	-1.900066
39C	3.007328	1.860324	1.531322
40C	2.532410	-1.064856	1.191231
41C	5.057033	0.191184	0.215277
42C	3.245586	-1.519946	2.471027
43C	5.429056	-1.051225	-0.605264
44C	1.546626	2.324912	1.627941
45H	1.388828	0.755536	-1.016298
46H	2.664212	-0.182146	-1.789689
47H	2.462237	2.075594	-2.863973
48H	2.753996	2.882384	-1.319979
49H	4.051720	1.948720	-2.096611
50H	3.656944	2.663296	1.162541
51H	3.393898	1.561318	2.513438
52H	2.540607	-1.852153	0.429323
53H	1.481143	-0.830381	1.398878
54H	5.492734	0.142735	1.220261
55H	5.443282	1.102826	-0.255208
56H	2.719444	-2.389381	2.880634
57H	4.285193	-1.813637	2.287247
58H	3.237214	-0.739155	3.239566
59H	6.519558	-1.125857	-0.680868
60H	5.062788	-1.971360	-0.137277
61H	5.027524	-1.001378	-1.623360
62H	1.474221	3.136152	2.360967
63H	1.184164	2.708788	0.670423
64H	0.875388	1.518575	1.939923

10h-003

1C	-0.988857	2.912558	-1.646636
2C	-1.316856	4.256411	-1.541743
3N	-1.910458	4.820191	-0.468053
4C	-2.186807	3.973576	0.544800
5C	-1.902023	2.613828	0.548061
6C	-1.271180	2.010510	-0.580011
7N	-0.904817	0.706759	-0.709375
8P	-1.216862	-0.468542	0.380134
9C	-0.476298	-1.949906	-0.416030
10O	-0.712557	-0.374461	1.818343
11C	-3.027805	-0.803825	0.407901
12C	-3.618144	-1.335187	1.564327
13C	-4.987862	-1.615350	1.596376
14C	-5.780807	-1.362588	0.471572
15C	-5.200388	-0.826049	-0.683492
16C	-3.830708	-0.549434	-0.715106
17C	-0.336460	-2.066013	-1.807784
18C	0.242444	-3.207462	-2.369995
19C	0.685494	-4.249239	-1.546344
20C	0.543983	-4.144620	-0.158253
21C	-0.034430	-3.000899	0.401869
22H	-0.509884	2.531713	-2.546179
23H	-1.091830	4.931252	-2.367778
24H	-2.665813	4.418922	1.416841
25H	-2.145194	2.018885	1.423679
26H	-3.000897	-1.518011	2.439965
27H	-5.435963	-2.026547	2.498232
28H	-6.846531	-1.578177	0.496031
29H	-5.814257	-0.619137	-1.557169
30H	-3.384015	-0.125357	-1.610726
31H	-0.664241	-1.250315	-2.445261
32H	0.349328	-3.283068	-3.449858
33H	1.135581	-5.137319	-1.984167
34H	0.885230	-4.950671	0.487555
35H	-0.131687	-2.910845	1.480600
36P	3.289088	0.442567	0.352449
37C	2.369737	0.273689	-1.208197
38C	2.857047	1.186292	-2.340871
39C	3.204136	2.154337	0.981245
40C	2.583912	-0.710304	1.573960
41C	5.055171	0.043780	0.087107
42C	3.272716	-0.668283	2.944655
43C	5.302155	-1.379290	-0.432788
44C	1.775661	2.662734	1.220961
45H	1.310957	0.466477	-0.984112
46H	2.442963	-0.782357	-1.492384

47H	2.243494	1.004435	-3.230164
48H	2.752221	2.245539	-2.081202
49H	3.902108	0.996083	-2.611562
50H	3.730925	2.785096	0.255172
51H	3.794401	2.171375	1.905623
52H	2.651986	-1.709216	1.127703
53H	1.514482	-0.479376	1.664684
54H	5.562113	0.205013	1.045997
55H	5.451173	0.791334	-0.610285
56H	2.790767	-1.394833	3.608107
57H	4.337140	-0.923848	2.886269
58H	3.179602	0.316991	3.414746
59H	6.378773	-1.542421	-0.554112
60H	4.926074	-2.138061	0.262440
61H	4.828156	-1.543143	-1.406922
62H	1.815892	3.674464	1.639094
63H	1.203513	2.708878	0.291218
64H	1.224416	2.027328	1.920913

10h-004

1C	0.428581	-2.609537	-2.376570
2C	0.248933	-3.984818	-2.387149
3N	0.349574	-4.782868	-1.301550
4C	0.656277	-4.147956	-0.152436
5C	0.855591	-2.778720	-0.026417
6C	0.742114	-1.925178	-1.165945
7N	0.873481	-0.571549	-1.186579
8P	1.213363	0.330837	0.131999
9C	1.308118	2.035803	-0.534162
10O	0.281325	0.317499	1.344282
11C	2.923254	-0.041553	0.709376
12C	3.247071	0.102033	2.066762
13C	4.542462	-0.168704	2.519056
14C	5.525176	-0.590332	1.616695
15C	5.207774	-0.742277	0.261842
16C	3.913607	-0.468483	-0.188971
17C	1.113323	3.107936	0.350525
18C	1.171021	4.427494	-0.107272
19C	1.424441	4.688244	-1.458627
20C	1.622079	3.624639	-2.346435
21C	1.567596	2.305504	-1.886014
22H	0.325532	-2.035629	-3.294893
23H	0.005938	-4.487711	-3.323246
24H	0.743278	-4.781366	0.730614
25H	1.083114	-2.363974	0.951120
26H	2.476092	0.416273	2.765459
27H	4.783425	-0.055865	3.573827
28H	6.532195	-0.804612	1.967286
29H	5.966040	-1.079039	-0.441322
30H	3.666524	-0.596851	-1.239877
31H	0.903535	2.904287	1.397384
32H	1.015630	5.249590	0.587762
33H	1.467432	5.713896	-1.817843
34H	1.817786	3.821958	-3.397986
35H	1.707026	1.479162	-2.576503
36P	-3.367745	0.133219	0.479831
37C	-2.366343	-1.237033	-0.172507
38C	-3.035022	-2.613900	-0.086670
39C	-2.456054	1.702351	0.313124
40C	-4.950430	0.230501	-0.430842
41C	-3.734722	-0.155596	2.248181
42C	-5.834417	1.416709	-0.022445
43C	-2.507675	-0.547844	3.085817
44C	-2.173379	2.110035	-1.138671
45H	-1.431634	-1.205763	0.394331
46H	-2.110146	-0.985541	-1.206887
47H	-3.275875	-2.886874	0.947157
48H	-3.955033	-2.662364	-0.680391
49H	-2.342902	-3.367490	-0.476408
50H	-1.519059	1.551592	0.861629
51H	-3.043917	2.466997	0.835381
52H	-5.470146	-0.720448	-0.263519
53H	-4.699990	0.275339	-1.497552
54H	-4.504484	-0.935857	2.290677
55H	-4.190893	0.766604	2.627177
56H	-6.760133	1.401768	-0.608295
57H	-6.109968	1.372180	1.037294
58H	-5.336994	2.375056	-0.207889
59H	-1.700199	0.185888	3.006296
60H	-2.803093	-0.629196	4.138056
61H	-2.102751	-1.515346	2.772317
62H	-1.614087	3.051192	-1.144781
63H	-1.558727	1.364386	-1.651778
64H	-3.096028	2.261934	-1.710887

10h-005

1C	-0.503442	2.887362	-1.746865
2C	-0.651023	4.265383	-1.679049
3N	-1.218560	4.926927	-0.648134
4C	-1.659662	4.147326	0.360251
5C	-1.560201	2.762424	0.399399
6C	-0.959743	2.054778	-0.684159
7N	-0.767907	0.710417	-0.775967
8P	-1.249881	-0.372897	0.347307
9C	-0.771700	-1.976819	-0.405586
10O	-0.708680	-0.311918	1.774543
11C	-3.090080	-0.415909	0.412548
12C	-3.737973	-0.713429	1.620540
13C	-5.134549	-0.757765	1.683327
14C	-5.895488	-0.502602	0.537377
15C	-5.255884	-0.201724	-0.670900
16C	-3.860590	-0.158302	-0.732262
17C	-0.546133	-3.071510	0.443889
18C	-0.177615	-4.314198	-0.079011
19C	-0.031201	-4.475653	-1.461786
20C	-0.258184	-3.390625	-2.315767
21C	-0.627500	-2.148223	-1.790484
22H	-0.036759	2.426726	-2.614944
23H	-0.294091	4.885923	-2.501250
24H	-2.120107	4.671390	1.197807
25H	-1.929013	2.227042	1.269470
26H	-3.142414	-0.899252	2.510597
27H	-5.627872	-0.986078	2.625526
28H	-6.981565	-0.533897	0.585650
29H	-5.843478	0.004501	-1.562606
30H	-3.366926	0.085149	-1.669646
31H	-0.645220	-2.939599	1.518250
32H	-0.001885	-5.153414	0.590188
33H	0.256981	-5.441272	-1.870923
34H	-0.143549	-3.509736	-3.390834
35H	-0.788267	-1.301933	-2.451094
36P	3.314539	0.132570	0.437579
37C	5.071534	-0.323340	0.208975
38C	5.891630	0.705943	-0.580924
39C	2.436277	-1.253685	1.226598
40C	3.216897	1.616269	1.499383
41C	2.553202	0.485442	-1.180008
42C	1.802618	2.204427	1.616762
43C	2.751931	-0.629027	-2.215644
44C	3.047514	-1.725637	2.552638
45H	5.076477	-1.297516	-0.294994
46H	5.495837	-0.478872	1.207893
47H	5.487269	0.862428	-1.586748
48H	5.928567	1.674726	-0.070856
49H	6.921422	0.346885	-0.687028
50H	2.409262	-2.067489	0.492676
51H	1.402614	-0.920646	1.380974
52H	3.916416	2.351458	1.084104
53H	3.608160	1.318956	2.480142
54H	2.971581	1.436291	-1.531607
55H	1.480587	0.640360	-0.995107
56H	1.815493	3.030644	2.336452
57H	1.454709	2.602431	0.659510
58H	1.070630	1.464907	1.957048
59H	2.325379	-1.577160	-1.872694
60H	2.230092	-0.353230	-3.138607
61H	3.808518	-0.788012	-2.459464
62H	2.428129	-2.532463	2.959983
63H	4.064823	-2.114253	2.428929
64H	3.069225	-0.921600	3.296822

10h-006

1C	-0.450325	-2.887141	1.721880
2C	-0.584529	-4.266252	1.648933
3N	-1.156957	-4.928555	0.621250
4C	-1.617136	-4.148686	-0.378335
5C	-1.532002	-2.762668	-0.411868
6C	-0.927152	-2.054118	0.668611
7N	-0.749145	-0.708178	0.765630
8P	-1.258159	0.376388	-0.344147
9C	-0.799562	1.983328	0.414712
10O	-0.727267	0.334545	-1.776009
11C	-3.099181	0.387650	-0.397399
12C	-3.759221	0.667616	-1.602993
13C	-5.156687	0.683245	-1.658540
14C	-5.906164	0.416894	-0.507631
15C	-5.254248	0.133648	0.698381

16C	-3.858081	0.119025	0.752605
17C	-0.677336	3.102711	-0.424024
18C	-0.325099	4.349488	0.099609
19C	-0.089369	4.490518	1.472365
20C	-0.210645	3.380505	2.315508
21C	-0.565650	2.133691	1.789659
22H	0.021190	-2.426100	2.587115
23H	-0.212178	-4.887016	2.464096
24H	-2.081469	-4.673419	-1.213307
25H	-1.915896	-2.227189	-1.275315
26H	-3.171950	0.861412	-2.496840
27H	-5.659539	0.897789	-2.598950
28H	-6.992898	0.425703	-0.550312
29H	-5.833029	-0.080991	1.593857
30H	-3.354422	-0.110952	1.688126
31H	-0.846028	2.989449	-1.491886
32H	-0.231831	5.208118	-0.561447
33H	0.186059	5.459700	1.881868
34H	-0.026567	3.483645	3.382575
35H	-0.646712	1.268043	2.439771
36P	3.307478	-0.107227	-0.454955
37C	5.074890	0.313300	-0.237432
38C	5.900815	-0.776317	0.460329
39C	2.419208	1.344243	-1.106397
40C	3.173021	-1.496859	-1.633363
41C	2.578222	-0.582325	1.145947
42C	1.770206	-2.117581	-1.706768
43C	2.855487	0.416098	2.278415
44C	3.048652	1.978863	-2.353369
45H	5.106333	1.251690	0.329857
46H	5.476275	0.529303	-1.234421
47H	5.527043	-0.984842	1.468293
48H	5.899610	-1.714305	-0.105734
49H	6.940761	-0.443389	0.550908
50H	2.356363	2.069397	-0.287206
51H	1.397595	1.008703	-1.321682
52H	3.918487	-2.242466	-1.333242
53H	3.485719	-1.101646	-2.607822
54H	2.961679	-1.579597	1.392500
55H	1.495485	-0.673211	0.976790
56H	1.758437	-2.885510	-2.488512
57H	1.496601	-2.599576	-0.763775
58H	0.999392	-1.376513	-1.940859
59H	2.504329	1.422551	2.027101
60H	2.312450	0.095774	3.174397
61H	3.920353	0.471114	2.530794
62H	2.413514	2.807298	-2.686236
63H	4.048083	2.381771	-2.154963
64H	3.119144	1.265355	-3.182119

10h-007

1C	-0.747571	2.863741	-1.861277
2C	-0.966490	4.232743	-1.805382
3N	-1.501325	4.882361	-0.749581
4C	-1.831313	4.099603	0.297821
5C	-1.652670	2.723207	0.351709
6C	-1.085169	2.028232	-0.757565
7N	-0.824002	0.694659	-0.838518
8P	-1.205573	-0.391583	0.320390
9C	-0.710788	-1.984378	-0.444356
10O	-0.595854	-0.296571	1.718141
11C	-3.037485	-0.496311	0.484394
12C	-3.605699	-0.835824	1.721162
13C	-4.994290	-0.924033	1.863018
14C	-5.827431	-0.670267	0.768087
15C	-5.267996	-0.326803	-0.468154
16C	-3.880221	-0.240251	-0.608676
17C	-0.321306	-3.041136	0.392933
18C	0.054330	-4.275199	-0.147132
19C	0.038843	-4.465814	-1.533330
20C	-0.354916	-3.418896	-2.374598
21C	-0.727952	-2.185554	-1.833088
22H	-0.313094	2.412609	-2.750803
23H	-0.699117	4.855575	-2.659182
24H	-2.263940	4.613771	1.156148
25H	-1.930411	2.185497	1.253487
26H	-2.954610	-1.019631	2.571795
27H	-5.425048	-1.185707	2.826920
28H	-6.907476	-0.734933	0.878019
29H	-5.911908	-0.119873	-1.319822
30H	-3.449844	0.037964	-1.567247
31H	-0.303049	-2.887081	1.468543
32H	0.358229	-5.085369	0.511924
33H	0.330503	-5.424645	-1.955751
34H	-0.365927	-3.561368	-3.452781

35H	-1.016189	-1.367460	-2.486321
36P	3.343242	0.215988	0.441976
37C	5.125247	-0.164039	0.256562
38C	5.868816	0.747871	-0.728688
39C	2.567842	-1.075509	1.466158
40C	3.186757	1.839881	1.263363
41C	2.540494	0.265184	-1.192768
42C	1.748931	2.377037	1.313940
43C	2.742809	-1.012204	-2.020083
44C	3.194463	-1.241462	2.857729
45H	5.196678	-1.214283	-0.050595
46H	5.564222	-0.094079	1.258897
47H	5.463706	0.664458	-1.743111
48H	5.821333	1.799525	-0.425627
49H	6.925258	0.459607	-0.765547
50H	2.629144	-2.007120	0.892015
51H	1.504068	-0.813573	1.550918
52H	3.848008	2.532997	0.729667
53H	3.601370	1.711473	2.270665
54H	2.940168	1.142690	-1.715515
55H	1.469745	0.448476	-1.022075
56H	1.724380	3.291648	1.916862
57H	1.384687	2.629586	0.315217
58H	1.051036	1.656140	1.751081
59H	2.320045	-1.889234	-1.520336
60H	2.223919	-0.901981	-2.977939
61H	3.800875	-1.206103	-2.231314
62H	2.659394	-2.031395	3.396582
63H	4.251893	-1.525878	2.810199
64H	3.107618	-0.323858	3.450414

10h-008

1C	-0.612732	2.755024	-2.162168
2C	-0.452660	4.130672	-2.098298
3N	-0.480129	4.855865	-0.958551
4C	-0.691945	4.144713	0.167087
5C	-0.863501	2.766814	0.219736
6C	-0.822184	1.990344	-0.977788
7N	-0.929082	0.637825	-1.078136
8P	-1.234651	-0.364377	0.175224
9C	-1.371422	-2.006661	-0.627068
10O	-0.265001	-0.463073	1.352481
11C	-2.919486	-0.012954	0.832477
12C	-3.183590	-0.177447	2.200046
13C	-4.457109	0.089962	2.713044
14C	-5.477606	0.525708	1.860946
15C	-5.220291	0.696054	0.495396
16C	-3.947608	0.428227	-0.015504
17C	-1.128098	-3.150880	0.148618
18C	-1.214274	-4.425981	-0.418316
19C	-1.547988	-4.569335	-1.769785
20C	-1.796680	-3.433251	-2.548193
21C	-1.710470	-2.158823	-1.979630
22H	-0.571514	2.241148	-3.119912
23H	-0.286933	4.696110	-3.015399
24H	-0.720800	4.719996	1.092794
25H	-1.010146	2.285576	1.182288
26H	-2.382553	-0.504486	2.857943
27H	-4.651674	-0.037292	3.775674
28H	-6.467505	0.736901	2.258932
29H	-6.008476	1.043037	-0.168871
30H	-3.746377	0.573369	-1.073971
31H	-0.857512	-3.037061	1.195315
32H	-1.018931	-5.305008	0.191832
33H	-1.614012	-5.560016	-2.213678
34H	-2.054912	-3.538896	-3.599548
35H	-1.886964	-1.275916	-2.586453
36P	3.445383	-0.124759	0.322012
37C	5.181134	0.325111	0.684346
38C	6.129863	-0.872613	0.826884
39C	2.422355	1.380616	0.346078
40C	3.389026	-0.907155	-1.328145
41C	2.821816	-1.290570	1.577656
42C	1.998601	-1.407073	-1.744349
43C	3.077909	-0.837881	3.022619
44C	2.808912	2.437939	-0.694826
45H	5.162909	0.922346	1.603804
46H	5.510625	0.990558	-0.122188
47H	5.818282	-1.544298	1.634217
48H	6.191393	-1.454583	-0.099361
49H	7.138133	-0.513657	1.061675
50H	2.485759	1.785797	1.362933
51H	1.392791	1.039294	0.213323
52H	4.115108	-1.728924	-1.306954
53H	3.769578	-0.161220	-2.036386

54H	3.285356	-2.263788	1.376449
55H	1.743267	-1.370062	1.392027
56H	2.058368	-1.847476	-2.746095
57H	1.624568	-2.177435	-1.063035
58H	1.261254	-0.599721	-1.773364
59H	2.615005	0.133646	3.227151
60H	2.632496	-1.564689	3.710714
61H	4.147857	-0.769682	3.250417
62H	2.122764	3.286318	-0.609190
63H	3.828685	2.810875	-0.543744
64H	2.725789	2.051667	-1.716103

10h-009

1C	-0.743478	2.771826	-2.205306
2C	-0.595383	4.148879	-2.143368
3N	-0.557735	4.867777	-0.999678
4C	-0.688866	4.148001	0.132607
5C	-0.841211	2.767890	0.187403
6C	-0.867209	1.998145	-1.014798
7N	-0.969119	0.645134	-1.114649
8P	-1.223546	-0.357735	0.148864
9C	-1.374009	-2.003243	-0.643379
10O	-0.216395	-0.440563	1.296020
11C	-2.889405	-0.025363	0.863077
12C	-3.084890	-0.125619	2.248074
13C	-4.341223	0.130222	2.807381
14C	-5.413932	0.488600	1.984238
15C	-5.226304	0.591768	0.600590
16C	-3.970544	0.336109	0.043609
17C	-1.153976	-3.144957	0.143346
18C	-1.249043	-4.422669	-0.415612
19C	-1.566905	-4.571708	-1.770509
20C	-1.791381	-3.438473	-2.559883
21C	-1.697324	-2.160934	-1.998941
22H	-0.758030	2.264044	-3.167058
23H	-0.496004	4.721154	-3.065780
24H	-0.665377	4.717791	1.061891
25H	-0.922789	2.279706	1.154106
26H	-2.244064	-0.394519	2.882007
27H	-4.481591	0.053804	3.883341
28H	-6.390555	0.690374	2.418179
29H	-6.056147	0.876093	-0.042360
30H	-3.825934	0.426284	-1.030128
31H	-0.894160	-3.028480	1.192643
32H	-1.072259	-5.299706	0.202958
33H	-1.639263	-5.564707	-2.208183
34H	-2.037260	-3.548243	-3.613785
35H	-1.855581	-1.279840	-2.613308
36P	3.473851	-0.123371	0.339405
37C	5.219112	0.348642	0.622044
38C	6.165467	-0.835628	0.861623
39C	2.461734	1.386835	0.216962
40C	3.395860	-1.070394	-1.222016
41C	2.858030	-1.154394	1.710434
42C	1.984303	-1.525871	-1.615184
43C	3.052454	-0.527391	3.098152
44C	2.743988	2.241466	-1.024877
45H	5.229403	1.037490	1.474817
46H	5.530218	0.927063	-0.255922
47H	5.889950	-1.400556	1.759100
48H	6.176980	-1.528101	0.012628
49H	7.186516	-0.463753	1.001982
50H	2.639442	1.957916	1.136209
51H	1.420876	1.052564	0.249077
52H	4.069196	-1.927111	-1.100041
53H	3.834860	-0.426072	-1.993299
54H	3.361382	-2.125820	1.636375
55H	1.789045	-1.297254	1.508800
56H	2.026034	-2.047312	-2.577993
57H	1.563769	-2.217551	-0.879794
58H	1.293678	-0.683505	-1.715710
59H	2.519661	0.425524	3.184264
60H	2.641407	-1.203082	3.856283
61H	4.109446	-0.359262	3.334887
62H	2.123696	3.142075	-0.986133
63H	3.793177	2.555380	-1.079901
64H	2.489679	1.707891	-1.946066

10h-010

1C	-0.699494	-1.672107	-2.429071
2C	-1.496585	-2.801291	-2.536295
3N	-1.684391	-3.707950	-1.551670

4C	-1.018446	-3.453851	-0.406906
5C	-0.200667	-2.352215	-0.186633
6C	-0.002810	-1.382289	-1.218021
7N	0.741150	-0.248382	-1.141825
8P	1.562069	0.220609	0.193775
9C	2.414593	1.749296	-0.348392
10O	0.817446	0.483420	1.500908
11C	2.925360	-0.976051	0.523093
12C	3.336088	-1.218648	1.842122
13C	4.368229	-2.124457	2.107865
14C	4.998463	-2.796789	1.055111
15C	4.591698	-2.562337	-0.263741
16C	3.560662	-1.656640	-0.527460
17C	2.692404	2.024353	-1.696005
18C	3.373731	3.192349	-2.052738
19C	3.787040	4.094992	-1.066424
20C	3.511902	3.828080	0.279407
21C	2.827995	2.662019	0.634864
22H	-0.601683	-0.986256	-3.267573
23H	-2.027150	-2.998226	-3.467958
24H	-1.158060	-4.180513	0.393761
25H	0.275099	-2.230173	0.781728
26H	2.835040	-0.702403	2.656905
27H	4.677678	-2.307382	3.134582
28H	5.799739	-3.502853	1.260819
29H	5.073771	-3.087953	-1.084848
30H	3.238996	-1.484848	-1.551709
31H	2.364272	1.326532	-2.460495
32H	3.581745	3.397695	-3.100467
33H	4.319639	5.001467	-1.344869
34H	3.827313	4.527443	1.050355
35H	2.604086	2.458199	1.678787
36P	-3.503731	0.711348	0.574168
37C	-3.691699	-0.836670	-0.367168
38C	-4.880791	-1.703268	0.062331
39C	-3.299453	0.341040	2.350967
40C	-2.041508	1.584829	-0.063278
41C	-5.000249	1.744155	0.384472
42C	-1.786585	2.956106	0.571360
43C	-5.298010	2.146106	-1.066372
44C	-2.172965	-0.660060	2.648342
45H	-2.748559	-1.379401	-0.251593
46H	-3.764406	-0.556245	-1.423532
47H	-4.889320	-2.618856	-0.538620
48H	-4.808868	-1.998945	1.115092
49H	-5.838233	-1.191392	-0.087634
50H	-4.268534	-0.025340	2.710881
51H	-3.115809	1.300953	2.848802
52H	-2.163455	1.661703	-1.149975
53H	-1.188558	0.923558	0.113201
54H	-4.854866	2.628200	1.016781
55H	-5.833263	1.176258	0.815522
56H	-0.865926	3.373944	0.150453
57H	-2.601099	3.662551	0.373823
58H	-1.643146	2.879719	1.654309
59H	-6.200414	2.766845	-1.095652
60H	-4.478339	2.726681	-1.503588
61H	-5.475166	1.270686	-1.701185
62H	-2.092366	-0.795464	3.733159
63H	-2.380860	-1.639486	2.204320
64H	-1.204671	-0.309006	2.275885

10h-011

1C	-0.699421	-1.672198	-2.436180
2C	-1.498995	-2.799703	-2.542539
3N	-1.689172	-3.705006	-1.557097
4C	-1.023270	-3.451111	-0.412282
5C	-0.203400	-2.350880	-0.192716
6C	-0.002774	-1.382523	-1.225072
7N	0.744068	-0.250446	-1.149757
8P	1.560781	0.219497	0.188052
9C	2.417721	1.746246	-0.352622
10O	0.810661	0.485171	1.491483
11C	2.921268	-0.978050	0.525558
12C	3.328086	-1.215925	1.846681
13C	4.358352	-2.121926	2.118867
14C	4.990591	-2.799255	1.070520
15C	4.587686	-2.569581	-0.250350
16C	3.558522	-1.663637	-0.520540
17C	2.701465	2.019282	-1.699394
18C	3.385923	3.185885	-2.054716
19C	3.796522	4.089089	-1.067792
20C	3.515465	3.824191	0.277215
21C	2.828373	2.659581	0.631238
22H	-0.599633	-0.987520	-3.275408

23H	-2.029536	-2.996457	-3.474255
24H	-1.164714	-4.176702	0.389041
25H	0.272012	-2.228779	0.775818
26H	2.825481	-0.695831	2.658059
27H	4.664812	-2.301089	3.147145
28H	5.790448	-3.505451	1.281234
29H	5.071323	-3.099108	-1.068015
30H	3.239885	-1.495558	-1.546356
31H	2.375558	1.320992	-2.464416
32H	3.598527	3.389660	-3.101827
33H	4.331588	4.994458	-1.345102
34H	3.828725	4.524015	1.048626
35H	2.599789	2.457425	1.674468
36P	-3.501501	0.713774	0.576024
37C	-3.688472	-0.833771	-0.366354
38C	-4.879156	-1.699817	0.059880
39C	-3.305918	0.343554	2.353887
40C	-2.035430	1.584744	-0.055157
41C	-4.996196	1.748362	0.381223
42C	-1.783996	2.957801	0.577081
43C	-5.289217	2.150048	-1.070657
44C	-2.179749	-0.655041	2.660548
45H	-2.745962	-1.377281	-0.249287
46H	-3.758646	-0.552433	-1.422668
47H	-4.887404	-2.614647	-0.542227
48H	-4.809457	-1.996868	1.112406
49H	-5.835866	-1.186913	-0.091232
50H	-4.276509	-0.025503	2.706921
51H	-3.128394	1.303705	2.853503
52H	-2.149590	1.658133	-1.142893
53H	-1.184142	0.923844	0.130671
54H	-4.851664	2.632432	1.013693
55H	-5.831239	1.181667	0.809930
56H	-0.860148	3.373635	0.161234
57H	-2.596545	3.664297	0.371938
58H	-1.647994	2.884559	1.661220
59H	-6.189954	2.773081	-1.102684
60H	-4.466980	2.728180	-1.506312
61H	-5.467044	1.274621	-1.705258
62H	-2.121717	-0.804465	3.745048
63H	-2.372294	-1.630008	2.200150
64H	-1.205372	-0.294547	2.313828

10h-012

1C	-0.526504	2.900245	-1.702166
2C	-0.533267	4.280930	-1.569068
3N	-0.849750	4.942524	-0.435055
4C	-1.182701	4.159204	0.610816
5C	-1.206266	2.770068	0.591773
6C	-0.864387	2.061785	-0.599710
7N	-0.801997	0.711169	-0.753806
8P	-1.301446	-0.369331	0.366769
9C	-0.947688	-1.981212	-0.437480
10O	-0.729497	-0.373439	1.780904
11C	-3.140701	-0.302789	0.478588
12C	-3.771846	-0.555040	1.705613
13C	-5.166483	-0.517374	1.806923
14C	-5.942694	-0.225779	0.680180
15C	-5.320028	0.030847	-0.547120
16C	-3.926731	-0.008053	-0.646716
17C	-0.875104	-3.126134	0.371775
18C	-0.601117	-4.377249	-0.187754
19C	-0.394440	-4.497258	-1.566845
20C	-0.468935	-3.361956	-2.381760
21C	-0.747907	-2.111538	-1.820690
22H	-0.265888	2.441689	-2.653130
23H	-0.270312	4.904614	-2.423676
24H	-1.443251	4.683215	1.530604
25H	-1.468606	2.226370	1.494587
26H	-3.163115	-0.770432	2.579925
27H	-5.646199	-0.711349	2.763785
28H	-7.027088	-0.194584	0.757972
29H	-5.919235	0.264654	-1.424210
30H	-3.445639	0.199933	-1.599075
31H	-1.020305	-3.030279	1.444549
32H	-0.544982	-5.255784	0.451067
33H	-0.179465	-5.469684	-2.004046
34H	-0.311740	-3.449732	-3.454561
35H	-0.798569	-1.227456	-2.448487
36P	3.398480	0.035986	0.312535
37C	4.950137	0.038512	1.280529
38C	5.971590	-1.024543	0.853956
39C	2.267019	1.286150	0.998073
40C	3.804336	0.436949	-1.422577
41C	2.635571	-1.618918	0.375970

42C	2.579678	0.565925	-2.338640
43C	2.233743	-2.070105	1.786831
44C	2.757102	2.731832	0.844889
45H	4.665960	-0.088653	2.331832
46H	5.370394	1.046524	1.183708
47H	5.579916	-2.039205	0.984086
48H	6.274016	-0.903416	-0.192297
49H	6.871566	-0.933043	1.471925
50H	2.110984	1.027628	2.051104
51H	1.308592	1.135047	0.494887
52H	4.481640	-0.349390	-1.776281
53H	4.379153	1.370601	-1.399467
54H	3.359572	-2.307993	-0.076024
55H	1.761252	-1.588266	-0.282969
56H	2.911643	0.828870	-3.349452
57H	2.016926	-0.370914	-2.400504
58H	1.893627	1.344950	-1.994452
59H	1.415874	-1.454752	2.173321
60H	1.876482	-3.104124	1.740212
61H	3.078434	-2.039707	2.485458
62H	2.013398	3.405692	1.282208
63H	3.710944	2.902047	1.357770
64H	2.872449	3.011773	-0.207493

10h-013

1C	0.357431	2.205818	-2.199708
2C	0.833176	3.506341	-2.268978
3N	0.820548	4.385151	-1.243224
4C	0.289690	3.917551	-0.095431
5C	-0.211844	2.634550	0.087218
6C	-0.195032	1.694106	-0.988284
7N	-0.617243	0.403191	-0.954417
8P	-1.379555	-0.308124	0.304872
9C	-1.932274	-1.911490	-0.393036
10O	-0.659015	-0.560754	1.627497
11C	-2.944360	0.602498	0.654308
12C	-3.452250	0.632725	1.961186
13C	-4.642118	1.311424	2.244182
14C	-5.333290	1.968930	1.220706
15C	-4.829990	1.947170	-0.085422
16C	-3.642232	1.266636	-0.366557
17C	-2.148774	-2.982304	0.487998
18C	-2.587561	-4.220065	0.008906
19C	-2.816127	-4.399466	-1.359889
20C	-2.605062	-3.335920	-2.244716
21C	-2.167418	-2.097924	-1.763567
22H	0.403645	1.556911	-3.071554
23H	1.256724	3.875156	-3.203161
24H	0.270739	4.619626	0.738296
25H	-0.601341	2.351858	1.060855
26H	-2.904250	0.129415	2.753346
27H	-5.026688	1.330005	3.261513
28H	-6.256691	2.500239	1.439703
29H	-5.359343	2.463832	-0.882730
30H	-3.249057	1.259841	-1.379967
31H	-1.958363	-2.845170	1.549269
32H	-2.747558	-5.043157	0.701654
33H	-3.156715	-5.362029	-1.734600
34H	-2.780069	-3.470332	-3.309824
35H	-1.992186	-1.276232	-2.451459
36P	3.418501	-0.483124	0.391073
37C	4.286929	-1.700736	1.442636
38C	5.217143	-2.648794	0.673450
39C	2.355457	0.574529	1.416498
40C	4.673891	0.538033	-0.462982
41C	2.392827	-1.348665	-0.849325
42C	4.082564	1.662860	-1.324663
43C	1.623113	-2.551840	-0.283316
44C	3.071804	1.285248	2.570716
45H	3.509407	-2.258645	1.977277
46H	4.844453	-1.130479	2.194745
47H	4.675828	-3.222983	-0.086514
48H	6.030520	-2.106417	0.179114
49H	5.668440	-3.362205	1.371821
50H	1.517372	-0.040003	1.766827
51H	1.914194	1.302687	0.727987
52H	5.274149	-0.147389	-1.073048
53H	5.336422	0.941870	0.312355
54H	3.057718	-1.648505	-1.668389
55H	1.684450	-0.608096	-1.240943
56H	4.895108	2.205500	-1.820580
57H	3.416513	1.272263	-2.100844
58H	3.517524	2.383292	-0.725017
59H	0.982119	-2.259859	0.553374
60H	0.974077	-2.958953	-1.065129

61H	2.297454	-3.349904	0.046269
62H	2.353578	1.933145	3.085254
63H	3.466826	0.576173	3.306875
64H	3.895645	1.917613	2.219971

10h-014

1C	0.430753	2.752417	1.885555
2C	0.363998	4.137548	1.853231
3N	0.632824	4.895080	0.768104
4C	0.992005	4.208066	-0.335308
5C	1.087442	2.824464	-0.418192
6C	0.799635	2.014910	0.721985
7N	0.811563	0.656222	0.780163
8P	1.309123	-0.328044	-0.426375
9C	1.010207	-2.001282	0.267913
10O	0.695977	-0.250751	-1.820948
11C	3.141739	-0.198687	-0.574379
12C	3.755260	-0.408587	-1.818279
13C	5.145336	-0.321726	-1.946819
14C	5.934402	-0.022585	-0.830811
15C	5.329147	0.192334	0.412926
16C	3.940212	0.103785	0.539968
17C	0.940748	-2.249443	1.647456
18C	0.693677	-3.541205	2.122990
19C	0.519521	-4.599996	1.224432
20C	0.594563	-4.362312	-0.152592
21C	0.837673	-3.069838	-0.626337
22H	0.202858	2.213719	2.802376
23H	0.079209	4.683338	2.752967
24H	1.213875	4.810387	-1.216501
25H	1.365909	2.361975	-1.360587
26H	3.136366	-0.628333	-2.684303
27H	5.611549	-0.482484	-2.916380
28H	7.015205	0.047558	-0.930121
29H	5.937948	0.432576	1.281613
30H	3.471826	0.279474	1.504988
31H	1.063279	-1.424964	2.343161
32H	0.636778	-3.720880	3.194291
33H	0.328018	-5.604521	1.594850
34H	0.460094	-5.180692	-0.856322
35H	0.877707	-2.878725	-1.695555
36P	-3.339612	0.046065	-0.209427
37C	-2.656059	-1.614429	-0.532853
38C	-3.507516	-2.765603	0.017456
39C	-3.414154	0.342377	1.594960
40C	-2.287620	1.277976	-1.040557
41C	-5.048857	0.161874	-0.847007
42C	-2.755670	2.728561	-0.876425
43C	-5.167796	0.006170	-2.369405
44C	-2.178657	-0.148389	2.363405
45H	-1.654772	-1.620294	-0.091851
46H	-2.515535	-1.701162	-1.615903
47H	-2.985202	-3.712484	-0.156900
48H	-3.671715	-2.671965	1.096959
49H	-4.484058	-2.823687	-0.476305
50H	-4.327641	-0.144455	1.957989
51H	-3.556370	1.421761	1.724634
52H	-2.252752	0.987149	-2.096661
53H	-1.276237	1.135633	-0.652417
54H	-5.443548	1.131595	-0.520224
55H	-5.628735	-0.608818	-0.324902
56H	-2.066512	3.386087	-1.415736
57H	-3.761449	2.887190	-1.283112
58H	-2.750633	3.041930	0.172698
59H	-6.223465	0.053103	-2.658958
60H	-4.639968	0.805323	-2.901005
61H	-4.769660	-0.954648	-2.713937
62H	-2.253708	0.171895	3.408913
63H	-2.113648	-1.241407	2.351346
64H	-1.246135	0.247012	1.947784

10h-015

1C	0.359511	-2.402923	1.774812
2C	0.704676	-3.746376	1.788333
3N	0.426846	-4.620475	0.797449
4C	-0.242692	-4.102100	-0.252867
5C	-0.634714	-2.774896	-0.373239
6C	-0.336722	-1.840640	0.664404
7N	-0.623775	-0.511775	0.673315
8P	-1.542710	0.252548	-0.444342
9C	-1.579249	1.977579	0.177366
10O	-1.153725	0.259039	-1.919181

11C	-3.279358	-0.344360	-0.287620
12C	-4.104772	-0.385209	-1.420892
13C	-5.428178	-0.826246	-1.318532
14C	-5.936820	-1.233965	-0.080660
15C	-5.117748	-1.200108	1.054144
16C	-3.796505	-0.757168	0.950578
17C	-1.380457	2.302040	1.528018
18C	-1.401739	3.636373	1.945442
19C	-1.627778	4.659945	1.017567
20C	-1.834871	4.343269	-0.329508
21C	-1.810445	3.008992	-0.745418
22H	0.618236	-1.761170	2.614341
23H	1.238897	-4.155886	2.645950
24H	-0.475525	-4.800566	-1.056665
25H	-1.152271	-2.449319	-1.270855
26H	-3.700777	-0.078554	-2.382145
27H	-6.059268	-0.856260	-2.203956
28H	-6.964885	-1.579638	-0.000567
29H	-5.506191	-1.523389	2.017251
30H	-3.160554	-0.739534	1.831999
31H	-1.191980	1.507890	2.244431
32H	-1.240237	3.877770	2.993777
33H	-1.642850	5.697729	1.342707
34H	-2.008786	5.134050	-1.055746
35H	-1.952511	2.761012	-1.793992
36P	3.494835	0.340760	-0.362965
37C	5.069173	1.271901	-0.344147
38C	5.464655	1.814697	1.035177
39C	2.168874	1.356937	0.357519
40C	3.152917	-0.098763	-2.102204
41C	3.661649	-1.175752	0.638131
42C	1.989623	-1.080196	-2.298578
43C	4.747623	-2.143011	0.150172
44C	1.880950	2.653306	-0.410635
45H	4.964078	2.086026	-1.071384
46H	5.837172	0.595226	-0.737347
47H	6.429872	2.327851	0.961726
48H	4.730990	2.535887	1.411320
49H	5.567976	1.013109	1.775072
50H	2.476721	1.569973	1.389108
51H	1.274884	0.720922	0.422578
52H	4.090988	-0.504978	-2.500806
53H	2.965311	0.844445	-2.629419
54H	2.676601	-1.655696	0.636766
55H	3.851454	-0.855589	1.669645
56H	1.890743	-1.302873	-3.367377
57H	2.163029	-2.026464	-1.776516
58H	1.037359	-0.660731	-1.962281
59H	4.751684	-3.031866	0.790389
60H	4.563564	-2.477016	-0.876689
61H	5.746581	-1.694422	0.193830
62H	1.102478	3.214745	0.114465
63H	2.767753	3.294342	-0.486474
64H	1.510273	2.446837	-1.419609

10h-016

1C	0.182632	2.385386	-2.092514
2C	0.516476	3.730356	-2.127531
3N	0.399949	4.578988	-1.082692
4C	-0.088229	4.031027	0.048012
5C	-0.451991	2.697634	0.195681
6C	-0.322145	1.790035	-0.899528
7N	-0.602402	0.459412	-0.896208
8P	-1.337348	-0.336789	0.329037
9C	-1.690419	-1.982749	-0.398508
10O	-0.651645	-0.523314	1.680342
11C	-3.000437	0.406650	0.614796
12C	-3.529343	0.443200	1.913015
13C	-4.790864	0.999191	2.149707
14C	-5.533810	1.526088	1.087965
15C	-5.011032	1.496134	-0.210487
16C	-3.751206	0.939001	-0.445210
17C	-1.927657	-3.057192	0.473149
18C	-2.209242	-4.330871	-0.028012
19C	-2.255851	-4.544445	-1.410546
20C	-2.022834	-3.478275	-2.286240
21C	-1.744284	-2.203350	-1.782518
22H	0.308509	1.765493	-2.977404
23H	0.907407	4.163326	-3.048313
24H	-0.190248	4.707338	0.896790
25H	-0.819413	2.350370	1.157010
26H	-2.941652	0.042251	2.734553
27H	-5.190921	1.024491	3.160922
28H	-6.513487	1.961672	1.270745
29H	-5.582112	1.910993	-1.037921

30H	-3.345068	0.925078	-1.453601
31H	-1.875864	-2.894267	1.546596
32H	-2.388084	-5.155672	0.658037
33H	-2.473508	-5.535413	-1.802378
34H	-2.056555	-3.639086	-3.361482
35H	-1.552103	-1.376824	-2.459830
36P	3.405328	-0.344994	0.367883
37C	4.471882	-1.355921	1.456606
38C	5.415976	-2.307736	0.707574
39C	2.337048	0.727496	1.376858
40C	4.489888	0.681451	-0.689280
41C	2.375855	-1.428500	-0.682470
42C	3.735295	1.643672	-1.617229
43C	1.744693	-2.608805	0.071267
44C	3.078516	1.576759	2.416944
45H	3.802191	-1.907454	2.127130
46H	5.040927	-0.655517	2.078986
47H	4.868750	-3.008760	0.067961
48H	6.129418	-1.759819	0.082152
49H	5.990334	-2.895367	1.432209
50H	1.569669	0.093106	1.835478
51H	1.801762	1.366224	0.666885
52H	5.114168	-0.011515	-1.265912
53H	5.157637	1.229681	-0.013660
54H	3.011012	-1.778849	-1.504670
55H	1.591089	-0.790543	-1.109058
56H	4.456436	2.204751	-2.222031
57H	3.066972	1.109192	-2.299906
58H	3.134971	2.365535	-1.055649
59H	1.110094	-2.265640	0.893078
60H	1.108023	-3.170960	-0.619099
61H	2.502654	-3.294201	0.465983
62H	2.354473	2.228117	2.918731
63H	3.559536	0.959769	3.184111
64H	3.840110	2.219557	1.960329

10h-017

1C	-0.324483	-2.004753	-2.479525
2C	-1.042098	-3.187302	-2.570179
3N	-1.310173	-4.007406	-1.529780
4C	-0.807751	-3.608385	-0.344242
5C	-0.078534	-2.443834	-0.137236
6C	0.190149	-1.558223	-1.225916
7N	0.838986	-0.366719	-1.167117
8P	1.491751	0.259884	0.193068
9C	2.227905	1.835418	-0.384701
10O	0.625600	0.530349	1.423856
11C	2.924122	-0.777564	0.712552
12C	3.232782	-0.905996	2.074898
13C	4.314166	-1.691880	2.486189
14C	5.095562	-2.359371	1.536937
15C	4.790947	-2.240033	0.175782
16C	3.710800	-1.453485	-0.233578
17C	2.426385	2.860370	0.553539
18C	2.988988	4.079854	0.165081
19C	3.359931	4.285988	-1.168246
20C	3.165115	3.268610	-2.109540
21C	2.603288	2.049019	-1.719868
22H	-0.158307	-1.393828	-3.363965
23H	-1.435174	-3.504754	-3.536070
24H	-1.011978	-4.264902	0.501897
25H	0.261741	-2.200630	0.864500
26H	2.614657	-0.395416	2.808708
27H	4.544005	-1.786001	3.545289
28H	5.934966	-2.973213	1.855387
29H	5.390714	-2.763817	-0.565065
30H	3.469468	-1.372656	-1.290492
31H	2.126721	2.701256	1.586270
32H	3.134426	4.867955	0.900468
33H	3.796167	5.234558	-1.472910
34H	3.448477	3.425350	-3.147970
35H	2.438446	1.263543	-2.451165
36P	-3.508019	0.641987	0.429839
37C	-3.403120	-0.774905	-0.712034
38C	-4.458425	-1.861943	-0.471802
39C	-2.117502	1.783141	0.146887
40C	-5.091381	1.515519	0.148049
41C	-3.461579	0.050406	2.158649
42C	-5.347703	2.678955	1.116282
43C	-2.313220	-0.927718	2.451792
44C	-1.892414	2.164321	-1.322734
45H	-2.393899	-1.184282	-0.605229
46H	-3.478496	-0.372072	-1.728242
47H	-4.371612	-2.296236	0.529946
48H	-5.478300	-1.481579	-0.597894

49H	-4.307113	-2.670428	-1.194567
50H	-1.222862	1.306294	0.568563
51H	-2.322886	2.670334	0.758636
52H	-5.888946	0.766308	0.217527
53H	-5.072045	1.867417	-0.890570
54H	-4.437183	-0.406143	2.365910
55H	-3.383277	0.944330	2.788626
56H	-6.290935	3.170750	0.853928
57H	-5.429491	2.332763	2.152427
58H	-4.554395	3.432988	1.067327
59H	-1.334995	-0.491022	2.226105
60H	-2.333816	-1.192218	3.515460
61H	-2.416830	-1.851681	1.874189
62H	-1.067566	2.882582	-1.379506
63H	-1.606481	1.294969	-1.922386
64H	-2.777223	2.630244	-1.773521

10h-018

1C	0.418162	1.909215	-2.831243
2C	1.372712	2.906498	-2.961678
3N	1.950800	3.559732	-1.928773
4C	1.523652	3.183340	-0.707115
5C	0.578879	2.195160	-0.460846
6C	-0.026282	1.486255	-1.543206
7N	-0.933852	0.478994	-1.457734
8P	-1.434913	-0.210746	-0.063936
9C	-2.785394	-1.323352	-0.604003
10O	-0.442540	-0.984524	0.804460
11C	-2.277749	1.040854	0.996620
12C	-2.192879	0.944992	2.393421
13C	-2.822464	1.891044	3.209087
14C	-3.541699	2.943839	2.633026
15C	-3.628904	3.047448	1.239599
16C	-2.999563	2.101058	0.426665
17C	-3.567385	-1.050958	-1.736979
18C	-4.615078	-1.904559	-2.093916
19C	-4.892898	-3.037958	-1.321069
20C	-4.117035	-3.316104	-0.190507
21C	-3.068886	-2.461732	0.165889
22H	0.005706	1.425804	-3.713857
23H	1.704480	3.205841	-3.955847
24H	1.976147	3.707590	0.135290
25H	0.314942	1.962970	0.565600
26H	-1.626677	0.129090	2.835452
27H	-2.750675	1.807937	4.291386
28H	-4.029853	3.681635	3.265643
29H	-4.181328	3.867899	0.787314
30H	-3.058928	2.190595	-0.655185
31H	-3.344012	-0.177744	-2.343030
32H	-5.211968	-1.686864	-2.976766
33H	-5.708255	-3.701357	-1.600353
34H	-4.325846	-4.198169	0.410688
35H	-2.459486	-2.678395	1.039506
36P	3.264074	-1.063323	0.473937
37C	2.318929	-1.048538	-1.080508
38C	2.831613	-2.027332	-2.143711
39C	4.992184	-0.553083	0.155956
40C	2.481485	0.078006	1.657409
41C	3.310259	-2.752447	1.167341
42C	3.082646	0.042972	3.068168
43C	1.927178	-3.329317	1.498274
44C	5.126945	0.871436	-0.401751
45H	2.338255	-0.018063	-1.450332
46H	1.281120	-1.257739	-0.801324
47H	2.211356	-1.930070	-3.041352
48H	3.869126	-1.821330	-2.431797
49H	2.765955	-3.067880	-1.806473
50H	5.412774	-1.288188	-0.540757
51H	5.539227	-0.660022	1.100530
52H	1.415093	-0.180145	1.654101
53H	2.566818	1.076310	1.215721
54H	3.945566	-2.705992	2.059956
55H	3.836029	-3.377657	0.436036
56H	2.571202	0.783917	3.692853
57H	2.950597	-0.935811	3.542763
58H	4.151569	0.287100	3.072861
59H	2.047151	-4.333062	1.921749
60H	1.391942	-2.711442	2.225324
61H	1.295614	-3.406337	0.608335
62H	6.182813	1.087598	-0.598696
63H	4.578746	0.996476	-1.341431
64H	4.758510	1.621239	0.306393

10h-019

1C	-0.806986	-1.634985	-2.441357
2C	-1.663453	-2.721579	-2.535946
3N	-1.833785	-3.653912	-1.572362
4C	-1.084481	-3.473767	-0.465795
5C	-0.203061	-2.420218	-0.260866
6C	-0.026842	-1.419105	-1.265709
7N	0.769189	-0.320905	-1.196771
8P	1.551446	0.147067	0.160966
9C	2.405776	1.685737	-0.349029
10O	0.760906	0.400901	1.444515
11C	2.916349	-1.034388	0.534497
12C	3.299220	-1.263319	1.864416
13C	4.333011	-2.157807	2.160316
14C	4.992222	-2.832993	1.127253
15C	4.613081	-2.612424	-0.202150
16C	3.580592	-1.717762	-0.496184
17C	2.686288	1.988846	-1.689945
18C	3.362337	3.167477	-2.021187
19C	3.767406	4.052845	-1.016044
20C	3.489212	3.758078	0.323359
21C	2.810481	2.581673	0.653293
22H	-0.727301	-0.925618	-3.262096
23H	-2.257157	-2.860731	-3.439676
24H	-1.207624	-4.223564	0.316072
25H	0.340199	-2.360266	0.677469
26H	2.775733	-0.745722	2.664153
27H	4.621239	-2.329825	3.195056
28H	5.794818	-3.530247	1.356458
29H	5.117839	-3.140294	-1.008041
30H	3.280473	-1.556553	-1.528737
31H	2.363764	1.304967	-2.469277
32H	3.572290	3.394763	-3.063966
33H	4.295770	4.967629	-1.274702
34H	3.797906	4.443910	1.109066
35H	2.584081	2.357413	1.692483
36P	-3.451984	0.779330	0.570113
37C	-3.407647	-1.041173	0.578739
38C	-4.594788	-1.704775	1.286399
39C	-3.452780	1.417117	2.282560
40C	-1.975023	1.379639	-0.298093
41C	-4.971469	1.369465	-0.255454
42C	-1.914814	2.899556	-0.486307
43C	-5.058538	0.979099	-1.737827
44C	-2.314915	0.855801	3.149445
45H	-2.458197	-1.317323	1.047900
46H	-3.338699	-1.365504	-0.465314
47H	-4.464153	-2.791978	1.257584
48H	-4.666138	-1.404007	2.337788
49H	-5.546191	-1.471145	0.795410
50H	-4.434595	1.192067	2.715614
51H	-3.381889	2.508798	2.200725
52H	-1.931099	0.855623	-1.258343
53H	-1.120410	1.026454	0.289230
54H	-4.996033	2.458934	-0.133132
55H	-5.820027	0.965697	0.309476
56H	-0.976752	3.153158	-0.992049
57H	-2.741133	3.275431	-1.100796
58H	-1.925073	3.430203	0.472585
59H	-5.999750	1.349316	-2.158848
60H	-4.237396	1.413304	-2.318191
61H	-5.035193	-0.107724	-1.873865
62H	-2.326963	1.353345	4.125757
63H	-2.435701	-0.219708	3.320541
64H	-1.330712	1.013541	2.694996

10h-020

1C	-0.999205	3.016137	-2.078643
2C	-0.950604	4.392561	-1.920757
3N	-0.942531	5.030413	-0.729132
4C	-0.996040	4.225289	0.350606
5C	-1.046551	2.837082	0.309493
6C	-1.042076	2.154279	-0.944156
7N	-1.050269	0.807896	-1.138077
8P	-1.195761	-0.289714	0.059271
9C	-1.150789	-1.895295	-0.828934
10O	-0.196004	-0.330854	1.215967
11C	-2.895664	-0.204369	0.767025
12C	-3.099616	-0.498683	2.123192
13C	-4.385461	-0.459984	2.672109
14C	-5.479794	-0.123141	1.868322
15C	-5.283462	0.178495	0.515448
16C	-3.998137	0.137836	-0.031875
17C	-0.851218	-3.054484	-0.094965

18C	-0.810799	-4.303359	-0.721274
19C	-1.068263	-4.406773	-2.093145
20C	-1.367734	-3.256815	-2.831696
21C	-1.411616	-2.008265	-2.202631
22H	-0.994134	2.576896	-3.073673
23H	-0.912761	5.034213	-2.801073
24H	-0.995152	4.728856	1.317674
25H	-1.073064	2.277243	1.239894
26H	-2.244103	-0.748862	2.745033
27H	-4.532414	-0.689376	3.725229
28H	-6.480002	-0.091465	2.294120
29H	-6.130234	0.449238	-0.111069
30H	-3.848098	0.380808	-1.080814
31H	-0.638747	-2.973484	0.968173
32H	-0.576076	-5.193026	-0.141158
33H	-1.036390	-5.377262	-2.583008
34H	-1.568620	-3.330897	-3.898156
35H	-1.637072	-1.114032	-2.775729
36P	3.424099	-0.113021	0.448877
37C	5.027335	0.043691	-0.414561
38C	5.913788	1.185511	0.101630
39C	2.469939	-1.470740	-0.299341
40C	3.760044	-0.484379	2.207399
41C	2.479372	1.441858	0.329832
42C	2.519559	-0.888088	3.017688
43C	2.404029	2.020757	-1.088692
44C	3.154125	-2.841699	-0.238138
45H	4.799464	0.171919	-1.479516
46H	5.535726	-0.922334	-0.309308
47H	5.424975	2.160612	-0.001380
48H	6.182398	1.045339	1.154484
49H	6.843434	1.216135	-0.477487
50H	2.253301	-1.181095	-1.334214
51H	1.515078	-1.470305	0.234725
52H	4.227167	0.414114	2.628307
53H	4.517054	-1.277867	2.225622
54H	2.945438	2.152683	1.022590
55H	1.479532	1.204344	0.712192
56H	2.807272	-1.030986	4.065598
57H	1.733016	-0.130022	2.971912
58H	2.089685	-1.825887	2.652605
59H	1.929030	1.323110	-1.785151
60H	1.791808	2.926983	-1.071199
61H	3.393486	2.288765	-1.475206
62H	2.489748	-3.590279	-0.683164
63H	4.098265	-2.859426	-0.794196
64H	3.356555	-3.149478	0.794243

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1C	-2.542445	-0.526165	-0.934553
2C	-3.928038	-0.484056	-0.818775
3N	-4.637634	-1.174870	0.090567
4C	-3.926860	-1.950562	0.923835
5C	-2.537672	-2.061745	0.906340
6C	-1.800604	-1.322169	-0.038624
7N	-0.397341	-1.383915	-0.073843
8P	0.528748	-0.152652	-0.840499
9C	-0.126045	1.404934	-0.157573
10O	0.517646	-0.161678	-2.347717
11C	2.210200	-0.368642	-0.172976
12C	2.501201	-0.252467	1.195961
13C	3.813292	-0.402751	1.646201
14C	4.842508	-0.664711	0.733249
15C	4.556957	-0.775212	-0.630602
16C	3.243094	-0.626421	-1.085236
17C	-0.591671	1.516738	1.161814
18C	-1.050829	2.745157	1.640275
19C	-1.048311	3.868250	0.804991
20C	-0.587041	3.760559	-0.510579
21C	-0.126277	2.532266	-0.992191
22C	0.245193	-2.599820	0.457758
23H	-2.058499	0.035756	-1.725129
24H	-4.501201	0.132525	-1.508345
25H	-4.497432	-2.515653	1.658765
26H	-2.050869	-2.704988	1.630812
27H	1.708876	-0.047265	1.910352
28H	4.034240	-0.312807	2.706740
29H	5.864514	-0.778540	1.086079
30H	5.354508	-0.974157	-1.341775
31H	3.013625	-0.706564	-2.143811
32H	-0.615771	0.644801	1.809957
33H	-1.418579	2.823352	2.660161
34H	-1.411077	4.822930	1.177586
35H	-0.589770	4.629295	-1.163916
36H	0.220280	2.441329	-2.017872

37H	-0.323554	-3.481037	0.145619
38H	1.254780	-2.694430	0.058641
39H	0.308450	-2.578955	1.552394

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1C	2.730420	-0.110640	-0.746012
2C	4.112576	-0.140019	-0.890906
3N	4.938518	-0.951884	-0.206507
4C	4.345563	-1.780350	0.665503
5C	2.971933	-1.838294	0.894718
6C	2.110502	-0.981574	0.177374
7N	0.725618	-0.995029	0.400783
8P	-0.352128	-0.165388	-0.667165
9C	-2.007357	-0.793203	-0.242563
10O	-0.024313	-0.365995	-2.122666
11C	-0.283215	1.582147	-0.162663
12C	0.155620	1.963583	1.113944
13C	0.170368	3.313641	1.474463
14C	-0.254423	4.286046	0.563006
15C	-0.690697	3.909354	-0.712292
16C	-0.704677	2.561158	-1.076684
17C	-2.903356	-0.078001	0.565793
18C	-4.174894	-0.596458	0.827656
19C	-4.555945	-1.827056	0.284576
20C	-3.666845	-2.539688	-0.528862
21C	-2.397563	-2.024340	-0.796149
22C	0.234050	-1.732545	1.576108
23H	2.158424	0.578639	-1.353442
24H	4.584520	0.535987	-1.601367
25H	5.004157	-2.446226	1.220697
26H	2.597185	-2.553156	1.616397
27H	0.496525	1.212035	1.820986
28H	0.517547	3.605369	2.462368
29H	-0.240340	5.336266	0.843630
30H	-1.015006	4.664523	-1.423712
31H	-1.033503	2.268858	-2.070474
32H	-2.615344	0.878787	0.991599
33H	-4.866290	-0.037358	1.452894
34H	-5.545382	-2.228194	0.489316
35H	-3.963761	-3.493123	-0.958011
36H	-1.712580	-2.572863	-1.437344
37H	0.326922	-2.815974	1.434385
38H	0.797016	-1.435455	2.467759
39H	-0.814965	-1.503518	1.751132

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1C	2.722157	-1.997030	0.495946
2C	3.708877	-2.159255	-0.474216
3N	3.631281	-1.683353	-1.727017
4C	2.502439	-1.019778	-2.030132
5C	1.449415	-0.808758	-1.146240
6C	1.544555	-1.289359	0.176781
7N	0.528576	-1.116970	1.124880
8P	-0.630206	0.162387	1.169194
9C	0.164290	1.592194	0.371971
10O	-1.044710	0.449080	2.589855
11C	-2.035837	-0.370605	0.142914
12C	-1.971466	-1.504054	-0.681421
13C	-3.082158	-1.883657	-1.440757
14C	-4.261805	-1.135756	-1.379951
15C	-4.335210	-0.010214	-0.550814
16C	-3.229119	0.369868	0.211249
17C	1.332501	2.103862	0.961256
18C	1.951989	3.231081	0.420622
19C	1.407433	3.857314	-0.706931
20C	0.241034	3.355369	-1.291141
21C	-0.380003	2.224013	-0.754987
22C	0.508339	-2.020606	2.291238
23H	2.887770	-2.408391	1.484386
24H	4.618267	-2.701827	-0.221991
25H	2.425045	-0.641894	-3.047809
26H	0.570681	-0.286986	-1.501971
27H	-1.061058	-2.094001	-0.728404
28H	-3.025237	-2.764332	-2.075338
29H	-5.124342	-1.431469	-1.971960
30H	-5.254360	0.567144	-0.493728
31H	-3.294349	1.238195	0.861898
32H	1.759040	1.619487	1.836300
33H	2.858884	3.620074	0.876306
34H	1.891813	4.734763	-1.127998
35H	-0.184954	3.839369	-2.166266
36H	-1.278359	1.832726	-1.223384

37H	-0.448401	-1.925839	2.804686
38H	0.624834	-3.055659	1.954334
39H	1.301919	-1.775326	3.006823

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1C	2.811226	1.084427	-0.777119
2C	4.180746	1.140120	-1.013351
3N	5.109957	0.513235	-0.268512
4C	4.646982	-0.210472	0.761298
5C	3.297003	-0.347554	1.083842
6C	2.331900	0.311701	0.299400
7N	0.962945	0.244001	0.617016
8P	-0.260236	0.064431	-0.588130
9C	-1.028860	-1.556318	-0.250207
10O	0.284215	0.143240	-1.988271
11C	-1.482709	1.351597	-0.187575
12C	-1.139532	2.467575	0.590369
13C	-2.070946	3.488217	0.800129
14C	-3.345758	3.401783	0.231816
15C	-3.690509	2.293926	-0.551046
16C	-2.762770	1.272429	-0.762066
17C	-2.101844	-1.737424	0.635749
18C	-2.608442	-3.018500	0.870800
19C	-2.043123	-4.124931	0.228747
20C	-0.972615	-3.949582	-0.655349
21C	-0.467541	-2.670356	-0.896783
22C	0.594693	-0.139061	1.989618
23H	2.130073	1.630423	-1.417046
24H	4.554733	1.735247	-1.844291
25H	5.394801	-0.719827	1.366729
26H	3.017521	-0.967353	1.928038
27H	-0.148941	2.536735	1.031434
28H	-1.800266	4.349740	1.405134
29H	-4.069175	4.196362	0.396296
30H	-4.679274	2.226129	-0.997191
31H	-3.035280	0.414799	-1.372236
32H	-2.547711	-0.884913	1.140315
33H	-3.443433	-3.150620	1.554182
34H	-2.438123	-5.120837	0.413539
35H	-0.534359	-4.806801	-1.160007
36H	0.355800	-2.530789	-1.592159
37H	-0.453554	0.106842	2.169579
38H	0.731563	-1.210864	2.178805
39H	1.197731	0.437218	2.697851

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1C	-2.579840	-1.762405	-0.925619
2C	-3.938454	-1.640378	-0.879153
3N	-4.558159	-0.788555	-0.004538
4C	-3.789828	-0.039405	0.839288
5C	-2.424598	-0.117249	0.846336
6C	-1.719349	-0.993890	-0.059901
7N	-0.404360	-1.146756	-0.163958
8P	0.692534	-0.271280	0.727250
9C	2.299683	-0.959600	0.198907
10O	0.580798	-0.233577	2.240760
11C	0.658012	1.442358	0.058434
12C	0.458416	1.694418	-1.308562
13C	0.437003	3.006365	-1.788644
14C	0.614490	4.078940	-0.906347
15C	0.813739	3.834718	0.456249
16C	0.835975	2.521199	0.936539
17C	2.498800	-1.522104	-1.071491
18C	3.761683	-1.991968	-1.442622
19C	4.835156	-1.903495	-0.549067
20C	4.641591	-1.346704	0.719543
21C	3.379007	-0.876269	1.091832
22C	-6.017998	-0.635888	-0.037847
23H	-2.130154	-2.454785	-1.629848
24H	-4.596278	-2.208598	-1.528168
25H	-4.329599	0.619489	1.510710
26H	-1.876871	0.485143	1.561772
27H	0.314519	0.865063	-1.996419
28H	0.280259	3.192550	-2.848559
29H	0.597205	5.099884	-1.280385
30H	0.950332	4.664863	1.145407
31H	0.983018	2.325745	1.995371
32H	1.664050	-1.603020	-1.761440
33H	3.906479	-2.431011	-2.426999
34H	5.816853	-2.270337	-0.839466
35H	5.470539	-1.282637	1.420470
36H	3.223100	-0.452369	2.080355

37H	-6.350715	-0.163249	0.887681
38H	-6.313671	-0.014331	-0.889629
39H	-6.486760	-1.619270	-0.123447

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1C	-2.437537	0.119811	0.849108
2C	-3.801872	0.037254	0.847908
3N	-4.574427	0.734109	-0.037223
4C	-3.959622	1.555998	-0.942659
5C	-2.601239	1.682847	-0.995096
6C	-1.736700	0.959437	-0.096096
7N	-0.422340	1.111593	-0.206891
8P	0.677758	0.267543	0.709979
9C	0.685817	-1.450471	0.051892
10O	0.543083	0.236243	2.221926
11C	2.279810	0.983728	0.203500
12C	2.481529	1.572913	-1.054306
13C	3.741336	2.065751	-1.406088
14C	4.808908	1.973549	-0.506042
15C	4.612805	1.389547	0.750012
16C	3.353396	0.897070	1.103343
17C	0.857188	-2.520605	0.941806
18C	0.865796	-3.837518	0.470448
19C	0.705073	-4.093791	-0.895003
20C	0.534550	-3.029833	-1.789137
21C	0.524699	-1.714555	-1.318043
22C	-6.039232	0.686658	0.052707
23H	-1.884573	-0.450233	1.586594
24H	-4.339356	-0.587330	1.553432
25H	-4.619166	2.092903	-1.615608
26H	-2.155791	2.339595	-1.735279
27H	1.651206	1.655329	-1.749332
28H	3.888127	2.525891	-2.380486
29H	5.788104	2.358178	-0.781518
30H	5.437140	1.322072	1.456042
31H	3.195706	0.452598	2.082521
32H	0.974599	-2.315801	2.002553
33H	0.996367	-4.660922	1.168817
34H	0.711981	-5.117391	-1.262082
35H	0.407931	-3.225453	-2.851398
36H	0.385496	-0.891968	-2.014993
37H	-6.468053	0.864545	-0.935678
38H	-6.349850	-0.300971	0.400307
39H	-6.401756	1.449212	0.750283

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1C	-2.620452	-1.646622	-1.007945
2C	-3.978571	-1.517664	-0.953670
3N	-4.591582	-0.705577	-0.038208
4C	-3.817367	-0.021342	0.855319
5C	-2.453212	-0.106233	0.855078
6C	-1.754220	-0.935473	-0.100787
7N	-0.440386	-1.088401	-0.213507
8P	0.665373	-0.254280	0.704023
9C	2.261673	-1.002687	0.225758
10O	0.511002	-0.198537	2.213662
11C	0.715233	1.455396	0.025795
12C	0.776040	2.539740	0.912518
13C	0.810056	3.850809	0.425288
14C	0.785631	4.086474	-0.952760
15C	0.725438	3.007709	-1.843826
16C	0.690715	1.698794	-1.357304
17C	2.409320	-1.848877	-0.883175
18C	3.665773	-2.370854	-1.207515
19C	4.783464	-2.047999	-0.431275
20C	4.642139	-1.204657	0.676853
21C	3.387255	-0.686793	1.004747
22C	-6.056281	-0.656040	0.052157
23H	-2.176642	-2.294888	-1.756556
24H	-4.639268	-2.044852	-1.633130
25H	-4.353522	0.595444	1.568657
26H	-1.898169	0.452180	1.599722
27H	0.789412	2.350002	1.982449
28H	0.855268	4.685082	1.121548
29H	0.812920	5.105070	-1.332545
30H	0.705578	3.187444	-2.916194
31H	0.640239	0.865240	-2.053690
32H	1.539787	-2.102696	-1.481334
33H	3.770320	-3.030586	-2.065757
34H	5.759876	-2.453443	-0.685998
35H	5.506839	-0.955309	1.287235
36H	3.277369	-0.041253	1.872585

37H	-6.364463	0.326715	0.415349
38H	-6.485358	-0.817201	-0.939007
39H	-6.420833	-1.428681	0.737492

10-PhNCO2-001

1C	3.327320	-1.164467	-0.689378
2C	4.378368	-2.043907	-0.452163
3N	4.237634	-3.329158	-0.083114
4C	2.968066	-3.754224	0.052036
5C	1.841202	-2.966740	-0.153802
6C	1.996245	-1.614396	-0.533224
7N	0.889900	-0.784209	-0.699044
8P	1.032268	0.898975	-1.012466
9C	-0.678323	1.450239	-1.302660
10O	1.933821	1.234901	-2.177258
11C	1.644932	1.649593	0.532505
12C	2.471717	2.780156	0.445721
13C	2.977460	3.367975	1.608436
14C	2.660319	2.828101	2.859830
15C	1.836024	1.700437	2.947600
16C	1.327482	1.109263	1.788158
17C	-1.410460	2.182208	-0.357310
18C	-2.700128	2.623162	-0.659847
19C	-3.266952	2.334978	-1.905937
20C	-2.538685	1.607873	-2.852748
21C	-1.245241	1.171389	-2.556587
22C	-0.481222	-1.372666	-0.514468
23O	-0.859521	-2.155665	-1.407417
24N	-1.033855	-0.939095	0.601605
25C	-2.371462	-1.183589	0.904056
26C	-3.377925	-1.600317	-0.003560
27C	-4.706183	-1.727799	0.410959
28C	-5.082786	-1.462982	1.733085
29C	-4.098844	-1.054026	2.643618
30C	-2.773333	-0.912676	2.234823
31H	3.547068	-0.151558	-1.003116
32H	5.401156	-1.688965	-0.570211
33H	2.840475	-4.794606	0.347381
34H	0.857258	-3.400980	-0.025531
35H	2.728938	3.184625	-0.529386
36H	3.622391	4.240533	1.536827
37H	3.058930	3.282203	3.764149
38H	1.592310	1.276658	3.918947
39H	0.680513	0.237126	1.842122
40H	-0.986207	2.390723	0.619846
41H	-3.266180	3.180213	0.082500
42H	-4.275409	2.670533	-2.135738
43H	-2.976638	1.376344	-3.820518
44H	-0.681281	0.607549	-3.294560
45H	-3.106855	-1.813356	-1.029888
46H	-5.456956	-2.041709	-0.312762
47H	-6.118506	-1.571603	2.047048
48H	-4.367243	-0.838937	3.676541
49H	-2.013490	-0.581576	2.939759

10-PhNCO2-002

1C	1.753044	2.973544	-0.268690
2C	2.852075	3.804828	-0.086682
3N	4.135591	3.414979	-0.194541
4C	4.320547	2.120571	-0.508649
5C	3.300393	1.198747	-0.717740
6C	1.954626	1.613322	-0.592967
7N	0.876110	0.746332	-0.742587
8P	1.065212	-0.944103	-0.975838
9C	1.671020	-1.604910	0.612388
10O	1.990323	-1.314809	-2.110674
11C	-0.628513	-1.550813	-1.260073
12C	-1.423313	-2.099833	-0.243623
13C	-2.701156	-2.579002	-0.536675
14C	-3.192946	-2.512468	-1.844959
15C	-2.402165	-1.969270	-2.862134
16C	-1.120579	-1.493744	-2.573521
17C	1.327251	-1.007345	1.834707
18C	1.825533	-1.533525	3.029471
19C	2.667327	-2.651331	3.009605
20C	3.011999	-3.247167	1.791164
21C	2.516327	-2.724766	0.593464
22C	-0.514849	1.305856	-0.610105
23O	-0.923689	1.973061	-1.579801
24N	-1.045393	0.975391	0.551305
25C	-2.382706	1.226269	0.849569
26C	-2.780571	0.966285	2.184390

27C	-4.101597	1.123252	2.600550
28C	-5.086366	1.540497	1.694269
29C	-4.714305	1.797186	0.369700
30C	-3.390201	1.651408	-0.053751
31H	0.754166	3.379464	-0.162998
32H	2.689192	4.851420	0.166215
33H	5.355283	1.794507	-0.603579
34H	3.553541	0.181408	-0.989651
35H	-1.056924	-2.135144	0.777265
36H	-3.316319	-2.991847	0.258850
37H	-4.192329	-2.877786	-2.069358
38H	-2.781480	-1.912647	-3.879401
39H	-0.505748	-1.073804	-3.364581
40H	0.668353	-0.142300	1.835436
41H	1.561334	-1.065828	3.974992
42H	3.057700	-3.054847	3.941103
43H	3.671176	-4.111826	1.772668
44H	2.793997	-3.172515	-0.356909
45H	-2.019741	0.631209	2.886368
46H	-4.366259	0.914808	3.635801
47H	-6.118923	1.662058	2.013913
48H	-5.465462	2.118738	-0.350274
49H	-3.122238	1.858012	-1.081970

10-PhNCO2-003

1C	-0.061758	-2.127802	1.301302
2C	0.199282	-3.460691	1.606316
3N	0.644881	-4.361293	0.710848
4C	0.827672	-3.924574	-0.544232
5C	0.583088	-2.612092	-0.954310
6C	0.135769	-1.682862	-0.010844
7N	-0.084397	-0.315728	-0.359180
8P	1.181752	0.670505	-0.962202
9C	1.107448	2.226766	-0.013155
10O	1.288746	0.880800	-2.452131
11C	2.689570	-0.174977	-0.345585
12C	2.962717	-0.343660	1.020625
13C	4.131943	-0.986549	1.430859
14C	5.042676	-1.461844	0.479612
15C	4.781719	-1.286265	-0.882452
16C	3.610128	-0.642818	-1.293120
17C	0.607600	2.286390	1.295800
18C	0.642690	3.487257	2.006690
19C	1.177319	4.638387	1.415657
20C	1.670525	4.583787	0.108486
21C	1.638183	3.381070	-0.604212
22C	-1.447057	0.217361	-0.471445
23O	-1.508212	1.372118	-0.954552
24N	-2.370768	-0.621189	-0.033301
25C	-3.724968	-0.315763	-0.059339
26C	-4.338884	0.869134	-0.549663
27C	-5.728413	1.024243	-0.514593
28C	-6.562634	0.027503	0.003705
29C	-5.974349	-1.147930	0.493601
30C	-4.591636	-1.313452	0.461085
31H	-0.420088	-1.444004	2.063041
32H	0.051043	-3.825926	2.620917
33H	1.185102	-4.659738	-1.262941
34H	0.740183	-2.317791	-1.987453
35H	2.262444	0.019238	1.767359
36H	4.331687	-1.118640	2.491501
37H	5.951590	-1.964971	0.800972
38H	5.486785	-1.650557	-1.625859
39H	3.400065	-0.504372	-2.349842
40H	0.167251	1.403124	1.749379
41H	0.242830	3.526842	3.017150
42H	1.200567	5.574383	1.968829
43H	2.077451	5.477019	-0.359667
44H	2.010396	3.339788	-1.624103
45H	-3.714635	1.654136	-0.956503
46H	-6.163371	1.944467	-0.902671
47H	-7.642083	0.160053	0.025085
48H	-6.598838	-1.941584	0.901012
49H	-4.138711	-2.228635	0.836994

10-PhNCO2-004

1C	-1.134288	-2.787727	1.305617
2C	-1.934359	-3.914059	1.147831
3N	-2.658854	-4.193007	0.049149
4C	-2.564136	-3.295549	-0.947681
5C	-1.790465	-2.140508	-0.905919
6C	-1.044035	-1.845766	0.257172

7N	-0.232694	-0.715663	0.368704
8P	-0.356143	0.578705	-0.750123
9C	-2.064312	1.191025	-0.540051
10O	-0.053500	0.230975	-2.186266
11C	0.752589	1.878685	-0.120516
12C	1.863145	2.209077	-0.909962
13C	2.720637	3.239100	-0.514445
14C	2.471533	3.941768	0.667961
15C	1.358895	3.618020	1.453748
16C	0.496567	2.595032	1.058707
17C	-2.724619	1.085961	0.693933
18C	-4.020078	1.590196	0.834166
19C	-4.661120	2.194451	-0.253296
20C	-4.005738	2.294442	-1.485732
21C	-2.708619	1.794451	-1.629895
22C	0.506067	-0.508202	1.690938
23O	-0.235329	-0.207274	2.650243
24N	1.808410	-0.619972	1.693501
25C	2.576551	-1.067271	0.620010
26C	3.749267	-0.347886	0.298581
27C	4.599582	-0.766327	-0.725593
28C	4.315896	-1.926847	-1.456800
29C	3.169565	-2.663512	-1.135282
30C	2.315190	-2.247736	-0.112247
31H	-0.599535	-2.639067	2.235680
32H	-1.999458	-4.635694	1.960714
33H	-3.139208	-3.514259	-1.846139
34H	-1.754852	-1.497510	-1.777008
35H	2.052696	1.654622	-1.823858
36H	3.585458	3.484650	-1.126003
37H	3.141386	4.740291	0.978605
38H	1.164309	4.159615	2.376023
39H	-0.358201	2.342171	1.677714
40H	-2.224993	0.606560	1.533369
41H	-4.530489	1.503887	1.790420
42H	-5.671588	2.581026	-0.142241
43H	-4.504591	2.757047	-2.334022
44H	-2.198748	1.860165	-2.587562
45H	3.965653	0.556042	0.861654
46H	5.488591	-0.181263	-0.955045
47H	4.977382	-2.254162	-2.255702
48H	2.936350	-3.574091	-1.684348
49H	1.442287	-2.844632	0.130847

10-PhNCO2-005

1C	1.780777	-2.147617	-0.904134
2C	2.549578	-3.305924	-0.944596
3N	2.640705	-4.202459	0.053420
4C	1.917615	-3.919075	1.151887
5C	1.122322	-2.789161	1.308426
6C	1.035640	-1.848393	0.258652
7N	0.228873	-0.714858	0.368475
8P	0.359394	0.578196	-0.750983
9C	-0.742955	1.883585	-0.121771
10O	0.055078	0.231208	-2.186972
11C	2.070485	1.182224	-0.541024
12C	2.731621	1.071802	0.692031
13C	4.029460	1.570002	0.831871
14C	4.671887	2.173811	-0.255008
15C	4.015535	2.279427	-1.486475
16C	2.716170	1.785259	-1.630290
17C	-0.477660	2.605504	1.051935
18C	-1.336181	3.631341	1.448056
19C	-2.454070	3.952290	0.668643
20C	-2.712112	3.244301	-0.508692
21C	-1.858485	2.211512	-0.905216
22C	-0.510557	-0.502770	1.689805
23O	0.230711	-0.201946	2.649147
24N	-1.813257	-0.611218	1.691863
25C	-2.582532	-1.058336	0.619160
26C	-2.322900	-2.238987	-0.113425
27C	-3.178462	-2.653880	-1.135840
28C	-4.324455	-1.916272	-1.456324
29C	-4.606703	-0.755761	-0.724519
30C	-3.755169	-0.338170	0.298994
31H	1.747522	-1.505596	-1.776058
32H	3.123574	-3.528176	-1.842870
33H	1.979860	-4.639962	1.965651
34H	0.588193	-2.637059	2.238315
35H	2.230601	0.593290	1.531117
36H	4.540554	1.479454	1.787369
37H	5.684165	2.555718	-0.144250
38H	4.515373	2.741897	-2.334256
39H	2.205470	1.855413	-2.587208
40H	0.381436	2.355203	1.665954

41H	-1.134597	4.177285	2.366262
42H	-3.121022	4.752888	0.980196
43H	-3.580912	3.487850	-1.115390
44H	-2.054789	1.653108	-1.815261
45H	-1.450544	-2.836913	0.128862
46H	-2.946436	-3.564588	-1.685202
47H	-4.986859	-2.242926	-2.254738
48H	-5.495566	-0.170083	-0.952975
49H	-3.970604	0.565620	0.862646

10-PhNCO2-006

1C	-0.672169	-2.393509	-1.013150
2C	-1.223872	-3.669605	-1.058745
3N	-1.948266	-4.229518	-0.074197
4C	-2.127938	-3.463656	1.016952
5C	-1.618080	-2.180316	1.176862
6C	-0.855467	-1.599350	0.140881
7N	-0.315896	-0.316287	0.273724
8P	0.950121	0.219357	-0.757986
9C	1.376950	1.908705	-0.219553
10O	0.603023	0.201172	-2.227431
11C	2.369133	-0.862846	-0.385327
12C	2.558909	-1.396118	0.898510
13C	3.668923	-2.204254	1.157896
14C	4.587502	-2.484760	0.140089
15C	4.395460	-1.958361	-1.142350
16C	3.287590	-1.148776	-1.406498
17C	2.167319	2.183450	0.906622
18C	2.504825	3.501734	1.218143
19C	2.060268	4.553107	0.408663
20C	1.285303	4.282875	-0.723232
21C	0.950788	2.964072	-1.041476
22C	-0.638328	0.443424	1.553114
23O	0.273199	0.436344	2.407414
24N	-1.835664	0.958320	1.673207
25C	-2.798840	0.963726	0.664418
26C	-4.099530	0.511924	0.982228
27C	-5.127712	0.535295	0.038402
28C	-4.894848	1.020256	-1.254708
29C	-3.616878	1.490848	-1.579184
30C	-2.586530	1.470197	-0.637184
31H	-0.129640	-2.018363	-1.871905
32H	-1.078364	-4.276350	-1.951359
33H	-2.715577	-3.904333	1.820827
34H	-1.814988	-1.639832	2.095215
35H	1.840793	-1.168586	1.682617
36H	3.812979	-2.618017	2.153046
37H	5.448920	-3.116548	0.344079
38H	5.103959	-2.181804	-1.936437
39H	3.126442	-0.746526	-2.403019
40H	2.501940	1.375808	1.546841
41H	3.110226	3.707120	2.097490
42H	2.321335	5.578897	0.658156
43H	0.942721	5.094761	-1.360030
44H	0.367980	2.749228	-1.932479
45H	-4.283304	0.136042	1.986301
46H	-6.115291	0.169582	0.313842
47H	-5.693843	1.036719	-1.992432
48H	-3.416015	1.879377	-2.576037
49H	-1.609743	1.856361	-0.902153

10-PhNCO-001

1C	0.188064	-2.218076	-0.623064
2C	1.550714	-2.181094	-0.725680
3N	2.292581	-1.183374	-0.158366
4C	1.645943	-0.207998	0.546690
5C	0.285572	-0.192983	0.690946
6C	-0.545198	-1.204039	0.085204
7N	-1.877309	-1.273483	0.115295
8P	-2.847052	-0.133205	0.822615
9C	-2.621086	1.436990	-0.114521
10O	-2.745775	0.148019	2.311968
11C	-4.530931	-0.698105	0.383918
12C	-5.595105	-0.324619	1.218984
13C	-6.906078	-0.693750	0.903187
14C	-7.164799	-1.438878	-0.252231
15C	-6.107534	-1.816414	-1.087982
16C	-4.796669	-1.447166	-0.772773
17C	-2.685963	2.658288	0.571375
18C	-2.505896	3.864652	-0.113053
19C	-2.259430	3.858554	-1.489929
20C	-2.193258	2.642763	-2.180873

21C	-2.373322	1.438182	-1.496433
22C	3.794510	-1.198802	-0.333465
23O	4.231523	-2.194065	-0.943935
24N	4.345033	-0.133252	0.195716
25C	5.721371	0.081916	0.182644
26C	6.722394	-0.808084	-0.283964
27C	8.074752	-0.456578	-0.221611
28C	8.482037	0.777732	0.295422
29C	7.504062	1.668263	0.760295
30C	6.154728	1.325024	0.706748
31H	-0.360462	-3.027595	-1.094525
32H	2.125649	-2.926979	-1.258978
33H	2.291970	0.544012	0.979013
34H	-0.158462	0.601194	1.280251
35H	-5.390621	0.246518	2.120897
36H	-7.722784	-0.403515	1.560177
37H	-8.183955	-1.728222	-0.498180
38H	-6.302686	-2.401616	-1.983825
39H	-3.976421	-1.751058	-1.416192
40H	-2.865022	2.655182	1.643368
41H	-2.552850	4.806672	0.428679
42H	-2.114596	4.795782	-2.022310
43H	-1.993657	2.633084	-3.249891
44H	-2.308606	0.496015	-2.034946
45H	6.428737	-1.766763	-0.691924
46H	8.819355	-1.162374	-0.586413
47H	9.536382	1.041517	0.336299
48H	7.795459	2.634803	1.167415
49H	5.396950	2.015898	1.070098

10-PhNCO-002

1C	0.187172	-2.213310	-0.613107
2C	1.549751	-2.176916	-0.716182
3N	2.292669	-1.181744	-0.145657
4C	1.646794	-0.206086	0.559909
5C	0.286168	-0.188439	0.701375
6C	-0.545269	-1.198794	0.095213
7N	-1.877454	-1.266606	0.124689
8P	-2.845064	-0.117340	0.820516
9C	-2.623381	1.436993	-0.143693
10O	-2.736521	0.187926	2.304636
11C	-4.530533	-0.690442	0.399052
12C	-5.590230	-0.309814	1.236558
13C	-6.902340	-0.685416	0.933358
14C	-7.166758	-1.443968	-0.211973
15C	-6.113990	-1.828514	-1.050189
16C	-4.801994	-1.452949	-0.747522
17C	-2.378427	1.414499	-1.525937
18C	-2.201019	2.607126	-2.231652
19C	-2.266911	3.834687	-1.561854
20C	-2.510542	3.864436	-0.184784
21C	-2.688010	2.669963	0.520903
22C	3.794062	-1.196569	-0.324659
23O	4.225548	-2.170055	-0.972964
24N	4.351908	-0.160774	0.253638
25C	5.725948	0.066147	0.213200
26C	6.691598	-0.663766	-0.526050
27C	8.042697	-0.304148	-0.486109
28C	8.484533	0.777181	0.283416
29C	7.542069	1.507360	1.021031
30C	6.193400	1.159399	0.983978
31H	-0.362030	-3.021594	-1.085895
32H	2.123966	-2.921600	-1.251943
33H	2.293867	0.543600	0.994824
34H	-0.158077	0.606647	1.289353
35H	-5.381324	0.271947	2.130604
36H	-7.715493	-0.389520	1.592232
37H	-8.186798	-1.738271	-0.448164
38H	-6.313513	-2.424079	-1.938202
39H	-3.985352	-1.762674	-1.392702
40H	-2.313826	0.463139	-2.048019
41H	-2.003592	2.578913	-3.300758
42H	-2.123787	4.762666	-2.110653
43H	-2.557076	4.815662	0.340654
44H	-2.864715	2.685431	1.593171
45H	6.371997	-1.506879	-1.124867
46H	8.758953	-0.883470	-1.066643
47H	9.537946	1.046493	0.309178
48H	7.860442	2.353060	1.627832
49H	5.463565	1.729569	1.554493

10-PhNCO-003

1C	-0.334908	-0.171617	0.653804
2C	-1.695479	-0.176784	0.510464
3N	-2.340674	-1.082372	-0.284145
4C	-1.596538	-2.017509	-0.947411
5C	-0.234456	-2.064774	-0.845636
6C	0.496514	-1.124424	-0.039940
7N	1.827448	-1.202000	-0.005481
8P	2.799317	-0.119043	0.782447
9C	4.480924	-0.772926	0.476707
10O	2.598965	0.177954	2.258790
11C	2.729838	1.452803	-0.175765
12C	2.644202	1.453490	-1.577377
13C	2.596769	2.659011	-2.281782
14C	2.632644	3.876564	-1.591419
15C	2.715738	3.883174	-0.195326
16C	2.764303	2.675669	0.509343
17C	4.786838	-1.598397	-0.616129
18C	6.099046	-2.032328	-0.826837
19C	7.117865	-1.643067	0.049741
20C	6.818928	-0.822657	1.143079
21C	5.507027	-0.389399	1.354553
22C	-3.842260	-1.086946	-0.460369
23O	-4.266468	-1.966567	-1.235391
24N	-4.408888	-0.141707	0.250044
25C	-5.787608	0.061839	0.257295
26C	-6.246434	1.141802	1.051690
27C	-7.600027	1.457177	1.150250
28C	-8.557333	0.702905	0.457302
29C	-8.125012	-0.368785	-0.330730
30C	-6.768352	-0.692513	-0.436818
31H	0.112785	0.563793	1.313028
32H	-2.343419	0.528656	1.012841
33H	-2.169556	-2.706444	-1.554205
34H	0.315443	-2.824877	-1.391924
35H	2.607188	0.510789	-2.117544
36H	2.526326	2.649098	-3.367069
37H	2.591926	4.814880	-2.139784
38H	2.738017	4.826721	0.345275
39H	2.818098	2.673568	1.594763
40H	3.994916	-1.909239	-1.290841
41H	6.324811	-2.675750	-1.674203
42H	8.138269	-1.981198	-0.115583
43H	7.605250	-0.522876	1.832032
44H	5.271739	0.240304	2.208670
45H	-5.505775	1.727742	1.591432
46H	-7.910820	2.295451	1.771120
47H	-9.614751	0.946288	0.531583
48H	-8.852884	-0.967681	-0.875902
49H	-6.455880	-1.525957	-1.052653

10-PhNCO-004

1C	-0.250946	-2.026330	-0.899860
2C	-1.613662	-1.980826	-0.991902
3N	-2.355631	-1.058627	-0.308447
4C	-1.707126	-0.162943	0.494933
5C	-0.345623	-0.156769	0.629751
6C	0.482969	-1.098735	-0.082057
7N	1.813718	-1.178091	-0.053985
8P	2.792435	-0.121987	0.760461
9C	4.466557	-0.801795	0.467166
10O	2.581493	0.156770	2.238981
11C	2.759861	1.465412	-0.173775
12C	2.500176	1.506673	-1.552836
13C	2.488334	2.727371	-2.233485
14C	2.739212	3.918423	-1.542573
15C	2.997844	3.884834	-0.168066
16C	3.006854	2.663606	0.512863
17C	4.786388	-1.555280	-0.672853
18C	6.090597	-2.017890	-0.869602
19C	7.087770	-1.730886	0.069503
20C	6.775165	-0.981780	1.208874
21C	5.470647	-0.519436	1.406043
22C	-3.858418	-1.067056	-0.472654
23O	-4.285679	-1.942124	-1.251275
24N	-4.423170	-0.129716	0.249683
25C	-5.802792	0.067108	0.269592
26C	-6.260457	1.139764	1.074477
27C	-7.614817	1.447173	1.186817
28C	-8.574138	0.692018	0.497599
29C	-8.142981	-0.372358	-0.300860
30C	-6.785570	-0.687933	-0.420920
31H	0.297312	-2.776553	-1.461258
32H	-2.188999	-2.661698	-1.605520
33H	-2.353415	0.533800	1.011371
34H	0.105598	0.570447	1.295897

35H	2.296217	0.584989	-2.091659
36H	2.277547	2.749421	-3.300224
37H	2.727375	4.868331	-2.072059
38H	3.186327	4.808416	0.374641
39H	3.194184	2.634346	1.583001
40H	4.010801	-1.789265	-1.396040
41H	6.326800	-2.605990	-1.753523
42H	8.101948	-2.092333	-0.084458
43H	7.544258	-0.761366	1.945597
44H	5.222973	0.053713	2.295669
45H	-5.518285	1.726205	1.611579
46H	-7.924673	2.279837	1.815652
47H	-9.632166	0.929098	0.582739
48H	-8.872317	-0.971949	-0.843315
49H	-6.474026	-1.515965	-1.044457

10-PhNCO-005

1C	0.137847	0.418629	-1.082765
2C	1.480202	0.682711	-1.139450
3N	2.401035	-0.060440	-0.460498
4C	1.962450	-1.111827	0.299266
5C	0.636846	-1.424413	0.399234
6C	-0.376626	-0.664765	-0.284348
7N	-1.654649	-1.010093	-0.125130
8P	-2.932614	-0.174389	-0.761091
9C	-4.375027	-1.166293	-0.225210
10O	-3.010480	0.120819	-2.249427
11C	-3.069378	1.401487	0.182460
12C	-2.653156	1.499889	1.519596
13C	-2.781641	2.706719	2.212475
14C	-3.329760	3.826405	1.575963
15C	-3.744766	3.736060	0.242989
16C	-3.614015	2.528791	-0.450422
17C	-5.558776	-1.071614	-0.973132
18C	-6.697981	-1.785848	-0.590802
19C	-6.663816	-2.602480	0.544697
20C	-5.486446	-2.701971	1.294494
21C	-4.347716	-1.985962	0.913696
22C	3.865042	0.301465	-0.573987
23O	4.098646	1.283507	-1.304801
24N	4.610710	-0.510724	0.136309
25C	5.997946	-0.395029	0.193046
26C	6.805910	0.561968	-0.472771
27C	8.196203	0.552119	-0.319806
28C	8.832272	-0.394795	0.489724
29C	8.047184	-1.347025	1.154927
30C	6.661708	-1.345597	1.008241
31H	-0.537776	1.037723	-1.662600
32H	1.893440	1.492472	-1.727102
33H	2.743987	-1.661733	0.805048
34H	0.333632	-2.266026	1.014216
35H	-2.219703	0.635217	2.015437
36H	-2.450601	2.774646	3.246252
37H	-3.428075	4.765799	2.115148
38H	-4.165184	4.605259	-0.257814
39H	-3.922481	2.456718	-1.490169
40H	-5.579172	-0.447305	-1.862597
41H	-7.608153	-1.708576	-1.181065
42H	-7.548170	-3.161841	0.841244
43H	-5.452801	-3.340463	2.174383
44H	-3.431065	-2.074273	1.489139
45H	6.334251	1.303863	-1.104211
46H	8.788472	1.299739	-0.845048
47H	9.914188	-0.392761	0.600757
48H	8.518020	-2.094515	1.790917
49H	6.054356	-2.085656	1.524799

10-PhNCO-006

1C	0.084629	0.276062	2.758639
2C	1.435764	0.299832	2.557080
3N	1.984637	0.206146	1.307852
4C	1.147330	0.093244	0.235399
5C	-0.213399	0.066061	0.371276
6C	-0.845111	0.148636	1.665861
7N	-2.147753	0.137834	1.933027
8P	-3.436666	-0.126248	0.932559
9C	-3.642088	1.316782	-0.183721
10O	-4.715481	-0.386287	1.703548
11C	-3.072423	-1.565355	-0.159128
12C	-3.018180	-2.830803	0.451216
13C	-2.728476	-3.971333	-0.300612
14C	-2.494747	-3.864335	-1.676659

15C	-2.550389	-2.611171	-2.293313
16C	-2.836463	-1.468203	-1.538753
17C	-2.744226	2.393694	-0.180096
18C	-2.951393	3.492041	-1.021705
19C	-4.057399	3.521959	-1.876055
20C	-4.962605	2.453634	-1.881605
21C	-4.758779	1.361025	-1.036165
22C	3.488560	0.237482	1.164181
23O	4.105677	0.371213	2.238982
24N	3.850047	0.115002	-0.090526
25C	5.186609	0.108059	-0.484984
26C	5.415799	0.021268	-1.880824
27C	6.702921	0.001947	-2.413877
28C	7.821166	0.065647	-1.570682
29C	7.616262	0.148669	-0.189530
30C	6.327981	0.170867	0.354901
31H	-0.306023	0.350045	3.768604
32H	2.153484	0.390018	3.362039
33H	1.644062	0.032174	-0.723319
34H	-0.809773	-0.013876	-0.528311
35H	-3.203258	-2.922732	1.518687
36H	-2.686169	-4.942726	0.186495
37H	-2.269467	-4.752035	-2.262995
38H	-2.369154	-2.519569	-3.361805
39H	-2.867237	-0.500445	-2.032077
40H	-1.885988	2.383334	0.484452
41H	-2.248970	4.322086	-1.007102
42H	-4.217731	4.375034	-2.531235
43H	-5.828639	2.475116	-2.539106
44H	-5.470096	0.538574	-1.038114
45H	4.549255	-0.030800	-2.536339
46H	6.835346	-0.063863	-3.492249
47H	8.827532	0.050883	-1.982647
48H	8.471782	0.198425	0.482084
49H	6.192900	0.237542	1.426785

10-PhNCO-007

1C	-0.087226	-0.045507	2.770907
2C	-1.438856	-0.029002	2.571473
3N	-1.986856	0.016729	1.319087
4C	-1.148642	0.048280	0.242010
5C	0.212515	0.029198	0.375383
6C	0.843381	-0.024373	1.671777
7N	2.146451	-0.041055	1.937402
8P	3.436948	-0.195317	0.916254
9C	3.081023	-1.528527	-0.304095
10O	4.717187	-0.518736	1.660169
11C	3.632443	1.346987	-0.061015
12C	2.725248	2.411749	0.037927
13C	2.928128	3.586294	-0.694904
14C	4.038177	3.705123	-1.535933
15C	4.952634	2.649421	-1.636356
16C	4.752693	1.479908	-0.899981
17C	2.840491	-1.305054	-1.668070
18C	2.563608	-2.375308	-2.525651
19C	2.521429	-3.680863	-2.028178
20C	2.759974	-3.913650	-0.668476
21C	3.040922	-2.845632	0.186099
22C	-3.491654	0.034761	1.178119
23O	-4.110371	-0.060011	2.256063
24N	-3.851073	0.150312	-0.077820
25C	-5.187375	0.185300	-0.471600
26C	-6.329728	0.129740	0.367521
27C	-7.617488	0.175093	-0.176745
28C	-7.820916	0.276638	-1.556877
29C	-6.701706	0.333752	-2.399266
30C	-5.415082	0.289990	-1.866434
31H	0.302806	-0.081117	3.783150
32H	-2.157564	-0.052468	3.380274
33H	-1.644980	0.093524	-0.717825
34H	0.809740	0.065148	-0.526634
35H	1.863618	2.333570	0.693475
36H	2.218516	4.405538	-0.606564
37H	4.195057	4.617605	-2.106509
38H	5.822061	2.740057	-2.283337
39H	5.471267	0.667353	-0.974836
40H	2.862659	-0.295020	-2.068304
41H	2.378915	-2.186117	-3.580556
42H	2.302783	-4.512388	-2.693943
43H	2.728716	-4.926678	-0.274359
44H	3.231219	-3.034247	1.239911
45H	-6.195840	0.050219	1.438692
46H	-8.473734	0.129392	0.494220
47H	-8.826886	0.309766	-1.968739
48H	-6.832986	0.412839	-3.476889

49H -4.547726 0.334954 -2.521396

10-PhNCO-008

1C	-0.607291	-2.637039	0.742397
2C	-1.968665	-2.764420	0.738491
3N	-2.756881	-2.032997	-0.102159
4C	-2.164025	-1.211032	-1.013534
5C	-0.806687	-1.051651	-1.075075
6C	0.064135	-1.722640	-0.142797
7N	1.384625	-1.566593	-0.032915
8P	2.226392	-0.393740	-0.845366
9C	1.604062	1.223383	-0.217855
10O	2.252436	-0.370526	-2.364272
11C	3.916591	-0.545962	-0.162954
12C	4.971472	0.040174	-0.880825
13C	6.277396	-0.007440	-0.386119
14C	6.542407	-0.645504	0.831004
15C	5.497249	-1.237364	1.548068
16C	4.189535	-1.186863	1.055073
17C	1.400982	1.444848	1.153999
18C	0.899789	2.667500	1.605905
19C	0.592018	3.680816	0.690045
20C	0.792293	3.467726	-0.676988
21C	1.298350	2.244017	-1.128506
22C	-4.274080	-2.157924	0.007530
23O	-4.660498	-3.328734	0.162017
24N	-4.983919	-1.063873	-0.111529
25C	-4.498984	0.225744	0.091931
26C	-4.934611	1.261637	-0.764576
27C	-4.507062	2.577844	-0.582860
28C	-3.640149	2.909402	0.466549
29C	-3.219651	1.898771	1.338887
30C	-3.646155	0.581393	1.164448
31H	-0.016284	-3.216920	1.444640
32H	-2.499821	-3.435456	1.402922
33H	-2.832829	-0.695236	-1.690804
34H	-0.395278	-0.402285	-1.838995
35H	4.767227	0.526744	-1.831172
36H	7.087179	0.447741	-0.951630
37H	7.558971	-0.685060	1.215564
38H	5.699134	-1.742238	2.490097
39H	3.379495	-1.655542	1.605264
40H	1.627806	0.658049	1.869258
41H	0.740411	2.827284	2.669843
42H	0.193153	4.629496	1.041729
43H	0.548422	4.249632	-1.392546
44H	1.447809	2.068290	-2.190540
45H	-5.604335	1.007278	-1.583198
46H	-4.850231	3.350035	-1.268899
47H	-3.300663	3.933251	0.602553
48H	-2.549640	2.135885	2.162654
49H	-3.312200	-0.189028	1.854600

10-001

1C	2.787355	-2.042696	-0.843624
2C	4.170538	-1.950316	-0.847653
3N	4.889028	-1.105384	-0.075331
4C	4.158153	-0.323283	0.745289
5C	2.771889	-0.333352	0.834413
6C	2.002721	-1.211900	0.010641
7N	0.647740	-1.315489	-0.031327
8P	-0.367962	-0.321059	0.775882
9C	-2.026607	-0.837406	0.180502
10O	-0.377811	-0.231767	2.297386
11C	-0.168737	1.387304	0.093075
12C	-0.438565	2.498483	0.905568
13C	-0.306883	3.796911	0.401935
14C	0.100758	3.996716	-0.921603
15C	0.378926	2.893703	-1.737401
16C	0.244012	1.597429	-1.232126
17C	-2.244705	-1.321688	-1.118838
18C	-3.532344	-1.668183	-1.538394
19C	-4.616871	-1.535434	-0.663035
20C	-4.407242	-1.056624	0.634326
21C	-3.118424	-0.708719	1.051867
22H	2.281856	-2.748556	-1.499138
23H	4.749431	-2.591640	-1.512866
24H	4.726083	0.358972	1.378517
25H	2.279183	0.327580	1.541777
26H	-0.741112	2.338376	1.937331
27H	-0.517295	4.650894	1.042314
28H	0.206590	5.005826	-1.313634

29H	0.705625	3.043227	-2.764210
30H	0.471606	0.742634	-1.863929
31H	-1.402382	-1.438776	-1.794826
32H	-3.688854	-2.046066	-2.546476
33H	-5.618014	-1.808088	-0.989541
34H	-5.244233	-0.958003	1.322192
35H	-2.947779	-0.345919	2.062126

10-002

1C	2.797124	-2.037378	-0.808701
2C	4.179164	-1.930992	-0.828071
3N	4.896156	-1.065160	-0.077867
4C	4.165158	-0.275842	0.735663
5C	2.779887	-0.298031	0.838008
6C	2.012114	-1.199402	0.038188
7N	0.658161	-1.317667	0.011047
8P	-0.365012	-0.312888	0.794324
9C	-2.018572	-0.849420	0.202119
10O	-0.380653	-0.187870	2.313503
11C	-0.177723	1.381880	0.075430
12C	-0.440221	2.508388	0.868912
13C	-0.320951	3.796793	0.337167
14C	0.067058	3.970944	-0.995826
15C	0.338011	2.852419	-1.792858
16C	0.215480	1.566274	-1.259461
17C	-3.140050	-0.541591	0.988358
18C	-4.424780	-0.896716	0.566361
19C	-4.601794	-1.567687	-0.648687
20C	-3.488711	-1.881667	-1.436822
21C	-2.204663	-1.522208	-1.015228
22H	2.292824	-2.759837	-1.446805
23H	4.758193	-2.577891	-1.487743
24H	4.732150	0.423365	1.350953
25H	2.286979	0.370700	1.537892
26H	-0.727926	2.367432	1.907665
27H	-0.525950	4.662849	0.962955
28H	0.162600	4.972114	-1.410210
29H	0.649281	2.982171	-2.827114
30H	0.436437	0.699547	-1.877341
31H	-2.998755	-0.032114	1.937968
32H	-5.284862	-0.656073	1.187426
33H	-5.600110	-1.848541	-0.976930
34H	-3.619874	-2.409700	-2.378887
35H	-1.339976	-1.772542	-1.622266

11-001

1C	-2.583021	-2.262166	-0.839985
2C	-3.973169	-2.304468	-0.831285
3N	-4.750170	-1.470701	-0.117681
4C	-4.108005	-0.557292	0.629263
5C	-2.723029	-0.426631	0.702532
6C	-1.922495	-1.297191	-0.057858
7N	-0.530262	-1.231081	-0.076782
8P	0.483590	-0.168457	0.795624
9C	2.111737	-0.669837	0.156372
10O	0.396450	-0.227170	2.297400
11C	0.074448	1.485153	0.155561
12C	0.259923	2.585623	1.006520
13C	-0.012702	3.877326	0.549346
14C	-0.473158	4.075740	-0.756528
15C	-0.664825	2.980344	-1.605905
16C	-0.392931	1.687747	-1.152611
17C	2.419128	-0.638902	-1.213702
18C	3.682063	-1.038923	-1.654323
19C	4.643266	-1.466525	-0.730434
20C	4.341400	-1.492499	0.634428
21C	3.077456	-1.094446	1.080109
22H	-2.016115	-2.966028	-1.444617
23H	-4.491938	-3.048497	-1.432826
24H	-4.736445	0.112688	1.212827
25H	-2.290367	0.329615	1.348096
26H	-0.063757	-2.010626	-0.532309
27H	0.605187	2.426568	2.024281
28H	0.129829	4.726070	1.213296
29H	-0.688445	5.081065	-1.109876
30H	-1.033441	3.130773	-2.617397
31H	-0.560435	0.839250	-1.809766
32H	1.680569	-0.296846	-1.934088
33H	3.917382	-1.013734	-2.715244
34H	5.626698	-1.776235	-1.075242
35H	5.087341	-1.822733	1.352681
36H	2.834987	-1.112964	2.138879

11-002

1C	1.316812	-1.471807	-0.810900
2C	2.266711	-2.080728	-1.628362
3N	3.462598	-2.523244	-1.208603
4C	3.730327	-2.352349	0.098823
5C	2.861662	-1.752000	1.003227
6C	1.611336	-1.287343	0.551316
7N	0.725519	-0.704592	1.454010
8P	-0.553328	0.418117	1.237075
9C	0.073106	1.771055	0.189421
10O	-0.958539	0.893748	2.608783
11C	-1.850190	-0.459344	0.318852
12C	-2.865861	0.278656	-0.313048
13C	-3.923595	-0.381272	-0.941142
14C	-3.975984	-1.779651	-0.941028
15C	-2.971842	-2.517956	-0.306745
16C	-1.912333	-1.861865	0.324388
17C	0.006527	1.771150	-1.212612
18C	0.546375	2.835229	-1.940123
19C	1.155160	3.903368	-1.274723
20C	1.221125	3.910376	0.123107
21C	0.681399	2.850359	0.853406
22H	0.366533	-1.169237	-1.232329
23H	2.045264	-2.224360	-2.684324
24H	4.698758	-2.711560	0.441694
25H	3.147980	-1.640325	2.046265
26H	1.054466	-0.679109	2.416956
27H	-2.832516	1.365148	-0.316280
28H	-4.705114	0.194883	-1.429538
29H	-4.799030	-2.291999	-1.432717
30H	-3.011272	-3.604160	-0.303481
31H	-1.133693	-2.439209	0.814328
32H	-0.472320	0.953993	-1.742719
33H	0.488055	2.828912	-3.025484
34H	1.573300	4.730448	-1.843000
35H	1.686931	4.742966	0.643911
36H	0.719650	2.861447	1.939349

11-003

1C	2.903765	-1.701491	-1.095133
2C	4.264337	-1.690082	-0.999878
3N	4.887536	-1.019671	0.015109
4C	4.162945	-0.350949	0.958286
5C	2.798483	-0.326455	0.915305
6C	2.071388	-1.009095	-0.136784
7N	0.756369	-1.051421	-0.291273
8P	-0.329531	-0.241895	0.672972
9C	-0.376754	1.483010	0.038025
10O	-0.155817	-0.230342	2.181053
11C	-1.934485	-0.975780	0.201614
12C	-2.145107	-1.616539	-1.029001
13C	-3.405868	-2.129788	-1.347629
14C	-4.464880	-2.006401	-0.441610
15C	-4.259969	-1.369751	0.787433
16C	-3.000077	-0.857444	1.107954
17C	-0.295549	1.767109	-1.335095
18C	-0.338342	3.088885	-1.785192
19C	-0.462711	4.139115	-0.867346
20C	-0.542425	3.862625	0.501162
21C	-0.500600	2.539137	0.952103
22H	2.426415	-2.239052	-1.907758
23H	4.913402	-2.197090	-1.705008
24H	5.899199	-1.027057	0.074397
25H	4.735658	0.148975	1.731541
26H	2.257059	0.199302	1.692608
27H	-1.320407	-1.722528	-1.727138
28H	-3.559604	-2.630641	-2.300648
29H	-5.444542	-2.407384	-0.690927
30H	-5.077884	-1.277367	1.498056
31H	-2.836588	-0.372443	2.066795
32H	-0.193349	0.955639	-2.051155
33H	-0.274285	3.300429	-2.850035
34H	-0.496029	5.167775	-1.218537
35H	-0.635966	4.675143	1.218001
36H	-0.555838	2.318451	2.014683

11-004

1C	-3.019448	-1.473927	1.092553
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2C	-4.022898	-1.849791	0.250000
3N	-3.894424	-1.692544	-1.102726
4C	-2.757388	-1.164901	-1.637409
5C	-1.718103	-0.771853	-0.842348
6C	-1.787135	-0.895783	0.599945
7N	-0.861658	-0.558306	1.480336
8P	0.582286	0.236269	1.281461
9C	1.733684	-0.842742	0.346717
10O	1.174567	0.652394	2.610152
11C	0.297193	1.721729	0.233664
12C	0.701803	1.832939	-1.105240
13C	0.433043	2.996471	-1.834093
14C	-0.246587	4.060001	-1.233244
15C	-0.653998	3.958153	0.102139
16C	-0.380486	2.798957	0.831243
17C	1.370791	-2.131772	-0.070062
18C	2.289890	-2.943051	-0.744175
19C	3.578992	-2.472073	-1.008591
20C	3.951821	-1.188969	-0.589917
21C	3.036368	-0.381506	0.087974
22H	-3.137352	-1.603536	2.163138
23H	-4.956465	-2.280853	0.593301
24H	-4.650977	-1.977177	-1.714374
25H	-2.732927	-1.083294	-2.718497
26H	-0.833640	-0.370807	-1.319091
27H	1.231335	1.015007	-1.586588
28H	0.757886	3.070709	-2.869371
29H	-0.454369	4.964726	-1.799628
30H	-1.178572	4.783606	0.577387
31H	-0.687438	2.731402	1.871994
32H	0.375775	-2.512287	0.139764
33H	1.998665	-3.942892	-1.057260
34H	4.293313	-3.102837	-1.532347
35H	4.956021	-0.821215	-0.786620
36H	3.335240	0.610919	0.416866

14-001

1C	3.453364	1.477360	0.087748
2C	4.789647	1.092509	0.097758
3N	5.201740	-0.183912	0.013422
4C	4.243851	-1.117132	-0.086111
5C	2.873102	-0.851073	-0.106828
6C	2.463534	0.486327	-0.018642
7N	1.124871	0.915730	-0.032872
8C	-0.022578	0.199258	-0.021819
9N	-0.053089	-1.109668	-0.006579
10S	-1.654235	-1.645636	0.024253
11C	-2.380750	-0.001691	0.014344
12C	-1.334017	0.918977	-0.022138
13O	-1.919266	-2.335414	1.297502
14O	-1.960074	-2.364408	-1.223600
15C	-3.716476	0.363871	0.028796
16C	-4.000745	1.735990	0.003347
17C	-2.966747	2.679642	-0.039926
18C	-1.623338	2.284392	-0.053549
19H	3.187130	2.528833	0.163686
20H	5.568345	1.847786	0.178902
21H	4.582921	-2.148593	-0.153970
22H	2.159327	-1.658290	-0.187123
23H	1.013443	1.922969	-0.013649
24H	-4.507959	-0.378837	0.057680
25H	-5.034719	2.068499	0.014507
26H	-3.208455	3.738321	-0.063356
27H	-0.845285	3.042428	-0.091632

14-002

1C	-3.419789	-1.055161	-0.902954
2C	-4.647292	-0.485892	-0.567775
3N	-4.822764	0.365195	0.455858
4C	-3.741124	0.654361	1.196305
5C	-2.470307	0.129363	0.963007
6C	-2.299868	-0.732535	-0.126938
7N	-1.063954	-1.341876	-0.438618
8C	0.200665	-0.903520	-0.201927
9N	1.145547	-1.800330	-0.049127
10S	2.639001	-1.043186	0.161758
11C	1.990222	0.626260	0.034382
12C	0.615782	0.533902	-0.200726
13O	3.524428	-1.335920	-0.978005
14O	3.140883	-1.333365	1.515077
15C	2.686645	1.823015	0.049625
16C	1.951645	2.990857	-0.194029

17C	0.580254	2.924048	-0.468321
18C	-0.100557	1.700815	-0.480512
19H	-3.333356	-1.726541	-1.752567
20H	-5.530934	-0.719531	-1.157470
21H	-3.896792	1.331503	2.033251
22H	-1.646165	0.381865	1.621586
23H	-1.113399	-2.334367	-0.659000
24H	3.756809	1.852991	0.230543
25H	2.455833	3.952939	-0.186773
26H	0.030426	3.836374	-0.681007
27H	-1.158388	1.676027	-0.710876

14-003

1C	-3.382444	1.511886	-0.000058
2C	-4.704934	1.159987	-0.000152
3N	-5.061455	-0.154326	-0.000103
4C	-4.127110	-1.138955	0.000004
5C	-2.786432	-0.843377	0.000103
6C	-2.346381	0.522596	0.000117
7N	-1.078746	0.992857	0.000011
8C	0.011753	0.217229	-0.000032
9N	0.072212	-1.114161	-0.000019
10S	1.665293	-1.634953	0.000001
11C	2.394158	0.006875	0.000016
12C	1.338303	0.914362	0.000007
13O	1.971299	-2.348959	-1.257821
14O	1.971270	-2.348970	1.257825
15C	3.727224	0.389000	0.000034
16C	3.992598	1.765462	0.000046
17C	2.944502	2.697581	0.000041
18C	1.607087	2.282879	0.000026
19H	-3.106255	2.560616	-0.000106
20H	-5.515426	1.879527	-0.000263
21H	-6.045837	-0.403872	-0.000170
22H	-4.503871	-2.155399	0.000010
23H	-2.067879	-1.649751	0.000170
24H	4.529511	-0.342939	0.000038
25H	5.022719	2.111299	0.000060
26H	3.175350	3.759565	0.000050
27H	0.792420	2.999908	0.000017

14-004

1C	-2.717531	-0.474527	1.207850
2C	-3.982076	0.108583	1.266031
3N	-4.780184	0.284651	0.199451
4C	-4.310269	-0.148367	-0.982890
5C	-3.064053	-0.748205	-1.155731
6C	-2.229170	-0.900648	-0.037922
7N	-0.995359	-1.547652	-0.156623
8C	0.132983	-0.954109	-0.183651
9N	1.301340	-1.720966	-0.283207
10S	2.738771	-0.874209	0.065833
11C	1.879933	0.687194	-0.002793
12C	0.500622	0.489761	-0.138127
13O	3.691084	-1.028855	-1.040552
14O	3.207196	-1.200098	1.422660
15C	2.476460	1.938490	0.058329
16C	1.631377	3.050436	-0.021931
17C	0.248506	2.884287	-0.169628
18C	-0.328764	1.611902	-0.230786
19H	-2.118152	-0.591537	2.105865
20H	-4.372991	0.455918	2.220469
21H	-4.965824	-0.007892	-1.840123
22H	-2.736443	-1.081219	-2.136150
23H	1.261219	-2.703635	-0.015751
24H	3.551381	2.050720	0.161542
25H	2.055674	4.049040	0.023564
26H	-0.391434	3.758789	-0.242039
27H	-1.398699	1.507765	-0.357417

14-005

1C	3.422916	-0.784803	-1.088023
2C	4.608319	-0.348195	-0.571665
3N	4.663621	0.214343	0.672029
4C	3.541272	0.345571	1.434617
5C	2.325171	-0.069575	0.971123
6C	2.197544	-0.654314	-0.342791
7N	1.073513	-1.128940	-0.856468
8C	-0.167559	-0.839848	-0.440043

9N	-1.050507	-1.796127	-0.208545
10S	-2.545402	-1.133148	0.186053
11C	-2.028805	0.582814	0.037904
12C	-0.685833	0.569897	-0.330412
13O	-2.882661	-1.465544	1.584575
14O	-3.549109	-1.460839	-0.845354
15C	-2.764937	1.747192	0.193943
16C	-2.096260	2.957145	-0.038716
17C	-0.748728	2.968486	-0.424843
18C	-0.031058	1.776099	-0.579640
19H	3.395286	-1.234486	-2.074624
20H	5.549433	-0.421824	-1.104198
21H	5.555911	0.523510	1.042135
22H	3.678365	0.787233	2.415272
23H	1.456199	0.029561	1.611545
24H	-3.813121	1.723902	0.476776
25H	-2.633275	3.895136	0.072471
26H	-0.253889	3.917276	-0.613659
27H	1.007036	1.793368	-0.894173

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1C	2.966592	3.371824	-1.350991
2C	2.933269	4.564362	-0.626647
3N	2.371602	4.684955	0.587058
4C	1.813079	3.585225	1.115505
5C	1.779062	2.348567	0.471887
6C	2.377489	2.238086	-0.786119
7N	2.346937	1.004554	-1.505083
8C	2.649392	-0.185215	-0.929658
9N	2.115396	-1.285111	-1.420458
10S	2.709073	-2.636706	-0.616089
11C	3.746590	-1.711053	0.515470
12C	3.625410	-0.354890	0.198604
13O	3.526784	-3.456450	-1.525706
14O	1.602597	-3.306715	0.090682
15C	4.592029	-2.200538	1.497586
16C	5.361448	-1.264728	2.200837
17C	5.284623	0.096655	1.884200
18C	4.426969	0.564860	0.881494
19C	1.609924	0.988153	-2.783513
20H	3.448700	3.327274	-2.322517
21H	3.387292	5.462190	-1.039386
22H	1.357330	3.697464	2.096646
23H	1.298654	1.496476	0.938452
24H	4.661843	-3.263971	1.706069
25H	6.034005	-1.602000	2.984179
26H	5.905995	0.808385	2.420186
27H	4.404842	1.622002	0.650932
28H	1.693386	1.970954	-3.245922
29H	2.047049	0.235736	-3.442153
30H	0.553905	0.755769	-2.617772
31P	-2.357960	-0.147142	0.141813
32C	-3.990217	0.266002	0.818277
33C	-1.141774	-0.018315	1.488699
34C	-2.365095	-1.818995	-0.554027
35C	-1.954776	1.032970	-1.181424
36C	-0.074740	-0.925740	1.578043
37C	0.870024	-0.782504	2.597246
38C	0.754501	0.256262	3.525127
39C	-0.313950	1.156093	3.440691
40C	-1.265507	1.020789	2.429009
41C	-3.431718	-2.698040	-0.303159
42C	-3.397167	-3.990870	-0.829445
43C	-2.307637	-4.408712	-1.600057
44C	-1.247459	-3.532205	-1.850985
45C	-1.272970	-2.237599	-1.334365
46C	-2.328828	0.753159	-2.506800
47C	-2.104986	1.703842	-3.504645
48C	-1.513322	2.930663	-3.187576
49C	-1.137566	3.207685	-1.869856
50C	-1.357198	2.263575	-0.866085
51C	-4.878675	1.069913	0.086911
52C	-6.146018	1.347310	0.604193
53C	-6.528914	0.826248	1.843379
54C	-5.643038	0.025942	2.573620
55C	-4.374299	-0.255788	2.066874
56H	0.033339	-1.743418	0.875040
57H	1.693446	-1.487439	2.660438
58H	1.492615	0.362976	4.315575
59H	-0.412624	1.959092	4.165923
60H	-2.102018	1.712242	2.382378
61H	-4.286447	-2.384081	0.287431
62H	-4.223413	-4.669382	-0.636307
63H	-2.283583	-5.417627	-2.002953
64H	-0.393137	-3.854762	-2.438608

65H	-0.439030	-1.571871	-1.533320
66H	-2.791958	-0.195037	-2.762061
67H	-2.392653	1.482868	-4.528694
68H	-1.340410	3.666866	-3.967940
69H	-0.666967	4.154539	-1.620306
70H	-1.055164	2.488404	0.150796
71H	-4.589010	1.484861	-0.873571
72H	-6.830247	1.973887	0.038839
73H	-7.515128	1.046777	2.242999
74H	-5.937230	-0.376552	3.538870
75H	-3.689031	-0.871628	2.642745

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1C	-4.071819	-2.556585	0.439344
2C	-3.886158	-3.771496	1.104818
3N	-2.851159	-4.594148	0.875907
4C	-1.955436	-4.219252	-0.050689
5C	-2.038314	-3.022500	-0.762570
6C	-3.112886	-2.172125	-0.498338
7N	-3.242091	-0.952418	-1.240386
8C	-3.108159	0.280566	-0.711835
9N	-3.440822	1.321412	-1.453043
10S	-3.108649	2.748255	-0.651349
11C	-2.605370	1.963951	0.879960
12C	-2.577830	0.581295	0.665373
13O	-4.337976	3.541197	-0.488576
14O	-1.943829	3.415312	-1.267315
15C	-2.235421	2.569333	2.068901
16C	-1.789039	1.734001	3.100862
17C	-1.701558	0.352765	2.900253
18C	-2.090212	-0.236483	1.690087
19C	-3.765053	-1.080696	-2.613596
20H	-4.927546	-1.925316	0.657461
21H	-4.605900	-4.098422	1.851550
22H	-1.127692	-4.902668	-0.225774
23H	-1.285581	-2.748755	-1.494962
24H	-2.285205	3.646833	2.192304
25H	-1.493224	2.164964	4.053075
26H	-1.322513	-0.283505	3.693334
27H	-2.001033	-1.306668	1.575624
28H	-3.266101	-0.366930	-3.268831
29H	-3.576202	-2.097524	-2.959142
30H	-4.843261	-0.883912	-2.625217
31P	2.251791	0.005812	-0.074886
32C	1.194718	-0.257024	-1.528826
33C	2.289287	1.764913	0.351899
34C	1.621921	-0.922688	1.353592
35C	3.920149	-0.578701	-0.482014
36C	1.166664	2.333442	0.977457
37C	1.154139	3.695633	1.271631
38C	2.258590	4.492276	0.951029
39C	3.378798	3.925054	0.336526
40C	3.399543	2.561933	0.032903
41C	0.874502	-2.094767	1.163182
42C	0.453354	-2.836409	2.268167
43C	0.777406	-2.415385	3.561036
44C	1.519236	-1.245207	3.752624
45C	1.941135	-0.494848	2.654352
46C	4.464440	-0.283982	-1.745217
47C	5.763789	-0.689835	-2.050104
48C	6.521379	-1.389288	-1.104034
49C	5.978749	-1.686267	0.149368
50C	4.679096	-1.283728	0.465290
51C	0.257303	0.710609	-1.926105
52C	-0.520492	0.492154	-3.065188
53C	-0.373514	-0.684369	-3.804030
54C	0.553576	-1.653200	-3.404944
55C	1.340318	-1.442923	-2.272446
56H	0.309653	1.720284	1.237020
57H	0.281357	4.132065	1.747921
58H	2.245885	5.554098	1.181485
59H	4.239884	4.540902	0.092414
60H	4.275234	2.130952	-0.441720
61H	0.609708	-2.427402	0.165548
62H	-0.135716	-3.736261	2.117451
63H	0.446422	-2.995114	4.418577
64H	1.766352	-0.911951	4.756751
65H	2.510427	0.416235	2.812940
66H	3.880139	0.252389	-2.487796
67H	6.182073	-0.461432	-3.026392
68H	7.532391	-1.705413	-1.346342
69H	6.562858	-2.234911	0.882963
70H	4.264231	-1.526262	1.438677
71H	0.128379	1.637243	-1.376805
72H	-1.241245	1.246228	-3.364055

73H	-0.976798	-0.846526	-4.693092
74H	0.673974	-2.567953	-3.978872
75H	2.072537	-2.191540	-1.983741

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1C	2.246450	-2.256398	-0.303144
2C	2.056045	-3.502774	0.293747
3N	3.061429	-4.310155	0.664014
4C	4.313142	-3.879060	0.436169
5C	4.614407	-2.646852	-0.146608
6C	3.554036	-1.815759	-0.514065
7N	3.804215	-0.547287	-1.124803
8C	3.237958	0.596901	-0.675683
9N	3.099414	1.611528	-1.504031
10S	2.421313	2.928100	-0.717268
11C	2.287538	2.115080	0.877308
12C	2.806391	0.823273	0.746998
13O	1.094494	3.209827	-1.295169
14O	3.379166	4.044056	-0.644810
15C	1.854900	2.652985	2.077932
16C	1.950827	1.840943	3.214665
17C	2.490572	0.553419	3.120047
18C	2.926440	0.033016	1.895229
19C	4.361727	-0.561113	-2.490148
20H	1.400842	-1.644539	-0.592737
21H	1.048643	-3.867340	0.478762
22H	5.115744	-4.545430	0.743201
23H	5.644408	-2.336975	-0.295290
24H	1.467742	3.664994	2.134300
25H	1.619533	2.220685	4.176938
26H	2.582812	-0.056111	4.014329
27H	3.354733	-0.960403	1.862578
28H	4.951496	-1.470011	-2.613195
29H	3.553696	-0.546396	-3.230192
30H	4.996700	0.314510	-2.636500
31P	-2.291605	-0.201436	-0.086657
32C	-4.011704	-0.429852	-0.623090
33C	-2.106584	1.540146	0.375670
34C	-1.913840	-1.273564	1.328088
35C	-1.140858	-0.651169	-1.415239
36C	-1.689226	1.920645	1.659156
37C	-1.606087	3.277505	1.981513
38C	-1.931633	4.248271	1.031728
39C	-2.352072	3.867419	-0.247742
40C	-2.448593	2.517436	-0.577225
41C	-2.900472	-2.048320	1.955137
42C	-2.550667	-2.873987	3.027468
43C	-1.227258	-2.926652	3.473233
44C	-0.243518	-2.152655	2.846934
45C	-0.580982	-1.329127	1.774773
46C	-1.088808	-1.996379	-1.829476
47C	-0.232522	-2.368231	-2.864432
48C	0.589780	-1.411473	-3.472217
49C	0.561129	-0.084522	-3.038607
50C	-0.307055	0.303953	-2.013748
51C	-4.340856	-1.075409	-1.824301
52C	-5.682961	-1.226715	-2.182720
53C	-6.693370	-0.738526	-1.350415
54C	-6.365498	-0.085186	-0.156863
55C	-5.029263	0.075563	0.207093
56H	-1.436409	1.176422	2.406996
57H	-1.285717	3.571575	2.977030
58H	-1.859561	5.302279	1.286124
59H	-2.602952	4.620723	-0.988748
60H	-2.785920	2.224522	-1.568102
61H	-3.929664	-2.020497	1.611853
62H	-3.314299	-3.478276	3.509059
63H	-0.959738	-3.572827	4.304867
64H	0.786861	-2.196712	3.186996
65H	0.191027	-0.738476	1.289646
66H	-1.706833	-2.747799	-1.344775
67H	-0.196825	-3.405403	-3.185453
68H	1.261999	-1.707223	-4.273136
69H	1.218026	0.656900	-3.481388
70H	-0.305589	1.337085	-1.685514
71H	-3.567875	-1.449786	-2.486811
72H	-5.934155	-1.723574	-3.115684
73H	-7.735524	-0.858337	-1.634056
74H	-7.148377	0.304797	0.487566
75H	-4.781533	0.596901	1.128069

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1C	3.366234	3.248719	-1.266801
2C	3.387363	4.424836	-0.515304
3N	2.751912	4.572921	0.658441
4C	2.058770	3.519811	1.117100
5C	1.965276	2.303175	0.442338
6C	2.640568	2.162061	-0.772410
7N	2.552983	0.948304	-1.519797
8C	2.703921	-0.273446	-0.948024
9N	2.115539	-1.312623	-1.501400
10S	2.520987	-2.722892	-0.681249
11C	3.541555	-1.908108	0.548433
12C	3.569485	-0.543240	0.249224
13O	3.336522	-3.597193	-1.540886
14O	1.312694	-3.306884	-0.072850
15C	4.252728	-2.482529	1.588838
16C	5.042264	-1.628958	2.369939
17C	5.117904	-0.263316	2.071241
18C	4.393716	0.292221	1.009436
19C	1.899692	1.016126	-2.840795
20H	3.910894	3.178825	-2.203288
21H	3.949696	5.285121	-0.870749
22H	1.540898	3.653504	2.064013
23H	1.384258	1.487345	0.854151
24H	4.206421	-3.549751	1.784112
25H	5.612560	-2.034738	3.200639
26H	5.754888	0.381860	2.669384
27H	4.487023	1.349296	0.795918
28H	2.029374	2.021521	-3.241551
29H	2.358910	0.290133	-3.514368
30H	0.831199	0.794596	-2.754461
31P	-2.404391	-0.026694	0.123578
32C	-4.000284	-0.432809	0.885085
33C	-1.997798	-1.338561	-1.059013
34C	-2.498524	1.577436	-0.721867
35C	-1.116971	0.110610	1.397024
36C	-1.509392	-1.034216	-2.338766
37C	-1.163572	-2.067965	-3.210801
38C	-1.306756	-3.399423	-2.814205
39C	-1.805038	-3.703668	-1.543308
40C	-2.153908	-2.679812	-0.664662
41C	-3.729154	2.192687	-0.995731
42C	-3.752243	3.427837	-1.649442
43C	-2.558301	4.048497	-2.027769
44C	-1.330745	3.433689	-1.756581
45C	-1.298483	2.202600	-1.104082
46C	-1.100567	1.245847	2.228451
47C	-0.143571	1.349294	3.237955
48C	0.804428	0.333951	3.413140
49C	0.796813	-0.784601	2.575759
50C	-0.162993	-0.903374	1.566580
51C	-4.226260	-0.238163	2.256551
52C	-5.480104	-0.531152	2.797845
53C	-6.504632	-1.014920	1.979097
54C	-6.277941	-1.213648	0.612752
55C	-5.028556	-0.927490	0.062666
56H	-1.401091	-0.004439	-2.662252
57H	-0.777565	-1.828951	-4.197627
58H	-1.026930	-4.200977	-3.492220
59H	-1.913280	-4.738265	-1.230958
60H	-2.540863	-2.926316	0.320128
61H	-4.662913	1.725094	-0.699473
62H	-4.705254	3.907074	-1.855616
63H	-2.583048	5.011619	-2.530245
64H	-0.399814	3.914814	-2.043978
65H	-0.343658	1.734011	-0.891937
66H	-1.821526	2.045980	2.084290
67H	-0.133698	2.225267	3.880502
68H	1.555230	0.422204	4.193857
69H	1.543474	-1.564262	2.692797
70H	-0.140842	-1.768913	0.914108
71H	-3.437166	0.128528	2.904759
72H	-5.652136	-0.385373	3.860632
73H	-7.477456	-1.243353	2.406128
74H	-7.070250	-1.596614	-0.024355
75H	-4.853571	-1.095716	-0.996197

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1C	2.068268	3.015752	0.031818
2C	2.690606	4.181190	-0.417092
3N	3.973996	4.481368	-0.163160
4C	4.680354	3.609397	0.572063
5C	4.153778	2.416462	1.074717
6C	2.823419	2.114751	0.782276
7N	2.210465	0.915990	1.277182
8C	2.567426	-0.323561	0.875530

9N	2.192852	-1.355881	1.604089
10S	2.620937	-2.791360	0.859897
11C	3.409228	-2.016609	-0.552236
12C	3.292765	-0.630205	-0.406389
13O	1.407983	-3.521630	0.444644
14O	3.595067	-3.519430	1.690214
15C	3.999211	-2.632406	-1.642621
16C	4.506510	-1.801238	-2.649372
17C	4.393324	-0.411047	-2.540135
18C	3.786707	0.187797	-1.428152
19C	1.404064	1.057405	2.503923
20H	1.029614	2.810830	-0.202481
21H	2.134788	4.902091	-1.012166
22H	5.716032	3.873876	0.772139
23H	4.765837	1.740718	1.663743
24H	4.062069	-3.714174	-1.712775
25H	4.983944	-2.240534	-3.520504
26H	4.781554	0.223510	-3.331692
27H	3.711061	1.265553	-1.386929
28H	0.996833	2.068415	2.530650
29H	0.593664	0.327635	2.496028
30H	2.025155	0.889203	3.391485
31P	-2.407057	0.054964	-0.135006
32C	-4.195889	-0.012379	-0.450333
33C	-2.102577	-0.760329	1.451413
34C	-1.507109	-0.795244	-1.458898
35C	-1.863851	1.790778	-0.107886
36C	-1.129980	-1.763836	1.562885
37C	-0.923585	-2.388742	2.795297
38C	-1.679625	-2.016199	3.908186
39C	-2.656723	-1.017898	3.794770
40C	-2.876934	-0.392607	2.569059
41C	-2.156149	-1.745764	-2.261916
42C	-1.435527	-2.428193	-3.244317
43C	-0.075787	-2.163764	-3.428231
44C	0.570587	-1.215126	-2.629486
45C	-0.138562	-0.531248	-1.642995
46C	-1.705045	2.469513	-1.330344
47C	-1.399265	3.831263	-1.334730
48C	-1.245029	4.519986	-0.126804
49C	-1.381832	3.842220	1.087893
50C	-1.688740	2.479715	1.102702
51C	-4.859500	1.044657	-1.093073
52C	-6.226197	0.943115	-1.361218
53C	-6.931943	-0.206206	-0.993269
54C	-6.272234	-1.258630	-0.349965
55C	-4.907482	-1.165730	-0.074277
56H	-0.531133	-2.071266	0.713191
57H	-0.165779	-3.161883	2.873501
58H	-1.514719	-2.505893	4.864260
59H	-3.252688	-0.734180	4.657849
60H	-3.652520	0.363292	2.477457
61H	-3.212617	-1.956529	-2.129576
62H	-1.939457	-3.164198	-3.864440
63H	0.482379	-2.696526	-4.193408
64H	1.626779	-1.013425	-2.771032
65H	0.372042	0.198727	-1.021774
66H	-1.823613	1.942694	-2.272884
67H	-1.280779	4.351285	-2.281228
68H	-1.006775	5.580098	-0.132773
69H	-1.243975	4.370341	2.027242
70H	-1.788255	1.966627	2.053099
71H	-4.327049	1.945983	-1.378222
72H	-6.737653	1.765392	-1.853782
73H	-7.995693	-0.279855	-1.202965
74H	-6.818656	-2.151192	-0.058192
75H	-4.405207	-1.983407	0.434505

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1C	3.471942	3.158148	-1.287298
2C	3.572364	4.346066	-0.561268
3N	2.928723	4.569257	0.596229
4C	2.144039	3.586447	1.062667
5C	1.965951	2.364893	0.412114
6C	2.655769	2.143950	-0.781896
7N	2.488652	0.920688	-1.506005
8C	2.639416	-0.297511	-0.928936
9N	1.993215	-1.331925	-1.425992
10S	2.459794	-2.744980	-0.646785
11C	3.560144	-1.935459	0.514390
12C	3.572957	-0.569945	0.216041
13O	3.214127	-3.611037	-1.569036
14O	1.303055	-3.341832	0.044218
15C	4.329793	-2.513956	1.509612
16C	5.162609	-1.663496	2.248278

17C	5.217253	-0.296154	1.954013
18C	4.434029	0.263347	0.936767
19C	1.738677	1.020469	-2.770674
20H	4.025653	3.021731	-2.211083
21H	4.207151	5.151637	-0.922732
22H	1.623651	3.783334	1.997109
23H	1.316503	1.605816	0.830004
24H	4.293579	-3.581689	1.703709
25H	5.779668	-2.072530	3.043138
26H	5.883635	0.348159	2.520259
27H	4.511028	1.322490	0.727988
28H	2.032224	1.942087	-3.275809
29H	1.973564	0.163198	-3.402219
30H	0.661162	1.041398	-2.577021
31P	-2.391401	-0.012316	0.128176
32C	-3.905017	-0.680569	0.875860
33C	-1.878763	-1.140198	-1.192326
34C	-2.700876	1.641744	-0.547446
35C	-1.101670	0.158862	1.397744
36C	-1.594014	-0.664104	-2.482137
37C	-1.186595	-1.558253	-3.473026
38C	-1.061092	-2.919407	-3.183317
39C	-1.357757	-3.395439	-1.902703
40C	-1.773435	-2.512935	-0.907624
41C	-4.005431	2.130488	-0.707526
42C	-4.202377	3.409110	-1.236916
43C	-3.107047	4.195642	-1.604597
44C	-1.804817	3.706975	-1.445009
45C	-1.598882	2.433763	-0.916525
46C	-1.132267	1.278914	2.249378
47C	-0.184691	1.401037	3.266299
48C	0.796873	0.417272	3.433134
49C	0.831351	-0.689177	2.580385
50C	-0.115375	-0.824689	1.561627
51C	-4.142358	-0.565872	2.254841
52C	-5.332817	-1.058266	2.793861
53C	-6.283233	-1.662652	1.965494
54C	-6.045725	-1.779372	0.591723
55C	-4.859078	-1.292136	0.043201
56H	-1.690731	0.390213	-2.719355
57H	-0.962065	-1.188126	-4.469571
58H	-0.730331	-3.609932	-3.954238
59H	-1.256141	-4.451604	-1.672879
60H	-2.012506	-2.892350	0.081277
61H	-4.862164	1.529797	-0.417744
62H	-5.213016	3.789703	-1.355075
63H	-3.265706	5.190888	-2.010947
64H	-0.950446	4.317415	-1.724602
65H	-0.586538	2.062694	-0.787693
66H	-1.882958	2.052990	2.117747
67H	-0.210046	2.266709	3.922339
68H	1.538765	0.518933	4.220658
69H	1.600776	-1.447001	2.693855
70H	-0.057876	-1.682150	0.902119
71H	-3.407832	-0.108005	2.909873
72H	-5.512692	-0.974871	3.862069
73H	-7.205857	-2.048429	2.390768
74H	-6.780203	-2.253667	-0.053192
75H	-4.676639	-1.392809	-1.023175

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1C	2.268051	-2.258324	-0.248148
2C	2.034731	-3.489704	0.363403
3N	3.012176	-4.320675	0.756480
4C	4.277919	-3.929372	0.535317
5C	4.621406	-2.715000	-0.062186
6C	3.589918	-1.857789	-0.451332
7N	3.880460	-0.605860	-1.077126
8C	3.326217	0.557560	-0.661013
9N	3.221611	1.556815	-1.512343
10S	2.546459	2.898859	-0.766328
11C	2.384212	2.126975	0.845796
12C	2.876303	0.821687	0.749229
13O	1.228838	3.175543	-1.368392
14O	3.512901	4.008375	-0.712305
15C	1.948730	2.698596	2.029142
16C	2.007672	1.906073	3.182050
17C	2.514113	0.603494	3.120950
18C	2.958241	0.050306	1.913321
19C	4.465064	-0.653036	-2.430188
20H	1.445617	-1.626286	-0.560112
21H	1.014768	-3.823054	0.539200
22H	5.057599	-4.614070	0.860515
23H	5.661793	-2.438457	-0.203878
24H	1.583047	3.719439	2.061576

25H	1.672036	2.312760	4.131544
26H	2.576544	0.008773	4.027794
27H	3.366315	-0.952126	1.907064
28H	5.131426	0.199656	-2.572629
29H	5.027249	-1.581617	-2.531609
30H	3.673493	-0.620392	-3.187204
31P	-2.308195	-0.183510	-0.104126
32C	-2.248589	-1.443210	1.200500
33C	-3.978082	-0.096704	-0.818216
34C	-1.943996	1.447280	0.599604
35C	-1.103907	-0.660364	-1.376734
36C	-4.316615	-0.820622	-1.972170
37C	-5.620675	-0.761051	-2.468103
38C	-6.585490	0.015332	-1.819384
39C	-6.247775	0.740173	-0.671660
40C	-4.947212	0.689232	-0.168972
41C	-2.049006	2.581761	-0.225850
42C	-1.835606	3.850128	0.310190
43C	-1.541405	3.996165	1.669945
44C	-1.450268	2.870961	2.492924
45C	-1.644375	1.593682	1.962979
46C	-1.086454	-2.000899	-1.807981
47C	-0.226521	-2.387200	-2.835424
48C	0.627765	-1.448324	-3.424898
49C	0.629228	-0.124511	-2.979029
50C	-0.236919	0.277294	-1.958136
51C	-0.992087	-1.859227	1.675830
52C	-0.915247	-2.799998	2.701741
53C	-2.086756	-3.332326	3.252567
54C	-3.335632	-2.922859	2.777015
55C	-3.422786	-1.978038	1.750922
56H	-3.574924	-1.417961	-2.491997
57H	-5.878125	-1.317429	-3.365060
58H	-7.598043	0.061033	-2.211084
59H	-6.993632	1.350307	-0.169872
60H	-4.689917	1.262224	0.717132
61H	-2.300789	2.480081	-1.277702
62H	-1.899497	4.721781	-0.334307
63H	-1.384000	4.987717	2.085949
64H	-1.225057	2.982516	3.549650
65H	-1.571425	0.727260	2.612241
66H	-1.732165	-2.740006	-1.342063
67H	-0.215786	-3.422188	-3.165172
68H	1.301240	-1.754453	-4.220897
69H	1.309511	0.603381	-3.408835
70H	-0.205743	1.307224	-1.621897
71H	-0.080050	-1.454939	1.248221
72H	0.056533	-3.121245	3.065953
73H	-2.024593	-4.069181	4.048922
74H	-4.245052	-3.340692	3.199494
75H	-4.397409	-1.671287	1.384693

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1C	5.608555	-0.981797	0.719631
2C	6.814112	-1.469022	0.210574
3N	6.898089	-2.500665	-0.642812
4C	5.749618	-3.087398	-1.015647
5C	4.491509	-2.675326	-0.574896
6C	4.422792	-1.591632	0.303859
7N	3.157542	-1.140437	0.792106
8C	2.772653	0.155081	0.736365
9N	1.853271	0.582934	1.577528
10S	1.461149	2.181510	1.256934
11C	2.579717	2.351222	-0.133752
12C	3.241737	1.132007	-0.304116
13O	1.866266	3.031439	2.389932
14O	0.057918	2.266642	0.813710
15C	2.743380	3.441729	-0.971979
16C	3.626791	3.292774	-2.048394
17C	4.288377	2.076955	-2.257279
18C	4.102158	0.988308	-1.396887
19C	2.420048	-2.046188	1.690207
20H	5.592951	-0.143739	1.409767
21H	7.754145	-1.010698	0.508947
22H	5.837191	-3.921288	-1.708368
23H	3.590635	-3.174408	-0.917102
24H	2.204353	4.369316	-0.804288
25H	3.790950	4.123235	-2.728990
26H	4.960591	1.969964	-3.103796
27H	4.621705	0.060405	-1.596039
28H	1.347233	-1.929555	1.525688
29H	2.719712	-3.070900	1.468586
30H	2.650171	-1.820556	2.737755
31P	-2.707434	-0.314608	-0.123535
32C	-1.143588	-0.487484	-1.030935

33C	-3.200734	1.424955	0.003259
34C	-4.027360	-1.196564	-1.005709
35C	-2.462586	-1.045596	1.518094
36C	-3.800047	2.039044	-1.111707
37C	-4.163103	3.383981	-1.049449
38C	-3.937733	4.116051	0.121919
39C	-3.349369	3.502853	1.231084
40C	-2.976801	2.158398	1.177132
41C	-3.725561	-2.135884	-2.003719
42C	-4.759592	-2.823111	-2.644353
43C	-6.089820	-2.578130	-2.292851
44C	-6.392047	-1.639595	-1.299793
45C	-5.366969	-0.946195	-0.656073
46C	-1.301315	-0.705526	2.234010
47C	-1.087193	-1.249242	3.500350
48C	-2.021013	-2.133586	4.051993
49C	-3.171521	-2.477035	3.335080
50C	-3.397733	-1.936816	2.066644
51C	-0.686337	0.528048	-1.882939
52C	0.499689	0.348941	-2.597504
53C	1.231693	-0.833649	-2.461814
54C	0.781737	-1.842560	-1.604678
55C	-0.402798	-1.674197	-0.887885
56H	-3.990294	1.472087	-2.018630
57H	-4.625801	3.856430	-1.911566
58H	-4.224214	5.163389	0.169546
59H	-3.171652	4.069366	2.140811
60H	-2.509821	1.698348	2.040357
61H	-2.696819	-2.329202	-2.290741
62H	-4.522484	-3.545040	-3.420932
63H	-6.891508	-3.112997	-2.794925
64H	-7.425582	-1.443856	-1.027937
65H	-5.611429	-0.213165	0.107744
66H	-0.567118	-0.029087	1.809429
67H	-0.188645	-0.981671	4.049619
68H	-1.850844	-2.557585	5.038148
69H	-3.893828	-3.169397	3.758611
70H	-4.289461	-2.218149	1.515511
71H	-1.231399	1.461339	-1.976710
72H	0.858354	1.142478	-3.246750
73H	2.159724	-0.962668	-3.011723
74H	1.353351	-2.758942	-1.486817
75H	-0.740920	-2.458831	-0.217042

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1C	2.148431	2.958848	-0.126811
2C	2.784006	4.087121	-0.647636
3N	4.071355	4.386533	-0.413852
4C	4.769398	3.552301	0.371336
5C	4.229538	2.398229	0.945830
6C	2.895328	2.095161	0.675241
7N	2.272792	0.938375	1.252172
8C	2.553668	-0.329337	0.880650
9N	2.135753	-1.314754	1.650520
10S	2.485191	-2.795019	0.957607
11C	3.300268	-2.114113	-0.487817
12C	3.255577	-0.719145	-0.391928
13O	1.234099	-3.480441	0.578891
14O	3.430106	-3.541209	1.806013
15C	3.866431	-2.797765	-1.550460
16C	4.424974	-2.029935	-2.580121
17C	4.384477	-0.633328	-2.519727
18C	3.798875	0.034596	-1.437173
19C	1.533879	1.155363	2.510472
20H	1.108297	2.747516	-0.353898
21H	2.236217	4.776842	-1.285979
22H	5.808736	3.815910	0.552624
23H	4.833177	1.750334	1.573836
24H	3.876521	-3.883116	-1.582768
25H	4.887090	-2.523887	-3.430019
26H	4.812909	-0.048301	-3.328591
27H	3.776072	1.115399	-1.436575
28H	1.248937	2.206680	2.561875
29H	0.643716	0.524815	2.533226
30H	2.165299	0.908400	3.371702
31P	-2.404688	0.067508	-0.107354
32C	-3.946972	-0.727160	-0.637977
33C	-1.111570	-0.405784	-1.290008
34C	-2.587385	1.873144	-0.127654
35C	-2.004607	-0.430312	1.590558
36C	-0.344522	0.572494	-1.944613
37C	0.613497	0.186757	-2.883452
38C	0.808816	-1.166339	-3.173175
39C	0.041465	-2.140158	-2.527665
40C	-0.924335	-1.765634	-1.594232

41C	-3.637277	2.483523	-0.829103
42C	-3.721670	3.877896	-0.871772
43C	-2.764148	4.661047	-0.221444
44C	-1.718176	4.052027	0.481931
45C	-1.628190	2.661488	0.533818
46C	-2.612112	0.260834	2.657251
47C	-2.366449	-0.140748	3.969718
48C	-1.521936	-1.228047	4.224848
49C	-0.918393	-1.910005	3.166272
50C	-1.154622	-1.516201	1.847381
51C	-4.856489	-1.228205	0.306775
52C	-6.055148	-1.800830	-0.124433
53C	-6.348021	-1.875103	-1.489250
54C	-5.439799	-1.379216	-2.431061
55C	-4.238582	-0.807053	-2.011455
56H	-0.492329	1.626582	-1.734572
57H	1.206388	0.945417	-3.386300
58H	1.561947	-1.462443	-3.897028
59H	0.194557	-3.193008	-2.745083
60H	-1.529226	-2.529432	-1.114304
61H	-4.388152	1.884818	-1.335453
62H	-4.538793	4.348888	-1.410888
63H	-2.834598	5.744796	-0.256736
64H	-0.975700	4.658719	0.993251
65H	-0.821171	2.195671	1.091471
66H	-3.269198	1.104463	2.467601
67H	-2.833647	0.395393	4.791163
68H	-1.329130	-1.535562	5.249190
69H	-0.244274	-2.739036	3.358323
70H	-0.649317	-2.046235	1.049080
71H	-4.635457	-1.186066	1.368696
72H	-6.754952	-2.194194	0.607615
73H	-7.280238	-2.324862	-1.820321
74H	-5.663132	-1.441230	-3.492554
75H	-3.535582	-0.431931	-2.749785

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1C	-2.210749	2.288636	-0.229094
2C	-1.952278	3.516718	0.379534
3N	-2.910131	4.381282	0.747175
4C	-4.182776	4.028819	0.503124
5C	-4.551777	2.823331	-0.096837
6C	-3.540853	1.931417	-0.461683
7N	-3.863460	0.691640	-1.097496
8C	-3.374926	-0.496856	-0.671618
9N	-3.306528	-1.501790	-1.520521
10S	-2.697183	-2.869595	-0.767013
11C	-2.531895	-2.108183	0.848939
12C	-2.960808	-0.781139	0.745347
13O	-1.379794	-3.194993	-1.346512
14O	-3.705030	-3.942285	-0.734391
15C	-2.150587	-2.702795	2.039427
16C	-2.201500	-1.912277	3.193945
17C	-2.643179	-0.586879	3.125645
18C	-3.030405	-0.009279	1.909902
19C	-4.425789	0.765650	-2.458781
20H	-1.401976	1.627760	-0.518491
21H	-0.926609	3.821509	0.571714
22H	-4.946958	4.739131	0.809509
23H	-5.597215	2.580103	-0.260381
24H	-1.831648	-3.739224	2.075911
25H	-1.909498	-2.337765	4.149482
26H	-2.698968	0.007728	4.033047
27H	-3.389482	1.011495	1.897882
28H	-4.967747	1.706277	-2.559187
29H	-3.623352	0.726727	-3.204137
30H	-5.107017	-0.071809	-2.619841
31P	2.351046	0.153522	-0.088821
32C	3.939481	-0.214616	-0.886530
33C	1.869425	-1.322201	0.849183
34C	2.514349	1.565015	1.036743
35C	1.124426	0.601694	-1.346813
36C	1.588075	-1.242355	2.222076
37C	1.299539	-2.407409	2.935574
38C	1.283542	-3.644775	2.286766
39C	1.559782	-3.724168	0.917904
40C	1.862163	-2.569179	0.198285
41C	3.772710	2.041108	1.431954
42C	3.854885	3.112245	2.325807
43C	2.690625	3.703041	2.824708
44C	1.434480	3.229790	2.426911
45C	1.342674	2.163204	1.533853
46C	1.167197	1.900957	-1.887148
47C	0.293773	2.250704	-2.916445
48C	-0.622706	1.313287	-3.406585

49C	-0.675141	0.029375	-2.858656
50C	0.194815	-0.332618	-1.827128
51C	4.202024	0.186226	-2.205767
52C	5.443259	-0.098011	-2.779771
53C	6.419349	-0.776931	-2.044894
54C	6.156256	-1.179898	-0.730880
55C	4.918479	-0.905078	-0.149776
56H	1.601474	-0.287401	2.737209
57H	1.088757	-2.344334	3.999244
58H	1.056396	-4.548217	2.846569
59H	1.542559	-4.683127	0.408404
60H	2.100043	-2.642357	-0.859100
61H	4.681367	1.589857	1.045548
62H	4.829700	3.484342	2.628169
63H	2.759678	4.535847	3.519351
64H	0.528765	3.692433	2.809081
65H	0.366233	1.802808	1.222939
66H	1.871699	2.633830	-1.504049
67H	0.325672	3.254992	-3.329435
68H	-1.301950	1.589558	-4.208549
69H	-1.399629	-0.695286	-3.214453
70H	0.124576	-1.329932	-1.407291
71H	3.448214	0.705205	-2.789606
72H	5.641976	0.205939	-3.803642
73H	7.382007	-0.998704	-2.497582
74H	6.911088	-1.713565	-0.160111
75H	4.714873	-1.232237	0.866108

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1C	4.533574	2.628583	-0.470863
2C	5.785095	3.065157	-0.907259
3N	6.943559	2.517098	-0.507704
4C	6.877876	1.504361	0.369412
5C	5.679522	0.994737	0.875427
6C	4.484694	1.562034	0.429286
7N	3.221278	1.094681	0.912785
8C	2.781058	-0.171279	0.751001
9N	1.786194	-0.594473	1.507022
10S	1.371308	-2.166814	1.106738
11C	2.582909	-2.328943	-0.205001
12C	3.285676	-1.124006	-0.295696
13O	0.009776	-2.219130	0.544673
14O	1.663965	-3.060891	2.240566
15C	2.770323	-3.398793	-1.064335
16C	3.723454	-3.243724	-2.078941
17C	4.428090	-2.041343	-2.208470
18C	4.217657	-0.973231	-1.327489
19C	2.505163	1.965331	1.860185
20H	3.621366	3.093460	-0.829800
21H	5.859474	3.886046	-1.616939
22H	7.826741	1.080598	0.689866
23H	5.679792	0.175143	1.587258
24H	2.197272	-4.315122	-0.957600
25H	3.908510	-4.058104	-2.773436
26H	5.154233	-1.928147	-3.008437
27H	4.771714	-0.054709	-1.467079
28H	1.434343	1.925762	1.653567
29H	2.686376	1.639173	2.890663
30H	2.868019	2.985677	1.733420
31P	-2.708277	0.328614	-0.130948
32C	-2.500262	-0.201605	1.587919
33C	-3.776257	1.797085	-0.199728
34C	-1.116624	0.788102	-0.876886
35C	-3.466598	-1.038042	-1.055548
36C	-3.826882	2.552475	-1.385119
37C	-4.663137	3.666359	-1.462058
38C	-5.445319	4.034538	-0.361592
39C	-5.389952	3.288675	0.819021
40C	-4.557487	2.169963	0.904857
41C	-0.435839	-0.102865	-1.719343
42C	0.787177	0.271324	-2.278200
43C	1.333968	1.526248	-1.998844
44C	0.658032	2.415199	-1.157300
45C	-0.566969	2.052158	-0.596706
46C	-4.485896	-0.795094	-1.990021
47C	-5.038176	-1.860698	-2.704280
48C	-4.578551	-3.163449	-2.490300
49C	-3.564630	-3.405199	-1.557120
50C	-3.005981	-2.349346	-0.836110
51C	-1.345466	0.136809	2.305212
52C	-1.209909	-0.276242	3.631114
53C	-2.222806	-1.020980	4.241356
54C	-3.376831	-1.358691	3.525105
55C	-3.518870	-0.955264	2.197479
56H	-3.215019	2.279999	-2.240413

57H	-4.700356	4.247012	-2.379584
58H	-6.093302	4.904688	-0.423900
59H	-5.990131	3.576681	1.677653
60H	-4.516303	1.603123	1.829470
61H	-0.845157	-1.082319	-1.938116
62H	1.313126	-0.423014	-2.926955
63H	2.288597	1.809332	-2.433360
64H	1.079864	3.391534	-0.935663
65H	-1.090869	2.752530	0.048213
66H	-4.859841	0.209637	-2.157481
67H	-5.831431	-1.670688	-3.422046
68H	-5.013662	-3.990394	-3.045263
69H	-3.208170	-4.417055	-1.384827
70H	-2.219020	-2.546122	-0.115169
71H	-0.538569	0.682995	1.832187
72H	-0.301516	-0.034707	4.175630
73H	-2.109690	-1.348955	5.271279
74H	-4.161846	-1.944393	3.995397
75H	-4.409412	-1.232884	1.640231

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1C	5.081535	-1.609191	0.974105
2C	6.146346	-2.417305	0.569639
3N	6.013225	-3.458152	-0.266159
4C	4.780940	-3.728801	-0.724750
5C	3.650624	-2.981511	-0.390292
6C	3.811504	-1.890965	0.467396
7N	2.677186	-1.105685	0.848317
8C	2.627397	0.236830	0.693926
9N	1.775913	0.931806	1.422454
10S	1.850361	2.555799	1.018014
11C	3.087917	2.355949	-0.262275
12C	3.416318	0.999503	-0.333735
13O	2.360175	3.329489	2.163360
14O	0.574452	2.997061	0.423650
15C	3.598239	3.320857	-1.114912
16C	4.493876	2.890889	-2.101945
17C	4.825469	1.535720	-2.213220
18C	4.291044	0.579721	-1.340956
19C	1.726302	-1.739166	1.779597
20H	5.238455	-0.778479	1.655329
21H	7.150034	-2.219649	0.938687
22H	4.693284	-4.577352	-1.399388
23H	2.676627	-3.233934	-0.797649
24H	3.308411	4.363604	-1.026558
25H	4.923275	3.613038	-2.790434
26H	5.507746	1.212122	-2.994047
27H	4.556449	-0.460793	-1.470666
28H	0.731537	-1.325904	1.624130
29H	1.718659	-2.812458	1.587671
30H	2.029562	-1.557091	2.816917
31P	-2.673891	-0.219087	-0.139966
32C	-2.147661	-1.120139	1.348850
33C	-3.410700	1.371337	0.322355
34C	-1.241920	0.069308	-1.218330
35C	-3.889167	-1.244569	-1.014472
36C	-2.565116	2.432381	0.691913
37C	-3.120364	3.645679	1.100029
38C	-4.509200	3.806434	1.139226
39C	-5.348490	2.752096	0.765485
40C	-4.805649	1.532553	0.355855
41C	-0.176949	-0.846453	-1.217133
42C	0.897678	-0.660470	-2.086146
43C	0.919760	0.439172	-2.949575
44C	-0.139625	1.350402	-2.951561
45C	-1.222918	1.169635	-2.090009
46C	-4.902531	-1.894143	-0.286474
47C	-5.863835	-2.648295	-0.959426
48C	-5.818467	-2.760676	-2.353583
49C	-4.809076	-2.119014	-3.076833
50C	-3.842244	-1.360415	-2.412457
51C	-1.848332	-0.425904	2.531673
52C	-1.410475	-1.130302	3.654908
53C	-1.270100	-2.519867	3.603568
54C	-1.568807	-3.212632	2.425385
55C	-2.008351	-2.518654	1.297484
56H	-1.485460	2.328823	0.653122
57H	-2.462476	4.462898	1.382494
58H	-4.937350	4.753765	1.456012
59H	-6.427371	2.877927	0.787042
60H	-5.467812	0.724829	0.060696
61H	-0.179307	-1.694584	-0.540110
62H	1.724715	-1.364119	-2.074399
63H	1.766552	0.591661	-3.612728
64H	-0.121682	2.210070	-3.615433

65H	-2.036600	1.888474	-2.093060
66H	-4.939861	-1.818954	0.796776
67H	-6.645197	-3.149064	-0.394577
68H	-6.567954	-3.350929	-2.873966
69H	-4.768770	-2.209923	-4.158666
70H	-3.058701	-0.870530	-2.982598
71H	-1.953943	0.652328	2.586733
72H	-1.178380	-0.588852	4.567602
73H	-0.930949	-3.063693	4.481227
74H	-1.464416	-4.293345	2.383834
75H	-2.247582	-3.064525	0.389052

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1C	5.629545	-1.017447	0.733294
2C	6.828527	-1.516679	0.220183
3N	6.899135	-2.548435	-0.634191
4C	5.743527	-3.123243	-1.003253
5C	4.491108	-2.698737	-0.557951
6C	4.436110	-1.614419	0.321131
7N	3.177261	-1.147823	0.813030
8C	2.802062	0.149962	0.744351
9N	1.886909	0.593771	1.582094
10S	1.505362	2.191561	1.243481
11C	2.617041	2.334892	-0.155337
12C	3.274357	1.110976	-0.309732
13O	1.923667	3.052670	2.363123
14O	0.100184	2.283584	0.806828
15C	2.778676	3.411404	-1.011788
16C	3.656522	3.243354	-2.089856
17C	4.315348	2.023302	-2.281519
18C	4.131030	0.948849	-1.403024
19C	2.438243	-2.039240	1.724214
20H	5.625280	-0.179872	1.424053
21H	7.774145	-1.068138	0.515689
22H	5.820127	-3.957471	-1.696900
23H	3.585040	-3.188860	-0.899077
24H	2.241924	4.342441	-0.856285
25H	3.818463	4.062144	-2.784964
26H	4.983917	1.901441	-3.128893
27H	4.648851	0.017442	-1.589769
28H	1.364878	-1.909563	1.572166
29H	2.722108	-3.068931	1.504268
30H	2.682839	-1.811239	2.768006
31P	-2.735784	-0.313306	-0.124776
32C	-1.163050	-0.492305	-1.014359
33C	-3.266423	1.419153	-0.120844
34C	-4.020920	-1.297667	-0.949731
35C	-2.485740	-0.915211	1.569306
36C	-3.934678	1.933636	-1.246603
37C	-4.304079	3.278342	-1.275765
38C	-4.013374	4.108656	-0.187203
39C	-3.352214	3.594854	0.931744
40C	-2.974210	2.251558	0.969651
41C	-3.678627	-2.301995	-1.868708
42C	-4.683157	-3.066639	-2.466780
43C	-6.024964	-2.834112	-2.152770
44C	-6.368080	-1.831208	-1.239440
45C	-5.372482	-1.060974	-0.638208
46C	-1.296329	-0.577096	2.237711
47C	-1.094504	-1.005526	3.549649
48C	-2.070127	-1.771676	4.196324
49C	-3.250572	-2.112983	3.528251
50C	-3.463142	-1.688960	2.214589
51C	-0.720074	0.503617	-1.896778
52C	0.473974	0.324218	-2.598120
53C	1.226917	-0.839253	-2.419681
54C	0.791596	-1.827197	-1.530880
55C	-0.399424	-1.657850	-0.825870
56H	-4.172703	1.291541	-2.089880
57H	-4.821272	3.675023	-2.145098
58H	-4.304867	5.155345	-0.211666
59H	-3.122293	4.237830	1.776636
60H	-2.447232	1.867939	1.835577
61H	-2.641298	-2.487223	-2.128680
62H	-4.413989	-3.839890	-3.180920
63H	-6.803633	-3.429168	-2.622329
64H	-7.410639	-1.644283	-0.997415
65H	-5.650027	-0.277239	0.061231
66H	-0.533394	0.015855	1.746932
67H	-0.172984	-0.738176	4.059633
68H	-1.910697	-2.104012	5.218723
69H	-4.007308	-2.713092	4.025955
70H	-4.379329	-1.966692	1.703299
71H	-1.284710	1.421131	-2.026588
72H	0.822438	1.102784	-3.270662

73H	2.159504	-0.969424	-2.961408
74H	1.379193	-2.727769	-1.378325
75H	-0.725769	-2.426020	-0.130676

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1C	-1.631953	2.980847	1.674605
2C	-1.203567	4.177134	1.098985
3N	-0.926734	4.320835	-0.207382
4C	-1.070754	3.237112	-0.984811
5C	-1.469738	1.987638	-0.508614
6C	-1.773362	1.859685	0.850216
7N	-2.176520	0.608294	1.401935
8C	-3.076134	-0.211678	0.801079
9N	-3.017658	-1.502346	1.051686
10S	-4.260518	-2.311217	0.261985
11C	-4.959414	-0.841567	-0.492590
12C	-4.200327	0.256729	-0.077017
13O	-5.200657	-2.891600	1.234953
14O	-3.678922	-3.216900	-0.746847
15C	-6.097582	-0.739056	-1.275380
16C	-6.494577	0.548390	-1.658671
17C	-5.771700	1.668834	-1.232559
18C	-4.627390	1.538853	-0.436526
19C	-1.329074	0.027552	2.461521
20H	-1.862070	2.929192	2.734274
21H	-1.086785	5.064519	1.716770
22H	-0.832112	3.362238	-2.038400
23H	-1.536226	1.138168	-1.178041
24H	-6.664477	-1.617740	-1.567275
25H	-7.379634	0.676830	-2.275040
26H	-6.105414	2.662695	-1.516759
27H	-4.102669	2.426987	-0.108548
28H	-0.800896	0.833678	2.966835
29H	-1.953331	-0.509009	3.178362
30H	-0.601551	-0.666969	2.031714
31P	2.641901	-0.286715	-0.147561
32C	3.938288	-1.422912	-0.710892
33C	2.229910	-0.725054	1.563995
34C	3.232265	1.425364	-0.221923
35C	1.190933	-0.433939	-1.232888
36C	2.197674	0.251779	2.570966
37C	1.870639	-0.113582	3.878749
38C	1.569088	-1.443269	4.183196
39C	1.614116	-2.420423	3.182387
40C	1.953834	-2.069371	1.876522
41C	4.594601	1.714681	-0.391595
42C	5.017291	3.046190	-0.425160
43C	4.088938	4.083088	-0.293789
44C	2.729298	3.794362	-0.128877
45C	2.298864	2.469048	-0.091020
46C	1.180505	0.277504	-2.446581
47C	0.125073	0.104746	-3.342798
48C	-0.918426	-0.775539	-3.036737
49C	-0.915308	-1.474614	-1.826213
50C	0.134027	-1.303609	-0.920416
51C	3.942010	-1.914224	-2.025398
52C	4.977577	-2.751513	-2.446172
53C	6.004032	-3.098680	-1.562916
54C	5.997256	-2.612715	-0.250680
55C	4.966569	-1.777348	0.180514
56H	2.424971	1.288881	2.346054
57H	1.850004	0.644378	4.657114
58H	1.307692	-1.721874	5.200471
59H	1.390439	-3.457020	3.417901
60H	2.008791	-2.839229	1.111449
61H	5.321518	0.916019	-0.502547
62H	6.071764	3.270258	-0.560185
63H	4.422552	5.116787	-0.326182
64H	2.000412	4.594862	-0.040265
65H	1.242378	2.250993	0.027444
66H	1.985818	0.963138	-2.692400
67H	0.120760	0.657343	-4.278177
68H	-1.737958	-0.910935	-3.737454
69H	-1.730582	-2.146563	-1.577842
70H	0.110130	-1.844455	0.019008
71H	3.144695	-1.658437	-2.715954
72H	4.976688	-3.135499	-3.462416
73H	6.806122	-3.752668	-1.894414
74H	6.790503	-2.887102	0.439035
75H	4.960352	-1.411399	1.203522

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1C	0.799654	2.799124	0.908744
2C	-0.190064	3.715410	1.167592
3N	-0.620473	4.602977	0.231269
4C	-0.036538	4.604614	-1.002161
5C	0.954213	3.714868	-1.321520
6C	1.424032	2.748976	-0.378751
7N	2.382183	1.899528	-0.816459
8C	2.901002	0.913256	-0.076833
9N	2.592463	0.581611	1.176943
10S	3.462368	-0.762044	1.665511
11C	4.343891	-0.983321	0.115521
12C	3.926845	0.039952	-0.731124
13O	4.392795	-0.410459	2.758087
14O	2.541521	-1.890638	1.924853
15C	5.270479	-1.946698	-0.254299
16C	5.796766	-1.856328	-1.550549
17C	5.395033	-0.829744	-2.418180
18C	4.455589	0.127936	-2.017959
19C	-1.643782	5.604457	0.573814
20H	1.088174	2.109423	1.687397
21H	-0.683851	3.765626	2.130934
22H	-0.405182	5.343574	-1.704257
23H	1.389295	3.736765	-2.314926
24H	5.576930	-2.734382	0.427702
25H	6.527056	-2.588548	-1.883898
26H	5.820312	-0.778219	-3.416905
27H	4.137908	0.922178	-2.685703
28H	-1.164332	6.494692	0.991944
29H	-2.197817	5.876264	-0.326199
30H	-2.333353	5.179881	1.305841
31P	-1.987819	-0.866569	-0.125985
32C	-1.608952	-0.056114	1.451921
33C	-0.484964	-1.487442	-0.927540
34C	-3.076087	-2.287095	0.175109
35C	-2.820590	0.346858	-1.191555
36C	0.117242	-2.648769	-0.412819
37C	1.285439	-3.139155	-0.994136
38C	1.849336	-2.484784	-2.092465
39C	1.244095	-1.337752	-2.613436
40C	0.078822	-0.832861	-2.034863
41C	-3.776758	-2.408672	1.384848
42C	-4.624753	-3.500252	1.585675
43C	-4.774306	-4.467238	0.587426
44C	-4.072618	-4.348125	-0.617545
45C	-3.220983	-3.263362	-0.826683
46C	-2.270912	1.636186	-1.317104
47C	-2.886260	2.572174	-2.147191
48C	-4.049373	2.234374	-2.848229
49C	-4.597857	0.955549	-2.719856
50C	-3.987143	0.008437	-1.893619
51C	-0.443344	-0.383033	2.158768
52C	-0.202716	0.209644	3.400695
53C	-1.115582	1.121843	3.935154
54C	-2.278097	1.450431	3.226361
55C	-2.528689	0.865632	1.985549
56H	-0.316632	-3.166924	0.437111
57H	1.759630	-4.022895	-0.578066
58H	2.767086	-2.861625	-2.534731
59H	1.685758	-0.825123	-3.462717
60H	-0.377747	0.061648	-2.445656
61H	-3.658474	-1.668797	2.170423
62H	-5.160001	-3.596874	2.526198
63H	-5.431125	-5.317442	0.750586
64H	-4.180987	-5.103121	-1.391364
65H	-2.667736	-3.183762	-1.758406
66H	-1.370622	1.906817	-0.774108
67H	-2.454870	3.563754	-2.248162
68H	-4.527034	2.967706	-3.492472
69H	-5.503018	0.691886	-3.259703
70H	-4.425811	-0.979735	-1.796893
71H	0.291413	-1.069392	1.753677
72H	0.708894	-0.035539	3.937680
73H	-0.920568	1.582712	4.900033
74H	-2.989597	2.160658	3.639237
75H	-3.430456	1.126139	1.438629

15g-Me-002

1C	-3.387828	-2.163731	1.469845
2C	-4.171189	-3.243056	1.157779
3N	-5.053584	-3.202039	0.119355
4C	-5.150486	-2.068545	-0.626316
5C	-4.379351	-0.960109	-0.374300
6C	-3.440897	-0.958662	0.705362
7N	-2.631862	0.049561	1.107254
8C	-2.416249	1.159724	0.397800

9N	-2.817668	1.421520	-0.847400
10S	-2.209649	2.886579	-1.371969
11C	-1.385082	3.305096	0.169336
12C	-1.575764	2.227044	1.030513
13O	-1.210124	2.667360	-2.441947
14O	-3.304340	3.830365	-1.674393
15C	-0.649144	4.429545	0.510847
16C	-0.069152	4.446308	1.787004
17C	-0.237659	3.365954	2.665055
18C	-0.995241	2.247198	2.297886
19C	-5.844232	-4.395777	-0.223751
20H	-2.708871	-2.225722	2.313190
21H	-4.136735	-4.171414	1.716356
22H	-5.872293	-2.093144	-1.435613
23H	-4.492672	-0.090021	-1.004695
24H	-0.524090	5.257682	-0.180241
25H	0.518445	5.306615	2.095844
26H	0.226002	3.398398	3.646931
27H	-1.125109	1.408715	2.972249
28H	-6.739418	-4.088077	-0.766000
29H	-5.247699	-5.066982	-0.849137
30H	-6.138212	-4.910794	0.692969
31P	2.126844	-0.655936	-0.117824
32C	3.449278	-1.894748	-0.249857
33C	1.728856	-0.393044	1.631050
34C	2.664873	0.918957	-0.836457
35C	0.689500	-1.297968	-1.019408
36C	2.555472	0.438603	2.406985
37C	2.304676	0.582727	3.771632
38C	1.235204	-0.097717	4.364403
39C	0.409856	-0.917677	3.590330
40C	0.650467	-1.066709	2.223200
41C	3.711532	0.950771	-1.772377
42C	4.076873	2.162818	-2.360453
43C	3.400218	3.338622	-2.022890
44C	2.360837	3.306418	-1.088597
45C	1.990981	2.102831	-0.488636
46C	0.363214	-2.662916	-0.906940
47C	-0.740280	-3.167249	-1.593922
48C	-1.518288	-2.318784	-2.390634
49C	-1.196641	-0.964296	-2.496840
50C	-0.092271	-0.448301	-1.815542
51C	4.243632	-2.217852	0.860910
52C	5.268079	-3.158406	0.729332
53C	5.501202	-3.776400	-0.502497
54C	4.707629	-3.456939	-1.609897
55C	3.680057	-2.521343	-1.488048
56H	3.385728	0.971449	1.952252
57H	2.942341	1.228039	4.369400
58H	1.040205	0.019664	5.427121
59H	-0.432874	-1.429921	4.045869
60H	-0.009651	-1.686443	1.625846
61H	4.246496	0.045112	-2.039380
62H	4.889144	2.185691	-3.081727
63H	3.682067	4.279824	-2.487231
64H	1.829571	4.216450	-0.828814
65H	1.185723	2.093788	0.239523
66H	0.969150	-3.328710	-0.298699
67H	-0.988592	-4.221875	-1.509921
68H	-2.377570	-2.714748	-2.925456
69H	-1.805513	-0.295401	-3.095754
70H	0.135419	0.607741	-1.912494
71H	4.066228	-1.749797	1.824012
72H	5.878000	-3.410752	1.592387
73H	6.297156	-4.510000	-0.599445
74H	4.882794	-3.940314	-2.567068
75H	3.057978	-2.290693	-2.348621

15g-Me-003

1C	0.873125	3.375743	-1.456861
2C	0.106120	4.451644	-1.094045
3N	-0.007172	4.836259	0.207896
4C	0.643388	4.125796	1.170768
5C	1.411668	3.028978	0.874156
6C	1.585977	2.610998	-0.484452
7N	2.400270	1.634984	-0.938428
8C	2.900120	0.660853	-0.178636
9N	2.478034	0.292294	1.033246
10S	3.336842	-1.037536	1.577761
11C	4.377972	-1.190539	0.120950
12C	4.001994	-0.173049	-0.751232
13O	4.133626	-0.674348	2.769079
14O	2.449995	-2.211599	1.715564
15C	5.366992	-2.117292	-0.173590
16C	6.003083	-1.992454	-1.416768

17C	5.642699	-0.971161	-2.308655
18C	4.637625	-0.051478	-1.985850
19C	-0.761123	6.045439	0.575541
20H	0.950752	3.105731	-2.504544
21H	-0.437471	5.047475	-1.817955
22H	0.517472	4.482419	2.187435
23H	1.898352	2.496406	1.679633
24H	5.637673	-2.903700	0.524807
25H	6.785950	-2.694631	-1.689988
26H	6.151614	-0.894792	-3.265768
27H	4.347789	0.735340	-2.675055
28H	-1.368371	5.841718	1.459565
29H	-0.065706	6.862776	0.788042
30H	-1.411464	6.328977	-0.252268
31P	-2.097187	-0.783052	-0.077047
32C	-0.613304	-1.104713	-1.066542
33C	-2.664348	0.933030	-0.281486
34C	-3.438919	-1.865935	-0.647324
35C	-1.740127	-1.101227	1.669426
36C	-3.347754	1.300151	-1.454455
37C	-3.798942	2.610773	-1.613892
38C	-3.586490	3.553836	-0.602368
39C	-2.914969	3.186545	0.566640
40C	-2.448457	1.880825	0.730362
41C	-3.146791	-3.044447	-1.351212
42C	-4.187080	-3.886769	-1.750224
43C	-5.512395	-3.558462	-1.450093
44C	-5.803660	-2.384377	-0.746772
45C	-4.771731	-1.536038	-0.344572
46C	-0.523651	-0.650940	2.209264
47C	-0.258781	-0.844451	3.565300
48C	-1.197833	-1.482447	4.381299
49C	-2.405436	-1.937046	3.840542
50C	-2.681616	-1.751104	2.484888
51C	-0.392152	-0.405604	-2.265303
52C	0.696788	-0.741703	-3.068953
53C	1.565027	-1.767792	-2.683155
54C	1.354462	-2.451318	-1.483298
55C	0.267806	-2.125033	-0.671673
56H	-3.540633	0.567153	-2.232818
57H	-4.329427	2.888965	-2.520392
58H	-3.953953	4.569660	-0.722462
59H	-2.757285	3.912304	1.359023
60H	-1.931589	1.608267	1.644615
61H	-2.120791	-3.304967	-1.592451
62H	-3.959633	-4.796322	-2.299322
63H	-6.318776	-4.214892	-1.766154
64H	-6.833047	-2.126495	-0.513675
65H	-5.003879	-0.623277	0.196512
66H	0.229918	-0.179590	1.585844
67H	0.690689	-0.512165	3.975128
68H	-0.983374	-1.637580	5.435408
69H	-3.130429	-2.444954	4.470624
70H	-3.616513	-2.117703	2.072946
71H	-1.050565	0.402225	-2.568569
72H	0.875788	-0.191361	-3.988377
73H	2.418846	-2.018837	-3.305832
74H	2.043871	-3.225949	-1.162821
75H	0.129892	-2.648424	0.267921

15g-Me-004

1C	0.887034	3.103243	1.796830
2C	0.318952	4.319445	1.526574
3N	0.285393	4.823450	0.260094
4C	0.823812	4.099594	-0.757616
5C	1.431373	2.885517	-0.546279
6C	1.501629	2.328443	0.767132
7N	2.028295	1.135181	1.128120
8C	2.928555	0.471841	0.398993
9N	3.573073	0.913123	-0.682168
10S	4.687864	-0.219261	-1.207254
11C	4.274396	-1.463936	0.023808
12C	3.299550	-0.907373	0.846645
13O	4.348742	-0.681992	-2.569710
14O	6.066424	0.273059	-1.004275
15C	4.780452	-2.742439	0.204073
16C	4.260503	-3.487170	1.272007
17C	3.279262	-2.944450	2.114607
18C	2.790331	-1.648486	1.911730
19C	-0.314623	6.146913	0.025104
20H	0.894495	2.731682	2.815784
21H	-0.126010	4.939281	2.297107
22H	0.753961	4.538726	-1.746269
23H	1.866775	2.366490	-1.388645
24H	5.544180	-3.150394	-0.451473

25H	4.626275	-4.494946	1.448854
26H	2.894141	-3.539815	2.938154
27H	2.031473	-1.225687	2.561205
28H	-0.320049	6.354611	-1.044961
29H	-1.340402	6.156961	0.401893
30H	0.274019	6.911782	0.538940
31P	-2.203488	-0.702610	-0.138067
32C	-0.670237	-1.331428	-0.866102
33C	-2.473612	1.033144	-0.595443
34C	-3.633699	-1.644118	-0.745107
35C	-2.066604	-0.845353	1.664428
36C	-2.802828	1.340986	-1.928266
37C	-3.031493	2.666551	-2.296050
38C	-2.949496	3.684226	-1.338387
39C	-2.632606	3.375661	-0.013660
40C	-2.387338	2.053356	0.362408
41C	-3.475539	-2.910376	-1.329437
42C	-4.600001	-3.622847	-1.752637
43C	-5.877695	-3.078108	-1.596428
44C	-6.035890	-1.812884	-1.020103
45C	-4.919089	-1.092026	-0.597332
46C	-0.851528	-0.481460	2.271901
47C	-0.729825	-0.545443	3.659784
48C	-1.807465	-0.975973	4.441916
49C	-3.012240	-1.344035	3.835049
50C	-3.147702	-1.280167	2.445941
51C	-0.006804	-0.629037	-1.884348
52C	1.164165	-1.152993	-2.434177
53C	1.667254	-2.375390	-1.981680
54C	1.006792	-3.075978	-0.968061
55C	-0.155329	-2.555193	-0.400635
56H	-2.891288	0.552692	-2.671407
57H	-3.283511	2.902459	-3.326181
58H	-3.140576	4.714762	-1.626255
59H	-2.575225	4.160739	0.734549
60H	-2.140329	1.825591	1.393837
61H	-2.488705	-3.341079	-1.464189
62H	-4.473595	-4.600388	-2.209596
63H	-6.749618	-3.635236	-1.928604
64H	-7.027377	-1.383769	-0.904955
65H	-5.048733	-0.104663	-0.163188
66H	-0.003355	-0.148862	1.678991
67H	0.209724	-0.261851	4.126532
68H	-1.706369	-1.029349	5.522632
69H	-3.847233	-1.686481	4.439980
70H	-4.085082	-1.573697	1.983789
71H	-0.380867	0.326291	-2.236152
72H	1.702395	-0.595961	-3.193647
73H	2.590753	-2.761068	-2.400483
74H	1.408750	-4.015539	-0.600474
75H	-0.645288	-3.090322	0.407771

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1C	4.358363	-1.181864	-0.316771
2C	5.019311	-2.351636	-0.597328
3N	4.749302	-3.510939	0.063202
4C	3.802614	-3.514839	1.043114
5C	3.120555	-2.374869	1.380449
6C	3.357714	-1.141691	0.703335
7N	2.653909	-0.064175	1.122570
8C	2.512903	1.054309	0.409469
9N	2.843987	1.240217	-0.869994
10S	2.311581	2.729475	-1.408261
11C	1.636236	3.264525	0.169697
12C	1.822248	2.211653	1.062559
13O	3.447388	3.577620	-1.822826
14O	1.225653	2.543996	-2.396560
15C	1.019618	4.456102	0.518847
16C	0.574867	4.577146	1.842795
17C	0.749084	3.528749	2.757554
18C	1.373598	2.334641	2.376600
19C	5.430843	-4.759348	-0.320265
20H	4.606377	-0.292635	-0.879300
21H	5.784604	-2.408803	-1.363927
22H	3.628727	-4.464994	1.535770
23H	2.382924	-2.413241	2.174617
24H	0.884474	5.258634	-0.199834
25H	0.088151	5.495060	2.161077
26H	0.395173	3.645432	3.778386
27H	1.509337	1.519639	3.078710
28H	5.470183	-5.425740	0.542797
29H	4.885167	-5.243364	-1.135881
30H	6.447542	-4.528948	-0.642441
31P	-2.191507	-0.574234	-0.140971
32C	-2.256045	1.150065	-0.695579

33C	-1.840333	-0.638082	1.638604
34C	-3.790382	-1.394410	-0.423306
35C	-0.876826	-1.439657	-1.050041
36C	-2.889158	-0.484874	2.563332
37C	-2.610808	-0.483437	3.930394
38C	-1.293288	-0.633569	4.378602
39C	-0.252380	-0.779436	3.457917
40C	-0.518846	-0.780925	2.087194
41C	-4.719943	-0.865275	-1.332345
42C	-5.924352	-1.534438	-1.561959
43C	-6.207029	-2.725820	-0.888232
44C	-5.285399	-3.250433	0.024273
45C	-4.080599	-2.588626	0.261459
46C	0.217694	-0.719110	-1.554491
47C	1.255355	-1.396601	-2.197383
48C	1.207575	-2.785180	-2.338506
49C	0.117312	-3.504506	-1.836182
50C	-0.926137	-2.837393	-1.194063
51C	-2.359223	2.187566	0.244546
52C	-2.438569	3.510695	-0.192959
53C	-2.410958	3.802622	-1.558994
54C	-2.300493	2.770194	-2.495654
55C	-2.223087	1.444763	-2.071014
56H	-3.914428	-0.372627	2.222073
57H	-3.422035	-0.367787	4.643882
58H	-1.080060	-0.633923	5.444361
59H	0.773736	-0.881500	3.799725
60H	0.307974	-0.874309	1.390091
61H	-4.518195	0.063852	-1.855532
62H	-6.641645	-1.119007	-2.264299
63H	-7.146104	-3.242356	-1.068189
64H	-5.505562	-4.171182	0.557591
65H	-3.379284	-2.996255	0.983706
66H	0.274319	0.359979	-1.468340
67H	2.098695	-0.826322	-2.571470
68H	2.017442	-3.307382	-2.841550
69H	0.072277	-4.584083	-1.951606
70H	-1.772099	-3.406130	-0.821843
71H	-2.363066	1.975159	1.308745
72H	-2.507120	4.311504	0.537502
73H	-2.460060	4.835040	-1.894543
74H	-2.257808	2.996098	-3.557153
75H	-2.119255	0.651381	-2.805754

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1C	-0.872245	3.313286	-1.453715
2C	-0.082501	4.370021	-1.083282
3N	0.020619	4.758586	0.218848
4C	-0.664895	4.071350	1.174331
5C	-1.455419	2.992607	0.870179
6C	-1.617404	2.570181	-0.488770
7N	-2.441437	1.604396	-0.948430
8C	-2.965229	0.644920	-0.184978
9N	-2.568066	0.291432	1.039059
10S	-3.431827	-1.033554	1.582402
11C	-4.455488	-1.195995	0.113294
12C	-4.062116	-0.189843	-0.764955
13O	-2.545993	-2.207137	1.735924
14O	-4.242324	-0.664557	2.762243
15C	-5.447893	-2.118230	-0.183808
16C	-6.068792	-2.000972	-1.435487
17C	-5.690144	-0.991836	-2.333566
18C	-4.681816	-0.076426	-2.008440
19C	0.790778	5.956835	0.590183
20H	-0.937321	3.038139	-2.500903
21H	0.491552	4.944751	-1.800421
22H	-0.548596	4.430271	2.191214
23H	-1.968034	2.477619	1.670719
24H	-5.733059	-2.895168	0.519418
25H	-6.854356	-2.699441	-1.710398
26H	-6.187901	-0.920898	-3.296924
27H	-4.378533	0.701750	-2.701715
28H	1.349874	5.761241	1.507732
29H	1.486179	6.200959	-0.213221
30H	0.108930	6.797468	0.749332
31P	2.154334	-0.768911	-0.082450
32C	1.735479	-0.823106	1.679846
33C	0.676435	-1.133287	-1.067884
34C	2.813180	0.874488	-0.496836
35C	3.443168	-1.993385	-0.453090
36C	0.514988	-0.556385	-2.339258
37C	-0.586415	-0.904603	-3.121062
38C	-1.525154	-1.824021	-2.642847
39C	-1.369219	-2.390998	-1.375679
40C	-0.272755	-2.049676	-0.583565

41C	2.577540	1.967531	0.350693
42C	3.083761	3.224907	0.015275
43C	3.814996	3.398118	-1.162878
44C	4.049669	2.309095	-2.009411
45C	3.557439	1.046356	-1.677558
46C	4.789207	-1.696900	-0.176104
47C	5.772679	-2.658917	-0.409621
48C	5.420909	-3.913609	-0.918853
49C	4.083032	-4.207111	-1.198465
50C	3.091522	-3.250969	-0.968828
51C	2.652999	-1.337003	2.611558
52C	2.335849	-1.321640	3.970884
53C	1.110444	-0.802006	4.402250
54C	0.196629	-0.296775	3.472544
55C	0.504598	-0.302029	2.112067
56H	1.230287	0.166094	-2.718855
57H	-0.716713	-0.446931	-4.097830
58H	-2.388794	-2.083045	-3.248705
59H	-2.110049	-3.080940	-0.985190
60H	-0.182023	-2.477820	0.408634
61H	2.015192	1.842088	1.270233
62H	2.911901	4.065734	0.680451
63H	4.210835	4.377715	-1.418194
64H	4.624935	2.438829	-2.921885
65H	3.763638	0.200494	-2.327709
66H	5.072902	-0.723950	0.214839
67H	6.812330	-2.426517	-0.195996
68H	6.189764	-4.659750	-1.100564
69H	3.807462	-5.178500	-1.599524
70H	2.056479	-3.486436	-1.195818
71H	3.600809	-1.754762	2.286886
72H	3.042568	-1.725939	4.690379
73H	0.863547	-0.803270	5.460629
74H	-0.766499	0.087358	3.796893
75H	-0.231236	0.072201	1.408159

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1C	-5.128002	-1.414309	1.563409
2C	-6.177120	-2.232908	1.239239
3N	-6.777633	-2.166797	0.015735
4C	-6.322791	-1.270220	-0.898841
5C	-5.266085	-0.430406	-0.638089
6C	-4.607248	-0.466089	0.629997
7N	-3.578600	0.304152	1.058953
8C	-2.862318	1.101087	0.261935
9N	-2.906219	1.172051	-1.068904
10S	-1.760383	2.243520	-1.645637
11C	-1.102605	2.692526	-0.031603
12C	-1.838427	1.981077	0.912888
13O	-0.755554	1.530158	-2.460498
14O	-2.410235	3.410174	-2.279403
15C	-0.100806	3.589987	0.306927
16C	0.158542	3.769700	1.672736
17C	-0.575925	3.069149	2.640500
18C	-1.577340	2.162838	2.270826
19C	-7.877614	-3.093436	-0.304401
20H	-4.680522	-1.486802	2.548964
21H	-6.581395	-2.964727	1.929768
22H	-6.839901	-1.256300	-1.851372
23H	-4.942384	0.255268	-1.407862
24H	0.459747	4.128314	-0.450088
25H	0.936519	4.462269	1.981804
26H	-0.361466	3.231321	3.693228
27H	-2.145677	1.614210	3.015048
28H	-8.326025	-2.804513	-1.255310
29H	-7.487871	-4.112567	-0.378628
30H	-8.635016	-3.044411	0.481629
31P	2.532051	-0.692409	-0.008544
32C	2.844306	1.030614	-0.479858
33C	1.020232	-1.319217	-0.790091
34C	3.911391	-1.739956	-0.552425
35C	2.367042	-0.756991	1.796481
36C	1.062204	-1.710124	-2.140330
37C	-0.098908	-2.163837	-2.765145
38C	-1.298270	-2.235438	-2.049841
39C	-1.337153	-1.858048	-0.705894
40C	-0.182495	-1.398867	-0.071080
41C	5.153743	-1.176185	-0.881692
42C	6.210564	-2.004904	-1.265609
43C	6.032803	-3.390041	-1.323065
44C	4.792918	-3.952523	-1.000159
45C	3.730629	-3.133454	-0.617070
46C	1.588041	0.224183	2.433814
47C	1.406760	0.174737	3.815326
48C	2.005972	-0.843010	4.565388

49C	2.787616	-1.814219	3.932256
50C	2.970454	-1.776957	2.547603
51C	2.294200	1.553579	-1.658923
52C	2.598665	2.862238	-2.040170
53C	3.443864	3.646800	-1.251475
54C	3.982708	3.128429	-0.067808
55C	3.685531	1.822936	0.322936
56H	1.991626	-1.663676	-2.700947
57H	-0.066160	-2.455023	-3.811250
58H	-2.203683	-2.579219	-2.542631
59H	-2.266657	-1.906273	-0.148054
60H	-0.229272	-1.107795	0.972868
61H	5.300565	-0.101124	-0.853677
62H	7.168921	-1.564351	-1.526045
63H	6.856675	-4.030795	-1.625862
64H	4.649253	-5.028200	-1.051113
65H	2.767942	-3.578106	-0.381142
66H	1.128464	1.023513	1.861333
67H	0.800046	0.933585	4.300953
68H	1.866673	-0.876613	5.642640
69H	3.260250	-2.600756	4.513936
70H	3.583306	-2.532679	2.066618
71H	1.608543	0.970809	-2.262010
72H	2.157496	3.268633	-2.945855
73H	3.674547	4.666015	-1.550375
74H	4.631578	3.740241	0.552920
75H	4.102271	1.428611	1.245424

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1C	-5.315937	-1.189102	1.617872
2C	-6.360245	-2.017707	1.305824
3N	-6.795851	-2.158392	0.019943
4C	-6.175744	-1.464724	-0.969405
5C	-5.119310	-0.619417	-0.720845
6C	-4.636968	-0.433618	0.612211
7N	-3.630868	0.367546	1.040390
8C	-2.875082	1.116782	0.232311
9N	-2.905073	1.174376	-1.099465
10S	-1.736735	2.222373	-1.677028
11C	-1.082324	2.672634	-0.062428
12C	-1.839267	1.984211	0.882320
13O	-0.741453	1.483491	-2.480595
14O	-2.361506	3.395591	-2.323414
15C	-0.070099	3.558397	0.276245
16C	0.179008	3.749023	1.642412
17C	-0.575814	3.070788	2.610375
18C	-1.588327	2.176953	2.240771
19C	-7.935295	-3.048739	-0.262467
20H	-5.000184	-1.096997	2.651634
21H	-6.892367	-2.594916	2.053713
22H	-6.563142	-1.610880	-1.971353
23H	-4.664812	-0.094225	-1.548145
24H	0.505457	4.080467	-0.480678
25H	0.964606	4.432987	1.951388
26H	-0.369488	3.241468	3.663394
27H	-2.174679	1.647887	2.985068
28H	-8.142064	-3.042544	-1.333024
29H	-7.690785	-4.066143	0.054093
30H	-8.816646	-2.695022	0.279004
31P	2.534685	-0.694461	0.006110
32C	2.855362	1.023298	-0.479074
33C	1.014927	-1.317104	-0.763080
34C	3.905082	-1.753762	-0.537435
35C	2.378276	-0.746264	1.812421
36C	1.046618	-1.719002	-2.110285
37C	-0.120643	-2.172505	-2.723748
38C	-1.315838	-2.231786	-2.000471
39C	-1.344977	-1.841335	-0.660022
40C	-0.183945	-1.383262	-0.036279
41C	5.149414	-1.199152	-0.875046
42C	6.199921	-2.036289	-1.257952
43C	6.014068	-3.420726	-1.305999
44C	4.772263	-3.974045	-0.974839
45C	3.716154	-3.146558	-0.592740
46C	1.611980	0.246165	2.447660
47C	1.438305	0.207801	3.830508
48C	2.032136	-0.810643	4.583880
49C	2.800394	-1.793734	3.952678
50C	2.975807	-1.767315	2.566819
51C	2.304611	1.539265	-1.660888
52C	2.616530	2.842201	-2.055340
53C	3.468723	3.628677	-1.276128
54C	4.007746	3.117636	-0.089361
55C	3.704039	1.817430	0.313965
56H	1.972846	-1.681715	-2.676882

57H	-0.095909	-2.473173	-3.767360
58H	-2.225954	-2.575980	-2.484302
59H	-2.271743	-1.878785	-0.096888
60H	-0.222316	-1.082727	1.005262
61H	5.302574	-0.124789	-0.854254
62H	7.159776	-1.602946	-1.524901
63H	6.833080	-4.068063	-1.607965
64H	4.622209	-5.049170	-1.018410
65H	2.751981	-3.584530	-0.350292
66H	1.156394	1.045990	1.872663
67H	0.841844	0.975718	4.314690
68H	1.898951	-0.835727	5.662128
69H	3.268587	-2.581059	4.536876
70H	3.578522	-2.532128	2.087397
71H	1.613222	0.955519	-2.256444
72H	2.175401	3.242906	-2.963604
73H	3.704978	4.643669	-1.584865
74H	4.662211	3.730989	0.523919
75H	4.121878	1.428673	1.238299

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1C	1.026992	3.631871	-1.177550
2C	0.112611	4.572804	-0.784343
3N	-0.371154	4.603656	0.490899
4C	0.068179	3.680635	1.389602
5C	0.976172	2.707655	1.055404
6C	1.518347	2.644929	-0.267954
7N	2.468554	1.806155	-0.732748
8C	2.907356	0.728090	-0.077674
9N	2.354947	0.143149	0.986490
10S	3.226917	-1.217051	1.427240
11C	4.459224	-1.076539	0.128196
12C	4.124655	0.047501	-0.621626
13O	3.824134	-1.034482	2.766003
14O	2.419633	-2.441278	1.228896
15C	5.541386	-1.892613	-0.166087
16C	6.317672	-1.539587	-1.278895
17C	5.998550	-0.410691	-2.048081
18C	4.898895	0.394938	-1.727780
19C	-1.302995	5.662549	0.913352
20H	1.391915	3.637202	-2.198971
21H	-0.267840	5.332140	-1.458083
22H	-0.347996	3.759994	2.387731
23H	1.269963	1.986264	1.804265
24H	5.777455	-2.765179	0.436021
25H	7.177003	-2.148585	-1.546080
26H	6.615179	-0.158123	-2.906519
27H	4.644448	1.267773	-2.320459
28H	-2.000984	5.256879	1.648278
29H	-0.743367	6.493084	1.354059
30H	-1.861734	6.017204	0.045888
31P	-2.062758	-0.778210	-0.142331
32C	-3.095092	-2.265799	-0.269792
33C	-0.803780	-0.815785	-1.447895
34C	-3.091681	0.698910	-0.382609
35C	-1.313658	-0.744767	1.505923
36C	0.433679	-1.432358	-1.209533
37C	1.364491	-1.531512	-2.244915
38C	1.070472	-1.015473	-3.509474
39C	-0.163861	-0.400796	-3.746833
40C	-1.105584	-0.302228	-2.721868
41C	-2.470345	1.930120	-0.657195
42C	-3.252114	3.068565	-0.850747
43C	-4.646151	2.991381	-0.760260
44C	-5.262519	1.769948	-0.475977
45C	-4.489866	0.620875	-0.289573
46C	-0.715023	-1.911810	2.009427
47C	-0.100095	-1.889467	3.260146
48C	-0.089530	-0.713882	4.015975
49C	-0.700374	0.442650	3.522916
50C	-1.311512	0.433398	2.268930
51C	-3.833628	-2.694236	0.846800
52C	-4.669290	-3.806505	0.738266
53C	-4.769604	-4.492245	-0.477090
54C	-4.030909	-4.068754	-1.586114
55C	-3.192510	-2.956211	-1.488284
56H	0.694915	-1.815375	-0.230645
57H	2.326158	-1.997411	-2.050812
58H	1.804681	-1.085348	-4.307808
59H	-0.395475	0.002588	-4.728898
60H	-2.062722	0.172735	-2.916035
61H	-1.388519	1.996805	-0.730373
62H	-2.772944	4.014290	-1.082397
63H	-5.249864	3.881228	-0.918001
64H	-6.344869	1.705083	-0.408816

65H	-4.979710	-0.326019	-0.084728
66H	-0.722168	-2.830835	1.431837
67H	0.383056	-2.786203	3.634899
68H	0.398585	-0.699160	4.986514
69H	-0.697075	1.355482	4.112796
70H	-1.778861	1.336915	1.893051
71H	-3.752792	-2.170685	1.794962
72H	-5.237010	-4.138240	1.603167
73H	-5.418099	-5.360576	-0.557170
74H	-4.101332	-4.606077	-2.527760
75H	-2.617264	-2.639881	-2.353217

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1C	-4.383840	2.322695	-1.306344
2C	-4.567239	3.644505	-0.996164
3N	-4.276842	4.129609	0.244634
4C	-3.787942	3.283029	1.191224
5C	-3.570606	1.950834	0.937938
6C	-3.864695	1.398677	-0.349420
7N	-3.750629	0.111012	-0.746896
8C	-3.082506	-0.822270	-0.067343
9N	-2.284653	-0.641158	0.987722
10S	-1.615139	-2.092665	1.478090
11C	-2.393228	-3.093440	0.205098
12C	-3.172491	-2.232314	-0.562115
13O	-0.147351	-2.082086	1.301148
14O	-2.107362	-2.454856	2.823800
15C	-2.281327	-4.451743	-0.051899
16C	-3.003852	-4.952180	-1.144107
17C	-3.798741	-4.102829	-1.928401
18C	-3.890914	-2.734334	-1.646242
19C	-4.425018	5.566664	0.532148
20H	-4.638948	1.967529	-2.299153
21H	-4.952279	4.362917	-1.710772
22H	-3.579006	3.725205	2.159258
23H	-3.183763	1.323577	1.728301
24H	-1.663842	-5.098836	0.564252
25H	-2.948507	-6.010827	-1.382606
26H	-4.350893	-4.514938	-2.768790
27H	-4.500062	-2.071912	-2.252924
28H	-3.493008	6.089233	0.295632
29H	-5.237305	5.972595	-0.073186
30H	-4.664437	5.700771	1.588338
31P	2.423752	0.321698	-0.130775
32C	3.372704	1.745800	-0.742280
33C	1.051210	0.054560	-1.285452
34C	3.495513	-1.142669	-0.061616
35C	1.813137	0.657137	1.541260
36C	0.650740	-1.242841	-1.635430
37C	-0.430431	-1.421509	-2.500239
38C	-1.109896	-0.314727	-3.014696
39C	-0.707119	0.979867	-2.670718
40C	0.369835	1.169613	-1.805904
41C	4.704150	-1.186544	-0.774614
42C	5.497993	-2.334288	-0.719404
43C	5.092302	-3.433611	0.043284
44C	3.889682	-3.387358	0.756359
45C	3.088583	-2.245590	0.710718
46C	2.707462	0.577947	2.623788
47C	2.254287	0.845922	3.915150
48C	0.913104	1.182974	4.131214
49C	0.024546	1.249046	3.055180
50C	0.468838	0.987978	1.758050
51C	3.845557	2.732806	0.135563
52C	4.606740	3.794169	-0.360785
53C	4.896800	3.874062	-1.725738
54C	4.420779	2.893032	-2.602775
55C	3.658071	1.831101	-2.116624
56H	1.165549	-2.108061	-1.233908
57H	-0.746620	-2.427355	-2.760432
58H	-1.958277	-0.459502	-3.677371
59H	-1.235453	1.841657	-3.068804
60H	0.679873	2.177385	-1.543805
61H	5.035730	-0.336352	-1.362075
62H	6.435334	-2.364155	-1.268056
63H	5.714528	-4.323692	0.085467
64H	3.573179	-4.238106	1.353593
65H	2.156256	-2.217268	1.265504
66H	3.745494	0.297942	2.465587
67H	2.945198	0.780534	4.751176
68H	0.559411	1.376120	5.140592
69H	-1.024368	1.474980	3.224163
70H	-0.242754	0.995098	0.941150
71H	3.621194	2.685591	1.196290
72H	4.969028	4.558333	0.321355

73H	5.489380	4.701220	-2.107492
74H	4.640695	2.954290	-3.665073
75H	3.284075	1.077457	-2.803824

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1C	3.396920	3.594895	-0.934987
2C	2.782691	4.799651	-0.714905
3N	1.763344	4.924356	0.184646
4C	1.356907	3.831174	0.882509
5C	1.937159	2.598473	0.710586
6C	3.002141	2.418099	-0.226295
7N	3.632150	1.266600	-0.555014
8C	3.414369	0.097920	0.055879
9N	2.687460	-0.128670	1.151514
10S	2.679922	-1.757296	1.530587
11C	3.685063	-2.276198	0.136411
12C	4.027346	-1.121082	-0.561558
13O	3.376520	-2.000850	2.810854
14O	1.303559	-2.292248	1.423524
15C	4.086026	-3.546127	-0.249931
16C	4.876132	-3.637689	-1.404316
17C	5.236252	-2.486807	-2.120944
18C	4.815593	-1.216826	-1.707515
19C	1.161553	6.245173	0.431698
20H	4.197780	3.529937	-1.664065
21H	3.067364	5.705477	-1.238969
22H	0.546465	3.985268	1.586263
23H	1.577112	1.766509	1.294943
24H	3.802182	-4.429870	0.313927
25H	5.214367	-4.612588	-1.744663
26H	5.851830	-2.583832	-3.011176
27H	5.087199	-0.323115	-2.260146
28H	1.837270	6.850443	1.043153
29H	0.980388	6.745835	-0.521943
30H	0.213626	6.114774	0.955642
31P	-2.400510	-0.321103	-0.134478
32C	-1.846636	0.723330	1.243150
33C	-0.955544	-0.814102	-1.109062
34C	-3.256774	-1.792414	0.493510
35C	-3.574775	0.600202	-1.171814
36C	-0.796911	-2.141831	-1.533276
37C	0.308338	-2.489748	-2.312494
38C	1.246470	-1.520027	-2.673086
39C	1.088676	-0.196078	-2.249586
40C	-0.002709	0.158949	-1.458758
41C	-3.014025	-2.267109	1.791629
42C	-3.648522	-3.430807	2.231600
43C	-4.519858	-4.120733	1.383970
44C	-4.761996	-3.647671	0.089600
45C	-4.134589	-2.485470	-0.359391
46C	-4.899045	0.758404	-0.724560
47C	-5.805660	1.495919	-1.486384
48C	-5.400562	2.073223	-2.694853
49C	-4.086776	1.910832	-3.143444
50C	-3.170882	1.176146	-2.386349
51C	-2.542905	1.891792	1.592263
52C	-2.118727	2.644897	2.689138
53C	-1.010414	2.234716	3.438046
54C	-0.316241	1.072660	3.085988
55C	-0.725278	0.316239	1.986386
56H	-1.512313	-2.905613	-1.246300
57H	0.440757	-3.522103	-2.623694
58H	2.112932	-1.796964	-3.266603
59H	1.831626	0.551635	-2.507108
60H	-0.103819	1.181607	-1.106146
61H	-2.339722	-1.741761	2.460043
62H	-3.459979	-3.794333	3.237816
63H	-5.012485	-5.024822	1.731749
64H	-5.440799	-4.180249	-0.570797
65H	-4.330496	-2.121450	-1.364023
66H	-5.224832	0.304300	0.206949
67H	-6.828215	1.613439	-1.138634
68H	-6.110871	2.642125	-3.288830
69H	-3.772254	2.348984	-4.086624
70H	-2.156591	1.049590	-2.750282
71H	-3.403992	2.219659	1.018996
72H	-2.657614	3.549664	2.957458
73H	-0.686193	2.821750	4.293441
74H	0.554973	0.757279	3.653154
75H	-0.164944	-0.571361	1.708094

15g-Me-012

1C	-1.335240	3.729364	-0.938500
2C	-0.258602	4.513287	-0.621784
3N	0.458401	4.306560	0.521415
4C	0.092463	3.301175	1.361943
5C	-0.967846	2.471333	1.092342
6C	-1.748453	2.654790	-0.092127
7N	-2.840634	1.959417	-0.481033
8C	-3.193851	0.781847	0.036598
9N	-2.487886	0.027314	0.881129
10S	-3.245433	-1.439560	1.134354
11C	-4.678399	-1.088856	0.109408
12C	-4.481214	0.178699	-0.432907
13O	-2.439301	-2.531226	0.539864
14O	-3.621189	-1.601113	2.553649
15C	-5.792021	-1.868841	-0.163058
16C	-6.750417	-1.324724	-1.029600
17C	-6.571440	-0.050993	-1.589294
18C	-5.434378	0.713455	-1.298928
19C	1.574557	5.208727	0.851458
20H	-1.884756	3.922023	-1.853653
21H	0.074813	5.330556	-1.251724
22H	0.692309	3.186581	2.256929
23H	-1.196229	1.675053	1.786084
24H	-5.918004	-2.854461	0.275135
25H	-7.641801	-1.898347	-1.268522
26H	-7.328113	0.348477	-2.259121
27H	-5.290023	1.698793	-1.730788
28H	1.182644	6.194621	1.117482
29H	2.129203	4.800521	1.696556
30H	2.237131	5.299280	-0.012331
31P	2.186891	-0.714037	-0.169294
32C	1.037685	-0.192559	-1.474410
33C	1.371625	-0.780704	1.450868
34C	2.814155	-2.368907	-0.564364
35C	3.564475	0.466366	-0.104779
36C	0.479802	-1.831151	1.730276
37C	-0.178007	-1.873312	2.958713
38C	0.051117	-0.879695	3.913974
39C	0.947695	0.158326	3.643367
40C	1.608172	0.212956	2.415171
41C	2.854231	-2.802707	-1.899042
42C	3.380647	-4.060037	-2.200641
43C	3.863221	-4.883142	-1.178266
44C	3.822238	-4.450666	0.151474
45C	3.299028	-3.195160	0.463531
46C	3.291731	1.846248	-0.094550
47C	4.341250	2.759917	-0.005356
48C	5.662831	2.305824	0.072666
49C	5.934528	0.935259	0.062312
50C	4.889248	0.011809	-0.026052
51C	-0.297114	-0.623613	-1.427191
52C	-1.168809	-0.285655	-2.462599
53C	-0.718261	0.477728	-3.542726
54C	0.614083	0.901167	-3.593823
55C	1.496938	0.566017	-2.565569
56H	0.285482	-2.609577	1.000442
57H	-0.882538	-2.673831	3.157968
58H	-0.470703	-0.914027	4.866320
59H	1.135141	0.927069	4.388253
60H	2.308306	1.018401	2.223009
61H	2.471599	-2.173730	-2.697188
62H	3.405488	-4.397835	-3.232844
63H	4.265822	-5.863917	-1.416934
64H	4.191077	-5.091350	0.947662
65H	3.260501	-2.868462	1.498513
66H	2.268487	2.202378	-0.164096
67H	4.128578	3.825086	-0.001809
68H	6.478548	3.021061	0.136850
69H	6.959790	0.580479	0.118103
70H	5.111363	-1.050853	-0.036499
71H	-0.674249	-1.204901	-0.595078
72H	-2.203785	-0.610011	-2.412520
73H	-1.404285	0.745003	-4.342027
74H	0.969640	1.491498	-4.434072
75H	2.530868	0.892201	-2.620238

15g-PhNCO2-001

1C	0.422491	-0.381274	3.079252
2C	-0.262466	-1.016515	4.113417
3N	0.096825	-2.199448	4.634636
4C	1.192920	-2.778675	4.116093
5C	1.952268	-2.231203	3.084272
6C	1.553076	-1.004678	2.543210
7N	2.276114	-0.366384	1.494629
8C	2.634530	-1.042030	0.378737

9N	2.135093	-2.239200	0.132870
10S	2.740127	-2.856656	-1.294991
11C	3.753343	-1.428250	-1.678346
12C	3.617073	-0.515823	-0.629320
13O	1.639224	-3.034259	-2.260998
14O	3.594750	-4.032710	-1.035422
15C	4.593639	-1.235381	-2.763614
16C	5.346689	-0.055304	-2.784683
17C	5.256382	0.861085	-1.728830
18C	4.399804	0.642207	-0.644174
19C	2.373619	1.138024	1.597009
20O	2.958760	1.558335	2.610523
21N	1.791675	1.705646	0.563731
22C	1.775048	3.094291	0.409595
23C	1.502984	3.571042	-0.894072
24C	1.398123	4.934220	-1.166059
25C	1.555603	5.875224	-0.139747
26C	1.828530	5.420941	1.155617
27C	1.943865	4.055954	1.434236
28H	0.073289	0.569786	2.692468
29H	-1.150867	-0.552969	4.537392
30H	1.483312	-3.733276	4.549868
31H	2.824437	-2.753527	2.709248
32H	4.668847	-1.972678	-3.557318
33H	6.014295	0.142606	-3.618664
34H	5.859967	1.764049	-1.747893
35H	4.357234	1.367613	0.157714
36H	1.367872	2.842191	-1.688011
37H	1.189973	5.263854	-2.182303
38H	1.472592	6.939490	-0.347186
39H	1.955932	6.138269	1.964437
40H	2.155317	3.723857	2.443084
41P	-2.597391	-0.084196	-0.485323
42C	-4.322516	-0.044399	-1.055667
43C	-2.353300	-1.606321	0.469500
44C	-1.471426	-0.052039	-1.906002
45C	-2.283359	1.363286	0.564917
46C	-1.138159	-2.300844	0.381925
47C	-0.929453	-3.433501	1.170059
48C	-1.925034	-3.874072	2.044210
49C	-3.141595	-3.186441	2.127616
50C	-3.361468	-2.054749	1.342769
51C	-1.927524	-0.435486	-3.178401
52C	-1.036421	-0.462923	-4.252475
53C	0.302818	-0.108914	-4.062536
54C	0.751322	0.278063	-2.797637
55C	-0.126682	0.309179	-1.714165
56C	-1.815338	2.560196	-0.001099
57C	-1.598894	3.673715	0.811423
58C	-1.857103	3.602755	2.182462
59C	-2.334633	2.415104	2.745867
60C	-2.545541	1.293591	1.943180
61C	-5.040582	1.161722	-1.053824
62C	-6.354438	1.187368	-1.527243
63C	-6.952593	0.016767	-2.002803
64C	-6.238270	-1.186247	-2.003631
65C	-4.926051	-1.222377	-1.530357
66H	-0.347902	-1.974476	-0.283901
67H	0.021145	-3.952244	1.102410
68H	-1.753713	-4.749675	2.664437
69H	-3.918622	-3.529151	2.805547
70H	-4.310819	-1.530618	1.408354
71H	-2.965689	-0.708038	-3.339008
72H	-1.390470	-0.761918	-5.235298
73H	0.996931	-0.138354	-4.898455
74H	1.790399	0.551371	-2.642744
75H	0.255443	0.630756	-0.746552
76H	-1.594879	2.623349	-1.061583
77H	-1.198605	4.583715	0.375282
78H	-1.669065	4.467055	2.813549
79H	-2.526076	2.353404	3.813734
80H	-2.893034	0.371034	2.396449
81H	-4.587272	2.074610	-0.679536
82H	-6.908814	2.121816	-1.519405
83H	-7.976057	0.039569	-2.367674
84H	-6.702024	-2.098425	-2.368957
85H	-4.381756	-2.162543	-1.527743

15g-PhNCO2-002

1C	1.795004	-2.588465	2.792517
2C	1.103618	-3.212208	3.826965
3N	0.166852	-2.607942	4.579376
4C	-0.086752	-1.319967	4.299282
5C	0.545047	-0.601152	3.285878
6C	1.505067	-1.249254	2.501948

7N	2.186070	-0.556263	1.466486
8C	2.376791	-1.139150	0.248640
9N	1.593770	-2.114592	-0.157395
10S	2.134170	-2.726383	-1.627103
11C	3.506696	-1.584652	-1.789861
12C	3.515788	-0.772822	-0.654740
13O	1.114253	-2.496605	-2.666671
14O	2.619158	-4.109454	-1.454275
15C	4.459443	-1.511537	-2.795476
16C	5.480661	-0.567712	-2.635487
17C	5.529961	0.239656	-1.490221
18C	4.557719	0.143178	-0.489609
19C	2.412909	0.916316	1.642183
20O	2.873614	1.261051	2.746089
21N	2.036358	1.566563	0.558244
22C	2.218924	2.941543	0.424726
23C	1.700782	3.512804	-0.763828
24C	1.802963	4.877253	-1.025724
25C	2.434864	5.729711	-0.109847
26C	2.957775	5.184057	1.067425
27C	2.853638	3.816752	1.343136
28H	2.534920	-3.138072	2.221431
29H	1.312988	-4.253269	4.063929
30H	-0.843782	-0.832631	4.910741
31H	0.284226	0.435423	3.110720
32H	4.419516	-2.164846	-3.661960
33H	6.246712	-0.469924	-3.399780
34H	6.337575	0.956871	-1.374130
35H	4.618461	0.776365	0.386991
36H	1.215483	2.851812	-1.476309
37H	1.389930	5.277725	-1.949768
38H	2.517754	6.795120	-0.311219
39H	3.452763	5.830971	1.789716
40H	3.252411	3.416477	2.266402
41P	-2.621456	0.097012	-0.403832
42C	-4.408056	0.165162	-0.736273
43C	-2.111935	-1.615037	-0.099720
44C	-1.705333	0.733928	-1.834960
45C	-2.287426	1.134249	1.046100
46C	-1.903478	-2.483269	-1.185402
47C	-1.535172	-3.807264	-0.949433
48C	-1.375112	-4.269162	0.360229
49C	-1.583345	-3.406337	1.439376
50C	-1.948207	-2.078953	1.214496
51C	-2.291926	1.665500	-2.708508
52C	-1.548406	2.171029	-3.775602
53C	-0.229238	1.748339	-3.977549
54C	0.351235	0.821176	-3.108898
55C	-0.380616	0.315905	-2.034221
56C	-3.144685	1.078889	2.160723
57C	-2.863149	1.853285	3.285863
58C	-1.737259	2.686626	3.301444
59C	-0.889482	2.742805	2.193042
60C	-1.159704	1.966924	1.063358
61C	-5.103605	-0.984390	-1.141448
62C	-6.467861	-0.903653	-1.430373
63C	-7.139579	0.317029	-1.317237
64C	-6.447934	1.463069	-0.910351
65C	-5.085744	1.391409	-0.616589
66H	-2.000177	-2.127593	-2.206441
67H	-1.349325	-4.468192	-1.790610
68H	-1.069147	-5.296578	0.538431
69H	-1.440537	-3.753257	2.457778
70H	-2.083920	-1.413032	2.058881
71H	-3.318269	1.990247	-2.569925
72H	-2.002206	2.888904	-4.453452
73H	0.344410	2.142277	-4.812471
74H	1.373859	0.488483	-3.257562
75H	0.075842	-0.403815	-1.366559
76H	-4.025753	0.443022	2.150654
77H	-3.524026	1.809310	4.147331
78H	-1.519833	3.287475	4.180593
79H	-0.006884	3.375583	2.202221
80H	-0.478589	2.003207	0.221749
81H	-4.593393	-1.938649	-1.226572
82H	-7.004201	-1.796964	-1.738605
83H	-8.201530	0.375090	-1.541226
84H	-6.968068	2.412350	-0.815433
85H	-4.558907	2.283075	-0.288387

15g-PhNCO2-003

1C	-2.437203	-2.758904	-2.508612
2C	-1.847535	-3.604222	-3.445624
3N	-0.774465	-3.275392	-4.185789
4C	-0.263361	-2.049693	-3.992263

5C	-0.771215	-1.127393	-3.078717
6C	-1.882607	-1.488703	-2.311057
7N	-2.435972	-0.569940	-1.376599
8C	-2.715607	-0.956453	-0.104600
9N	-2.207379	-2.069240	0.383732
10S	-2.729860	-2.316846	1.954669
11C	-3.731555	-0.831988	2.036506
12C	-3.641301	-0.195332	0.797551
13O	-1.574073	-2.249102	2.871615
14O	-3.576944	-3.522320	2.037785
15C	-4.536255	-0.385712	3.074302
16C	-5.298012	0.764702	2.838045
17C	-5.253440	1.402653	1.590677
18C	-4.433298	0.931011	0.560540
19C	-2.373979	0.888798	-1.746502
20O	-2.869438	1.177559	-2.851156
21N	-1.768210	1.571916	-0.798015
22C	-1.664715	2.960606	-0.841240
23C	-1.095293	3.560536	0.308400
24C	-0.905895	4.937747	0.397394
25C	-1.282399	5.774640	-0.662719
26C	-1.852526	5.200905	-1.804200
27C	-2.044551	3.818725	-1.903779
28H	-3.301503	-3.087154	-1.942297
29H	-2.261677	-4.596385	-3.612430
30H	0.606852	-1.788722	-4.590325
31H	-0.299383	-0.158582	-2.960772
32H	-4.581327	-0.912160	4.023096
33H	-5.939126	1.155579	3.623368
34H	-5.864276	2.283982	1.416495
35H	-4.420014	1.440536	-0.394814
36H	-0.804639	2.908537	1.126975
37H	-0.463572	5.361650	1.297159
38H	-1.136484	6.850370	-0.598190
39H	-2.152006	5.836222	-2.636056
40H	-2.478466	3.392186	-2.799122
41P	2.660671	-0.091463	0.369126
42C	1.675367	0.731163	1.652379
43C	2.279847	0.572979	-1.274187
44C	4.409547	0.206620	0.765507
45C	2.320172	-1.870957	0.336690
46C	1.545922	1.757422	-1.422336
47C	1.293968	2.258322	-2.701887
48C	1.776751	1.586192	-3.827023
49C	2.503374	0.398305	-3.679322
50C	2.749491	-0.116751	-2.407564
51C	4.847566	-0.025075	2.082043
52C	6.185709	0.183272	2.414835
53C	7.088862	0.629577	1.443147
54C	6.652072	0.869973	0.137812
55C	5.313692	0.660189	-0.206079
56C	1.065404	-2.289548	-0.136567
57C	0.751639	-3.647060	-0.163222
58C	1.691121	-4.589880	0.264913
59C	2.944483	-4.174772	0.726930
60C	3.264274	-2.815896	0.768348
61C	2.047578	2.024882	2.061452
62C	1.311037	2.675822	3.050096
63C	0.204618	2.044819	3.630951
64C	-0.164651	0.761364	3.222134
65C	0.569224	0.097997	2.236438
66H	1.147062	2.279087	-0.559973
67H	0.698036	3.159560	-2.810038
68H	1.570021	1.974868	-4.820631
69H	2.865541	-0.134439	-4.554154
70H	3.292292	-1.052100	-2.300137
71H	4.149218	-0.361150	2.843608
72H	6.520060	0.002048	3.432698
73H	8.130260	0.795241	1.706453
74H	7.348936	1.226267	-0.615853
75H	4.984019	0.859124	-1.220709
76H	0.332016	-1.567114	-0.475995
77H	-0.229732	-3.954851	-0.509157
78H	1.445243	-5.648273	0.240487
79H	3.676077	-4.907141	1.057401
80H	4.239969	-2.504096	1.127047
81H	2.906999	2.519492	1.617500
82H	1.598758	3.676135	3.361962
83H	-0.369660	2.557126	4.398444
84H	-1.021923	0.261538	3.662074
85H	0.267989	-0.901706	1.947507

15g-PhNCO2-004

1C	1.656137	-2.360477	3.021605
2C	1.123097	-2.621232	4.281442

3N	0.670744	-1.678735	5.125155
4C	0.769162	-0.408322	4.704462
5C	1.287675	-0.033759	3.466948
6C	1.732596	-1.029603	2.586043
7N	2.279990	-0.655835	1.330862
8C	2.166406	-1.420766	0.218139
9N	1.304288	-2.416568	0.165197
10S	1.423036	-3.233547	-1.284512
11C	2.681796	-2.164452	-1.977130
12C	3.020488	-1.219353	-1.005354
13O	0.147948	-3.143007	-2.020609
14O	1.966180	-4.589784	-1.066706
15C	3.290134	-2.249311	-3.218923
16C	4.306030	-1.326844	-3.495411
17C	4.690118	-0.388422	-2.529308
18C	4.062237	-0.327499	-1.279793
19C	2.898969	0.723468	1.256217
20O	3.901057	0.885037	1.975424
21N	2.213131	1.492941	0.439356
22C	2.647939	2.784834	0.123009
23C	1.737271	3.586851	-0.606587
24C	2.064137	4.878183	-1.015280
25C	3.321092	5.420876	-0.716709
26C	4.235479	4.643658	0.001169
27C	3.912063	3.350095	0.424002
28H	1.990118	-3.178827	2.397973
29H	1.055428	-3.650134	4.628613
30H	0.410386	0.357351	5.389483
31H	1.339834	1.015254	3.200790
32H	2.991559	-3.001423	-3.943011
33H	4.807021	-1.349329	-4.459197
34H	5.492939	0.309977	-2.747998
35H	4.396130	0.403070	-0.555232
36H	0.760292	3.176195	-0.841881
37H	1.333959	5.464238	-1.570195
38H	3.579890	6.427870	-1.035130
39H	5.216532	5.047562	0.244727
40H	4.630275	2.773342	0.992408
41P	-2.579589	0.313721	-0.267232
42C	-2.127103	1.852263	0.586883
43C	-4.320552	0.393882	-0.780703
44C	-1.555590	0.082718	-1.749885
45C	-2.349941	-1.064532	0.883779
46C	-4.687519	1.204094	-1.870395
47C	-6.026905	1.293413	-2.249327
48C	-7.003409	0.575526	-1.549395
49C	-6.639206	-0.233529	-0.469619
50C	-5.300157	-0.328132	-0.082221
51C	-0.218213	0.511281	-1.748982
52C	0.563416	0.330509	-2.890305
53C	0.025559	-0.282042	-4.024648
54C	-1.297502	-0.731859	-4.016104
55C	-2.091208	-0.553815	-2.882589
56C	-2.632421	-0.893998	2.251667
57C	-2.487472	-1.971985	3.123074
58C	-2.071619	-3.216815	2.635476
59C	-1.793429	-3.383210	1.277375
60C	-1.924687	-2.308185	0.396490
61C	-2.910068	3.012789	0.470471
62C	-2.514532	4.182341	1.122535
63C	-1.343375	4.200746	1.886794
64C	-0.567343	3.044984	2.005166
65C	-0.957435	1.870015	1.364019
66H	-3.932233	1.754213	-2.424292
67H	-6.305701	1.918555	-3.093178
68H	-8.045795	0.643742	-1.849348
69H	-7.394331	-0.797443	0.071098
70H	-5.026603	-0.965374	0.752819
71H	0.241957	0.966194	-0.876932
72H	1.596759	0.663829	-2.879347
73H	0.640904	-0.422586	-4.909444
74H	-1.714729	-1.226750	-4.888857
75H	-3.117021	-0.908496	-2.887936
76H	-2.948692	0.071311	2.635949
77H	-2.683286	-1.837619	4.182961
78H	-1.946185	-4.049824	3.321858
79H	-1.441323	-4.339696	0.902015
80H	-1.658145	-2.436426	-0.646967
81H	-3.825103	3.012359	-0.112287
82H	-3.123086	5.078041	1.032208
83H	-1.033187	5.115207	2.385260
84H	0.351951	3.058273	2.582278
85H	-0.346486	0.981388	1.464021

1C	1.514563	0.296032	3.324802
2C	1.180764	-0.081788	4.624343
3N	1.497024	-1.267396	5.165898
4C	2.192219	-2.114485	4.387811
5C	2.574705	-1.840679	3.077093
6C	2.215016	-0.607792	2.516687
7N	2.570582	-0.239488	1.190004
8C	2.507346	-1.118430	0.162735
9N	1.883204	-2.272797	0.301005
10S	1.994358	-3.183084	-1.091247
11C	2.908887	-1.955615	-2.022513
12C	3.155584	-0.874863	-1.172436
13O	0.644125	-3.417809	-1.638391
14O	2.834054	-4.377467	-0.867851
15C	3.377750	-2.036838	-3.323740
16C	4.145783	-0.964451	-3.792309
17C	4.438992	0.116643	-2.951048
18C	3.956266	0.172002	-1.638549
19C	2.839617	1.234792	0.973467
20O	3.806711	1.688587	1.610607
21N	1.964423	1.749601	0.139742
22C	1.990352	3.114000	-0.171177
23C	1.387364	3.501779	-1.389263
24C	1.273624	4.843829	-1.751515
25C	1.752460	5.850427	-0.903801
26C	2.355950	5.484219	0.304747
27C	2.483422	4.141048	0.668710
28H	1.227556	1.274544	2.956258
29H	0.624517	0.606110	5.257999
30H	2.460755	-3.068766	4.836130
31H	3.130756	-2.575615	2.508730
32H	3.160497	-2.897641	-3.948967
33H	4.528513	-0.979583	-4.809017
34H	5.054819	0.932154	-3.319560
35H	4.210221	1.016446	-1.011667
36H	1.000190	2.727992	-2.045619
37H	0.803227	5.104942	-2.697550
38H	1.660580	6.897849	-1.181232
39H	2.737162	6.252769	0.974799
40H	2.959996	3.877117	1.605200
41P	-2.636532	-0.064209	-0.153668
42C	-1.672208	-0.396247	-1.653739
43C	-4.396148	-0.293982	-0.543011
44C	-2.129139	-1.180231	1.176782
45C	-2.347718	1.639782	0.408641
46C	-5.231131	-1.025403	0.315219
47C	-6.588436	-1.161743	0.012822
48C	-7.115064	-0.573793	-1.140350
49C	-6.282193	0.149616	-2.001208
50C	-4.925435	0.288949	-1.708836
51C	-1.374956	-2.325174	0.885418
52C	-0.988900	-3.174123	1.925906
53C	-1.346023	-2.881749	3.243155
54C	-2.095955	-1.734673	3.532882
55C	-2.489182	-0.881102	2.504390
56C	-1.215690	1.902751	1.196772
57C	-0.934967	3.208943	1.595881
58C	-1.777153	4.255880	1.213493
59C	-2.908999	3.994784	0.434188
60C	-3.199162	2.690715	0.029309
61C	-0.421140	0.218846	-1.819538
62C	0.323902	-0.041340	-2.969904
63C	-0.166336	-0.912172	-3.946145
64C	-1.402040	-1.540982	-3.769332
65C	-2.158065	-1.288823	-2.624076
66H	-4.833043	-1.494178	1.209392
67H	-7.230170	-1.732483	0.678389
68H	-8.171041	-0.683705	-1.372830
69H	-6.686027	0.601266	-2.903226
70H	-4.283209	0.838909	-2.391359
71H	-1.057500	-2.544682	-0.128714
72H	-0.381321	-4.045642	1.702246
73H	-1.023456	-3.533245	4.050564
74H	-2.358445	-1.498260	4.560199
75H	-3.055037	0.018152	2.732255
76H	-0.549082	1.099534	1.485932
77H	-0.046671	3.409042	2.186529
78H	-1.547784	5.273652	1.517057
79H	-3.568133	4.806512	0.138304
80H	-4.083847	2.504425	-0.570430
81H	-0.006687	0.879465	-1.063499
82H	1.294946	0.429355	-3.090628
83H	0.422024	-1.113546	-4.837432
84H	-1.777101	-2.234219	-4.517222
85H	-3.115852	-1.783486	-2.494084

15g-PhNCO2-006

1C	1.848996	-2.071427	3.139443
2C	1.365709	-2.233822	4.435287
3N	0.920603	-1.231325	5.211538
4C	0.971880	-0.000724	4.679431
5C	1.437760	0.276255	3.396127
6C	1.878301	-0.781835	2.588608
7N	2.380653	-0.509661	1.289051
8C	2.225466	-1.365253	0.249238
9N	1.355316	-2.352882	0.309596
10S	1.438898	-3.306926	-1.058098
11C	2.677378	-2.308231	-1.882498
12C	3.043848	-1.280624	-1.009850
13O	0.144004	-3.290986	-1.763159
14O	1.994863	-4.634619	-0.725678
15C	3.254793	-2.507595	-3.126003
16C	4.263798	-1.616528	-3.510545
17C	4.672808	-0.594739	-2.644032
18C	4.077323	-0.419335	-1.389571
19C	2.946920	0.879694	1.077305
20O	3.957265	1.141808	1.754389
21N	2.221091	1.541233	0.204121
22C	2.530038	2.859682	-0.148347
23C	1.862660	3.373205	-1.285788
24C	2.044383	4.689009	-1.707749
25C	2.897568	5.548606	-1.003338
26C	3.564672	5.059440	0.124510
27C	3.394557	3.738135	0.550008
28H	2.183079	-2.933327	2.577053
29H	1.336110	-3.229778	4.872251
30H	0.618505	0.813710	5.308801
31H	1.454490	1.299701	3.040051
32H	2.939490	-3.322125	-3.771251
33H	4.740786	-1.728615	-4.480297
34H	5.470309	0.078139	-2.946136
35H	4.427448	0.371692	-0.739395
36H	1.190408	2.717876	-1.831218
37H	1.513947	5.046766	-2.588162
38H	3.039294	6.576823	-1.327676
39H	4.232590	5.712043	0.683982
40H	3.924788	3.377356	1.422182
41P	-2.583596	0.230765	-0.224621
42C	-2.298012	-1.031165	1.040677
43C	-1.613840	-0.133873	-1.715981
44C	-4.342251	0.260773	-0.679938
45C	-2.101358	1.846611	0.449726
46C	-2.180443	-0.873787	-2.767566
47C	-1.422272	-1.148088	-3.906336
48C	-0.103881	-0.693860	-3.998016
49C	0.464751	0.022527	-2.942061
50C	-0.282131	0.302289	-1.797706
51C	-5.291492	-0.411208	0.104786
52C	-6.643766	-0.354588	-0.242331
53C	-7.051008	0.368113	-1.366987
54C	-6.104738	1.034963	-2.153542
55C	-4.752457	0.981875	-1.816005
56C	-0.904935	1.940187	1.179351
57C	-0.481185	3.178947	1.658530
58C	-1.244201	4.324254	1.417790
59C	-2.441621	4.230713	0.701169
60C	-2.874599	2.995740	0.215233
61C	-1.891037	-2.316426	0.655784
62C	-1.719502	-3.303307	1.628372
63C	-1.939861	-3.008548	2.975285
64C	-2.337183	-1.722356	3.359697
65C	-2.520832	-0.731199	2.396953
66H	-3.203237	-1.232418	-2.705935
67H	-1.862648	-1.722097	-4.717080
68H	0.484640	-0.911050	-4.885617
69H	1.495644	0.359841	-2.995321
70H	0.196386	0.841911	-0.985994
71H	-4.983865	-0.980368	0.976562
72H	-7.375357	-0.879568	0.365735
73H	-8.103610	0.408509	-1.634657
74H	-6.417043	1.592656	-3.032204
75H	-4.021350	1.490579	-2.438199
76H	-0.300109	1.060829	1.364678
77H	0.453459	3.250258	2.205418
78H	-0.904387	5.288462	1.786151
79H	-3.040305	5.118832	0.517823
80H	-3.808800	2.936048	-0.332720
81H	-1.670964	-2.543737	-0.381743
82H	-1.382258	-4.291877	1.330002
83H	-1.785311	-3.773626	3.731353
84H	-2.487065	-1.487130	4.409518
85H	-2.822229	0.266852	2.701657

15g-PhNCO2-007

1C	-3.726543	-0.857765	-2.870814
2C	-4.054678	-1.684044	-3.942955
3N	-4.195743	-3.016464	-3.855820
4C	-4.018736	-3.551112	-2.635176
5C	-3.689658	-2.821778	-1.496414
6C	-3.518933	-1.432042	-1.607424
7N	-3.193581	-0.616451	-0.501708
8C	-2.455195	-1.053878	0.558653
9N	-1.639812	-2.078628	0.462849
10S	-0.942233	-2.413510	1.953185
11C	-1.747066	-1.070340	2.825133
12C	-2.576027	-0.418395	1.911766
13O	0.517275	-2.223021	1.872425
14O	-1.416789	-3.716661	2.458104
15C	-1.668903	-0.734650	4.167134
16C	-2.479238	0.319290	4.606776
17C	-3.340865	0.973376	3.716052
18C	-3.404965	0.609759	2.366426
19C	-3.397782	0.873053	-0.636784
20O	-4.566739	1.251223	-0.825315
21N	-2.236860	1.489838	-0.551301
22C	-2.167947	2.884499	-0.497042
23C	-0.962180	3.483085	-0.928705
24C	-0.752402	4.857314	-0.822544
25C	-1.739590	5.684416	-0.271672
26C	-2.940645	5.108778	0.159489
27C	-3.161933	3.733866	0.043994
28H	-3.627886	0.209558	-3.027882
29H	-4.204984	-1.246554	-4.928033
30H	-4.145089	-4.629335	-2.559673
31H	-3.553585	-3.335613	-0.553509
32H	-1.011415	-1.267402	4.847530
33H	-2.446802	0.622384	5.649546
34H	-3.975340	1.778134	4.076617
35H	-4.087828	1.120829	1.698350
36H	-0.187046	2.844170	-1.343387
37H	0.187305	5.283805	-1.168434
38H	-1.577763	6.756131	-0.184894
39H	-3.720341	5.737424	0.585689
40H	-4.104574	3.309196	0.368771
41P	2.670821	-0.060692	-0.287336
42C	1.499347	-1.012936	-1.291481
43C	3.310346	1.271613	-1.348887
44C	1.907776	0.696654	1.170443
45C	4.038626	-1.122158	0.260008
46C	3.470405	2.571696	-0.845718
47C	3.965050	3.579881	-1.677025
48C	4.302121	3.295140	-3.003241
49C	4.143294	1.998486	-3.505498
50C	3.645559	0.986669	-2.684409
51C	0.571090	1.115099	1.124603
52C	0.034739	1.812726	2.206987
53C	0.814800	2.077358	3.334766
54C	2.145270	1.647944	3.384097
55C	2.698802	0.963523	2.301146
56C	3.800955	-2.074945	1.267665
57C	4.838136	-2.909215	1.685918
58C	6.108600	-2.797074	1.110201
59C	6.345064	-1.845779	0.113817
60C	5.313724	-1.006318	-0.314377
61C	1.496221	-2.416191	-1.274559
62C	0.603482	-3.114244	-2.088824
63C	-0.284334	-2.421905	-2.916267
64C	-0.279857	-1.024406	-2.933450
65C	0.606988	-0.317136	-2.124642
66H	3.199095	2.805133	0.179047
67H	4.077915	4.587894	-1.287475
68H	4.681110	4.083678	-3.648127
69H	4.398402	1.775677	-4.537897
70H	3.508549	-0.014294	-3.083620
71H	-0.069667	0.906382	0.273306
72H	-0.998999	2.137448	2.163952
73H	0.384418	2.612714	4.177116
74H	2.754327	1.847044	4.261926
75H	3.735018	0.641919	2.341841
76H	2.818156	-2.165151	1.719924
77H	4.651272	-3.645756	2.462562
78H	6.913677	-3.448161	1.440810
79H	7.331871	-1.751782	-0.331237
80H	5.510076	-0.268298	-1.085508
81H	2.175776	-2.966386	-0.633682
82H	0.595358	-4.200337	-2.064793
83H	-0.988626	-2.967302	-3.538293
84H	-0.974965	-0.482050	-3.565427

85H 0.600469 0.767553 -2.148882

15g-PhNCO2-008

1C -3.692917 -2.773858 -1.589413
2C -4.002856 -3.475781 -2.750906
3N -4.145429 -2.913636 -3.963556
4C -3.988858 -1.581199 -4.018996
5C -3.675153 -0.781914 -2.922689
6C -3.501634 -1.384977 -1.667883
7N -3.185455 -0.596589 -0.539046
8C -2.472634 -1.066287 0.523495
9N -1.683043 -2.111140 0.424122
10S -1.009680 -2.482546 1.914363
11C -1.792318 -1.134015 2.798089
12C -2.595218 -0.448557 1.885777
13O 0.455038 -2.326435 1.848820
14O -1.519604 -3.780950 2.396750
15C -1.723730 -0.823525 4.146750
16C -2.516928 0.239403 4.595409
17C -3.353156 0.927244 3.705873
18C -3.407207 0.589514 2.349184
19C -3.388816 0.894942 -0.643818
20O -4.554764 1.271525 -0.854964
21N -2.233790 1.514952 -0.512219
22C -2.173565 2.909071 -0.435370
23C -0.937808 3.511299 -0.767606
24C -0.739096 4.885472 -0.644113
25C -1.768943 5.711153 -0.174849
26C -2.999132 5.132720 0.158610
27C -3.208560 3.757207 0.026464
28H -3.586027 -3.308096 -0.654221
29H -4.143219 -4.553728 -2.701072
30H -4.112023 -1.121353 -4.997619
31H -3.558379 0.286639 -3.055034
32H -1.086558 -1.382611 4.825320
33H -2.491462 0.523266 5.643787
34H -3.975185 1.738905 4.072621
35H -4.070467 1.128486 1.683323
36H -0.131862 2.873890 -1.120595
37H 0.224655 5.313698 -0.913178
38H -1.616933 6.783280 -0.076169
39H -3.811993 5.759684 0.520537
40H -4.173714 3.331857 0.273840
41P 2.688176 -0.056964 -0.285203
42C 3.994908 -1.220046 0.203742
43C 3.416690 1.310339 -1.238583
44C 1.481657 -0.875957 -1.360839
45C 1.932588 0.632648 1.210378
46C 3.769403 1.103373 -2.583931
47C 4.352841 2.138527 -3.314970
48C 4.581497 3.381149 -2.713035
49C 4.224963 3.589557 -1.377876
50C 3.642938 2.557796 -0.637236
51C 1.364432 -2.274296 -1.380767
52C 0.430843 -2.875864 -2.225413
53C -0.386280 -2.092101 -3.043612
54C -0.266596 -0.699417 -3.026032
55C 0.663251 -0.087125 -2.188666
56C 2.720838 0.824536 2.358751
57C 2.171471 1.458670 3.473791
58C 0.848363 1.912451 3.440638
59C 0.069985 1.719502 2.297418
60C 0.601671 1.071713 1.182294
61C 5.264060 -1.168113 -0.393470
62C 6.245705 -2.086308 -0.013448
63C 5.966540 -3.052869 0.957111
64C 4.702028 -3.102663 1.553817
65C 3.714014 -2.189779 1.183209
66H 3.580879 0.145843 -3.061438
67H 4.621777 1.976147 -4.355100
68H 5.030371 4.187369 -3.287212
69H 4.391480 4.556027 -0.910142
70H 3.360079 2.732237 0.395989
71H 1.983983 -2.893560 -0.742079
72H 0.330470 -3.957485 -2.228046
73H -1.127309 -2.562522 -3.683849
74H -0.908354 -0.086041 -3.650126
75H 0.747310 0.995262 -2.184266
76H 3.751450 0.483800 2.387898
77H 2.778102 1.600380 4.364331
78H 0.421818 2.408605 4.308556
79H -0.958941 2.060694 2.267047
80H -0.038069 0.914181 0.319246
81H 5.495168 -0.418141 -1.143036
82H 7.228331 -2.041415 -0.475112

83H	6.733934	-3.764233	1.250911
84H	4.480772	-3.851559	2.309329
85H	2.735143	-2.234337	1.650193

15g-PhNCO2-009

1C	-0.453949	-1.023842	2.993584
2C	0.260911	-0.832536	4.175575
3N	0.030428	0.151519	5.056808
4C	-0.972766	0.990995	4.749662
5C	-1.750324	0.898019	3.599852
6C	-1.493858	-0.134378	2.678525
7N	-2.251674	-0.181500	1.476355
8C	-2.418546	-1.269387	0.693850
9N	-1.823705	-2.418363	0.968098
10S	-2.136702	-3.558673	-0.203644
11C	-3.172901	-2.497654	-1.199877
12C	-3.276487	-1.261573	-0.553920
13O	-2.912063	-4.685052	0.350662
14O	-0.884523	-3.904207	-0.908468
15C	-3.810541	-2.812981	-2.388656
16C	-4.616103	-1.823601	-2.963429
17C	-4.770818	-0.588245	-2.325010
18C	-4.115766	-0.295563	-1.122510
19C	-2.801836	1.164132	1.021078
20O	-3.895091	1.494799	1.514582
21N	-1.985316	1.695058	0.148281
22C	-2.243933	2.960301	-0.391965
23C	-2.864747	4.026314	0.296998
24C	-2.983742	5.285540	-0.296913
25C	-2.506898	5.518469	-1.592572
26C	-1.901011	4.465971	-2.290345
27C	-1.767773	3.210011	-1.697331
28H	-0.193610	-1.839970	2.340621
29H	1.074085	-1.514573	4.415185
30H	-1.169564	1.788464	5.463249
31H	-2.545108	1.614243	3.434706
32H	-3.691137	-3.788786	-2.850053
33H	-5.133451	-2.022811	-3.897894
34H	-5.416275	0.167206	-2.764210
35H	-4.287625	0.663212	-0.656337
36H	-3.242904	3.861859	1.299669
37H	-3.458573	6.091996	0.258727
38H	-2.608145	6.499386	-2.050714
39H	-1.526669	4.624726	-3.299953
40H	-1.281648	2.399869	-2.233344
41P	2.530970	0.057894	-0.422592
42C	4.233887	0.404042	-0.963054
43C	1.882522	1.478870	0.495504
44C	1.479004	-0.262466	-1.864258
45C	2.583751	-1.427524	0.615762
46C	1.870866	1.478459	1.899224
47C	1.408884	2.601735	2.586522
48C	0.956469	3.720062	1.880866
49C	0.963301	3.719591	0.483299
50C	1.424284	2.603197	-0.212904
51C	0.093076	-0.052425	-1.773108
52C	-0.720753	-0.385352	-2.858027
53C	-0.165779	-0.928503	-4.019424
54C	1.215415	-1.131968	-4.108449
55C	2.041694	-0.798780	-3.034536
56C	3.555987	-1.537771	1.626988
57C	3.581325	-2.671079	2.438792
58C	2.649473	-3.698234	2.240432
59C	1.693146	-3.591917	1.228160
60C	1.655272	-2.457758	0.413590
61C	5.086606	-0.669354	-1.275110
62C	6.382880	-0.417868	-1.726677
63C	6.834558	0.898865	-1.864867
64C	5.988754	1.966694	-1.550227
65C	4.688797	1.724656	-1.100591
66H	2.194693	0.608992	2.459293
67H	1.385957	2.588908	3.671895
68H	0.579376	4.585707	2.418862
69H	0.584358	4.575014	-0.067357
70H	1.402939	2.602349	-1.298612
71H	-0.365844	0.389355	-0.890176
72H	-1.790759	-0.216958	-2.788087
73H	-0.808339	-1.190466	-4.856054
74H	1.651738	-1.547659	-5.012612
75H	3.113057	-0.954425	-3.114765
76H	4.288968	-0.749374	1.776021
77H	4.328566	-2.753272	3.223432
78H	2.671952	-4.580077	2.875356
79H	0.963558	-4.379046	1.065140
80H	0.898888	-2.394348	-0.359670

81H	4.746379	-1.694340	-1.158222
82H	7.038916	-1.250642	-1.964793
83H	7.846778	1.091697	-2.210453
84H	6.339442	2.990406	-1.648621
85H	4.044012	2.561411	-0.851060

15g-PhNCO2-010

1C	-0.758895	-1.285585	3.228133
2C	-0.153570	-1.054297	4.463918
3N	-0.311944	0.053187	5.201456
4C	-1.132794	0.984222	4.685344
5C	-1.794025	0.860696	3.469325
6C	-1.611932	-0.302956	2.692861
7N	-2.274082	-0.387993	1.443152
8C	-2.231119	-1.430900	0.580798
9N	-1.432833	-2.464024	0.778361
10S	-1.580101	-3.593103	-0.438227
11C	-2.780980	-2.665963	-1.379829
12C	-3.077638	-1.495248	-0.674110
13O	-2.169949	-4.841216	0.083337
14O	-0.299463	-3.720297	-1.161646
15C	-3.365329	-3.022321	-2.583907
16C	-4.316544	-2.145421	-3.117198
17C	-4.655546	-0.977604	-2.425787
18C	-4.052864	-0.643630	-1.206966
19C	-2.985227	0.891336	1.012030
20O	-4.131087	1.041935	1.472190
21N	-2.190844	1.589632	0.241140
22C	-2.583230	2.811624	-0.315444
23C	-3.881657	3.376532	-0.293685
24C	-4.136148	4.597690	-0.927394
25C	-3.120577	5.295457	-1.588932
26C	-1.829440	4.750678	-1.611323
27C	-1.568103	3.532111	-0.988702
28H	-0.551265	-2.200027	2.698003
29H	0.509291	-1.813902	4.871211
30H	-1.273314	1.886430	5.277287
31H	-2.443255	1.663795	3.146134
32H	-3.094749	-3.944664	-3.089367
33H	-4.799346	-2.379117	-4.061992
34H	-5.406502	-0.308138	-2.835794
35H	-4.367192	0.258341	-0.703205
36H	-4.679058	2.857484	0.222915
37H	-5.143919	5.007829	-0.897643
38H	-3.328526	6.245351	-2.075709
39H	-1.022138	5.278777	-2.115090
40H	-0.564459	3.117201	-1.000944
41P	2.537784	0.209974	-0.357036
42C	2.030601	1.805251	0.349152
43C	1.433748	-0.267986	-1.713616
44C	4.217225	0.342422	-1.044320
45C	2.515109	-1.033694	0.958235
46C	1.913043	-1.103055	-2.738958
47C	1.064541	-1.469608	-3.783348
48C	-0.254711	-1.005337	-3.810490
49C	-0.731773	-0.188183	-2.783079
50C	0.104059	0.179976	-1.726869
51C	5.319553	-0.209888	-0.374352
52C	6.599810	-0.076466	-0.918035
53C	6.785456	0.604062	-2.124350
54C	5.686618	1.150134	-2.796827
55C	4.404340	1.017115	-2.264311
56C	1.971966	-2.302554	0.714411
57C	2.018850	-3.274660	1.716943
58C	2.599834	-2.983123	2.952648
59C	3.125469	-1.709083	3.201134
60C	3.082557	-0.730497	2.209845
61C	2.565505	3.010296	-0.138762
62C	2.131665	4.225571	0.391784
63C	1.169259	4.246271	1.406666
64C	0.638533	3.049230	1.891256
65C	1.063384	1.828328	1.366936
66H	2.937273	-1.463592	-2.727359
67H	1.434345	-2.119062	-4.572060
68H	-0.913402	-1.290016	-4.626764
69H	-1.759461	0.160859	-2.789533
70H	-0.305714	0.793975	-0.929140
71H	5.189890	-0.749135	0.558256
72H	7.449317	-0.511532	-0.398726
73H	7.783009	0.703297	-2.544113
74H	5.824809	1.672652	-3.739455
75H	3.553430	1.424698	-2.803351
76H	1.490949	-2.537220	-0.228415
77H	1.581762	-4.251463	1.530121
78H	2.627130	-3.740974	3.731451

79H	3.556090	-1.473005	4.170266
80H	3.477481	0.261199	2.412479
81H	3.320049	3.010581	-0.918443
82H	2.547366	5.154930	0.012082
83H	0.827856	5.194593	1.812654
84H	-0.120269	3.056652	2.666919
85H	0.635113	0.908601	1.749736

15g-PhNCO2-011

1C	-1.909408	0.067718	2.809033
2C	-1.763340	0.369275	4.160417
3N	-2.043887	1.567951	4.698054
4C	-2.498933	2.511330	3.857384
5C	-2.681256	2.316178	2.488747
6C	-2.376075	1.064626	1.943655
7N	-2.480343	0.828598	0.543407
8C	-3.070977	-0.304086	0.074860
9N	-3.857964	-1.028151	0.841256
10S	-4.387913	-2.393536	0.018922
11C	-3.472482	-2.048399	-1.485304
12C	-2.786261	-0.848479	-1.294798
13O	-5.844516	-2.313947	-0.191014
14O	-3.867610	-3.614892	0.663796
15C	-3.346523	-2.835025	-2.619830
16C	-2.469150	-2.383356	-3.613669
17C	-1.748053	-1.195320	-3.436359
18C	-1.895728	-0.419335	-2.281894
19C	-2.205558	1.971460	-0.404511
20O	-3.071078	2.149664	-1.281739
21N	-1.072370	2.562423	-0.096956
22C	-0.628904	3.699928	-0.770817
23C	-1.214448	4.304146	-1.912889
24C	-0.623817	5.422983	-2.509215
25C	0.557337	5.976934	-2.004070
26C	1.144963	5.394045	-0.873048
27C	0.562389	4.281319	-0.270133
28H	-1.654838	-0.919246	2.441237
29H	-1.391195	-0.390852	4.844419
30H	-2.730235	3.478615	4.298443
31H	-3.043436	3.126385	1.866002
32H	-3.895503	-3.765901	-2.727500
33H	-2.340434	-2.964856	-4.522475
34H	-1.057612	-0.864346	-4.206917
35H	-1.319264	0.488947	-2.169770
36H	-2.125085	3.887098	-2.323145
37H	-1.096783	5.864919	-3.384603
38H	1.008426	6.846143	-2.476864
39H	2.061172	5.810025	-0.457961
40H	1.019874	3.830069	0.606194
41P	2.518069	-0.809052	0.100770
42C	1.218687	-1.983612	0.572895
43C	4.125658	-1.650525	0.052498
44C	2.185184	-0.139549	-1.551522
45C	2.549834	0.508497	1.345707
46C	5.199048	-1.040154	-0.620361
47C	6.452166	-1.653304	-0.624615
48C	6.639059	-2.873075	0.035269
49C	5.570523	-3.482817	0.698971
50C	4.312475	-2.875631	0.710835
51C	1.551995	1.103373	-1.694387
52C	1.261388	1.589306	-2.971202
53C	1.597597	0.838519	-4.100367
54C	2.231229	-0.402239	-3.958492
55C	2.528794	-0.895045	-2.688016
56C	3.761109	0.970929	1.886658
57C	3.742469	1.979919	2.851503
58C	2.525847	2.521492	3.281577
59C	1.322130	2.063290	2.738819
60C	1.330014	1.059367	1.771302
61C	0.439127	-2.621709	-0.405463
62C	-0.539725	-3.538215	-0.019204
63C	-0.743967	-3.822720	1.334004
64C	0.038627	-3.194782	2.308117
65C	1.016526	-2.272448	1.933925
66H	5.058656	-0.097551	-1.142273
67H	7.279742	-1.179521	-1.145342
68H	7.615890	-3.349308	0.027382
69H	5.711719	-4.433089	1.206550
70H	3.487697	-3.359968	1.224451
71H	1.271464	1.692449	-0.829659
72H	0.765619	2.550468	-3.070998
73H	1.368115	1.219254	-5.092185
74H	2.496372	-0.985287	-4.836319
75H	3.028748	-1.854112	-2.584802
76H	4.709595	0.548340	1.570122

77H	4.678884	2.336037	3.272219
78H	2.516216	3.302173	4.037882
79H	0.373581	2.484915	3.056674
80H	0.388962	0.730132	1.347266
81H	0.572089	-2.394017	-1.457866
82H	-1.162574	-4.007760	-0.773843
83H	-1.529776	-4.511418	1.625954
84H	-0.124962	-3.405881	3.361290
85H	1.604613	-1.771675	2.697405

15g-PhNCO2-012

1C	-4.939414	-0.739182	-2.091957
2C	-5.433753	-1.062092	-3.353224
3N	-4.925801	-0.593339	-4.506046
4C	-3.877984	0.238981	-4.403806
5C	-3.300610	0.622988	-3.194724
6C	-3.836643	0.120914	-2.002333
7N	-3.286288	0.504221	-0.751384
8C	-3.128844	-0.394412	0.263984
9N	-3.063315	-1.682768	0.013996
10S	-2.926795	-2.553775	1.442148
11C	-2.982585	-1.122464	2.518094
12C	-3.098653	0.008363	1.709450
13O	-1.609458	-3.218626	1.487281
14O	-4.115040	-3.404674	1.641637
15C	-2.986822	-1.082666	3.904346
16C	-3.117006	0.175295	4.503144
17C	-3.261922	1.325369	3.714439
18C	-3.261544	1.255752	2.317818
19C	-2.637636	1.853541	-0.658921
20O	-3.305120	2.807786	-1.097456
21N	-1.446901	1.744620	-0.103339
22C	-0.698367	2.878955	0.222518
23C	0.285772	2.697496	1.220596
24C	1.131513	3.733600	1.608521
25C	1.027319	4.994398	1.006774
26C	0.056801	5.192876	0.018768
27C	-0.800615	4.159497	-0.371640
28H	-5.400543	-1.157485	-1.204679
29H	-6.287584	-1.730749	-3.440425
30H	-3.470141	0.617997	-5.338786
31H	-2.450778	1.295890	-3.188631
32H	-2.901152	-1.989167	4.496207
33H	-3.119541	0.257787	5.586497
34H	-3.378365	2.292999	4.194307
35H	-3.382225	2.158471	1.731707
36H	0.363924	1.718661	1.682734
37H	1.878774	3.554756	2.379117
38H	1.690282	5.804673	1.300906
39H	-0.036883	6.166332	-0.459482
40H	-1.548436	4.332422	-1.135653
41P	2.792353	-0.549803	-0.309256
42C	2.119903	-0.492426	1.375558
43C	3.094793	1.138932	-0.911485
44C	4.383691	-1.425015	-0.269180
45C	1.645880	-1.441569	-1.393815
46C	4.296657	1.788055	-0.575435
47C	4.506912	3.109045	-0.972047
48C	3.525034	3.787731	-1.700774
49C	2.332332	3.143084	-2.036501
50C	2.111790	1.822210	-1.644284
51C	4.691603	-2.275403	0.803819
52C	5.896592	-2.982133	0.803809
53C	6.791306	-2.844973	-0.261325
54C	6.482590	-2.000791	-1.334073
55C	5.281976	-1.290621	-1.342580
56C	0.287261	-1.077300	-1.434480
57C	-0.583183	-1.775015	-2.271750
58C	-0.115021	-2.826465	-3.064472
59C	1.233056	-3.191535	-3.019044
60C	2.115811	-2.505359	-2.183351
61C	2.682447	0.403441	2.301341
62C	2.198964	0.442771	3.608078
63C	1.154583	-0.405052	3.995765
64C	0.602683	-1.300332	3.077326
65C	1.082210	-1.351085	1.766588
66H	5.067939	1.270288	-0.013255
67H	5.436953	3.606238	-0.710028
68H	3.686765	4.819493	-2.001118
69H	1.561093	3.669002	-2.590385
70H	1.175312	1.344199	-1.906092
71H	4.002842	-2.385834	1.635858
72H	6.134121	-3.636307	1.638132
73H	7.729076	-3.394170	-0.256485
74H	7.176631	-1.893126	-2.163066

75H	5.049218	-0.635304	-2.177135
76H	-0.104590	-0.271352	-0.816995
77H	-1.632512	-1.508257	-2.287710
78H	-0.805267	-3.366010	-3.707677
79H	1.599816	-4.015523	-3.625081
80H	3.157288	-2.806844	-2.147246
81H	3.477015	1.081462	2.005417
82H	2.626764	1.145230	4.318143
83H	0.768794	-0.361430	5.010860
84H	-0.210951	-1.958047	3.362437
85H	0.629582	-2.048319	1.070604

15g-PhNCO-001

1C	1.079479	-3.543663	-1.418519
2C	-0.286405	-3.684076	-1.382163
3N	-1.022288	-3.197982	-0.347924
4C	-0.387211	-2.619490	0.707179
5C	0.973420	-2.446406	0.723321
6C	1.769321	-2.852407	-0.386189
7N	3.111618	-2.668656	-0.523849
8C	3.758111	-1.672303	0.066623
9N	3.215955	-0.637138	0.726942
10S	4.375869	0.464200	1.162065
11C	5.771258	-0.457153	0.499039
12C	5.248523	-1.613620	-0.075224
13O	4.465501	0.583514	2.635025
14O	4.187187	1.736157	0.423911
15C	7.125179	-0.154812	0.500404
16C	7.983524	-1.079111	-0.111041
17C	7.477922	-2.249780	-0.695826
18C	6.105634	-2.527972	-0.686797
19C	-2.546010	-3.276839	-0.428038
20O	-2.972520	-3.930780	-1.395216
21N	-3.087418	-2.596466	0.548693
22C	-4.468923	-2.482632	0.707839
23C	-5.468824	-3.076721	-0.100199
24C	-6.822938	-2.842092	0.159836
25C	-7.226217	-2.019087	1.216688
26C	-6.246179	-1.431794	2.028541
27C	-4.895085	-1.661715	1.778824
28H	1.633373	-3.919671	-2.272117
29H	-0.857498	-4.157217	-2.170437
30H	-1.034318	-2.288834	1.507430
31H	1.425998	-1.964731	1.577052
32H	7.504926	0.755105	0.955694
33H	9.052466	-0.884559	-0.130751
34H	8.163273	-2.951342	-1.163881
35H	5.708607	-3.430695	-1.140537
36H	-5.175832	-3.710596	-0.927388
37H	-7.571063	-3.310664	-0.476972
38H	-8.281834	-1.842206	1.408276
39H	-6.537426	-0.790754	2.858299
40H	-4.132914	-1.201267	2.402960
41P	-1.040425	1.915047	-0.308704
42C	-0.937077	1.236436	1.370458
43C	-2.760798	1.827185	-0.877899
44C	-0.489675	3.645094	-0.276486
45C	0.034027	1.007500	-1.454374
46C	-3.338796	2.904156	-1.569551
47C	-4.650915	2.800456	-2.036125
48C	-5.385054	1.630929	-1.814349
49C	-4.809997	0.559701	-1.123498
50C	-3.499334	0.652107	-0.652916
51C	-0.530150	4.377194	0.920333
52C	-0.141486	5.718426	0.924305
53C	0.288120	6.329097	-0.257610
54C	0.330472	5.599080	-1.450253
55C	-0.056016	4.258429	-1.464191
56C	1.420605	1.233893	-1.422974
57C	2.254415	0.530550	-2.291950
58C	1.715191	-0.391977	-3.191545
59C	0.335077	-0.617047	-3.223316
60C	-0.509805	0.078209	-2.357631
61C	0.275132	0.691805	1.820615
62C	0.384633	0.247197	3.138911
63C	-0.709554	0.334546	4.004379
64C	-1.919303	0.874135	3.553473
65C	-2.037075	1.331909	2.240424
66H	-2.778314	3.817736	-1.741799
67H	-5.098877	3.635935	-2.567265
68H	-6.407769	1.555303	-2.174531
69H	-5.377443	-0.347604	-0.940618
70H	-3.067650	-0.185975	-0.112682
71H	-0.849969	3.907934	1.845669
72H	-0.165592	6.280423	1.853836

73H	0.596825	7.371094	-0.248798
74H	0.671351	6.069179	-2.368631
75H	-0.011383	3.693700	-2.390939
76H	1.862160	1.940186	-0.727556
77H	3.325533	0.701117	-2.249745
78H	2.370872	-0.943755	-3.859822
79H	-0.087354	-1.337934	-3.917355
80H	-1.578495	-0.106644	-2.391542
81H	1.129363	0.586260	1.160762
82H	1.327174	-0.172954	3.478845
83H	-0.622442	-0.020575	5.027871
84H	-2.773705	0.937591	4.221745
85H	-2.979279	1.750038	1.900474

15g-PhNCO-002

1C	-1.353110	-3.621876	1.280245
2C	0.016953	-3.729767	1.311178
3N	0.798753	-3.109068	0.390610
4C	0.213048	-2.391490	-0.606391
5C	-1.145972	-2.220746	-0.669979
6C	-1.993865	-2.804604	0.312826
7N	-3.349610	-2.673775	0.352970
8C	-3.957365	-1.545948	0.026368
9N	-3.369190	-0.348224	-0.141824
10S	-4.498331	0.829346	-0.425708
11C	-5.930354	-0.258078	-0.362363
12C	-5.449073	-1.537924	-0.097893
13O	-4.335515	1.405492	-1.782140
14O	-4.525732	1.812366	0.682682
15C	-7.277921	0.026520	-0.528595
16C	-8.172441	-1.046924	-0.418633
17C	-7.708424	-2.343785	-0.151716
18C	-6.342217	-2.602765	0.012695
19C	2.318836	-3.217574	0.521487
20O	2.698774	-3.831182	1.532040
21N	2.909556	-2.633375	-0.489180
22C	4.299763	-2.586684	-0.610285
23C	5.245200	-2.871654	0.404300
24C	6.615104	-2.734571	0.158252
25C	7.088615	-2.317514	-1.090570
26C	6.163048	-2.033054	-2.103588
27C	4.796218	-2.160238	-1.864584
28H	-1.946459	-4.122029	2.038478
29H	0.552542	-4.289014	2.067298
30H	0.897536	-1.956588	-1.319279
31H	-1.556425	-1.609086	-1.461854
32H	-7.625191	1.034629	-0.734889
33H	-9.237631	-0.870158	-0.541419
34H	-8.422013	-3.159397	-0.070256
35H	-5.977175	-3.603516	0.222335
36H	4.898936	-3.199323	1.376583
37H	7.319374	-2.958945	0.957163
38H	8.155965	-2.218271	-1.272795
39H	6.508247	-1.704721	-3.081873
40H	4.077169	-1.930659	-2.647755
41P	1.248688	1.845006	0.171062
42C	0.501895	3.473001	0.458733
43C	0.613618	1.208929	-1.408396
44C	3.053905	1.990787	0.098212
45C	0.802827	0.753748	1.552546
46C	1.463208	0.561458	-2.320885
47C	0.939901	0.052729	-3.510736
48C	-0.422942	0.187490	-3.795343
49C	-1.267933	0.839553	-2.892187
50C	-0.753357	1.354270	-1.702178
51C	3.673589	3.249090	0.041529
52C	5.066389	3.328407	-0.031628
53C	5.837656	2.162004	-0.048582
54C	5.219939	0.908205	0.008454
55C	3.830457	0.818434	0.085081
56C	1.715957	0.506127	2.591491
57C	1.325080	-0.266609	3.686864
58C	0.025935	-0.776497	3.758763
59C	-0.884558	-0.519465	2.729593
60C	-0.502160	0.238491	1.623243
61C	0.121864	3.850870	1.755895
62C	-0.418782	5.119364	1.975927
63C	-0.579855	6.008564	0.909471
64C	-0.201499	5.631576	-0.383865
65C	0.338051	4.365938	-0.614419
66H	2.520814	0.443743	-2.113045
67H	1.599827	-0.452332	-4.210799
68H	-0.826246	-0.215820	-4.720618
69H	-2.330119	0.942351	-3.089854
70H	-1.420119	1.866353	-1.016200

71H	3.082272	4.159294	0.058005
72H	5.545890	4.302683	-0.072100
73H	6.921082	2.228747	-0.105602
74H	5.811603	-0.001444	-0.009280
75H	3.359007	-0.158521	0.134956
76H	2.724392	0.904571	2.554904
77H	2.038903	-0.468817	4.480523
78H	-0.274413	-1.378921	4.612114
79H	-1.893697	-0.916677	2.774428
80H	-1.228209	0.404765	0.834751
81H	0.234273	3.160687	2.586573
82H	-0.721799	5.406501	2.978992
83H	-1.008396	6.992093	1.083328
84H	-0.333476	6.318735	-1.215061
85H	0.618358	4.075415	-1.623075

15g-PhNCO-003

1C	0.675750	-3.363943	-1.561173
2C	-0.687634	-3.515642	-1.492220
3N	-1.393674	-3.082597	-0.414161
4C	-0.730673	-2.534320	0.635557
5C	0.630781	-2.348750	0.625584
6C	1.403630	-2.730819	-0.512435
7N	2.743298	-2.568242	-0.704432
8C	3.505850	-1.795081	0.065262
9N	3.112903	-1.005680	1.072346
10S	4.387209	-0.122517	1.672988
11C	5.624661	-0.798628	0.555860
12C	4.966699	-1.713813	-0.262632
13O	4.673784	-0.500019	3.074884
14O	4.182172	1.322879	1.423085
15C	6.979569	-0.521176	0.449299
16C	7.694891	-1.213332	-0.537819
17C	7.052237	-2.139701	-1.372455
18C	5.681823	-2.398296	-1.244958
19C	-2.922487	-3.163947	-0.449738
20O	-3.372801	-3.831457	-1.396029
21N	-3.432822	-2.467775	0.531451
22C	-4.806668	-2.299753	0.693458
23C	-5.829521	-2.826214	-0.132974
24C	-7.172626	-2.537151	0.127604
25C	-7.544624	-1.727960	1.206534
26C	-6.542961	-1.207021	2.037149
27C	-5.201953	-1.488574	1.783686
28H	1.207877	-3.709352	-2.441505
29H	-1.278356	-3.966661	-2.278987
30H	-1.355634	-2.236410	1.464096
31H	1.098404	-1.887314	1.483034
32H	7.465723	0.199294	1.100603
33H	8.759274	-1.028593	-0.655597
34H	7.627725	-2.664567	-2.130361
35H	5.178430	-3.112022	-1.889439
36H	-5.560528	-3.452253	-0.973996
37H	-7.937963	-2.954193	-0.524548
38H	-8.592347	-1.511053	1.400500
39H	-6.808984	-0.578715	2.885003
40H	-4.423073	-1.079456	2.423399
41P	-0.729664	2.003605	-0.324866
42C	-1.975640	1.021761	-1.205361
43C	-0.387881	1.273042	1.299169
44C	0.801785	2.061695	-1.294500
45C	-1.382386	3.684005	-0.106227
46C	0.862198	1.466860	1.909980
47C	1.094259	0.944523	3.183149
48C	0.088219	0.237649	3.847512
49C	-1.155413	0.042795	3.236232
50C	-1.397924	0.555945	1.962384
51C	1.121996	3.190634	-2.065865
52C	2.277497	3.185536	-2.849393
53C	3.110520	2.062275	-2.867036
54C	2.793369	0.941170	-2.094905
55C	1.644576	0.938319	-1.304522
56C	-1.131547	4.388829	1.081182
57C	-1.600929	5.696760	1.221344
58C	-2.317241	6.301434	0.184230
59C	-2.569560	5.598164	-0.998891
60C	-2.105742	4.290805	-1.148073
61C	-1.585810	0.071560	-2.162719
62C	-2.554565	-0.707287	-2.796533
63C	-3.905107	-0.549787	-2.475977
64C	-4.294798	0.396528	-1.524052
65C	-3.336003	1.185258	-0.888940
66H	1.665848	1.985007	1.397299
67H	2.069885	1.073772	3.641621
68H	0.278710	-0.176530	4.834131

69H	-1.932246	-0.526036	3.740054
70H	-2.353879	0.366909	1.484694
71H	0.485640	4.069659	-2.055714
72H	2.528183	4.062312	-3.440236
73H	4.011452	2.063619	-3.474867
74H	3.442035	0.070693	-2.095981
75H	1.423292	0.078224	-0.683679
76H	-0.580520	3.924944	1.893472
77H	-1.408600	6.239244	2.142944
78H	-2.682540	7.318690	0.298257
79H	-3.130155	6.064478	-1.804414
80H	-2.311592	3.746594	-2.065752
81H	-0.540135	-0.065709	-2.416883
82H	-2.250655	-1.448015	-3.530114
83H	-4.651860	-1.175382	-2.955446
84H	-5.342675	0.509334	-1.262308
85H	-3.647977	1.918418	-0.150690

15g-PhNCO-004

1C	0.754184	-2.965161	-1.827011
2C	-0.613368	-3.082953	-1.769971
3N	-1.285473	-2.963091	-0.594094
4C	-0.586332	-2.773207	0.556604
5C	0.778486	-2.627536	0.560839
6C	1.512416	-2.678728	-0.658634
7N	2.858736	-2.520979	-0.796446
8C	3.572709	-1.757933	0.018017
9N	3.097943	-0.934356	0.965708
10S	4.312114	-0.012072	1.613727
11C	5.642688	-0.743824	0.646226
12C	5.054927	-1.692778	-0.186996
13O	4.487684	-0.289204	3.057061
14O	4.124752	1.414151	1.252121
15C	7.003115	-0.472423	0.645641
16C	7.798037	-1.207755	-0.244574
17C	7.226108	-2.167986	-1.092559
18C	5.848592	-2.418811	-1.074516
19C	-2.814747	-2.957508	-0.618464
20O	-3.305961	-3.279337	-1.715031
21N	-3.285974	-2.544001	0.527444
22C	-4.653370	-2.382401	0.754989
23C	-5.708598	-2.838946	-0.070992
24C	-7.040304	-2.593873	0.277093
25C	-7.366763	-1.889544	1.440936
26C	-6.331891	-1.437533	2.270449
27C	-5.002066	-1.684253	1.934651
28H	1.259525	-3.047729	-2.783223
29H	-1.233817	-3.255464	-2.640047
30H	-1.187852	-2.717219	1.451635
31H	1.279916	-2.444436	1.501080
32H	7.434555	0.275071	1.304860
33H	8.869549	-1.029465	-0.276929
34H	7.863014	-2.724577	-1.774903
35H	5.399200	-3.157004	-1.731478
36H	-5.475915	-3.377392	-0.981139
37H	-7.831982	-2.958531	-0.374958
38H	-8.405736	-1.701077	1.700579
39H	-6.562385	-0.890692	3.182612
40H	-4.198977	-1.331527	2.577657
41P	-0.809405	1.928806	-0.339481
42C	-0.434716	1.159266	1.259679
43C	-0.580833	3.723284	-0.161885
44C	0.272568	1.312563	-1.661107
45C	-2.529185	1.574553	-0.787680
46C	-0.140617	4.493813	-1.249344
47C	-0.018793	5.878123	-1.113371
48C	-0.332214	6.495432	0.101462
49C	-0.766799	5.727759	1.186826
50C	-0.891795	4.343359	1.060576
51C	1.562117	0.849759	-1.360517
52C	2.412768	0.458212	-2.396170
53C	1.981519	0.515804	-3.723428
54C	0.692344	0.969785	-4.022901
55C	-0.163168	1.373923	-2.997613
56C	-2.847167	0.332973	-1.363615
57C	-4.177035	0.012256	-1.632344
58C	-5.190980	0.925534	-1.328686
59C	-4.875789	2.166068	-0.765280
60C	-3.546698	2.495829	-0.491721
61C	-1.330147	0.238028	1.825695
62C	-1.034355	-0.338418	3.062292
63C	0.149499	-0.010792	3.728106
64C	1.043880	0.903004	3.160900
65C	0.753268	1.496422	1.933973
66H	0.116364	4.023793	-2.193631

67H	0.328256	6.471065	-1.955134
68H	-0.231251	7.572640	0.204818
69H	-1.003977	6.203791	2.134311
70H	-1.222389	3.753255	1.910356
71H	1.909283	0.766101	-0.337314
72H	3.407379	0.094784	-2.158987
73H	2.645482	0.200357	-4.524058
74H	0.350481	1.010095	-5.053549
75H	-1.160959	1.727132	-3.240227
76H	-2.065419	-0.383176	-1.594660
77H	-4.413454	-0.960019	-2.052176
78H	-6.227567	0.663724	-1.522695
79H	-5.663584	2.877547	-0.533091
80H	-3.310768	3.460874	-0.053448
81H	-2.243035	-0.048640	1.313926
82H	-1.728050	-1.055093	3.493515
83H	0.381720	-0.473102	4.683914
84H	1.976069	1.142957	3.662894
85H	1.456196	2.204813	1.507120

15g-PhNCO-005

1C	1.324664	-2.211920	1.216318
2C	-0.018812	-2.297834	1.481411
3N	-0.886903	-2.855057	0.597376
4C	-0.410485	-3.431364	-0.538106
5C	0.930868	-3.422130	-0.832483
6C	1.852718	-2.739653	0.005539
7N	3.162985	-2.680030	-0.363580
8C	3.908899	-1.618213	-0.108790
9N	3.454697	-0.410454	0.268305
10S	4.697619	0.673291	0.404875
11C	6.004731	-0.475970	-0.055892
12C	5.389147	-1.698627	-0.314032
13O	4.860132	1.119285	1.809595
14O	4.565238	1.758075	-0.596118
15C	7.374492	-0.280694	-0.158089
16C	8.147698	-1.385607	-0.540645
17C	7.547171	-2.625633	-0.805008
18C	6.161652	-2.795145	-0.694581
19C	-2.379655	-2.755668	0.892505
20O	-2.650257	-2.530188	2.084729
21N	-3.069698	-2.869521	-0.213148
22C	-4.465191	-2.805447	-0.212251
23C	-5.312843	-2.968917	0.909235
24C	-6.701186	-2.880518	0.769667
25C	-7.287900	-2.620845	-0.473853
26C	-6.459367	-2.464121	-1.593253
27C	-5.074810	-2.560948	-1.464334
28H	1.967222	-1.711141	1.928348
29H	-0.468092	-1.902540	2.381566
30H	-1.159996	-3.861416	-1.188411
31H	1.280530	-3.884634	-1.749162
32H	7.829372	0.683265	0.050582
33H	9.225206	-1.278195	-0.632313
34H	8.167912	-3.467626	-1.099500
35H	5.690466	-3.751933	-0.897688
36H	-4.877164	-3.153220	1.883343
37H	-7.329512	-3.011268	1.648731
38H	-8.368379	-2.546984	-0.570919
39H	-6.895132	-2.265591	-2.570362
40H	-4.429190	-2.437273	-2.330891
41P	-1.196653	1.872357	-0.073711
42C	-0.761222	0.732126	-1.417775
43C	-0.431835	1.394436	1.501245
44C	-0.577803	3.524085	-0.506614
45C	-3.001306	1.915360	0.105573
46C	0.954052	1.563781	1.668352
47C	1.560652	1.185632	2.865447
48C	0.786200	0.660961	3.905541
49C	-0.594752	0.508651	3.747570
50C	-1.208393	0.868226	2.546057
51C	-0.355647	3.858774	-1.851513
52C	0.086254	5.141372	-2.181646
53C	0.305452	6.088859	-1.177225
54C	0.085629	5.755158	0.163394
55C	-0.354117	4.475223	0.503604
56C	-3.722284	0.708027	0.131971
57C	-5.106502	0.731372	0.303718
58C	-5.773973	1.951651	0.449573
59C	-5.058432	3.152617	0.422144
60C	-3.672478	3.140142	0.249743
61C	0.532687	0.189930	-1.480831
62C	0.903237	-0.581082	-2.582843
63C	-0.007114	-0.821511	-3.615427
64C	-1.298304	-0.289769	-3.547682

65C	-1.678142	0.492602	-2.456024
66H	1.561994	1.985943	0.874452
67H	2.636581	1.290837	2.968377
68H	1.260888	0.369058	4.838787
69H	-1.198551	0.097548	4.551791
70H	-2.278061	0.730318	2.431039
71H	-0.513212	3.125670	-2.636864
72H	0.266199	5.395300	-3.222648
73H	0.654970	7.084369	-1.438021
74H	0.262608	6.487287	0.946423
75H	-0.511948	4.219335	1.547430
76H	-3.217529	-0.245174	0.007740
77H	-5.655522	-0.204576	0.320079
78H	-6.852798	1.965088	0.581291
79H	-5.576206	4.101812	0.530702
80H	-3.126896	4.078100	0.224065
81H	1.257593	0.341774	-0.688655
82H	1.902853	-1.003124	-2.619057
83H	0.285590	-1.429758	-4.467383
84H	-2.013691	-0.481904	-4.342591
85H	-2.680586	0.906482	-2.419174

15g-PhNCO-006

1C	0.957972	-2.229099	1.302396
2C	-0.396797	-2.200147	1.522934
3N	-1.275163	-2.775776	0.661444
4C	-0.801751	-3.477529	-0.405215
5C	0.543449	-3.559700	-0.663147
6C	1.486487	-2.867427	0.146216
7N	2.794749	-2.895065	-0.230589
8C	3.638534	-1.916993	0.068123
9N	3.334224	-0.731904	0.620614
10S	4.660782	0.260410	0.666189
11C	5.808605	-0.922679	-0.054914
12C	5.074615	-2.074617	-0.327514
13O	5.034103	0.580578	2.062805
14O	4.472494	1.424166	-0.233034
15C	7.162492	-0.801732	-0.333101
16C	7.793965	-1.910878	-0.912719
17C	7.073143	-3.080856	-1.195275
18C	5.705809	-3.174002	-0.908271
19C	-2.766107	-2.547577	0.890692
20O	-3.032369	-1.984550	1.968479
21N	-3.462085	-2.940197	-0.142942
22C	-4.854179	-2.816772	-0.167386
23C	-5.699552	-2.694925	0.960917
24C	-7.084405	-2.588115	0.804252
25C	-7.670353	-2.591333	-0.466523
26C	-6.844811	-2.720506	-1.591158
27C	-5.463374	-2.838829	-1.442476
28H	1.610072	-1.722977	1.998710
29H	-0.844750	-1.693844	2.367731
30H	-1.559020	-3.926011	-1.033445
31H	0.888263	-4.109884	-1.532174
32H	7.710250	0.109704	-0.111626
33H	8.854316	-1.861674	-1.145645
34H	7.584455	-3.927248	-1.646089
35H	5.141369	-4.074632	-1.128996
36H	-5.264497	-2.676041	1.952469
37H	-7.710730	-2.496843	1.689701
38H	-8.748190	-2.501926	-0.578833
39H	-7.279792	-2.731940	-2.588464
40H	-4.822879	-2.942949	-2.315354
41P	-0.865597	2.074437	-0.122714
42C	-0.286937	3.759870	-0.481777
43C	-0.481579	1.668177	1.602606
44C	-2.660354	1.979736	-0.369396
45C	-0.026338	0.950705	-1.273644
46C	-1.394831	1.998479	2.619839
47C	-1.064254	1.748726	3.952186
48C	0.173380	1.180825	4.274701
49C	1.079864	0.854324	3.262311
50C	0.755966	1.090989	1.925415
51C	-3.313747	2.931327	-1.169557
52C	-4.684631	2.811338	-1.406494
53C	-5.402916	1.747915	-0.850996
54C	-4.753514	0.803346	-0.050034
55C	-3.384112	0.914056	0.194560
56C	1.358820	1.084153	-1.475181
57C	2.013397	0.228505	-2.359979
58C	1.295258	-0.752769	-3.048738
59C	-0.082506	-0.885237	-2.848985
60C	-0.748803	-0.038655	-1.961744
61C	-0.110398	4.686663	0.557356
62C	0.294747	5.989955	0.261402

63C	0.524644	6.370861	-1.063867
64C	0.352844	5.446429	-2.099631
65C	-0.051568	4.141926	-1.813940
66H	-2.358136	2.437708	2.378878
67H	-1.775529	1.994366	4.735904
68H	0.427184	0.987699	5.313737
69H	2.039929	0.405842	3.502502
70H	1.463827	0.796461	1.158791
71H	-2.765259	3.761865	-1.602636
72H	-5.188368	3.550429	-2.023625
73H	-6.468985	1.653979	-1.040464
74H	-5.304321	-0.027234	0.379926
75H	-2.899488	0.175659	0.826505
76H	1.934489	1.838939	-0.948749
77H	3.085849	0.327832	-2.493847
78H	1.810956	-1.421428	-3.732920
79H	-0.642407	-1.652265	-3.376312
80H	-1.817570	-0.154844	-1.813307
81H	-0.271624	4.398293	1.591497
82H	0.438078	6.702981	1.068602
83H	0.845051	7.384593	-1.289457
84H	0.538865	5.736924	-3.130013
85H	-0.172910	3.426831	-2.622477

15g-PhNCO-007

1C	0.243998	-2.081088	1.110012
2C	-1.100410	-1.953559	1.373819
3N	-2.053024	-2.430958	0.536502
4C	-1.673905	-3.090077	-0.593939
5C	-0.349692	-3.259632	-0.908264
6C	0.685040	-2.737411	-0.077031
7N	1.965290	-2.929479	-0.503191
8C	3.021107	-2.329991	0.041117
9N	3.025939	-1.397186	1.001063
10S	4.570268	-0.853168	1.297583
11C	5.376428	-1.914503	0.090269
12C	4.372261	-2.666357	-0.514879
13O	4.990896	-1.195222	2.674223
14O	4.704757	0.571683	0.916438
15C	6.716813	-2.023649	-0.249840
16C	7.045165	-2.945540	-1.253487
17C	6.049503	-3.712816	-1.876393
18C	4.703094	-3.580664	-1.514641
19C	-3.521145	-2.147159	0.867395
20O	-3.682034	-1.454420	1.886936
21N	-4.306829	-2.695443	-0.020141
22C	-5.688347	-2.502651	-0.007056
23C	-6.408840	-1.604295	0.818482
24C	-7.794810	-1.473592	0.687732
25C	-8.508584	-2.224797	-0.252010
26C	-7.809116	-3.120912	-1.071634
27C	-6.426814	-3.253738	-0.952220
28H	0.953946	-1.659661	1.806364
29H	-1.476718	-1.449357	2.252943
30H	-2.487460	-3.449972	-1.208210
31H	-0.081299	-3.788897	-1.816811
32H	7.478532	-1.423208	0.238817
33H	8.083570	-3.065475	-1.550562
34H	6.328623	-4.420998	-2.652039
35H	3.927815	-4.170135	-1.993769
36H	-5.876073	-1.017255	1.555550
37H	-8.321829	-0.774412	1.334678
38H	-9.586922	-2.118197	-0.342490
39H	-8.343468	-3.717463	-1.808340
40H	-5.883355	-3.945036	-1.592592
41P	-0.154785	2.361993	-0.223124
42C	1.128336	1.938734	-1.432296
43C	-0.376374	4.163855	-0.165417
44C	-1.733671	1.613799	-0.715783
45C	0.340788	1.752363	1.410613
46C	-1.130265	4.802423	-1.166077
47C	-1.266622	6.190862	-1.150315
48C	-0.657261	6.944299	-0.140961
49C	0.089131	6.309119	0.855893
50C	0.232280	4.919652	0.848329
51C	-1.757597	0.506749	-1.579492
52C	-2.976771	-0.088266	-1.905915
53C	-4.168964	0.408920	-1.373181
54C	-4.146476	1.512457	-0.515450
55C	-2.934215	2.120062	-0.186968
56C	1.699498	1.716257	1.765705
57C	2.067369	1.283643	3.040326
58C	1.090164	0.890973	3.958798
59C	-0.263019	0.926968	3.604341
60C	-0.642632	1.354166	2.331940

61C	1.509856	2.853725	-2.426996
62C	2.460805	2.481545	-3.379047
63C	3.030424	1.204756	-3.342750
64C	2.654889	0.297306	-2.348120
65C	1.707966	0.659789	-1.390984
66H	-1.611689	4.223108	-1.948885
67H	-1.850861	6.681730	-1.923807
68H	-0.768695	8.025302	-0.129478
69H	0.558107	6.891583	1.644098
70H	0.807405	4.434217	1.630957
71H	-0.838367	0.106043	-1.994481
72H	-2.993393	-0.952238	-2.563270
73H	-5.111990	-0.073443	-1.610649
74H	-5.071515	1.894959	-0.093591
75H	-2.927002	2.980283	0.476377
76H	2.474058	1.985569	1.055351
77H	3.120001	1.231797	3.300374
78H	1.383743	0.542253	4.945373
79H	-1.024606	0.606387	4.310004
80H	-1.693577	1.354796	2.061273
81H	1.082037	3.850645	-2.459458
82H	2.760308	3.192808	-4.143904
83H	3.773638	0.919948	-4.082764
84H	3.102955	-0.690566	-2.308153
85H	1.446684	-0.039544	-0.605537

15g-PhNCO-008

1C	0.360180	-3.027733	-1.851087
2C	-1.005630	-3.148988	-1.775133
3N	-1.670038	-2.934615	-0.608703
4C	-0.966186	-2.643933	0.515522
5C	0.402529	-2.522092	0.505779
6C	1.134732	-2.671612	-0.709956
7N	2.474755	-2.513423	-0.902588
8C	3.286273	-1.963323	-0.003260
9N	2.960056	-1.432238	1.181969
10S	4.282226	-0.730584	1.907953
11C	5.448873	-1.136784	0.601852
12C	4.733918	-1.830616	-0.370992
13O	4.630515	-1.431923	3.163420
14O	4.088613	0.733198	2.014359
15C	6.800821	-0.846666	0.489275
16C	7.451743	-1.288233	-0.670820
17C	6.750767	-1.989898	-1.663279
18C	5.385257	-2.266917	-1.524441
19C	-3.196431	-2.972401	-0.618097
20O	-3.685402	-3.529885	-1.615860
21N	-3.666961	-2.349103	0.429752
22C	-5.033853	-2.174184	0.646140
23C	-6.090779	-2.620258	-0.185116
24C	-7.420999	-2.347255	0.150501
25C	-7.744768	-1.629891	1.306713
26C	-6.708427	-1.184664	2.138897
27C	-5.380227	-1.451239	1.813025
28H	0.858766	-3.184721	-2.801979
29H	-1.630491	-3.398420	-2.622790
30H	-1.561695	-2.496185	1.405996
31H	0.909908	-2.284428	1.427859
32H	7.331770	-0.301817	1.264391
33H	8.511214	-1.084171	-0.800455
34H	7.276991	-2.323046	-2.553887
35H	4.835686	-2.803394	-2.291548
36H	-5.860611	-3.179960	-1.082890
37H	-8.213726	-2.704075	-0.504559
38H	-8.782550	-1.424755	1.558167
39H	-6.937699	-0.627669	3.045329
40H	-4.573609	-1.106503	2.455929
41P	-0.508911	2.045174	-0.283749
42C	1.239945	2.104477	-0.759562
43C	-0.690408	1.241463	1.328738
44C	-1.158614	3.736297	-0.122660
45C	-1.426988	1.175018	-1.586877
46C	-1.937973	1.275643	1.979516
47C	-2.085405	0.656923	3.219163
48C	-0.992802	0.017226	3.818481
49C	0.248061	-0.001350	3.177917
50C	0.405946	0.609217	1.931345
51C	-1.829793	4.353869	-1.189521
52C	-2.277649	5.670002	-1.056967
53C	-2.057498	6.371082	0.132611
54C	-1.392463	5.754657	1.197755
55C	-0.943238	4.439072	1.075553
56C	-2.536327	0.373048	-1.276855
57C	-3.283502	-0.201614	-2.307358
58C	-2.921275	0.006168	-3.640464

59C	-1.806060	0.792052	-3.950655
60C	-1.060053	1.381465	-2.929890
61C	2.004374	3.257308	-0.520588
62C	3.356691	3.273880	-0.867137
63C	3.943977	2.151359	-1.457343
64C	3.181326	1.004720	-1.698000
65C	1.833561	0.972016	-1.342904
66H	-2.783585	1.785730	1.527190
67H	-3.050591	0.676216	3.717263
68H	-1.111450	-0.464226	4.785687
69H	1.099571	-0.494311	3.637966
70H	1.374775	0.576209	1.446397
71H	-2.015595	3.815445	-2.113655
72H	-2.802730	6.143346	-1.882061
73H	-2.409223	7.394622	0.232224
74H	-1.225064	6.294392	2.125834
75H	-0.434595	3.964026	1.909479
76H	-2.815700	0.166591	-0.249960
77H	-4.135622	-0.827097	-2.062784
78H	-3.501413	-0.453603	-4.436140
79H	-1.514741	0.947250	-4.985966
80H	-0.196468	1.990239	-3.180156
81H	1.555671	4.137321	-0.070547
82H	3.948208	4.164513	-0.673983
83H	4.997446	2.165558	-1.723785
84H	3.635432	0.128224	-2.148527
85H	1.255536	0.071098	-1.522360

15g-PhNCO-009

1C	0.497089	-2.268959	1.203171
2C	-0.850190	-2.182095	1.464635
3N	-1.787995	-2.596910	0.576734
4C	-1.388690	-3.163165	-0.595943
5C	-0.058974	-3.293170	-0.908069
6C	0.956890	-2.812788	-0.031382
7N	2.248243	-2.939368	-0.447599
8C	3.242767	-2.206617	0.044292
9N	3.137582	-1.165885	0.879436
10S	4.608591	-0.430318	1.104040
11C	5.541610	-1.552871	0.051736
12C	4.629879	-2.477782	-0.452613
13O	5.042820	-0.538174	2.515277
14O	4.598602	0.939545	0.539063
15C	6.892311	-1.568314	-0.263514
16C	7.331428	-2.578435	-1.130682
17C	6.430604	-3.520748	-1.648825
18C	5.070685	-3.479255	-1.317087
19C	-3.264544	-2.351897	0.908350
20O	-3.444311	-1.748882	1.980348
21N	-4.030287	-2.821115	-0.039436
22C	-5.413729	-2.645706	-0.032782
23C	-6.179173	-1.970822	0.950161
24C	-7.563640	-1.838176	0.805676
25C	-8.230550	-2.363690	-0.306089
26C	-7.486203	-3.037392	-1.284040
27C	-6.106064	-3.175315	-1.147777
28H	1.194633	-1.894151	1.938475
29H	-1.242633	-1.758480	2.378652
30H	-2.191317	-3.482175	-1.246264
31H	0.226342	-3.743466	-1.853280
32H	7.580025	-0.832508	0.142784
33H	8.382066	-2.630082	-1.403472
34H	6.794791	-4.294724	-2.319191
35H	4.368249	-4.203186	-1.718161
36H	-5.680897	-1.552814	1.815310
37H	-8.126405	-1.314681	1.576572
38H	-9.307780	-2.255570	-0.407629
39H	-7.983738	-3.457286	-2.155979
40H	-5.528178	-3.696185	-1.908078
41P	-0.393505	2.285786	-0.205508
42C	0.136664	1.658424	1.409821
43C	-2.020791	1.605632	-0.635470
44C	-0.536235	4.095913	-0.147924
45C	0.824154	1.809056	-1.461238
46C	-3.179106	2.170850	-0.072491
47C	-4.428178	1.619192	-0.358770
48C	-4.529780	0.511728	-1.206056
49C	-3.379206	-0.048031	-1.767851
50C	-2.124019	0.493357	-1.486314
51C	0.160394	4.830599	0.823855
52C	0.069961	6.224372	0.834551
53C	-0.710506	6.885668	-0.118234
54C	-1.404631	6.153814	-1.087824
55C	-1.320868	4.761125	-1.106502
56C	1.373673	0.517199	-1.425144

57C	2.258846	0.112864	-2.424063
58C	2.605012	0.993267	-3.452751
59C	2.067254	2.284180	-3.482994
60C	1.176561	2.697054	-2.490680
61C	-0.818861	1.213827	2.338810
62C	-0.405666	0.784718	3.600475
63C	0.952460	0.792556	3.935708
64C	1.903022	1.226263	3.007183
65C	1.501902	1.659454	1.743066
66H	-3.111005	3.034228	0.583205
67H	-5.320466	2.051013	0.085841
68H	-5.501193	0.074460	-1.415518
69H	-3.457124	-0.916191	-2.414378
70H	-1.238105	0.048107	-1.927797
71H	0.765018	4.326443	1.571284
72H	0.606675	6.789861	1.591307
73H	-0.781272	7.970067	-0.103649
74H	-2.014482	6.664718	-1.827860
75H	-1.867869	4.199632	-1.858439
76H	1.137916	-0.160101	-0.613287
77H	2.682669	-0.886039	-2.386964
78H	3.301599	0.676965	-4.224695
79H	2.345193	2.974501	-4.274754
80H	0.771250	3.703465	-2.520018
81H	-1.872529	1.176512	2.081932
82H	-1.145623	0.427024	4.311281
83H	1.271866	0.444427	4.914554
84H	2.960441	1.202766	3.252303
85H	2.255946	1.959458	1.022190

15g-PhNCO-010

1C	0.158318	-2.012804	1.101198
2C	-1.185297	-1.856654	1.353713
3N	-2.141392	-2.414078	0.572104
4C	-1.767263	-3.188287	-0.484666
5C	-0.443989	-3.395482	-0.780277
6C	0.594440	-2.792079	-0.010621
7N	1.872530	-3.041285	-0.413171
8C	2.936335	-2.406071	0.070872
9N	2.955254	-1.388253	0.940686
10S	4.507052	-0.837129	1.182881
11C	5.296446	-2.016001	0.077848
12C	4.282240	-2.810622	-0.451306
13O	4.928115	-1.055318	2.584609
14O	4.658733	0.544320	0.671890
15C	6.634535	-2.171251	-0.253482
16C	6.949848	-3.186986	-1.166612
17C	5.944059	-3.999097	-1.711671
18C	4.600268	-3.818443	-1.361385
19C	-3.607561	-2.094293	0.878472
20O	-3.767389	-1.370377	1.876250
21N	-4.392723	-2.648668	-0.005840
22C	-5.771263	-2.435326	-0.012624
23C	-6.490244	-1.522301	0.798096
24C	-7.872810	-1.374900	0.649499
25C	-8.584490	-2.122504	-0.294610
26C	-7.886450	-3.032010	-1.100638
27C	-6.507660	-3.182066	-0.963012
28H	0.870568	-1.525132	1.750531
29H	-1.558460	-1.266899	2.179031
30H	-2.583295	-3.606643	-1.057262
31H	-0.178318	-4.019230	-1.627600
32H	7.404194	-1.535704	0.174711
33H	7.985873	-3.345784	-1.453631
34H	6.213182	-4.780915	-2.416949
35H	3.817035	-4.441637	-1.781116
36H	-5.958761	-0.937616	1.538017
37H	-8.398783	-0.665307	1.285863
38H	-9.660148	-2.002550	-0.399185
39H	-8.419177	-3.625597	-1.840910
40H	-5.965252	-3.883883	-1.592739
41P	-0.070473	2.383683	-0.223771
42C	0.422620	1.782051	1.414354
43C	-1.626943	1.603644	-0.739869
44C	-0.327685	4.180875	-0.158928
45C	1.233311	1.989175	-1.420246
46C	-2.848392	2.080925	-0.232417
47C	-4.040491	1.448301	-0.586836
48C	-4.022811	0.348549	-1.449330
49C	-2.809931	-0.119991	-1.961178
50C	-1.610921	0.500645	-1.609354
51C	0.266905	4.942351	0.859250
52C	0.099741	6.328976	0.873811
53C	-0.656803	6.956166	-0.120494
54C	-1.251241	6.197429	-1.134699

55C	-1.090436	4.811615	-1.157735
56C	1.847716	0.727247	-1.367248
57C	2.821770	0.392082	-2.307177
58C	3.182097	1.305565	-3.301404
59C	2.573407	2.564178	-3.352114
60C	1.600703	2.912108	-2.413316
61C	-0.562866	1.391095	2.336291
62C	-0.186472	0.963537	3.609467
63C	1.166337	0.920363	3.964596
64C	2.145608	1.308887	3.046745
65C	1.780443	1.743036	1.771777
66H	-2.873233	2.937959	0.434573
67H	-4.981642	1.808184	-0.181221
68H	-4.950877	-0.151902	-1.707114
69H	-2.794225	-0.979901	-2.624142
70H	-0.675916	0.123591	-2.010769
71H	0.850141	4.463009	1.639681
72H	0.557738	6.915378	1.665560
73H	-0.787743	8.034915	-0.103237
74H	-1.842978	6.682069	-1.906419
75H	-1.560440	4.228428	-1.944549
76H	1.601766	0.021956	-0.581467
77H	3.309703	-0.576095	-2.248076
78H	3.946187	1.042269	-4.028073
79H	2.861415	3.280815	-4.116405
80H	1.145256	3.896455	-2.454059
81H	-1.613794	1.398633	2.065885
82H	-0.950044	0.648659	4.315554
83H	1.457659	0.569654	4.951111
84H	3.197731	1.250321	3.307755
85H	2.556763	2.008542	1.062242

15g-PhNCO-011

1C	0.299815	-2.229891	1.163617
2C	-1.043664	-2.112842	1.428775
3N	-1.993520	-2.480157	0.530943
4C	-1.609977	-3.021088	-0.659644
5C	-0.284695	-3.189355	-0.970418
6C	0.743741	-2.776414	-0.074870
7N	2.031071	-2.981922	-0.466222
8C	3.060234	-2.314913	0.039737
9N	3.012139	-1.261110	0.866831
10S	4.523030	-0.613289	1.090074
11C	5.398737	-1.823237	0.087015
12C	4.435333	-2.690179	-0.423099
13O	4.939847	-0.691090	2.507299
14O	4.600774	0.731429	0.467947
15C	6.752089	-1.941166	-0.193782
16C	7.137947	-2.997078	-1.031061
17C	6.183774	-3.881438	-1.556341
18C	4.822791	-3.735903	-1.260354
19C	-3.464081	-2.242932	0.890183
20O	-3.635199	-1.786417	2.033666
21N	-4.239717	-2.556703	-0.113282
22C	-5.626916	-2.399359	-0.059891
23C	-6.370703	-1.792427	0.982098
24C	-7.760766	-1.671763	0.885597
25C	-8.453306	-2.145067	-0.233342
26C	-7.729641	-2.749120	-1.270536
27C	-6.344013	-2.870786	-1.184965
28H	1.009216	-1.888270	1.903800
29H	-1.424364	-1.706260	2.355751
30H	-2.420157	-3.294004	-1.321569
31H	-0.011635	-3.625835	-1.925474
32H	7.480877	-1.248648	0.217133
33H	8.188502	-3.129958	-1.275361
34H	6.507218	-4.692164	-2.203828
35H	4.079165	-4.413937	-1.667402
36H	-5.854335	-1.421638	1.858203
37H	-8.306544	-1.201113	1.701361
38H	-9.534586	-2.049080	-0.296362
39H	-8.247791	-3.126797	-2.149678
40H	-5.781530	-3.336881	-1.990884
41P	-0.216205	2.289223	-0.194545
42C	0.362791	1.164389	-1.497945
43C	0.383288	1.782258	1.441884
44C	0.420424	3.953572	-0.538748
45C	-2.029107	2.314649	-0.208734
46C	1.732277	1.996077	1.776245
47C	2.214997	1.569777	3.012447
48C	1.358830	0.941231	3.921691
49C	0.013987	0.742738	3.596630
50C	-0.478535	1.159436	2.358779
51C	0.792882	4.308999	-1.844323
52C	1.233831	5.607464	-2.108424

53C	1.305464	6.548339	-1.076706
54C	0.935337	6.193686	0.225133
55C	0.493161	4.898836	0.498814
56C	-2.731478	1.096795	-0.231444
57C	-4.125432	1.097405	-0.209890
58C	-4.823338	2.308781	-0.168779
59C	-4.127107	3.521016	-0.150329
60C	-2.730332	3.530125	-0.170386
61C	1.657062	0.626521	-1.420089
62C	2.135134	-0.172795	-2.458531
63C	1.332326	-0.439164	-3.570782
64C	0.043886	0.099224	-3.649906
65C	-0.444022	0.905262	-2.619821
66H	2.409253	2.482325	1.081358
67H	3.263140	1.713651	3.254863
68H	1.741887	0.603373	4.880914
69H	-0.656238	0.258516	4.301659
70H	-1.524181	0.997035	2.121284
71H	0.749407	3.580927	-2.648779
72H	1.527548	5.879280	-3.118571
73H	1.653482	7.556611	-1.285331
74H	0.994473	6.922263	1.029116
75H	0.213870	4.627339	1.512869
76H	-2.196247	0.153158	-0.268904
77H	-4.661483	0.154734	-0.223564
78H	-5.910048	2.304219	-0.152537
79H	-4.668222	4.462904	-0.122855
80H	-2.199323	4.476791	-0.159479
81H	2.291855	0.801419	-0.559967
82H	3.132230	-0.595905	-2.386724
83H	1.706996	-1.072032	-4.371000
84H	-0.585215	-0.108379	-4.511271
85H	-1.443960	1.320520	-2.693995

15g-PhNCO-012

1C	0.130737	-2.114288	1.070574
2C	-1.209763	-1.963941	1.338380
3N	-2.172364	-2.493426	0.543621
4C	-1.806566	-3.229082	-0.542545
5C	-0.485828	-3.434686	-0.850748
6C	0.557060	-2.864061	-0.064328
7N	1.835769	-3.130937	-0.449975
8C	2.896240	-2.469671	0.000193
9N	2.906487	-1.352377	0.741220
10S	4.466733	-0.838017	1.016958
11C	5.264438	-2.146579	0.076764
12C	4.249795	-2.964689	-0.412622
13O	4.811206	-0.942278	2.452487
14O	4.701017	0.481960	0.389228
15C	6.611232	-2.380541	-0.160097
16C	6.934465	-3.504272	-0.932990
17C	5.928079	-4.343780	-1.433918
18C	4.576041	-4.082737	-1.180007
19C	-3.636452	-2.191177	0.874080
20O	-3.790704	-1.516267	1.906641
21N	-4.424984	-2.694866	-0.037089
22C	-5.804759	-2.490643	-0.024648
23C	-6.548903	-1.770500	0.942747
24C	-7.933503	-1.625080	0.810178
25C	-8.620954	-2.181629	-0.273432
26C	-7.897666	-2.898025	-1.236641
27C	-6.517755	-3.048618	-1.112906
28H	0.849265	-1.645555	1.727455
29H	-1.577841	-1.402308	2.185800
30H	-2.627350	-3.620248	-1.127366
31H	-0.227569	-4.032829	-1.718590
32H	7.380913	-1.724756	0.236427
33H	7.976989	-3.727637	-1.143120
34H	6.203134	-5.210794	-2.028654
35H	3.793269	-4.728194	-1.565727
36H	-6.034808	-1.332745	1.788876
37H	-8.480184	-1.068284	1.569193
38H	-9.697903	-2.062933	-0.365529
39H	-8.411440	-3.341226	-2.087356
40H	-5.955837	-3.603861	-1.860772
41P	-0.023477	2.466712	-0.193414
42C	0.584742	1.825180	1.389155
43C	-1.501708	1.560956	-0.726717
44C	-0.477534	4.215516	0.003609
45C	1.269973	2.309590	-1.456090
46C	-2.752098	1.872525	-0.163610
47C	-3.884891	1.157006	-0.552401
48C	-3.779320	0.139274	-1.505287
49C	-2.536680	-0.169960	-2.065180
50C	-1.395437	0.533078	-1.677977

51C	0.090729	4.977643	1.036436
52C	-0.228065	6.332334	1.153905
53C	-1.110380	6.928008	0.247680
54C	-1.678884	6.168765	-0.780656
55C	-1.366636	4.814469	-0.905996
56C	2.091192	1.170118	-1.473308
57C	3.040425	1.021892	-2.485933
58C	3.172120	1.997739	-3.477221
59C	2.358483	3.135869	-3.454866
60C	1.408496	3.297657	-2.445915
61C	-0.318906	1.246936	2.295433
62C	0.138326	0.790591	3.531736
63C	1.491584	0.906114	3.865767
64C	2.390161	1.483988	2.964833
65C	1.943129	1.947094	1.727184
66H	-2.844393	2.668156	0.570303
67H	-4.847303	1.386681	-0.104700
68H	-4.661273	-0.420880	-1.797982
69H	-2.451765	-0.968501	-2.796409
70H	-0.435118	0.278073	-2.114808
71H	0.777124	4.522490	1.749760
72H	0.210311	6.917957	1.957240
73H	-1.359056	7.981565	0.344763
74H	-2.369023	6.627497	-1.483396
75H	-1.818781	4.230174	-1.702213
76H	2.020680	0.414270	-0.697504
77H	3.687448	0.150376	-2.486393
78H	3.916201	1.878232	-4.260448
79H	2.467300	3.902274	-4.217522
80H	0.788837	4.188611	-2.431682
81H	-1.367426	1.134656	2.039972
82H	-0.561422	0.332207	4.225203
83H	1.849049	0.532100	4.821420
84H	3.445436	1.549388	3.209181
85H	2.657886	2.367253	1.027488

15g-001

1C	0.943007	2.854131	1.100504
2C	-0.027240	3.815874	1.379057
3N	-0.468079	4.741362	0.508271
4C	0.105041	4.716903	-0.711897
5C	1.083841	3.809394	-1.093362
6C	1.542101	2.823517	-0.184647
7N	2.509177	1.956466	-0.660602
8C	2.956252	0.908874	-0.002361
9N	2.588568	0.458445	1.219940
10S	3.367616	-0.946701	1.594269
11C	4.311074	-1.066472	0.069148
12C	3.978391	0.050477	-0.690984
13O	2.406052	-2.074307	1.706281
14O	4.271981	-0.780886	2.758180
15C	5.209900	-2.036152	-0.354676
16C	5.801132	-1.851416	-1.611339
17C	5.485620	-0.727570	-2.391476
18C	4.570879	0.230929	-1.940708
19H	1.226697	2.138697	1.859206
20H	-0.487304	3.834621	2.365755
21H	-0.245733	5.466605	-1.419837
22H	1.506586	3.843553	-2.094043
23H	5.446815	-2.898835	0.261683
24H	6.513736	-2.583408	-1.982481
25H	5.960117	-0.601468	-3.361443
26H	4.316589	1.098281	-2.541691
27P	-2.093478	-0.566790	-0.125689
28C	-2.998205	0.783944	-0.930570
29C	-3.158059	-2.035073	-0.019514
30C	-0.636180	-1.012240	-1.107367
31C	-1.637228	-0.027110	1.542431
32C	-3.291659	-2.870545	-1.141821
33C	-4.141776	-3.975657	-1.086332
34C	-4.857069	-4.252232	0.083967
35C	-4.721208	-3.423394	1.201625
36C	-3.872470	-2.315068	1.155391
37C	-0.167420	-0.162106	-2.121140
38C	0.965688	-0.520324	-2.852443
39C	1.631557	-1.717214	-2.575727
40C	1.164516	-2.564596	-1.566600
41C	0.031403	-2.218643	-0.831968
42C	-2.522476	0.791803	2.267832
43C	-2.203281	1.164482	3.573069
44C	-1.007905	0.725538	4.155814
45C	-0.128940	-0.081520	3.430364
46C	-0.437406	-0.460977	2.122447
47C	-4.170049	0.533588	-1.661635
48C	-4.830402	1.592161	-2.289766

49C	-4.327887	2.893212	-2.188600
50C	-3.161172	3.141812	-1.457874
51C	-2.493450	2.092079	-0.827365
52H	-2.731502	-2.665529	-2.049794
53H	-4.240173	-4.621627	-1.954487
54H	-5.515317	-5.116094	0.125714
55H	-5.268923	-3.641502	2.114370
56H	-3.765346	-1.683209	2.031703
57H	-0.669456	0.774470	-2.338921
58H	1.336986	0.147771	-3.623909
59H	2.524155	-1.982166	-3.134952
60H	1.691315	-3.486058	-1.337301
61H	-0.324377	-2.881830	-0.048928
62H	-3.445026	1.146840	1.817604
63H	-2.882685	1.804076	4.130003
64H	-0.757547	1.025063	5.170205
65H	0.811097	-0.405944	3.866376
66H	0.275316	-1.064655	1.573586
67H	-4.571859	-0.471847	-1.738466
68H	-5.739750	1.398557	-2.852343
69H	-4.847590	3.714511	-2.675114
70H	-2.768931	4.150066	-1.367139
71H	-1.593045	2.295287	-0.256125

15g-002

1C	-2.988145	3.121176	-0.544864
2C	-2.809986	4.470706	-0.838162
3N	-2.086005	5.329538	-0.097358
4C	-1.527538	4.816433	1.015494
5C	-1.656680	3.490931	1.411531
6C	-2.391810	2.579635	0.618526
7N	-2.490188	1.277011	1.082610
8C	-2.780395	0.249744	0.313593
9N	-2.933766	0.228358	-1.029731
10S	-3.168699	-1.308036	-1.577669
11C	-3.170492	-2.097510	0.039324
12C	-2.922756	-1.094047	0.971403
13O	-2.010704	-1.781387	-2.378583
14O	-4.489952	-1.457024	-2.234682
15C	-3.371139	-3.425576	0.388014
16C	-3.311022	-3.744093	1.750795
17C	-3.049002	-2.750650	2.706816
18C	-2.851449	-1.417596	2.326742
19H	-3.567462	2.495091	-1.210563
20H	-3.268654	4.886899	-1.734272
21H	-0.945669	5.509550	1.621881
22H	-1.186040	3.143955	2.326481
23H	-3.564555	-4.186033	-0.362947
24H	-3.467326	-4.771714	2.068879
25H	-3.005243	-3.020119	3.759107
26H	-2.657338	-0.642963	3.061984
27P	2.050792	-0.151775	-0.056113
28C	1.156783	1.065059	-1.053823
29C	1.376479	-1.818002	-0.290858
30C	3.800500	-0.204601	-0.553477
31C	1.937955	0.326305	1.691835
32C	1.633779	-2.493606	-1.497349
33C	1.121575	-3.775007	-1.694657
34C	0.363344	-4.388481	-0.691838
35C	0.116157	-3.720528	0.509485
36C	0.616731	-2.433633	0.714279
37C	4.399624	0.889743	-1.195931
38C	5.756399	0.843022	-1.524723
39C	6.516243	-0.289398	-1.217249
40C	5.919098	-1.382736	-0.580785
41C	4.564363	-1.344995	-0.248466
42C	0.702435	0.767844	2.195398
43C	0.587131	1.094454	3.547065
44C	1.694341	0.991309	4.394979
45C	2.925002	0.557967	3.890949
46C	3.051910	0.223865	2.540878
47C	0.334769	0.661300	-2.116878
48C	-0.287564	1.628310	-2.908493
49C	-0.099352	2.985603	-2.641917
50C	0.701390	3.388091	-1.567270
51C	1.328457	2.433311	-0.769193
52H	2.230902	-2.025395	-2.275027
53H	1.311430	-4.291224	-2.631525
54H	-0.037677	-5.386204	-0.849656
55H	-0.476856	-4.190883	1.286782
56H	0.412809	-1.922978	1.649433
57H	3.818031	1.770519	-1.448545
58H	6.215346	1.690376	-2.026649
59H	7.570764	-0.323016	-1.478263
60H	6.504770	-2.267290	-0.345588

61H	4.106629	-2.200418	0.239774
62H	-0.171325	0.859971	1.555676
63H	-0.371771	1.432499	3.930017
64H	1.599966	1.252484	5.445822
65H	3.789073	0.483574	4.545566
66H	4.012847	-0.106236	2.158589
67H	0.134653	-0.386825	-2.310235
68H	-0.946662	1.311579	-3.711151
69H	-0.600655	3.733111	-3.250182
70H	0.817344	4.442956	-1.336934
71H	1.932098	2.750774	0.076400

15g-003

1C	0.947182	2.907583	1.016962
2C	0.106040	3.975776	1.323824
3N	-0.148725	5.013774	0.508240
4C	0.474262	4.986474	-0.686804
5C	1.321144	3.967182	-1.099418
6C	1.590857	2.871824	-0.244947
7N	2.423232	1.887957	-0.753325
8C	2.878755	0.867656	-0.059532
9N	2.662352	0.562864	1.241820
10S	3.423191	-0.841163	1.658734
11C	4.132167	-1.172484	0.041029
12C	3.741434	-0.124304	-0.786403
13O	2.434874	-1.891013	2.016621
14O	4.490936	-0.615396	2.662314
15C	4.908906	-2.237490	-0.394420
16C	5.304570	-2.230279	-1.738239
17C	4.924423	-1.180974	-2.590207
18C	4.140444	-0.119199	-2.123369
19H	1.099749	2.116339	1.736859
20H	-0.395563	3.995373	2.290508
21H	0.271711	5.825949	-1.350419
22H	1.782196	3.997745	-2.083041
23H	5.194645	-3.043159	0.275849
24H	5.913847	-3.043965	-2.122904
25H	5.244721	-1.194322	-3.628831
26H	3.840101	0.693702	-2.776962
27P	-2.052163	-0.555835	-0.106937
28C	-1.965383	0.827134	-1.278380
29C	-1.672496	-0.018020	1.580534
30C	-3.746553	-1.218240	-0.100123
31C	-0.892743	-1.847103	-0.636846
32C	-2.621384	0.736348	2.297151
33C	-2.321962	1.174662	3.585747
34C	-1.086766	0.857543	4.166049
35C	-0.152597	0.100048	3.457261
36C	-0.439187	-0.340750	2.162800
37C	-4.601304	-1.010303	-1.193653
38C	-5.884991	-1.560721	-1.184806
39C	-6.318253	-2.316809	-0.091510
40C	-5.468850	-2.520561	1.001170
41C	-4.185774	-1.971658	1.002576
42C	0.361222	-1.488170	-1.161566
43C	1.261049	-2.485466	-1.538696
44C	0.924508	-3.833035	-1.384174
45C	-0.319892	-4.190161	-0.857386
46C	-1.232101	-3.201581	-0.485196
47C	-2.164280	2.144305	-0.836307
48C	-2.187940	3.188563	-1.761811
49C	-2.003404	2.926714	-3.122024
50C	-1.791632	1.616411	-3.562333
51C	-1.774890	0.564061	-2.646261
52H	-3.587466	0.972722	1.859943
53H	-3.052695	1.760259	4.137035
54H	-0.856508	1.201216	5.171094
55H	0.808563	-0.147657	3.897078
56H	0.306371	-0.922789	1.633995
57H	-4.277994	-0.418306	-2.044278
58H	-6.545919	-1.392678	-2.030716
59H	-7.318644	-2.741465	-0.087412
60H	-5.804125	-3.102295	1.855469
61H	-3.535221	-2.125452	1.858720
62H	0.638306	-0.444699	-1.277115
63H	2.228591	-2.207403	-1.942394
64H	1.634320	-4.603709	-1.672899
65H	-0.584960	-5.236984	-0.736891
66H	-2.199140	-3.490565	-0.086056
67H	-2.281508	2.366429	0.218264
68H	-2.329234	4.206168	-1.412183
69H	-2.010891	3.744676	-3.837695
70H	-1.636027	1.410554	-4.617870
71H	-1.607821	-0.450291	-2.995605

15g-004

1C	1.195299	2.763083	1.376611
2C	0.162146	3.632544	1.718912
3N	-0.433943	4.488830	0.870755
4C	0.037006	4.487916	-0.391436
5C	1.070119	3.672102	-0.836578
6C	1.689023	2.758592	0.049414
7N	2.718449	1.986771	-0.464811
8C	3.128367	0.863561	0.081699
9N	2.620083	0.226100	1.162561
10S	3.344504	-1.237331	1.390039
11C	4.490676	-1.105398	0.010622
12C	4.242177	0.121359	-0.598627
13O	2.384587	-2.348187	1.169391
14O	4.078063	-1.288031	2.678837
15C	5.451678	-1.998980	-0.442398
16C	6.195343	-1.619983	-1.567471
17C	5.962308	-0.386834	-2.196533
18C	4.984099	0.493837	-1.719916
19H	1.606365	2.094350	2.120060
20H	-0.217478	3.631334	2.740027
21H	-0.444952	5.177824	-1.082485
22H	1.408129	3.724094	-1.868387
23H	5.620669	-2.950117	0.054517
24H	6.960591	-2.287675	-1.954642
25H	6.552087	-0.112483	-3.067492
26H	4.796142	1.446957	-2.204522
27P	-2.212031	-0.493722	-0.166408
28C	-2.732642	1.098099	-0.866337
29C	-1.801380	-0.316999	1.587383
30C	-3.569991	-1.697383	-0.295114
31C	-0.781080	-1.084079	-1.111542
32C	-2.836688	-0.177663	2.531449
33C	-2.520370	-0.012475	3.878870
34C	-1.180297	0.006631	4.288602
35C	-0.157291	-0.138024	3.349682
36C	-0.462016	-0.299189	1.995983
37C	-4.591262	-1.533545	-1.243209
38C	-5.595054	-2.498446	-1.354417
39C	-5.584210	-3.623020	-0.523827
40C	-4.568959	-3.784839	0.424810
41C	-3.562552	-2.825431	0.544276
42C	0.173466	-0.156415	-1.560994
43C	1.289296	-0.601323	-2.269016
44C	1.464252	-1.964888	-2.519446
45C	0.517119	-2.888695	-2.067854
46C	-0.607381	-2.454320	-1.364767
47C	-3.082599	2.170328	-0.032814
48C	-3.511922	3.374113	-0.596104
49C	-3.591399	3.512470	-1.983693
50C	-3.232776	2.446865	-2.817121
51C	-2.800883	1.241785	-2.264509
52H	-3.877510	-0.204242	2.220380
53H	-3.317880	0.095961	4.609060
54H	-0.937993	0.130892	5.340969
55H	0.884364	-0.123904	3.657026
56H	0.352143	-0.399506	1.287796
57H	-4.614451	-0.661155	-1.888187
58H	-6.386630	-2.366414	-2.086978
59H	-6.368428	-4.370436	-0.611873
60H	-4.560359	-4.654887	1.075631
61H	-2.781112	-2.953464	1.287763
62H	0.057173	0.903398	-1.357633
63H	2.028444	0.120055	-2.600857
64H	2.343993	-2.307280	-3.057915
65H	0.654664	-3.949983	-2.255553
66H	-1.337548	-3.180131	-1.021147
67H	-3.004894	2.084199	1.045777
68H	-3.760849	4.207822	0.053530
69H	-3.918850	4.453741	-2.417140
70H	-3.280571	2.555281	-3.897218
71H	-2.509914	0.424570	-2.917902

15g-005

1C	-1.480369	3.118538	-0.419628
2C	-0.736547	4.285842	-0.582790
3N	0.106341	4.796459	0.332322
4C	0.215891	4.099566	1.481399
5C	-0.469049	2.920550	1.744602
6C	-1.362184	2.382089	0.786062
7N	-1.966989	1.182476	1.112463
8C	-2.950810	0.636461	0.430460

9N	-3.605666	1.124870	-0.648441
10S	-4.780580	0.080088	-1.155372
11C	-4.449792	-1.196446	0.067633
12C	-3.423590	-0.717749	0.875634
13O	-4.495589	-0.425065	-2.522205
14O	-6.139293	0.641624	-0.961994
15C	-5.040113	-2.440520	0.244886
16C	-4.558253	-3.231718	1.295696
17C	-3.527069	-2.765829	2.126816
18C	-2.951810	-1.506020	1.925417
19H	-2.142232	2.784279	-1.207077
20H	-0.823607	4.845623	-1.513279
21H	0.900336	4.506452	2.224437
22H	-0.318163	2.394835	2.682426
23H	-5.840073	-2.786687	-0.403502
24H	-4.991271	-4.213305	1.469939
25H	-3.172566	-3.394760	2.939711
26H	-2.154324	-1.138589	2.563191
27P	2.240535	-0.494002	-0.158899
28C	3.479415	-1.823252	-0.231757
29C	1.992361	0.012832	1.565744
30C	2.826998	0.941905	-1.098672
31C	0.695487	-1.123105	-0.862657
32C	2.910441	0.889271	2.171443
33C	2.746222	1.244816	3.510118
34C	1.671985	0.731960	4.246018
35C	0.755519	-0.131288	3.640352
36C	0.909356	-0.491274	2.300537
37C	3.817471	0.799570	-2.083815
38C	4.218728	1.913550	-2.823852
39C	3.638999	3.163556	-2.583592
40C	2.654649	3.305365	-1.600289
41C	2.245618	2.198378	-0.856030
42C	0.277968	-2.429706	-0.549697
43C	-0.932722	-2.905848	-1.051996
44C	-1.725934	-2.087040	-1.862349
45C	-1.309238	-0.791007	-2.175462
46C	-0.100443	-0.303544	-1.677929
47C	4.408238	-1.991750	0.807052
48C	5.383621	-2.986787	0.710302
49C	5.434599	-3.814820	-0.414926
50C	4.507345	-3.650215	-1.449361
51C	3.529791	-2.658241	-1.362080
52H	3.740218	1.300489	1.603483
53H	3.452143	1.927820	3.974469
54H	1.542403	1.017599	5.286574
55H	-0.094835	-0.508380	4.201445
56H	0.174704	-1.135642	1.830394
57H	4.278231	-0.164593	-2.274369
58H	4.987229	1.803716	-3.584165
59H	3.956277	4.028235	-3.160617
60H	2.200633	4.271517	-1.402166
61H	1.483653	2.316969	-0.092662
62H	0.892373	-3.070254	0.076647
63H	-1.260729	-3.910712	-0.800685
64H	-2.678970	-2.444505	-2.238835
65H	-1.944541	-0.153601	-2.779687
66H	0.206195	0.708925	-1.919423
67H	4.373553	-1.360081	1.689052
68H	6.098832	-3.116585	1.517920
69H	6.192736	-4.590526	-0.484302
70H	4.540067	-4.295017	-2.323279
71H	2.809557	-2.542233	-2.166740

15g-006

1C	1.040991	2.703705	1.338041
2C	0.057358	3.624919	1.693338
3N	-0.400219	4.607411	0.898412
4C	0.162068	4.681048	-0.324251
5C	1.151444	3.819473	-0.779494
6C	1.632110	2.778698	0.051759
7N	2.626039	1.972999	-0.480341
8C	3.051465	0.861967	0.081919
9N	2.604779	0.269144	1.212973
10S	3.341310	-1.185586	1.457351
11C	4.407379	-1.112858	0.011978
12C	4.129327	0.092233	-0.627116
13O	2.361742	-2.295749	1.337666
14O	4.146735	-1.190779	2.702839
15C	5.339124	-2.027635	-0.459657
16C	6.022367	-1.693311	-1.635932
17C	5.761122	-0.481340	-2.294533
18C	4.812779	0.420823	-1.798218
19H	1.342745	1.939476	2.039560
20H	-0.396662	3.560516	2.681725

21H	-0.207129	5.473573	-0.973484
22H	1.566476	3.935544	-1.777285
23H	5.530777	-2.961611	0.061031
24H	6.762688	-2.378881	-2.039901
25H	6.304964	-0.240910	-3.204563
26H	4.601492	1.356382	-2.306661
27P	-2.174806	-0.500497	-0.174720
28C	-2.514961	1.070116	-1.019294
29C	-1.764764	-0.238081	1.567842
30C	-3.647947	-1.568123	-0.227372
31C	-0.798707	-1.301708	-1.041531
32C	-2.765237	0.198181	2.457640
33C	-2.446578	0.414849	3.796752
34C	-1.140846	0.188025	4.253193
35C	-0.155508	-0.257077	3.370608
36C	-0.461956	-0.472474	2.024492
37C	-4.642897	-1.393372	-1.201435
38C	-5.740126	-2.256872	-1.233993
39C	-5.848740	-3.292439	-0.300907
40C	-4.859750	-3.464763	0.673246
41C	-3.761157	-2.605175	0.715143
42C	0.257881	-0.509175	-1.521898
43C	1.328892	-1.113621	-2.178654
44C	1.361250	-2.501438	-2.342215
45C	0.315189	-3.290336	-1.855509
46C	-0.769110	-2.695341	-1.208010
47C	-2.758715	2.247889	-0.298834
48C	-3.050994	3.429702	-0.983455
49C	-3.099239	3.441415	-2.379120
50C	-2.841967	2.269849	-3.100234
51C	-2.546860	1.085515	-2.426462
52H	-3.781917	0.361136	2.109773
53H	-3.215511	0.756831	4.484204
54H	-0.896183	0.357729	5.298598
55H	0.859098	-0.431399	3.716073
56H	0.318709	-0.811220	1.354572
57H	-4.575806	-0.587171	-1.924919
58H	-6.511295	-2.115024	-1.986234
59H	-6.705302	-3.960840	-0.328796
60H	-4.943067	-4.264257	1.404318
61H	-3.001789	-2.737750	1.480699
62H	0.253575	0.567622	-1.385049
63H	2.142829	-0.498486	-2.547119
64H	2.206057	-2.967028	-2.842728
65H	0.340250	-4.369724	-1.977063
66H	-1.579399	-3.316495	-0.838970
67H	-2.697629	2.263110	0.783492
68H	-3.215856	4.342887	-0.420052
69H	-3.319441	4.365759	-2.906792
70H	-2.861427	2.278642	-4.186690
71H	-2.330242	0.184158	-2.992856

15g-007

1C	1.393582	2.988967	1.192809
2C	0.477257	3.978518	1.541112
3N	-0.181470	4.757153	0.664391
4C	0.099554	4.544217	-0.635845
5C	1.005909	3.595511	-1.092590
6C	1.692404	2.767079	-0.174052
7N	2.619282	1.880590	-0.695105
8C	3.051613	0.817199	-0.056307
9N	2.626411	0.326327	1.132708
10S	3.383877	-1.090968	1.498431
11C	4.420125	-1.145337	0.029000
12C	4.108388	-0.015216	-0.720793
13O	2.436290	-2.234946	1.500974
14O	4.210714	-0.962816	2.723686
15C	5.349961	-2.093748	-0.376173
16C	5.994430	-1.872480	-1.600444
17C	5.698228	-0.735992	-2.369824
18C	4.752769	0.201540	-1.938624
19H	1.873045	2.400863	1.964029
20H	0.254150	4.152068	2.593294
21H	-0.435113	5.170160	-1.348861
22H	1.197135	3.480850	-2.156241
23H	5.569547	-2.968464	0.229582
24H	6.732471	-2.586951	-1.955664
25H	6.212144	-0.583155	-3.315528
26H	4.513700	1.079070	-2.531249
27P	-2.203711	-0.521843	-0.114049
28C	-1.717497	-0.554239	1.631811
29C	-3.407973	-1.847122	-0.430359
30C	-2.988309	1.065430	-0.514051
31C	-0.742722	-0.759282	-1.159590
32C	-4.757460	-1.662257	-0.080884

33C	-5.672637	-2.698198	-0.272045
34C	-5.248970	-3.918602	-0.809018
35C	-3.908010	-4.102845	-1.158073
36C	-2.984896	-3.071475	-0.971014
37C	-2.635908	2.216039	0.207144
38C	-3.205389	3.445443	-0.130372
39C	-4.118842	3.530476	-1.184475
40C	-4.462004	2.385417	-1.912166
41C	-3.899631	1.152022	-1.581916
42C	0.258560	-1.665477	-0.771643
43C	1.345623	-1.894113	-1.614676
44C	1.443663	-1.220863	-2.834953
45C	0.455974	-0.306779	-3.213808
46C	-0.638329	-0.072188	-2.381056
47C	-2.590721	-1.072527	2.604162
48C	-2.220096	-1.042193	3.948790
49C	-0.983114	-0.506614	4.326597
50C	-0.113634	-0.000952	3.357300
51C	-0.477306	-0.017748	2.010362
52H	-5.095953	-0.716782	0.332543
53H	-6.714781	-2.550389	-0.002232
54H	-5.964265	-4.723203	-0.957697
55H	-3.576387	-5.048275	-1.578417
56H	-1.947005	-3.223835	-1.250117
57H	-1.918763	2.166160	1.020692
58H	-2.915937	4.332521	0.424021
59H	-4.560273	4.489591	-1.442675
60H	-5.168404	2.449898	-2.735445
61H	-4.172272	0.266729	-2.149243
62H	0.221536	-2.167952	0.188630
63H	2.126904	-2.576273	-1.296328
64H	2.302748	-1.390152	-3.477952
65H	0.543390	0.237392	-4.150145
66H	-1.391128	0.651594	-2.677300
67H	-3.545375	-1.505510	2.322628
68H	-2.893404	-1.447488	4.699356
69H	-0.694055	-0.495983	5.374293
70H	0.858637	0.395355	3.635230
71H	0.228205	0.359234	1.279380

15g-008

1C	3.845024	2.811897	0.795396
2C	3.675504	4.149311	1.139675
3N	3.049903	5.060388	0.369561
4C	2.590714	4.617280	-0.814481
5C	2.723191	3.306518	-1.263883
6C	3.351208	2.348087	-0.443496
7N	3.516267	1.052855	-0.915923
8C	3.230813	0.015361	-0.172063
9N	2.639627	0.026321	1.051272
10S	2.327624	-1.500097	1.569675
11C	3.034145	-2.345621	0.145115
12C	3.498631	-1.355896	-0.715353
13O	0.864371	-1.744304	1.656085
14O	3.088769	-1.840401	2.798245
15C	3.146149	-3.702094	-0.129216
16C	3.766633	-4.061044	-1.332904
17C	4.247752	-3.077684	-2.211331
18C	4.115872	-1.716883	-1.912595
19H	4.343104	2.130061	1.476315
20H	4.053590	4.511774	2.094562
21H	2.085877	5.354508	-1.437351
22H	2.333053	3.012654	-2.234777
23H	2.772148	-4.453315	0.560617
24H	3.879136	-5.112144	-1.586125
25H	4.729289	-3.379115	-3.138173
26H	4.479039	-0.950988	-2.591160
27P	-2.274018	0.013074	-0.061238
28C	-2.672878	-1.113451	1.305257
29C	-1.628569	1.589115	0.557176
30C	-1.034703	-0.732083	-1.153052
31C	-3.804008	0.313159	-0.996553
32C	-0.302525	1.635978	1.019670
33C	0.213804	2.836279	1.506744
34C	-0.578596	3.987705	1.526770
35C	-1.896695	3.941042	1.060917
36C	-2.427041	2.744800	0.573093
37C	-0.865170	-2.123979	-1.185985
38C	0.047435	-2.686430	-2.079107
39C	0.794631	-1.867163	-2.929693
40C	0.638568	-0.478370	-2.884607
41C	-0.276003	0.093581	-2.000738
42C	-4.996080	0.575550	-0.298147
43C	-6.167983	0.849798	-1.003645
44C	-6.158096	0.861654	-2.402892

45C	-4.974450	0.597667	-3.097737
46C	-3.795745	0.322952	-2.399664
47C	-2.010392	-0.996479	2.535932
48C	-2.295496	-1.899109	3.561949
49C	-3.232498	-2.916678	3.364371
50C	-3.890903	-3.036745	2.135307
51C	-3.615912	-2.138005	1.104542
52H	0.337479	0.759141	0.991719
53H	1.243380	2.867327	1.847059
54H	-0.162767	4.922865	1.892218
55H	-2.511361	4.837255	1.065357
56H	-3.446347	2.723072	0.201367
57H	-1.416543	-2.766252	-0.507390
58H	0.190393	-3.763024	-2.092675
59H	1.518000	-2.308881	-3.608202
60H	1.242979	0.162040	-3.520203
61H	-0.378806	1.173898	-1.958773
62H	-5.012998	0.561774	0.788113
63H	-7.087254	1.050912	-0.460255
64H	-7.073367	1.072285	-2.949943
65H	-4.965362	0.600327	-4.184325
66H	-2.882962	0.113687	-2.948609
67H	-1.268193	-0.223725	2.696415
68H	-1.774629	-1.808811	4.510900
69H	-3.448874	-3.618114	4.165938
70H	-4.619271	-3.827772	1.978566
71H	-4.134141	-2.235464	0.154963

15g-009

1C	0.977221	2.513663	1.150267
2C	-0.014585	3.444706	1.455810
3N	-0.239319	4.583821	0.779887
4C	0.577576	4.812937	-0.267722
5C	1.600797	3.958950	-0.657535
6C	1.842290	2.757659	0.053588
7N	2.898053	1.981798	-0.396354
8C	3.199335	0.792215	0.078437
9N	2.545004	0.074960	1.021571
10S	3.241734	-1.406541	1.235216
11C	4.560280	-1.179538	0.034194
12C	4.387227	0.088358	-0.514197
13O	2.334274	-2.498862	0.801535
14O	3.791209	-1.556811	2.604772
15C	5.578827	-2.042055	-0.348154
16C	6.462520	-1.587035	-1.335360
17C	6.306897	-0.312185	-1.901874
18C	5.269404	0.536590	-1.497994
19H	1.080991	1.620452	1.750108
20H	-0.674390	3.255476	2.300590
21H	0.399299	5.734557	-0.820231
22H	2.231446	4.206315	-1.507531
23H	5.686977	-3.026022	0.099224
24H	7.276658	-2.227989	-1.663554
25H	7.004874	0.021422	-2.665476
26H	5.144859	1.523718	-1.932085
27P	-2.269024	-0.478459	-0.161943
28C	-3.708930	-1.586791	-0.130237
29C	-1.485685	-0.453912	1.472636
30C	-1.082683	-1.060843	-1.403029
31C	-2.854983	1.182926	-0.599170
32C	-0.530473	-1.427840	1.806452
33C	0.043397	-1.423534	3.078384
34C	-0.333217	-0.459078	4.016148
35C	-1.284154	0.511544	3.682946
36C	-1.860296	0.520703	2.413019
37C	-1.513977	-1.873369	-2.465800
38C	-0.601539	-2.271522	-3.443423
39C	0.735720	-1.867594	-3.362622
40C	1.163531	-1.066535	-2.301039
41C	0.260063	-0.657848	-1.319444
42C	-4.065807	1.656109	-0.062634
43C	-4.494568	2.950336	-0.358776
44C	-3.723532	3.772548	-1.187564
45C	-2.521634	3.301000	-1.721526
46C	-2.082415	2.008632	-1.430312
47C	-3.790225	-2.610962	0.825788
48C	-4.878985	-3.485760	0.812548
49C	-5.884370	-3.342660	-0.148461
50C	-5.804340	-2.321117	-1.101090
51C	-4.720605	-1.442177	-1.095150
52H	-0.196938	-2.161162	1.080702
53H	0.806196	-2.157093	3.319100
54H	0.128964	-0.450888	4.999653
55H	-1.564815	1.274279	4.404123
56H	-2.577486	1.293117	2.157142

57H	-2.545933	-2.202879	-2.531817
58H	-0.934194	-2.904514	-4.261689
59H	1.445854	-2.187113	-4.120841
60H	2.203930	-0.766840	-2.224138
61H	0.614326	-0.059727	-0.486850
62H	-4.671789	1.020421	0.577075
63H	-5.429474	3.315060	0.057878
64H	-4.057149	4.782017	-1.412610
65H	-1.916076	3.939607	-2.357679
66H	-1.143648	1.657385	-1.845818
67H	-3.016601	-2.725317	1.579015
68H	-4.941094	-4.275232	1.556535
69H	-6.731141	-4.024028	-0.153950
70H	-6.585413	-2.205133	-1.847585
71H	-4.669134	-0.646154	-1.832417

15g-010

1C	0.991454	2.508032	1.180879
2C	-0.039620	3.406194	1.453538
3N	-0.310890	4.510363	0.737270
4C	0.502720	4.741597	-0.312494
5C	1.562446	3.918931	-0.671498
6C	1.845871	2.748296	0.074509
7N	2.917099	1.986595	-0.363020
8C	3.226870	0.799069	0.113916
9N	2.578613	0.078595	1.056467
10S	3.267853	-1.407589	1.249702
11C	4.582685	-1.175649	0.045791
12C	4.413029	0.099197	-0.487225
13O	2.348464	-2.488747	0.809813
14O	3.820179	-1.577694	2.615923
15C	5.596734	-2.037514	-0.349526
16C	6.479775	-1.573834	-1.333373
17C	6.327474	-0.291980	-1.884535
18C	5.293495	0.555360	-1.468672
19H	1.125967	1.636654	1.806750
20H	-0.694361	3.216287	2.301893
21H	0.288973	5.637063	-0.894635
22H	2.184569	4.163946	-1.528381
23H	5.702170	-3.027351	0.085253
24H	7.290756	-2.213827	-1.671092
25H	7.024918	0.048112	-2.645776
26H	5.170972	1.547673	-1.891445
27P	-2.277638	-0.472984	-0.183900
28C	-3.572020	-1.746038	-0.157837
29C	-1.530776	-0.334655	1.461129
30C	-1.004280	-0.921942	-1.394728
31C	-3.049134	1.108696	-0.640220
32C	-0.447035	-1.157677	1.804413
33C	0.090583	-1.087401	3.090415
34C	-0.444673	-0.202185	4.028976
35C	-1.522632	0.621273	3.683822
36C	-2.067993	0.560636	2.401900
37C	-1.245992	-1.913892	-2.359528
38C	-0.267614	-2.202307	-3.312655
39C	0.944975	-1.505726	-3.309266
40C	1.186952	-0.523745	-2.344757
41C	0.221097	-0.234718	-1.381705
42C	-4.344093	1.405221	-0.178333
43C	-4.914166	2.647118	-0.460757
44C	-4.199514	3.595831	-1.199443
45C	-2.913798	3.300777	-1.660112
46C	-2.335397	2.060755	-1.384687
47C	-3.600644	-2.703344	0.867894
48C	-4.573759	-3.705598	0.852656
49C	-5.514865	-3.756025	-0.179431
50C	-5.487966	-2.800798	-1.201899
51C	-4.521429	-1.794945	-1.194383
52H	0.007304	-1.825249	1.080396
53H	0.945641	-1.706574	3.342913
54H	-0.011784	-0.140872	5.023952
55H	-1.929397	1.323157	4.406818
56H	-2.889645	1.219137	2.138855
57H	-2.179290	-2.466904	-2.368822
58H	-0.452246	-2.976261	-4.052663
59H	1.705675	-1.734602	-4.050920
60H	2.128954	0.014682	-2.329554
61H	0.431122	0.503991	-0.617102
62H	-4.906492	0.674726	0.395806
63H	-5.914839	2.872241	-0.102209
64H	-4.644166	4.563994	-1.413679
65H	-2.352906	4.036653	-2.228776
66H	-1.335746	1.849445	-1.748456
67H	-2.874626	-2.671186	1.674488
68H	-4.594290	-4.444037	1.649494

69H	-6.271264	-4.536593	-0.186621
70H	-6.221089	-2.835310	-2.003255
71H	-4.511417	-1.052218	-1.987534

15g-011

1C	2.296773	2.813657	0.540099
2C	2.017036	4.168699	0.696876
3N	2.779141	5.169651	0.220896
4C	3.882447	4.795002	-0.456871
5C	4.248231	3.473245	-0.682676
6C	3.450440	2.418171	-0.179980
7N	3.835483	1.128704	-0.501594
8C	3.358925	0.048707	0.075619
9N	2.512934	-0.043965	1.131240
10S	2.193318	-1.620196	1.499507
11C	3.169893	-2.338644	0.174498
12C	3.767617	-1.277569	-0.498281
13O	0.750558	-1.919693	1.312250
14O	2.742806	-2.005415	2.822947
15C	3.348702	-3.667511	-0.185589
16C	4.175599	-3.923539	-1.286903
17C	4.791396	-2.868476	-1.978872
18C	4.592709	-1.537948	-1.592735
19H	1.634739	2.072521	0.960579
20H	1.123934	4.467979	1.244626
21H	4.503053	5.602843	-0.842065
22H	5.145229	3.238979	-1.250122
23H	2.866453	-4.473416	0.360273
24H	4.343584	-4.949201	-1.605001
25H	5.431439	-3.089951	-2.829193
26H	5.061173	-0.717383	-2.126896
27P	-2.319263	-0.011215	-0.130401
28C	-2.745970	-1.648530	0.525062
29C	-1.975088	1.151565	1.218391
30C	-0.850332	-0.120328	-1.184247
31C	-3.738555	0.584479	-1.098392
32C	-0.729486	1.075434	1.863397
33C	-0.444234	1.941345	2.919458
34C	-1.391474	2.884643	3.329714
35C	-2.628765	2.964591	2.681602
36C	-2.926366	2.101111	1.625302
37C	-0.440531	-1.354824	-1.709367
38C	0.679295	-1.412447	-2.540005
39C	1.389522	-0.247875	-2.844115
40C	0.987125	0.980977	-2.312738
41C	-0.128474	1.049240	-1.479413
42C	-5.038983	0.404181	-0.593947
43C	-6.133884	0.890519	-1.308890
44C	-5.938940	1.555119	-2.524790
45C	-4.646927	1.732906	-3.027454
46C	-3.544540	1.249607	-2.318375
47C	-2.321163	-2.038216	1.803576
48C	-2.622870	-3.319074	2.270194
49C	-3.339772	-4.210253	1.467284
50C	-3.760252	-3.823417	0.189707
51C	-3.466795	-2.545051	-0.284432
52H	0.015084	0.354994	1.543319
53H	0.524045	1.880164	3.408113
54H	-1.162938	3.562156	4.148284
55H	-3.362161	3.703705	2.992469
56H	-3.885865	2.179695	1.123890
57H	-0.966963	-2.268099	-1.453076
58H	1.012735	-2.371938	-2.925265
59H	2.274767	-0.300320	-3.471104
60H	1.556951	1.880950	-2.520681
61H	-0.418370	2.002778	-1.048250
62H	-5.197743	-0.117722	0.345646
63H	-7.137489	0.747862	-0.917622
64H	-6.794147	1.929894	-3.081066
65H	-4.492796	2.244031	-3.973816
66H	-2.546112	1.385231	-2.721893
67H	-1.748902	-1.362729	2.428665
68H	-2.288640	-3.618680	3.259496
69H	-3.570939	-5.206727	1.834863
70H	-4.317116	-4.514441	-0.437325
71H	-3.800840	-2.248670	-1.274554

15g-012

1C	2.251680	2.834900	0.676376
2C	1.904741	4.176452	0.817010
3N	2.551169	5.202539	0.235346
4C	3.607282	4.868820	-0.533689

5C	4.032899	3.563964	-0.749566
6C	3.354104	2.481456	-0.140199
7N	3.795148	1.210500	-0.462046
8C	3.358282	0.106746	0.102836
9N	2.498844	-0.033623	1.141978
10S	2.219023	-1.627359	1.470051
11C	3.257882	-2.288003	0.162281
12C	3.831083	-1.194411	-0.479150
13O	0.793310	-1.968220	1.231464
14O	2.739626	-2.019138	2.803017
15C	3.496155	-3.603314	-0.213479
16C	4.361734	-3.809902	-1.295307
17C	4.954246	-2.721306	-1.954870
18C	4.694098	-1.405566	-1.554748
19H	1.676718	2.071643	1.177718
20H	1.049770	4.442024	1.438128
21H	4.135225	5.696809	-1.004643
22H	4.886111	3.361480	-1.391829
23H	3.031279	-4.435869	0.306824
24H	4.577783	-4.823205	-1.623828
25H	5.624895	-2.904848	-2.790487
26H	5.143707	-0.558898	-2.063724
27P	-2.310735	-0.049203	-0.140376
28C	-2.658676	-1.744433	0.403936
29C	-2.016963	1.038150	1.282453
30C	-0.839996	-0.007624	-1.194526
31C	-3.765929	0.532274	-1.061799
32C	-0.762340	0.978774	1.911639
33C	-0.506807	1.785012	3.021224
34C	-1.491636	2.655857	3.497865
35C	-2.737205	2.721386	2.864212
36C	-3.006392	1.914649	1.756551
37C	-0.300163	-1.189442	-1.722172
38C	0.829375	-1.125592	-2.539921
39C	1.420255	0.107691	-2.826592
40C	0.886595	1.285227	-2.293449
41C	-0.239164	1.232841	-1.473580
42C	-5.046889	0.292791	-0.532029
43C	-6.175059	0.762228	-1.204893
44C	-6.033212	1.465081	-2.406737
45C	-4.761214	1.697100	-2.937126
46C	-3.625327	1.232903	-2.268775
47C	-2.237553	-2.193383	1.663624
48C	-2.488240	-3.513398	2.044057
49C	-3.150694	-4.383159	1.174006
50C	-3.567183	-3.936488	-0.085496
51C	-3.324898	-2.619127	-0.473883
52H	0.012312	0.318402	1.537596
53H	0.466953	1.735241	3.500439
54H	-1.286213	3.288176	4.357737
55H	-3.499702	3.405493	3.226809
56H	-3.972933	1.982698	1.267621
57H	-0.732718	-2.153429	-1.477721
58H	1.262873	-2.042937	-2.928220
59H	2.314274	0.151336	-3.441855
60H	1.363585	2.240301	-2.489578
61H	-0.631444	2.148223	-1.039812
62H	-5.163833	-0.259935	0.396322
63H	-7.162894	0.576140	-0.792292
64H	-6.914117	1.827032	-2.930407
65H	-4.648042	2.235996	-3.873807
66H	-2.642939	1.411612	-2.693991
67H	-1.706136	-1.533278	2.339081
68H	-2.156452	-3.859355	3.018954
69H	-3.342288	-5.409948	1.474927
70H	-4.081637	-4.611206	-0.764365
71H	-3.656329	-2.275889	-1.450074

15-Me2-001

1C	3.207872	0.780184	1.014662
2C	4.485518	0.219986	0.941434
3N	4.908827	-0.533888	-0.083344
4C	4.041196	-0.753346	-1.084745
5C	2.744553	-0.239959	-1.113875
6C	2.323839	0.543693	-0.038264
7N	1.016554	1.147629	-0.029446
8C	-0.071382	0.346590	0.024051
9N	0.104428	-0.957555	0.130124
10S	-1.354818	-1.760508	0.147771
11C	-2.357363	-0.280106	0.027970
12C	-1.499817	0.825563	-0.035427
13O	-1.555500	-2.429360	1.446388
14O	-1.498409	-2.587161	-1.065556
15C	-3.738201	-0.197062	-0.007479
16C	-4.301649	1.080878	-0.110353

17C	-3.476353	2.207073	-0.175243
18C	-2.079723	2.096315	-0.139723
19C	0.972634	2.618336	-0.059534
20H	2.912077	1.378660	1.871215
21H	5.197308	0.383037	1.747625
22H	4.400117	-1.367099	-1.907814
23H	2.080540	-0.452509	-1.944869
24H	-4.356550	-1.088277	0.041673
25H	-5.381422	1.194614	-0.139809
26H	-3.921096	3.194866	-0.255117
27H	-1.492172	3.000731	-0.194634
28H	1.999043	2.983147	-0.049461
29H	0.498531	2.972613	-0.979084
30H	0.456585	3.018346	0.817106

15-Me-001

1C	2.966317	-1.609422	-0.047769
2C	4.296243	-1.285070	-0.044811
3N	4.709285	0.015263	-0.010319
4C	3.779549	1.005741	0.025658
5C	2.429768	0.744794	0.022607
6C	1.951475	-0.603319	-0.011972
7N	0.671184	-1.044561	-0.013672
8C	-0.397625	-0.242598	-0.006760
9N	-0.424027	1.091309	-0.012702
10S	-2.001316	1.652829	-0.010773
11C	-2.773768	0.030824	0.003551
12C	-1.742379	-0.904396	0.004162
13O	-2.285584	2.384230	1.242662
14O	-2.295900	2.366194	-1.272189
15C	-4.116543	-0.316009	0.012613
16C	-4.418423	-1.684808	0.023882
17C	-3.395337	-2.644405	0.025678
18C	-2.047502	-2.265233	0.015535
19C	6.147910	0.321650	0.049742
20H	2.672726	-2.653244	-0.078447
21H	5.080458	-2.033521	-0.069957
22H	4.164705	2.018651	0.055679
23H	1.736795	1.573145	0.045336
24H	-4.899106	0.437084	0.011262
25H	-5.457366	-2.003195	0.031605
26H	-3.654023	-3.699923	0.035040
27H	-1.252261	-3.003809	0.016436
28H	6.301338	1.374050	-0.191919
29H	6.526536	0.116958	1.055558
30H	6.679920	-0.295416	-0.677840

15-Me-002

1C	2.973030	-1.038691	-1.231731
2C	4.202684	-0.608644	-0.821390
3N	4.377372	0.065529	0.356284
4C	3.293733	0.299275	1.151488
5C	2.033883	-0.101457	0.798585
6C	1.799747	-0.794361	-0.440260
7N	0.631108	-1.278947	-0.843201
8C	-0.576859	-0.899026	-0.412953
9N	-1.503718	-1.799044	-0.119566
10S	-2.950285	-1.048974	0.281474
11C	-2.353627	0.631767	0.057254
12C	-1.024377	0.539500	-0.348721
13O	-3.995607	-1.360334	-0.714116
14O	-3.275151	-1.310616	1.698418
15C	-3.029837	1.834836	0.190123
16C	-2.314086	3.002543	-0.107153
17C	-0.981470	2.934483	-0.536592
18C	-0.325392	1.704365	-0.667886
19C	5.731199	0.443936	0.787151
20H	2.876989	-1.569998	-2.172541
21H	5.101091	-0.780402	-1.403977
22H	3.491408	0.819744	2.082175
23H	1.212819	0.100229	1.477265
24H	-4.068747	1.870889	0.504249
25H	-2.802709	3.968507	-0.013762
26H	-0.449420	3.850876	-0.777144
27H	0.700530	1.662699	-1.017572
28H	6.255253	-0.430330	1.186427
29H	6.284404	0.844169	-0.065662
30H	5.663917	1.210867	1.560447

15-PhNCO2-001

1C	0.423876	2.860402	-0.960714
2C	0.120874	4.218237	-1.036591
3N	-0.719289	4.850488	-0.199922
4C	-1.289971	4.103619	0.758743
5C	-1.056669	2.739363	0.925575
6C	-0.177125	2.098185	0.047239
7N	0.050382	0.696735	0.162791
8C	1.300009	0.184220	0.145269
9N	2.355595	0.971408	0.252955
10S	3.767087	0.089743	0.125471
11C	2.959764	-1.498916	-0.071996
12C	1.580480	-1.279136	-0.058050
13O	4.529455	0.164783	1.387227
14O	4.491565	0.450846	-1.110875
15C	3.542021	-2.737523	-0.288862
16C	2.678823	-3.817151	-0.511822
17C	1.292521	-3.621808	-0.531004
18C	0.729244	-2.359897	-0.308058
19C	-1.140827	-0.150824	0.549225
20O	-1.009029	-0.799338	1.604975
21N	-2.099582	-0.012017	-0.337549
22C	-3.344630	-0.623502	-0.177610
23C	-3.760118	-1.453097	0.895178
24C	-5.049595	-1.995253	0.919111
25C	-5.963197	-1.742324	-0.109176
26C	-5.566140	-0.925402	-1.177290
27C	-4.285246	-0.378039	-1.208373
28H	1.110641	2.410344	-1.668184
29H	0.574721	4.828611	-1.814688
30H	-1.969147	4.621199	1.433187
31H	-1.550766	2.193048	1.722341
32H	4.620723	-2.861549	-0.295540
33H	3.089661	-4.808364	-0.683092
34H	0.634435	-4.464798	-0.722148
35H	-0.345509	-2.242754	-0.335324
36H	-3.067534	-1.665062	1.699464
37H	-5.339421	-2.626795	1.757373
38H	-6.962379	-2.170866	-0.081143
39H	-6.259823	-0.712107	-1.988411
40H	-3.979219	0.259677	-2.034677

15-PhNCO2-002

1C	-2.207161	-1.553615	1.653374
2C	-3.262079	-2.428536	1.393814
3N	-3.537972	-2.929734	0.180184
4C	-2.734341	-2.549371	-0.828100
5C	-1.657222	-1.678979	-0.681460
6C	-1.384265	-1.167035	0.591684
7N	-0.348377	-0.212111	0.810070
8C	0.906907	-0.427337	0.374692
9N	1.256727	-1.597139	-0.135024
10S	2.835920	-1.564106	-0.665579
11C	3.144134	0.135107	-0.185037
12C	1.967481	0.640985	0.372830
13O	2.890805	-1.697209	-2.136721
14O	3.660369	-2.506991	0.115857
15C	4.297424	0.881408	-0.364656
16C	4.259390	2.221491	0.039168
17C	3.088972	2.761299	0.585644
18C	1.936872	1.984734	0.758898
19C	-0.691229	0.923930	1.796812
20O	-0.026608	0.900130	2.845644
21N	-1.662962	1.722005	1.446135
22C	-2.226045	1.728446	0.166595
23C	-3.624554	1.601820	0.034856
24C	-4.235008	1.632303	-1.219816
25C	-3.469691	1.806391	-2.380100
26C	-2.083132	1.957651	-2.262234
27C	-1.468288	1.924076	-1.008497
28H	-2.035950	-1.181172	2.658061
29H	-3.915757	-2.741596	2.205463
30H	-2.970677	-2.952783	-1.810521
31H	-1.057286	-1.398109	-1.538212
32H	5.188526	0.445128	-0.806054
33H	5.141301	2.844995	-0.079737
34H	3.068670	3.804776	0.887403
35H	1.053074	2.434549	1.189969
36H	-4.217898	1.457382	0.934596
37H	-5.314460	1.515058	-1.292657
38H	-3.946158	1.828864	-3.357312
39H	-1.473416	2.103358	-3.151988
40H	-0.392112	2.048052	-0.928357

15-PhNCO2-003

1C	3.501016	0.659419	-0.211452
2C	4.786970	0.268396	0.156259
3N	5.154008	-1.003422	0.378457
4C	4.197068	-1.933775	0.219612
5C	2.882610	-1.655756	-0.145802
6C	2.508492	-0.320274	-0.362963
7N	1.205061	0.047629	-0.774213
8C	0.093967	-0.598432	-0.341729
9N	0.112121	-1.365452	0.729492
10S	-1.419861	-1.958366	1.054235
11C	-2.210365	-1.169575	-0.349751
12C	-1.222111	-0.482110	-1.054883
13O	-1.902256	-1.414953	2.336962
14O	-1.452583	-3.427171	0.894833
15C	-3.529552	-1.255862	-0.764058
16C	-3.861392	-0.619807	-1.967202
17C	-2.878877	0.039924	-2.716247
18C	-1.552485	0.111759	-2.275590
19C	1.097447	1.366451	-1.586667
20O	1.717966	1.329800	-2.661680
21N	0.376788	2.331335	-1.084621
22C	-0.219241	2.322686	0.179662
23C	-1.581044	2.682694	0.277379
24C	-2.234257	2.708334	1.510191
25C	-1.545951	2.387014	2.686540
26C	-0.190639	2.051384	2.607597
27C	0.468356	2.028692	1.377057
28H	3.286982	1.709201	-0.377454
29H	5.560941	1.023257	0.280422
30H	4.496605	-2.965759	0.391560
31H	2.171168	-2.465124	-0.249029
32H	-4.270305	-1.800009	-0.185920
33H	-4.885575	-0.654492	-2.328387
34H	-3.146635	0.507137	-3.659835
35H	-0.810386	0.618990	-2.879210
36H	-2.120194	2.917761	-0.636950
37H	-3.289524	2.971224	1.551066
38H	-2.057778	2.391501	3.645710
39H	0.361213	1.796309	3.509802
40H	1.520343	1.764860	1.338038

15-PhNCO2-004

1C	1.816165	1.963408	-1.470663
2C	2.619125	2.998441	-0.993623
3N	2.773275	3.290402	0.308866
4C	2.114888	2.513810	1.185902
5C	1.298445	1.446886	0.818445
6C	1.127380	1.172442	-0.544121
7N	0.347330	0.077692	-0.985862
8C	-0.888784	-0.203405	-0.537136
9N	-1.347848	-1.439654	-0.627680
10S	-2.887992	-1.547499	0.002809
11C	-3.029498	0.193745	0.415576
12C	-1.841299	0.817353	0.029820
13O	-2.868851	-2.385773	1.219161
14O	-3.872511	-1.906137	-1.036472
15C	-4.120470	0.870037	0.937632
16C	-4.006314	2.259268	1.072415
17C	-2.839967	2.916141	0.661307
18C	-1.752897	2.209167	0.133193
19C	1.029748	-0.875562	-2.039262
20O	0.462666	-0.865672	-3.137803
21N	2.138487	-1.445526	-1.660280
22C	2.556193	-1.512369	-0.331425
23C	3.866857	-1.106823	-0.001208
24C	4.334250	-1.183795	1.311253
25C	3.512132	-1.679399	2.332336
26C	2.218321	-2.108771	2.012883
27C	1.745665	-2.034923	0.700685
28H	1.725910	1.775470	-2.535781
29H	3.161379	3.629014	-1.695214
30H	2.260995	2.744713	2.239032
31H	0.822413	0.829980	1.572378
32H	-5.028761	0.344667	1.217583
33H	-4.834785	2.830549	1.482085
34H	-2.774227	3.997248	0.747221
35H	-0.871600	2.746948	-0.192131
36H	4.501057	-0.712378	-0.791789
37H	5.344574	-0.850041	1.540158
38H	3.877606	-1.739832	3.354823
39H	1.569877	-2.510621	2.789456
40H	0.744653	-2.379384	0.458781

15-PhNCO2-005

1C	-2.699780	-1.444073	-0.551009
2C	-3.933690	-1.920162	-0.113463
3N	-4.860813	-1.161308	0.493956
4C	-4.553902	0.136487	0.666551
5C	-3.346874	0.712886	0.280211
6C	-2.375109	-0.097290	-0.325972
7N	-1.144480	0.449597	-0.729492
8C	0.003643	-0.278494	-0.750486
9N	0.891124	-0.092000	-1.700534
10S	2.232312	-1.076126	-1.451657
11C	1.636405	-1.791739	0.083526
12C	0.382283	-1.239012	0.341800
13O	3.446088	-0.275146	-1.215420
14O	2.291597	-2.087668	-2.525161
15C	2.284903	-2.659465	0.948295
16C	1.624486	-2.981621	2.140681
17C	0.377043	-2.416844	2.437780
18C	-0.252359	-1.537901	1.549394
19C	-1.191179	1.830896	-1.452465
20O	-2.060917	1.899953	-2.332965
21N	-0.331153	2.722575	-1.046993
22C	0.472200	2.582371	0.084221
23C	1.866140	2.765580	-0.034754
24C	2.702558	2.681328	1.078454
25C	2.175399	2.422744	2.350520
26C	0.792746	2.254887	2.488297
27C	-0.047743	2.336029	1.375467
28H	-2.010350	-2.107557	-1.063099
29H	-4.194926	-2.964600	-0.272580
30H	-5.314215	0.750101	1.145544
31H	-3.167608	1.769594	0.446008
32H	3.267607	-3.059309	0.716631
33H	2.092860	-3.661040	2.847411
34H	-0.110581	-2.657456	3.378349
35H	-1.207736	-1.096753	1.806705
36H	2.280393	2.946589	-1.022868
37H	3.775771	2.805355	0.949154
38H	2.829410	2.354273	3.216643
39H	0.362285	2.059202	3.468880
40H	-1.119821	2.210825	1.497279

15-PhNCO-001

1C	0.077301	-0.853797	0.013635
2C	-1.265257	-1.161694	0.015315
3N	-2.229780	-0.207716	0.012040
4C	-1.864081	1.105635	0.007882
5C	-0.544254	1.475355	0.006656
6C	0.503910	0.507538	0.008820
7N	1.774107	0.998670	0.006507
8C	2.870725	0.246121	0.002631
9N	2.963721	-1.090254	0.000144
10S	4.559545	-1.573403	-0.006195
11C	5.259147	0.082197	-0.005098
12C	4.186134	0.968438	0.000178
13O	4.889251	-2.280014	-1.264731
14O	4.897475	-2.285339	1.247130
15C	6.584814	0.491445	-0.008415
16C	6.823929	1.872335	-0.006149
17C	5.757125	2.783695	-0.000748
18C	4.428582	2.342102	0.002356
19C	-3.696761	-0.648666	0.012343
20O	-3.853029	-1.881805	0.023870
21N	-4.491083	0.389191	0.000146
22C	-5.880860	0.262931	-0.004157
23C	-6.626221	-0.942685	-0.012201
24C	-8.024427	-0.914703	-0.017475
25C	-8.726631	0.294920	-0.014653
26C	-8.002413	1.494973	-0.007320
27C	-6.609198	1.477227	-0.002433
28H	0.798563	-1.658051	0.015788
29H	-1.631241	-2.180486	0.018906
30H	-2.683678	1.810910	0.005539
31H	-0.286802	2.529567	0.003558
32H	7.401200	-0.224862	-0.012624
33H	7.847091	2.238686	-0.008557
34H	5.966761	3.850213	0.000986
35H	3.598663	3.041510	0.006414
36H	-6.103280	-1.890541	-0.015280
37H	-8.569401	-1.857141	-0.023867
38H	-9.814116	0.304399	-0.018407

39H	-8.526221	2.449009	-0.005388
40H	-6.047968	2.409055	0.003064

15-PhNCO-002

1C	-0.437293	-1.631708	-0.969680
2C	-1.709405	-1.207068	-0.695566
3N	-1.975008	-0.344004	0.329436
4C	-0.946898	0.089881	1.109637
5C	0.349011	-0.295832	0.886912
6C	0.677036	-1.170738	-0.199487
7N	1.904499	-1.630833	-0.467254
8C	3.052680	-1.021491	-0.192761
9N	4.115295	-1.718333	0.210490
10S	5.447066	-0.729105	0.378819
11C	4.621779	0.786666	-0.120911
12C	3.305048	0.450348	-0.426488
13O	6.500824	-1.079068	-0.599237
14O	5.864016	-0.666068	1.796808
15C	5.139797	2.064822	-0.268676
16C	4.271995	3.051255	-0.755075
17C	2.949169	2.733247	-1.093025
18C	2.455000	1.432479	-0.939022
19C	-3.380027	0.159638	0.630025
20O	-3.435069	0.980419	1.564454
21N	-4.255564	-0.383378	-0.176598
22C	-5.617087	-0.085472	-0.106802
23C	-6.438123	-0.724644	-1.067414
24C	-7.815569	-0.517447	-1.107240
25C	-8.431194	0.338738	-0.183821
26C	-7.636915	0.978163	0.773536
27C	-6.253667	0.777534	0.820558
28H	-0.267413	-2.317743	-1.793088
29H	-2.574826	-1.516865	-1.264833
30H	-1.233184	0.757062	1.912501
31H	1.126472	0.067895	1.549746
32H	6.174169	2.289018	-0.025063
33H	4.632420	4.068382	-0.883102
34H	2.295544	3.507258	-1.486016
35H	1.434291	1.199879	-1.220710
36H	-5.962464	-1.391015	-1.783545
37H	-8.412589	-1.026985	-1.861198
38H	-9.505972	0.502515	-0.211251
39H	-8.096991	1.646568	1.499451
40H	-5.657262	1.283056	1.569078

15-PhNCO-003

1C	-1.217893	0.617933	-1.323667
2C	-2.478909	0.077275	-1.334501
3N	-2.719654	-1.157440	-0.819796
4C	-1.695900	-1.875341	-0.299558
5C	-0.413098	-1.379146	-0.231208
6C	-0.116243	-0.082658	-0.751569
7N	1.089388	0.548663	-0.802148
8C	2.203688	0.085146	-0.244140
9N	2.359123	-1.004737	0.519092
10S	3.950254	-1.179826	0.984737
11C	4.558157	0.284245	0.138240
12C	3.460670	0.867712	-0.487638
13O	4.535335	-2.405400	0.395193
14O	4.090247	-1.032679	2.451325
15C	5.840938	0.808599	0.070456
16C	6.008176	1.985773	-0.671289
17C	4.915239	2.591726	-1.309306
18C	3.631497	2.039272	-1.225002
19C	-4.134536	-1.794199	-0.864211
20O	-4.110300	-2.965174	-1.267945
21N	-5.142292	-1.035972	-0.534468
22C	-5.057470	0.137561	0.212354
23C	-5.863444	1.236443	-0.157809
24C	-5.852179	2.420448	0.580952
25C	-5.045237	2.543663	1.719651
26C	-4.257933	1.454559	2.111478
27C	-4.265743	0.266847	1.377205
28H	-1.053406	1.599783	-1.754906
29H	-3.331446	0.596953	-1.752504
30H	-1.955800	-2.863718	0.060839
31H	0.363426	-1.984608	0.213824
32H	6.678115	0.329725	0.569804
33H	6.995449	2.433101	-0.750826
34H	5.068639	3.505062	-1.878250
35H	2.781909	2.503251	-1.715671
36H	-6.492200	1.142456	-1.040321

37H	-6.478381	3.252739	0.265510
38H	-5.036847	3.466435	2.294429
39H	-3.633061	1.526081	2.999501
40H	-3.657352	-0.572759	1.702809

15-PhNCO-004

1C	0.964473	-2.598499	-1.126599
2C	2.308732	-2.469077	-0.893981
3N	2.786737	-1.710035	0.128690
4C	1.913958	-1.119099	0.988137
5C	0.557279	-1.226224	0.826785
6C	0.011069	-1.936680	-0.290933
7N	-1.296608	-2.092445	-0.532941
8C	-2.270211	-1.250362	-0.210416
9N	-3.472717	-1.714888	0.135575
10S	-4.547762	-0.468299	0.379852
11C	-3.390563	0.854795	0.010972
12C	-2.176311	0.256145	-0.320386
13O	-4.972833	-0.423133	1.796506
14O	-5.632474	-0.489633	-0.627116
15C	-3.603255	2.225062	-0.015233
16C	-2.523099	3.030376	-0.398354
17C	-1.297186	2.453180	-0.755732
18C	-1.113731	1.065650	-0.729462
19C	4.310564	-1.546914	0.288701
20O	4.922458	-2.621699	0.204371
21N	4.754430	-0.341786	0.526887
22C	4.053793	0.830948	0.252972
23C	4.093219	1.885384	1.191382
24C	3.447120	3.097218	0.943117
25C	2.754049	3.305116	-0.256691
26C	2.725812	2.277795	-1.207113
27C	3.368041	1.062008	-0.963332
28H	0.616223	-3.195268	-1.963068
29H	3.060720	-2.947966	-1.509864
30H	2.355102	-0.564847	1.807244
31H	-0.099712	-0.757437	1.551047
32H	-4.566225	2.653933	0.246259
33H	-2.640917	4.110288	-0.425364
34H	-0.471180	3.090331	-1.058189
35H	-0.159647	0.642265	-1.020420
36H	4.633011	1.728291	2.122322
37H	3.486558	3.886223	1.691623
38H	2.254535	4.251408	-0.449418
39H	2.205283	2.423936	-2.151837
40H	3.347816	0.280482	-1.718528

15-PhNCO-005

1C	-1.162218	-1.361977	-1.557445
2C	-2.395638	-1.468882	-0.969931
3N	-2.535049	-1.652084	0.371704
4C	-1.428379	-1.761874	1.151053
5C	-0.165794	-1.626985	0.634449
6C	0.026980	-1.383953	-0.765491
7N	1.223544	-1.274898	-1.357621
8C	2.326226	-0.780452	-0.810207
9N	3.523982	-1.293637	-1.096547
10S	4.736099	-0.424441	-0.354596
11C	3.656878	0.787496	0.418342
12C	2.352973	0.461405	0.053357
13O	5.610708	0.235154	-1.349474
14O	5.415446	-1.254833	0.664473
15C	3.982925	1.900670	1.179374
16C	2.926349	2.724809	1.587982
17C	1.607573	2.431502	1.213745
18C	1.308161	1.304276	0.439659
19C	-3.923214	-1.735388	1.035559
20O	-4.042983	-2.716606	1.783889
21N	-4.789703	-0.814896	0.708729
22C	-4.463229	0.410789	0.130418
23C	-5.269483	0.905771	-0.917483
24C	-5.012623	2.146865	-1.501674
25C	-3.949666	2.941428	-1.052742
26C	-3.156052	2.475091	0.001846
27C	-3.409797	1.235007	0.591921
28H	-1.086857	-1.227822	-2.631394
29H	-3.315139	-1.411239	-1.538999
30H	-1.614391	-1.954782	2.201212
31H	0.687889	-1.716436	1.297276
32H	5.012573	2.128304	1.439337
33H	3.134361	3.606868	2.187645
34H	0.802707	3.092942	1.523121

35H	0.285290	1.104932	0.141432
36H	-6.095460	0.291375	-1.268124
37H	-5.646697	2.495819	-2.314361
38H	-3.749732	3.907213	-1.510151
39H	-2.334499	3.084389	0.374455
40H	-2.794236	0.894783	1.420737

15-001

1C	3.430866	1.483479	-0.040079
2C	4.766591	1.104984	-0.043509
3N	5.189119	-0.174967	-0.002882
4C	4.221458	-1.107295	0.043954
5C	2.852781	-0.840518	0.050169
6C	2.407443	0.504954	0.007088
7N	1.107387	0.980357	0.008302
8C	0.033803	0.219695	0.006803
9N	-0.049885	-1.131865	-0.000510
10S	-1.624876	-1.629920	-0.012334
11C	-2.354502	0.013330	-0.002255
12C	-1.297287	0.917840	0.008720
13O	-1.962341	-2.338233	-1.272703
14O	-1.973173	-2.359876	1.232536
15C	-3.688086	0.399961	-0.004301
16C	-3.953609	1.775253	0.006443
17C	-2.902265	2.705506	0.018637
18C	-1.566648	2.287223	0.019357
19H	3.156397	2.534708	-0.072663
20H	5.546267	1.864857	-0.080337
21H	4.560368	-2.142286	0.077178
22H	2.143347	-1.655627	0.086628
23H	-4.490870	-0.331846	-0.013772
24H	-4.983401	2.123237	0.005669
25H	-3.130743	3.768382	0.027422
26H	-0.748846	3.001025	0.028028

15-002

1C	-3.258970	-0.924628	-1.057529
2C	-4.486483	-0.339127	-0.767021
3N	-4.773565	0.299429	0.384184
4C	-3.779099	0.346624	1.292123
5C	-2.514364	-0.198513	1.103911
6C	-2.205924	-0.849351	-0.116943
7N	-1.015711	-1.490161	-0.355390
8C	0.179664	-0.989737	-0.184262
9N	1.251121	-1.816321	-0.083704
10S	2.648097	-0.981218	0.106202
11C	1.914786	0.656258	0.021502
12C	0.543374	0.485719	-0.163728
13O	3.247948	-1.219000	1.444302
14O	3.579550	-1.170948	-1.035584
15C	2.541665	1.894298	0.046144
16C	1.736461	3.024597	-0.136180
17C	0.359678	2.882665	-0.356534
18C	-0.246482	1.620575	-0.377475
19H	-3.097939	-1.430281	-2.005742
20H	-5.291113	-0.383886	-1.500000
21H	-4.012181	0.852746	2.228262
22H	-1.765869	-0.125971	1.887702
23H	3.615187	1.979791	0.188592
24H	2.184668	4.014664	-0.122614
25H	-0.251193	3.766733	-0.519867
26H	-1.309840	1.538378	-0.564977

22-Me-001

1P	-0.000441	-0.034082	0.783501
2C	-0.007808	-0.060812	2.597892
3C	-1.454484	-0.914975	0.155835
4C	-0.068825	1.691650	0.233794
5C	1.518029	-0.802120	0.158260
6C	-1.869747	-0.702686	-1.170178
7C	-2.957687	-1.412700	-1.677314
8C	-3.634846	-2.331980	-0.868254
9C	-3.222473	-2.543723	0.450428
10C	-2.132136	-1.839571	0.966678
11C	1.111082	2.383423	-0.083868
12C	1.048559	3.735994	-0.426379
13C	-0.182195	4.398628	-0.450884
14C	-1.357694	3.709894	-0.132526
15C	-1.306204	2.358482	0.210413

16C	1.762960	-0.781601	-1.226476
17C	2.914870	-1.377476	-1.736847
18C	3.825846	-1.996127	-0.872405
19C	3.584082	-2.017238	0.503514
20C	2.432127	-1.421320	1.024745
21H	0.030470	-1.082961	2.983091
22H	0.857368	0.503123	2.959122
23H	-0.922543	0.429792	2.943772
24H	-1.354397	0.016503	-1.800767
25H	-3.277897	-1.245000	-2.701842
26H	-4.483997	-2.881286	-1.265815
27H	-3.747463	-3.256092	1.080655
28H	-1.820790	-2.016800	1.991420
29H	2.071073	1.876091	-0.071417
30H	1.961880	4.269246	-0.675210
31H	-0.226625	5.450454	-0.720358
32H	-2.315303	4.222508	-0.153723
33H	-2.224368	1.829327	0.449485
34H	1.061719	-0.298699	-1.901917
35H	3.102211	-1.357773	-2.806744
36H	4.723107	-2.460036	-1.273040
37H	4.290606	-2.495533	1.175986
38H	2.260819	-1.446085	2.096211

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1P	0.004479	0.001360	-1.239514
2C	-1.076571	1.267578	-0.425071
3C	-0.557059	-1.567662	-0.429134
4C	1.643236	0.300674	-0.427788
5C	-1.842270	1.027801	0.727460
6C	-2.636225	2.040096	1.276833
7C	-2.670467	3.307583	0.687056
8C	-1.912093	3.557154	-0.462105
9C	-1.128887	2.541959	-1.017504
10C	-1.666675	-2.216807	-0.999711
11C	-2.167059	-3.397856	-0.446300
12C	-1.551712	-3.960342	0.677658
13C	-0.438720	-3.331252	1.244106
14C	0.053927	-2.141083	0.697599
15C	1.826015	1.100091	0.712174
16C	3.101121	1.276423	1.260001
17C	4.209987	0.651370	0.681203
18C	4.039410	-0.146575	-0.455579
19C	2.767530	-0.311932	-1.009988
20H	-1.821885	0.050514	1.201518
21H	-3.224520	1.837067	2.168851
22H	-3.287852	4.093286	1.115795
23H	-1.937010	4.537832	-0.931372
24H	-0.551560	2.743233	-1.918065
25H	-2.145874	-1.793462	-1.880628
26H	-3.029972	-3.882011	-0.897489
27H	-1.934404	-4.884104	1.104883
28H	0.046323	-3.763471	2.116405
29H	0.914655	-1.660814	1.154718
30H	0.974240	1.587272	1.178335
31H	3.225485	1.900236	2.142187
32H	5.200038	0.788498	1.109315
33H	4.896349	-0.632747	-0.915886
34H	2.647860	-0.925061	-1.901303

22-002

1P	0.006713	0.003314	-1.236682
2C	-1.080326	1.264291	-0.422103
3C	-0.549738	-1.569120	-0.429330
4C	1.644514	0.306454	-0.424801
5C	-1.131905	2.540682	-1.010665
6C	-1.924056	3.550895	-0.459099
7C	-2.691430	3.294678	0.682533
8C	-2.656435	2.025974	1.269403
9C	-1.854061	1.018333	0.723636
10C	-1.657264	-2.220582	-1.001085
11C	-2.154823	-3.403624	-0.449287
12C	-1.538571	-3.965642	0.674270
13C	-0.427573	-3.334274	1.241991
14C	0.062002	-2.142011	0.697146
15C	2.771319	-0.296276	-1.012192
16C	4.043134	-0.126347	-0.459337
17C	4.211146	0.666648	0.681256
18C	3.099684	1.281875	1.265501
19C	1.824627	1.101212	0.718733
20H	-0.548032	2.746807	-1.905825
21H	-1.949152	4.532860	-0.925676

22H	-3.315858	4.076591	1.107960
23H	-3.251143	1.818123	2.156072
24H	-1.834281	0.039509	1.194408
25H	-2.137702	-1.797051	-1.881157
26H	-3.016402	-3.889348	-0.901391
27H	-1.918904	-4.890988	1.100207
28H	0.058139	-3.766356	2.114007
29H	0.921200	-1.659918	1.155064
30H	2.653598	-0.905085	-1.906762
31H	4.902269	-0.604318	-0.924087
32H	5.201227	0.807301	1.108194
33H	3.221816	1.901690	2.150854
34H	0.971061	1.581484	1.188946

22-PPh3PhNCO-001

1P	-0.707110	0.040046	0.081590
2C	-0.699563	-1.691097	-0.464988
3C	-1.058299	1.107335	-1.351558
4C	-2.043791	0.264274	1.288513
5C	-1.316786	-2.076093	-1.664032
6C	-1.326128	-3.422697	-2.038627
7C	-0.723382	-4.382606	-1.220568
8C	-0.104292	-3.997506	-0.025551
9C	-0.087888	-2.654980	0.353509
10C	-0.000927	1.495850	-2.190937
11C	-0.263697	2.279453	-3.316220
12C	-1.572992	2.676793	-3.607833
13C	-2.625472	2.290715	-2.771644
14C	-2.372112	1.507597	-1.642938
15C	-2.890897	-0.795962	1.646559
16C	-3.898684	-0.592624	2.593200
17C	-4.064033	0.663668	3.183309
18C	-3.221245	1.722370	2.825739
19C	-2.211437	1.527926	1.882554
20C	0.970401	0.571681	0.855595
21O	0.896826	1.381362	1.798769
22N	1.914696	-0.018547	0.169057
23C	3.278694	0.195276	0.419347
24C	3.828022	0.999828	1.445667
25C	5.214542	1.119215	1.584434
26C	6.087345	0.453731	0.717467
27C	5.553937	-0.345721	-0.302308
28C	4.173435	-0.473215	-0.446725
29H	-1.782367	-1.334868	-2.307270
30H	-1.801673	-3.717985	-2.970233
31H	-0.729843	-5.428846	-1.515504
32H	0.373442	-4.740461	0.607533
33H	0.409576	-2.358090	1.272460
34H	1.015125	1.185869	-1.965053
35H	0.556501	2.582240	-3.961769
36H	-1.772528	3.288219	-4.484248
37H	-3.643394	2.600044	-2.993763
38H	-3.192672	1.216416	-0.993507
39H	-2.769274	-1.775167	1.193593
40H	-4.551783	-1.416948	2.867349
41H	-4.847872	0.818489	3.920415
42H	-3.345593	2.699460	3.285035
43H	-1.553346	2.348028	1.615164
44H	3.167085	1.523562	2.125113
45H	5.613879	1.742856	2.381945
46H	7.163818	0.554174	0.833618
47H	6.216727	-0.872324	-0.985899
48H	3.754858	-1.095698	-1.234160

22-PPh3PhNCO-002

P	0.613766	-0.008051	0.336586
C	-0.223681	-1.253904	-0.702724
C	2.400296	-0.372418	0.243649
C	0.395336	1.648816	-0.375520
C	0.286246	-2.558389	-0.740743
C	-0.343401	-3.523957	-1.522397
C	-1.477056	-3.195180	-2.269951
C	-1.992212	-1.898114	-2.219102
C	-1.374256	-0.929173	-1.433628
C	3.212511	0.320769	-0.662305
C	4.567912	0.009300	-0.759640
C	5.119159	-0.988900	0.046196
C	4.309404	-1.677281	0.953167
C	2.954302	-1.371407	1.056315
C	0.389511	2.739886	0.501084
C	0.280878	4.031773	-0.006831
C	0.178406	4.237986	-1.384939

C	0.197581	3.148216	-2.258837
C	0.311462	1.852380	-1.759585
C	0.099483	-0.014704	2.228180
O	1.099571	-0.058687	2.966701
N	-1.162524	0.077417	2.534052
C	-2.257622	0.025156	1.661355
C	-2.977495	-1.179407	1.490651
C	-4.113224	-1.236388	0.685882
C	-4.576491	-0.092797	0.026417
C	-3.893171	1.113871	0.201877
C	-2.759808	1.176645	1.015213
H	1.168606	-2.831417	-0.168925
H	0.057309	-4.534404	-1.547419
H	-1.964702	-3.951910	-2.880738
H	-2.889106	-1.639120	-2.776304
H	-1.814645	0.060021	-1.363202
H	2.802812	1.103815	-1.293990
H	5.192077	0.553376	-1.464568
H	6.178450	-1.225766	-0.027569
H	4.732321	-2.448957	1.591798
H	2.339469	-1.897512	1.778950
H	0.459063	2.588306	1.575809
H	0.268819	4.875773	0.678175
H	0.086757	5.248129	-1.777857
H	0.127051	3.303957	-3.332627
H	0.343357	1.015095	-2.450563
H	-2.628545	-2.071932	2.005862
H	-4.639338	-2.182521	0.570613
H	-5.463902	-0.138903	-0.602733
H	-4.249811	2.018924	-0.287631
H	-2.255861	2.126734	1.169468

23-001

1N	-2.433104	-0.746220	0.000000
2C	-2.424412	0.619780	-0.000003
3C	-1.274293	1.377432	0.000001
4C	-0.010622	0.729053	0.000000
5C	-0.007880	-0.700751	0.000000
6C	-1.266383	-1.364778	0.000002
7C	1.232237	1.419591	0.000001
8C	2.417623	0.713469	-0.000001
9C	2.418084	-0.707268	0.000000
10C	1.227449	-1.403219	0.000000
11H	-3.402242	1.095151	0.000000
12H	-1.329875	2.463243	0.000002
13H	-1.287387	-2.454770	-0.000001
14H	1.233132	2.507185	0.000002
15H	3.365426	1.245945	-0.000001
16H	3.364250	-1.242031	0.000000
17H	1.217597	-2.491046	0.000000

23-Me-001

1N	-2.024200	-0.181178	0.000213
2C	-1.804439	1.180181	0.000163
3C	-0.534301	1.682506	0.000032
4C	0.586427	0.808667	-0.000062
5C	0.329609	-0.601787	-0.000016
6C	-1.005793	-1.042574	0.000136
7C	1.927470	1.261724	-0.000203
8C	2.962013	0.346538	-0.000306
9C	2.706124	-1.049962	-0.000272
10C	1.412571	-1.523073	-0.000129
11C	-3.424949	-0.657556	0.000341
12H	-2.692133	1.800375	0.000228
13H	-0.388666	2.757840	-0.000002
14H	-1.251743	-2.099067	0.000188
15H	2.127181	2.329626	-0.000234
16H	3.990510	0.696304	-0.000417
17H	3.539447	-1.746399	-0.000358
18H	1.204827	-2.589549	-0.000100
19H	-3.436424	-1.747203	0.000351
20H	-3.925917	-0.280821	0.894959
21H	-3.926070	-0.280840	-0.894200

23-PhNCO-001

1N	0.648319	-0.819449	-0.000043
2C	1.435528	-1.943046	-0.000062
3C	2.800332	-1.845480	0.000000

4C	3.428919	-0.572223	0.000087
5C	2.582631	0.584044	0.000111
6C	1.188503	0.397700	0.000043
7C	4.835208	-0.391966	0.000153
8C	5.365944	0.882359	0.000240
9C	4.525288	2.027844	0.000263
10C	3.155605	1.886536	0.000199
11C	-0.911036	-1.027124	-0.000135
12O	-1.237479	-2.220885	-0.000223
13N	-1.503878	0.127780	-0.000074
14C	-2.897997	0.251210	-0.000101
15C	-3.835296	-0.808912	-0.000168
16C	-5.207557	-0.539873	-0.000162
17C	-5.687295	0.773769	-0.000085
18C	-4.768433	1.831397	-0.000011
19C	-3.398817	1.572863	-0.000015
20H	0.892689	-2.878402	-0.000132
21H	3.398312	-2.751662	-0.000019
22H	0.483085	1.220023	0.000056
23H	5.482513	-1.264869	0.000135
24H	6.444214	1.017049	0.000292
25H	4.971500	3.018135	0.000334
26H	2.500966	2.754071	0.000217
27H	-3.483798	-1.833224	-0.000224
28H	-5.908811	-1.372136	-0.000217
29H	-6.756486	0.971497	-0.000081
30H	-5.120368	2.860938	0.000054
31H	-2.684222	2.392745	0.000046

23-PhNCO-002

1N	0.063352	1.182865	-0.344578
2C	-0.006799	0.278500	-1.371553
3C	1.024157	-0.589844	-1.609608
4C	2.176072	-0.575912	-0.778093
5C	2.225448	0.388180	0.280966
6C	1.130300	1.259922	0.438702
7C	3.268021	-1.465234	-0.943756
8C	4.352198	-1.391865	-0.092674
9C	4.399576	-0.433115	0.954275
10C	3.356263	0.446824	1.140799
11C	-1.155607	2.210591	-0.070596
12O	-0.743800	3.368479	-0.007248
13N	-2.330129	1.677033	-0.003239
14C	-2.595057	0.319077	0.193210
15C	-3.582733	-0.303402	-0.597377
16C	-3.905767	-1.648404	-0.411809
17C	-3.263061	-2.406514	0.575655
18C	-2.300039	-1.792565	1.383937
19C	-1.972495	-0.446768	1.202968
20H	-0.912186	0.302584	-1.963305
21H	0.951994	-1.292884	-2.433593
22H	1.111827	2.025643	1.207552
23H	3.237292	-2.199492	-1.744408
24H	5.185703	-2.076973	-0.222465
25H	5.266674	-0.397642	1.607642
26H	3.381599	1.186600	1.936487
27H	-4.084035	0.285632	-1.361714
28H	-4.665909	-2.107211	-1.040544
29H	-3.518084	-3.453346	0.720151
30H	-1.803255	-2.361452	2.167185
31H	-1.236650	0.024599	1.849453

23-PhNCO-003

1N	0.036426	1.466052	-0.152822
2C	0.827660	2.052452	0.798872
3C	2.047212	1.521389	1.120919
4C	2.518547	0.358881	0.451852
5C	1.679133	-0.218836	-0.554899
6C	0.433145	0.385884	-0.813969
7C	3.769881	-0.247392	0.728229
8C	4.158624	-1.374490	0.031983
9C	3.323985	-1.944797	-0.965314
10C	2.102817	-1.378742	-1.258582
11C	-1.373587	2.173071	-0.489032
12O	-1.219065	3.383257	-0.653775
13N	-2.397417	1.389689	-0.576153
14C	-2.476057	0.082258	-0.091774
15C	-3.084576	-0.902973	-0.896607
16C	-3.221275	-2.215560	-0.441957
17C	-2.767760	-2.579824	0.832311
18C	-2.183488	-1.605425	1.649299
19C	-2.043037	-0.290392	1.199947

20H	0.420962	2.945988	1.255003
21H	2.652324	1.995564	1.887364
22H	-0.246369	-0.013242	-1.558189
23H	4.412828	0.184705	1.490341
24H	5.117887	-1.837301	0.247808
25H	3.654240	-2.833364	-1.495547
26H	1.451851	-1.807193	-2.015784
27H	-3.441381	-0.619384	-1.883817
28H	-3.688605	-2.957821	-1.085674
29H	-2.878897	-3.601720	1.185963
30H	-1.841156	-1.866817	2.648459
31H	-1.601566	0.461305	1.849423