Supplementary Information

for

Inductive Effects Through Alkyl Groups - How Long is Long Enough?

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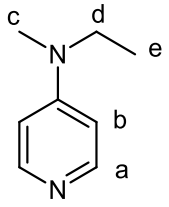
0. General Information

All air and water sensitive manipulations were carried out under a nitrogen atmosphere using standard Schlenk techniques. Calibrated flasks for kinetic measurements were dried in the oven at 120 °C for at least 12 hours prior to use and then assembled quickly while still hot, cooled under a nitrogen stream and sealed with a rubber septum. All commercial chemicals were of reagent grade and were used as received unless otherwise noted. $CDCl_3$ was refluxed for at least one hour over CaH_2 and subsequently distilled. ^1H and ^{13}C NMR spectra were recorded on Varian 300 or Varian INOVA 400 machines at room temperature. All ^1H chemical shifts are reported in ppm (δ) relative to TMS (0.00); ^{13}C chemical shifts are reported in ppm (δ) relative to $CDCl_3$ (77.16). ^1H NMR kinetic data were measured on a Varian Mercury 200 MHz spectrometer at 23 °C. HRMS spectra (ESI-MS) were carried out using a Thermo Finnigan LTQ FT instrument. IR spectra were measured on a Perkin-Elmer FT-IR BX spectrometer mounting ATR technology. Analytical TLC were carried out using aluminum sheets silica gel Si 60 F254.

1. Catalyst Synthesis

N-ethyl-*N*-methylpyridin-4-amine (**1b**)



To 1.50 g (9.99 mmol) 4-Chloropyridine hydrochloride was added 6.51 g (20 mmol) Cs_2CO_3 in an oven dried pressure tube. After addition of 4.29 mL (50 mmol) *N*-methylethylamine, 0.23 g (0.20 mmol) $Pd(PPh_3)_4$ and 2 mL dist. water the pressure tube was closed and heated for 72 h at 120 °C in an oilbath. The brown suspension was poured into DCM, filtered and extracted three times with dist. water. After drying over $MgSO_4$, filtration and evaporation of the solvent the crude product was purified by column chromatography on silica ($CHCl_3$/MeOH, 10:1) yielding 870 mg (64 %) of a yellow liquid.

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 8.17 (dd, *J* = 5.0 Hz, 1.6 Hz, 2H, H_a), 6.45 (dd, *J* = 5.0 Hz, 1.6 Hz, 2H, H_b), 3.38 (q, *J* = 7.1 Hz, 2H, H_d), 2.91 (s, 3H, H_c), 1.12 (t, *J* = 7.1 Hz, 2H, H_e).

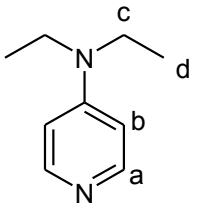
^{13}C-NMR (101 MHz, $CDCl_3$): δ = 149.9 (C_a), 106.4 (C_b), 45.6 (C_d), 36.5 (C_c), 11.2 (C_e).

MS (EI) m/z (%): 136 (M^+, 30), 121 (M^+-CH_3, 100), 78 ($C_5H_4N^+$).

HRMS (EI): $C_8H_{12}N_2$ calc. 137.1037 g/mol $[M+H]^+$, found 137.0988 g/mol $[M+H]^+$.

IR (ATR): $\tilde{\nu}$ = 2928 (w), 2850 (w), 1594 (vs), 1514 (vs), 1466 (w), 1371 (vs), 1230 (vs), 1210 (vs), 1110 (w), 1080 (w), 998 (vs), 799 (vs), 810 (vs), 736 (s).

N,*N*-diethylpyridine-4-amine (**1c**)

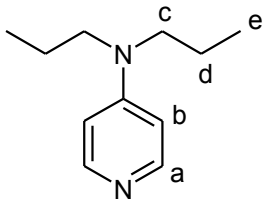


To 1.50 g (9.99 mmol) 4-chlorpyridine hydrochloride was added 6.51 g (20 mmol) Cs_2CO_3 in a oven dried pressure tube. After adding 2.08 mL (20 mmol) diethylamine the pressure tube was closed and heated for 5 days at 170 °C in an oil bath. The brown solution was poured into DCM, filtered and the solvent was evaporated. Column chromatography (silica, EA/Net_3, 20:1) followed by distillation of the brown crude product yielded 220 mg (20 %) of a pale yellow solid.

^{1}H-NMR (300 MHz, $CDCl_3$): δ = 8.19 (dd, *J* = 5.0 Hz, 1.6 Hz, 2H, H_a), 6.47 (dd, *J* = 5.0 Hz, 1.6 Hz, 2H, H_b), 3.37 (q, *J* = 10.5 Hz, 4.5 Hz, 4H, H_c), 1.19 (t, *J* = 7.1 Hz, 6H, H_d).

^{13}C-NMR (75 MHz, $CDCl_3$): *δ* = 149.9 (C_a), 106.2 (C_b), 43.7 (C_c), 12.3 (C_d). (in agreement with literature[9])

N,*N*-dipropylpyridin-4-amine (**1d**)

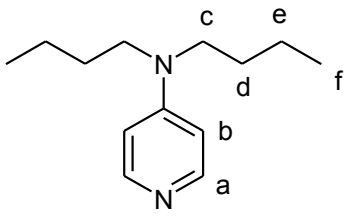


To 1.00 g (6.66 mmol) 4-chloropyridine hydrochloride was added 3.25 g (9.99 mmol) Cs_2CO_3 into an oven dried pressure tube. After adding 0.46 mL (3.33 mmol) dipropylamine the pressure tube was closed and heated for 3 days at 170 °C oil bath temperature. The warm brown solution was poured into DCM, filtered and the solvent was evaporated. Column chromatography (Silica, EA/Net_3, 20:1) of the brown crude mixture yielded 230 mg (38 %) of a pale yellow solid.

^{1}H-NMR (300 MHz, $CDCl_3$): δ = 8.14 (dd, *J* = 5.0 Hz, 1.6 Hz, 2H, H_a), 6.40 (dd, *J* = 5.0 Hz, 1.6 Hz, 2H, H_b), 3.21 (t, *J* = 7.5 Hz, 4H, H_c), 1.70 – 1.48 (m, 4H, H_d), 0.91 (t, *J* = 7.4, 6H, H_e).

^{13}C-NMR (75 MHz, $CDCl_3$): *δ* = 149.9 (C_a), 106.3 (C_b), 51.8 (C_c), 20.1 (C_d), 11.2 (C_e). (in agreement with literature[10])

N,*N*-dibutylpyridin-4-amine (**1e**)

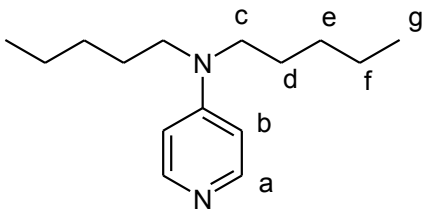


To 1.00 g (6.66 mmol) 4-chloropyridin hydrochloride was added 2.49 mL (14.6 mmol) dibutylamine into a oven dried microwave vial. After addition of 2.68 mL (33.3 mmol) pyridine the vial was closed with a septum cap and the reaction mixture was heated for 2h at 170 °C (200 W). The brown residue was taken up in DCM and was washed three times with sat. K_2CO_3 solution. The collected organic phase was dried over $MgSO_4$ and filtered. After evaporation of the solvent the crude mixture was purified two times by column chromatography (silica, EA/IH, 5:1) and yielded 240 mg (18 %) of a pale brown oil.

^{1}H-NMR (300 MHz, $CDCl_3$): δ = 8.16 (d, *J* = 3.3 Hz, 2H, H_a), 6.43 (d, *J* = 3.3 Hz, 2H, H_b), 3.26 (t, *J* = 7.6 Hz, 4H, H_c), 1.68 – 1.44 (m, 4H, H_d), 1.43-1.25 (m, 4H, H_e), 0.95 (t, *J* = 7.3 Hz, 6H, H_f).

^{13}C-NMR (75 MHz, $CDCl_3$): *δ* = 149.9 (C_a), 106.3 (C_b), 49.9 (C_c), 29.0 (C_d), 20.2 (C_e), 13.9 (C_f). (in agreement with literature[11])

N,*N*-dipentylpyridin-4-amine (**1f**)

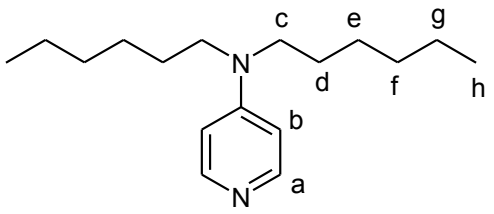


To 2.00 g (13.3 mmol) 4-chloropyridine hydrochloride was added 3.75 mL (46.6 mmol) pyridine in a oven dried pressure tube. After addition of 3.26 mL (15.98 mmol) dipentylamine the reaction mixture was heated for 22h at 185 °C. The brown crude mixture was taken up in DCM and washed with sat. K_2CO_3 solution. The collected organic phase was dried over $MgSO_4$, filtered and the solvent was evaporated under reduced pressure. After column chromatography (Silica, EA/Net_3, 10:1) of the brown mixture the product was distilled three times at 140 °C (4 mbar) to give 190 mg (6 %) of a pale yellow viscous liquid.

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 8.15 (d, *J* = 6.6 Hz, 2H, H_a), 6.40 (d, *J* = 6.6 Hz, 2H, H_b), 3.26 (t, *J* = 7.6 Hz, 4H, H_c), 1.65 – 1.48 (m, 4H, H_d), 1.44 – 1.19 (m, 8H, H_e, H_f), 0.90 (t, *J* = 7.1 Hz, 6H, H_g).

^{13}C-NMR (75 MHz, $CDCl_3$): *δ* = 149.8 (C_a), 106.4 (C_b), 50.1 (C_c), 29.1 (C_e), 26.6 (C_d), 22.5 (C_f), 14.0 (C_g). (in agreement with literature[12])

N,*N*-dihexylpyridin-4-amine (**1g**)

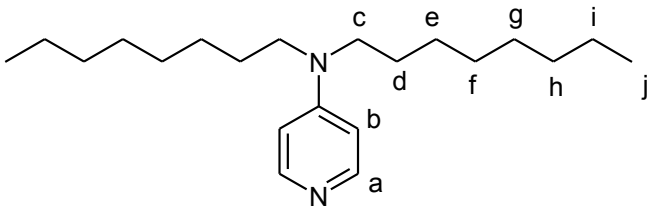


In a pressure tube 2.00 g (13.3 mmol) of 4-chloropyridine hydrochloride were suspended in 3.75 mL (46.6 mmol) pyridine. After addition of 6.21 mL (26.6 mmol) dihexylamine the pressure tube was closed and heated at 185 °C in an oil bath. After 22 h reaction time the residue was dissolved in DCM and washed three times with sat. K_2CO_3-solution. After drying the organic layer over $MgSO_4$ and filtration, the solvent was evaporated at reduced pressure. Column chromatography (Silica, EA/NEt_3 10:1) followed by a distillation (130 °C, 10 mbar) gave 570 mg (16%) of a pale yellow viscous liquid.

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 8.15 (dd, *J* = 5.0 Hz, 1.6 Hz, 2H, H_a), 6.40 (dd, *J* = 5.0 Hz, 1.6 Hz, 2H, H_b), 3.26 (t, *J* = 7.5 Hz, 4H, H_c), 1.61 – 1.49 (m, 4H, H_d), 1.39 – 1.18 (m, 12H, H_e, H_f, H_g), 0.90 (t, *J* = 7.1 Hz, 6H, H_h).

^{13}C-NMR (75 MHz, $CDCl_3$): *δ* = 149.8 (C_a), 106.4 (C_b), 50.1(C_c), 31.6 (C_e), 26.9 (C_d), 26.7 (C_f), 22.6 (C_g), 14.0 (C_h). (in agreement with literature[11])

N,N -Dioktylpyridin-4-amine (**1h**)



In a pressure tube 2.00 g (13.3 mmol) of 4-chloropyridine hydrochloride were suspended in 3.75 mL (46.6 mmol) pyridine. After addition of 8.10 mL (26.6 mmol) dioktylamine the pressure tube was sealed and heated at 160 °C in an oil bath. After 18 h the residue was dissolved in DCM and washed three times with sat. K_2CO_3-solution. After drying the organic layer over $MgSO_4$ and filtration, the solvent was evaporated at reduced pressure. Column chromatography on Silica (EA/NEt_3 10:1) and on basic AlOx. (EA/IH 1:10 → 10:1) yielded 610 mg (14 %) of a brown viscous liquid.

^{1}H-NMR (300 MHz, $CDCl_3$): δ = 8.16 (dd, *J* = 5.0 Hz, 1.6 Hz, 2H, H_a), 6.40 (dd, *J* = 5.0 Hz, 1.6 Hz, 2H, H_b), 3.33 – 3.14 (t, *J* = 7.7 Hz, 4H, H_c), 1.72 – 1.41 (m, 4H, H_d), 1.41 – 1.18 (m, 20H, H_e, H_f, H_g, H_h, H_i), 1.01 – 0.76 (m, *J* = 6.0 Hz, 3H, H_j).

^{13}C-NMR (75 MHz, $CDCl_3$): *δ* = 149.9 (C_a), 106.3 (C_b), 50.1 (C_c), 31.8 (C_e), 29.4 (C_f), 29.3 (C_g), 27.0 (C_d), 26.9 (C_h), 22.6 (C_i), 14.1 (C_j).

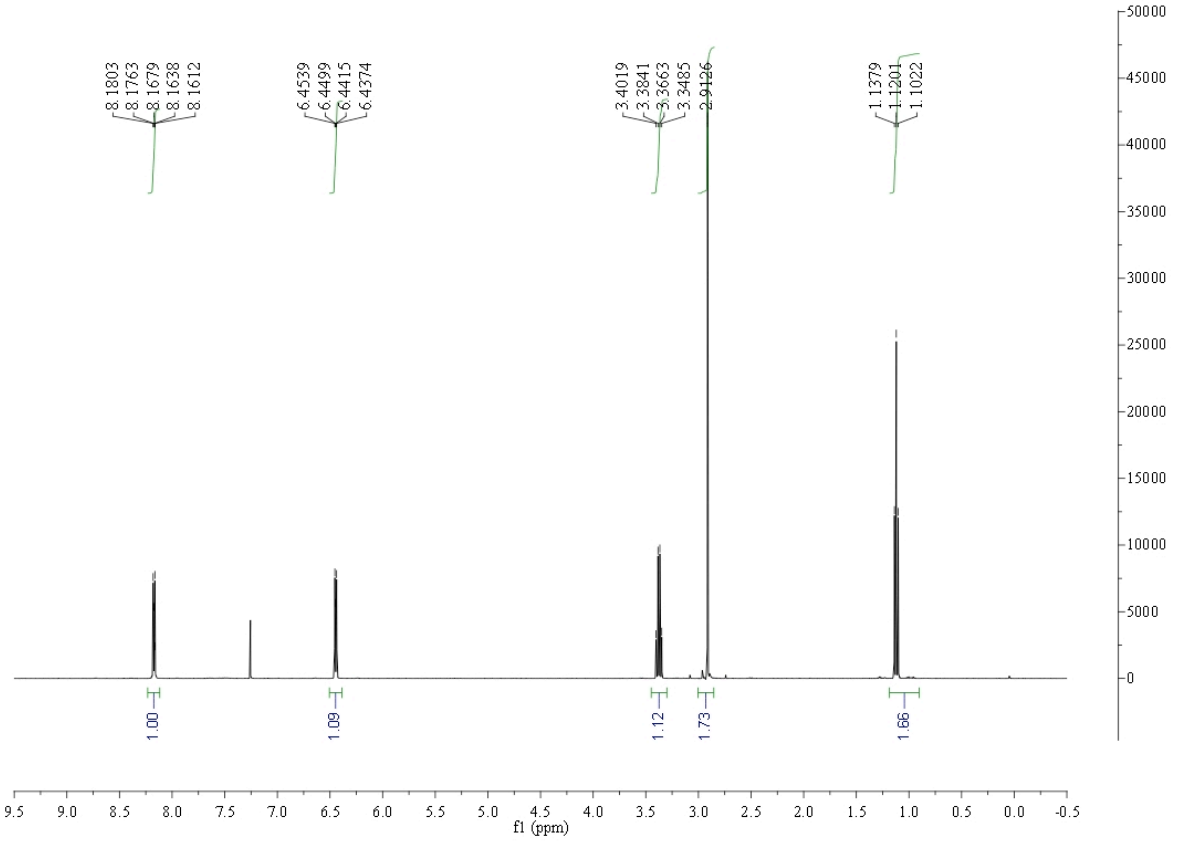
MS (EI) m/z (%): 318 (M^+, 13), 219 ($C_{14}H_{23}N_2$, 100), 121 ($C_7H_9N_2$, 30).

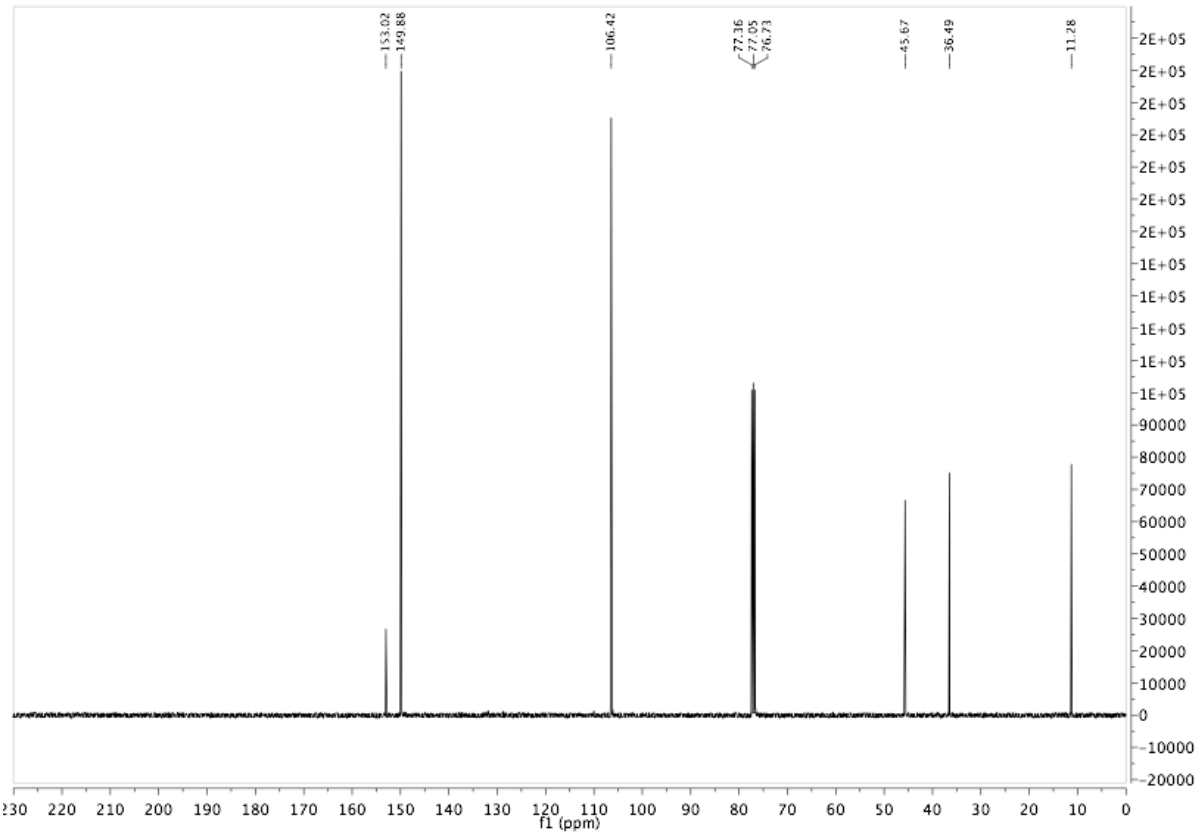
HRMS (EI): $C_{21}H_{38}N_2$ calc. 318.3035 g/mol [M^+], found 318.3030 g/mol [M]$^+$.

IR (ATR): $\tilde{\nu}$ = 2923 (vs), 2854 (s), 1593 (vs), 1512 (vs), 1466 (s), 1371 (s), 1228 (s), 1104 (w), 986 (s), 799 (vs), 734 (w).

2. ^{1}H and ^{13}C NMR spectra of synthesized catalysts

1b:





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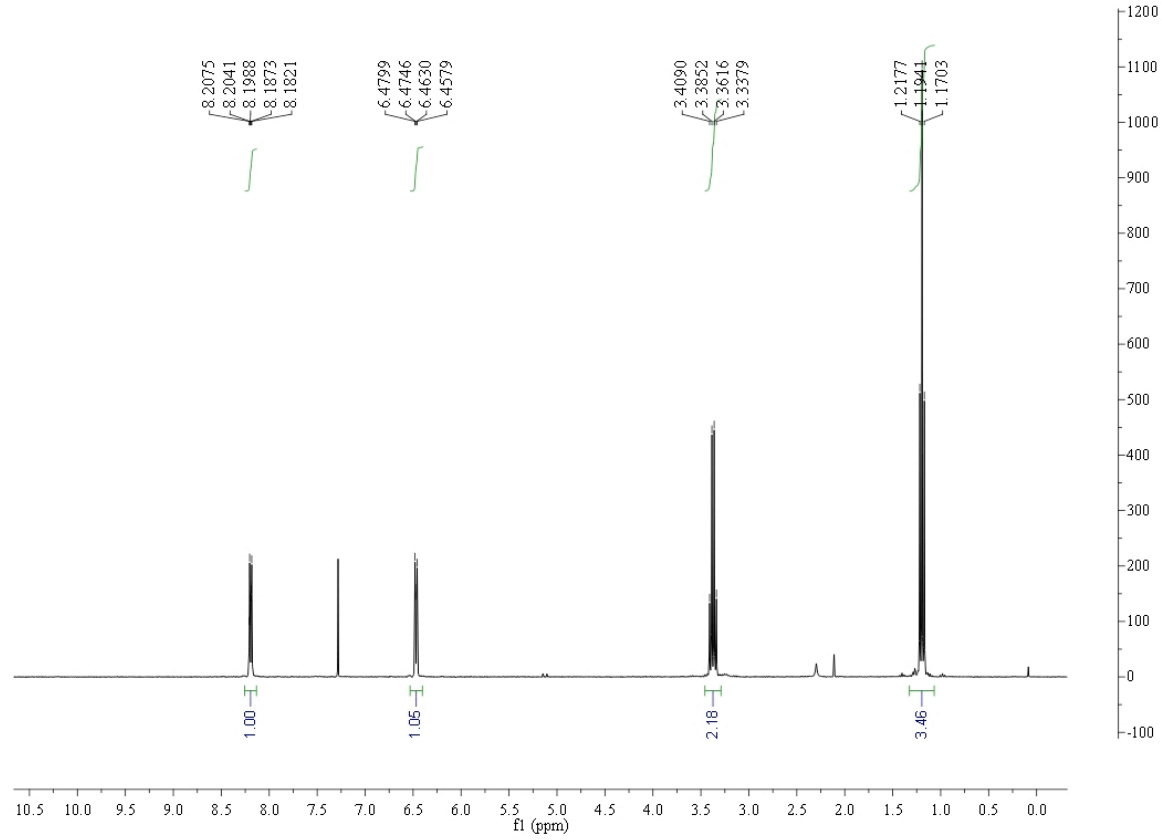
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8.1988
8.1873
8.1821
6.4799
6.4746
6.4630
6.4579
3.4090
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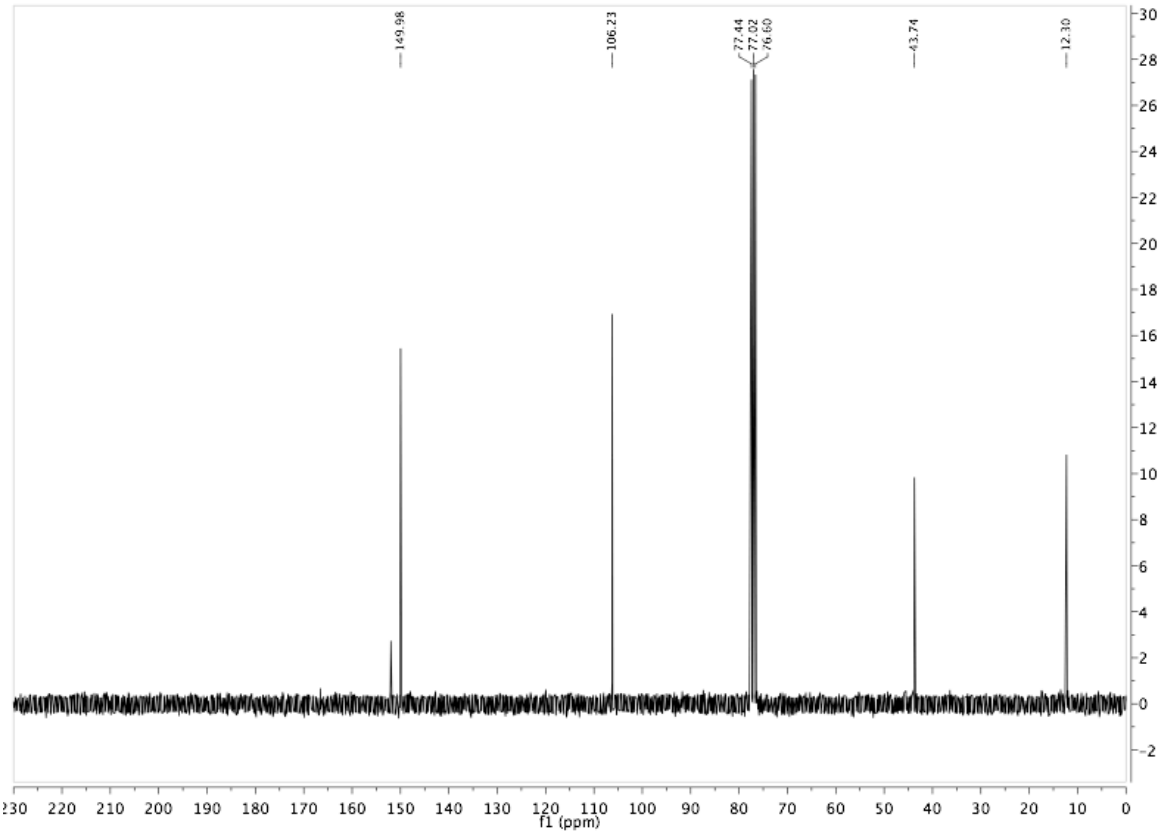
1.1703
1.00
1.05
2.18
3.46
f1 (ppm)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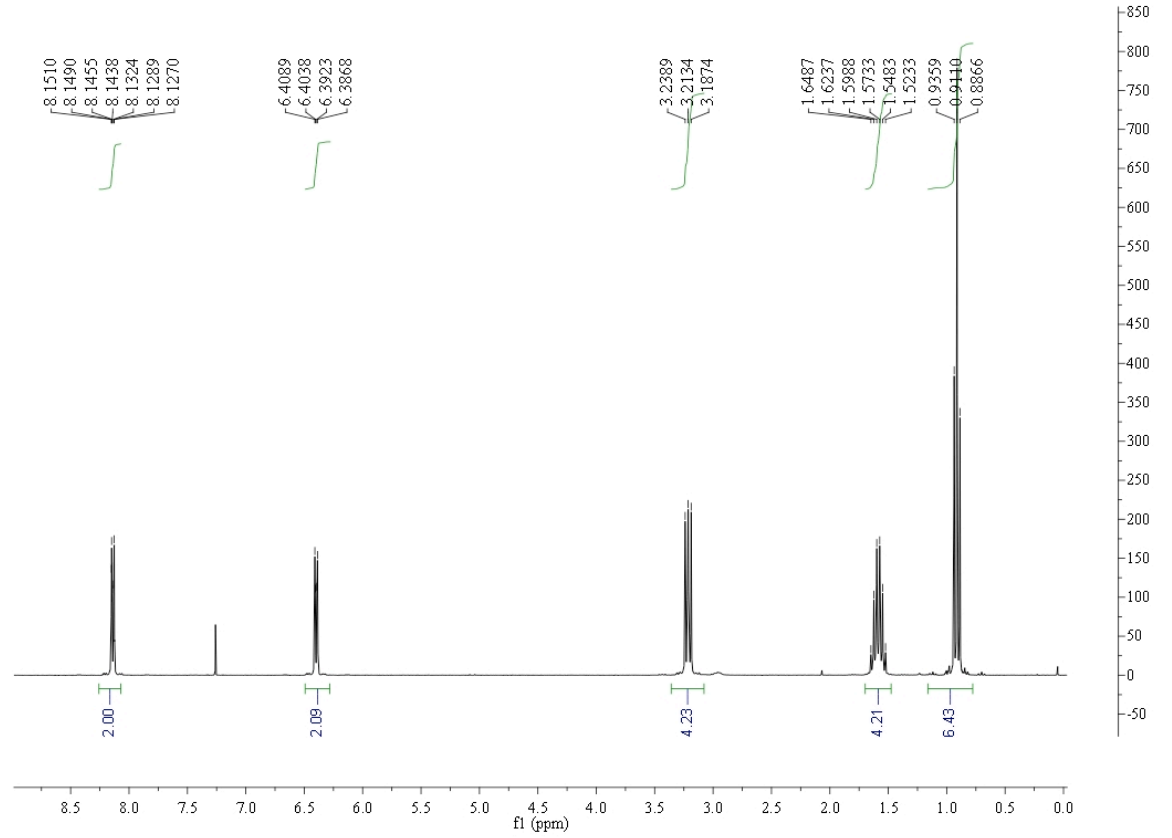
f1 (ppm)

1d: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6.3868
3.2389
3.2134
3.1874
1.6487
1.6237
1.5988
1.5733
1.5483
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0.9359
0.9110
0.8866
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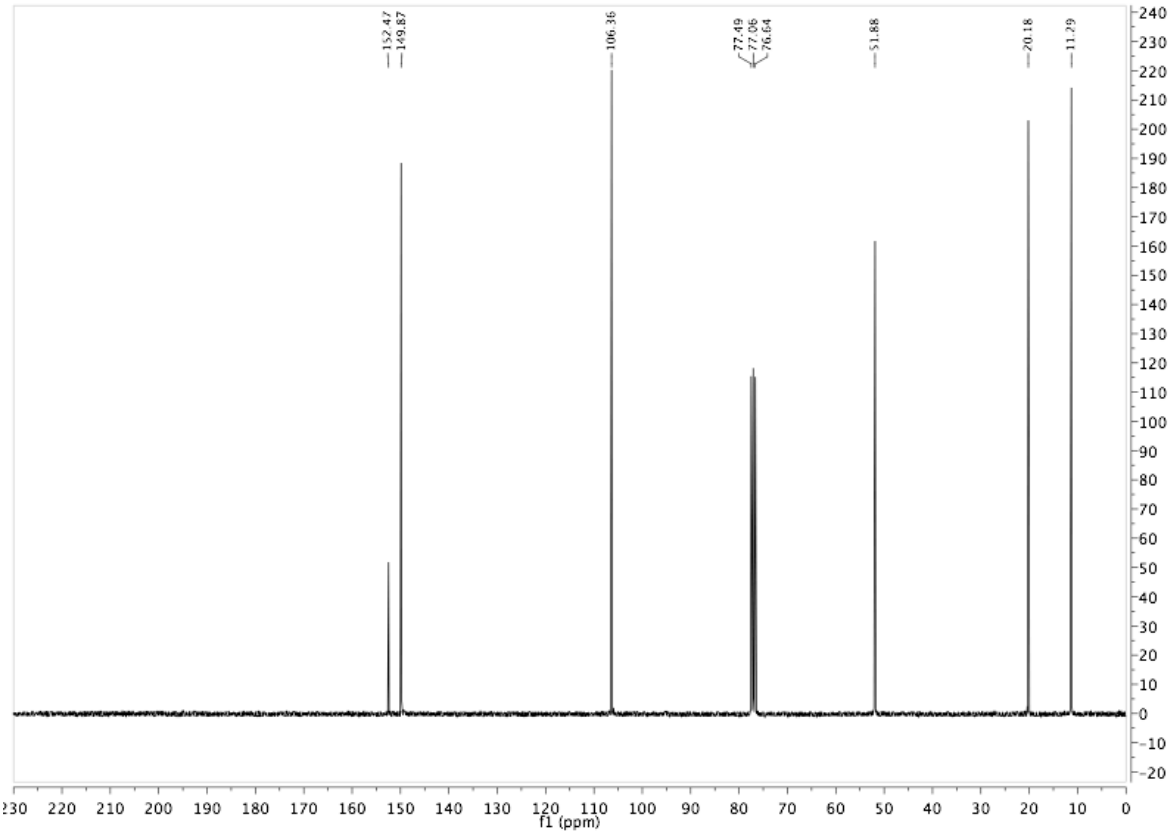
2.09
4.23
4.21
6.43
f1 (ppm)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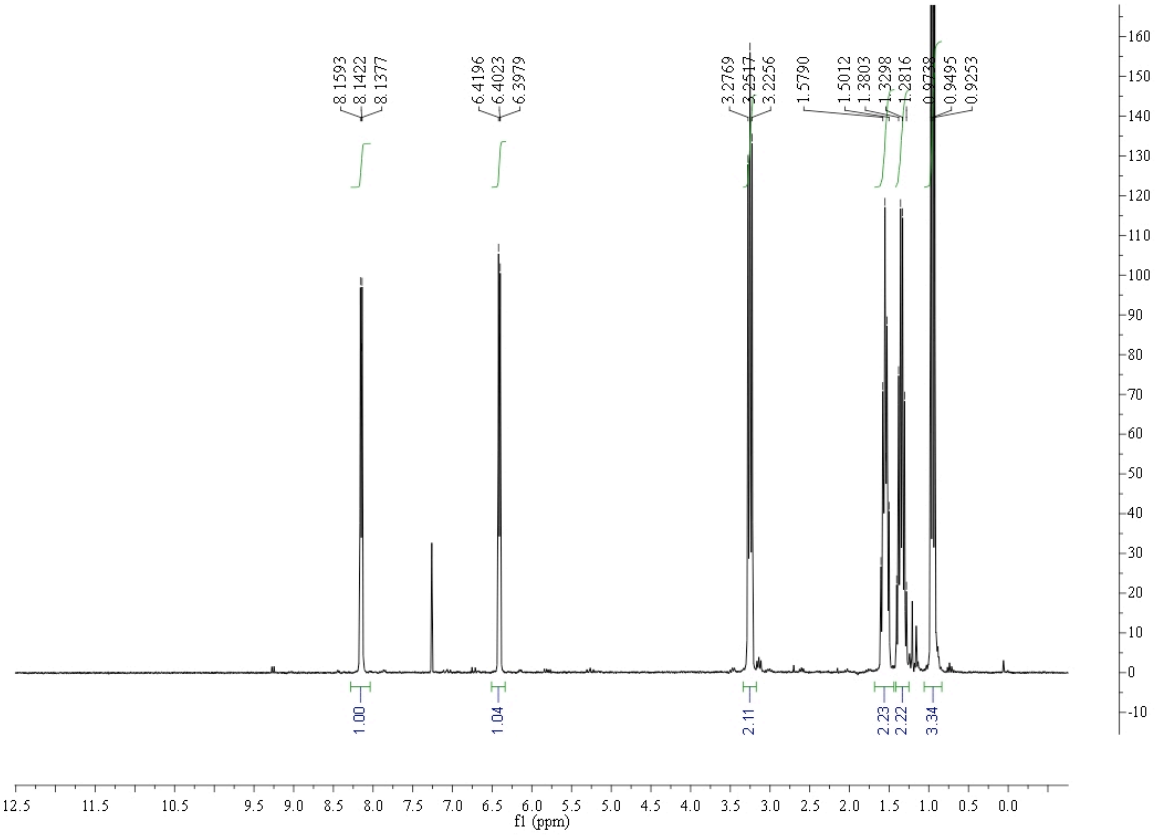
f1 (ppm)

1e: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6.3979
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3.2256
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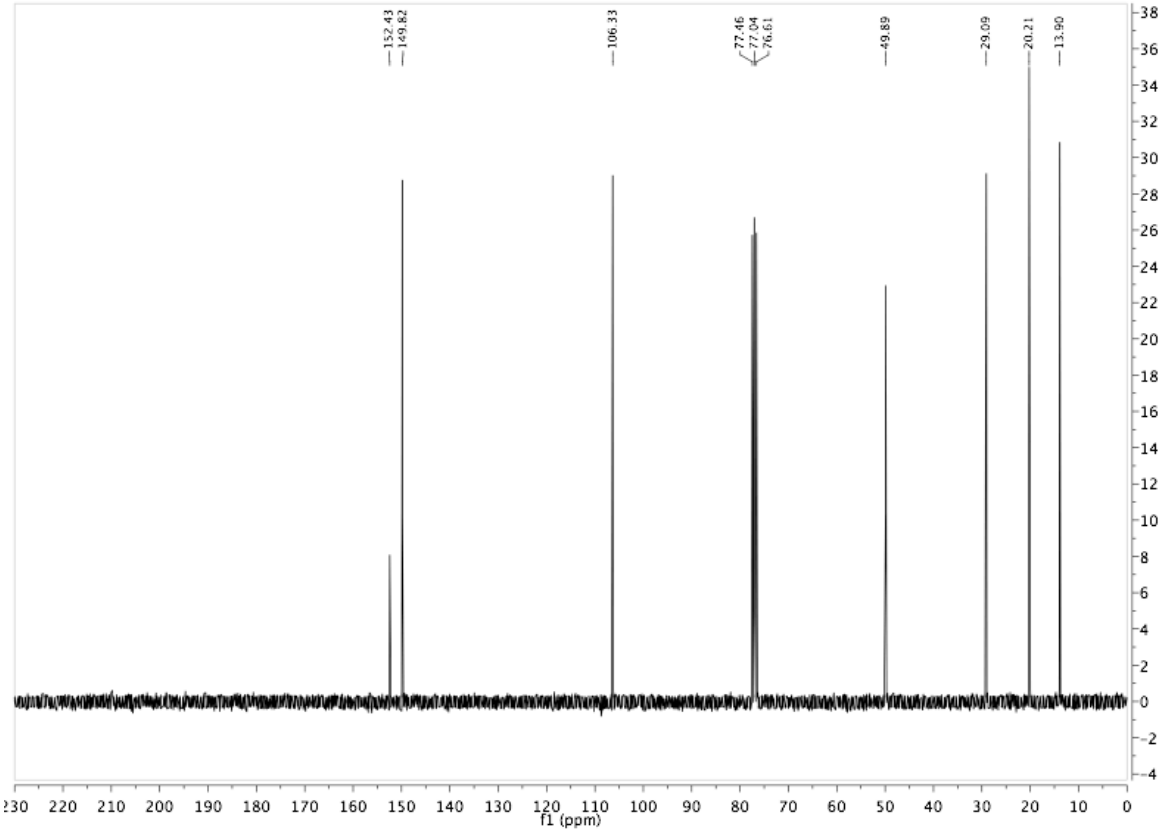
1.5012
1.3803
1.3298
1.2816
0.9495
0.9253
1.00
1.04
2.11
2.23
2.22
3.34
f1 (ppm)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76.61
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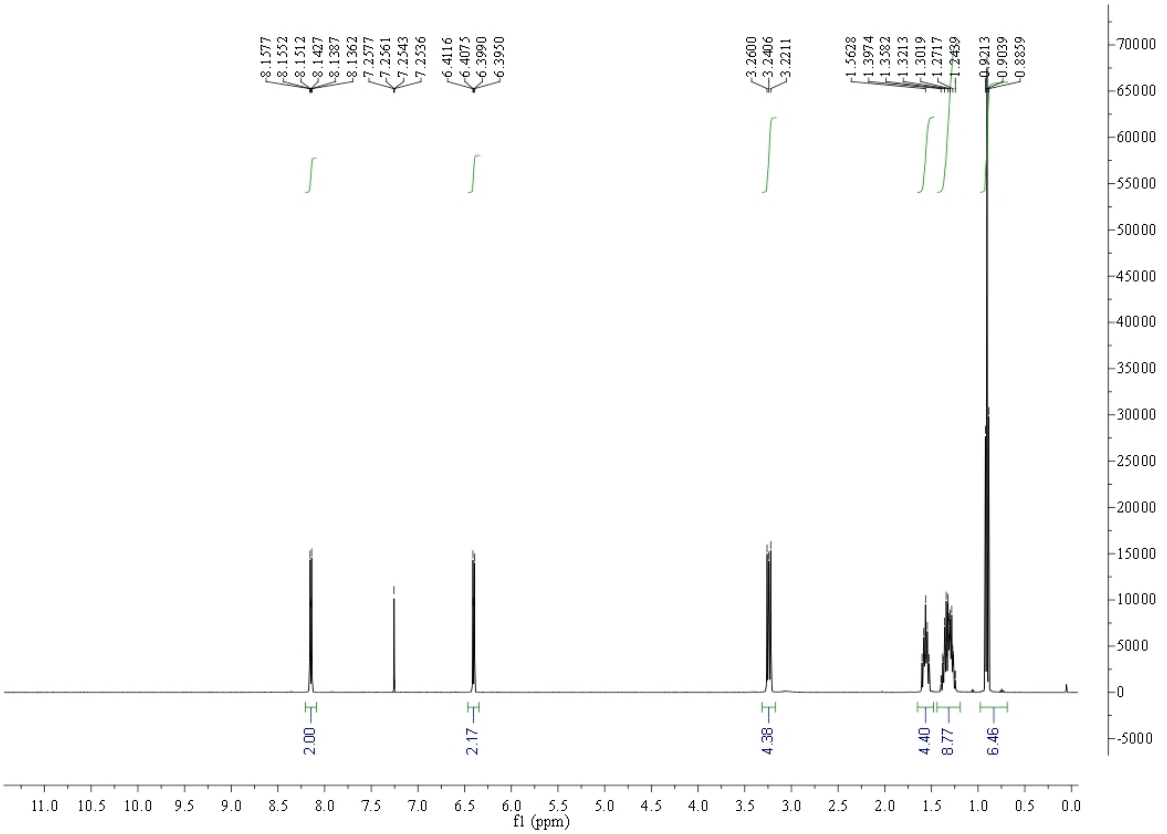
29.09
20.21
13.90
f1 (ppm)

1f: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6.4075
6.3990
6.3950
3.2600
3.2406
3.2211
1.5628
1.3974
1.3582
1.3213
1.3019
1.2717
1.2459
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0.9039
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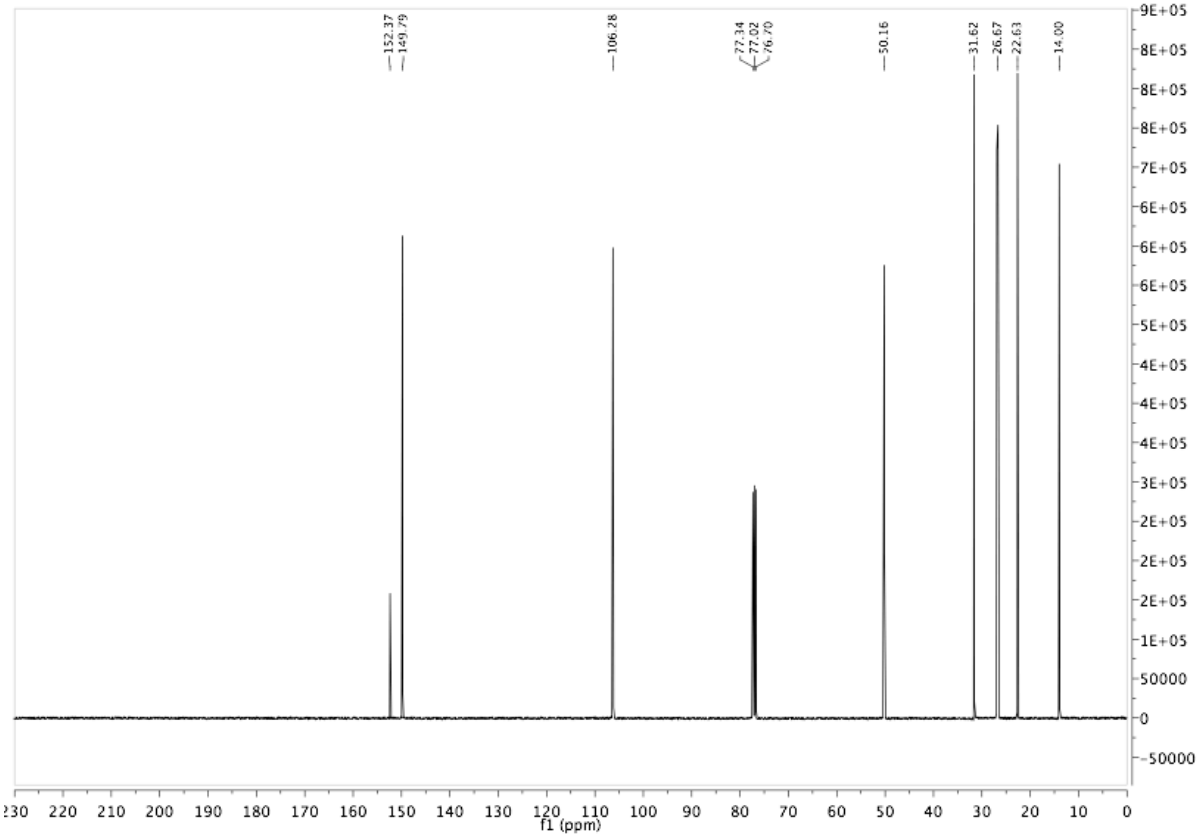
4.40
8.77
6.46
f1 (ppm)


152.37
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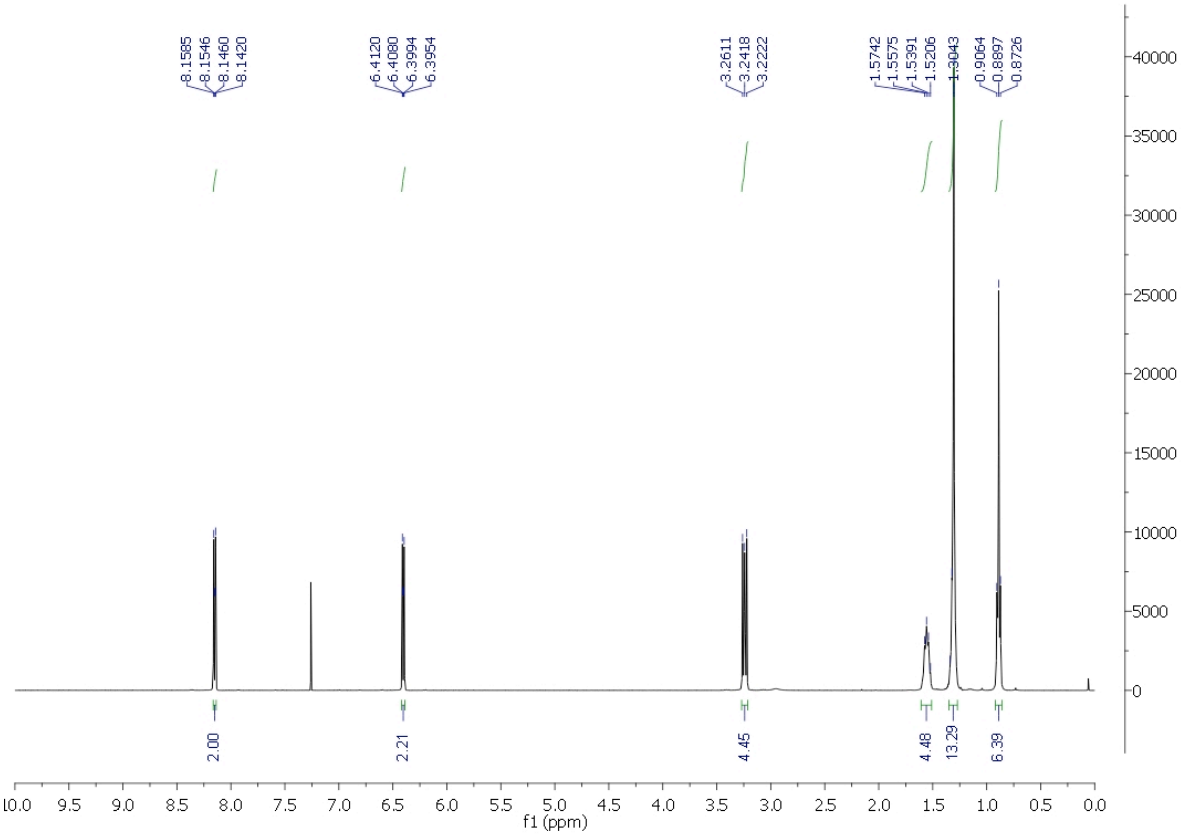
22.63
14.00
f1 (ppm)

1g: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8.1420
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6.3994
6.3954
3.2611
3.2418
3.2222
1.5742
1.5575
1.5391
1.5206
1.3043
0.9064
0.8897
0.8726
2.00
2.21
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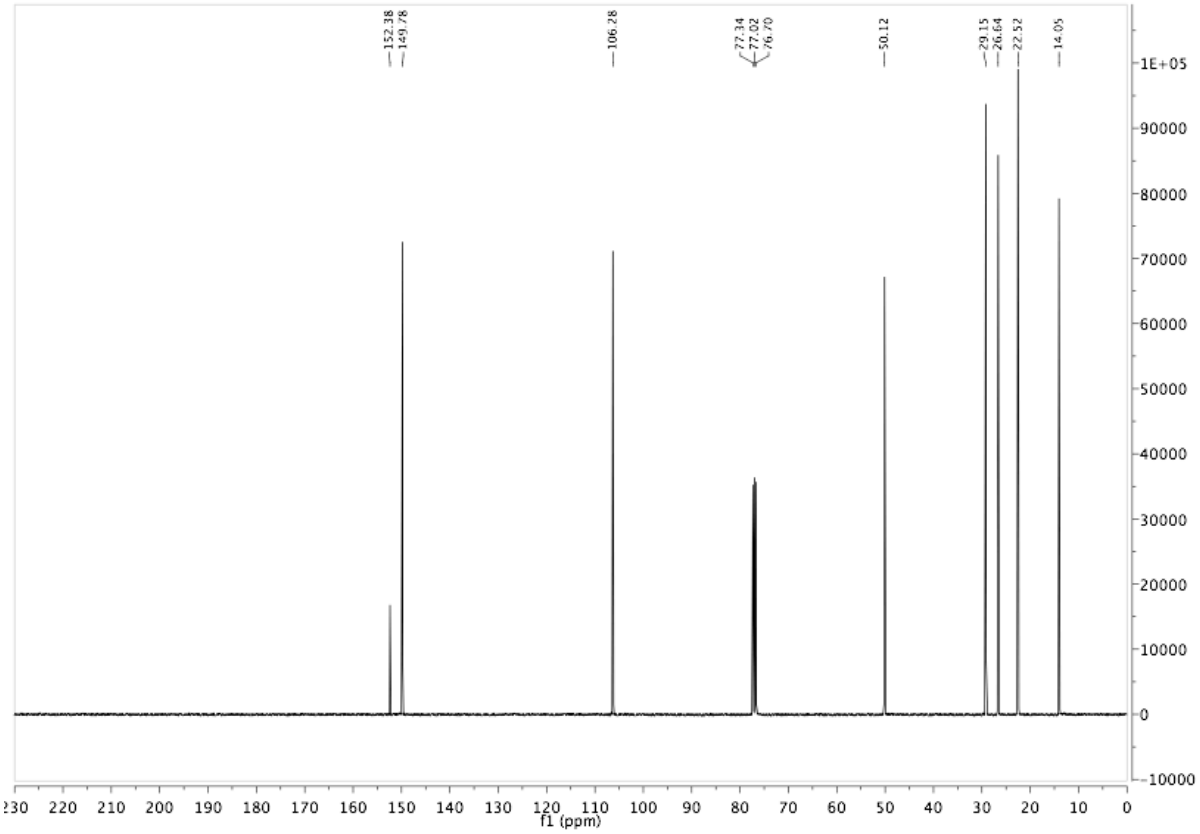
4.48
13.29
6.39
f1 (ppm)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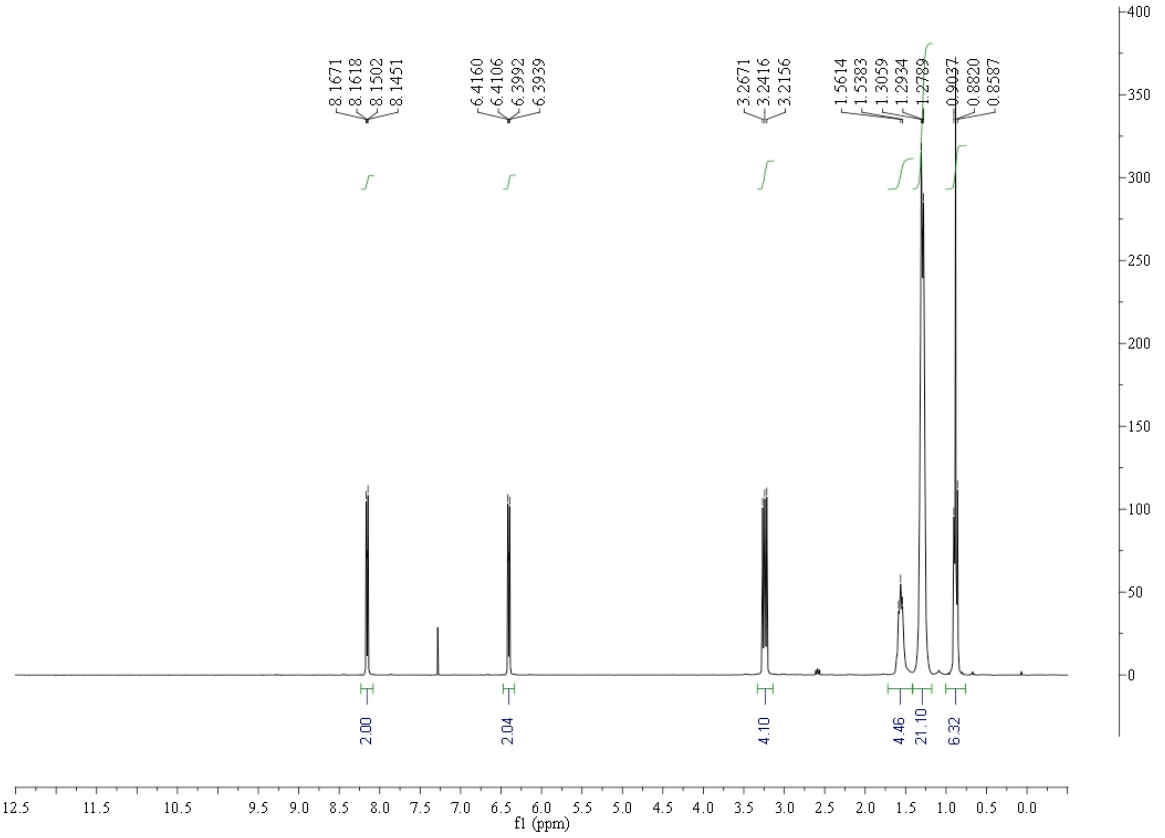
106.28
77.34
77.02
76.70
50.12
29.15
26.64
22.52
14.05
f1 (ppm)

1h: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8.1451
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6.4106
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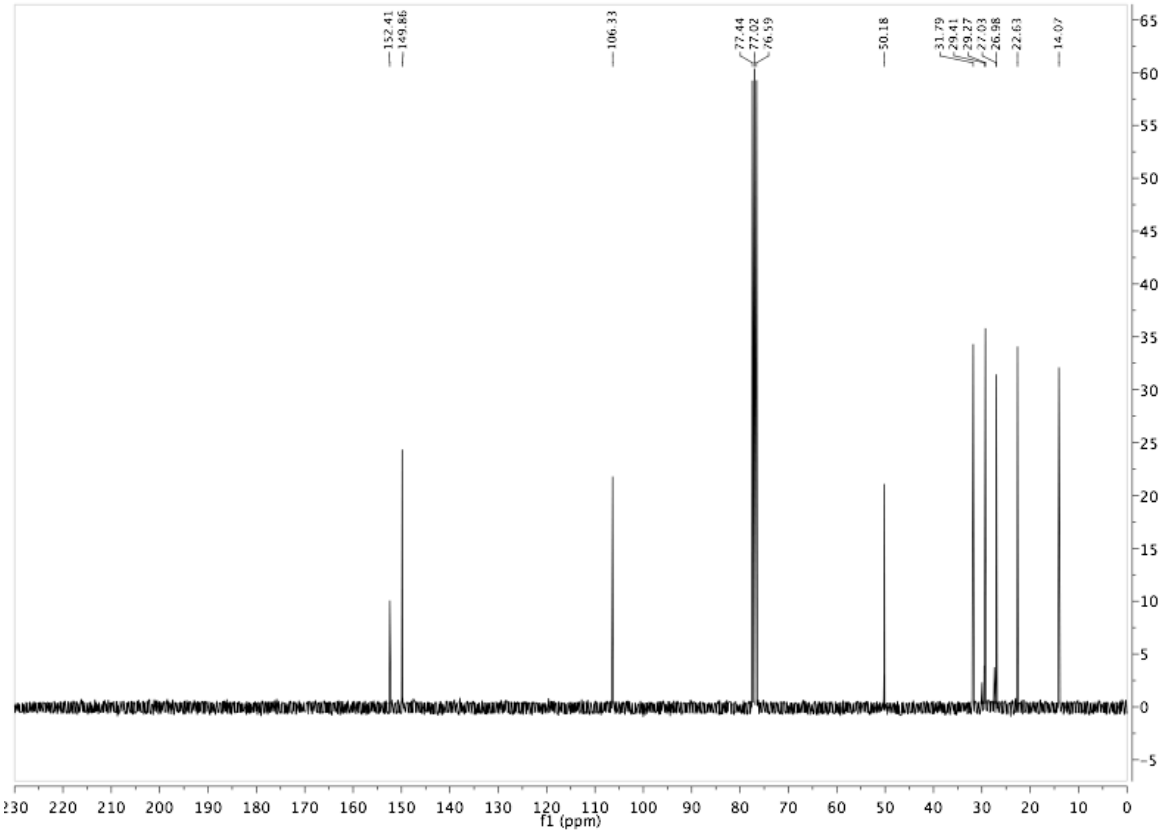
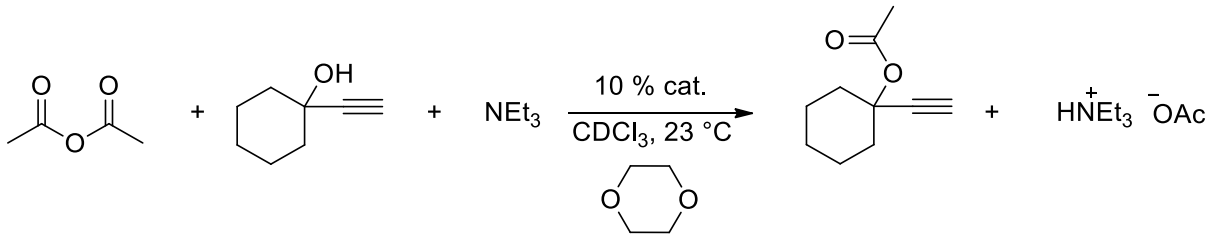
3.2156
1.5614
1.5383
1.3059
1.2934
1.2789
0.9037
0.8820
0.8587
2.00
2.04
4.10
4.46
21.10
6.32
f1 (ppm)


152.41
149.86
106.33
77.44
77.02
76.59
50.18
31.79
29.41
29.27
27.03
26.98
22.63
14.07
f1 (ppm)

3. Conduction and evaluation of kinetic measurements

3.1 Kinetic measurements using ^1H NMR spectroscopy

The benchmark reaction was carried out using stock solutions. The preparation of these stock solutions is carried out as follows: 3 *mmol* of the alcohol **4** and 9 *mmol* triethylamine are mixed in a graduated 5 *mL* measurement flask. In the same way 6 *mmol* anhydride and 1.5 *mmol* dioxane (internal Standard) are mixed in another graduated 5 *mL* measurement flask. In a third graduated 5 *mL* measurement flask 0.3 *mmol* of the catalyst is weighed in. After this every graduated 5 *mL* measurement flask is filled up to 5 *mL* with freshly distilled $CDCl_3$ and sealed with a septum. After shaking the 5 *mL* measurement flasks 200 *µL* of every stocksolution is transferred into a ovendried and degassed NMR-tube. The concentrations of the stocksolutions are: alcohol **4**: 0.6 *M*; anhydride: 1.2 *M*; triethylamine: 1.8 *M*; dioxane: 0.3 *M*; catalyst: 0.06 *M*.



Scheme S1. ^1H NMR benchmark reaction; acylation of a tertiary alcohol **4** in $CDCl_3$.

Concentrations used in the benchmark reaction: alcohol **4**: 0.2 *M*; anhydride: 0.4 *M*; triethylamine: 0.6 *M*; dioxane: 0.1 *M*; catalyst: 0.02 *M*.

Calculation of conversion:

$$Conversion = \left[\frac{4I_{ester}}{I_{ester} + I_{anhydride} + I_{ammoniumacestate}}\right] * 100\ \%$$

The used abbreviations are: = Singlett of $-CH_3$ at 1.9 *ppm*; = Singlett of 4 $-CH_2$ groups at 3.6 *ppm*; = Singlett of $-CH_3$ at 2.1 *ppm*; = Singlett of alkine proton at 2.3 *ppm*; = Singlett of $-CH_3$ at 1.8 *ppm*.
Figure S1 shows a ^1H NMR of a kinetic measurement where the different substrates are designated to the chemical shifts.

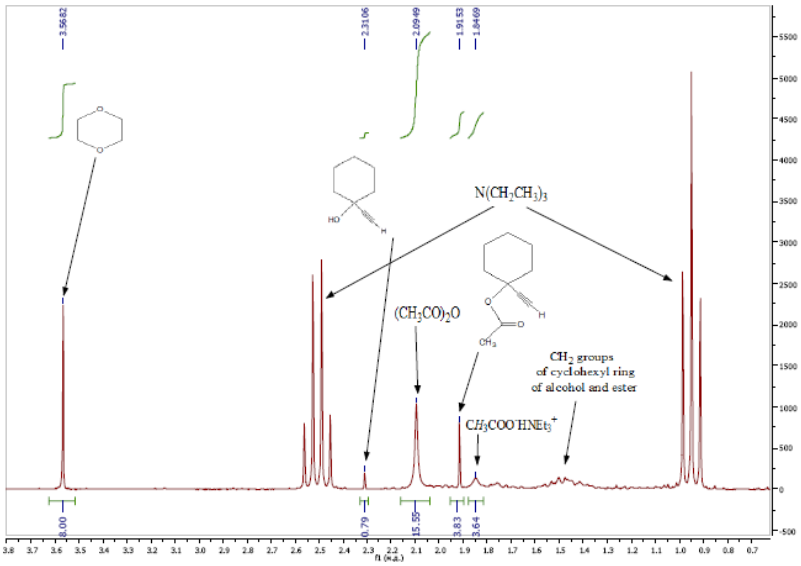


Figure S1. ^{1}H NMR (200 *MHz*) spectrum of reaction mixture for the benchmark reaction.

The experimental Data were fitted with a second order rate law:

$$conversion\ [\%] = c_1 * \left(1 - \frac{1}{2\exp\left(k\left(t - t_0\right)\right) - 1}\right) * 100$$

The resulting plot is depicted in Figure S2.

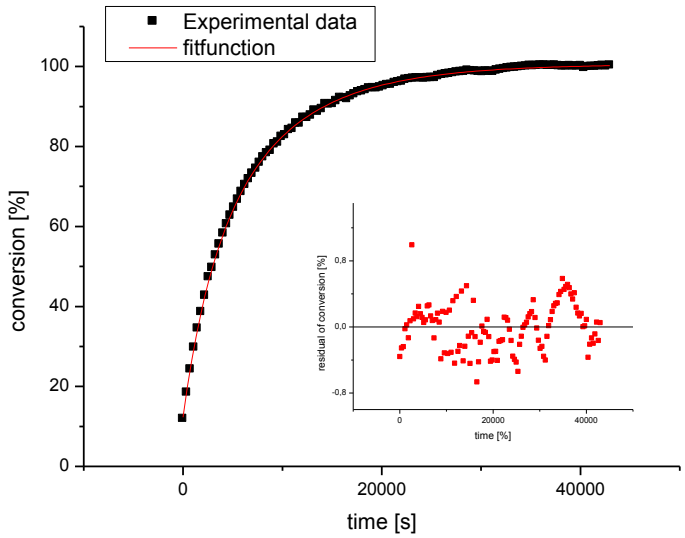


Figure S2. Results for the reaction of tertiary alcohol **4** and Ac_2O catalyzed by 10% PPY in $CDCl_3$.

Finally the kinetic half-life time is calculated by the following formula:

$$t_{1/2} = \frac{\ln 1.5}{k_2[ROH]_0}$$

3.2 Kinetic measurements using UV/vis spectroscopy

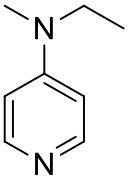
Materials. Benzoyl chloride (**6**) and benzylamine (**8**) were purchased and purified by distillation prior to use.
Acetonitrile (> 99.9%, extra dry) was purchased and used without further purification.

Kinetics. The kinetics of the reactions of the pyridines **1b–h** with benzoyl chloride (**6**) and that of 1-benzoylpyridinium chlorides **7b–h** with benzylamine (**8**) in acetonitrile at 20 °C were monitored by UV/Vis spectroscopy.
The stock solutions of the 1-benzoylpyridinium chlorides **7b–h** were prepared by mixing benzoyl chloride (**6**) with 1.0 equivalents of the pyridines **1b–h** in acetonitrile.
Stopped-flow spectrophotometer systems (Applied Photophysics SX.18MV-R or Hi-Tech SF-61DX2) were used for the investigation of the reactions. The kinetic runs were initiated by mixing equal volumes of acetonitrile solutions of the electrophiles and the nucleophiles. The temperature of the solutions during the kinetic studies was maintained to 20 °C within ± 0.1 °C by using circulating bath cryostats.
Benzoyl chloride (**6**) was used in large excess (more than 8 equivalents) relative to the pyridines **1b–h** to ensure first-order conditions with $k_{obs} = k_2[Nu]_0 + k_0$. For the reactions of 1-benzoyl pyridinium chlorides **7b–h** with benzylamine (**8**), the latter was used in excess. The first-order rate constants k_{obs} (s^{-1}) were obtained by least-squares fitting of the single-exponential curve $A_t = A_0e^{-kobst} + C$ or $A_t = A_0(1–e^{-kobst}) + C$ to the absorbances of the 1-benzoyl pyridinium chlorides **7b–h** at or close to λ_{max}. The slopes of the plot of k_{obs} versus the concentrations yielded the second order rate constant k_2 (M^{-1} s^{-1}).

4. Data of kinetics

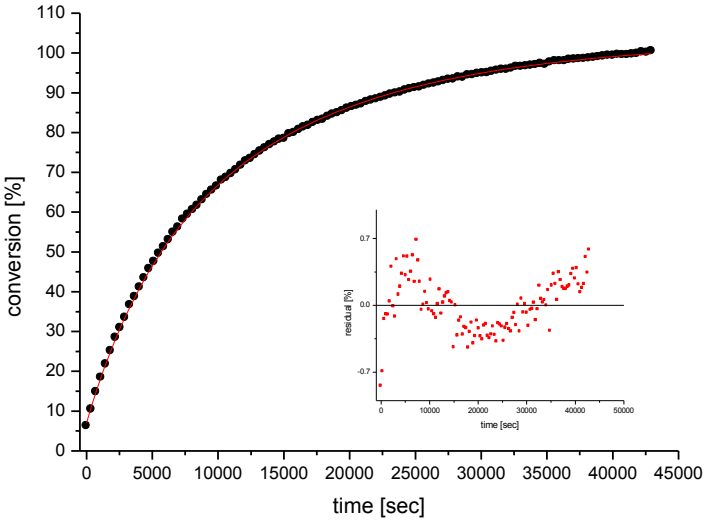
*4.1 Kinetics of the reactions of pyridines (**1a** – **1h**) with alcohol **4***

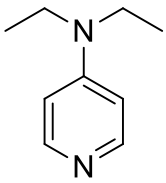
Kinetics of the reactions of catalysts **1a–h** with alcohol **4.** All time specifications are in minutes if not stated different. For every measurement the experimental data and the fit curve together with the residuals are depicted. Every experiment was done at least twice and the resulting kinetic half-life times are given with standard deviations.



1b

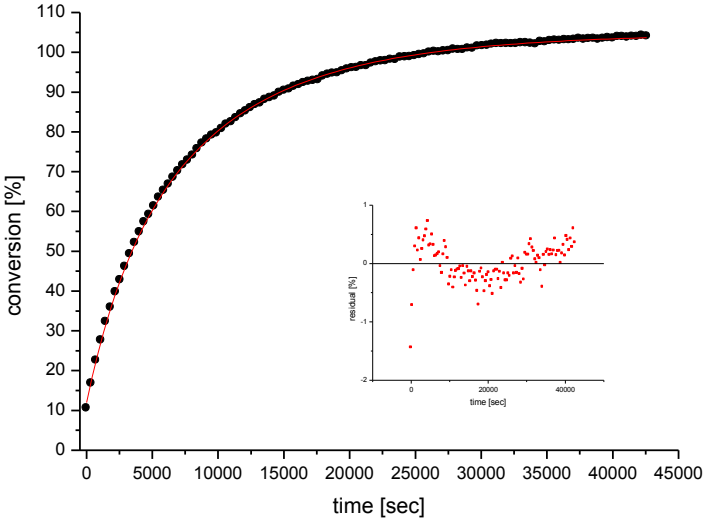
1) 110.1
2) 110.4
   = 110.3 ± 0.2

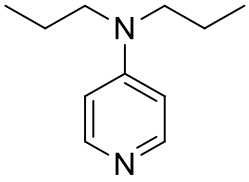




1c

1) 74.3
2) 75.4
   = 74.9 ± 0.6

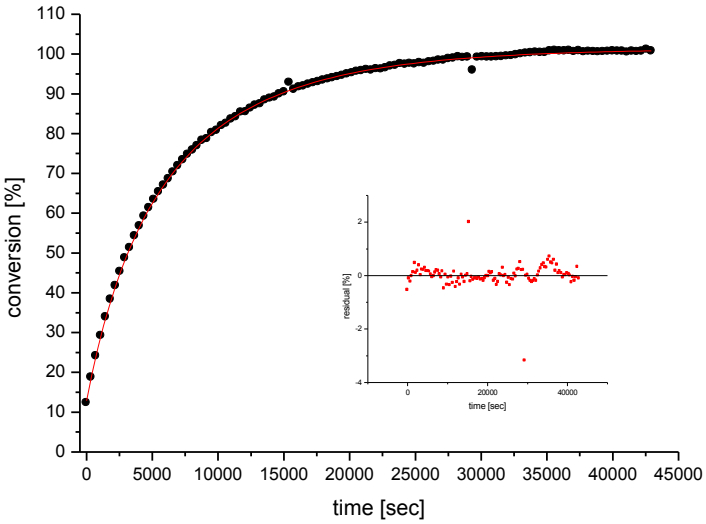


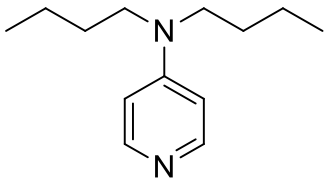


1d

1) 65.1
2) 65.8

= 65.5 ± 0.4

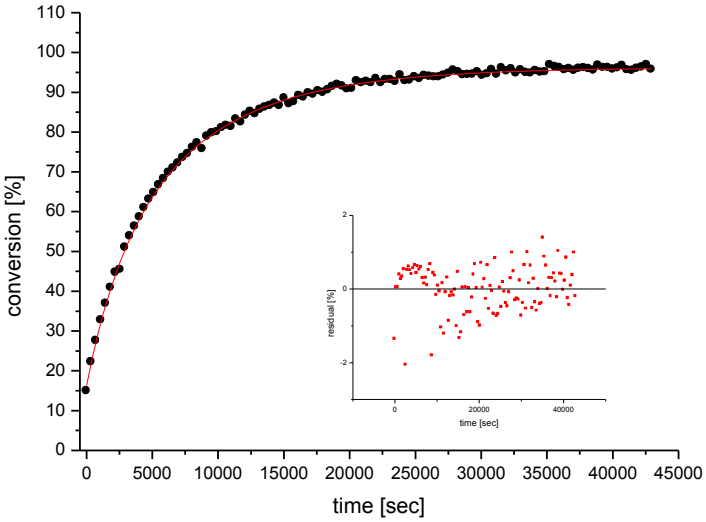


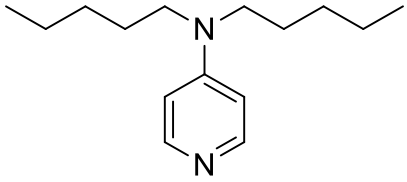


1e

1) 57.1
2) 60.3

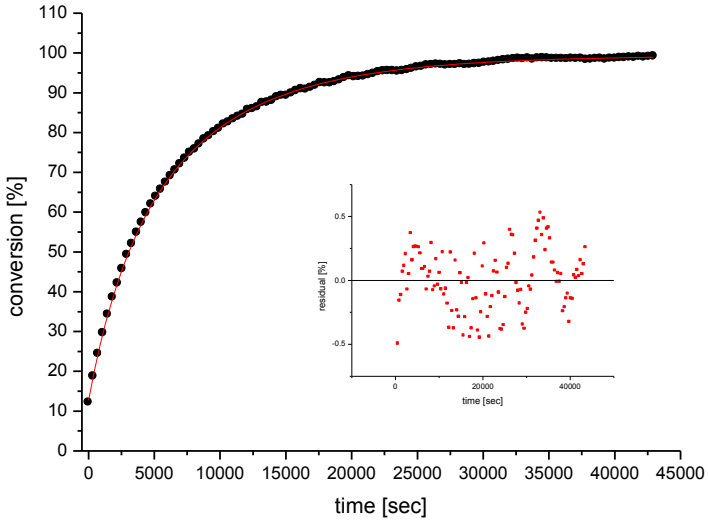
= 58.7 ± 1.6

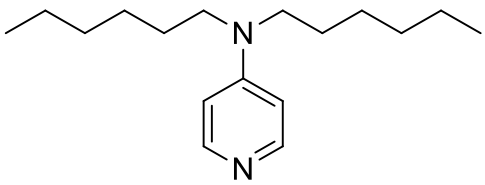




1f

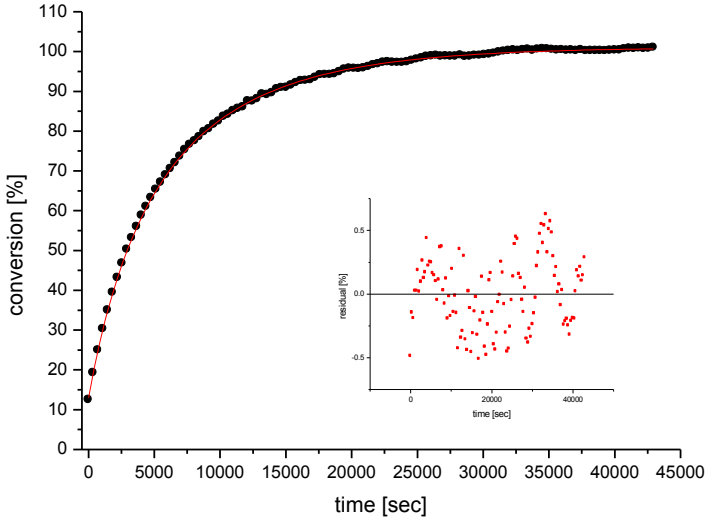
1) 61.1
2) 60.4
   = 60.8 ± 0.3

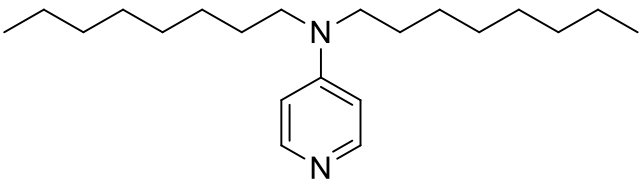




1g

1) 60.8
2) 61.2
   = 61.0 ± 0.2

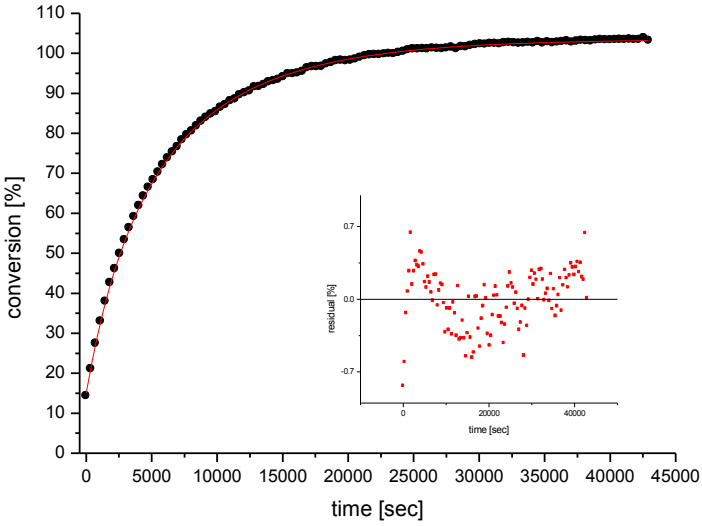




1h

1) 58.6
2) 59.5

= 59.1 ± 0.5



*4.2 Kinetics of the reactions of pyridines (**1a** – **1h**) with benzoyl chloride (**6**)*

Table S1: Rate constants for the reactions of 4-(ethylmethylamino)pyridine (**1b**) with benzoyl chloride (**6**) in CH_3CN (20 °C, λ = 320 nm).

$[\mathbf{1b}]_0$/M	$[\mathbf{6}]_0$/M	$[\mathbf{6}]_0/[\mathbf{1b}]_0$	k_{obs}/s^{-1}
3.69×10^{-5}	7.75×10^{-4}	21	2.92×10^{1}
3.69×10^{-5}	1.10×10^{-3}	30	3.94×10^{1}
3.69×10^{-5}	1.49×10^{-3}	40	5.30×10^{1}
3.69×10^{-5}	1.87×10^{-3}	51	6.57×10^{1}
3.69×10^{-5}	2.26×10^{-3}	61	7.89×10^{1}
$k_2 = 3.36 \times 10^4\ M^{-1}\ s^{-1}$			

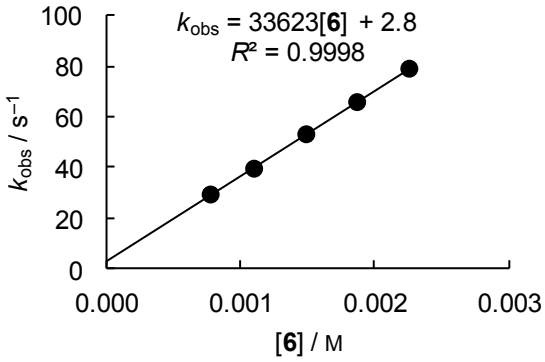


Table S2: Rate constants for the reactions of 4-(diethylamino)pyridine (**1c**) with benzoyl chloride (**6**) in CH_3CN (20 °C, λ = 320 nm).

$[\mathbf{1c}]_0$/M	$[\mathbf{6}]_0$/M	$[\mathbf{6}]_0/[\mathbf{1c}]_0$	k_{obs}/s^{-1}
3.71×10^{-5}	7.75×10^{-4}	21	3.46×10^{1}
3.71×10^{-5}	1.10×10^{-3}	30	4.71×10^{1}
3.71×10^{-5}	1.49×10^{-3}	40	6.32×10^{1}
3.71×10^{-5}	1.87×10^{-3}	50	7.79×10^{1}
3.71×10^{-5}	2.26×10^{-3}	61	9.51×10^{1}
$k_2 = 4.06 \times 10^4\ M^{-1}\ s^{-1}$			

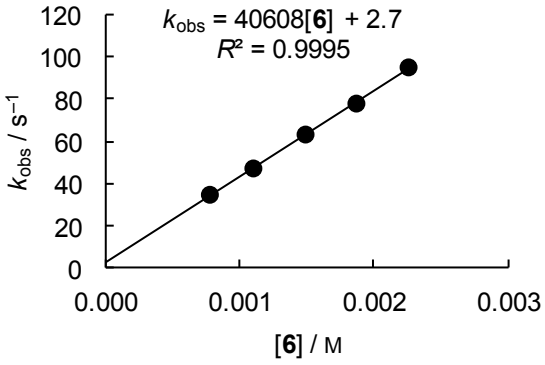


Table S3: Rate constants for the reactions of 4-(di-*n*-butylamino)pyridine (**1e**) with benzoyl chloride (**6**) in CH_3CN (20 °C, λ = 320 nm).

$[\mathbf{1e}]_0$/M	$[\mathbf{6}]_0$/M	$[\mathbf{6}]_0/[\mathbf{1e}]_0$	k_{obs}/s^{-1}
3.42×10^{-5}	7.24×10^{-4}	21	3.30×10^{1}
3.42×10^{-5}	1.11×10^{-3}	32	4.95×10^{1}
3.42×10^{-5}	1.45×10^{-3}	42	6.42×10^{1}
3.42×10^{-5}	1.83×10^{-3}	54	7.98×10^{1}
3.42×10^{-5}	2.22×10^{-3}	65	9.47×10^{1}
$k_2 = 4.14 \times 10^4\ M^{-1}\ s^{-1}$			

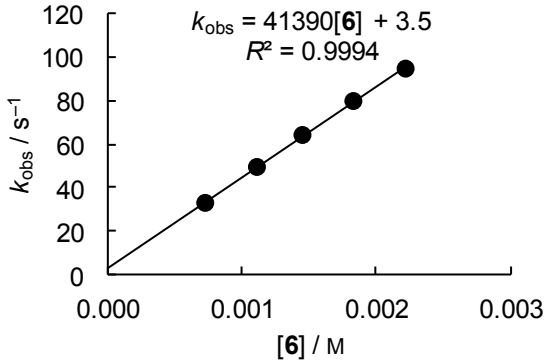


Table S4: Rate constants for the reactions of 4-(di-*n*-hexylamino)pyridine (**1g**) with benzoyl chloride (**6**) in CH_3CN (20 °C, λ = 320 nm).

$[\mathbf{1g}]_0$/M	$[\mathbf{6}]_0$/M	$[\mathbf{6}]_0/[\mathbf{1g}]_0$	k_{obs}/s^{-1}
3.40×10^{-5}	6.79×10^{-4}	20	3.28×10^{1}
3.40×10^{-5}	1.02×10^{-3}	30	4.70×10^{1}
3.40×10^{-5}	1.36×10^{-3}	40	6.16×10^{1}
3.40×10^{-5}	1.70×10^{-3}	50	7.54×10^{1}
3.40×10^{-5}	2.04×10^{-3}	60	8.88×10^{1}
$k_2 = 4.13 \times 10^{4}$ M^{-1} s^{-1}			

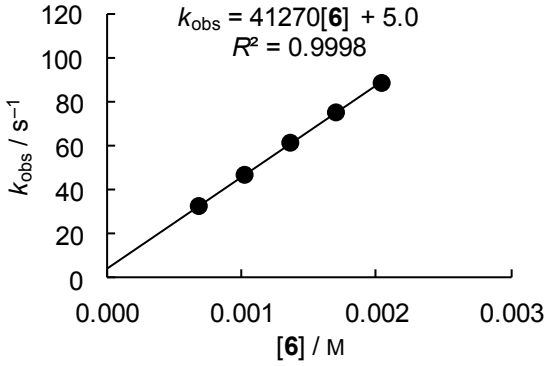
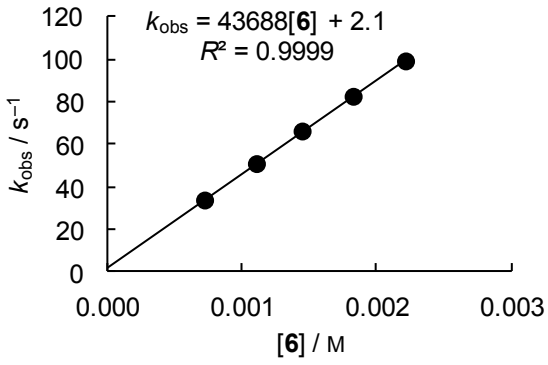


Table S5: Rate constants for the reactions of 4-(di-*n*-oktylamino)pyridine (**1h**) with benzoyl chloride (**6**) in CH_3CN (20 °C, λ = 320 nm).

$[\mathbf{1h}]_0$/M	$[\mathbf{6}]_0$/M	$[\mathbf{6}]_0/[\mathbf{1h}]_0$	k_{obs}/s^{-1}
3.70×10^{-5}	7.24×10^{-4}	20	3.35×10^{1}
3.70×10^{-5}	1.11×10^{-3}	30	5.06×10^{1}
3.70×10^{-5}	1.45×10^{-3}	39	6.59×10^{1}
3.70×10^{-5}	1.83×10^{-3}	49	8.22×10^{1}
3.70×10^{-5}	2.22×10^{-3}	60	9.88×10^{1}
$k_2 = 4.37 \times 10^{4}$ M^{-1} s^{-1}			



4.3 Kinetics of the reactions of N-benzoyl pyridinium chlorides (7) with benzylamine (8).

Table S6: Rate constants for the reactions of 1-benzoyl 4-(ethylmethylamino)pyridinium chloride (**7b**) generated from benzoyl chloride (**6**) and 4-(ethylmethylamino)pyridine (**1b**, 1.0 equiv.) with benzylamine (**8**) in CH_3CN (20 °C, λ = 320 nm).

$[\mathbf{7b}]_0$/M	$[\mathbf{8}]_0$/M	$[\mathbf{8}]_0/[\mathbf{7b}]_0$	k_{obs}/s^{-1}
3.32×10^{-5}	6.41×10^{-4}	19	2.69×10^{-1}
3.32×10^{-5}	1.28×10^{-3}	39	5.29×10^{-1}
3.32×10^{-5}	1.92×10^{-3}	58	7.89×10^{-1}
3.32×10^{-5}	2.56×10^{-3}	77	1.06
3.32×10^{-5}	3.20×10^{-3}	96	1.32
	$k_2 = 4.11 \times 10^2$ M^{-1} s^{-1}		

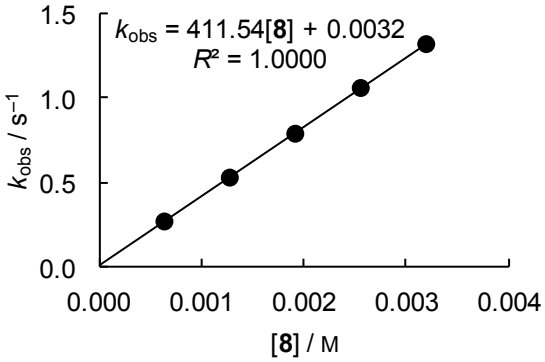


Table S7: Rate constants for the reactions of 1-benzoyl 4-(diethylamino)pyridinium chloride (**7c**) generated from benzoyl chloride (**6**) and 4-(diethylamino)pyridine (**1c**, 1.0 equiv.) with benzylamine (**8**) in CH_3CN (20 °C, λ = 320 nm).

$[\mathbf{7c}]_0$/M	$[\mathbf{8}]_0$/M	$[\mathbf{8}]_0/[\mathbf{7c}]_0$	k_{obs}/s^{-1}
3.23×10^{-5}	6.41×10^{-4}	20	2.53×10^{-1}
3.23×10^{-5}	1.28×10^{-3}	40	4.89×10^{-1}
3.23×10^{-5}	1.92×10^{-3}	59	7.26×10^{-1}
3.23×10^{-5}	2.56×10^{-3}	79	9.72×10^{-1}
3.23×10^{-5}	3.20×10^{-3}	99	1.22
	$k_2 = 3.78 \times 10^2$ M^{-1} s^{-1}		

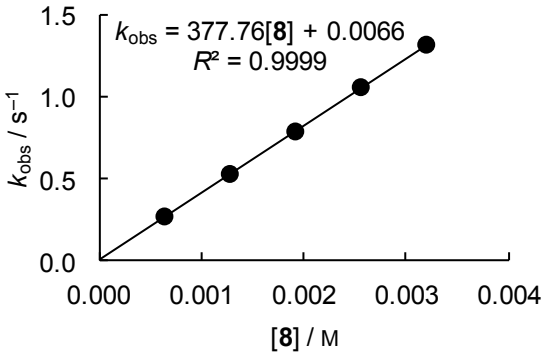


Table S8:. Rate constants for the reactions of 1-benzoyl 4-(di-*n*-butylamino)pyridinium chloride (**7e**) generated from benzoyl chloride (**6**) and 4-(di-*n*-butylamino)pyridine (**1e**, 1.0 equiv.) with benzylamine (**8**) in CH_3CN (20 °C, λ = 320 nm).

$[\mathbf{7e}]_0$/M	$[\mathbf{8}]_0$/M	$[\mathbf{8}]_0/[\mathbf{7e}]_0$	k_{obs}/s^{-1}
3.28×10^{-5}	6.26×10^{-4}	19	2.28×10^{-1}
3.28×10^{-5}	1.25×10^{-3}	38	4.64×10^{-1}
3.28×10^{-5}	1.88×10^{-3}	57	6.95×10^{-1}
3.28×10^{-5}	2.51×10^{-3}	77	9.27×10^{-1}
3.28×10^{-5}	3.13×10^{-3}	95	1.15
	$k_2 = 3.68 \times 10^2\ M^{-1}\ s^{-1}$		

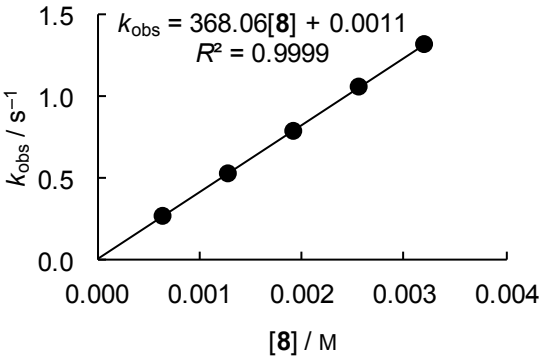


Table S9: Rate constants for the reactions of 1-benzoyl 4-(di-*n*-hexylamino)pyridinium chloride (**7g**) generated from benzoyl chloride (**6**) and 4-(di-*n*-hexylamino)pyridine (**1g**, 1.0 equiv.) with benzylamine (**8**) in CH_3CN (20 °C, λ = 320 nm).

$[\mathbf{7g}]_0$/M	$[\mathbf{8}]_0$/M	$[\mathbf{8}]_0/[\mathbf{7g}]_0$	k_{obs}/s^{-1}
3.40×10^{-5}	6.92×10^{-4}	20	2.47×10^{-1}
3.40×10^{-5}	1.39×10^{-3}	41	4.96×10^{-1}
3.40×10^{-5}	2.08×10^{-3}	61	7.37×10^{-1}
3.40×10^{-5}	2.67×10^{-3}	79	9.48×10^{-1}
3.40×10^{-5}	3.36×10^{-3}	99	1.19
	$k_2 = 3.53 \times 10^2\ M^{-1}\ s^{-1}$		

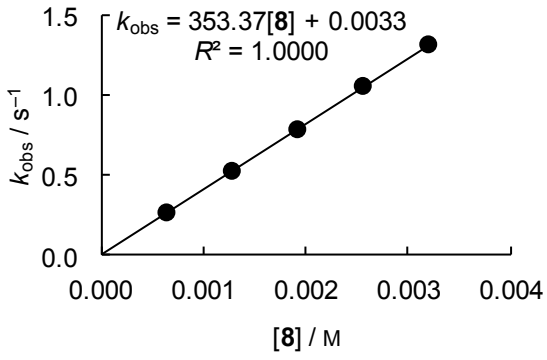
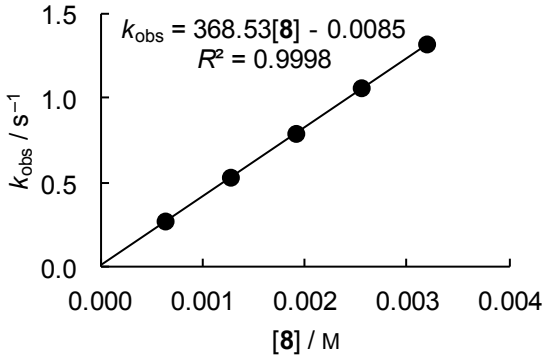


Table S10: Rate constants for the reactions of 1-benzoyl 4-(di-*n*-oktylamino)pyridinium chloride (**7h**) generated from benzoyl chloride (**6**) and 4-(di-*n*-oktylamino)pyridine (**1h**, 1.0 equiv.) with benzylamine (**8**) in CH_3CN (20 °C, λ = 320 nm).

$[\mathbf{7h}]_0$/M	$[\mathbf{8}]_0$/M	$[\mathbf{8}]_0/[\mathbf{7h}]_0$	k_{obs}/s^{-1}
3.28×10^{-5}	6.26×10^{-4}	19	2.23×10^{-1}
3.28×10^{-5}	1.25×10^{-3}	38	4.53×10^{-1}
3.28×10^{-5}	1.88×10^{-3}	57	6.85×10^{-1}
3.28×10^{-5}	2.51×10^{-3}	77	9.09×10^{-1}
3.28×10^{-5}	3.13×10^{-3}	95	1.15
	$k_2 = 3.69 \times 10^2\ M^{-1}\ s^{-1}$		



5. Additional correlations

Table S11. N-C bond lengths r(N-C) of the acetylated catalysts **10a**–**h.**

Acetylated catalyst	r(N-C) [pm]
10a	148.29
10b	148.08
10c	147.86
10d	147.69
10e	147.64
10f	147.53
10g	147.54
10h	147.48

Stronger electron donating effects of longer alkyl substituents may also be reflected in the overal charge of the pyridine nitrogen atom, which is often portrayed as the "formal" center of positive charge in acylpyridinium ions. Practically any population analysis method shows that the pyridine nitrogen atoms in acylpyridinium ions **10** carry a negative partial charge and that the formal positive charge is not helpful in understanding the charge distribution in this type of system. However, the partial charge of the pyridinium nitrogen atom does vary with the size of the alkyl substituents in the expected manner, assuming slightly more negative values with longer alkyl substituents. The magnitude of these variations is, however, very small and does not lend itself to quantitative analysis (see Table S12 and Figure S3). The same is true for analysis of the acyl group charge in acylpyridinium ions **10a**–**h**, even though the variations are slightly larger (see Table S13 and Figure S4).

Table S12. Mulliken charges q(N) on the pyridinium nitrogen atom of the acylated catalysts **10a**–**h.**

Acetylated catalyst	q(N)
10a	-0.781
10b	-0.782
10c	-0.783
10d	-0.783
10e	-0.783
10f	-0.783
10g	-0.783
10h	-0.783

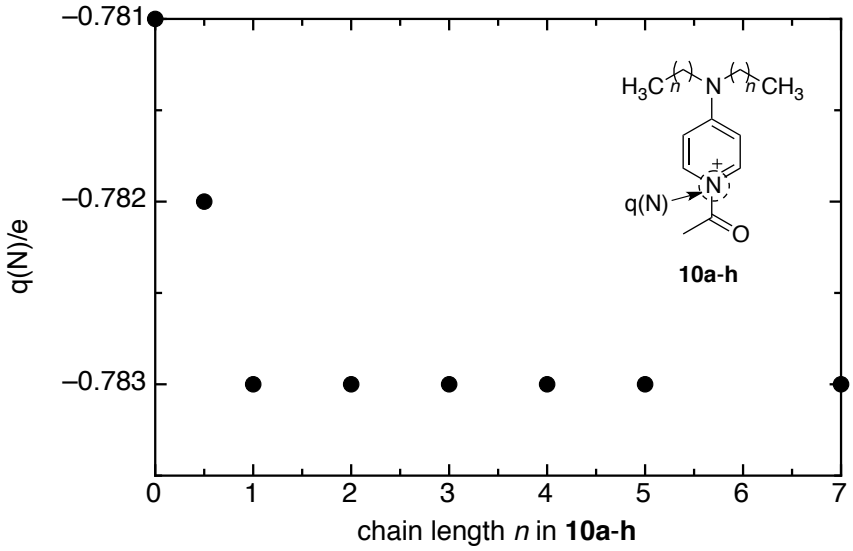


Figure S3. Mulliken charges q(N) on the pyridinium nitrogen atom in the best conformers of **10a – h**.

Table S13. Mulliken charges q(N) on the pyridinium nitrogen atom of the acylated catalysts **10a**–**h**.

Acetylated catalyst	q($COCH_3$) in **10a – 10h**
10a	0.383
10b	0.381
10c	0.378
10d	0.377
10e	0.377
10f	0.375
10g	0.375
10h	0.375

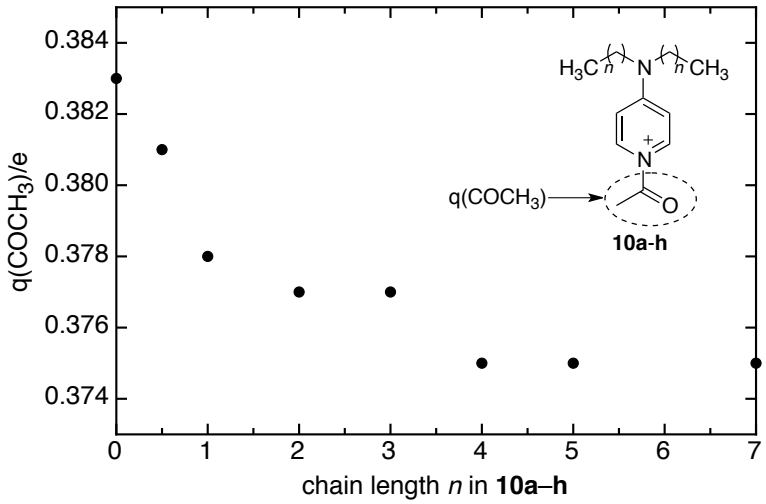


Figure S4. Mulliken charges q($COCH_3$) of the whole acyl group in **10a – h** for the best conformers.

Table S14. ^{1}H NMR shifts $\delta(^1H,CH_3)$ of the terminal CH_3 groups in pyridines **1a**–**h**.

Catalyst	$\delta(^1H,CH_3)$ [ppm]
1a	2.9799
1b	2.0204
1c	1.172
1d	0.9123
1e	0.9484
1f	0.9077
1g	0.8896
1h	0.8585

6. Calculation of inductive effects by an increment-based method

Adapted method for calculation of σ^*-values from Galkin *et al*.[6]

The calculation of σ^*-values and $\log\frac{k_X}{k_H}$ was performed according to Eq. (1) and Eq. (2). The models surveyed can be found in the main text in Figure 9.

Table S15. Electronegativity χ and covalent radii R for nitrogen, carbon and hydrogen atoms.

	N	C	H
χ	3.04	2.55	2.20
R [pm]	71	sp^3: 76	31
		sp^2: 73	
		sp: 69	

[a] Pauling scale[13]; [b] data from Ref.[14]

The bond lengths in **1a**–**h** necessary for the determination of r_i in Eq. (1) are given in Figure S5.

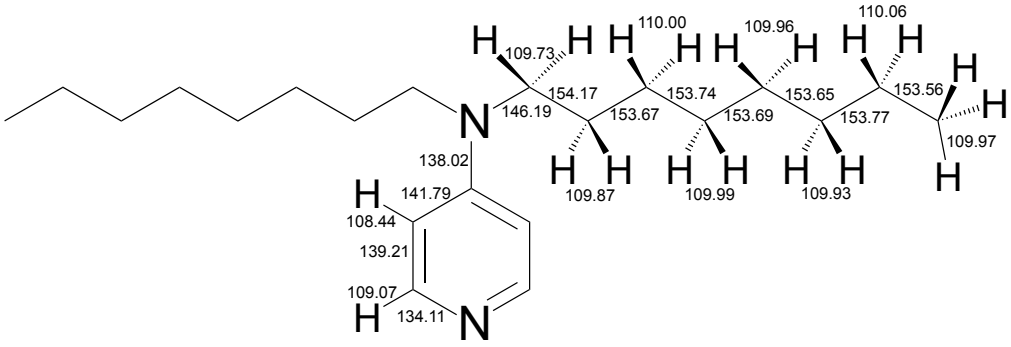


Figure S5. Bond length in **1a**–**1h**.

Plotting the σ^*-values from Table 5 in the main text vs. the alkyl chain length in **1a**–**h** for models 1–3 leads to Figures S6 – S8.

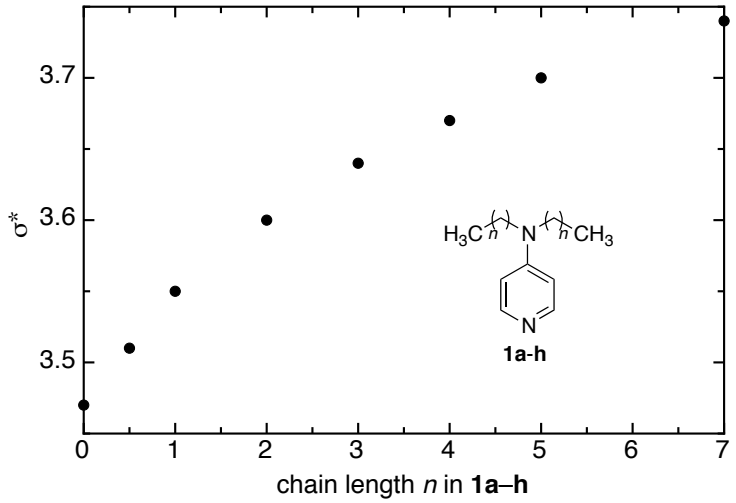


Figure S6. σ^*-values vs. chain length *n* in **1a**–**h** for model 1.

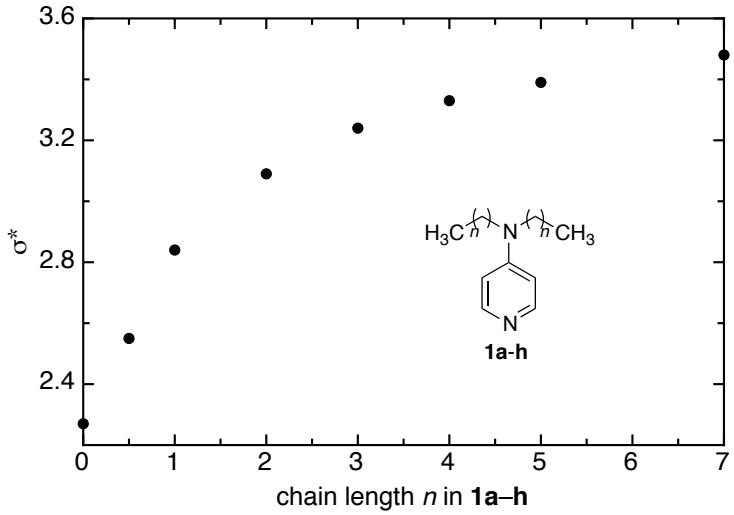


Figure S7. σ^*-values vs. chain length *n* in **1a**–**h** for model 2.

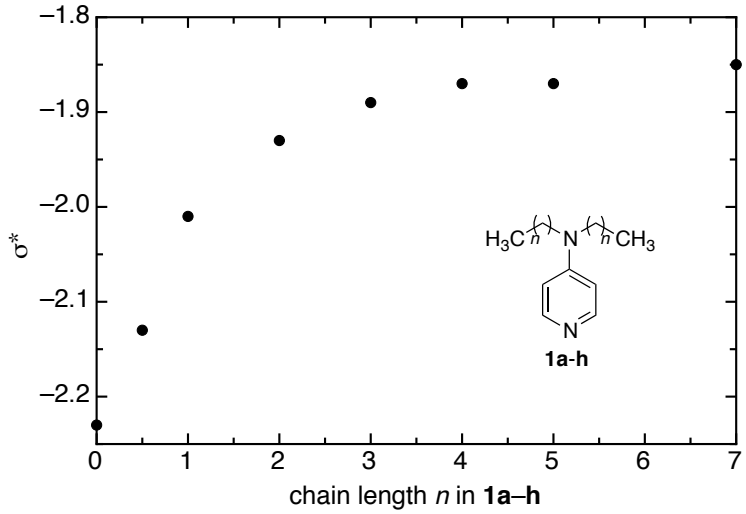


Figure S8. σ^*-values vs. chain length *n* in **1a**–**h** for model 3.

In the following part the σ* value of **1a** for model 1 will be calculated exemplarily:

$$\sigma^* = 7.840 \cdot \sum_i \Delta\chi_i \frac{R_i^2}{r_i^2}$$

Point of reference in model 1 is the pyridine nitrogen. From there on the single contributions of every atom will be added. Since **1a** is symmetric, the summation will be done for one half of the molecule and the contributions can then be doubled.

$$\sigma^* = 7.840 \cdot \left(\left(0.49 \cdot \frac{73^2}{134.11^2} + 0.84 \cdot \frac{31^2}{243.18^2} + 0.49 \cdot \frac{73^2}{273.32^2} + 0.84 \cdot \frac{31^2}{381.76^2} + 0.49 \cdot \frac{73^2}{415.11^2} + 0 \cdot \frac{71^2}{553.13^2} + 0.49 \cdot \frac{76^2}{699.32^2} + 0.84 \frac{31^2}{809.05^2}\right) \cdot 2\right)$$

$$= 7.840 \cdot ((1.45 \cdot 10^{-1} + 1.37 \cdot 10^{-2} + 3.50 \cdot 10^{-2} + 5.54 \cdot 10^{-3} + 1.51 \cdot 10^{-2} + 0 + 5.79 \cdot 10^{-3} + 1.23 \cdot 10^{-3}) \cdot 2) = 7.840 \cdot 0.443 = 3.47$$

–> $\sigma^*_{(1a)} = 3.47$

Table S16. R^2-values together with the values for ρ σ^* properties for model 2 with exception of the ^{1}H NMR correlation in which the σ^* values for model 3 were used.

	σ^* (model 2)	model 1		model 2		model 3	
		R^2	ρ	R^2	ρ	R^2	ρ
1	$\log(k_2)$[a]	0.7727	1.42	0.9202	0.33	0.9731	1.07
2	$\log(k_{2(X)}/k_{2(\mathbf{1a})})$[b]	0.7727	1.42	0.9202	0.33	0.9731	1.07
3	$\log(k_2$(benzoylation)) [c]	0.8664	0.51	0.8752	0.12	0.9655	0.40
4	$\log(k_2$(aminolysis)) [d]	0.9370	-0.29	0.8262	0.09	0.8217	-0.37
5	$\Delta H_{298,ave}$ gas phase [e]	0.9333	-70.8	0.9935	-15.91	0.9889	-48.9
6	$\Delta H_{298,ave}$ solvation [f]	0.7847	-24.7	0.8968	-5.76	0.9301	-18.0
7	$\Delta H_{298,best}$ gas phase [g]	0.8892	-63.9	0.9809	-14.61	0.9942	-45.3
8	$\Delta H_{298,best}$ solvation [h]	0.6663	-21.3	0.7955	-5.07	0.8488	-16.2
9	$\Delta H_{298,best}$ only electrostatic [i]	0.9257	-25.0	0.9599	-5.56	0.9310	-16.8
10	$\Delta H_{298,best}$ only non-electrostatic [j]	0.9620	-69.00	0.9911	-15.26	0.9622	-46.3
11	r(N-C) [k]	0.9216	-2.96	0.9925	-0.67	0.9923	-2.06
12	q(N)[l]	0.5856	-6.03×10^{-3}	0.7696	-1.51×10^{-3}	0.8538	-4.88×10^{-3}
13	q($COCH_3$)[m]	0.8887	-2.97×10^{-2}	0.9657	-6.74×10^{-3}	0.9691	-2.08×10^{-2}
14	^{1}H NMR shifts[n]	0.6863	-6.75	0.8554	-1.64	0.9236	-5.25
		$\Delta\sigma^*$		$\Delta\sigma^*$		$\Delta\sigma^*$	
15	$\log(k_2)$[a]	0.7727	1.42	0.9202	0.33	0.9731	1.07
16	$\log(k_{2(X)}/k_{2(\mathbf{1a})})$[b]	0.7727	1.42	0.9202	0.33	0.9731	1.07

[a] Observed reaction rates in reaction (**I**) according to Scheme 2; [b] Observed reaction rates of **1a**–**h** in reaction (**I**) according to Scheme 2 in relation to the reaction rate obtained for **1a**; [c] Observed reaction rates for benzoylation reaction (**II**) according to Scheme 4; [d] Observed reaction rates for aminolysis reaction (**III**) according to Scheme 4; [e] Boltzmann averaged ΔH_{298} at MP2-5 level of theory: "MP2-5": MP2/6-31+G(2d,p)//B98/6-31G(d); [f] Boltzmann averaged ΔH_{298} at MP2-5 level of theory with PCM/UAHF/RHF/6-31G(d) solvation energies for chloroform; [g] Energetically best conformer used for the calculation of ΔH_{298} at MP2-5 level of theory; [h] Energetically best conformer used for the calculation of ΔH_{298} at MP2-5 level of theory with inclusion of solvent effects as described above; [i] Acetylation enthalpies for **1a–h** according to Scheme 5 including only the electrostatic term for the solvent contribution; [j] Acetylation enthalpies for **1a–h** according to Scheme 5 including only the non electrostatic term for the solvent contribution; [k] N-C bond length of the pyridine nitrogen and the carbonyl group in **11a**–**h**; [l] Mulliken charges on N in **10a**–**h**; [m] Mulliken charges for the whole acyl cation in **10a**–**h**; [n] ^{1}H NMR shifts of terminal CH_3-group in **1a–h.**

The plots for R^2-values better than 0.90 in Table S16 are given in the following section.

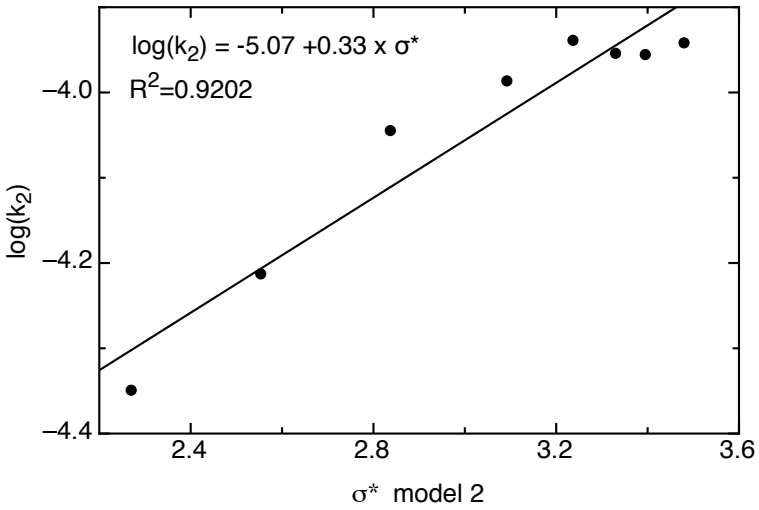


Figure S9. Observed log(k_2) values for acylation reaction (**I**) vs. σ^*-value determined for model 2.

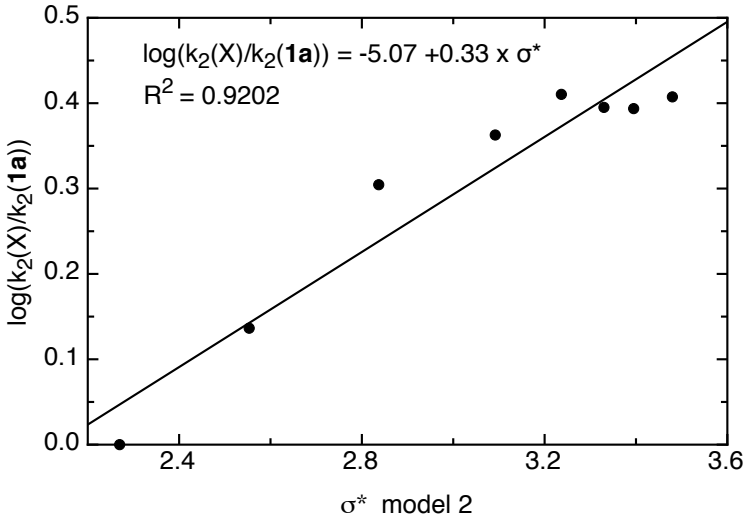


Figure S10. Observed log(k_2(X)/k_2(**1a**)) values for acylation reaction (**I**) vs. σ^*-value determined for model 2 with X=**1a**–**h**.

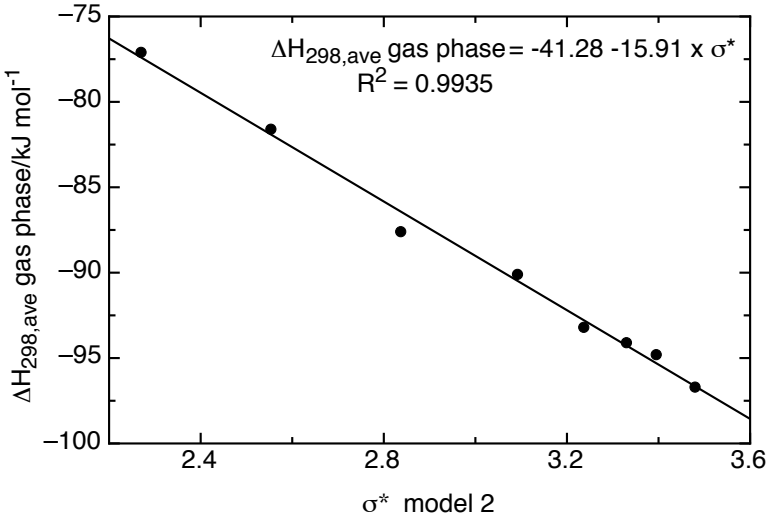


Figure S11. Boltzmann averaged ΔH_{298} in the gas phase at MP2-5 level of theory ($\Delta H_{298,ave.}$ (gas phase)) vs. σ^*-value determined for model 2.

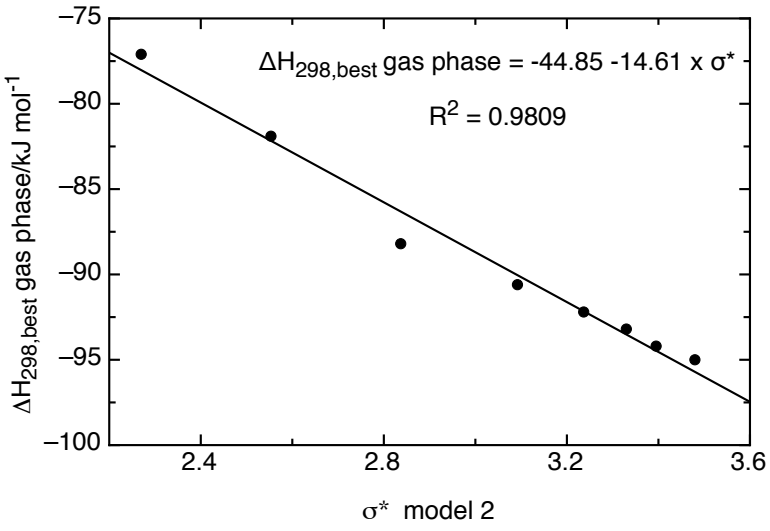


Figure S12. ΔH_{298} for the best conformer in the gas phase at MP2-5 level of theory ($\Delta H_{298,best}$ (gas phase)) vs. σ^*-value determined for model 2.

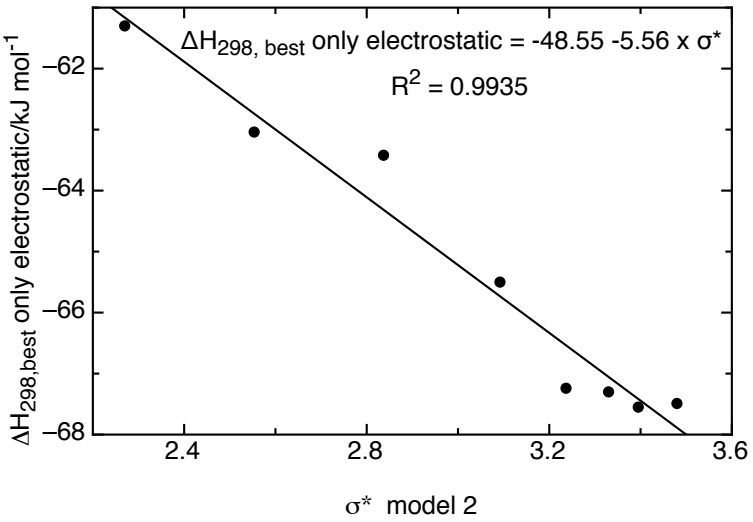


Figure S13. $\Delta H_{298,best}$ (only electrostatic) for **1a–h** according to Scheme 5 including only the electrostatic term for the solvent contribution at MP2-5 level of theory vs. σ^*-value determined for model 2.

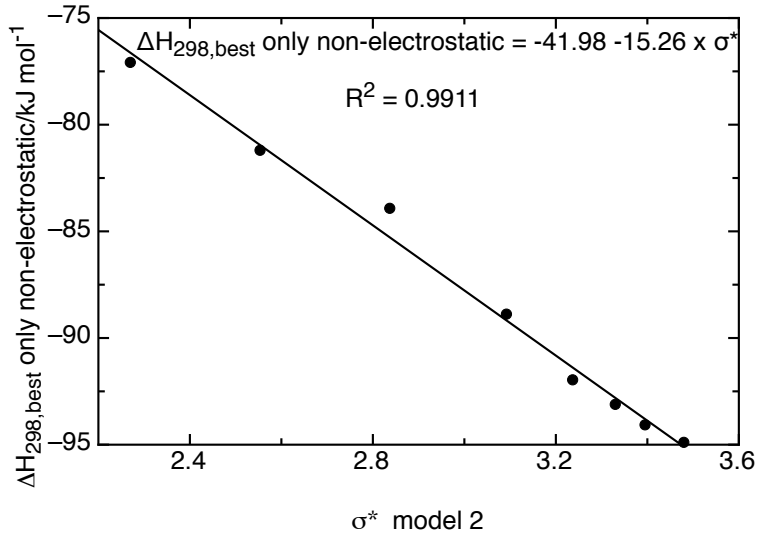


Figure S14. $\Delta H_{298,best}$ (only non-electrostatic) for **1a–h** according to Scheme 5 including only the non electrostatic term for the solvent contribution at MP2-5 level of theory vs. σ^*-value determined for model 2.

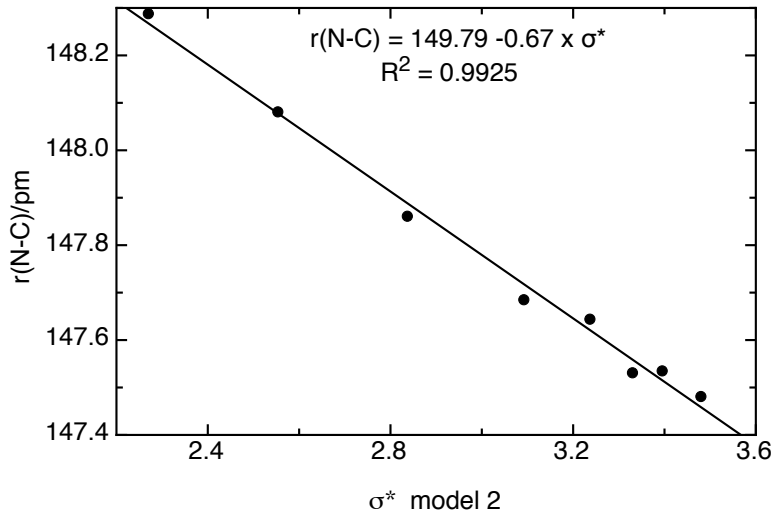


Figure S15. N-C bond length (r(N-C)) of the pyridine nitrogen and the carbonyl group in **10a**–**h** in [pm] vs. σ^*-value determined for model 2.

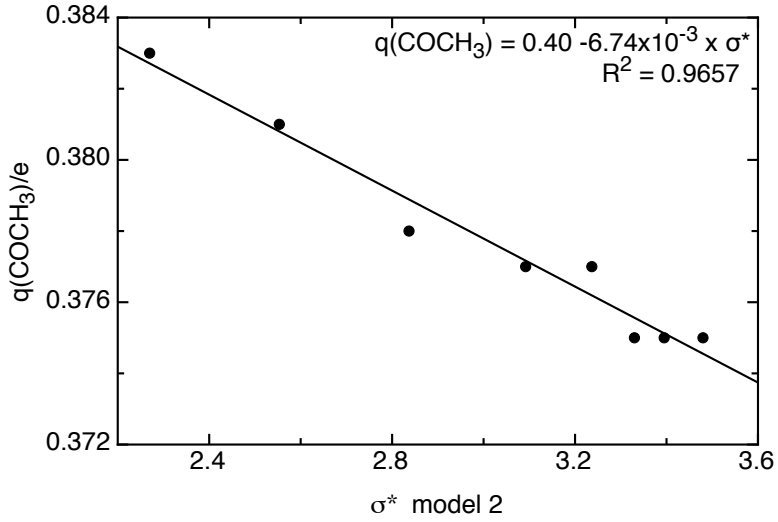


Figure S16. Charge of the whole acyl group (q($COCH_3$) in **10a**–**h** in [pm] vs. σ^*-value determined for model 2.

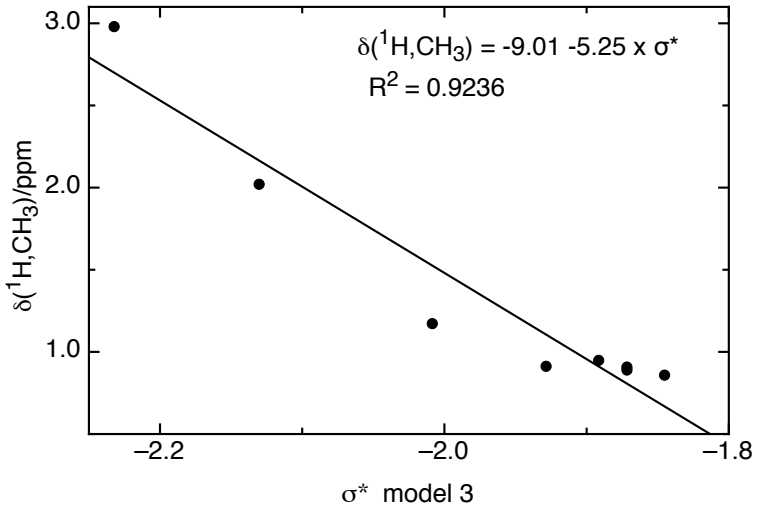


Figure S17. ^{1}H NMR shifts of terminal CH_3-group (δ^1H,CH_3) in **1a**–**h** in [ppm] vs. σ^*-value determined for model 2.

7. Theoretical procedures

Following a recently developed protocol for the calculation of cation affinity values,[15,16,2b] geometry optimizations have been performed in the gas phase at B98/6-31G(d) level. Thermal corrections to 289.15 K and 1 atm have been calculated at the same level of theory using the rigid rotor/harmonic oscillator model. Single point energies calculated at the MP2(FC)/6-31+G(2d,p) level have then been combined with thermal corrections obtained previously to calculate enthalpies (H_{298}) and free energies (G_{298}) at 298.15 K. Solvent effects in chloroform have subsequently been determined through single point calculations with the PCM/UAHF/RHF/6-31G(d) continuum solvation model. Partial atomic charges have been calculated using the Mulliken population analysis at the B98/6-31G(d) level. For selected systems calculations have been repeated using the G3(MP2)B3 compound scheme developed by Curtiss *et al.*[17,18] All quantum mechanical calculations have been performed with Gaussian 03.[19]

Table S17. Acetylation enthalpies [kJ/mol] for pyridines **1a–h** according to Scheme 5 for the Boltzmann-averaged, selected and best conformers calculated at MP2-5 level of theory or G3MP2B3 in the gas phase and in $CHCl_3$ solution.

catalyst	$\Delta H_{298,ave}$ [kJ/mol]		$\Delta H_{298,best}$ [kJ/mol]		$\Delta H_{298,sel}$ [kJ/mol]		$\Delta H_{298,sel}$ G3MP2B3 [kJ/mol]
	gas phase	$CHCl_3$	gas phase	$CHCl_3$	gas phase	$CHCl_3$	gas phase
1a	–77.1	–61.2	–77.1	–61.2	–77.1	–61.2	–81.8
1b	–81.6	–63.3	–81.9	–63.6	–81.3	–62.9	–86.6
1c	–87.6	–67.1	–88.2	–67.8	–88.2	–67.7	–92.6
1d	–90.1	–66.1	–90.6	–66.1	–88.9	–65.5	–93.9
1e	–93.2	–67.9	–92.2	–67.1	–92.1	–67.1	–97.3
1f	–94.1	–67.8	–93.2	–67.6	–93.2	–67.1	–98.6
1g	–94.8	–68.1	–94.2	–67.4	–94.2	–67.4	–99.6
1h	–96.7	–68.5	–95.0	–68.2	–95.0	–67.4	–

Table S18. Calculated energies of conformers for catalysts **1a** – **1h**, as calculated at MP2/6-31+G(2d,p)//B98/6-31G(d) level with inclusion of solvent effects at PCM/UAHF/RHF/6-31G(d).

Conf		**E_{tot} B98/6-31G(d)**	**H_{298} B98/6-31G(d)**	**E_{tot} MP2(FC)/6-31+G(2d.p)**	**$G_{solv.}$ kcal/mol**	**H_{298} MP2-5 with-out solvation**	**H_{298} MP2-5 with solvation**
Pyr							
1		-248.181767	-248.087628	-247.589433	-2.15	-247.495294	-247.498720
Pyr-Ac$^+$							
1	ac	-401.140005	-400.991697	-400.215517	-34.07	-400.067209	-400.121503
1a							
1		-382.100962	-381.928960	-381.179975	-3.27	-381.007973	-381.013184
1a-Ac$^+$							
1	ac	-535.091159	-534.864305	-533.836114	-31.39	-533.609261	-533.659284
1b							
1		-421.400415	-421.198543	-420.374849	-2.84	-420.172978	-420.177503
1b-Ac$^+$							
1	ac1	-574.392288	-574.135480	-573.032902	-30.37	-572.776094	-572.824492
1	ac2	-574.392332	-574.135258	-573.032926	-30.37	-572.775852	-572.824249
1c							
4		-460.699626	-460.467717	-459.569493	-2.29	-459.337583	-459.341233

5		-460.698872	-460.467017	-459.568777	-2.39	-459.336921	-459.340730
2		-460.695706	-460.463514	-459.566589	-2.54	-459.334396	-459.338444
12		-460.695601	-460.463698	-459.566199	-2.53	-459.334296	-459.338328
10		-460.688598	-460.457621	-459.563361	-1.71	-459.332384	-459.335109
1c-Ac$^+$							
4	ac1	-613.693223	-613.406531	-612.229788	-29.32	-611.943096	-611.989821
4	ac2	-613.693223	-613.406527	-612.229789	-29.32	-611.943093	-611.989817
12	ac2	-613.691702	-613.404882	-612.228221	-29.54	-611.941402	-611.988477
12	ac1	-613.691702	-613.404881	-612.228221	-29.54	-611.941400	-611.988475
5	ac1	-613.691701	-613.404880	-612.228221	-29.54	-611.941399	-611.988474
10	ac2	-613.691702	-613.404879	-612.228221	-29.54	-611.941399	-611.988474
10	ac1	-613.691702	-613.404879	-612.228221	-29.54	-611.941399	-611.988474
5	ac2	-613.691701	-613.404879	-612.228221	-29.54	-611.941398	-611.988473
2	ac1	-613.688778	-613.401873	-612.225068	-29.50	-611.938163	-611.985174
2	ac2	-613.688797	-613.401760	-612.224973	-29.51	-611.937936	-611.984963
1d							
37		-539.292811	-539.001043	-537.954451	-0.71	-537.662683	-537.663814
34		-539.293771	-539.002066	-537.954231	-0.65	-537.662525	-537.663561
29		-539.288540	-538.997719	-537.952842	-0.86	-537.662021	-537.663391
7		-539.294761	-539.003085	-537.953964	-0.67	-537.662288	-537.663356
48		-539.292832	-539.001072	-537.953309	-0.82	-537.661549	-537.662856
49		-539.292832	-539.001067	-537.953310	-0.82	-537.661545	-537.662852
9		-539.294028	-539.002224	-537.953368	-0.62	-537.661564	-537.662552
64		-539.292137	-539.000246	-537.953085	-0.66	-537.661193	-537.662245
61		-539.291362	-538.999336	-537.952841	-0.86	-537.660814	-537.662185
111		-539.290465	-538.998527	-537.952504	-0.91	-537.660566	-537.662017
62		-539.291992	-539.000333	-537.952415	-0.69	-537.660756	-537.661856
85		-539.290007	-538.998114	-537.951373	-1.03	-537.659480	-537.661121
18		-539.288610	-538.996981	-537.951579	-0.50	-537.659950	-537.660747
3		-539.289875	-538.997982	-537.951279	-0.61	-537.659386	-537.660358
103		-539.288696	-538.996917	-537.950548	-0.85	-537.658770	-537.660124
15		-539.288720	-538.996971	-537.950657	-0.71	-537.658908	-537.660039
11		-539.290276	-538.998313	-537.950527	-0.87	-537.658564	-537.659950
24		-539.288889	-538.997060	-537.949759	-0.88	-537.657931	-537.659333
70		-539.287980	-538.996108	-537.949538	-0.96	-537.657666	-537.659196
90		-539.287099	-538.995070	-537.949661	-0.93	-537.657632	-537.659114
84		-539.287698	-538.995852	-537.949137	-0.86	-537.657291	-537.658661
39		-539.282774	-538.992967	-537.948055	0.48	-537.658248	-537.657483
60		-539.286580	-538.994778	-537.946978	-1.00	-537.655175	-537.656769
44		-539.283056	-538.991938	-537.947933	0.25	-537.656815	-537.656416
40		-539.283243	-538.992118	-537.947716	0.11	-537.656590	-537.656415
36		-539.283164	-538.992152	-537.946893	-0.16	-537.655882	-537.656137
78		-539.283972	-538.992085	-537.945907	-0.91	-537.654020	-537.655470
97		-539.284282	-538.992454	-537.945351	-1.04	-537.653523	-537.655180
1d-Ac$^+$							
7	ac1	-692.289974	-691.943339	-690.615729	-26.79	-690.269095	-690.311787

7	ac2	-692.289974	-691.943337	-690.615730	-26.76	-690.269093	-690.311738
37	ac1	-692.287303	-691.940567	-690.615189	-27.04	-690.268453	-690.311544
37	ac2	-692.287303	-691.940567	-690.615188	-26.99	-690.268451	-690.311463
3	ac2	-692.288154	-691.941357	-690.615007	-27.08	-690.268210	-690.311365
49	ac1	-692.288154	-691.941361	-690.615006	-27.06	-690.268213	-690.311336
48	ac2	-692.288154	-691.941360	-690.615006	-27.06	-690.268212	-690.311335
61	ac1	-692.286569	-691.939824	-690.614546	-27.18	-690.267802	-690.311116
29	ac2	-692.286568	-691.939820	-690.614543	-27.18	-690.267795	-690.311109
48	ac1	-692.288187	-691.941145	-690.615072	-27.03	-690.268030	-690.311105
3	ac1	-692.288187	-691.941143	-690.615073	-27.03	-690.268028	-690.311103
49	ac2	-692.288187	-691.941143	-690.615072	-27.03	-690.268028	-690.311103
61	ac2	-692.286537	-691.939772	-690.614502	-27.21	-690.267736	-690.311098
29	ac1	-692.286537	-691.939773	-690.614501	-27.20	-690.267737	-690.311083
34	ac1	-692.288586	-691.941676	-690.615390	-26.73	-690.268480	-690.311077
34	ac2	-692.288597	-691.941614	-690.615430	-26.75	-690.268447	-690.311076
97	ac1	-692.288597	-691.941612	-690.615428	-26.75	-690.268444	-690.311073
64	ac1	-692.286900	-691.940493	-690.614412	-26.93	-690.268005	-690.310921
85	ac1	-692.285608	-691.938989	-690.613568	-27.40	-690.266949	-690.310614
85	ac2	-692.285608	-691.938989	-690.613565	-27.40	-690.266946	-690.310610
70	ac1	-692.286889	-691.940040	-690.614345	-26.97	-690.267496	-690.310475
64	ac2	-692.286889	-691.940039	-690.614344	-26.95	-690.267494	-690.310442
9	ac1	-692.288461	-691.941910	-690.614291	-26.75	-690.267740	-690.310369
9	ac2	-692.288461	-691.941902	-690.614291	-26.74	-690.267732	-690.310345
36	ac2	-692.288461	-691.941893	-690.614291	-26.74	-690.267723	-690.310336
36	ac1	-692.288461	-691.941884	-690.614290	-26.74	-690.267713	-690.310326
111	ac1	-692.283859	-691.937527	-690.611734	-27.65	-690.265401	-690.309465
111	ac2	-692.283916	-691.937315	-690.611746	-27.60	-690.265145	-690.309128
44	ac2	-692.285609	-691.938952	-690.612229	-27.13	-690.265572	-690.308806
84	ac2	-692.285610	-691.938929	-690.612235	-27.13	-690.265553	-690.308788
62	ac1	-692.285610	-691.938928	-690.612233	-27.13	-690.265550	-690.308785
39	ac2	-692.285610	-691.938927	-690.612233	-27.13	-690.265550	-690.308784
40	ac1	-692.285610	-691.938927	-690.612231	-27.13	-690.265548	-690.308782
40	ac2	-692.285608	-691.938916	-690.612201	-27.14	-690.265509	-690.308759
62	ac2	-692.285608	-691.938908	-690.612201	-27.14	-690.265501	-690.308751
39	ac1	-692.285608	-691.938914	-690.612201	-27.13	-690.265507	-690.308742
44	ac1	-692.285608	-691.938909	-690.612200	-27.13	-690.265501	-690.308736
90	ac2	-692.283154	-691.936353	-690.611439	-27.37	-690.264639	-690.308256
84	ac1	-692.285370	-691.938743	-690.611773	-27.05	-690.265146	-690.308253
103	ac1	-692.283154	-691.936350	-690.611439	-27.37	-690.264635	-690.308252
103	ac2	-692.283157	-691.936285	-690.611441	-27.38	-690.264569	-690.308202
90	ac1	-692.283158	-691.936290	-690.611437	-27.37	-690.264569	-690.308186
18	ac2	-692.282474	-691.936592	-690.610834	-27.00	-690.264952	-690.307980
11	ac2	-692.285079	-691.938428	-690.610697	-26.84	-690.264047	-690.306819
18	ac1	-692.282456	-691.935470	-690.610702	-27.03	-690.263717	-690.306792
11	ac1	-692.285122	-691.938269	-690.610738	-26.84	-690.263885	-690.306657
15	ac1	-692.283077	-691.936148	-690.610344	-27.05	-690.263414	-690.306521

24	ac2	-692.283507	-691.936583	-690.610270	-27.07	-690.263346	-690.306484
15	ac2	-692.283062	-691.936053	-690.610135	-27.11	-690.263126	-690.306329
24	ac1	-692.283544	-691.936533	-690.610128	-27.07	-690.263117	-690.306256
70	ac2	-692.282045	-691.936105	-690.608755	-27.15	-690.262815	-690.306081
60	ac2	-692.281448	-691.934966	-690.607755	-27.08	-690.261274	-690.304428
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97	ac2	-692.278860	-691.933027	-690.605483	-26.94	-690.259650	-690.302582
78	ac1	-692.278316	-691.931537	-690.605588	-27.33	-690.258809	-690.302362
78	ac2	-692.278300	-691.931328	-690.605602	-27.39	-690.258630	-690.302279

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37		-617.887497	-617.535936	-616.338253	-0.06	-615.986692	-615.986788
34		-617.888418	-617.536743	-616.337923	-0.12	-615.986248	-615.986439
7		-617.889328	-617.537918	-616.337281	-0.31	-615.985872	-615.986366
49		-617.887503	-617.536024	-616.337133	-0.27	-615.985654	-615.986084
48		-617.887503	-617.536023	-616.337133	-0.27	-615.985653	-615.986083
61		-617.886098	-617.534293	-616.336942	-0.17	-615.985137	-615.985408
29		-617.886098	-617.534293	-616.336942	-0.16	-615.985137	-615.985392
9		-617.888537	-617.536890	-616.336840	-0.09	-615.985194	-615.985337
64		-617.886754	-617.535081	-616.337112	0.17	-615.985439	-615.985169
111		-617.885263	-617.533778	-616.337062	0.30	-615.985577	-615.985099
85		-617.884861	-617.533215	-616.335796	-0.34	-615.984151	-615.984693
62		-617.886578	-617.535001	-616.336191	0.10	-615.984614	-615.984455
18		-617.883333	-617.531687	-616.335538	0.22	-615.983892	-615.983542
3		-617.884456	-617.532879	-616.334928	-0.04	-615.983351	-615.983415
103		-617.883482	-617.531926	-616.335214	0.19	-615.983658	-615.983355
15		-617.883332	-617.532020	-616.334445	-0.05	-615.983134	-615.983213
11		-617.884930	-617.533132	-616.334057	-0.39	-615.982260	-615.982881
90		-617.881854	-617.530280	-616.334320	0.14	-615.982746	-615.982523
24		-617.883652	-617.532095	-616.333598	-0.24	-615.982042	-615.982424
70		-617.882691	-617.530994	-616.333345	-0.28	-615.981647	-615.982093
84		-617.882538	-617.530945	-616.333182	0.23	-615.981588	-615.981222
60		-617.881288	-617.529397	-616.331193	-0.17	-615.979302	-615.979573
44		-617.877742	-617.526908	-616.331997	1.18	-615.981163	-615.979282
40		-617.877946	-617.526987	-616.331377	0.74	-615.980418	-615.979239
39		-617.877946	-617.526986	-616.331375	0.78	-615.980415	-615.979172
36		-617.877798	-617.526769	-616.330099	0.20	-615.979070	-615.978751
78		-617.878773	-617.527280	-616.330025	-0.08	-615.978532	-615.978660
97		-617.879200	-617.527580	-616.329631	0.05	-615.978011	-615.977931

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37	ac1	-770.882953	-770.476564	-769.000087	-26.00	-768.593698	-768.635132
49	ac1	-770.883688	-770.477305	-768.999787	-26.18	-768.593405	-768.635125
7	ac1	-770.885523	-770.479189	-769.000042	-25.98	-768.593708	-768.635110
7	ac2	-770.885523	-770.479188	-769.000042	-25.98	-768.593707	-768.635109
48	ac2	-770.883688	-770.477305	-768.999788	-26.09	-768.593406	-768.634983
3	ac2	-770.883688	-770.477305	-768.999787	-26.09	-768.593404	-768.634981

49	ac2	-770.883729	-770.477103	-768.999863	-26.18	-768.593236	-768.634957
97	ac2	-770.884158	-770.477758	-769.000061	-25.89	-768.593661	-768.634919
34	ac1	-770.884158	-770.477752	-769.000064	-25.89	-768.593658	-768.634916
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48	ac1	-770.883729	-770.477103	-768.999864	-26.09	-768.593238	-768.634815
97	ac1	-770.884205	-770.477612	-769.000120	-25.89	-768.593527	-768.634785
34	ac2	-770.884205	-770.477613	-769.000117	-25.89	-768.593525	-768.634784
29	ac2	-770.882224	-770.475606	-768.999500	-26.09	-768.592882	-768.634459
61	ac1	-770.882224	-770.475607	-768.999500	-26.06	-768.592883	-768.634412
78	ac1	-770.882224	-770.475609	-768.999496	-26.06	-768.592881	-768.634410
44	ac1	-770.882224	-770.475609	-768.999496	-26.06	-768.592881	-768.634410
29	ac1	-770.882223	-770.475542	-768.999468	-26.09	-768.592787	-768.634364
78	ac2	-770.882223	-770.475542	-768.999470	-26.06	-768.592789	-768.634319
61	ac2	-770.882223	-770.475542	-768.999468	-26.06	-768.592787	-768.634316
85	ac2	-770.881310	-770.474556	-768.998826	-26.31	-768.592072	-768.634000
85	ac1	-770.881310	-770.474553	-768.998825	-26.31	-768.592069	-768.633996
70	ac1	-770.882399	-770.475943	-768.999355	-25.67	-768.592899	-768.633807
64	ac2	-770.882399	-770.475940	-768.999358	-25.66	-768.592899	-768.633790
70	ac2	-770.882440	-770.475846	-768.999408	-25.67	-768.592814	-768.633722
64	ac1	-770.882440	-770.475846	-768.999410	-25.66	-768.592816	-768.633708
36	ac1	-770.883970	-770.477420	-768.998717	-25.82	-768.592167	-768.633314
9	ac2	-770.883970	-770.477391	-768.998717	-25.82	-768.592139	-768.633285
36	ac2	-770.883970	-770.477391	-768.998716	-25.82	-768.592138	-768.633284
9	ac1	-770.883969	-770.477367	-768.998703	-25.82	-768.592101	-768.633248
111	ac1	-770.879564	-770.472902	-768.997235	-26.00	-768.590573	-768.632007
111	ac2	-770.879594	-770.473007	-768.997110	-26.00	-768.590523	-768.631957
44	ac2	-770.881161	-770.474504	-768.997058	-26.06	-768.590400	-768.631930
84	ac1	-770.881092	-770.474569	-768.997012	-25.94	-768.590489	-768.631827
39	ac2	-770.881091	-770.474552	-768.997018	-25.93	-768.590479	-768.631801
62	ac2	-770.881092	-770.474565	-768.997014	-25.91	-768.590487	-768.631777
40	ac2	-770.881094	-770.474583	-768.997012	-25.90	-768.590501	-768.631775
84	ac2	-770.881161	-770.474504	-768.997032	-25.94	-768.590375	-768.631713
39	ac1	-770.881159	-770.474494	-768.997044	-25.93	-768.590380	-768.631702
62	ac1	-770.881159	-770.474492	-768.997047	-25.91	-768.590380	-768.631670
40	ac1	-770.881162	-770.474504	-768.997051	-25.90	-768.590393	-768.631668
103	ac1	-770.878753	-770.472094	-768.997007	-25.87	-768.590347	-768.631574
90	ac2	-770.878754	-770.472092	-768.997002	-25.83	-768.590340	-768.631503
103	ac2	-770.878818	-770.472181	-768.996826	-25.87	-768.590189	-768.631415
90	ac1	-770.878818	-770.472182	-768.996826	-25.83	-768.590190	-768.631353
18	ac2	-770.877930	-770.471492	-768.995613	-25.88	-768.589175	-768.630417
18	ac1	-770.877949	-770.471321	-768.995605	-25.88	-768.588977	-768.630219
15	ac1	-770.878637	-770.472070	-768.994911	-26.16	-768.588344	-768.630032
15	ac2	-770.878633	-770.471913	-768.994844	-26.16	-768.588124	-768.629813
11	ac2	-770.880689	-770.473966	-768.995119	-25.96	-768.588396	-768.629766
11	ac1	-770.880730	-770.473881	-768.995142	-25.96	-768.588293	-768.629663
24	ac2	-770.879108	-770.472413	-768.994858	-26.02	-768.588162	-768.629628

24	ac1	-770.879111	-770.472384	-768.994856	-26.02	-768.588128	-768.629594
60	ac2	-770.877088	-770.470609	-768.992628	-25.84	-768.586149	-768.627328
60	ac1	-770.877050	-770.470539	-768.992558	-25.84	-768.586047	-768.627226
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37		-696.482340	-696.071133	-694.722029	0.33	-694.310821	-694.310295
34		-696.483260	-696.071916	-694.721441	0.15	-694.310098	-694.309858
7		-696.484181	-696.073018	-694.720709	-0.16	-694.309546	-694.309801
49		-696.482373	-696.071012	-694.720715	0.09	-694.309353	-694.309210
48		-696.482373	-696.071012	-694.720715	0.09	-694.309353	-694.309210
9		-696.483414	-696.072035	-694.720319	0.06	-694.308940	-694.308845
61		-696.480912	-696.069542	-694.720705	0.35	-694.309335	-694.308777
29		-696.480912	-696.069540	-694.720705	0.36	-694.309334	-694.308760
64		-696.481634	-696.070227	-694.720769	0.63	-694.309362	-694.308358
111		-696.480197	-696.068619	-694.721312	1.12	-694.309733	-694.307949
62		-696.481385	-696.070047	-694.719829	0.58	-694.308491	-694.307567
85		-696.479643	-696.068124	-694.719517	0.28	-694.307998	-694.307552
18		-696.478062	-696.066949	-694.719268	0.73	-694.308156	-694.306992
3		-696.479281	-696.067812	-694.718389	0.21	-694.306920	-694.306585
11		-696.479785	-696.068111	-694.717483	-0.23	-694.305809	-694.306176
103		-696.478244	-696.066897	-694.719325	1.20	-694.307978	-694.306066
15		-696.478181	-696.066749	-694.718044	0.39	-694.306612	-694.305990
90		-696.476792	-696.065473	-694.718583	0.97	-694.307264	-694.305718
70		-696.477485	-696.066199	-694.716876	0.07	-694.305590	-694.305478
24		-696.478507	-696.066812	-694.717192	0.19	-694.305496	-694.305194
84		-696.477414	-696.065926	-694.717468	1.17	-694.305980	-694.304115
60		-696.476117	-696.064578	-694.714720	0.36	-694.303182	-694.302608
39		-696.472716	-696.061987	-694.714791	1.00	-694.304062	-694.302468
40		-696.472716	-696.061987	-694.714791	1.00	-694.304062	-694.302468
36		-696.472619	-696.061808	-694.713426	0.33	-694.302615	-694.302089
44		-696.472569	-696.061847	-694.715684	1.88	-694.304962	-694.301966
78		-696.473556	-696.062231	-694.713777	0.51	-694.302452	-694.301639
97		-696.473976	-696.062556	-694.713476	0.72	-694.302056	-694.300909
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7	ac2	-849.480922	-849.014921	-847.384012	-25.62	-846.918011	-846.958839
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37	ac1	-849.478322	-849.012227	-847.384344	-25.35	-846.918249	-846.958646
97	ac1	-849.478322	-849.012228	-847.384346	-25.33	-846.918252	-846.958618
37	ac2	-849.478322	-849.012226	-847.384346	-25.33	-846.918250	-846.958616
34	ac1	-849.479604	-849.013299	-847.384208	-25.35	-846.917903	-846.958301
97	ac2	-849.479604	-849.013300	-847.384207	-25.35	-846.917902	-846.958300
34	ac2	-849.479582	-849.013234	-847.384164	-25.29	-846.917816	-846.958118
49	ac2	-849.479151	-849.012711	-847.383968	-25.46	-846.917528	-846.958102
48	ac1	-849.479151	-849.012711	-847.383968	-25.46	-846.917528	-846.958101
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49	ac1	-849.479198	-849.012736	-847.383889	-25.35	-846.917427	-846.957825
48	ac2	-849.479198	-849.012736	-847.383890	-25.34	-846.917428	-846.957810

3	ac2	-849.479198	-849.012735	-847.383890	-25.34	-846.917427	-846.957809
29	ac2	-849.477591	-849.011049	-847.383845	-25.29	-846.917302	-846.957605
78	ac1	-849.477591	-849.011044	-847.383846	-25.29	-846.917299	-846.957601
61	ac1	-849.477591	-849.011046	-847.383844	-25.29	-846.917299	-846.957601
29	ac1	-849.477612	-849.011094	-847.383736	-25.15	-846.917218	-846.957297
61	ac2	-849.477612	-849.011095	-847.383735	-25.14	-846.917218	-846.957282
78	ac2	-849.477612	-849.011094	-847.383735	-25.14	-846.917217	-846.957280
64	ac2	-849.477863	-849.011613	-847.383611	-24.88	-846.917361	-846.957009
70	ac1	-849.477864	-849.011604	-847.383602	-24.89	-846.917342	-846.957006
36	ac2	-849.479357	-849.012896	-847.382722	-25.44	-846.916261	-846.956802
36	ac1	-849.479355	-849.012858	-847.382709	-25.44	-846.916212	-846.956753
9	ac1	-849.479356	-849.012846	-847.382703	-25.44	-846.916193	-846.956735
9	ac2	-849.479355	-849.012844	-847.382701	-25.44	-846.916189	-846.956731
64	ac1	-849.477838	-849.011204	-847.383695	-24.87	-846.917060	-846.956693
70	ac2	-849.477838	-849.011206	-847.383692	-24.87	-846.917060	-846.956693
85	ac2	-849.476766	-849.010179	-847.383068	-25.18	-846.916481	-846.956608
85	ac1	-849.476769	-849.010196	-847.383059	-25.17	-846.916486	-846.956597
111	ac2	-849.475063	-849.008757	-847.382159	-24.85	-846.915853	-846.955454
111	ac1	-849.475134	-849.008906	-847.382069	-24.81	-846.915841	-846.955378
44	ac1	-849.476558	-849.010249	-847.381290	-25.19	-846.914981	-846.955124
62	ac2	-849.476558	-849.010245	-847.381291	-25.19	-846.914978	-846.955121
84	ac1	-849.476559	-849.010243	-847.381288	-25.19	-846.914972	-846.955115
40	ac2	-849.476560	-849.010215	-847.381298	-25.18	-846.914953	-846.955080
39	ac1	-849.476544	-849.010234	-847.381236	-25.19	-846.914926	-846.955069
62	ac1	-849.476544	-849.010235	-847.381234	-25.19	-846.914925	-846.955068
84	ac2	-849.476544	-849.010235	-847.381233	-25.19	-846.914924	-846.955067
40	ac1	-849.476544	-849.010234	-847.381233	-25.19	-846.914923	-846.955066
44	ac2	-849.476544	-849.010233	-847.381232	-25.19	-846.914921	-846.955064
39	ac2	-849.476561	-849.010206	-847.381294	-25.17	-846.914939	-846.955050
103	ac1	-849.474216	-849.007951	-847.381679	-24.26	-846.915415	-846.954075
90	ac2	-849.474215	-849.007957	-847.381686	-24.25	-846.915428	-846.954073
90	ac1	-849.474214	-849.007811	-847.381668	-24.35	-846.915265	-846.954070
103	ac2	-849.474214	-849.007809	-847.381669	-24.24	-846.915264	-846.953893
18	ac1	-849.473375	-849.006825	-847.379943	-25.08	-846.913394	-846.953361
18	ac2	-849.473359	-849.006705	-847.379932	-25.14	-846.913278	-846.953341
11	ac1	-849.476075	-849.009630	-847.379077	-25.53	-846.912632	-846.953317
11	ac2	-849.476115	-849.009448	-847.379123	-25.54	-846.912456	-846.953156
15	ac1	-849.474018	-849.007577	-847.378995	-25.46	-846.912554	-846.953127
15	ac2	-849.474042	-849.007690	-847.379043	-25.37	-846.912691	-846.953121
24	ac2	-849.474476	-849.007948	-847.378972	-25.32	-846.912444	-846.952794
24	ac1	-849.474493	-849.007961	-847.378971	-25.32	-846.912439	-846.952789
60	ac2	-849.472437	-849.006138	-847.376824	-25.00	-846.910525	-846.950365
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37		-775.077114	-774.606103	-773.105282	0.52	-772.634271	-772.633443
34		-775.078023	-774.606780	-773.104714	0.31	-772.633471	-772.632977

7		-775.078966	-774.607937	-773.103913	0.01	-772.632884	-772.632868
49		-775.077165	-774.605877	-773.103996	0.38	-772.632708	-772.632103
48		-775.077165	-774.605877	-773.103996	0.38	-772.632708	-772.632103
9		-775.078201	-774.607185	-773.103496	0.24	-772.632481	-772.632098
61		-775.075663	-774.604455	-773.103938	0.50	-772.632730	-772.631933
29		-775.075663	-774.604455	-773.103938	0.50	-772.632730	-772.631933
64		-775.076394	-774.605194	-773.104146	0.92	-772.632946	-772.631480
111		-775.075012	-774.604033	-773.105047	1.73	-772.634068	-772.631311
85		-775.074404	-774.603150	-773.102919	0.61	-772.631665	-772.630693
62		-775.076159	-774.605002	-773.103139	0.83	-772.631982	-772.630659
18		-775.072911	-774.601738	-773.102542	0.92	-772.631369	-772.629903
3		-775.074020	-774.602807	-773.101697	0.38	-772.630484	-772.629879
11		-775.074476	-774.603224	-773.100630	-0.05	-772.629378	-772.629457
15		-775.072893	-774.601748	-773.101289	0.56	-772.630144	-772.629252
103		-775.073017	-774.601979	-773.102846	1.68	-772.631808	-772.629131
24		-775.073221	-774.602233	-773.100450	0.38	-772.629462	-772.628857
70		-775.072215	-774.601113	-773.100151	0.28	-772.629049	-772.628603
90		-775.071637	-774.600371	-773.102270	1.63	-772.631004	-772.628406
84		-775.072132	-774.602009	-773.101007	1.58	-772.630884	-772.628366
60		-775.070936	-774.599473	-773.098304	0.68	-772.626841	-772.625757
40		-775.067548	-774.596946	-773.098038	1.22	-772.627436	-772.625492
39		-775.067548	-774.596946	-773.098038	1.22	-772.627436	-772.625492
36		-775.067379	-774.596759	-773.096633	0.51	-772.626013	-772.625200
44		-775.067345	-774.596797	-773.098864	2.10	-772.628316	-772.624969
78		-775.068356	-774.597283	-773.097051	0.73	-772.625977	-772.624814
97		-775.068752	-774.597451	-773.096752	0.92	-772.625451	-772.623985
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97	ac2	-928.073384	-927.547455	-925.767939	-24.99	-925.242010	-925.281834
7	ac1	-928.076042	-927.549910	-925.767587	-25.28	-925.241454	-925.281741
7	ac2	-928.076042	-927.549910	-925.767586	-25.28	-925.241454	-925.281740
3	ac1	-928.074230	-927.548259	-925.767633	-25.13	-925.241661	-925.281708
49	ac2	-928.074229	-927.548225	-925.767629	-25.09	-925.241625	-925.281609
48	ac1	-928.074229	-927.548115	-925.767627	-25.14	-925.241513	-925.281576
34	ac1	-928.074752	-927.548676	-925.767664	-25.02	-925.241588	-925.281460
34	ac2	-928.074718	-927.548335	-925.767783	-25.05	-925.241400	-925.281320
29	ac2	-928.072730	-927.546791	-925.767454	-24.97	-925.241515	-925.281307
48	ac2	-928.074306	-927.548057	-925.767565	-25.02	-925.241317	-925.281189
3	ac2	-928.074305	-927.548052	-925.767562	-25.02	-925.241309	-925.281181
78	ac2	-928.072748	-927.546815	-925.767348	-24.88	-925.241415	-925.281064
29	ac1	-928.072748	-927.546814	-925.767347	-24.88	-925.241413	-925.281062
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44	ac1	-928.071729	-927.548258	-925.764802	-24.71	-925.241331	-925.280709
64	ac1	-928.072887	-927.546931	-925.767365	-24.50	-925.241409	-925.280453
70	ac2	-928.072879	-927.546848	-925.767396	-24.51	-925.241365	-925.280425

64	ac2	-928.072979	-927.546932	-925.767368	-24.42	-925.241321	-925.280237
85	ac1	-928.071891	-927.545536	-925.766876	-24.85	-925.240520	-925.280121
85	ac2	-928.071891	-927.545534	-925.766875	-24.85	-925.240518	-925.280119
70	ac1	-928.072993	-927.546779	-925.767378	-24.43	-925.241164	-925.280096
78	ac1	-928.072730	-927.545520	-925.767456	-24.98	-925.240246	-925.280054
9	ac1	-928.074473	-927.548127	-925.766283	-25.07	-925.239937	-925.279888
36	ac1	-928.074473	-927.548126	-925.766282	-25.07	-925.239934	-925.279886
36	ac2	-928.074473	-927.548126	-925.766281	-25.07	-925.239934	-925.279886
9	ac2	-928.074474	-927.548126	-925.766280	-25.07	-925.239932	-925.279884
61	ac1	-928.072730	-927.545326	-925.767458	-24.98	-925.240054	-925.279863
62	ac1	-928.071692	-927.546914	-925.764769	-24.71	-925.239991	-925.279368
60	ac1	-928.067640	-927.546755	-925.760630	-24.54	-925.239744	-925.278851
111	ac2	-928.070298	-927.544162	-925.766203	-24.07	-925.240067	-925.278425
103	ac1	-928.069379	-927.544135	-925.765584	-23.77	-925.240340	-925.278220
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84	ac1	-928.071729	-927.545520	-925.764817	-24.71	-925.238608	-925.277986
62	ac2	-928.071729	-927.545518	-925.764815	-24.71	-925.238604	-925.277982
40	ac2	-928.071728	-927.545516	-925.764810	-24.71	-925.238597	-925.277975
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40	ac1	-928.071692	-927.545327	-925.764766	-24.70	-925.238400	-925.277762
90	ac2	-928.069378	-927.543128	-925.765569	-23.77	-925.239319	-925.277199
90	ac1	-928.069396	-927.543037	-925.765641	-23.74	-925.239282	-925.277114
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11	ac2	-928.071192	-927.545119	-925.762680	-25.20	-925.236606	-925.276765
18	ac1	-928.068461	-927.542095	-925.763644	-24.74	-925.237277	-925.276703
11	ac1	-928.071158	-927.544845	-925.762607	-25.18	-925.236294	-925.276421
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15	ac1	-928.069150	-927.542761	-925.762708	-25.11	-925.236319	-925.276334
18	ac2	-928.068444	-927.542191	-925.763609	-24.34	-925.237356	-925.276144
97	ac1	-928.074725	-927.543136	-925.767795	-25.02	-925.236207	-925.276079
24	ac1	-928.069608	-927.543125	-925.762615	-24.97	-925.236132	-925.275924
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49	ac1	-928.074305	-927.541400	-925.767549	-25.02	-925.234645	-925.274517
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37		-932.266633	-931.675706	-929.871618	0.86	-929.280691	-929.279321
34		-932.267584	-931.676735	-929.871007	0.62	-929.280157	-929.279169
7		-932.268490	-931.677826	-929.870241	0.3	-929.279577	-929.279099
48		-932.266627	-931.675837	-929.870194	0.55	-929.279404	-929.278527
9		-932.267523	-931.676782	-929.869797	0.55	-929.279056	-929.278180
64		-932.265849	-931.675225	-929.870497	1.29	-929.279873	-929.277817
29		-932.265275	-931.674129	-929.870283	0.86	-929.279138	-929.277767
49		-932.266627	-931.675837	-929.870194	1.11	-929.279404	-929.277635

61		-932.265275	-931.674129	-929.870284	1.25	-929.279138	-929.277146
62		-932.265691	-931.675106	-929.869398	1.3	-929.278813	-929.276741
18		-932.262441	-931.671620	-929.868907	1.25	-929.278086	-929.276094
3		-932.263599	-931.672752	-929.867876	0.68	-929.277029	-929.275945
11		-932.264023	-931.673166	-929.866920	0.25	-929.276063	-929.275664
84		-932.261739	-931.671219	-929.867507	0.83	-929.276986	-929.275664
15		-932.262439	-931.671744	-929.867598	0.9	-929.276903	-929.275469
90		-932.259869	-931.668931	-929.868179	1.35	-929.277241	-929.275090
44		-932.256791	-931.666843	-929.865284	0.55	-929.275336	-929.274459
103		-932.262536	-931.671875	-929.869183	2.57	-929.278522	-929.274427
24		-932.262878	-931.671605	-929.866768	0.72	-929.275495	-929.274347
85		-932.263894	-931.673230	-929.869220	2.7	-929.278556	-929.274253
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60		-932.260404	-931.669408	-929.864619	0.85	-929.273623	-929.272269
39		-932.256972	-931.666930	-929.864384	1.56	-929.274342	-929.271856
40		-932.256972	-931.666930	-929.864384	1.56	-929.274342	-929.271856
36		-932.256900	-931.666625	-929.862979	0.8	-929.272703	-929.271428
78		-932.257787	-931.667183	-929.863427	2.45	-929.272823	-929.268918
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49	ac1	-1085.264081	-1084.618509	-1082.534323	-24.59	-1081.888751	-1081.927938
48	ac2	-1085.264081	-1084.618507	-1082.534323	-24.59	-1081.888750	-1081.927937
78	ac2	-1085.264081	-1084.618503	-1082.534329	-24.58	-1081.888751	-1081.927922
34	ac2	-1085.264589	-1084.618904	-1082.534414	-24.52	-1081.888729	-1081.927804
97	ac1	-1085.263339	-1084.617439	-1082.534699	-24.45	-1081.888800	-1081.927763
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37	ac1	-1085.263339	-1084.617439	-1082.534697	-24.45	-1081.888798	-1081.927761
97	ac2	-1085.264551	-1084.618863	-1082.534380	-24.49	-1081.888691	-1081.927718
34	ac1	-1085.264551	-1084.618858	-1082.534377	-24.49	-1081.888684	-1081.927711
61	ac2	-1085.262641	-1084.617019	-1082.534355	-24.34	-1081.888733	-1081.927521
29	ac1	-1085.262641	-1084.617013	-1082.534358	-24.34	-1081.888730	-1081.927519
49	ac2	-1085.264174	-1084.618364	-1082.534312	-24.47	-1081.888502	-1081.927497
48	ac1	-1085.264174	-1084.618370	-1082.534312	-24.46	-1081.888507	-1081.927487
3	ac1	-1085.264171	-1084.618396	-1082.534265	-24.47	-1081.888490	-1081.927485
78	ac1	-1085.264175	-1084.618355	-1082.534313	-24.46	-1081.888493	-1081.927472
29	ac2	-1085.262645	-1084.616861	-1082.534254	-24.24	-1081.888470	-1081.927099
61	ac1	-1085.262644	-1084.616852	-1082.534256	-24.24	-1081.888464	-1081.927093
64	ac1	-1085.262863	-1084.617245	-1082.534038	-23.88	-1081.888420	-1081.926476
64	ac2	-1085.262821	-1084.617029	-1082.534127	-23.90	-1081.888336	-1081.926423
36	ac1	-1085.264411	-1084.618581	-1082.533066	-24.59	-1081.887236	-1081.926423
70	ac1	-1085.262812	-1084.617025	-1082.534122	-23.90	-1081.888335	-1081.926422
36	ac2	-1085.264411	-1084.618578	-1082.533067	-24.59	-1081.887234	-1081.926421
9	ac1	-1085.264411	-1084.618578	-1082.533067	-24.59	-1081.887234	-1081.926420
9	ac2	-1085.264411	-1084.618578	-1082.533067	-24.59	-1081.887234	-1081.926420

85	ac1	-1085.261796	-1084.615900	-1082.533640	-24.23	-1081.887744	-1081.926357
85	ac2	-1085.261796	-1084.615900	-1082.533640	-24.23	-1081.887744	-1081.926357
70	ac2	-1085.262929	-1084.617058	-1082.534044	-23.79	-1081.888174	-1081.926085
40	ac1	-1085.261489	-1084.616993	-1082.531337	-24.12	-1081.886841	-1081.925279
39	ac1	-1085.261483	-1084.617035	-1082.531221	-24.10	-1081.886774	-1081.925179
62	ac1	-1085.261505	-1084.615887	-1082.531588	-24.15	-1081.885970	-1081.924456
11	ac2	-1085.260903	-1084.616703	-1082.529286	-24.69	-1081.885086	-1081.924432
40	ac2	-1085.260969	-1084.616419	-1082.530516	-24.03	-1081.885966	-1081.924260
62	ac2	-1085.261522	-1084.615725	-1082.531324	-24.14	-1081.885527	-1081.923997
39	ac2	-1085.261519	-1084.615716	-1082.531336	-24.13	-1081.885532	-1081.923986
44	ac1	-1085.260718	-1084.616142	-1082.530322	-23.84	-1081.885745	-1081.923737
44	ac2	-1085.260804	-1084.616039	-1082.530209	-23.90	-1081.885444	-1081.923531
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18	ac1	-1085.258456	-1084.612395	-1082.530400	-24.21	-1081.884339	-1081.922920
103	ac2	-1085.259352	-1084.613363	-1082.532555	-22.75	-1081.886566	-1081.922820
11	ac1	-1085.261055	-1084.615165	-1082.529333	-24.70	-1081.883443	-1081.922805
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3	ac2	-1085.259822	-1084.614063	-1082.529602	-24.37	-1081.883843	-1081.922679
90	ac1	-1085.258084	-1084.612235	-1082.531866	-22.82	-1081.886017	-1081.922383
24	ac1	-1085.259526	-1084.613586	-1082.529353	-24.42	-1081.883414	-1081.922329
24	ac2	-1085.259541	-1084.613451	-1082.529344	-24.42	-1081.883254	-1081.922170
90	ac2	-1085.258050	-1084.612082	-1082.531967	-22.69	-1081.886000	-1081.922158
60	ac2	-1085.257466	-1084.611582	-1082.527388	-23.92	-1081.881505	-1081.919623
60	ac1	-1085.257429	-1084.611476	-1082.527322	-23.91	-1081.881368	-1081.919472

Additional calculations on the G3MP2B3-level have been performed for the best conformations for every catalyst. The results are given in Table S19.

Table S19. Calculated energies of selected conformers for catalysts **1a** – **1h**, as calculated at G3MP2B3 level of theory.

Conf	MP2(FC)/G3MP2 Large	MP2(FC)/6-31G(d)	QCISD(T)/6-31G(d)	E_{tot} G3MP2B3	H_{298} G3MP2B3
Pyr					
1	-247.743288	-247.480917	-247.549940	-247.812311	-247.718172
Pyr-Ac$^+$					
1.ac1	-400.461686	-400.042094	-400.145167	-400.564760	-400.416452
1a					
1	-381.426640	-380.994471	-381.105670	-381.537838	-381.365836
1a-Ac$^+$					
1.ac1	-534.179287	-533.590508	-533.736587	-534.325366	-534.098512

1b					
1	-420.647244	-420.163547	-420.290752	-420.774449	-420.572577
1b-Ac$^+$					
1.ac1	-573.401787	-572.761082	-572.923180	-573.563885	-573.307078
1.ac2	-573.401825	-572.761099	-572.923205	-573.563930	-573.306856
1c					
2	-459.864610	-459.328721	-459.471985	-460.007873	-459.778963
4	-459.867600	-459.332188	-459.475461	-460.010873	-459.778359
5	-459.866988	-459.331545	-459.474772	-460.010214	-459.775670
10	-459.859945	-459.326362	-459.468987	-460.002570	-459.775681
12	-459.864144	-459.328336	-459.471765	-460.007574	-459.771592
1c-Ac$^+$					
2.ac1	-612.620092	-611.926956	-612.105155	-612.798291	-612.515775
2.ac2	-612.620139	-611.926978	-612.105177	-612.798338	-612.515775
4.ac1	-612.624426	-611.931767	-612.109807	-612.802466	-612.515770
4.ac2	-612.624427	-611.931767	-612.109807	-612.802467	-612.514142
5.ac1	-612.622920	-611.930223	-612.108264	-612.800961	-612.514141
5.ac2	-612.622920	-611.930223	-612.108264	-612.800961	-612.514139
10.ac1	-612.622920	-611.932233	-612.108265	-612.798952	-612.514138
10.ac2	-612.622920	-611.930223	-612.108265	-612.800962	-612.512129
12.ac1	-612.622919	-611.930223	-612.108265	-612.800961	-612.511385
12.ac2	-612.622920	-611.930223	-612.108265	-612.800962	-612.511301
1d					
37	-538.304079	-537.664430	-537.839791	-538.479440	-538.187672
1d-Ac$^+$					
37.ac1	-691.061455	-690.264508	-690.474739	-691.271686	-690.924950
1e					
37	-616.739297	-615.996176	-616.204117	-616.947239	-616.595678
1e-Ac$^+$					
37.ac1	-769.497867	-768.597309	-768.840086	-769.740644	-769.334256
1f					
37	-695.174685	-694.327902	-694.568382	-695.415165	-695.003958
1f-Ac$^+$					
37.ac1	-847.933799	-846.929534	-847.204868	-848.209132	-847.743037
1g					
37	-773.609585	-772.659269	-772.932352	-773.882668	-773.411657
1g-Ac$^+$					
37.ac1	-926.369072	-925.261247	-925.569174	-926.676999	-926.151110

Table S20. Solvation energy data $\Delta G_{solv.}$ divided into electrostatic and non electrostatic terms for neutral caltalysts **1a-h** and acylated catalysts **10a-h**.

	$\Delta G_{solv.}$					
catalyst	total		electrostatic		non electrostatic	
	1	**10**	**1**	**10**	**1**	**10**
a	-3.27	-31.39	-2.93	-32.10	-0.33	+0.71
b	-2.84	-30.37	-2.92	-31.51	+0.08	+1.14
c	-2.29	-29.32	-2.87	-30.93	+0.59	+1.61
d	-0.71	-26.78	-2.74	-29.97	+2.03	+3.19
e	-0.06	-26.00	-2.73	-29.73	+2.67	+3.74
f	+0.33	-25.62	-2.74	-29.40	+3.08	+3.78
g	+0.52	-25.00	-2.74	-29.32	+3.26	+4.32
h	+0.86	-24.84	-2.76	-29.10	+3.62	+4.26

In order to explore the similarities and differences of the preferred conformations in **1a** - **1h** the following part shows the conformational analysis of the five best conformations of these catalyst systems. Figure S18 shows the terminology for the evaluation of the different conformations whereas Table S21 shows the results of the evaluation.

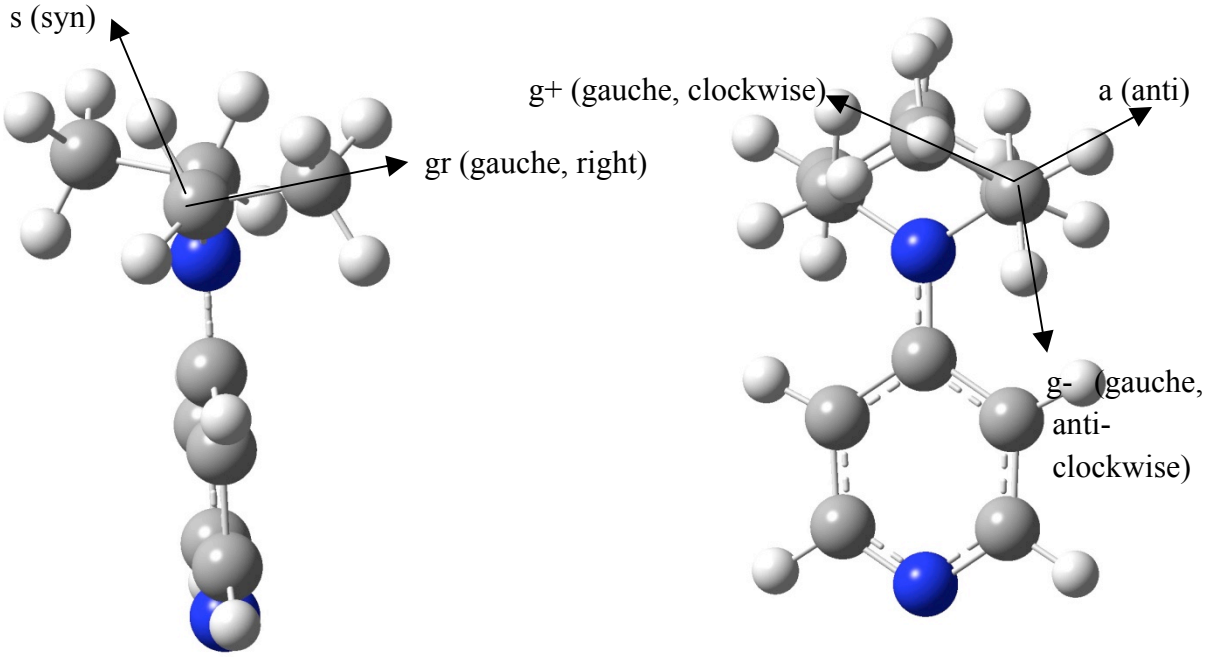

Figure S18. Terminology for the conformational analysis on the example of the preferred conformation for **1d** with tw = twisted; oop = out of plane.

As could be seen in Figure S18 the preferred conformation for longer alkyl groups in **1d** – **1h** is a "twisted" gauche conformation. As this is true for all catalyst conformations this conformations was named for reasons of simplicity "g" (=gauche). For the assignment of the conformers the pyridine ring was adjusted to a position shown in Figure S18 left were the pyridine ring heads out of the plane. If the alkylgroup heads to the right hand side the assignment is "gr" and in reverse "gl". Afterwards the pyridine ring is turned like shown in Figure S17 right and the relative orientation of the alkyl chain towards the nitrogen in 4-position is determined. Finally the carbon-carbon bonds are analysed with g=gauche, a=anti and s=syn. Table S21 shows the results in that way, that every column show an additional C-atom beginning from the C-atom next to the nitrogen in 4-position.

Table S21. Conformational analysis of the DMAP-derivatives **1b** – **1h** and acylated derivatives **10b** – **10h**.

system	**conformer**	**Orientation of C-atom:**							
		2		**3**		**4**		**5**	**6**	**7**	**8**
1b	1	gr									
10b	1ac1	gr									
	1ac2	gr									
1c	4	gr	gr								
	5	gr	gl								
	2	gl	s								
	12	gr	gl,s,tw								
	10	oop,a	oop,a								
10c	4ac1	gr	gr								
	4ac2	gr	gr								
	12ac2	gr	gl								
	12ac1	gr	gl								
	5ac1	gr	gl								
1d	37	gl	gl	g+	g+						
	34	gr	gr	g+	a						
	29	gr	gr	g-	g+						
	7	gl	gl	a	a						
	48	gr	gr	g+	a						
10d	7ac1	gl	gl	a	a						
	7ac2	gl	gl	a	a						
	37ac1	gl	gl	g+	g+						
	37ac2	gl	gl	g+	g+						
	3ac2	gl	gl	a	g-						
1e	37	gl	gl	g+	g+	a	a				
	34	gr	gr	g+	a	a	a				
	7	gl	gl	a	a	a	a				
	49	gl	gl	g-	a	a	a				
	48	gr	gr	a	g-	a	a				
10e	37ac2	gl	gl	g+	g+	a	a				
	37ac1	gl	gl	g+	g+	a	a				

	49ac1	gl	gl	a	g-	a	a				
	7ac1	gl	gl	a	a	a	a				
	7ac2	gl	gl	a	a	a	a				
1f	37	gl	gl	g+	g+	a	a	a			
	34	gr	gr	g+	a	a	a	a			
	7	gl	gl	a	a	a	a	a			
	49	gl	gl	g-	a	a	a	a			
	48	gr	gr	a	g-	a	a	a			
10f	7ac2	gl	gl	a	a	a	a	a			
	7ac1	gl	gl	a	a	a	a	a			
	37ac1	gl	gl	g+	g+	a	a	a			
	97ac1	gr	gr	g+	g+	a	a	a			
	37ac2	gl	gl	g+	g+	a	a	a			
1g	37	gl	gl	g+	g+	a	a	a	a		
	34	gr	gr	g+	a	a	a	a	a		
	7	gl	gl	a	a	a	a	a	a		
	49	gl	gl	g-	a	a	a	a	a		
	48	gr	gr	a	g-	a	a	a	a		
10g	37ac2	gl	gl	g+	g+	a	a	a	a		
	37ac1	gl	gl	g+	g+	a	a	a	a		
	97ac2	gl	gl	g+	g+	a	a	a	a		
	7ac1	gr	gr	a	a	a	a	a	a		
	7ac2	gl	gl	a	a	a	a	a	a		
1h	37	gl	gl	g+	g+	a	a	a	a	a	a
	34	gr	gr	g+	a	a	a	a	a	a	a
	7	gl	gl	a	a	a	a	a	a	a	a
	48	gr	gr	g-	a	a	a	a	a	a	a
	9	gl	gr	a	a	a	a	a	a	a	a
10h	7ac1	gl	gl	a	a	a	a	a	a	a	a
	7ac2	gl	gl	a	a	a	a	a	a	a	a
	49ac1	gl	gl	g-	a	a	a	a	a	a	a
	48ac2	gr	gr	g-	a	a	a	a	a	a	a
	78ac2	gl	gl	g-	a	a	a	a	a	a	a

Table S21 shows that the preferred conformation of all unacylated catalyst systems **1d** – **1h** is "gl, gl, g+, g+". Figure S19 shows this conformation for **1d** from front view (left) and top view (right). Figure S20 shows the same preferred conformation for **1f** in which now 5 C-atoms are on every side of the nitrogen atom.

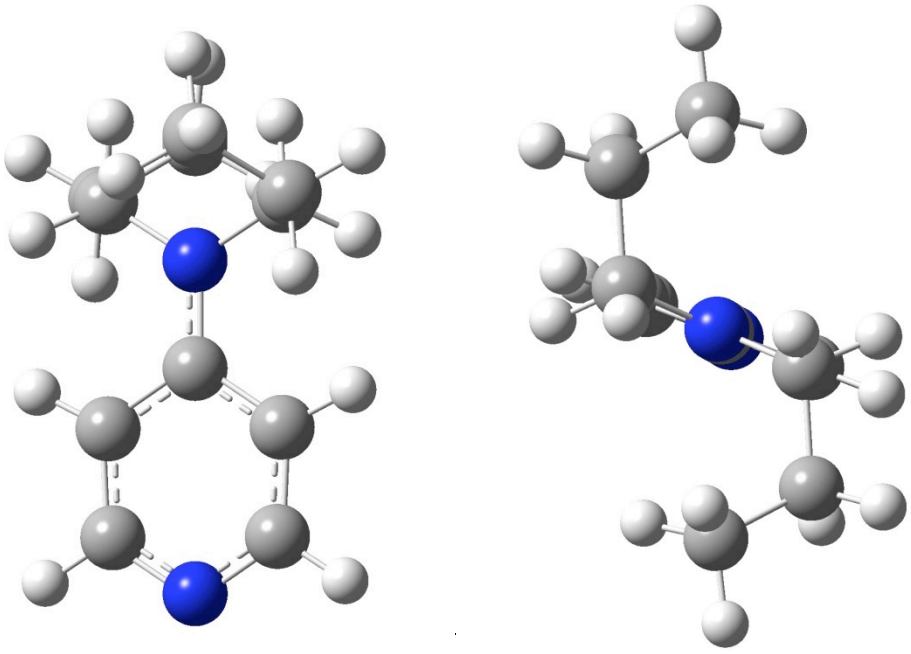

Figure S19. Preferred conformation for the unacylated catalyst **1d** from front view (right) and top view (left).

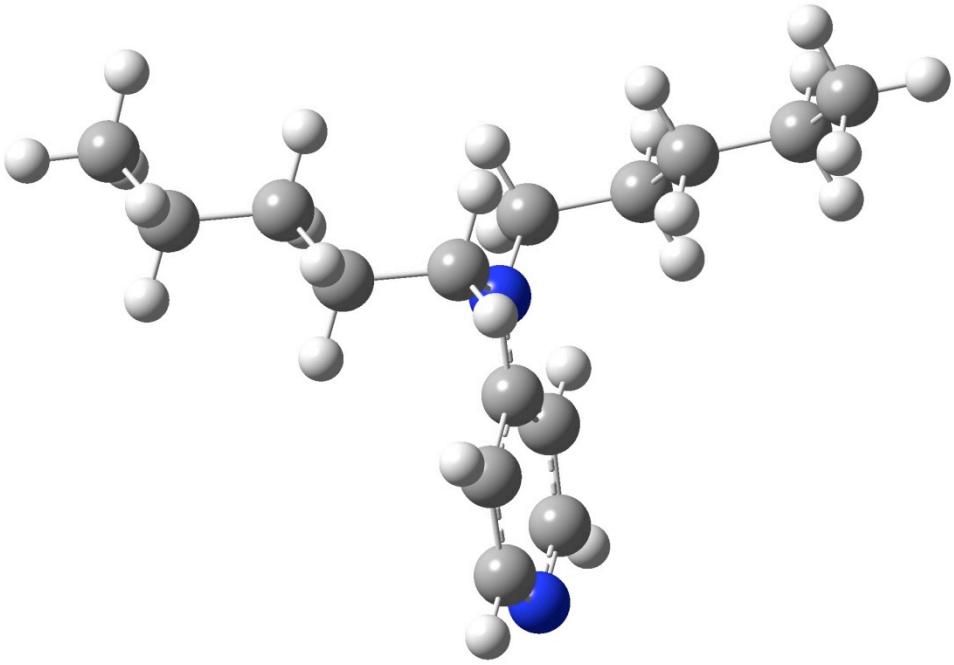

Figure S20. Another view for the preferred conformation now for **1f**.

8. References

References 1 – 12 like in the main text and additionally:

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9. Archive entries

pyridin

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pyridin.ac1

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1a.1.ac1

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\C,0,1.2254912396,-0.0663894323,2.0882110309\C,0,2.3977575529,-0.06226
29048,1.2590081485\C,0,2.287887838,-0.0412399048,-0.1008603877\H,0,-1.
0127405399,-0.012167826,-0.5055312715\H,0,-0.9724389357,-0.0486501461,
1.9300260597\H,0,3.3916834003,-0.0755954752,1.6884552864\H,0,3.1422808
155,-0.0373379688,-0.7682533584\N,0,1.2985987467,-0.0866772136,3.42465
01668\N,0,1.0688918336,-0.0232509351,-0.7302725469\C,0,2.6050282794,-0
.1061832697,4.1011423516\H,0,3.1863932563,0.7890355707,3.8517146497\H,
0,3.1736102467,-1.0017255366,3.8248645845\H,0,2.4436567958,-0.12118010
56,5.1787376398\C,0,0.0752411763,-0.0903413059,4.2411177359\H,0,0.3541
846929,-0.1081190997,5.2944010866\H,0,-0.5192045315,0.8123779681,4.057
6352793\H,0,-0.5318086296,-0.9786789162,4.0306985357\C,0,1.0662737193,
-0.0010134625,-2.2129828906\O,0,2.1291640225,-0.0009023227,-2.76709931
67\C,0,-0.2786913528,0.0192160548,-2.8926959857\H,0,-0.856099164,0.909
9365012,-2.6163493162\H,0,-0.0957132127,0.035174904,-3.9685781553\H,0,
-0.8679953335,-0.8721723003,-2.6449583629\\Version=IA32L-G03RevD.01\St
ate=1-A\HF=-531.9964222\MP2=-533.8361142\RMSD=2.693e-09\Thermal=0.\PG=
C01 [X(C9H13N2O1)]\\@

1b.1

1\1\GINC-NODE-21\SP\RMP2-FC\6-31+G(2d,p)\C8H12N2\ZIP08\26-Aug-2010\0\\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=r

ead\\sp of d15ap1 MP2-5/6-31+G(2d,p)\\0,1\C,0,-0.0418231561,0.19619398
13,0.0658543946\C,0,-0.0022267567,0.3233263035,1.4520860249\C,0,2.2187
101404,-0.1035902541,1.5350514607\C,0,2.3102635069,-0.2561351402,0.154
6376194\C,0,1.1498375993,-0.0948668036,-0.6430280406\H,0,-0.9880555318
,0.3272683312,-0.4477027864\H,0,-0.9240994796,0.5522686955,1.988064914
9\H,0,3.1175725934,-0.2273623344,2.1401641336\H,0,3.2722776237,-0.5038
864556,-0.2808900952\N,0,1.09509811,0.1837652893,2.2096486939\N,0,1.16
54966954,-0.1967990857,-2.0192597092\C,0,-0.0921212293,-0.1780481053,-
2.7512781437\H,0,-0.6178657939,0.7768056179,-2.6140294082\H,0,0.117779
7144,-0.2940084877,-3.8179431558\H,0,-0.7699398011,-0.9897719634,-2.44
48194616\C,0,2.3656084964,-0.6163703978,-2.7389180768\H,0,3.2343970903
,-0.1091493707,-2.3038592611\H,0,2.2804049104,-0.2370194562,-3.7645241
014\C,0,2.5887829724,-2.137974394,-2.7627665999\H,0,1.7524778727,-2.64
80810525,-3.2565997232\H,0,3.5076510238,-2.3822385353,-3.3110243637\H,
0,2.6773151313,-2.5389813422,-1.7465116064\\Version=IA32L-G03RevD.01\S
tate=1-A\HF=-418.8550441\MP2=-420.3748493\RMSD=7.125e-09\Thermal=0.\PG
=C01 [X(C8H12N2)]\\@

1b.1.ac1

1\1\GINC-NODE-25\SP\RMP2-FC\6-31+G(2d,p)\C10H15N2O1(1+)\ZIP08\29-Aug-2
010\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check
guess=read\\sp of d15ap1.ac1 MP2-5/6-31+G(2d,p)\\1,1\C,0,-0.0070173387
,-0.0120860116,0.038235804\C,0,-0.0315024617,0.0224955715,1.401372699\
C,0,2.3267647523,-0.0481961706,1.503345156\C,0,2.4212098315,-0.0804959
786,0.1420335216\C,0,1.239289212,-0.0584258301,-0.6770220002\H,0,-0.95
47445828,0.0138799747,-0.4844912328\H,0,-0.948423822,0.0685907549,1.97
75641139\H,0,3.2115363429,-0.0714543333,2.1263979361\H,0,3.4108027927,
-0.1437098367,-0.2918161027\N,0,1.1187649532,0.0062795983,2.1493735436
\N,0,1.2820303052,-0.0776897488,-2.0141229926\C,0,0.043102651,-0.16399
20576,-2.8026640946\H,0,-0.5292252239,0.7694201201,-2.737457951\H,0,0.
3074715452,-0.3368303397,-3.8468038781\H,0,-0.5781718288,-1.0001686338
,-2.4654459978\C,0,2.5512998994,-0.0557016578,-2.7740903822\H,0,3.2814
656312,0.5443647894,-2.2236878113\H,0,2.3487376817,0.4891079113,-3.701
5215736\C,0,3.0896369678,-1.4592198965,-3.0775079857\H,0,2.3675546454,
-2.0442028821,-3.6583107112\H,0,4.0104310553,-1.3791947989,-3.66586604
37\H,0,3.3162043071,-2.0115522055,-2.1581450868\C,0,0.9779161149,0.048
2955648,3.6228745056\O,0,-0.1329965763,0.0871996337,4.0724806403\C,0,2
.2507076494,0.0400296116,4.4306134242\H,0,2.8828407831,0.9048818742,4.
1952447883\H,0,1.964992521,0.0850560196,5.4830214704\H,0,2.8299960271,
-0.8754229754,4.2584001443\\Version=IA32L-G03RevD.01\State=1-A\HF=-571
.0387989\MP2=-573.0329019\RMSD=2.477e-09\Thermal=0.\PG=C01 [X(C10H15N2
O1)]\\@

1b.1.ac2

1\1\GINC-NODE-25\SP\RMP2-FC\6-31+G(2d,p)\C10H15N2O1(1+)\ZIP08\29-Aug-2
010\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check
guess=read\\sp of d15ap1.ac2 MP2-5/6-31+G(2d,p)\\1,1\C,0,-0.0420168514
,-0.0278410011,0.0184194676\C,0,-0.0833751998,0.0020722117,1.382807133
3\C,0,2.2739118378,-0.0572283649,1.514078447\C,0,2.3850510494,-0.08394
54489,0.155536872\C,0,1.214916794,-0.0652404173,-0.6795387262\H,0,-0.9
827973333,-0.0046455903,-0.5167296328\H,0,-1.0256139792,0.0413854663,1
.9142109908\H,0,3.1292006561,-0.0760128581,2.1796222033\H,0,3.38040498
22,-0.1397592803,-0.2663170817\N,0,1.0551750779,-0.0108849738,2.144836
4963\N,0,1.276421193,-0.0794064502,-2.0159018247\C,0,0.0513916515,-0.1
710348701,-2.8243433874\H,0,-0.5276619758,0.7588577485,-2.7670179461\H
,0,0.3336266266,-0.3398280736,-3.8644668052\H,0,-0.570265048,-1.012138
9063,-2.4999711001\C,0,2.5579397467,-0.0462452431,-2.7556457986\H,0,3.
2755361716,0.5542956342,-2.1897058926\H,0,2.366856821,0.5029025323,-3.
6829738869\C,0,3.1089351958,-1.445076894,-3.0578215664\H,0,2.400940768
6,-2.0303601114,-3.6554657861\H,0,4.0398545486,-1.3560451992,-3.628642

1951\H,0,3.3222884431,-2.0015255835,-2.1378825622\C,0,1.0519614197,0.0
17191747,3.6252729962\O,0,2.1137717119,-0.0044519148,4.1820023709\C,0,
-0.2926977572,0.0719993467,4.3044987522\H,0,-0.9018641814,-0.807727637
9,4.0633036324\H,0,-0.1097564449,0.091831791,5.3803240517\H,0,-0.85021
63824,0.9732144841,4.0214166241\\Version=IA32L-G03RevD.01\State=1-A\HF
=-571.0388282\MP2=-573.032926\RMSD=2.378e-09\Thermal=0.\PG=C01 [X(C10H
15N2O1)]\\@

1c.1

1\1\GINC-YIN\SP\RMP2-FC\6-31+G(2d,p)\C9H14N2\RAMAN\01-Jun-2010\0\\#P M
P2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=read\
\sp of d2ap4 mp2-5 on 2p 900 MB\\0,1\C,0,0.339189923,0.1045160185,-0.0
508099047\C,0,0.3656013428,0.7393099621,1.2168153949\C,0,1.4942523264,
0.6195134241,2.0226630601\C,0,2.5780335356,-0.6569790112,0.5027038833\
C,0,1.5113758215,-0.6172319268,-0.3907792768\H,0,-0.469080179,1.333490
2525,1.5728140506\H,0,1.5024570966,1.1139081434,2.9948677958\H,0,3.473
3451866,-1.2170137287,0.2298275118\H,0,1.5954063939,-1.156613535,-1.32
80525134\N,0,-0.749397333,0.1835555428,-0.8934037159\C,0,-1.9911970846
,0.835997293,-0.4836599029\H,0,-2.812160956,0.3495292182,-1.0260243976
\H,0,-2.1728693774,0.6341273198,0.578719102\C,0,-0.719279545,-0.381464
8868,-2.2408082108\H,0,0.2790349976,-0.2383662498,-2.6712922146\H,0,-1
.4017169083,0.2132635383,-2.8615566375\C,0,-1.1247114037,-1.8633202162
,-2.299951123\H,0,-2.1427781468,-2.0042004805,-1.9162639211\H,0,-1.096
9932169,-2.2282303897,-3.3346918687\H,0,-0.4499754987,-2.4815437006,-1
.6970700162\C,0,-2.0150499368,2.3487800793,-0.7568257536\H,0,-1.211322
1899,2.8603261453,-0.2152509811\H,0,-1.883139428,2.5535957376,-1.82648
52635\H,0,-2.9738370802,2.7809249113,-0.4428430073\N,0,2.6055513747,-0
.0601764947,1.7034763805\\Version=AM64L-G03RevD.01\State=1-A\HF=-457.8
949688\MP2=-459.5694926\RMSD=7.552e-09\Thermal=0.\PG=C01 [X(C9H14N2)]\
\@

1c.2

1\1\GINC-SOLARIS\SP\RMP2-FC\6-31+G(2d,p)\C9H14N2\RAMAN\01-Jun-2010\0\\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=r
ead\\sp of d2ap5 mp2-5 on 2p 900 MB\\0,1\C,0,0.043799593,0.0708259709,
0.0113427808\C,0,0.0511431903,0.1147670253,1.4288394754\C,0,1.25714917
03,0.0047726336,2.115526873\C,0,2.4547377863,-0.1616170977,0.205011406
\C,0,1.3193371286,-0.0614370313,-0.5942983384\H,0,-0.8625828562,0.2346
10918,2.0001716667\H,0,1.2471358229,0.0348427174,3.2057453841\H,0,3.42
86092035,-0.2682520973,-0.2743446539\H,0,1.4390764347,-0.0852243914,-1
.671694566\N,0,-1.1229968953,0.1331961691,-0.7255399503\C,0,-2.4159409
418,0.3184961883,-0.0676391258\H,0,-3.1861118349,-0.0429471772,-0.7592
498246\H,0,-2.4653846008,-0.3395729766,0.8095636663\C,0,-1.0868915557,
0.1343370558,-2.1875767828\H,0,-2.0722371025,-0.1968037999,-2.53623704
23\H,0,-0.3748415862,-0.6296499819,-2.5256705392\C,0,-0.7450969092,1.4
920261143,-2.826721367\H,0,0.2227277149,1.8643862129,-2.4728032456\H,0
,-0.6971908586,1.3942967725,-3.9190106633\H,0,-1.5049735956,2.24417161
9,-2.585400103\C,0,-2.7328921571,1.7675302621,0.34283565\H,0,-2.791978
7552,2.4221325207,-0.5343061586\H,0,-3.6973018358,1.810102147,0.865372
7101\H,0,-1.96249397,2.1677189175,1.0113640489\N,0,2.4631148028,-0.134
4974836,1.5457586378\\Version=AM64L-G03RevD.01\State=1-A\HF=-457.89333
05\MP2=-459.5687767\RMSD=7.330e-09\Thermal=0.\PG=C01 [X(C9H14N2)]\\@

1c.3

1\1\GINC-AZAZEL\SP\RMP2-FC\6-31+G(2d,p)\C9H14N2\RAMAN\01-Jun-2010\0\\#
P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=re
ad\\sp of d2ap2 mp2-5 on 2p 900 MB\\0,1\C,0,0.1204952814,-0.018553618,
-0.0215299426\C,0,0.1936686273,-0.5019124275,1.3099510695\C,0,1.389352
5827,-0.4071177792,2.0154580402\C,0,2.4673064564,0.5454610791,0.272797
9558\C,0,1.3329580686,0.5060574621,-0.5355310533\H,0,-0.6620453529,-0.

9465103703,1.8052962906\H,0,1.4267785594,-0.7768044855,3.0408357395\H,
0,3.3912302919,0.9557369017,-0.136732555\H,0,1.4132304956,0.8726836173
,-1.5518843709\N,0,-1.0542962473,-0.0379495871,-0.7607536634\C,0,-2.15
71212171,-0.9005729121,-0.3328087841\H,0,-2.3241105731,-0.7463327928,0
.7380594606\H,0,-3.0704150883,-0.548762293,-0.8194028658\C,0,-0.986876
2308,0.3742631945,-2.1693995566\H,0,-0.376129524,-0.3339611611,-2.7570
063594\H,0,-0.4665006294,1.3387342236,-2.201681882\C,0,-2.3435563401,0
.5617690012,-2.8553787096\H,0,-2.9823739701,1.256333166,-2.2969752563\
H,0,-2.1711634551,0.9889988378,-3.8502705058\H,0,-2.8858602336,-0.3803
031247,-2.9945476987\C,0,-1.9459935214,-2.3946213821,-0.6322557929\H,0
,-1.8368155537,-2.5679092347,-1.7103080976\H,0,-1.0448103882,-2.773129
7821,-0.1362076867\H,0,-2.8045236419,-2.980710768,-0.2802334451\N,0,2.
5323452697,0.1072739067,1.5370874381\\Version=AM64L-G03RevD.01\State=1
-A\HF=-457.8906497\MP2=-459.5665887\RMSD=7.804e-09\Thermal=0.\PG=C01 [
X(C9H14N2)]\\@

1c.4

1\1\GINC-YIN\SP\RMP2-FC\6-31+G(2d,p)\C9H14N2\RAMAN\01-Jun-2010\0\\#P M
P2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=read\
\sp of d2ap12 mp2-5 on 2p 900 MB\\0,1\C,0,-0.0125435738,0.0225245261,0
.014113817\C,0,0.0230518973,-0.1955250788,1.4135081046\C,0,1.249746150
2,-0.2685237207,2.0696517744\C,0,2.4138237552,0.0787175136,0.163821628
4\C,0,1.2558661379,0.1663590817,-0.6034918157\H,0,-0.8810864807,-0.280
2462738,2.0056111255\H,0,1.2602797963,-0.4335706723,3.147730005\H,0,3.
3817010295,0.1860493382,-0.3272488281\H,0,1.3516174907,0.3203820331,-1
.6726626654\N,0,-1.186479132,0.090578039,-0.7200554229\C,0,-1.18327908
63,0.7575256833,-2.0267077497\H,0,-2.1367584722,1.2914810047,-2.131063
7465\H,0,-0.4048605932,1.5311365317,-2.0269199578\C,0,-2.4905338379,-0
.103544737,-0.0843890599\H,0,-2.9096352916,0.8637599619,0.2455398661\H
,0,-2.3452079764,-0.7110168418,0.8111038121\C,0,-3.5101817579,-0.83082
62656,-0.9723887127\H,0,-3.1326310811,-1.8151724725,-1.2724046314\H,0,
-4.4401261242,-0.975103091,-0.4087624248\H,0,-3.7599557108,-0.26538460
45,-1.8772841516\C,0,-0.9876987858,-0.1856833767,-3.225028433\H,0,-0.9
661491462,0.3901203041,-4.1595482133\H,0,-0.0471150839,-0.7416870441,-
3.1429939464\H,0,-1.8012568297,-0.916142414,-3.2908902286\N,0,2.449720
7715,-0.1387224155,1.4867021665\\Version=AM64L-G03RevD.01\State=1-A\HF
=-457.8906718\MP2=-459.566199\RMSD=7.121e-09\Thermal=0.\PG=C01 [X(C9H1
4N2)]\\@

1c.5

1\1\GINC-SOLARIS\SP\RMP2-FC\6-31+G(2d,p)\C9H14N2\RAMAN\23-Jun-2010\0\\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=r
ead\\sp of d2ap10reop mp2-5 on 2p 900 MB\\0,1\C\C,1,1.40520059\C,2,1.3
9527517,1,119.39502618\C,3,2.27533299,2,92.34947272,1,0.88616915,0\C,4
,1.39766394,3,92.439566,2,-0.62879843,0\H,2,1.08584307,1,119.88159342,
5,177.56829601,0\H,3,1.09008144,2,119.85740131,1,179.99192683,0\H,4,1.
0903226,3,147.86038036,2,179.4913522,0\H,5,1.08655119,4,119.48624275,3
,-179.77069629,0\N,1,1.42855599,2,119.61520986,3,179.55580676,0\C,10,1
.4796447,1,114.01147711,2,-83.98057285,0\H,11,1.09739571,10,106.082874
28,1,-178.09746175,0\H,11,1.10721427,10,110.74119466,1,-62.69292622,0\
C,10,1.47127847,1,115.46930483,2,145.13777659,0\H,14,1.09737197,10,106
.10007293,1,-179.23464497,0\H,14,1.10725075,10,112.63803116,1,65.33001
374,0\C,14,1.53163432,10,112.80195387,1,-60.37205284,0\H,17,1.09541516
,14,112.07442342,10,65.04566299,0\H,17,1.09681404,14,109.83757821,10,-
174.97807109,0\H,17,1.09600626,14,110.1946954,10,-55.41066978,0\C,11,1
.53076303,10,115.09828978,1,61.99404362,0\H,21,1.09488736,11,112.22657
192,10,-66.09073698,0\H,21,1.09646784,11,110.80634212,10,55.43423667,0
\H,21,1.09711797,11,109.0801247,10,174.58221579,0\N,4,1.33915025,3,31.
94314312,2,179.84570535,0\\Version=AM64L-G03RevD.01\State=1-A\HF=-457.
8866335\MP2=-459.5633614\RMSD=3.419e-09\Thermal=0.\PG=C01 [X(C9H14N2)]

\\@

1c.1.ac1

1\1\GINC-GOLEM\SP\RMP2-FC\6-31+G(2d,p)\C11H17N2O1(1+)\RAMAN\10-Jul-201
0\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check gu
ess=read\\sp of d2ap4.ac1 mp2-5 on 2p 900 MB\\1,1\C,0,-0.0104187226,0.
001982288,0.0071882934\C,0,-0.0192655032,-0.0229492585,1.4466319418\C,
0,1.1468628896,-0.0165793546,2.1550844316\C,0,2.4230769727,0.033748608
3,0.169494355\C,0,1.2957444442,0.0309595709,-0.5966168104\H,0,-0.94585
63056,-0.0271862045,2.0057991043\H,0,1.143824884,-0.0271383218,3.23745
15324\H,0,3.4242158983,0.0478634181,-0.2460460874\H,0,1.4204187171,0.0
314251398,-1.6717042285\N,0,-1.1353608557,-0.0013421797,-0.7158457758\
C,0,-2.4741965127,-0.1112554548,-0.095294882\H,0,-3.1163827914,-0.6028
732051,-0.8329806372\H,0,-2.4168488343,-0.792392888,0.7593733384\C,0,-
1.1255127592,0.1052975309,-2.1923176003\H,0,-0.3248794497,0.7868660289
,-2.4953084159\H,0,-2.0639972086,0.594803002,-2.4716146464\C,0,-1.0033
464283,-1.2557510582,-2.889077541\H,0,-1.8280192931,-1.9205288733,-2.6
078948844\H,0,-1.0384275474,-1.1146620009,-3.9749990857\H,0,-0.0611881
242,-1.756767343,-2.6389557928\C,0,-3.0618057045,1.248405675,0.3035646
273\H,0,-2.4436683377,1.7532062347,1.054864873\H,0,-3.1511692318,1.911
3411,-0.5644729647\H,0,-4.0634844961,1.1049943525,0.7236418451\N,0,2.3
723677098,0.011340863,1.5413572432\C,0,3.6573253852,0.017788026,2.2728
910203\O,0,4.665444021,0.0456522069,1.6235146019\C,0,3.5866272197,-0.0
118257435,3.7786604583\H,0,3.0830513682,-0.916702809,4.1400038565\H,0,
4.6129526503,-0.0048402155,4.1498730528\H,0,3.0591098945,0.8648456731,
4.1740107242\\Version=AM64L-G03RevD.01\State=1-A\HF=-610.080645\MP2=-6
12.2297885\RMSD=2.173e-09\Thermal=0.\PG=C01 [X(C11H17N2O1)]\\@

1c.2.ac2

1\1\GINC-GOLEM\SP\RMP2-FC\6-31+G(2d,p)\C11H17N2O1(1+)\RAMAN\11-Jul-201
0\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check gu
ess=read\\sp of d2ap4.ac2 mp2-5 on 2p 900 MB\\1,1\C,0,0.0022683894,-0.
0009471113,-0.012938583\C,0,0.0132435952,-0.0273482936,1.4260390925\C,
0,1.1869427453,-0.0257233811,2.1190130435\C,0,2.4385467931,0.024365301
7,0.1177536793\C,0,1.3004127704,0.026316164,-0.6348660016\H,0,-0.90601
51731,-0.0293282845,1.9973006825\H,0,1.2381266593,-0.0377707802,3.2017
771015\H,0,3.4162351227,0.0366798711,-0.3465811907\H,0,1.411090332,0.0
288040849,-1.7114336221\N,0,-1.1315388487,-0.0021137495,-0.7219291087\
C,0,-2.4623143585,-0.1114549554,-0.0828539414\H,0,-3.1139082286,-0.604
394125,-0.8114304776\H,0,-2.3926649196,-0.7910740893,0.7719116857\C,0,
-1.1418753447,0.1051219461,-2.1977348807\H,0,-0.3465722166,0.788137329
7,-2.5118273456\H,0,-2.0845442116,0.593372644,-2.4646983754\C,0,-1.027
6926048,-1.2554486141,-2.8969127964\H,0,-1.8483615532,-1.9206887802,-2
.6055085474\H,0,-1.0764821649,-1.1142073772,-3.9822960955\H,0,-0.08254
43831,-1.7565371045,-2.6581992886\C,0,-3.0443841604,1.2486712847,0.322
2261708\H,0,-2.4181556764,1.7526066213,1.0673009747\H,0,-3.1430433819,
1.9117736195,-0.5447460121\H,0,-4.0414285594,1.1055503294,0.7532403025
\N,0,2.4061062115,-0.0011691305,1.4880138144\C,0,3.6157039776,-0.00290
08203,2.338153786\O,0,3.4584137232,-0.0290401967,3.5270318765\C,0,4.94
75103008,0.0289315154,1.6320514223\H,0,5.0572647336,0.9329539348,1.020
7716202\H,0,5.7208833835,0.0254091842,2.4021562798\H,0,5.0825187283,-0
.8485766914,0.9879310867\\Version=AM64L-G03RevD.01\State=1-A\HF=-610.0
806487\MP2=-612.2297889\RMSD=2.350e-09\Thermal=0.\PG=C01 [X(C11H17N2O1
)]\\@

1c.3.ac2

1\1\GINC-GOLEM\SP\RMP2-FC\6-31+G(2d,p)\C11H17N2O1(1+)\RAMAN\10-Jul-201
0\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check gu
ess=read\\sp of d2ap12.ac2 mp2-5 on 2p 900 MB\\1,1\C,0,-0.0592439813,0
.1908040491,-0.1715058468\C,0,-0.1174836624,-0.1050800229,1.2358791262

\C,0,1.0212263079,-0.2392627896,1.973641851\C,0,2.3686838676,0.1436655
961,0.0743904849\C,0,1.2683391405,0.289750618,-0.7197084819\H,0,-1.062
131493,-0.2307852971,1.7484456229\H,0,1.0192054013,-0.4534426347,3.036
3495715\H,0,3.3680485614,0.2228800863,-0.333927853\H,0,1.4332412966,0.
4770366562,-1.7725465562\N,0,-1.1585399049,0.3720855407,-0.9147471012\
C,0,-1.0711153802,0.6674245755,-2.3644408149\H,0,-1.996661463,1.183385
5963,-2.6332556216\H,0,-0.2640007992,1.3905060442,-2.5235801038\C,0,-2
.5146510216,0.2377375293,-0.3301944306\H,0,-3.189204879,0.804383612,-0
.9772921156\H,0,-2.5261432144,0.7457119271,0.6401592716\C,0,-2.9988139
383,-1.213560302,-0.2042928722\H,0,-2.3360240204,-1.8149737004,0.42812
54552\H,0,-3.9977649222,-1.2216833687,0.2461302993\H,0,-3.0662870584,-
1.6974385874,-1.1839983185\C,0,-0.884500373,-0.5769116595,-3.243804237
2\H,0,-0.8121706753,-0.2696610694,-4.2932238893\H,0,0.0270987547,-1.12
82878763,-2.9864604879\H,0,-1.7337936361,-1.2613852578,-3.15077435\N,0
,2.2692922622,-0.1135654866,1.4167602625\C,0,3.4367838641,-0.275443529
8,2.3101531327\O,0,3.222075681,-0.5130002443,3.4659937572\C,0,4.800615
8888,-0.1228345341,1.6860224775\H,0,4.9321947888,0.8729964775,1.245636
0699\H,0,5.5360293603,-0.2597969596,2.4807459176\H,0,4.9737411093,-0.8
762185534,0.907721072\\Version=AM64L-G03RevD.01\State=1-A\HF=-610.0783
347\MP2=-612.2282211\RMSD=2.466e-09\Thermal=0.\PG=C01 [X(C11H17N2O1)]\
\@

1c.4.ac2

1\1\GINC-YANG\SP\RMP2-FC\6-31+G(2d,p)\C11H17N2O1(1+)\RAMAN\10-Jul-2010
\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check gue
ss=read\\sp of d2ap12.ac1 mp2-5 on 2p 900 MB\\1,1\C,0,-0.0656306608,0.
2270997126,-0.1485069991\C,0,-0.1357578912,-0.0302584529,1.2663090057\
C,0,0.9984632279,-0.1343797743,2.018215741\C,0,2.3594839315,0.20868839
37,0.1209380328\C,0,1.2662575191,0.3222104457,-0.6858475027\H,0,-1.084
0224489,-0.1531240876,1.7726983076\H,0,0.9488245225,-0.3226533528,3.08
30171102\H,0,3.3777231554,0.282775375,-0.2436489179\H,0,1.4395315695,0
.4845353386,-1.7415525511\N,0,-1.1596684294,0.3778505621,-0.9061876911
\C,0,-1.0589247053,0.6150076717,-2.366486371\H,0,-1.9952969513,1.09090
27932,-2.6690779833\H,0,-0.2706811958,1.3544414294,-2.5444192207\C,0,-
2.5203489622,0.2671390695,-0.3293423592\H,0,-3.1844868637,0.8336951251
,-0.9874091332\H,0,-2.5325301591,0.7876084465,0.6342760205\C,0,-3.0215
087494,-1.1769204321,-0.1878661695\H,0,-2.3656353402,-1.7780047124,0.4
522789631\H,0,-4.0216146865,-1.1696465625,0.2600659225\H,0,-3.09211080
87,-1.6712108267,-1.1621121155\C,0,-0.8235230102,-0.6586132712,-3.1905
430667\H,0,-0.7486163622,-0.3923078153,-4.2508835573\H,0,0.1019560963,
-1.1698793966,-2.9024007978\H,0,-1.652263563,-1.3649739861,-3.07760855
13\N,0,2.2489498118,-0.0128045887,1.4708893284\C,0,3.5004819922,-0.116
4233859,2.2521042088\O,0,4.5362758325,-0.0073989105,1.6573309595\C,0,3
.3624617458,-0.3475426668,3.7354883675\H,0,2.8550922684,-1.2963433026,
3.9493190428\H,0,4.3708991072,-0.3842046309,4.1512779829\H,0,2.8061019
833,0.4644454903,4.21924664\\Version=AM64L-G03RevD.01\State=1-A\HF=-61
0.0783328\MP2=-612.2282206\RMSD=2.522e-09\Thermal=0.\PG=C01 [X(C11H17N
2O1)]\\@

1c.5.ac1

1\1\GINC-GOLEM\SP\RMP2-FC\6-31+G(2d,p)\C11H17N2O1(1+)\RAMAN\10-Jul-201
0\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check gu
ess=read\\sp of d2ap5.ac1 mp2-5 on 2p 900 MB\\1,1\C,0,-0.0075503554,0.
0242069017,0.0119759797\C,0,-0.0144812557,0.0289742643,1.4516689357\C,
0,1.1522972663,0.0171712129,2.1596197796\C,0,2.4271692449,0.0319548523
,0.173657244\C,0,1.2988754687,0.0446917325,-0.5917073408\H,0,-0.939342
8817,0.0468608868,2.0129831458\H,0,1.1502751554,0.0153599006,3.2420827
511\H,0,3.4280892684,0.0382958886,-0.2427094102\H,0,1.4247240712,0.072
0640975,-1.6661030423\N,0,-1.1341194599,-0.0083207655,-0.7116027838\C,
0,-2.4676065922,-0.020167292,-0.0651099722\H,0,-3.1572624794,-0.472762
7947,-0.7825067182\H,0,-2.4321368573,-0.7011738255,0.7919756372\C,0,-1

.0987414765,0.0150120809,-2.1937535065\H,0,-2.0444387032,-0.4149999996
,-2.5337646461\H,0,-0.3140450566,-0.669768485,-2.5330170052\C,0,-0.910
7730488,1.4164421583,-2.7914736265\H,0,0.0233626637,1.8834268489,-2.45
9424631\H,0,-0.8830122115,1.3405706274,-3.8843225169\H,0,-1.7384257792
,2.0796199231,-2.5199967334\C,0,-2.9719185108,1.3693136174,0.349090668
9\H,0,-3.0906528063,2.0251474998,-0.5193811218\H,0,-3.9503579864,1.268
7956284,0.8322792436\H,0,-2.2916965251,1.8590675154,1.0552695681\N,0,2
.3771785694,0.0122499108,1.5450436855\C,0,3.6624029864,-0.003071321,2.
2766225023\O,0,4.6706037295,0.0096789674,1.6270828104\C,0,3.5909092915
,-0.0372304522,3.7821607337\H,0,3.0634111615,-0.9298439652,4.139779091
\H,0,4.6170821631,-0.0583974147,4.1532217389\H,0,3.0868339897,0.851542
2445,4.1813466559\\Version=AM64L-G03RevD.01\State=1-A\HF=-610.0783322\
MP2=-612.2282208\RMSD=2.583e-09\Thermal=0.\PG=C01 [X(C11H17N2O1)]\\@

1d.1

1\1\GINC-NODE-28\SP\RMP2-FC\6-31+G(2d,p)\C11H18N2\ZIP08\06-Aug-2010\0\
\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=
read\\sp of d3ap37 MP2-5/6-31+G(2d,p)\\0,1\C,0,0.0126165156,0.06855707
5,-0.0428585818\C,0,-0.0131874721,0.0744698151,1.3489654755\C,0,1.2032
965356,0.0006147983,2.0744651705\C,0,2.3754943472,-0.0723585101,1.2793
151654\C,0,2.2687344893,-0.0648521851,-0.1086405334\H,0,-0.9308590578,
0.1236788679,-0.5873346546\H,0,-0.972197029,0.1390319505,1.8508006595\
H,0,3.3620818672,-0.1374487731,1.7244170326\H,0,3.1789228413,-0.119310
1562,-0.7071638292\N,0,1.2435020247,-0.0001804705,3.4548237235\N,0,1.1
196708635,0.0022644052,-0.7969811319\C,0,2.51456369,-0.1421447898,4.16
80604858\H,0,3.2625347451,0.5257571273,3.7189672348\H,0,2.3573622388,0
.2244110619,5.1889394693\C,0,0.0161206314,0.1409578513,4.2410006021\H,
0,0.2324577361,-0.2267734675,5.2505752541\H,0,-0.756763955,-0.52643054
87,3.8354388766\C,0,3.0646698433,-1.5830378251,4.224928934\H,0,3.23970
81704,-1.9471866859,3.2042080991\H,0,4.0476503121,-1.5439950116,4.7173
897966\C,0,-0.5296562339,1.5817804843,4.3314451228\H,0,-1.4822981521,1
.5421683905,4.880259118\H,0,-0.7638082207,1.9470873,3.3230611482\C,0,0
.4266163599,2.5654035345,5.01988778\H,0,0.655430048,2.2503925028,6.047
3575089\H,0,1.3726081964,2.6466989604,4.4706635847\H,0,-0.0144572946,3
.5681388383,5.070389073\C,0,2.1500917269,-2.5674954433,4.9667624817\H,
0,2.5933454591,-3.5702635811,4.9903592104\H,0,1.9814918645,-2.25366273
01,6.0061684811\H,0,1.1737269861,-2.6482184636,4.4734551028\\Version=I
A32L-G03RevD.01\State=1-A\HF=-535.9698216\MP2=-537.954451\RMSD=7.430e-
09\Thermal=0.\PG=C01 [X(C11H18N2)]\\@

1d.2

1\1\GINC-NODE-31\SP\RMP2-FC\6-31+G(2d,p)\C11H18N2\ZIP08\06-Aug-2010\0\
\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=
read\\sp of d3ap34 MP2-5/6-31+G(2d,p)\\0,1\C,0,0.0077693821,0.03812246
14,-0.0175812956\C,0,-0.0115400403,0.0186096387,1.3742610975\C,0,1.210
547557,-0.0137205216,2.092939567\C,0,2.3813188515,-0.0209371907,1.2923
939855\C,0,2.2671847152,-0.0045895883,-0.0948250085\H,0,-0.9396819081,
0.0625577232,-0.5573996443\H,0,-0.9695839059,0.0185740717,1.881921548\
H,0,3.3723570745,-0.0289124718,1.7326730569\H,0,3.1758376397,-0.011394
8019,-0.6981048979\N,0,1.2547835562,-0.0420468787,3.4727297924\N,0,1.1
129005111,0.0253577867,-0.7771512661\C,0,2.5297288569,-0.0160407318,4.
188044295\H,0,2.3592119561,-0.4452254408,5.1827862173\H,0,3.2392941152
,-0.6902397525,3.6907834967\C,0,0.033173111,0.0881636698,4.2688262575\
H,0,-0.6246088201,0.8388207237,3.8104149572\H,0,0.3224209924,0.4955412
552,5.2462374206\C,0,3.1441697794,1.3900568002,4.3361104205\H,0,3.2772
789974,1.8335997004,3.3405645263\H,0,2.4306502782,2.0339691215,4.87012
02273\C,0,-0.740199803,-1.2309333699,4.4779088121\H,0,-1.0440289836,-1
.6322508682,3.5021632306\H,0,-1.6659194623,-0.9919165459,5.0221465212\
C,0,0.0516829621,-2.2998813646,5.2430938248\H,0,-0.5456977714,-3.21023
89612,5.3730582728\H,0,0.9649140686,-2.5759756427,4.7021505425\H,0,0.3

40421548,-1.9457732197,6.2423760822\C,0,4.4840809149,1.3585088915,5.08
47115432\H,0,5.2237015896,0.7467367875,4.5510945883\H,0,4.9010849936,2
.3667814176,5.1910789718\H,0,4.3689534109,0.9366402881,6.0922107012\\V
ersion=IA32L-G03RevD.01\State=1-A\HF=-535.971555\MP2=-537.9542305\RMSD
=5.915e-09\Thermal=0.\PG=C01 [X(C11H18N2)]\\@

1d.3

1\1\GINC-NODE-28\SP\RMP2-FC\6-31+G(2d,p)\C11H18N2\ZIP08\05-Aug-2010\0\
\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=
read\\sp of d3ap29_1 MP2-5/6-31+G(2d,p)\\0,1\C,0,0.1701591557,-0.77117
05992,0.2157950095\C,0,0.175029248,-0.5622957104,1.5916095213\C,0,1.33
84079359,-0.0529029022,2.2232349093\C,0,2.4312123786,0.1947387539,1.35
24337283\C,0,2.3029997849,-0.0615483517,-0.0100385265\H,0,-0.73365315,
-1.1622373485,-0.2530730826\H,0,-0.7173422332,-0.8116396267,2.15371537
88\H,0,3.3736639304,0.585088191,1.7189134977\H,0,3.1540581895,0.132953
2782,-0.6639647344\N,0,1.4167262115,0.1884585874,3.5818040896\N,0,1.20
13507883,-0.535242224,-0.6091951753\C,0,0.3169796804,-0.0961711049,4.5
067652668\H,0,0.2923011354,0.7123484071,5.2485064462\H,0,-0.6348743169
,-0.0359505086,3.969687551\C,0,2.6495785898,0.7038995543,4.1811376801\
H,0,3.5109362999,0.1499036668,3.7837062617\H,0,2.6100648106,0.47016373
69,5.2524337856\C,0,0.4291429648,-1.4441236347,5.2503257608\H,0,1.3787
802704,-1.4636541454,5.805230751\H,0,-0.3675107792,-1.4686242765,6.009
0021507\C,0,2.8752717331,2.2211099114,4.0050119428\H,0,2.9419011822,2.
4602162319,2.9359561786\H,0,3.856186219,2.4605410362,4.4418463324\C,0,
1.7924487526,3.0959788289,4.6518733847\H,0,2.0185229384,4.1600990857,4
.5131387164\H,0,0.8098594138,2.9054453132,4.2033118038\H,0,1.717361573
3,2.9103276119,5.7321677562\C,0,0.3331555423,-2.6889897012,4.357883971
5\H,0,0.458771959,-3.6015207104,4.9535999554\H,0,-0.6427366833,-2.7501
391648,3.8590994194\H,0,1.1057721154,-2.6854474469,3.5803674345\\Versi
on=IA32L-G03RevD.01\State=1-A\HF=-535.9679687\MP2=-537.9528417\RMSD=7.
733e-09\Thermal=0.\PG=C01 [X(C11H18N2)]\\@

1d.4

1\1\GINC-NODE-31\SP\RMP2-FC\6-31+G(2d,p)\C11H18N2\ZIP08\06-Aug-2010\0\
\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=
read\\sp of d3ap7 MP2-5/6-31+G(2d,p)\\0,1\C,0,0.2690110149,0.654284714
1,-0.3107690389\C,0,0.4449875963,0.8310837815,1.0586307754\C,0,1.46456
80238,0.1123162892,1.7328327987\C,0,2.2392229769,-0.7490486253,0.91511
72422\C,0,1.9666790101,-0.8334151631,-0.4472781692\H,0,-0.5181932933,1
.2140120569,-0.817450836\H,0,-0.1973883667,1.5315133176,1.5813315352\H
,0,3.0350960224,-1.3600787752,1.3270562661\H,0,2.5693216102,-1.5006116
728,-1.0648434019\N,0,1.6870071569,0.2418714056,3.0876097428\N,0,1.001
4818835,-0.1573319691,-1.0877425967\C,0,0.8168645002,1.0559304961,3.93
2429273\H,0,-0.221966715,0.9549275661,3.5922681809\H,0,0.8430041429,0.
6284541531,4.9440950286\C,0,2.804032217,-0.4286045711,3.7480991782\H,0
,3.0868827747,0.1786290731,4.6188144799\H,0,3.6780592694,-0.4236975888
,3.0839170789\C,0,1.2159880732,2.5428493405,3.9948492869\H,0,2.2542694
252,2.616392219,4.3489953425\H,0,1.2054455404,2.9617573269,2.979807373
5\C,0,2.4901566971,-1.8656913188,4.2068026825\H,0,2.1910484459,-2.4646
202155,3.3363341952\H,0,1.6203634792,-1.8410458168,4.8788945173\C,0,3.
6827118785,-2.5217358391,4.9168099638\H,0,4.5571571171,-2.582114184,4.
2550531598\H,0,3.979409058,-1.9520972314,5.8077684887\H,0,3.4389599369
,-3.5408696776,5.239136876\C,0,0.2905152324,3.3541434186,4.9124527553\
H,0,0.5926287096,4.4074571024,4.9471142354\H,0,-0.7500043132,3.3176470
222,4.5628679674\H,0,0.3090419488,2.9678256552,5.9404301139\\Version=I
A32L-G03RevD.01\State=1-A\HF=-535.9733103\MP2=-537.9539638\RMSD=2.386e
-09\Thermal=0.\PG=C01 [X(C11H18N2)]\\@

1d.5

1\1\GINC-NODE-31\SP\RMP2-FC\6-31+G(2d,p)\C11H18N2\ZIP08\06-Aug-2010\0\

\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=
read\\sp of d3ap48 MP2-5/6-31+G(2d,p)\\0,1\C,0,0.1382940765,-0.7432314
035,-0.3410340983\C,0,-0.0099235481,-0.6362516229,1.0392552991\C,0,0.9
504634037,0.081748918,1.797232872\C,0,2.0111603521,0.6438328872,1.0425
680242\C,0,2.0506876287,0.460682793,-0.3364798085\H,0,-0.6085549236,-1
.299530908,-0.9089100812\H,0,-0.8601133482,-1.1193455186,1.5078472373\
H,0,2.7896216426,1.237222811,1.5082598086\H,0,2.8729377711,0.900535811
4,-0.902158729\N,0,0.8418786431,0.2315204397,3.1670367203\N,0,1.144067
0714,-0.2182024166,-1.0552342779\C,0,1.918646716,0.7747752681,3.997489
6894\H,0,2.0317018055,0.1154449471,4.8706077222\H,0,2.8661066648,0.712
5181719,3.4528377581\C,0,-0.2770780087,-0.3568804505,3.9014322281\H,0,
-1.2062722754,-0.1942702862,3.3407324699\H,0,-0.3902179511,0.208623212
2,4.8356968636\C,0,1.6774461513,2.2159713214,4.4924239147\H,0,0.736553
3203,2.2430222925,5.0613787488\H,0,2.4752032499,2.4589230243,5.2100383
827\C,0,-0.1041580109,-1.8531032083,4.2306347376\H,0,0.8195467122,-1.9
86404609,4.811765954\H,0,0.0334034644,-2.4160967012,3.2984409653\C,0,-
1.2990778362,-2.4130212457,5.0156057015\H,0,-1.1573723123,-3.475182349
9,5.2473062393\H,0,-1.437639273,-1.8797126182,5.9656766588\H,0,-2.2314
731326,-2.3186371889,4.4429897904\C,0,1.6339021929,3.2742174095,3.3823
855405\H,0,0.857985007,3.0420812855,2.6436600019\H,0,1.4177392956,4.26
552535,3.7991367663\H,0,2.59372833,3.3391677786,2.8535689104\\Version=
IA32L-G03RevD.01\State=1-A\HF=-535.9702465\MP2=-537.9533089\RMSD=6.440
e-09\Thermal=0.\PG=C01 [X(C11H18N2)]\\@

1d.1.ac1

1\1\GINC-NODE-28\SP\RMP2-FC\6-31+G(2d,p)\C13H21N2O1(1+)\ZIP08\07-Aug-2
010\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check
guess=read\\sp of d3ap7.ac1 MP2-5/6-31+G(2d,p)\\1,1\C,0,-0.0251965261,
-0.045825337,0.0101166035\C,0,0.0001674465,-0.0455184554,1.3725197617\
C,0,1.2470479749,-0.0046364,2.0911555862\C,0,2.427254145,0.0343209634,
1.2668405176\C,0,2.3326637717,0.0309556511,-0.0939799925\H,0,-0.942234
2026,-0.069727676,-0.5673951642\H,0,-0.9493103115,-0.0587168453,1.8916
895204\H,0,3.4183739265,0.048524785,1.7011036849\H,0,3.2179865813,0.05
33594727,-0.7163444924\N,0,1.3059172408,-0.003187447,3.426731581\N,0,1
.124136038,-0.0084170823,-0.7410288581\C,0,0.0944431302,-0.1092894712,
4.2693158814\H,0,-0.614695525,-0.7969248725,3.7962541212\H,0,0.4067932
714,-0.5894174534,5.2030864698\C,0,2.5851336769,0.1025184533,4.1613286
48\H,0,2.355430869,0.5849610336,5.1175817506\H,0,3.2525607734,0.788084
3322,3.6280785961\C,0,-0.5581502721,1.2525265339,4.5646486451\H,0,0.18
64542464,1.9136150832,5.0287432766\H,0,-0.8532205568,1.7310322106,3.62
04738132\C,0,3.2580613198,-1.2601298062,4.4025297703\H,0,3.4706011683,
-1.7408973907,3.437463952\H,0,2.55378469,-1.9188581961,4.9286877422\C,
0,4.5510478795,-1.1145248152,5.218360364\H,0,5.2826595423,-0.478387450
4,4.7040677543\H,0,4.3542120079,-0.6733074486,6.2031749878\H,0,5.01472
67052,-2.0934316222,5.3787621708\C,0,-1.7775171653,1.1047387877,5.4867
619763\H,0,-2.2291579988,2.0826641038,5.6833246581\H,0,-2.5474592014,0
.4655742207,5.0364021132\H,0,-1.4974334281,0.6663091246,6.45250589\C,0
,0.9802317893,-0.0121580688,-2.2108441538\O,0,-0.1312644231,-0.0516287
159,-2.6609627083\C,0,2.2502900319,0.0349072507,-3.0224648691\H,0,2.88
76495769,-0.8352249683,-2.8230827134\H,0,1.9608908434,0.0283266057,-4.
0747791643\H,0,2.8258296039,0.9456261069,-2.8167139766\\Version=IA32L-
G03RevD.01\State=1-A\HF=-688.1604523\MP2=-690.6157294\RMSD=1.652e-09\T
hermal=0.\PG=C01 [X(C13H21N2O1)]\\@

1d.2.ac2

1\1\GINC-NODE-28\SP\RMP2-FC\6-31+G(2d,p)\C13H21N2O1(1+)\ZIP08\09-Aug-2
010\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check
guess=read\\sp of d3ap7.ac2 MP2-5/6-31+G(2d,p)\\1,1\C,0,-0.0722033032,
-0.02911849,0.0218544875\C,0,-0.0354126248,-0.0351820527,1.3854594311\
C,0,1.2186142503,0.002365306,2.092516206\C,0,2.3905556029,0.0449289686

,1.2573393948\C,0,2.2847421706,0.0479102066,-0.101197584\H,0,-1.013249
0692,-0.0504383149,-0.5125465335\H,0,-0.9801614788,-0.0503887474,1.913
0247471\H,0,3.385576741,0.0573259006,1.6827912706\H,0,3.14192605,0.073
1366318,-0.7642421606\N,0,1.2885368295,-0.001723069,3.4275303004\N,0,1
.0684968239,0.0117493622,-0.7383491474\C,0,0.0859971433,-0.109128913,4
.2816277706\H,0,-0.6296186879,-0.7938585141,3.8138170457\H,0,0.4066738
756,-0.5933014254,5.2104362835\C,0,2.5754710603,0.1029718002,4.1497594
522\H,0,2.3545026667,0.581130113,5.1102579704\H,0,3.2357314175,0.79172
82295,3.6120053935\C,0,-0.5607048022,1.2528883162,4.5890962275\H,0,0.1
909629858,1.9108584933,5.0460903048\H,0,-0.8653732355,1.7353570218,3.6
499110387\C,0,3.2535686238,-1.2592707757,4.3781322229\H,0,3.4565048274
,-1.7357594007,3.4089678309\H,0,2.557094231,-1.9215142677,4.9103134933
\C,0,4.5559382774,-1.1130081605,5.1790098356\H,0,5.2789831836,-0.47277
96378,4.6579743278\H,0,4.3700012806,-0.6765496795,6.1680812281\H,0,5.0
244320697,-2.0912119882,5.3292996448\C,0,-1.7689563009,1.1054031239,5.
5255510587\H,0,-2.215075269,2.0838848639,5.7318000682\H,0,-2.546720451
7,0.4700525492,5.0830183627\H,0,-1.4780212064,0.6623798294,6.485949664
9\C,0,1.0704402169,0.0183833389,-2.2152831205\O,0,2.1335417026,0.05887
27545,-2.7699979577\C,0,-0.2717681959,-0.0272263326,-2.9011195313\H,0,
-0.8869691355,0.8423960947,-2.6396036352\H,0,-0.0849277445,-0.01847857
96,-3.9763761533\H,0,-0.8248794453,-0.9384524935,-2.642813159\\Version
=IA32L-G03RevD.01\State=1-A\HF=-688.1604514\MP2=-690.6157299\RMSD=1.68
4e-09\Thermal=0.\PG=C01 [X(C13H21N2O1)]\\@

1d.3.ac1

1\1\GINC-NODE-31\SP\RMP2-FC\6-31+G(2d,p)\C13H21N2O1(1+)\ZIP08\07-Aug-2
010\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check
guess=read\\sp of d3ap37.ac1 MP2-5/6-31+G(2d,p)\\1,1\C,0,-0.0230448225
,0.028950936,-0.0139320671\C,0,-0.0002885315,0.0261780616,1.3488045336
\C,0,1.244970353,0.0037184902,2.0712146118\C,0,2.4268149962,-0.0127531
782,1.2480908754\C,0,2.3350738315,-0.0034629212,-0.1131564082\H,0,-0.9
399000936,0.0437544153,-0.5917687301\H,0,-0.9513492681,0.0466229024,1.
8643634745\H,0,3.4172368183,-0.0381108648,1.6829450561\H,0,3.222135479
2,-0.013949473,-0.7333181084\N,0,1.3009394358,-0.001624528,3.408198195
2\N,0,1.127819834,0.0161075618,-0.7628941087\C,0,2.5956661056,-0.04108
11857,4.1297037533\H,0,3.2879413414,0.6582018207,3.6472333796\H,0,2.40
58146347,0.3584750522,5.1297213799\C,0,0.0693773419,0.0310415112,4.234
3371759\H,0,0.3422322618,-0.3741095628,5.2126951098\H,0,-0.6590334639,
-0.6664707031,3.8056798305\C,0,3.2141258063,-1.4489982743,4.2340232853
\H,0,3.4182744127,-1.841623835,3.2283689951\H,0,4.1905243599,-1.325382
5849,4.7219492251\C,0,-0.5409198911,1.4368200563,4.3975642388\H,0,-1.4
726576774,1.3076639264,4.9648425005\H,0,-0.8300753969,1.8339358102,3.4
149369885\C,0,0.3670524836,2.4451207854,5.11530839\H,0,0.6461830137,2.
092192309,6.1165206566\H,0,1.2869619864,2.641506944,4.5503329469\H,0,-
0.1514959824,3.4021595701,5.2367538635\C,0,2.3664551583,-2.4591113105,
5.0198893348\H,0,2.8902414475,-3.4182715137,5.0922292713\H,0,2.1736338
256,-2.1109366749,6.0428106641\H,0,1.401720943,-2.6494629385,4.5331801
265\C,0,0.987491614,0.024147728,-2.2335167032\O,0,-0.1233900949,0.0458
233221,-2.6861927833\C,0,2.2602472533,0.0036876735,-3.0419425054\H,0,2
.852335855,-0.8967251606,-2.8377661264\H,0,1.9734893276,0.0083906985,-
4.0950096756\H,0,2.8808080344,0.8848850113,-2.8380596802\\Version=IA32
L-G03RevD.01\State=1-A\HF=-688.1563024\MP2=-690.6151888\RMSD=2.020e-09
\Thermal=0.\PG=C01 [X(C13H21N2O1)]\\@

1d.4.ac1

1\1\GINC-NODE-31\SP\RMP2-FC\6-31+G(2d,p)\C13H21N2O1(1+)\ZIP08\09-Aug-2
010\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check
guess=read\\sp of d3ap37.ac2 MP2-5/6-31+G(2d,p)\\1,1\C,0,-0.0769383465
,0.0143075559,0.0021056689\C,0,-0.038361922,0.0182217666,1.3659220382\
C,0,1.2166284393,-0.0014385824,2.072442541\C,0,2.3872630193,-0.0210170

752,1.2344213991\C,0,2.2798791058,-0.0184046552,-0.1242694949\H,0,-1.0
191231375,0.0271904704,-0.5305388802\H,0,-0.982760392,0.0417892065,1.8
934007293\H,0,3.3831731002,-0.0434698925,1.6567907255\H,0,3.137403796,
-0.0308926171,-0.7870161937\N,0,1.2884943253,-0.0013866617,3.408674808
8\N,0,1.062802517,-0.0026427629,-0.7599363259\C,0,2.5932608353,-0.0373
750694,4.1133732045\H,0,3.2776998183,0.6619006219,3.6200070796\H,0,2.4
151595648,0.3637740927,5.1149439622\C,0,0.0685342595,0.035238798,4.250
5787899\H,0,0.352807058,-0.3681710834,5.2263723708\H,0,-0.6668672575,-
0.6621909825,3.833684287\C,0,3.2158180274,-1.4438007135,4.2119063108\H
,0,3.4086617633,-1.8373710409,3.2045417546\H,0,4.1979832944,-1.3168299
278,4.6871451148\C,0,-0.5366401402,1.4427335487,4.4189012054\H,0,-1.46
23009237,1.3171581229,4.9969066432\H,0,-0.8352685623,1.8394733312,3.43
88054601\C,0,0.3823176822,2.4495884589,5.1247462968\H,0,0.6710113053,2
.0973998868,6.1234407056\H,0,1.2966968091,2.6415773184,4.5495205959\H,
0,-0.1316571662,3.4085963492,5.2500748219\C,0,2.3807940472,-2.45458356
35,5.0102125402\H,0,2.9079320157,-3.4122909736,5.0772007046\H,0,2.2001
014401,-2.1054781831,6.0350881847\H,0,1.4103921006,-2.6483987478,4.536
1280036\C,0,1.06215833,-0.0048641286,-2.2372586675\O,0,2.1247703049,-0
.0247217677,-2.7939500951\C,0,-0.2819225132,0.018775841,-2.9204622048\
H,0,-0.8514984412,0.918365548,-2.6571713569\H,0,-0.0969573133,0.018243
8128,-3.9960967966\H,0,-0.8805203043,-0.8632291483,-2.6617715179\\Vers
ion=IA32L-G03RevD.01\State=1-A\HF=-688.1563034\MP2=-690.6151876\RMSD=1
.958e-09\Thermal=0.\PG=C01 [X(C13H21N2O1)]\\@

1d.5.ac1

1\1\GINC-NODE-25\SP\RMP2-FC\6-31+G(2d,p)\C13H21N2O1(1+)\ZIP08\10-Aug-2
010\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check
guess=read\\sp of d3ap3.ac2 MP2-5/6-31+G(2d,p)\\1,1\C,0,-0.0395888406,
0.1378200111,0.1923431583\C,0,-0.032744136,0.3577674912,1.5386765807\C
,0,1.169495488,0.1852024814,2.314683614\C,0,2.3235234797,-0.2284948393
,1.5600265523\C,0,2.2500371887,-0.4320632229,0.2148642512\H,0,-0.94099
00083,0.2724193725,-0.3916052871\H,0,-0.9586764006,0.6803066033,1.9962
214736\H,0,3.2747210912,-0.4141916424,2.0400735742\H,0,3.0959329318,-0
.750348429,-0.3834399621\N,0,1.1975245011,0.394674562,3.6360899733\N,0
,1.0836943195,-0.2543604055,-0.4885233211\C,0,-0.0136147471,0.79149247
21,4.3883637183\H,0,-0.873624001,0.2261606831,4.013356856\H,0,0.138462
3744,0.4604042509,5.4206196022\C,0,2.4315342683,0.32444406,4.452528378
6\H,0,2.3799326168,1.1687691769,5.1498472286\H,0,3.2999289147,0.507932
7546,3.8148040877\C,0,-0.2806198507,2.3074577361,4.3590017957\H,0,0.60
37500272,2.8341341435,4.7426205519\H,0,-0.4132420921,2.6409741052,3.32
06061831\C,0,2.5880298856,-0.9907409432,5.2400542337\H,0,1.7161835347,
-1.1266432582,5.8945127916\H,0,3.4489648924,-0.8523668497,5.9077343151
\C,0,2.7934399691,-2.2447981329,4.3800107299\H,0,2.8938960218,-3.12845
21511,5.0193729787\H,0,1.9456098138,-2.4236291029,3.7067594944\H,0,3.7
071368339,-2.1746343161,3.7755900464\C,0,-1.5146543668,2.6764391307,5.
1953643414\H,0,-2.4193952585,2.1829225428,4.8181213957\H,0,-1.38635888
65,2.387410024,6.2457164267\H,0,-1.6875974938,3.7572672373,5.166134206
3\C,0,1.1166640277,-0.5040750512,-1.9432636864\O,0,2.1610756818,-0.844
4792558,-2.4260965384\C,0,-0.1731095471,-0.3092927538,-2.6999559044\H,
0,-0.5350577504,0.7230403577,-2.6201147657\H,0,0.0312429379,-0.5330413
052,-3.7484573688\H,0,-0.957862927,-0.9848680657,-2.3381441201\\Versio
n=IA32L-G03RevD.01\State=1-A\HF=-688.1575019\MP2=-690.6150065\RMSD=1.7
55e-09\Thermal=0.\PG=C01 [X(C13H21N2O1)]\\@

1e.1

1\1\GINC-NODE17\SP\RMP2-FC\6-31+G(2d,p)\C13H22N2\ZIP08\06-Aug-2010\0\\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=r
ead\\sp of d4ap37 MP2-5/6-31+G(2d,p)\\0,1\C,0,-0.0016644086,0.01936998
44,-0.0386543721\C,0,-0.0017043582,0.0205457633,1.3534275455\C,0,1.230
2968957,0.0000807181,2.0561253214\C,0,2.3894783003,-0.0175952262,1.238

8027985\C,0,2.2563630823,-0.0113203462,-0.146886367\H,0,-0.956714736,0
.0333746071,-0.5652967945\H,0,-0.9530207176,0.0433439564,1.8728175936\
H,0,3.3860848392,-0.0421292043,1.6647865993\H,0,3.1566929751,-0.023228
4669,-0.7624623337\N,0,1.2963727392,-0.0024501041,3.4353893801\N,0,1.0
92814581,0.0053482889,-0.8136388891\C,0,2.5869069047,-0.0625908972,4.1
254018566\H,0,3.2836524119,0.6455478782,3.6563624425\H,0,2.4271141888,
0.3054632032,5.145485484\C,0,0.0777192537,0.0549387503,4.2458234395\H,
0,0.3342293191,-0.3168155881,5.2446074271\H,0,-0.6607953374,-0.6516030
571,3.8429490038\C,0,3.2266060789,-1.4655355821,4.1853935802\H,0,3.384
0928061,-1.8409728192,3.1648589777\H,0,4.2252420056,-1.3575371908,4.63
68922399\C,0,-0.553072372,1.4575411772,4.371822698\H,0,-1.5039914084,1
.3477149715,4.916322075\H,0,-0.8073330617,1.8366795219,3.3723970733\C,
0,0.3324935174,2.4868734657,5.0924479282\H,0,0.5944508572,2.10838534,6
.0929653064\H,0,1.277580704,2.6011156546,4.5431237683\C,0,2.4138025505
,-2.4976488782,4.9836073417\H,0,2.2487600999,-2.122867478,6.0059624463
\H,0,1.4205090841,-2.6100435922,4.5267335754\C,0,-0.346033661,3.857922
6807,5.2276268447\H,0,-1.2803415249,3.7831180174,5.7997669863\H,0,0.30
48274936,4.575885212,5.7416486812\H,0,-0.5919031281,4.2749522415,4.242
2352416\C,0,3.1018995759,-3.8690669109,5.0482866606\H,0,4.0866378204,-
3.7961948435,5.5287567848\H,0,2.5030309676,-4.5890155426,5.6195477869\
H,0,3.2523653415,-4.2824486521,4.0423852671\\Version=AM64L-G03RevD.01\
State=1-A\HF=-614.0478378\MP2=-616.338253\RMSD=6.163e-09\Thermal=0.\PG
=C01 [X(C13H22N2)]\\@

1e.2

1\1\GINC-NODE-31\SP\RMP2-FC\6-31+G(2d,p)\C11H18N2\ZIP08\06-Aug-2010\0\
\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=
read\\sp of d3ap34 MP2-5/6-31+G(2d,p)\\0,1\C,0,0.0077693821,0.03812246
14,-0.0175812956\C,0,-0.0115400403,0.0186096387,1.3742610975\C,0,1.210
547557,-0.0137205216,2.092939567\C,0,2.3813188515,-0.0209371907,1.2923
939855\C,0,2.2671847152,-0.0045895883,-0.0948250085\H,0,-0.9396819081,
0.0625577232,-0.5573996443\H,0,-0.9695839059,0.0185740717,1.881921548\
H,0,3.3723570745,-0.0289124718,1.7326730569\H,0,3.1758376397,-0.011394
8019,-0.6981048979\N,0,1.2547835562,-0.0420468787,3.4727297924\N,0,1.1
129005111,0.0253577867,-0.7771512661\C,0,2.5297288569,-0.0160407318,4.
188044295\H,0,2.3592119561,-0.4452254408,5.1827862173\H,0,3.2392941152
,-0.6902397525,3.6907834967\C,0,0.033173111,0.0881636698,4.2688262575\
H,0,-0.6246088201,0.8388207237,3.8104149572\H,0,0.3224209924,0.4955412
552,5.2462374206\C,0,3.1441697794,1.3900568002,4.3361104205\H,0,3.2772
789974,1.8335997004,3.3405645263\H,0,2.4306502782,2.0339691215,4.87012
02273\C,0,-0.740199803,-1.2309333699,4.4779088121\H,0,-1.0440289836,-1
.6322508682,3.5021632306\H,0,-1.6659194623,-0.9919165459,5.0221465212\
C,0,0.0516829621,-2.2998813646,5.2430938248\H,0,-0.5456977714,-3.21023
89612,5.3730582728\H,0,0.9649140686,-2.5759756427,4.7021505425\H,0,0.3
40421548,-1.9457732197,6.2423760822\C,0,4.4840809149,1.3585088915,5.08
47115432\H,0,5.2237015896,0.7467367875,4.5510945883\H,0,4.9010849936,2
.3667814176,5.1910789718\H,0,4.3689534109,0.9366402881,6.0922107012\\V
ersion=IA32L-G03RevD.01\State=1-A\HF=-535.971555\MP2=-537.9542305\RMSD
=5.915e-09\Thermal=0.\PG=C01 [X(C11H18N2)]\\@

1e.3

1\1\GINC-NODE23\SP\RMP2-FC\6-31+G(2d,p)\C13H22N2\ZIP08\06-Aug-2010\0\\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=r
ead\\sp of d4ap7 MP2-5/6-31+G(2d,p)\\0,1\C,0,-0.0008469359,0.021779151
,-0.0163189225\C,0,-0.0008007347,0.0226533442,1.3756110703\C,0,1.23179
33726,-0.0000747343,2.076591742\C,0,2.3914118695,-0.0197140767,1.26045
59679\C,0,2.2578611994,-0.0131962153,-0.1250368158\H,0,-0.9556414886,0
.0412412063,-0.5432550515\H,0,-0.9511443574,0.057696556,1.8972840693\H
,0,3.3874317656,-0.0566798909,1.6883590142\H,0,3.1576683055,-0.0303339
555,-0.7412562999\N,0,1.2980378816,-0.0028706751,3.453740164\N,0,1.093

8462635,0.0057542499,-0.7912566778\C,0,0.0974793052,-0.1067364844,4.27
93059738\H,0,-0.6219934463,-0.7768984095,3.7919227529\H,0,0.3829291827
,-0.6050711492,5.2157710769\C,0,2.5723225481,0.0978045455,4.1606696681
\H,0,2.3781913552,0.5922280573,5.1222536375\H,0,3.2418321916,0.7700982
843,3.6092364326\C,0,-0.564894403,1.2469306689,4.6006624938\H,0,0.1667
135853,1.8902092953,5.1124569087\H,0,-0.8206447016,1.7576838005,3.6616
041095\C,0,3.2621973207,-1.2570535782,4.4113849381\H,0,3.4265014936,-1
.7638963239,3.4500204412\H,0,2.5829682048,-1.9025633171,4.988408217\C,
0,4.5967869065,-1.1083521476,5.160217247\H,0,5.2707104208,-0.461852807
5,4.577780712\H,0,4.4238769616,-0.5884366348,6.1150066137\C,0,-1.82145
10849,1.0948693812,5.4735505501\H,0,-2.5483031569,0.4506330489,4.95585
16016\H,0,-1.5577666594,0.5710630301,6.405178331\C,0,-2.4809629307,2.4
395991073,5.8122378117\H,0,-3.3717116954,2.3001512995,6.4369634181\H,0
,-1.7877004736,3.0932410976,6.3576922739\H,0,-2.7896507337,2.968950544
6,4.9014286439\C,0,5.2854888738,-2.4543418471,5.4284792464\H,0,6.23213
64172,-2.3173010563,5.9653584636\H,0,4.647665098,-3.1103512033,6.03528
54208\H,0,5.5051842339,-2.9798831059,4.4900685137\\Version=AM64L-G03Re
vD.01\State=1-A\HF=-614.0512673\MP2=-616.3372815\RMSD=2.288e-09\Therma
l=0.\PG=C01 [X(C13H22N2)]\\@

1e.4

1\1\GINC-NODE17\SP\RMP2-FC\6-31+G(2d,p)\C13H22N2\ZIP08\06-Aug-2010\0\\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=r
ead\\sp of d4ap49 MP2-5/6-31+G(2d,p)\\0,1\C,0,0.0057823404,0.018664227
,0.0016230922\C,0,0.0036328047,0.0103171728,1.3933432898\C,0,1.2333956
265,0.0035811834,2.099257798\C,0,2.3933508953,0.0129282756,1.282502136
\C,0,2.2630680958,0.0280972866,-0.1036233485\H,0,-0.9489362633,0.02456
59972,-0.5256949969\H,0,-0.9492820059,0.031773539,1.9095157133\H,0,3.3
902278903,-0.0017239401,1.7087395607\H,0,3.1650780698,0.0350158075,-0.
7168527418\N,0,1.3071403212,0.005472093,3.4789647163\N,0,1.1012402227,
0.0277566084,-0.7726720455\C,0,0.1436943765,-0.2163163226,4.3400129822
\H,0,-0.6493245166,-0.7034315244,3.7635743506\H,0,0.4365366528,-0.9397
968422,5.1148776096\C,0,2.5995967898,0.0120224993,4.1625805747\H,0,2.4
379805269,0.4270351937,5.1661396916\H,0,3.2741044168,0.7134870709,3.65
55224358\C,0,-0.3942239502,1.0550758772,5.0279846619\H,0,-1.1555420643
,0.7436661326,5.7600874937\H,0,0.418080433,1.5158715637,5.6112762806\C
,0,3.2605416866,-1.3755080057,4.2849645504\H,0,3.3887198317,-1.8082678
251,3.2831543964\H,0,2.5816870659,-2.0502092168,4.8280483408\C,0,4.616
9571396,-1.3184792943,5.0067782044\H,0,5.2920314003,-0.6428699388,4.45
97175814\H,0,4.4820127603,-0.8737872101,6.0046479185\C,0,-0.9933423991
,2.1048720584,4.0788798396\H,0,-0.2509996079,2.3731662531,3.3151529755
\H,0,-1.8473256236,1.6660983564,3.5412030702\C,0,-1.454171261,3.370436
0705,4.8170885807\H,0,-1.8841008957,4.1015342063,4.121604161\H,0,-2.21
73673589,3.136352659,5.5713194713\H,0,-0.6145087657,3.8544900892,5.333
5540115\C,0,5.2777123965,-2.6975723627,5.1464808001\H,0,6.2432723902,-
2.6262412982,5.6620112193\H,0,4.6413354481,-3.3842860127,5.7199222476\
H,0,5.4550632907,-3.1519903154,4.1630192905\\Version=AM64L-G03RevD.01\
State=1-A\HF=-614.0482204\MP2=-616.337133\RMSD=8.982e-09\Thermal=0.\PG
=C01 [X(C13H22N2)]\\@

1e.5

1\1\GINC-NODE17\SP\RMP2-FC\6-31+G(2d,p)\C13H22N2\ZIP08\06-Aug-2010\0\\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=r
ead\\sp of d4ap48 MP2-5/6-31+G(2d,p)\\0,1\C,0,-0.0055057985,0.01443493
43,0.0051449803\C,0,-0.0033652776,0.0054740343,1.3974313126\C,0,1.2290
102669,0.0037438309,2.1002276139\C,0,2.3860604401,0.0110397965,1.28055
63205\C,0,2.2515805281,0.0127296105,-0.1046772797\H,0,-0.9617484113,0.
0155359263,-0.5195634944\H,0,-0.9551451296,-0.0103327931,1.9165868202\
H,0,3.3836477667,0.0380090717,1.7036786877\H,0,3.1518159468,0.01916628
58,-0.7204058495\N,0,1.2867496497,0.011977725,3.4806718417\N,0,1.08744

78493,0.014616457,-0.7713365086\C,0,2.5275890863,-0.2018709713,4.22818
90987\H,0,2.3123962584,-0.9225342578,5.0306423727\H,0,3.2640056973,-0.
6892071844,3.5811683076\C,0,0.0651167233,0.0176636889,4.2840373014\H,0
,-0.6570886367,0.7145350766,3.8402905364\H,0,0.3198880703,0.4379796098
,5.2658273639\C,0,3.1237915258,1.0745663606,4.8561634805\H,0,2.3689143
913,1.5355592938,5.511942865\H,0,3.9523785127,0.7691581868,5.513982420
8\C,0,-0.5761402318,-1.3713776812,4.4748778922\H,0,0.1537158712,-2.041
289532,4.9539747839\H,0,-0.7973673464,-1.8093328294,3.4917255303\C,0,-
1.8580138323,-1.3152514856,5.3220949715\H,0,-1.6304755696,-0.865337635
7,6.3006189041\H,0,-2.5844959571,-0.6444578146,4.8386613587\C,0,3.6261
448637,2.1216833122,3.8496842324\H,0,2.8136041658,2.3838946141,3.15877
47708\H,0,4.4267661999,1.6830673985,3.2352517397\C,0,4.1504038017,3.39
22785889,4.5350375647\H,0,4.9827019977,3.1643084,5.2143291845\H,0,4.50
95745418,4.1214017764,3.7985471248\H,0,3.3618661029,3.8760967056,5.126
8197966\C,0,-2.4974441764,-2.6957789305,5.5301446028\H,0,-3.409887763,
-2.6250843424,6.1348054761\H,0,-2.7658019758,-3.1554817087,4.570038865
\H,0,-1.806933573,-3.3776791195,6.0435585072\\Version=AM64L-G03RevD.01
\State=1-A\HF=-614.0482204\MP2=-616.3371329\RMSD=8.983e-09\Thermal=0.\
PG=C01 [X(C13H22N2)]\\@

1e.1.ac

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1\1\GINC-NODE15\SP\RMP2-FC\6-31+G(2d,p)\C15H25N2O1(1+)\ZIP08\18-Aug-20
10\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check g
uess=read\\sp of d4ap37.ac2 MP2-5/6-31+G(2d,p)\\1,1\C,0,-0.0757037759,
0.0135610438,0.0083584341\C,0,-0.0383736016,0.0182216473,1.3720416662\
C,0,1.2163250856,0.0013211416,2.079735735\C,0,2.3879123992,-0.01491518
43,1.2424297056\C,0,2.28157847,-0.0138266221,-0.1161641448\H,0,-1.0174
326774,0.0242450504,-0.5250497564\H,0,-0.9830379451,0.0429099138,1.898
6781106\H,0,3.3831593161,-0.0368910875,1.6660249537\H,0,3.1393118195,-
0.0250961761,-0.7786122773\N,0,1.2872245616,0.0005902813,3.4154671841\
N,0,1.0647897646,-0.0016341942,-0.7530145918\C,0,2.5921409537,-0.02283
1794,4.1210682937\H,0,3.2657870606,0.6913916566,3.6342078454\H,0,2.406
3067207,0.3685881452,5.1249657388\C,0,0.0662266572,0.022468841,4.25676
59158\H,0,0.357609685,-0.3735169809,5.2334147539\H,0,-0.6570344515,-0.
6891684915,3.8422667317\C,0,3.2367520626,-1.4193204655,4.2114740984\H,
0,3.4290913667,-1.8109130311,3.2022317284\H,0,4.221614373,-1.278882749
1,4.6796553073\C,0,-0.5629809497,1.4193285684,4.4210167403\H,0,-1.4925
231596,1.2787934728,4.9912354698\H,0,-0.8608105992,1.8148478617,3.4390
918661\C,0,0.325790642,2.4505983377,5.1376705405\H,0,0.630145469,2.051
7044903,6.1169125238\H,0,1.2485910947,2.6112555495,4.5610279005\C,0,2.
4309854845,-2.4541613301,5.0157311988\H,0,2.2336987161,-2.0593625947,6
.0236618961\H,0,1.4513985097,-2.6137576984,4.5412941413\C,0,-0.3891404
915,3.7955560497,5.3340905443\H,0,-1.2949992342,3.6771574586,5.9415378
08\H,0,0.2626583426,4.5148718353,5.8420661888\H,0,-0.6845770894,4.2329
178527,4.3717276672\C,0,3.163876634,-3.799118275,5.1283749226\H,0,4.12
99163618,-3.6819237887,5.6348845893\H,0,2.5713847581,-4.5213461715,5.7
008189783\H,0,3.3542768333,-4.2319046401,4.137906785\C,0,1.065381106,-
0.0048814515,-2.2294502945\O,0,2.1284781788,-0.015808894,-2.785867815\
C,0,-0.2782551615,0.0048498041,-2.9141902868\H,0,-0.8547936452,0.90187
10234,-2.6571978988\H,0,-0.0921480719,-0.0007501365,-3.9896036481\H,0,
-0.8707083975,-0.8797582302,-2.6504673194\\Version=AM64L-G03RevD.01\St
ate=1-A\HF=-766.2351721\MP2=-769.000087\RMSD=1.939e-09\Thermal=0.\PG=C
01 [X(C15H25N2O1)]\\@
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1e.2.ac

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1\1\GINC-NODE19\SP\RMP2-FC\6-31+G(2d,p)\C15H25N2O1(1+)\ZIP08\17-Aug-20
10\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check g
uess=read\\sp of d4ap37.ac1 MP2-5/6-31+G(2d,p)\\1,1\C,0,-0.0240368773,
0.0240118664,-0.0057367712\C,0,-0.0001201983,0.0199951015,1.3567968025
\C,0,1.2460834279,0.0009410945,2.078304826\C,0,2.4274498574,-0.0129801
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053,1.2539477852\C,0,2.3343589933,-0.0032134548,-0.1070396811\H,0,-0.9
411207455,0.0375278279,-0.5831837007\H,0,-0.9503557636,0.040122082,1.8
735942851\H,0,3.418094147,-0.0393840503,1.6878515411\H,0,3.2208332677,
-0.0116534824,-0.7279939476\N,0,1.3030882044,-0.0033338954,3.414693904
2\N,0,1.1263595482,0.0145235584,-0.7559358224\C,0,2.5988573919,-0.0280
344316,4.1354353113\H,0,3.2792829694,0.6853580925,3.6564402303\H,0,2.4
021167731,0.3641972228,5.1369338477\C,0,0.0715330376,0.0171159193,4.24
17872086\H,0,0.3523619111,-0.3779969723,5.2218767835\H,0,-0.6456024699
,-0.6954618455,3.8188246761\C,0,3.2407540058,-1.4253305731,4.233580157
1\H,0,3.4431709082,-1.8171808676,3.2262093274\H,0,4.2206294273,-1.2866
627169,4.712708107\C,0,-0.5613639398,1.4130877499,4.3985665001\H,0,-1.
4969741086,1.270657567,4.9582245399\H,0,-0.849264518,1.8083519486,3.41
37878763\C,0,0.3176788923,2.4451686876,5.1259440925\H,0,0.6104486512,2
.0466738147,6.1088989964\H,0,1.2474033578,2.6068407233,4.5605887349\C,
0,2.424548689,-2.4594290266,5.0282327931\H,0,2.2154780326,-2.064243273
1,6.0336083159\H,0,1.4507201711,-2.6181014745,4.542053667\C,0,-0.40101
36827,3.7894692404,5.313198993\H,0,-1.3143259083,3.6700440768,5.909117
1665\H,0,0.2434532833,4.5096564495,5.8292848543\H,0,-0.6850172782,4.22
60138606,4.3470968906\C,0,3.1547652455,-3.8049841968,5.1502294207\H,0,
4.1148710738,-3.6886237781,5.668157479\H,0,2.5546858922,-4.5261719763,
5.7159936663\H,0,3.3561833477,-4.2389017801,4.1623751698\C,0,0.9847520
489,0.0232900974,-2.225542815\O,0,-0.1266288837,0.0360075021,-2.677831
9935\C,0,2.2568445078,0.0164834662,-3.0355154079\H,0,2.8552127214,-0.8
813378998,-2.8381301594\H,0,1.9688751166,0.026059018,-4.0882086396\H,0
,2.871856673,0.9002577236,-2.8262660595\\Version=AM64L-G03RevD.01\Stat
e=1-A\HF=-766.2351723\MP2=-769.0000869\RMSD=1.960e-09\Thermal=0.\PG=C0
1 [X(C15H25N2O1)]\\@

1e.3.ac

1\1\GINC-NODE19\SP\RMP2-FC\6-31+G(2d,p)\C15H25N2O1(1+)\ZIP08\17-Aug-20
10\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check g
uess=read\\sp of d4ap49.ac1 MP2-5/6-31+G(2d,p)\\1,1\C,0,-0.0471984783,
-0.0296546787,0.0417332081\C,0,-0.01207065,-0.0576206221,1.4033038175\
C,0,1.2386093339,-0.0398889203,2.1165089515\C,0,2.4122860812,0.0114501
374,1.2815566829\C,0,2.3087930765,0.0368100897,-0.0782614015\H,0,-0.96
93171511,-0.0351553201,-0.5278565144\H,0,-0.958988245,-0.0672985178,1.
9258295835\H,0,3.4072176604,0.0147459077,1.7065896123\H,0,3.1905316379
,0.0691602082,-0.705169532\N,0,1.3183875958,-0.0664131419,3.4514277626
\N,0,1.0965006558,0.0155575086,-0.7183482213\C,0,0.1439414372,-0.22306
48715,4.3408741532\H,0,-0.6588840963,-0.7264022161,3.7959382738\H,0,0.
4573150908,-0.9151639216,5.1311835282\C,0,2.6196262162,-0.0195548797,4
.1559670502\H,0,2.4190971125,0.3919416429,5.1502273335\H,0,3.274150795
9,0.7024626697,3.6558721019\C,0,-0.3498069451,1.0940283435,4.969475111
4\H,0,-1.0969337119,0.8175361236,5.72694958\H,0,0.4764743198,1.5674683
763,5.5195843431\C,0,3.2924100828,-1.397901316,4.2837537748\H,0,3.4773
650818,-1.8174888363,3.2842612662\H,0,2.6021031515,-2.0905966459,4.786
211388\C,0,4.6133629091,-1.3208344849,5.0703602948\H,0,5.2954400229,-0
.6153188633,4.5727915159\H,0,4.4172472521,-0.9076395569,6.0702952488\C
,0,-0.964022128,2.1067102889,3.9891744364\H,0,-0.229419452,2.370611961
1,3.2140427\H,0,-1.8183460439,1.6433243961,3.472389014\C,0,-1.43518189
46,3.3861111479,4.6969375825\H,0,-1.8740699418,4.0908962173,3.98199219
15\H,0,-2.1950047665,3.1614601545,5.4556372567\H,0,-0.6002900793,3.892
4359473,5.197536749\C,0,5.2962844688,-2.6895177839,5.2042145566\H,0,6.
2318333778,-2.6043198624,5.7678440977\H,0,4.652137506,-3.4046349903,5.
7310182802\H,0,5.5353038018,-3.1131730847,4.2204582877\C,0,0.942964416
2,0.042780113,-2.1855276666\O,0,-0.1716391289,0.0225281755,-2.62990063
94\C,0,2.2080081098,0.0942117758,-3.0052230508\H,0,2.8405909966,-0.783
6136482,-2.8252529626\H,0,1.9112060019,0.1077168538,-4.0554064445\H,0,
2.7918519577,0.9971065051,-2.7884650104\\Version=AM64L-G03RevD.01\Stat
e=1-A\HF=-766.2363423\MP2=-768.9997875\RMSD=1.929e-09\Thermal=0.\PG=C0
1 [X(C15H25N2O1)]\\@

1e.4.ac

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1\1\GINC-NODE19\SP\RMP2-FC\6-31+G(2d,p)\C15H25N2O1(1+)\ZIP08\17-Aug-20
 10\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check g
 uess=read\\sp of d4ap7.ac1 MP2-5/6-31+G(2d,p)\\1,1\C,0,-0.0291440815,-
 0.0507302845,0.0017051846\C,0,-0.0031262112,-0.0557495261,1.3639506525
 \C,0,1.2441646619,-0.0107132768,2.082236948\C,0,2.4240410979,0.0339661
 082,1.2571812336\C,0,2.3288091423,0.0327306162,-0.1033685556\H,0,-0.94
 64783035,-0.0743631602,-0.5751497358\H,0,-0.9524524138,-0.0721735722,1
 .8834725074\H,0,3.4153332176,0.0473821794,1.6911841906\H,0,3.213802858
 ,0.0573976849,-0.7260270635\N,0,1.3041061598,-0.0102035855,3.417081137
 \N,0,1.1198526311,-0.0074748231,-0.750238695\C,0,0.0969668464,-0.14072
 49195,4.2624132717\H,0,-0.6041176981,-0.8322124348,3.7835179533\H,0,0.
 4204649276,-0.6286321246,5.1882842932\C,0,2.5805255176,0.123743512,4.1
 519580374\H,0,2.3401659923,0.6168642292,5.1001239704\H,0,3.2371660917,
 0.8125240001,3.6099870398\C,0,-0.5732247562,1.2074452868,4.5790691393\
 H,0,0.1627413539,1.8747575138,5.0502057258\H,0,-0.8810996793,1.6968053
 535,3.6435276357\C,0,3.2764813182,-1.2227206518,4.4159510026\H,0,3.496
 0393675,-1.7202492668,3.4598971802\H,0,2.5871080257,-1.885409872,4.958
 4085419\C,0,4.5736863325,-1.0468078241,5.2257070462\H,0,5.2560337494,-
 0.37614975,4.6825303049\H,0,4.3421729288,-0.5470382765,6.1774932749\C,
 0,-1.7895966539,1.0376469988,5.5067975656\H,0,-2.51893459,0.3629918475
 ,5.0344124389\H,0,-1.4706292754,0.5455618268,6.4370965752\C,0,-2.46549
 98481,2.3758097628,5.8386438309\H,0,-3.324455545,2.2237804704,6.501401
 5763\H,0,-1.7693505019,3.0572629851,6.3435336469\H,0,-2.8272450689,2.8
 755138582,4.9310802508\C,0,5.2776658125,-2.3825868875,5.5044070178\H,0
 ,6.1930332892,-2.2261709167,6.0856367872\H,0,4.6304471444,-3.060363604
 6,6.0749653198\H,0,5.5559260835,-2.8889597951,4.571392353\C,0,0.975859
 7455,-0.0050437497,-2.2190154381\O,0,-0.1354714738,-0.0446624493,-2.67
 01123187\C,0,2.2458059803,0.0480862232,-3.0308057738\H,0,2.8836869387,
 -0.8229625904,-2.8369672513\H,0,1.9561562427,0.0479261609,-4.083055531
 3\H,0,2.8210874395,0.9576802965,-2.8194121005\\Version=AM64L-G03RevD.0
 1\State=1-A\HF=-766.2393438\MP2=-769.000042\RMSD=1.733e-09\Thermal=0.\
 PG=C01 [X(C15H25N2O1)]\\@
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1e.5.ac

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1\1\GINC-NODE19\SP\RMP2-FC\6-31+G(2d,p)\C15H25N2O1(1+)\ZIP08\18-Aug-20
 10\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check g
 uess=read\\sp of d4ap7.ac2 MP2-5/6-31+G(2d,p)\\1,1\C,0,-0.0695141207,-
 0.031136602,0.0120181658\C,0,-0.0336701821,-0.0350735899,1.3754461382\
 C,0,1.2200042961,0.0083000688,2.0834373315\C,0,2.3925365241,0.05505946
 42,1.2487898385\C,0,2.2875450288,0.0527269709,-0.1096823335\H,0,-1.010
 2587032,-0.0548718416,-0.5227227635\H,0,-0.9786639652,-0.0496554621,1.
 9026332298\H,0,3.3873513813,0.0707283354,1.6747763563\H,0,3.1452872079
 ,0.0777545118,-0.7718364452\N,0,1.2886361267,0.0051111391,3.4178749474
 \N,0,1.0716870576,0.0106601756,-0.7479011475\C,0,0.0888067939,-0.13052
 06415,4.2719038132\H,0,-0.6169037546,-0.8183745556,3.7942615417\H,0,0.
 4193315356,-0.6254654307,5.1915411977\C,0,2.5715155705,0.1341095273,4.
 1434874992\H,0,2.3385424651,0.6200487908,5.0971764083\H,0,3.2232438953
 ,0.8267223158,3.6007702283\C,0,-0.5784795902,1.2153043433,4.6042806036
 \H,0,0.1599371712,1.8770776477,5.0790889934\H,0,-0.8891010793,1.714615
 1938,3.6747768076\C,0,3.2690139012,-1.2145965522,4.3913553278\H,0,3.48
 5455381,-1.7019314905,3.429506245\H,0,2.5817623309,-1.8830191164,4.929
 6964966\C,0,4.5690020657,-1.0465558,5.198138732\H,0,5.2494969786,-0.37
 06836678,4.6592805877\H,0,4.3409956985,-0.5566033536,6.1558961258\C,0,
 -1.7916748828,1.0376448033,5.5348819834\H,0,-2.5231146205,0.3677763931
 ,5.0587563296\H,0,-1.4695337568,0.5362582831,6.4590552543\C,0,-2.46563
 98409,2.3727589862,5.8824586325\H,0,-3.3207693592,2.215085362,6.548851
 5536\H,0,-1.7665365823,3.0496857704,6.3892483959\H,0,-2.832487663,2.88
 07144833,4.9814792294\C,0,5.2737357564,-2.3852828279,5.4604454554\H,0,
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6.1924534102,-2.2344991834,6.0378394732\H,0,4.6294116035,-3.0680334712
,6.0284363365\H,0,5.5465175502,-2.8828812505,4.5211781977\C,0,1.074103
2993,0.0110442839,-2.2239115704\O,0,2.1370313777,0.0515794265,-2.77938
04695\C,0,-0.2679195217,-0.0405148387,-2.9100717506\H,0,-0.8843127831,
0.8298444924,-2.6537606324\H,0,-0.0808052302,-0.0378091358,-3.98530575
45\H,0,-0.8200660054,-0.950833014,-2.6465367784\\Version=AM64L-G03RevD
.01\State=1-A\HF=-766.2393418\MP2=-769.0000423\RMSD=1.787e-09\Thermal=
0.\PG=C01 [X(C15H25N2O1)]\\@

1f.1

1\1\GINC-NODE11\SP\RMP2-FC\6-31+G(2d,p)\C15H26N2\ZIP08\25-Aug-2010\0\\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=r
ead\\sp of d5ap37 MP2-5/6-31+G(2d,p)\\0,1\C,0,0.0014867751,-0.01645941
62,0.0236060982\C,0,0.0013212044,-0.0177323691,1.4156315125\C,0,1.2333
979044,-0.0000661134,2.1184253738\C,0,2.3926011911,0.020405548,1.30106
78093\C,0,2.2592800064,0.0242580522,-0.0845535698\H,0,-0.9535421003,-0
.0320336188,-0.5030596191\H,0,-0.9501710928,-0.0283832922,1.9354548191
\H,0,3.3894565134,0.0293113068,1.7275270399\H,0,3.159553088,0.04193999
95,-0.7000981652\N,0,1.2995116585,-0.0026122162,3.4975716883\N,0,1.095
8245125,0.0052292411,-0.7513748222\C,0,2.5909752144,-0.0397516187,4.18
72997346\H,0,3.273261426,0.6855923901,3.7232784684\H,0,2.4235330637,0.
3173455932,5.2098877405\C,0,0.0799530219,0.0317594668,4.3078049334\H,0
,0.3443783439,-0.3290799126,5.3083626208\H,0,-0.6437228645,-0.69198442
58,3.9085023403\C,0,3.2592352099,-1.4298316156,4.2375712437\H,0,3.4377
762748,-1.7887123781,3.2145863446\H,0,4.2495784316,-1.3062471894,4.702
9517227\C,0,-0.5801809201,1.4215292439,4.4268984141\H,0,-1.5214962783,
1.2960548669,4.9844047276\H,0,-0.8556791396,1.784159416,3.4270131944\C
,0,0.2930932516,2.4765193867,5.1246466715\H,0,0.5735451251,2.117926334
7,6.1286179957\H,0,1.2315667579,2.6018771329,4.5642983252\C,0,2.456516
9288,-2.4875553513,5.0117347567\H,0,2.2734190467,-2.1327225414,6.03924
12415\H,0,1.4687377943,-2.6110232977,4.5432420846\C,0,-0.4020904844,3.
8424575033,5.2525972659\H,0,-1.3431010934,3.72053,5.8100434727\H,0,-0.
6832409042,4.1987997035,4.2503928899\C,0,3.1605276351,-3.8538235852,5.
0675779869\H,0,4.1505611444,-3.7337658211,5.5329092119\H,0,3.344475279
2,-4.2064234614,4.0417729996\C,0,2.3571799497,-4.9121271593,5.83723587
61\H,0,2.8824527893,-5.8749190225,5.8581565104\H,0,2.1866908877,-4.601
5133231,6.8767081889\H,0,1.3752269402,-5.0768655661,5.3742711178\C,0,0
.4713908599,4.8980518764,5.9457751434\H,0,-0.0492960141,5.8606702458,6
.0203968747\H,0,0.7404760041,4.583633449,6.9630184918\H,0,1.4045846628
,5.0646657892,5.3916121463\\Version=AM64L-G03RevD.01\State=1-A\HF=-692
.1259876\MP2=-694.7220286\RMSD=7.521e-09\Thermal=0.\PG=C01 [X(C15H26N2
)]\\@

1f.2

1\1\GINC-NODE11\SP\RMP2-FC\6-31+G(2d,p)\C15H26N2\ZIP08\25-Aug-2010\0\\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=r
ead\\sp of d5ap34 MP2-5/6-31+G(2d,p)\\0,1\C,0,0.0014849685,0.020958083
3,0.0009900851\C,0,0.0006956629,0.0141042392,1.3931028442\C,0,1.232520
6896,0.0051076163,2.0961123015\C,0,2.3923291026,0.0063012502,1.2797826
421\C,0,2.259886982,0.0088632376,-0.105867943\H,0,-0.9533316057,0.0275
52196,-0.5262125847\H,0,-0.9510050248,0.0062595555,1.9123326392\H,0,3.
3893247564,0.0151222023,1.7063634541\H,0,3.1605993207,0.0094499573,-0.
7209923944\N,0,1.295432386,-0.0095483889,3.4753419314\N,0,1.0963890707
,0.0167548038,-0.7732637214\C,0,2.5789873761,0.0569545885,4.1736261356
\H,0,2.4307408649,-0.3644375232,5.1751404755\H,0,3.2976382239,-0.60601
3503,3.6751570928\C,0,0.0836587232,0.1244435592,4.2863172609\H,0,-0.58
53723607,0.8640606496,3.8259621802\H,0,0.3835020998,0.5489753969,5.252
9657291\C,0,3.1578387322,1.4803400475,4.295048828\H,0,3.2657355082,1.9
147729398,3.2913986446\H,0,2.4343093258,2.1132493577,4.8307777919\C,0,
-0.6802268391,-1.1945449521,4.5259022162\H,0,-0.9761833306,-1.62506727

76,3.5592214133\H,0,-1.612366372,-0.9486821979,5.0581273633\C,0,0.1059
531791,-2.2447567868,5.3265713977\H,0,1.0393077286,-2.4842468995,4.795
8611615\H,0,0.3987150945,-1.8216374304,6.3015312988\C,0,4.5103224622,1
.5056373734,5.0252969351\H,0,5.2308058444,0.8719112302,4.4839166754\H,
0,4.3979403155,1.0545865592,6.0243159867\C,0,-0.6885210397,-3.54124633
15,5.5580660972\H,0,-1.6283598441,-3.3031465519,6.0788524578\H,0,-0.97
61675368,-3.965971241,4.5848083845\C,0,5.094174146,2.9208398369,5.1726
757116\H,0,4.376336283,3.5531319503,5.7163412402\H,0,5.2054246495,3.37
14605902,4.1752268384\C,0,6.447095014,2.9398204676,5.8985426959\H,0,6.
8371576693,3.9611634722,5.9884237967\H,0,6.3590283144,2.5249203619,6.9
114989589\H,0,7.1941758681,2.3427831781,5.3589165485\C,0,0.0925849436,
-4.5891126937,6.3639322438\H,0,0.3653786529,-4.2036537108,7.3554933365
\H,0,-0.4987131086,-5.5012715415,6.511303859\H,0,1.0210000438,-4.87190
70465,5.8503604116\\Version=AM64L-G03RevD.01\State=1-A\HF=-692.1277179
\MP2=-694.7214411\RMSD=2.869e-09\Thermal=0.\PG=C01 [X(C15H26N2)]\\@

1f.3

1\1\GINC-NODE10\SP\RMP2-FC\6-31+G(2d,p)\C15H26N2\ZIP08\25-Aug-2010\0\\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=r
ead\\sp of d5ap7 MP2-5/6-31+G(2d,p)\\0,1\C,0,-0.0000065834,-0.00086888
11,0.0002690747\C,0,-0.0000166165,-0.0008517743,1.3921841465\C,0,1.232
7811475,-0.0000595744,2.0931782923\C,0,2.3925827347,0.0033969701,1.277
0703163\C,0,2.2589375126,0.0082870059,-0.1084050284\H,0,-0.9549985684,
0.0003030141,-0.5266881246\H,0,-0.9507766751,0.0153925871,1.9140337775
\H,0,3.3890499833,-0.0145108402,1.7051680618\H,0,3.1589253205,0.009121
7805,-0.7246161533\N,0,1.2990427061,-0.0024753471,3.4702851954\N,0,1.0
947933283,0.0049728012,-0.7746698379\C,0,0.1007693079,-0.13077941,4.29
56930456\H,0,-0.6059441759,-0.8134041737,3.806992615\H,0,0.3956578593,
-0.6253959945,5.2311933863\C,0,2.5710532032,0.1231291754,4.1772730413\
H,0,2.367430513,0.6143956517,5.1385015141\H,0,3.2276902556,0.807595631
7,3.6253828794\C,0,-0.587753968,1.2093742593,4.6197703903\H,0,0.130452
1923,1.8639036605,5.1360669949\H,0,-0.8494201654,1.7180897657,3.681299
5836\C,0,3.2872941413,-1.2180361578,4.429022106\H,0,3.4575475936,-1.72
34049963,3.4679789997\H,0,2.6218793633,-1.8745010251,5.0095976672\C,0,
4.6210242613,-1.040720322,5.1725692199\H,0,5.2832689712,-0.3855676691,
4.584471984\H,0,4.4434990678,-0.5178589103,6.1261126231\C,0,-1.8439484
492,1.0292285693,5.4873313091\H,0,-2.5597242468,0.3760402412,4.9632500
709\H,0,-1.5757649316,0.5030471674,6.4175760333\C,0,-2.5359839251,2.35
68177033,5.8390969293\H,0,-1.82321605,3.0069731046,6.3681339885\H,0,-2
.8004138175,2.8838256346,4.910235337\C,0,5.3434266046,-2.3694154294,5.
4515834506\H,0,4.6846610556,-3.0215451902,6.0443525248\H,0,5.517330238
7,-2.8931173293,4.4997756868\C,0,6.678883504,-2.1838356623,6.186397267
2\H,0,6.5319502888,-1.6929700212,7.1577054239\H,0,7.1704922707,-3.1471
915539,6.3695454049\H,0,7.3690714894,-1.561938133,5.6010873993\C,0,-3.
794716956,2.1684427082,6.6981325781\H,0,-3.5552582534,1.6741621555,7.6
490920852\H,0,-4.2662718923,3.1310724548,6.9310638022\H,0,-4.53805807,
1.5485214068,6.1796295952\\Version=AM64L-G03RevD.01\State=1-A\HF=-692.
1294341\MP2=-694.7207094\RMSD=2.207e-09\Thermal=0.\PG=C01 [X(C15H26N2)
]\\@

1f.4

1\1\GINC-NODE19\SP\RMP2-FC\6-31+G(2d,p)\C15H26N2\ZIP08\25-Aug-2010\0\\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=r
ead\\sp of d5ap49 MP2-5/6-31+G(2d,p)\\0,1\C,0,-0.007505757,0.001343906
1,-0.005556921\C,0,-0.0027297463,0.0013373896,1.3861369494\C,0,1.23030
99682,-0.0025495285,2.0861066634\C,0,2.386364938,0.001638561,1.2638270
309\C,0,2.2492079237,0.0081248678,-0.1217126922\H,0,-0.9648126854,0.00
51938718,-0.528198147\H,0,-0.9526064709,0.0277237396,1.9075256915\H,0,
3.3850626886,-0.0107240431,1.6859042745\H,0,3.1481892716,0.0105933314,
-0.7394338694\N,0,1.3094232488,0.0060802836,3.4655087038\N,0,1.0841734

654,0.0044798263,-0.7851649395\C,0,0.1487974979,-0.2135172453,4.331267
8842\H,0,-0.6449858472,-0.7043389636,3.7592620078\H,0,0.445425801,-0.9
326828673,5.1088439036\C,0,2.6034068979,0.0245003182,4.1458851401\H,0,
2.4409959309,0.4459509487,5.1466212372\H,0,3.2732850072,0.7260647885,3
.6332237377\C,0,-0.3899263833,1.0603888195,5.0147961265\H,0,-1.1469283
626,0.7496162051,5.7515329638\H,0,0.4235445327,1.5257176227,5.59227325
02\C,0,3.2718151389,-1.3587027858,4.2782940103\H,0,3.4115843809,-1.793
5529819,3.2790037637\H,0,2.5908626003,-2.0348997667,4.8166547628\C,0,4
.6203376002,-1.2903807486,5.0132649745\H,0,5.2977175846,-0.6093264082,
4.4737260687\H,0,4.4731849327,-0.8467647257,6.0110594248\C,0,-0.995918
0228,2.1025719189,4.0620969616\H,0,-0.2567951578,2.3713397194,3.293984
4218\H,0,-1.850475746,1.658138412,3.5277090957\C,0,-1.4651454783,3.374
8556608,4.7879821609\H,0,-2.1977304026,3.1029247921,5.5631103795\H,0,-
0.6116212616,3.8245384747,5.3178301425\C,0,5.299602745,-2.6618628943,5
.1646805237\H,0,4.6239072553,-3.3424259432,5.7040784921\H,0,5.44779221
54,-3.103469967,4.167974618\C,0,6.6462076539,-2.587441158,5.8986403567
\H,0,6.5233322488,-2.1822339356,6.9118842517\H,0,7.1064759285,-3.57909
02262,5.9887627951\H,0,7.3527661197,-1.9381298664,5.3647969457\C,0,-2.
0829738179,4.4125013441,3.8396006718\H,0,-2.9618717215,4.0034185172,3.
3239224146\H,0,-2.4020271442,5.3103348708,4.3833430244\H,0,-1.36286931
01,4.7232991034,3.0714268048\\Version=AM64L-G03RevD.01\State=1-A\HF=-6
92.1263588\MP2=-694.7207146\RMSD=9.669e-09\Thermal=0.\PG=C01 [X(C15H26
N2)]\\@

1f.5

1\1\GINC-NODE22\SP\RMP2-FC\6-31+G(2d,p)\C15H26N2\ZIP08\25-Aug-2010\0\\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=r
ead\\sp of d5ap48 MP2-5/6-31+G(2d,p)\\0,1\C,0,0.0066458182,-0.00538060
21,-0.0136461326\C,0,0.0018910241,-0.0052651324,1.378672711\C,0,1.2309
108012,-0.0025932781,2.0872825045\C,0,2.3917807472,0.0007253509,1.2732
004164\C,0,2.2641881821,-0.0062152822,-0.1126230232\H,0,-0.9470085123,
-0.0081381428,-0.543069243\H,0,-0.952102774,-0.0178915187,1.8938771772
\H,0,3.3868566405,0.0319768602,1.7017509543\H,0,3.1674397635,-0.002702
5572,-0.7239572018\N,0,1.2833095053,0.0127447525,3.467899174\N,0,1.103
3131453,-0.009573037,-0.7848728807\C,0,2.5216262802,-0.1997596377,4.22
03800236\H,0,2.3023339173,-0.9157321052,5.0260513729\H,0,3.2588083669,
-0.6915455943,3.5778087969\C,0,0.059845236,0.031491153,4.2681671181\H,
0,-0.6577404292,0.7288896951,3.8182146683\H,0,0.3154895207,0.458324680
2,5.2469059898\C,0,3.1192859586,1.0788261515,4.8435109543\H,0,2.363097
6176,1.5451022028,5.49351979\H,0,3.9437977955,0.7735429556,5.506379849
7\C,0,-0.5890091197,-1.3526173088,4.4701183888\H,0,0.1419723611,-2.024
4936288,4.9444803763\H,0,-0.8219380764,-1.7927895208,3.4907289693\C,0,
-1.861715421,-1.2838261843,5.3296819483\H,0,-1.621603791,-0.8348776303
,6.3068382686\H,0,-2.5892662516,-0.6070900999,4.8537838844\C,0,3.62896
93926,2.1176689287,3.8325531416\H,0,2.8193912631,2.3808334349,3.136950
258\H,0,4.4300963632,1.6726010016,3.2214307449\C,0,4.161480717,3.39467
91949,4.5044653144\H,0,4.9652283421,3.1283711013,5.2076868649\H,0,3.36
09367702,3.8449747256,5.1109473685\C,0,-2.5196033904,-2.6561443906,5.5
515311541\H,0,-2.7606491348,-3.1030812792,4.5755475641\H,0,-1.79374432
18,-3.3323938098,6.0274470807\C,0,-3.7905145746,-2.5812536511,6.409876
3718\H,0,-4.2373071702,-3.5735306456,6.5480774534\H,0,-3.5729920074,-2
.1706935922,7.4049034202\H,0,-4.5464796332,-1.9363010949,5.9425736483\
C,0,4.6833675142,4.4290361212,3.4967016073\H,0,5.050132725,5.330332115
2,4.0033618732\H,0,5.5103997882,4.0194703276,2.9017159836\H,0,3.892593
5914,4.7342780592,2.7990335506\\Version=AM64L-G03RevD.01\State=1-A\HF=
-692.1263588\MP2=-694.7207146\RMSD=9.672e-09\Thermal=0.\PG=C01 [X(C15H
26N2)]\\@

1f.1.ac

1\1\GINC-NODE10\SP\RMP2-FC\6-31+G(2d,p)\C17H29N2O1(1+)\ZIP08\04-Sep-20

10\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check g
uess=read\\sp of d5ap7.ac2 MP2-5/6-31+G(2d,p)\\1,1\C,0,-0.0319818393,-
0.0558168741,-0.0119047114\C,0,-0.0049573136,-0.0658633564,1.350186253
8\C,0,1.2424576282,-0.0134709761,2.0680359177\C,0,2.4216337234,0.04020
70351,1.2422933396\C,0,2.3255236662,0.0435326518,-0.118107064\H,0,-0.9
497426424,-0.0839641266,-0.5877736852\H,0,-0.9537193775,-0.0916987048,
1.8703591211\H,0,3.4130915596,0.0572176361,1.6757777708\H,0,3.20963411
06,0.0754054519,-0.7417557538\N,0,1.3030373178,-0.0145004235,3.4026037
364\N,0,1.1163164496,-0.0011458133,-0.7644631649\C,0,0.0967804149,-0.1
518053253,4.2484568781\H,0,-0.5990327821,-0.8499658906,3.7715569514\H,
0,0.4242512585,-0.634533295,5.1755646203\C,0,2.579111064,0.1259386996,
4.1371056199\H,0,2.3366909066,0.6189206779,5.084809309\H,0,3.232497453
,0.8170187352,3.5942131164\C,0,-0.5834066373,1.1923228959,4.5613536311
\H,0,0.1496294613,1.867405846,5.025917313\H,0,-0.8981921469,1.67419267
04,3.6242505699\C,0,3.2814139535,-1.217107834,4.4020548496\H,0,3.49736
3528,-1.716432661,3.4461464077\H,0,2.596725373,-1.8801453002,4.9498937
159\C,0,4.5816339166,-1.0327425364,5.2042641342\H,0,5.2627164336,-0.36
56319239,4.6531125633\H,0,4.3556334848,-0.525266465,6.1544601006\C,0,-
1.7940287753,1.0166587189,5.4946853387\H,0,-2.5200917811,0.3302327061,
5.0318537847\H,0,-1.4673855649,0.5355233635,6.4292061053\C,0,-2.491249
1305,2.3480796811,5.8246224213\H,0,-1.762818077,3.0334048219,6.2823612
084\H,0,-2.8206786889,2.8261143334,4.8902106671\C,0,5.2977436612,-2.36
30069212,5.4960012605\H,0,4.6168436904,-3.025658707,6.0499082844\H,0,5
.5191585305,-2.8717307925,4.5459392689\C,0,6.5956509829,-2.1744898913,
6.2939496942\H,0,6.3999010613,-1.700309324,7.2641510255\H,0,7.08199076
5,-3.1377373527,6.4852685082\H,0,7.3086749099,-1.5419581405,5.74962824
46\C,0,-3.6924256948,2.1713674789,6.7639422424\H,0,-3.3866135642,1.728
8395474,7.7205862416\H,0,-4.1673294087,3.1353718944,6.9787104802\H,0,-
4.452395725,1.5159481928,6.3193216463\C,0,0.9723463059,0.0086896772,-2
.2326966231\O,0,-0.1385187846,-0.0351223056,-2.6847500447\C,0,2.242319
2551,0.0743302082,-3.0437172334\H,0,2.8853881645,-0.7939270325,-2.8546
269022\H,0,1.953138434,0.0784680575,-4.0960857933\H,0,2.8119996813,0.9
861483873,-2.8268079555\\Version=AM64L-G03RevD.01\State=1-A\HF=-844.31
80435\MP2=-847.3840125\RMSD=7.028e-09\Thermal=0.\PG=C01 [X(C17H29N2O1)
]\\@

1f.2.ac

1\1\GINC-NODE13\SP\RMP2-FC\6-31+G(2d,p)\C17H29N2O1(1+)\ZIP08\03-Sep-20
10\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check g
uess=read\\sp of d5ap7.ac1 MP2-5/6-31+G(2d,p)\\1,1\C,0,-0.0670426272,-
0.0327767533,-0.0034741626\C,0,-0.0322737136,-0.0345969653,1.359863047
4\C,0,1.220650945,0.0161855481,2.0689424231\C,0,2.393503781,0.07141825
86,1.2350040691\C,0,2.2898209353,0.0665154204,-0.1234226537\H,0,-1.006
8671148,-0.0624325222,-0.5396386268\H,0,-0.9776071308,-0.0534362936,1.
8863542677\H,0,3.38777818,0.0953616895,1.6619240054\H,0,3.1481399112,0
.0969370778,-0.7845553342\N,0,1.2883253855,0.0121522337,3.4031765589\N
,0,1.0746446626,0.0145266391,-0.7626219505\C,0,0.0885603559,-0.1313006
906,4.2561333012\H,0,-0.6140468465,-0.8203936639,3.7757840866\H,0,0.42
06494464,-0.6278670161,5.1743279568\C,0,2.5701644724,0.1464261994,4.12
99356577\H,0,2.3332876755,0.6256740403,5.0859738746\H,0,3.217228789,0.
8463997498,3.5910791122\C,0,-0.5848050783,1.2106135065,4.5924067449\H,
0,0.1495022403,1.8717404264,5.0743379016\H,0,-0.8915975899,1.713470005
5,3.6635749703\C,0,3.276891326,-1.1987965964,4.3711443654\H,0,3.500388
6731,-1.6770373382,3.4063731899\H,0,2.5915586502,-1.875756056,4.901188
7102\C,0,4.5713610831,-1.0265083809,5.1849156174\H,0,5.2500594121,-0.3
384808923,4.657139504\H,0,4.33584856,-0.548676656,6.1481018579\C,0,-1.
801881409,1.02298428,5.5152299732\H,0,-2.5326136242,0.3572487375,5.029
9434092\H,0,-1.4854891518,0.512625206,6.4376796829\C,0,-2.4869743625,2
.3519192541,5.8786996673\H,0,-1.7559773853,3.0134462544,6.3661133461\H
,0,-2.7994032167,2.8632059748,4.955977963\C,0,5.2964448736,-2.35912721
31,5.4418969593\H,0,4.6149672223,-3.0459811412,5.9649937268\H,0,5.5345

777069,-2.833935352,4.4785632273\C,0,6.5822166703,-2.1857804589,6.2623
310711\H,0,6.3696966708,-1.7466566137,7.2454512452\H,0,7.0751796906,-3
.1505527632,6.4271547435\H,0,7.2962865039,-1.5287948646,5.7492133476\C
,0,-3.701578079,2.1602470352,6.7978383656\H,0,-3.4127425785,1.68351229
68,7.7432245042\H,0,-4.1675723288,3.1226108544,7.038008293\H,0,-4.4636
048335,1.5287209824,6.3232051919\C,0,1.0771451214,0.0103169501,-2.2379
000685\O,0,2.1395353461,0.0561515674,-2.7942526854\C,0,-0.2647571983,-
0.0525692275,-2.9236381492\H,0,-0.8864886534,0.8149818533,-2.670700884
8\H,0,-0.0777967023,-0.0529577694,-3.9988886904\H,0,-0.811277388,-0.96
51763822,-2.6563177305\\Version=AM64L-G03RevD.01\State=1-A\HF=-844.318
0428\MP2=-847.3840118\RMSD=7.061e-09\Thermal=0.\PG=C01 [X(C17H29N2O1)]
\\@

1f.3.ac

1\1\GINC-NODE24\SP\RMP2-FC\6-31+G(2d,p)\C17H29N2O1(1+)\ZIP08\03-Sep-20
10\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check g
uess=read\\sp of d5ap37.ac1 MP2-5/6-31+G(2d,p)\\1,1\C,0,-0.0765587342,
0.0138812712,-0.0140901279\C,0,-0.0382638067,0.0187875607,1.3493701198
\C,0,1.2167968183,-0.0011648351,2.0565377197\C,0,2.3881107065,-0.02106
78888,1.218580264\C,0,2.2811006661,-0.0192638955,-0.139830144\H,0,-1.0
186041833,0.0258588548,-0.546969593\H,0,-0.9824864881,0.0433746631,1.8
7708884\H,0,3.3833472468,-0.0433385695,1.6426714301\H,0,3.138037818,-0
.0319615276,-0.8034626858\N,0,1.2877047113,-0.0014340038,3.3919932677\
N,0,1.0637460285,-0.0038274267,-0.7760602107\C,0,2.5920615848,-0.04007
36732,4.0973372134\H,0,3.2747718611,0.6646844031,3.6094109646\H,0,2.41
20015141,0.3545753517,5.1008727016\C,0,0.0666776921,0.035815863,4.2326
60751\H,0,0.3529124393,-0.3596641539,5.2108473192\H,0,-0.6641508889,-0
.6691121361,3.8201760298\C,0,3.2175401921,-1.4453932478,4.1866631633\H
,0,3.4036346197,-1.8372163623,3.1761944311\H,0,4.2046796971,-1.3187398
393,4.653978315\C,0,-0.5464120795,1.4405687651,4.3906848374\H,0,-1.476
977442,1.3129269368,4.962277111\H,0,-0.8411227808,1.8337707424,3.40677
49324\C,0,0.3553409695,2.4642856405,5.1009506341\H,0,0.6541221258,2.06
9407968,6.0846949572\H,0,1.2825527232,2.6102787671,4.525473301\C,0,2.3
97553154,-2.4693580801,4.9895433891\H,0,2.2078068061,-2.076078945,6.00
06916862\H,0,1.4130283712,-2.6139773866,4.5181431622\C,0,-0.3338760793
,3.8269499156,5.2917644455\H,0,-1.2601685881,3.6851469525,5.8672374136
\H,0,-0.6375761202,4.2191363866,4.3096661856\C,0,3.1022716059,-3.83283
05867,5.1021909247\H,0,4.0853754804,-3.6925288814,5.5744531827\H,0,3.2
979380083,-4.2231783524,4.092355071\C,0,2.2884255895,-4.8591951907,5.9
025200265\H,0,2.8160389988,-5.8177677436,5.9628825246\H,0,2.1097025204
,-4.5117983777,6.9282190043\H,0,1.3119776638,-5.0444842858,5.436004131
6\C,0,0.5612719222,4.8524020845,6.0013581104\H,0,0.042808108,5.8104762
376,6.1203914163\H,0,0.8499851032,4.503006895,7.0009417377\H,0,1.48142
58585,5.0392024281,5.4323735945\C,0,1.0635272827,-0.0072615686,-2.2518
767326\O,0,2.1260958643,-0.0257820369,-2.8092946991\C,0,-0.2803992976,
0.0129196759,-2.9360219851\H,0,-0.8515234246,0.912239241,-2.6751229742
\H,0,-0.0947809724,0.0101969651,-4.0115013906\H,0,-0.8777189951,-0.869
3460793,-2.6753480366\\Version=AM64L-G03RevD.01\State=1-A\HF=-844.3138
633\MP2=-847.3843438\RMSD=1.892e-09\Thermal=0.\PG=C01 [X(C17H29N2O1)]\
\@

1f.4.ac

1\1\GINC-NODE10\SP\RMP2-FC\6-31+G(2d,p)\C17H29N2O1(1+)\ZIP08\04-Sep-20
10\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check g
uess=read\\sp of d5ap97.ac1 MP2-5/6-31+G(2d,p)\\1,1\C,0,-0.0343480846,
-0.442820341,0.6837235369\C,0,-0.065572305,0.0431038806,1.9578548815\C
,0,1.1395798849,0.4809439109,2.6147989724\C,0,2.3408128181,0.357573315
8,1.8297129735\C,0,2.3045074847,-0.1419352654,0.5624702267\H,0,-0.9391
975269,-0.7694173075,0.1876015724\H,0,-1.025297251,0.0820989559,2.4559
053743\H,0,3.3026630458,0.6621060787,2.2207973805\H,0,3.1861516066,-0.

2519271827,-0.0584301872\N,0,1.1414810021,0.9660177647,3.8610620052\N,
0,1.1325427877,-0.545340389,-0.029768583\C,0,-0.1070087819,1.067676975
8,4.6547644466\H,0,0.077745834,1.8199193,5.4262449502\H,0,-0.897207085
3,1.4751504641,4.0138919375\C,0,2.3932878829,1.4271017989,4.5097239282
\H,0,3.1818180435,0.6927583041,4.3102018827\H,0,2.2122030219,1.3953176
186,5.5874267699\C,0,-0.5492383378,-0.257253496,5.3052890261\H,0,-1.51
61090183,-0.0598723481,5.7902225831\H,0,-0.7431145606,-1.0102987704,4.
527550733\C,0,2.8351199342,2.8422221,4.0897898266\H,0,3.0235247454,2.8
696252486,3.0067612122\H,0,3.8048105092,3.0235493665,4.5752680131\C,0,
1.854588756,3.9654520576,4.4671779283\H,0,0.8856027624,3.7998079662,3.
9711446786\H,0,1.6624258844,3.93625061,5.5512991624\C,0,0.434916461,-0
.8313041898,6.3385064442\H,0,0.6326686523,-0.0762064871,7.1154720305\H
,0,1.400902389,-1.0475465627,5.8565140632\C,0,2.3790963094,5.360829309
1,4.0848419976\H,0,3.3459783429,5.5306866153,4.5803180508\H,0,2.577653
6746,5.3885031553,3.0030680269\C,0,-0.0896571226,-2.1157370878,7.00434
31685\H,0,-1.0542313925,-1.9032599971,7.4878138023\H,0,-0.2926720043,-
2.868436856,6.2279494033\C,0,1.4043113617,6.4861471923,4.4586793481\H,
0,1.2165534629,6.5061993454,5.5398956873\H,0,1.8058471175,7.4647394668
,4.1723128713\H,0,0.4381287181,6.3607431888,3.9525312598\C,0,0.8881953
762,-2.6924941435,8.0375521\H,0,0.4865959538,-3.6055177023,8.491409414
8\H,0,1.8519427393,-2.9450133085,7.5763070295\H,0,1.0806858995,-1.9751
979677,8.845656989\C,0,1.2074358285,-1.0675178024,-1.4080903891\O,0,2.
286698191,-1.1067415643,-1.9313114472\C,0,-0.0869208199,-1.5093471674,
-2.0437180338\H,0,-0.8010659813,-0.6802951756,-2.1199777564\H,0,0.1517
52323,-1.8650507124,-3.0475249721\H,0,-0.55535053,-2.3244036857,-1.478
6772772\\Version=AM64L-G03RevD.01\State=1-A\HF=-844.3138622\MP2=-847.3
843461\RMSD=1.861e-09\Thermal=0.\PG=C01 [X(C17H29N2O1)]\\@

1f.4.ac

1\1\GINC-NODE10\SP\RMP2-FC\6-31+G(2d,p)\C17H29N2O1(1+)\ZIP08\04-Sep-20
10\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check g
uess=read\\sp of d5ap37.ac2 MP2-5/6-31+G(2d,p)\\1,1\C,0,-0.0240764553,
0.0271018987,-0.0289946891\C,0,-0.0008294699,0.0243072943,1.3334224858
\C,0,1.2451734897,0.0018719932,2.0555753604\C,0,2.4269431099,-0.015431
2108,1.2316913945\C,0,2.3348140765,-0.0059291801,-0.1291664102\H,0,-0.
9404856917,0.041834081,-0.6076907262\H,0,-0.9509938602,0.0449163278,1.
8507325822\H,0,3.4172516174,-0.0415982239,1.6667259592\H,0,3.221643562
3,-0.0159104121,-0.7496402787\N,0,1.3021584279,-0.0023881207,3.3916902
618\N,0,1.1269334538,0.0140913588,-0.7786584265\C,0,2.5979138508,-0.04
21245225,4.1117104686\H,0,3.2860422246,0.6643157801,3.6335982433\H,0,2
.4065056661,0.3500761914,5.1140723044\C,0,0.0711614021,0.0334643306,4.
2185597796\H,0,0.3462724844,-0.3645513064,5.1989392618\H,0,-0.65506751
82,-0.6698167139,3.7956597269\C,0,3.2231578387,-1.4472650318,4.2057612
023\H,0,3.4220715475,-1.8372743411,3.1968657107\H,0,4.2042753607,-1.32
12924621,4.6858682109\C,0,-0.5429245503,1.4382592998,4.3720848688\H,0,
-1.4798505282,1.3098769316,4.9329427896\H,0,-0.8266173948,1.832665086,
3.3855978447\C,0,0.3510938166,2.460509811,5.0940482258\H,0,0.639407559
7,2.0642657562,6.0804377945\H,0,1.2845214677,2.6076474793,4.5288193677
\C,0,2.3935341735,-2.473390349,4.9959662704\H,0,2.1906638658,-2.081746
2873,6.005129159\H,0,1.4153277042,-2.6175985095,4.5116886283\C,0,-0.34
01992965,3.822873536,5.2797004076\H,0,-1.2713925488,3.6802125773,5.846
915425\H,0,-0.6355862403,4.2155164567,4.2953187329\C,0,3.0975740549,-3
.8366104362,5.1152996896\H,0,4.0750077535,-3.696563046,5.5993518915\H,
0,3.3051979999,-4.2257274675,4.1073120221\C,0,2.2746436972,-4.86430993
74,5.9045943523\H,0,2.8018220074,-5.8227907066,5.9699969371\H,0,2.0837
830352,-4.5181395874,6.9284780386\H,0,1.3038467125,-5.0492231266,5.426
3868055\C,0,0.5481749081,4.8481704327,5.9979280299\H,0,0.0282465777,5.
8059319325,6.1130248509\H,0,0.8283185154,4.4983437857,6.9998402029\H,0
,1.4732252791,5.0358666965,5.4371515534\C,0,0.9861763411,0.0225019554,
-2.2477180017\O,0,-0.1247793307,0.0425799152,-2.701028816\C,0,2.258601
1263,0.005052461,-3.0571831488\H,0,2.8519534866,-0.8950364448,-2.85518

67761\H,0,1.9710882108,0.0114845204,-4.1099947511\H,0,2.8781752344,0.8
865450384,-2.8516798041\\Version=AM64L-G03RevD.01\State=1-A\HF=-844.31
38621\MP2=-847.3843464\RMSD=2.017e-09\Thermal=0.\PG=C01 [X(C17H29N2O1)
]\\@

1g.1

1\1\GINC-NODE11\SP\RMP2-FC\6-31+G(2d,p)\C17H30N2\ZIP08\16-Oct-2010\0\\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=r
ead\\sp of d6ap37 MP2-5/6-31+G(2d,p)\\0,1\C,0,-0.0008612061,0.00164042
27,-0.0183173317\C,0,-0.0009031108,0.0017299524,1.3737069883\C,0,1.231
4169253,0.0000327204,2.076297911\C,0,2.3907117131,0.0008402649,1.25881
12021\C,0,2.257231308,0.0055068517,-0.1267908074\H,0,-0.9560974936,0.0
011599592,-0.54487079\H,0,-0.9523031832,0.0072582398,1.8937809847\H,0,
3.3875836019,-0.0062478211,1.6852684709\H,0,3.1575935499,0.007869503,-
0.7424834203\N,0,1.2976698848,-0.0022399167,3.4554065112\N,0,1.0935520
444,0.0047615914,-0.7934671364\C,0,2.5888052951,-0.0535941334,4.144673
969\H,0,3.2803307153,0.6596526002,3.6756867537\H,0,2.4275043463,0.3120
339593,5.1653116651\C,0,0.0785610738,0.0466434431,4.2654321992\H,0,0.3
368990523,-0.3223133129,5.2646997358\H,0,-0.6548491318,-0.6651665793,3
.8625509806\C,0,3.2376931137,-1.4526847639,4.2012903602\H,0,3.40198557
73,-1.8221104115,3.179685777\H,0,4.2336688959,-1.3401452612,4.65730994
59\C,0,-0.5616904777,1.4454377584,4.3885899561\H,0,-1.509383611,1.3312
420195,4.9376107434\H,0,-0.8230985425,1.8181945199,3.3886592237\C,0,0.
3223204965,2.4821320346,5.1003596208\H,0,0.5843283733,2.1138857952,6.1
057474781\H,0,1.2690820631,2.5917577407,4.5509353868\C,0,2.4258191669,
-2.4918532838,4.9911105647\H,0,2.2614523633,-2.1269563344,6.0181898895
\H,0,1.4307325807,-2.5998210246,4.5346153331\C,0,-0.3495738276,3.85971
81114,5.2254219696\H,0,-1.3025404118,3.7539262013,5.7677995502\H,0,-0.
6087454141,4.2289396756,4.2208207181\C,0,3.1063897476,-3.8697371869,5.
0466588664\H,0,4.1069766873,-3.7655790994,5.4955325123\H,0,3.268008548
6,-4.2356124745,4.0206311934\C,0,2.3028581334,-4.9154614071,5.83731177
83\H,0,2.1432126395,-4.5499591346,6.8631447486\H,0,1.3028921021,-5.017
94726,5.3894180071\C,0,0.52621406,4.9029639821,5.9388417999\H,0,0.7834
029561,4.5341157154,6.9434395799\H,0,1.4786561974,5.007080446,5.397493
4964\C,0,2.9864372149,-6.2896418759,5.8838036422\H,0,3.9760710537,-6.2
237328465,6.3552640435\H,0,2.3915747784,-7.0131778699,6.454989632\H,0,
3.1269982607,-6.6956025093,4.873257972\C,0,-0.1495437755,6.2768758619,
6.055165929\H,0,-1.0894364782,6.209260132,6.6191019735\H,0,0.497447014
2,6.9986238728,6.5690743\H,0,-0.3862642304,6.6861350714,5.064088575\\V
ersion=AM64L-G03RevD.01\State=1-A\HF=-770.2040654\MP2=-773.105282\RMSD
=1.955e-09\Thermal=0.\PG=C01 [X(C17H30N2)]\\@

1g.2

1\1\GINC-NODE14\SP\RMP2-FC\6-31+G(2d,p)\C17H30N2\ZIP08\16-Oct-2010\0\\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=r
ead\\sp of d6ap34 MP2-5/6-31+G(2d,p)\\0,1\C,0,0.0223399406,-0.01564126
37,-0.0032794611\C,0,0.008963759,-0.0067014253,1.3887645778\C,0,1.2342
635676,-0.0017871862,2.1026064543\C,0,2.4015701321,-0.0035637815,1.296
7892091\C,0,2.2817226045,-0.0178641859,-0.0898914338\H,0,-0.9276803063
,-0.0195948636,-0.5391027457\H,0,-0.9471697565,-0.0133947556,1.9000426
223\H,0,3.3941226,0.0163493738,1.7330308717\H,0,3.1878819533,-0.019960
5688,-0.6969631616\N,0,1.2857376933,-0.0013888004,3.4822427966\N,0,1.1
243272769,-0.0236674468,-0.7676485938\C,0,2.5641762024,0.0766339589,4.
1887247813\H,0,2.4106748665,-0.3331192214,5.1942502728\H,0,3.287643353
4,-0.5906008618,3.702841584\C,0,0.0665735087,0.1311320929,4.2821815448
\H,0,-0.603079592,0.8635648513,3.8112320563\H,0,0.3565842564,0.5645349
263,5.2480298816\C,0,3.1394169578,1.5026741334,4.2961636576\H,0,3.2371
478411,1.9307472482,3.2887946708\H,0,2.4185247135,2.1369359398,4.83381
66815\C,0,-0.6914346973,-1.1904279062,4.5265897102\H,0,-0.9901376248,-
1.6237318761,3.5620779232\H,0,-1.622060826,-0.9470517759,5.0625655528\

C,0,0.1034976048,-2.2360504371,5.324813558\H,0,1.0303673796,-2.4765157
514,4.7836697543\H,0,0.4073922872,-1.8065836065,6.2934283714\C,0,4.498
6054288,1.5363809449,5.0137173636\H,0,5.2166893148,0.9069069119,4.4643
401708\H,0,4.398635722,1.0836513068,6.0131997898\C,0,-0.6868550698,-3.
5317039067,5.5728566843\H,0,-1.6161598419,-3.295109649,6.1149479937\H,
0,-0.9966732432,-3.9583987933,4.6060570011\C,0,5.0749081198,2.95499601
55,5.155826163\H,0,4.363740881,3.581650538,5.7166973119\H,0,5.16449695
05,3.4126811367,4.1582321762\C,0,6.4438289287,2.9904089045,5.855189113
5\H,0,6.3552286641,2.5274076513,6.8496953567\H,0,7.1550499125,2.368942
458,5.2903938372\C,0,0.1051807654,-4.5874034526,6.361978057\H,0,0.4166
980862,-4.1603173215,7.3273198558\H,0,1.0320615694,-4.8250426311,5.818
5146424\C,0,7.008225189,4.4111353448,6.000070196\H,0,6.334940404,5.045
9785385,6.591312119\H,0,7.98514506,4.4041823031,6.4991693155\H,0,7.136
8378092,4.887598365,5.0191153436\C,0,-0.6905871554,-5.8777283189,6.606
3116025\H,0,-0.0999945672,-6.6113030757,7.1690601556\H,0,-1.6059734839
,-5.6757153583,7.1783355087\H,0,-0.988275728,-6.3442763285,5.657910334
9\\Version=AM64L-G03RevD.01\State=1-A\HF=-770.2057689\MP2=-773.104714\
RMSD=2.775e-09\Thermal=0.\PG=C01 [X(C17H30N2)]\\@

1g.3

1\1\GINC-NODE24\SP\RMP2-FC\6-31+G(2d,p)\C17H30N2\ZIP08\15-Oct-2010\0\\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=r
ead\\sp of d6ap7 MP2-5/6-31+G(2d,p)\\0,1\C,0,0.0006131261,-0.000611627
8,0.0132130245\C,0,0.0006551671,-0.0007888937,1.4051362101\C,0,1.23343
64836,-0.0000223769,2.1062639095\C,0,2.3931791651,0.0034761333,1.28998
26318\C,0,2.2595341642,0.0082987326,-0.0955013482\H,0,-0.9544035758,0.
0006769527,-0.5136950126\H,0,-0.9502704899,0.0151997528,1.9266564442\H
,0,3.3897951855,-0.0142208356,1.7176996853\H,0,3.15952885,0.009068116,
-0.7116990488\N,0,1.2997210014,-0.0025014207,3.4833489405\N,0,1.095386
2642,0.0051407704,-0.7617892324\C,0,0.1007645909,-0.1285043468,4.30832
54474\H,0,-0.6046660116,-0.8138079544,3.8214791311\H,0,0.3950413375,-0
.6191574308,5.2460331199\C,0,2.5723915909,0.1207445155,4.1898045143\H,
0,2.3696222805,0.6079728742,5.1531985075\H,0,3.2279191506,0.8079164734
,3.6399216865\C,0,-0.5879996792,1.2129941439,4.6253263402\H,0,0.129015
8357,1.8684490953,5.1421756956\H,0,-0.8449284323,1.7188377293,3.684056
2386\C,0,3.2881881005,-1.2217644456,4.4343637204\H,0,3.4534346598,-1.7
241787465,3.470956802\H,0,2.6240174528,-1.8791965586,5.0153336488\C,0,
4.6257879959,-1.0499266336,5.1727511944\H,0,5.2852600242,-0.3918500766
,4.5848465227\H,0,4.4528469168,-0.5321880109,6.1297981218\C,0,-1.84852
4184,1.0382751802,5.4881525071\H,0,-2.5615294253,0.3822017007,4.963947
2935\H,0,-1.5845496636,0.5171315435,6.4222978326\C,0,-2.5409046813,2.3
684570284,5.8279482584\H,0,-1.831531654,3.0227402774,6.3586883057\H,0,
-2.8001689175,2.8922392586,4.8945798495\C,0,5.3473763061,-2.3811997623
,5.4396927683\H,0,4.6921485775,-3.037508282,6.0337613094\H,0,5.5157013
591,-2.9015814622,4.4838622866\C,0,6.6910120158,-2.2114790031,6.168127
063\H,0,6.5224837556,-1.6913656692,7.1233119485\H,0,7.3446431816,-1.55
55394284,5.5735016453\C,0,-3.8083908532,2.1958906724,6.6814576412\H,0,
-3.548985965,1.6723806433,7.6141656463\H,0,-4.5162276306,1.5419774419,
6.1500121456\C,0,-4.4945570454,3.5282803433,7.0155561647\H,0,-5.393072
7911,3.3728839415,7.6255028885\H,0,-3.8211165298,4.1912831796,7.574820
1838\H,0,-4.797702195,4.0572340159,6.1023123983\C,0,7.4058663245,-3.54
49404569,6.4299894276\H,0,7.6198008494,-4.0705600806,5.4899579434\H,0,
8.3588404567,-3.3915786408,6.9513665112\H,0,6.7891432669,-4.21006325,7
.0489687956\\Version=AM64L-G03RevD.01\State=1-A\HF=-770.2074961\MP2=-7
73.1039133\RMSD=1.867e-09\Thermal=0.\PG=C01 [X(C17H30N2)]\\@

1g.4

1\1\GINC-NODE11\SP\RMP2-FC\6-31+G(2d,p)\C17H30N2\ZIP08\16-Oct-2010\0\\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=r
ead\\sp of d6ap49 MP2-5/6-31+G(2d,p)\\0,1\C,0,0.0042679971,0.015367959

2,0.0032899854\C,0,0.0012761895,0.0072072421,1.3949874221\C,0,1.2306986356,0.0062428729,2.1013842539\C,0,2.3911976862,0.0216959715,1.2855196911\C,0,2.2615047133,0.0362375886,-0.1006231515\H,0,-0.9501331727,0.0166467449,-0.5247207443\H,0,-0.9515233301,0.0253000226,1.9117117686\H,0,3.3877312909,0.0118992224,1.7129262699\H,0,3.1638041006,0.0478321683,-0.7133981756\N,0,1.3031799681,0.0076753155,3.4809614034\N,0,1.1001289802,0.0299217799,-0.770329688\C,0,0.1395737232,-0.2188876978,4.3406198556\H,0,-0.6483147098,-0.7145251436,3.7642726497\H,0,0.4368486634,-0.9361035094,5.1196449213\C,0,2.5944340751,0.0285017069,4.1666623255\H,0,2.4273012012,0.4473623278,5.167672636\H,0,3.2644262688,0.7323262755,3.6570351845\C,0,-0.4089930473,1.0521922926,5.0213209537\H,0,-1.1631861637,0.7380177226,5.7594561793\H,0,0.401659692,1.5249144343,5.5971261221\C,0,3.266000535,-1.3532266642,4.2978768387\H,0,3.4065625893,-1.7864136371,3.2980277612\H,0,2.5864895897,-2.031536255,4.835349457\C,0,4.6145857439,-1.2828975501,5.0328665253\H,0,5.2903505998,-0.6008031498,4.4927295634\H,0,4.4664230219,-0.8390083432,6.0302742429\C,0,-1.0227777562,2.0877003948,4.0661488416\H,0,-0.2899446726,2.3490442662,3.2895422808\H,0,-1.8820502929,1.6395382003,3.5429682636\C,0,-1.483595119,3.3656860471,4.787215634\H,0,-2.2085951522,3.1023290592,5.5738569865\H,0,-0.6238877341,3.8204777175,5.3045027864\C,0,5.2948742399,-2.6536897851,5.1841171248\H,0,4.6208202588,-3.3364035597,5.7250261397\H,0,5.4435753318,-3.0973930092,4.1872748784\C,0,6.6450852085,-2.5876551181,5.9168729721\H,0,6.4955371639,-2.1451295574,6.9133740585\H,0,7.3177055191,-1.9047448088,5.3762562629\C,0,-2.1142321381,4.403526841,3.8441481805\H,0,-2.9762835609,3.9506606899,3.3316774232\H,0,-1.3914668025,4.6623118447,3.0561551928\C,0,-2.5627731055,5.6805224135,4.5696734374\H,0,-3.0102213567,6.4000375396,3.872825696\H,0,-3.3092960024,5.4549204331,5.342951775\H,0,-1.714417657,6.1745471785,5.0618050534\C,0,7.3176874014,-3.960482894,6.0616850408\H,0,8.2767167373,-3.8820901866,6.5886125067\H,0,6.6813933567,-4.6551871864,6.6259550464\H,0,7.5114462315,-4.411512699,5.0794330407\\Version=AM64L-G03RevD.01\State=1-A\HF=-770.2044334\MP2=-773.1039962\RMSD=2.697e-09\Thermal=0.\PG=C01 [X(C17H30N2)]\\@

1g.5

1\1\GINC-NODE24\SP\RMP2-FC\6-31+G(2d,p)\C17H30N2\ZIP08\16-Oct-2010\0\\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=read\\sp of d6ap48 MP2-5/6-31+G(2d,p)\\0,1\C,0,-0.0037474778,0.0223335105,0.0080685464\C,0,-0.0009939086,0.0138720977,1.4003129785\C,0,1.231874858,0.00626114,2.1021738044\C,0,2.3885460723,0.0081369157,1.2820608663\C,0,2.2532064652,0.0097338718,-0.1030665335\H,0,-0.9602626139,0.0279322881,-0.5161635642\H,0,-0.95232686,0.0026531428,1.9205930325\H,0,3.3860839802,0.0319465366,1.7057464499\H,0,3.153065243,0.0118158904,-0.7194498657\N,0,1.2908944182,0.013939211,3.482371788\N,0,1.0887028086,0.016867268,-0.7690175684\C,0,2.5318393215,-0.2045618809,4.22845243\H,0,2.3127698148,-0.9191234203,5.0353362085\H,0,3.2632725347,-0.7001876427,3.58195316\C,0,0.0706200538,0.0335439026,4.2876683486\H,0,-0.6475200129,0.7326472238,3.8410053516\H,0,0.3305520854,0.457687577,5.2664107452\C,0,3.1377100247,1.0715917111,4.8483529735\H,0,2.3836489411,1.5442265406,5.4965688375\H,0,3.9598782446,0.7634972643,5.5127878739\C,0,-0.5800617735,-1.3498579681,4.4881798025\H,0,0.1500992887,-2.02327974,4.9615546587\H,0,-0.8133681727,-1.7882350199,3.5081285282\C,0,-1.852918954,-1.2807153666,5.3477680302\H,0,-1.6123211984,-0.8316140213,6.3246163835\H,0,-2.5796224978,-0.6035149355,4.8713644616\C,0,3.6538814066,2.1046970544,3.8346356221\H,0,2.8495188428,2.3598663539,3.1301130781\H,0,4.461239627,1.6570329675,3.2340639181\C,0,4.1762286851,3.3876358436,4.5030354586\H,0,4.9737439936,3.1304715729,5.2183132124\H,0,3.3678467629,3.8419088267,5.0977397669\C,0,-2.5104141157,-2.6531183164,5.5690159752\H,0,-2.7514966742,-3.1020321523,4.5927810317\H,0,-1.7853370106,-3.3309407847,6.0463515562\C,0,-3.7850834609,-2.588286582,6.4265568397\H,0,-3.5431848072,-2.1405523458,7.4023780631\H,0,-4.5087049421,-1.9102583895,5.9493769157\C,0,4.7103397843,4.4231798664,3.4997574474\H,0,5.521540628

8,3.9708789637,2.9096526483\H,0,3.9149547092,4.6757351194,2.7829095479
\C,0,-4.4355346499,-3.9627280939,6.6406686941\H,0,-3.7457694619,-4.652
5732064,7.1448737014\H,0,-5.3403994965,-3.8851638757,7.2560862661\H,0,
-4.7200828237,-4.419038586,5.6832750544\C,0,5.2208298892,5.7051353435,
4.1737629851\H,0,6.0382819897,5.4857648612,4.8736208587\H,0,5.59729799
58,6.422856857,3.4344007904\H,0,4.4211487843,6.1985890476,4.7420713905
\\Version=AM64L-G03RevD.01\State=1-A\HF=-770.2044334\MP2=-773.1039961\
RMSD=2.695e-09\Thermal=0.\PG=C01 [X(C17H30N2)]\\@

1g.1.ac

1\1\GINC-NODE23\SP\RMP2-FC\6-31+G(2d,p)\C19H33N2O1(1+)\ZIP08\13-Nov-20
10\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check g
uess=read\\sp of d6ap37.ac2 MP2-5/6-31+G(2d,p)\\1,1\C,0,-1.2666768835,
-2.7301695689,-1.1570890447\C,0,-0.5251732238,-1.5872364919,-1.1712406
069\C,0,-0.4612799956,-0.7280646332,-0.0169328547\C,0,-1.2273141453,-1
.1749504297,1.1187899724\C,0,-1.9453415906,-2.333732192,1.0694893056\H
,0,-1.3401521253,-3.4000491164,-2.0058445635\H,0,0.0171751554,-1.35430
64235,-2.0779272437\H,0,-1.2601820034,-0.6037576536,2.0370483225\H,0,-
2.5199762645,-2.6726653419,1.9217801349\N,0,0.2564025239,0.3997682891,
-0.0000917617\N,0,-1.9809125844,-3.123282183,-0.0515500397\C,0,0.29945
90774,1.2753485405,1.1957445271\H,0,0.4213934565,0.6475481452,2.085749
6941\H,0,1.2155235858,1.8663345722,1.1121364761\C,0,1.0470133525,0.831
2983757,-1.1787598832\H,0,1.1919059723,1.9097846558,-1.0734274167\H,0,
0.4378828089,0.6907559699,-2.0786974774\C,0,-0.9191432488,2.2082449206
,1.3372981671\H,0,-1.8386622637,1.6125623947,1.4321152389\H,0,-0.79716
94309,2.7392711449,2.29230307\C,0,2.4100709269,0.1262619509,-1.3172435
706\H,0,2.8432757768,0.4694541328,-2.2676646546\H,0,2.2614966718,-0.95
83932774,-1.4205192133\C,0,3.4019679671,0.4003768921,-0.1738469236\H,0
,3.5440899867,1.4870559939,-0.064892641\H,0,2.9844390313,0.0403049715,
0.779202152\C,0,-1.0857498227,3.2293715938,0.1991377127\H,0,-0.1587670
448,3.8145571309,0.0939255865\H,0,-1.2364342141,2.7027860015,-0.755890
6921\C,0,4.7685904475,-0.2677454962,-0.4050339867\H,0,5.1908237055,0.0
900873851,-1.3564115886\H,0,4.6279514555,-1.353901053,-0.5198676754\C,
0,-2.2653780314,4.1898265277,0.4316391558\H,0,-2.1146887708,4.72660874
59,1.3806323491\H,0,-3.1920199692,3.6069295261,0.5515181785\C,0,-2.447
8933851,5.2076741953,-0.7065233668\H,0,-1.5202338212,5.7867770293,-0.8
263132014\H,0,-2.5996174439,4.6688253036,-1.6540285526\C,0,5.772062668
5,-0.0010378331,0.7293716354\H,0,5.9109004408,1.0845550604,0.841871025
3\H,0,5.3480043231,-0.3578233942,1.6802410465\C,0,-3.6234057981,6.1659
014141,-0.4671355737\H,0,-3.4810069505,6.7454601347,0.4539710359\H,0,-
3.7289328098,6.87618698,-1.2953228777\H,0,-4.569979711,5.6177104025,-0
.3740372901\C,0,7.1331311382,-0.6702050902,0.4908696844\H,0,7.59646538
99,-0.3066309899,-0.4353167679\H,0,7.8255579644,-0.4617058522,1.314641
7718\H,0,7.0305854011,-1.7599877951,0.4075659664\C,0,-2.7462177851,-4.
3812688446,-0.1434525972\O,0,-2.6994252328,-4.9885032144,-1.1774848031
\C,0,-3.5263295242,-4.7988325069,1.0780472504\H,0,-4.2841883817,-4.052
8005611,1.3465973189\H,0,-4.0246425525,-5.7392045355,0.8361755214\H,0,
-2.8681979458,-4.956074659,1.9412839844\\Version=AM64L-G03RevD.01\Stat
e=1-A\HF=-922.3923377\MP2=-925.7679439\RMSD=2.247e-09\Thermal=0.\PG=C0
1 [X(C19H33N2O1)]\\@

1g.2.ac

1\1\GINC-NODE12\SP\RMP2-FC\6-31+G(2d,p)\C19H33N2O1(1+)\ZIP08\11-Nov-20
10\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check g
uess=read\\sp of d6ap37.ac1 MP2-5/6-31+G(2d,p)\\1,1\C,0,-0.0826739313,
0.0261584122,-0.035463218\C,0,-0.043544034,0.0224410823,1.3280971603\C
,0,1.2119396454,-0.0041167638,2.0343718152\C,0,2.3825478039,-0.0233725
563,1.195927655\C,0,2.2747307097,-0.0136540799,-0.1625879599\H,0,-1.02
46958985,0.0446421105,-0.5679989697\H,0,-0.9871393597,0.0474481377,1.8
566987538\H,0,3.3780281171,-0.0520434887,1.6187701506\H,0,3.1312720128
,-0.0251313547,-0.8266418677\N,0,1.2838943301,-0.008886356,3.369560614

3\N,0,1.0572933323,0.0098718894,-0.7979121906\C,0,2.5884355885,-0.0443
030893,4.0742119814\H,0,3.2714339638,0.6558873171,3.5803256216\H,0,2.4
088085712,0.3591884523,5.0744687859\C,0,0.0645107237,0.0216915902,4.21
24638281\H,0,0.3529030041,-0.3786419874,5.1881230741\H,0,-0.6653106668
,-0.6828014497,3.797324645\C,0,3.2140902999,-1.4489939341,4.1761880512
\H,0,3.400905506,-1.8496981422,3.1693708429\H,0,4.2004472062,-1.317187
783,4.6435188373\C,0,-0.5513591882,1.4247423447,4.3800369237\H,0,-1.48
04464442,1.2919400368,4.9527444662\H,0,-0.8486159527,1.8240236303,3.39
95641785\C,0,0.352062129,2.443714403,5.0952941157\H,0,0.6471660079,2.0
435304683,6.0779313635\H,0,1.2805902631,2.5872126948,4.5214525497\C,0,
2.394193064,-2.4661154249,4.9882686095\H,0,2.198734906,-2.059619461,5.
9931055356\H,0,1.4124606684,-2.619703616,4.5143045083\C,0,-0.331534198
7,3.8084186924,5.2899778988\H,0,-1.2605101405,3.6704727018,5.863989485
6\H,0,-0.6325741191,4.208470665,4.3090902172\C,0,3.1033908779,-3.82494
53269,5.1222648191\H,0,4.0831973529,-3.6764426809,5.6011279095\H,0,3.3
093820713,-4.2290776211,4.1188007486\C,0,2.2929887403,-4.8532697379,5.
9290081466\H,0,2.0874931385,-4.4468608745,6.9305138048\H,0,1.313585874
,-5.0007869556,5.4491548006\C,0,0.5623394473,4.8348342748,6.0057120362
\H,0,0.8584422089,4.4347847629,6.9867868319\H,0,1.4927475289,4.9675089
283,5.4330851723\C,0,3.0087836728,-6.2050741952,6.0613553252\H,0,3.975
5214017,-6.0932598304,6.568816536\H,0,2.4076965854,-6.9151586229,6.641
0221099\H,0,3.1980509173,-6.6524557016,5.076882044\C,0,-0.1237766387,6
.1955613279,6.19259298\H,0,-1.0384117941,6.0992671338,6.7915949324\H,0
,0.5374346286,6.9041764679,6.7046233035\H,0,-0.4020792431,6.6360579046
,5.2263128146\C,0,1.057140998,0.0163277492,-2.2743652622\O,0,2.1198126
95,-0.0037748757,-2.8314808834\C,0,-0.2868831139,0.0458791802,-2.95771
81682\H,0,-0.8532705905,0.9467755933,-2.6918900762\H,0,-0.1023307638,0
.04742132,-4.03341539\H,0,-0.8882308057,-0.8346043036,-2.7006688189\\V
ersion=AM64L-G03RevD.01\State=1-A\HF=-922.3922771\MP2=-925.767969\RMSD
=2.227e-09\Thermal=0.\PG=C01 [X(C19H33N2O1)]\\@

1g.3.ac

1\1\GINC-NODE20\SP\RMP2-FC\6-31+G(2d,p)\C19H33N2O1(1+)\ZIP08\14-Nov-20
10\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check g
uess=read\\sp of d6ap97.ac2 MP2-5/6-31+G(2d,p)\\1,1\C,0,-0.8648074428,
2.8845421121,-1.1553725903\C,0,-0.2916298117,1.6486143993,-1.169434621
6\C,0,-0.3547699649,0.7868782703,-0.0177280488\C,0,-1.0578141319,1.333
3450658,1.1149232732\C,0,-1.6070230032,2.581069533,1.0654594433\H,0,-0
.8387019645,3.5606596253,-2.0023405426\H,0,0.2183708074,1.3436475833,-
2.0736106085\H,0,-1.1777534732,0.7697638421,2.0306275981\H,0,-2.134198
1199,2.9937390987,1.9160755467\N,0,0.1964427722,-0.4306416081,0.000201
9261\N,0,-1.524258478,3.37120155,-0.0528153716\C,0,0.9221381462,-0.969
3286814,-1.1766784308\H,0,0.9182545103,-2.0570327126,-1.0672581999\H,0
,0.3396026964,-0.7478990356,-2.0783058044\C,0,0.1096453112,-1.30284354
29,1.1967586581\H,0,0.3121719306,-0.6975376032,2.0877255852\H,0,0.9348
214373,-2.0156908821,1.1196262651\C,0,2.3701687583,-0.4598712358,-1.31
46180526\H,0,2.7552571686,-0.8688092339,-2.2598459893\H,0,2.3755433434
,0.6336846215,-1.4285530929\C,0,-1.2289382254,-2.0541524357,1.32882640
1\H,0,-2.0565870845,-1.3336498477,1.3994438105\H,0,-1.1979447464,-2.58
33524001,2.2920409937\C,0,-1.521742226,-3.0593216854,0.2012443997\H,0,
-1.5736814658,-2.5335486688,-0.7645075367\H,0,-0.6888037356,-3.7759561
263,0.1252234802\C,0,3.3109006416,-0.8585374347,-0.16436418\H,0,3.2951
561694,-1.9527659631,-0.0411707611\H,0,2.9496659931,-0.4286797165,0.78
24926351\C,0,-2.8337986033,-3.832012344,0.422313534\H,0,-2.784899199,-
4.3612389718,1.3860519729\H,0,-3.6683147256,-3.1182066093,0.5049983457
\C,0,4.7594122446,-0.3974895008,-0.4028855273\H,0,5.126377355,-0.83029
86934,-1.3458863382\H,0,4.775690842,0.6950802212,-0.5393292176\C,0,-3.
1359171274,-4.8420980325,-0.6977949779\H,0,-2.301260883,-5.5546343951,
-0.7759637347\H,0,-3.1806029506,-4.3127504791,-1.6615204274\C,0,5.7141
045181,-0.7832765534,0.7397906781\H,0,5.351656908,-0.3411710859,1.6802
107309\H,0,5.6873233133,-1.8739126358,0.8812112221\C,0,7.1599181254,-0

.3336688637,0.4855687166\H,0,7.8157572402,-0.624288142,1.3144037365\H,
0,7.559640971,-0.7857529745,-0.431094987\H,0,7.222791069,0.7567738649,
0.3749948161\C,0,-4.4460608865,-5.6101265313,-0.4724625292\H,0,-4.6334
533408,-6.31883093,-1.2874222091\H,0,-4.41552312,-6.1797729147,0.46515
73263\H,0,-5.303157038,-4.9262686314,-0.4204119653\C,0,-2.1060281641,4
.7239151125,-0.1440738857\O,0,-1.9614138828,5.325250964,-1.1732980472\
C,0,-2.8366138609,5.236317331,1.0720380845\H,0,-2.1712502722,5.3054174
603,1.9413226379\H,0,-3.2074053729,6.2337021189,0.829536308\H,0,-3.685
3890431,4.5919230153,1.3316948329\\Version=AM64L-G03RevD.01\State=1-A\
HF=-922.3922587\MP2=-925.7679387\RMSD=2.438e-09\Thermal=0.\PG=C01 [X(C
19H33N2O1)]\\@

1g.4.ac

1\1\GINC-NODE13\SP\RMP2-FC\6-31+G(2d,p)\C19H33N2O1(1+)\ZIP08\11-Nov-20
10\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check g
uess=read\\sp of d6ap7.ac1 MP2-5/6-31+G(2d,p)\\1,1\C,0,-0.0685240873,-
0.0442736079,-0.0066948831\C,0,-0.0366822122,-0.0620986337,1.356576664
\C,0,1.2143024939,-0.0080467287,2.0690304264\C,0,2.3888892379,0.056233
793,1.2381146266\C,0,2.288154883,0.067420935,-0.1203837711\H,0,-1.0068
173874,-0.0750786849,-0.5454070875\H,0,-0.9829627468,-0.0966204428,1.8
805796601\H,0,3.3819819891,0.0771542165,1.6678176572\H,0,3.1475997373,
0.108444112,-0.779565703\N,0,1.2796644806,-0.0163601938,3.403267603\N,
0,1.0744139336,0.0206773536,-0.7627760604\C,0,0.0769296386,-0.15259513
17,4.2537681294\H,0,-0.621247282,-0.8513426889,3.7807504966\H,0,0.4068
575665,-0.6338829209,5.1806869679\C,0,2.5607591642,0.1209566009,4.1308
891336\H,0,2.3228149618,0.6006760315,5.0864183757\H,0,3.2062761212,0.8
218049587,3.5913024896\C,0,-0.6001083419,1.1934263216,4.5645641269\H,0
,0.1352935613,1.8678590815,5.0260213295\H,0,-0.9140299248,1.6738192537
,3.6263207752\C,0,3.2702071423,-1.2225602275,4.3723212799\H,0,3.479664
1698,-1.7084803866,3.4082049381\H,0,2.5925112046,-1.8950644947,4.91755
17843\C,0,4.5774008115,-1.0439522059,5.1647969458\H,0,5.2479136563,-0.
3629434965,4.6178297954\H,0,4.3572859155,-0.5538738058,6.1254095721\C,
0,-1.8113691449,1.0262548838,5.4993193268\H,0,-2.5367647093,0.33507666
16,5.0424461897\H,0,-1.4847427183,0.5537616234,6.4380553374\C,0,-2.507
3810082,2.3612749016,5.8144446244\H,0,-1.7797150547,3.0530061057,6.266
0161544\H,0,-2.8369868368,2.8314999572,4.8748292086\C,0,5.3044156038,-
2.3742338741,5.4253757357\H,0,4.6349665131,-3.0531325511,5.9757025978\
H,0,5.5207421785,-2.8665947951,4.4645026854\C,0,6.6135157061,-2.199922
0963,6.2138119945\H,0,6.3952271084,-1.7073855394,7.1729503932\H,0,7.28
02142505,-1.5196846686,5.6630456562\C,0,-3.713609879,2.2058039969,6.75
61593564\H,0,-3.3816050116,1.7390575958,7.6953044526\H,0,-4.4380632949
,1.5106680676,6.3061024423\C,0,-4.4049858189,3.5418001615,7.0626838135
\H,0,-5.2578591996,3.3994319087,7.7363301819\H,0,-3.7129380645,4.24517
6348,7.5435795419\H,0,-4.7787098233,4.0152627668,6.1454250227\C,0,7.33
60320253,-3.5296750093,6.4717337524\H,0,7.5997356619,-4.0277759002,5.5
29666799\H,0,8.262252267,-3.372111067,7.0363979569\H,0,6.7058870261,-4
.218597024,7.0490395362\C,0,1.0808961794,0.04217013,-2.237658315\O,0,2
.1448274307,0.0996078267,-2.7901418811\C,0,-0.2586927835,-0.0101546613
,-2.9285484074\H,0,-0.8850191686,0.8486129327,-2.6577584646\H,0,-0.068
6595703,0.0146224193,-4.0029864314\H,0,-0.801973266,-0.9310320299,-2.6
838621999\\Version=AM64L-G03RevD.01\State=1-A\HF=-922.3964569\MP2=-925
.7675867\RMSD=3.172e-09\Thermal=0.\PG=C01 [X(C19H33N2O1)]\\@

1g.5.ac

1\1\GINC-NODE23\SP\RMP2-FC\6-31+G(2d,p)\C19H33N2O1(1+)\ZIP08\12-Nov-20
10\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check g
uess=read\\sp of d6ap7.ac2 MP2-5/6-31+G(2d,p)\\1,1\C,0,-0.0298407146,-
0.057212062,-0.0098470396\C,0,-0.0000803412,-0.0510381125,1.3520880133
\C,0,1.248653982,0.0104832549,2.0669956991\C,0,2.4257090988,0.06735839
1,1.2382700169\C,0,2.3269080633,0.0545534815,-0.1218474521\H,0,-0.9484

488746,-0.0960142661,-0.583869147\H,0,-0.9474868674,-0.0737842842,1.87
47890854\H,0,3.417810382,0.1000829705,1.6694053935\H,0,3.2093440051,0.
0874780508,-0.7477691153\N,0,1.3112960306,0.0139323279,3.401389596\N,0
,1.1168440063,-0.0078304965,-0.7652881766\C,0,0.1057153456,-0.12635110
87,4.2478022135\H,0,-0.5885853329,-0.8253254565,3.7698773406\H,0,0.433
9713517,-0.6095733567,5.1743720333\C,0,2.5899262598,0.1473734856,4.133
3743425\H,0,2.3502935333,0.6253333089,5.0893047163\H,0,3.2397443445,0.
8479039732,3.5981781195\C,0,-0.5771601167,1.2161090697,4.5610219824\H,
0,0.1499294992,1.887021169,5.0406336718\H,0,-0.8786031587,1.7051759545
,3.6232280786\C,0,3.2933625841,-1.1996242022,4.3731848672\H,0,3.516072
2921,-1.6765858974,3.4075075401\H,0,2.6053449372,-1.8758492114,4.90041
26484\C,0,4.5884742644,-1.0355909261,5.1884473081\H,0,5.2667896941,-0.
3422723645,4.6670454638\H,0,4.3530907324,-0.5669683178,6.1559924108\C,
0,-1.801865466,1.034416757,5.4752225926\H,0,-2.5218344303,0.3547409401
,4.9933318695\H,0,-1.4900797306,0.5415223398,6.4086282674\C,0,-2.50066
20337,2.3635288866,5.8087550325\H,0,-1.7812960704,3.0412948532,6.29359
69285\H,0,-2.809176538,2.8584377492,4.874743989\C,0,5.3115418037,-2.37
15282158,5.4302285618\H,0,4.6303602006,-3.0654937616,5.9462829466\H,0,
5.5500813273,-2.8377165263,4.4615204937\C,0,6.6020756251,-2.2192926559
,6.2532305763\H,0,6.3610707144,-1.756762345,7.2217623302\H,0,7.2801253
208,-1.5217790817,5.739106699\C,0,-3.7272068002,2.1862260536,6.7197491
98\H,0,-3.4168684254,1.6913127473,7.6519175904\H,0,-4.4437995858,1.506
9816586,6.2342873028\C,0,-4.4219286055,3.5147956528,7.0499933115\H,0,-
5.2889230634,3.3551345778,7.7014410474\H,0,-3.7390709768,4.20270618,7.
5652242004\H,0,-4.7760161634,4.0150924604,6.1392468782\C,0,7.319857239
6,-3.5561355184,6.4866467508\H,0,7.6045249174,-4.0254183559,5.53589022
77\H,0,8.2330474999,-3.4160926734,7.0765043427\H,0,6.676995995,-4.2620
210965,7.0282971577\C,0,0.9692032632,-0.0238263271,-2.2328626642\O,0,-
0.142726476,-0.0796437621,-2.6811650117\C,0,2.2365079747,0.0316304384,
-3.0485974702\H,0,2.8857081978,-0.8281224537,-2.8425393208\H,0,1.94449
81844,0.0112249137,-4.1000053733\H,0,2.8008958747,0.9516003492,-2.8532
564361\\Version=AM64L-G03RevD.01\State=1-A\HF=-922.3964566\MP2=-925.76
75863\RMSD=3.260e-09\Thermal=0.\PG=C01 [X(C19H33N2O1)]\\@

1h.1

1\1\GINC-NODE13\SP\RMP2-FC\6-31+G(2d,p)\C21H38N2\ZIP08\08-Jul-2011\0\\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=r
ead\\sp of d8ap37 MP2-5/6-31+G(2d,p)\\0,1\C,0,-0.3397207321,3.79863572
77,-1.0782454907\C,0,-0.3624654111,2.408235675,-1.1410778161\C,0,-0.00
0110676,1.6475139473,-0.0000297685\C,0,0.3621676508,2.4082304017,1.141
0461062\C,0,0.3392826773,3.7986305122,1.0782645804\H,0,-0.6186028938,4
.3705127829,-1.9641801942\H,0,-0.6627474688,1.9339571227,-2.0686292385
\H,0,0.6624982576,1.9339482954,2.0685799783\H,0,0.6181075035,4.3705032
465,1.9642201262\N,0,-0.000041543,0.2669181642,-0.0000557679\N,0,-0.00
02554598,4.5203354706,0.0000227731\C,0,0.4340653915,-0.4843515779,1.17
97632453\H,0,-0.028209122,-0.0520302241,2.0778099543\H,0,0.0238976865,
-1.4966508459,1.0889252433\C,0,-0.4340631309,-0.4843493775,-1.17990751
87\H,0,-0.0237897337,-1.4966092977,-1.0891085588\H,0,0.0281696055,-0.0
519426927,-2.0779347909\C,0,1.9635686451,-0.5695199565,1.3677337267\H,
0,2.3763386392,0.4426791608,1.4776375272\H,0,2.1530319907,-1.089795986
9,2.3195526422\C,0,-1.9635564489,-0.5696721992,-1.3678873514\H,0,-2.15
29609284,-1.0899278879,-2.3197291601\H,0,-2.3764343416,0.4424874117,-1
.4777491866\C,0,-2.6999214316,-1.2943348058,-0.2296810567\H,0,-2.28605
20203,-2.3088299429,-0.1091128065\H,0,-2.5140763014,-0.7662007195,0.71
71382924\C,0,2.7000073265,-1.2940555756,0.2294943622\H,0,2.2862459443,
-2.3085898352,0.1088844605\H,0,2.5141032311,-0.7659012433,-0.717302095
2\C,0,-4.2170330379,-1.3918493089,-0.4627869637\H,0,-4.4074236794,-1.9
305761636,-1.4043969911\H,0,-4.6275192633,-0.3794123932,-0.6008722312\
C,0,4.2171303224,-1.3914171927,0.4625904094\H,0,4.4075831465,-1.930162
3223,1.4041773892\H,0,4.6275081417,-0.3789417606,0.6007155433\C,0,4.96
62299627,-2.0901263613,-0.684200044\H,0,4.5506214069,-3.0999830942,-0.

8293191738\H,0,4.7808211077,-1.5451753001,-1.6231868423\C,0,-4.9660630
652,-2.0906859025,0.6839713116\H,0,-4.5503459558,-3.1005034303,0.82905
2372\H,0,-4.7807185322,-1.5457522972,1.6229808581\C,0,6.4820232749,-2.
1945508716,-0.4488211144\H,0,6.6684308355,-2.7468529788,0.4858787803\H
,0,6.8968322551,-1.1857640684,-0.2951114975\C,0,-6.4818436439,-2.19526
577,0.448579065\H,0,-6.6681848689,-2.7475498087,-0.4861447171\H,0,-6.8
967619814,-1.1865180236,0.2949083446\C,0,-7.2342355164,-2.8813566851,1
.6008186857\H,0,-6.817495193,-3.8878727571,1.7576259928\H,0,-7.0519714
447,-2.3260495374,2.5332828652\C,0,-8.7463228133,-2.9861483211,1.35456
18502\H,0,-8.9599332174,-3.5672632888,0.4475760987\H,0,-9.255657331,-3
.4765754042,2.1934831937\H,0,-9.1956770384,-1.992542063,1.2250350426\C
,0,7.2344827077,-2.8805120319,-1.6010937869\H,0,6.817846829,-3.8870646
274,-1.7579443053\H,0,7.0521572948,-2.325182468,-2.5335326557\C,0,8.74
6581825,-2.9851565959,-1.3548470912\H,0,8.9602567802,-3.5662924677,-0.
4478899432\H,0,9.2559650761,-3.475489799,-2.1937937237\H,0,9.195831759
6,-1.9915091353,-1.225274289\\Version=AM64L-G03RevD.01\State=1-A\HF=-9
26.3601634\MP2=-929.8716183\RMSD=7.857e-09\Thermal=0.\PG=C01 [X(C21H38
N2)]\\@

1h.2

1\1\GINC-NODE20\SP\RMP2-FC\6-31+G(2d,p)\C21H38N2\ZIP08\08-Jul-2011\0\\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=r
ead\\sp of d8ap34 MP2-5/6-31+G(2d,p)\\0,1\C,0,-1.2167153722,4.16735748
12,0.2979302221\C,0,-1.1858649018,2.844770717,0.73124672\C,0,-0.337378
831,1.9124015018,0.0814075174\C,0,0.4288980096,2.4392312484,-0.9896595
141\C,0,0.304200715,3.7831088356,-1.3301815608\H,0,-1.8738184305,4.873
3212765,0.8073498839\H,0,-1.8245522828,2.5529516351,1.5573818651\H,0,1
.1222819355,1.8229505725,-1.5513555739\H,0,0.8992476986,4.1743726163,-
2.1563670428\N,0,-0.2688216707,0.5872871523,0.4617555449\N,0,-0.496835
3038,4.6671656849,-0.7171524147\C,0,0.6696295588,-0.3359093751,-0.1761
063896\H,0,0.286376399,-1.3518192817,-0.0228262561\H,0,0.6575857967,-0
.1742997128,-1.2617479668\C,0,-0.9850159283,0.1047956756,1.6439756972\
H,0,-0.9143164426,0.8525459484,2.4455996117\H,0,-0.4505994682,-0.78162
95568,2.0091227305\C,0,2.1106517084,-0.243759681,0.3628738966\H,0,2.48
4495005,0.7805070997,0.2261247353\H,0,2.0962340143,-0.4259305662,1.448
0411188\C,0,-2.464049613,-0.2592665441,1.3972538528\H,0,-3.0053857361,
0.6309174629,1.0483698668\H,0,-2.9059690743,-0.5343561102,2.3675715547
\C,0,-2.675118741,-1.4031811895,0.3925742715\H,0,-2.2317523897,-1.1229
130669,-0.574304367\H,0,-2.1356569005,-2.3004970513,0.7371968653\C,0,3
.0581323595,-1.2446212286,-0.3184428063\H,0,3.0594498739,-1.0661596113
,-1.4055649175\H,0,2.6737881436,-2.2675035352,-0.1778554738\C,0,-4.158
3756664,-1.7534540819,0.1857549852\H,0,-4.6038864699,-2.037647464,1.15
21848552\H,0,-4.6992706221,-0.8542241983,-0.1479224476\C,0,4.501093480
1,-1.1688383324,0.2082345983\H,0,4.4994580093,-1.3364817462,1.29669555
38\H,0,4.8889067931,-0.1495552587,0.0566167881\C,0,5.4479171464,-2.179
5237945,-0.4599518059\H,0,5.0618047219,-3.1990235803,-0.3023170879\H,0
,5.4441920434,-2.0164700388,-1.5492925524\C,0,-4.3819125912,-2.8859566
657,-0.8299891971\H,0,-3.8359946017,-3.7841014871,-0.5001529372\H,0,-3
.94099104,-2.5980993164,-1.797356831\C,0,6.8925497128,-2.0980313633,0.
0602459764\H,0,6.896711054,-2.2558049813,1.1504862515\H,0,7.2806752732
,-1.0800771485,-0.1020921513\C,0,-5.8644458759,-3.2394200407,-1.033015
1568\H,0,-6.3049353242,-3.5309500952,-0.0663016463\H,0,-6.4116502204,-
2.3407501131,-1.3589342525\C,0,7.8392925866,-3.1131035002,-0.601397264
3\H,0,7.452424161,-4.1301854857,-0.4366590965\H,0,7.8342807206,-2.9565
926983,-1.6907166817\C,0,9.2801141379,-3.0223348144,-0.0780403744\H,0,
9.9312211114,-3.7566841783,-0.5684318462\H,0,9.7041183501,-2.025626126
2,-0.2587420523\H,0,9.3207258188,-3.2085947869,1.00350259\C,0,-6.09099
98754,-4.3672292579,-2.0533183175\H,0,-5.5434399866,-5.2650727206,-1.7
28847317\H,0,-5.6534317011,-4.0745418379,-3.0197054397\C,0,-7.57418717
2,-4.7144954444,-2.2473870965\H,0,-7.7041210896,-5.521094618,-2.979690
2945\H,0,-8.0303318131,-5.0424520849,-1.3037274529\H,0,-8.1408194122,-

3.8441525677,-2.6043326303\\Version=AM64L-G03RevD.01\State=1-A\HF=-926
.3618664\MP2=-929.8710066\RMSD=9.738e-09\Thermal=0.\PG=C01 [X(C21H38N2
)]\\@

1h.3

1\1\GINC-NODE13\SP\RMP2-FC\6-31+G(2d,p)\C21H38N2\ZIP08\08-Jul-2011\0\\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=r
ead\\sp of d8ap7 MP2-5/6-31+G(2d,p)\\0,1\C,0,1.0078799737,4.0767613453
,0.5126509792\C,0,1.0686040071,2.6864487591,0.5407654719\C,0,0.0000375
596,1.9267675556,-0.000035783\C,0,-1.0685029198,2.6864448825,-0.540893
798\C,0,-1.0077340026,4.0767572796,-0.512881134\H,0,1.837279398,4.6489
568027,0.9302528638\H,0,1.9467491723,2.2113932514,0.9646242525\H,0,-1.
946662692,2.2113865713,-0.9647188749\H,0,-1.8371142797,4.6489496213,-0
.9305252683\N,0,0.0000102789,0.5481006705,0.0000148916\N,0,0.000084827
5,4.7982782415,-0.000141138\C,0,1.0504299591,-0.2181410571,0.666070245
1\H,0,1.3498283826,0.299801218,1.5860919419\H,0,0.6098889397,-1.170960
5766,0.98951074\C,0,-1.0504213089,-0.2181416915,-0.6660215257\H,0,-0.6
099121547,-1.1710026674,-0.9893825416\H,0,-1.3497683581,0.2997508053,-
1.5860886055\C,0,2.2819862272,-0.4955588652,-0.2175110675\H,0,1.960662
0349,-1.0477725704,-1.1134686816\H,0,2.6927799172,0.4591505351,-0.5747
96393\C,0,-2.2820205426,-0.4954464321,0.2175355873\H,0,-2.6927745386,0
.4593033114,0.5747581189\H,0,-1.9607574172,-1.0476320018,1.113532239\C
,0,-3.3707164688,-1.2907793758,-0.5214944209\H,0,-3.6880943651,-0.7307
485736,-1.4154986519\H,0,-2.9470630542,-2.2387246243,-0.8899228\C,0,3.
3706645068,-1.2909172829,0.5215173184\H,0,3.6881333429,-0.7308470351,1
.4154642391\H,0,2.9469624759,-2.2388060552,0.8900353511\C,0,4.60083718
13,-1.5903446973,-0.3512716824\H,0,4.2856775721,-2.1598353857,-1.23959
90982\H,0,5.0177641201,-0.6431574836,-0.7274463044\C,0,-4.6009626044,-
1.5900533615,0.3512432404\H,0,-4.2859012556,-2.159507412,1.2396289452\
H,0,-5.0178393427,-0.6428080194,0.7273270964\C,0,-5.6996764613,-2.3697
744017,-0.3901536475\H,0,-5.2822007185,-3.3162359324,-0.7686795374\H,0
,-6.0145583448,-1.7981771047,-1.2774705101\C,0,5.6995363153,-2.3701009
767,0.3901097278\H,0,5.2820064187,-3.3164971472,0.76873953\H,0,6.01453
10133,-1.7984612356,1.2773589557\C,0,6.9292470091,-2.670394661,-0.4824
868145\H,0,6.6161967761,-3.2461521591,-1.3679045432\H,0,7.3443257146,-
1.7243999977,-0.8647845895\C,0,-6.9294765578,-2.6698928593,0.482376711
\H,0,-7.3444983022,-1.7238321652,0.8645728115\H,0,-6.6165433068,-3.245
6121114,1.367860734\C,0,8.0320556435,-3.4430819951,0.2601234574\H,0,8.
3443731736,-2.8673708912,1.1445659833\H,0,7.6180070696,-4.3888569648,0
.6413876552\C,0,9.2573933917,-3.737240156,-0.6172696613\H,0,9.71347384
67,-2.8081502261,-0.9842197152\H,0,10.0249515938,-4.2887790842,-0.0601
445987\H,0,8.9820631839,-4.3398045905,-1.4931097021\C,0,-8.0323005033,
-3.4425358568,-0.2602571377\H,0,-7.6183097124,-4.388376601,-0.64142074
88\H,0,-8.3445002071,-2.8668618556,-1.1447655149\C,0,-9.257730336,-3.7
365166556,0.6170665662\H,0,-10.0252989495,-4.288023635,0.0599242182\H,
0,-8.9825214494,-4.3390441676,1.4929701739\H,0,-9.7137512626,-2.807357
8506,0.9839163041\\Version=AM64L-G03RevD.01\State=1-A\HF=-926.3635878\
MP2=-929.8702414\RMSD=2.249e-09\Thermal=0.\PG=C01 [X(C21H38N2)]\\@

1h.4

1\1\GINC-NODE13\SP\RMP2-FC\6-31+G(2d,p)\C21H38N2\ZIP08\08-Jul-2011\0\\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=r
ead\\sp of d8ap48 MP2-5/6-31+G(2d,p)\\0,1\C,0,-0.0296619113,3.68694168
76,-0.8995991513\C,0,0.327090384,2.3507225867,-0.7383551243\C,0,-0.408
0416592,1.5282035717,0.1534243819\C,0,-1.4780613502,2.1757871635,0.821
6304023\C,0,-1.7303978666,3.5226508831,0.5790529886\H,0,0.5464527006,4
.3056853258,-1.5888469831\H,0,1.1754880761,1.9706317913,-1.2968143886\
H,0,-2.127287925,1.642323372,1.5064373819\H,0,-2.558104454,4.005045730
2,1.1004443078\N,0,-0.108837168,0.1922177856,0.3390054163\N,0,-1.03716
79526,4.3022672847,-0.2641796942\C,0,-0.6950736406,-0.611689588,1.4135

936771\H,0,0.1212643782,-1.1727063177,1.8916679906\H,0,-1.0940228373,0
.0506570456,2.1883528617\C,0,0.9915788159,-0.4430012669,-0.3846447456\
H,0,0.9865923332,-0.1003081214,-1.4268231658\H,0,0.7783540519,-1.51943
45133,-0.4245857794\C,0,-1.7755453001,-1.6106490536,0.9515651409\H,0,-
1.346303924,-2.2687422572,0.1805725972\H,0,-2.0148553964,-2.260959338,
1.8074335845\C,0,2.379764419,-0.2224372834,0.2489586905\H,0,2.36150670
37,-0.589917146,1.2860282266\H,0,2.5878010625,0.8548042616,0.307772394
3\C,0,3.500756201,-0.9320648845,-0.5280806538\H,0,3.267597166,-2.00580
37003,-0.6091031544\H,0,3.531479092,-0.5478042032,-1.5600167575\C,0,-3
.066833761,-0.9746187677,0.4133730283\H,0,-2.8243453607,-0.2912774819,
-0.4130484045\H,0,-3.5275634123,-0.357654023,1.2009066563\C,0,-4.08718
21305,-2.0205761582,-0.0666645292\H,0,-4.3202132221,-2.7086458728,0.76
15884919\H,0,-3.6301158343,-2.6377701536,-0.8563806867\C,0,4.885646491
8,-0.7628665536,0.1189860707\H,0,5.1191817847,0.3098640573,0.203079006
2\H,0,4.8527730614,-1.1501276197,1.1494705319\C,0,6.0115817961,-1.4703
633075,-0.6530602901\H,0,5.7709644626,-2.541177838,-0.7469187294\H,0,6
.0528459125,-1.0751265513,-1.6803043834\C,0,-5.3924133187,-1.404004756
7,-0.5963781401\H,0,-5.8449913807,-0.7795038942,0.1899910989\H,0,-5.16
12448315,-0.7238323407,-1.4309618303\C,0,7.3919275326,-1.3167628214,0.
0067904242\H,0,7.3499603399,-1.7123864754,1.0340481561\H,0,7.633543834
2,-0.2463189439,0.1018240305\C,0,-6.4151283361,-2.4533651146,-1.062012
7419\H,0,-6.6454372306,-3.1327064358,-0.2258123446\H,0,-5.9632313948,-
3.0794993268,-1.8477875918\C,0,8.5201547581,-2.0243707439,-0.761818034
6\H,0,8.2773433507,-3.0934580898,-0.8584419629\H,0,8.564913024,-1.6268
165752,-1.7870402237\C,0,9.8934543993,-1.8697960881,-0.0922784343\H,0,
9.8879670009,-2.2888707229,0.9228123524\H,0,10.6768956361,-2.384681190
5,-0.6622153685\H,0,10.1779772603,-0.8121533893,-0.0125663423\C,0,-7.7
227683285,-1.8419380491,-1.5918262774\H,0,-8.1718593734,-1.2129752976,
-0.8083137229\H,0,-7.4939347077,-1.16792847,-2.4311022878\C,0,-8.74022
50327,-2.8985307121,-2.0460489074\H,0,-9.0145520239,-3.5653117426,-1.2
176510327\H,0,-9.6609525579,-2.4332473785,-2.4196171293\H,0,-8.3300393
366,-3.5223241567,-2.851532186\\Version=AM64L-G03RevD.01\State=1-A\HF=
-926.360551\MP2=-929.8701936\RMSD=9.005e-09\Thermal=0.\PG=C01 [X(C21H3
8N2)]\\@

1h.5

1\1\GINC-NODE20\SP\RMP2-FC\6-31+G(2d,p)\C21H38N2\ZIP08\08-Jul-2011\0\\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=r
ead\\sp of d8ap9 MP2-5/6-31+G(2d,p)\\0,1\C,0,-1.1302002352,4.174113058
1,-0.7292868608\C,0,-1.197075076,2.9606493784,-0.0505108499\C,0,0.0001
001371,2.3027169135,0.3314163669\C,0,1.1973870661,2.9605723675,-0.0502
918491\C,0,1.1307154344,4.1740408938,-0.7290789481\H,0,-2.058945394,4.
6708795247,-1.0127509081\H,0,-2.1725000651,2.5411821535,0.1696635108\H
,0,2.1727448168,2.5410498785,0.1700747863\H,0,2.0595447665,4.670750164
3,-1.0123673554\N,0,0.0000049544,1.1166011078,1.0385990621\N,0,0.00031
00449,4.8044724729,-1.0803548976\C,0,1.2541701138,0.4481091042,1.38154
10715\H,0,1.9736748851,1.1983892639,1.7374231393\H,0,1.0516472559,-0.2
047764119,2.2400224009\C,0,-1.2542576983,0.4482757585,1.3815019102\H,0
,-1.9737128182,1.1986681777,1.7372391009\H,0,-1.0518835502,-0.20453756
87,2.2400746332\C,0,1.8863349395,-0.3849183371,0.2479976215\H,0,1.1793
05253,-1.168452222,-0.0595911028\H,0,2.0418928615,0.2546892554,-0.6319
439603\C,0,-1.8864084012,-0.3848097923,0.2479928397\H,0,-1.1794296358,
-1.1684468979,-0.0594511829\H,0,-2.0418280991,0.2547211101,-0.63202958
27\C,0,-3.217943433,-1.0264164813,0.6717724019\H,0,-3.0555639916,-1.65
00881103,1.5654710956\H,0,-3.9248582968,-0.237740613,0.9749704596\C,0,
3.217774129,-1.0266949381,0.6718204629\H,0,3.0552663869,-1.6504320688,
1.5654496141\H,0,3.9247436636,-0.2381158016,0.975144743\C,0,-3.8576996
446,-1.8837833328,-0.4330908185\H,0,-3.1461666463,-2.6650079808,-0.743
3498614\H,0,-4.0323785048,-1.258797738,-1.3226090058\C,0,3.8575358313,
-1.8840164872,-0.433074284\H,0,3.1459814514,-2.6651861509,-0.743422782
6\H,0,4.0322835126,-1.2589741304,-1.3225390589\C,0,5.1791377807,-2.543

1737441,-0.0046933524\H,0,5.0020173779,-3.1653793494,0.886873827\H,0,5
.8921673524,-1.7626335034,0.3043032697\C,0,-5.1793500289,-2.5428515896
,-0.0047222605\H,0,-5.0022850233,-3.165040741,0.8868677845\H,0,-5.8923
448287,-1.7622638402,0.3042327858\C,0,5.8158847073,-3.4061199435,-1.10
64670565\H,0,5.0997300979,-4.1820285263,-1.4204932627\H,0,6.0005697419
,-2.7834996838,-1.9961287049\C,0,-5.8161123466,-3.4058001119,-1.106485
9809\H,0,-5.0999597603,-4.1817096503,-1.4205143958\H,0,-6.0008063189,-
2.7831850182,-1.9961493951\C,0,7.1307632657,-4.0767165412,-0.675184008
4\H,0,6.9454483005,-4.6973911071,0.2145989874\H,0,7.847701763,-3.30206
6709,-0.3637183708\C,0,7.7571193118,-4.9401637956,-1.7797486519\H,0,8.
6917816461,-5.4054046613,-1.4424718888\H,0,7.0753389124,-5.7442105018,
-2.0874466461\H,0,7.984808567,-4.3395516216,-2.6704268042\C,0,-7.13098
70365,-4.0763949577,-0.6751880269\H,0,-7.8479096876,-3.3017496085,-0.3
636756879\H,0,-6.9456516244,-4.6971017999,0.2145683584\C,0,-7.75737790
6,-4.9398028802,-1.7797642854\H,0,-7.075628973,-5.7438733072,-2.087468
7981\H,0,-8.6920609327,-5.4050083706,-1.4424960692\H,0,-7.9850395113,-
4.3391704164,-2.6704360378\\Version=AM64L-G03RevD.01\State=1-A\HF=-926
.3618216\MP2=-929.8697966\RMSD=2.706e-09\Thermal=0.\PG=C01 [X(C21H38N2
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1h.1.ac

1\1\GINC-NODE26\SP\RMP2-FC\6-31+G(2d,p)\C23H41N2O1(1+)\ZIP08\27-Aug-20
11\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check g
uess=read\\sp of d8ap7.ac1 MP2-5/6-31+G(2d,p)\\1,1\C,0,-0.0381534653,-
0.0604995258,-0.0577718022\C,0,-0.0084796152,-0.0637436516,1.304129516
3\C,0,1.2401909269,-0.0020954733,2.0193385593\C,0,2.417217525,0.060271
2927,1.1908491809\C,0,2.3182962786,0.0569830318,-0.1693277103\H,0,-0.9
562872918,-0.097833137,-0.6325834108\H,0,-0.955845853,-0.0933374146,1.
8265955918\H,0,3.4094183225,0.0902293283,1.6219331431\H,0,3.2011229592
,0.0953347735,-0.7942737818\N,0,1.3031949426,-0.0026584315,3.353568036
5\N,0,1.1082207288,-0.0020996584,-0.8131810069\C,0,0.0981635206,-0.143
7506143,4.2007364099\H,0,-0.5958412918,-0.8438249934,3.7240229772\H,0,
0.4274992341,-0.6257149401,5.1275448766\C,0,2.5811810149,0.1365784672,
4.0854407079\H,0,2.3395864659,0.6158973753,5.040190806\H,0,3.228306226
4,0.8384508698,3.5488012483\C,0,-0.5847343948,1.1988477594,4.512997616
7\H,0,0.1444799282,1.8722489592,4.9858619318\H,0,-0.8918249615,1.68422
80827,3.5751481135\C,0,3.2901280601,-1.2067025317,4.3294185535\H,0,3.5
102662249,-1.6887399229,3.365652434\H,0,2.6069133745,-1.8821763422,4.8
638301932\C,0,4.5882785431,-1.0323748951,5.1377275894\H,0,5.2631303907
,-0.3434609887,4.6060936958\H,0,4.3560511434,-0.5536731983,6.101112272
5\C,0,-1.804015262,1.0208139721,5.4353104681\H,0,-2.5256345729,0.33648
31258,4.9626503677\H,0,-1.4858099192,0.5353892224,6.3704218538\C,0,-2.
5023995942,2.3518167858,5.7625493634\H,0,-1.778817108,3.0353377688,6.2
326685966\H,0,-2.8202679683,2.836005551,4.8261655654\C,0,5.3151332199,
-2.3642548541,5.3910345842\H,0,4.6377106923,-3.0525203851,5.9193019019
\H,0,5.5477418616,-2.8412594011,4.4262453992\C,0,6.6103966835,-2.19928
36499,6.2038875129\H,0,6.3751601018,-1.7255475673,7.1695201463\H,0,7.2
847562039,-1.5056330113,5.6777266701\C,0,-3.7194051709,2.1820607898,6.
6875765359\H,0,-3.3992444791,1.6991626519,7.6238557262\H,0,-4.44025055
21,1.4945097517,6.2182246609\C,0,-4.4213789858,3.5105896264,7.01359991
6\H,0,-3.700011475,4.198893885,7.4813077047\H,0,-4.7422398993,3.992994
528,6.0769003412\C,0,7.3412584327,-3.5288576529,6.4531314051\H,0,7.577
5740518,-4.0017972046,5.4868829098\H,0,6.6659808547,-4.2233314913,6.97
70820298\C,0,-5.6375041372,3.3439558313,7.9401936603\H,0,-6.3563792568
,2.6538263856,7.4735335327\H,0,-5.3158818353,2.8646700038,8.876962863\
C,0,-6.3355510373,4.6739690111,8.2578010439\H,0,-6.7004982468,5.158714
973,7.3427555865\H,0,-7.1954786937,4.5226981988,8.9211099334\H,0,-5.64
96265183,5.373076055,8.7539846712\C,0,8.6353251523,-3.3677865116,7.268
488144\H,0,8.398076127,-2.898922732,8.2351865061\H,0,9.3080029139,-2.6
708222109,6.7463408566\C,0,9.3616975036,-4.6989034032,7.5084447557\H,0
,10.27756831,-4.5518392656,8.0931298196\H,0,8.7245617789,-5.4047733858

,8.0572618343\H,0,9.6435908577,-5.1735533809,6.5593669525\C,0,0.9598298917,-0.0051686355,-2.2805071737\O,0,-0.1521544341,-0.0623561609,-2.7286989842\C,0,2.2261407759,0.0648319286,-3.096899459\H,0,2.8770925151,-0.7967667197,-2.904298079\H,0,1.9328230381,0.0591655067,-4.1481156836\H,0,2.789305014,0.9826855466,-2.8886603559\\Version=AM64L-G03RevD.01\State=1-A\HF=-1078.5529514\MP2=-1082.5342746\RMSD=7.366e-10\Thermal=0.\PG=C01 [X(C23H41N2O1)]\\@

1h.2.ac

1\1\GINC-NODE15\SP\RMP2-FC\6-31+G(2d,p)\C23H41N2O1(1+)\ZIP08\27-Jul-2011\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=read\\sp of d8ap7.ac2 MP2-5/6-31+G(2d,p)\\1,1\C,0,-0.0654316601,-0.0457737645,-0.0545897003\C,0,-0.0329913186,-0.0540978542,1.3087729707\C,0,1.2183201895,0.0054050224,2.020358577\C,0,2.3923736756,0.0698939609,1.188530173\C,0,2.2908350037,0.0716829216,-0.1699077092\H,0,-1.0043184738,-0.0819661172,-0.5917989052\H,0,-0.9791040936,-0.0858086466,1.8332306544\H,0,3.3856305634,0.0977147872,1.6175008263\H,0,3.1493996744,0.111292327,-0.8302644621\N,0,1.2840301963,0.0010479502,3.3544537192\N,0,1.0770708228,0.0158855055,-0.8116915729\C,0,0.0824026348,-0.1410996814,4.2054307938\H,0,-0.6134976022,-0.8411171084,3.7310103399\H,0,0.4146971785,-0.6238712849,5.1307276147\C,0,2.5650394826,0.1392318214,4.0822055134\H,0,2.3265367962,0.6177337256,5.0381753268\H,0,3.2100620008,0.8411688508,3.5434725864\C,0,-0.5995293284,1.2011520692,4.5214408375\H,0,0.1320796708,1.8747898747,4.9900594103\H,0,-0.9113493058,1.6866712351,3.5851152907\C,0,3.2745747242,-1.2043896145,4.3223436482\H,0,3.4898841168,-1.6862599699,3.3575102153\H,0,2.5941351047,-1.8796529754,4.8607157111\C,0,4.576997528,-1.029546279,5.1236727709\H,0,5.2498959147,-0.3433438907,4.586285889\H,0,4.350357012,-0.547637822,6.0868569393\C,0,-1.8138574175,1.0236391838,5.4503359025\H,0,-2.536876665,0.3365476885,4.9836342926\H,0,-1.4900378069,0.5414668282,6.3851330912\C,0,-2.5127188726,2.3544541819,5.777306391\H,0,-1.7874564747,3.0409216124,6.2403772833\H,0,-2.8370816496,2.8349192873,4.8411440335\C,0,5.3033980732,-2.3616244857,5.3772546643\H,0,4.6282893653,-3.0470187076,5.9122761787\H,0,5.5296089611,-2.8422781787,4.4128408277\C,0,6.603790975,-2.1950766745,6.1815148407\H,0,6.3752844558,-1.7157230377,7.1460443655\H,0,7.2762479016,-1.5056486701,5.647542486\C,0,-3.7237055718,2.1862902115,6.7105182926\H,0,-3.3966422063,1.7090983823,7.6472819606\H,0,-4.4457156784,1.4944256114,6.2492352156\C,0,-4.4269497356,3.5148138784,7.033814265\H,0,-3.7042316115,4.2075170581,7.4927907538\H,0,-4.7551667262,3.9912010235,6.0965407547\C,0,7.3336517893,-3.5246754602,6.4335411795\H,0,7.562832731,-4.0035256021,5.468527877\H,0,6.6605088521,-4.2148567335,6.9659068803\C,0,-5.636482821,3.3505481698,7.9694451964\H,0,-6.3564401785,2.6553474894,7.5120066284\H,0,-5.3072910636,2.8782373858,8.9070919315\C,0,-6.3361514861,4.6806503309,8.2830689833\H,0,-6.7080830964,5.1586741763,7.3672822405\H,0,-7.1914633225,4.5312996262,8.9527253895\H,0,-5.6489983848,5.384653077,8.7705065975\C,0,8.6333026729,-3.3612615406,7.2394606136\H,0,8.4033688503,-2.8855316737,8.2046050886\H,0,9.3040666742,-2.6692593089,6.7083857367\C,0,9.3584428581,-4.692315102,7.4834831846\H,0,10.2782172941,-4.543352763,8.0615508268\H,0,8.7233139363,-5.393397422,8.0407409205\H,0,9.6335890525,-5.1735781944,6.5357733724\C,0,1.0835591962,0.024404524,-2.2864676479\O,0,2.1472605123,0.0834572383,-2.8393747225\C,0,-0.255454799,-0.0427707491,-2.9774578084\H,0,-0.8846813845,0.8180008095,-2.7199085026\H,0,-0.0646638623,-0.0331524602,-4.0519947813\H,0,-0.7961432378,-0.9614835259,-2.7193979693\\Version=AM64L-G03RevD.01\State=1-A\HF=-1078.5529514\MP2=-1082.5342746\RMSD=1.375e-09\Thermal=0.\PG=C01 [X(C23H41N2O1)]\\@

1h.3.ac

1\1\GINC-NODE24\SP\RMP2-FC\6-31+G(2d,p)\C23H41N2O1(1+)\ZIP08\27-Aug-2011\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check g

uess=read\\sp of d8ap49.ac1 MP2-5/6-31+G(2d,p)\\1,1\C,0,-0.0684339414,
-0.0114205336,0.0611397955\C,0,-0.0622660316,-0.0688986059,1.421976140
5\C,0,1.1730474687,-0.0639322437,2.1614993427\C,0,2.3644085949,0.01364
65603,1.3533016724\C,0,2.2898553272,0.0679239612,-0.0073949252\H,0,-0.
9784711137,-0.0070755039,-0.5274293988\H,0,-1.0196801894,-0.0897570035
,1.924400627\H,0,3.3490503017,0.0129147818,1.8015244357\H,0,3.18357734
93,0.1188027748,-0.6159066027\N,0,1.2256587494,-0.124347609,3.49630551
57\N,0,1.0911349309,0.0535458931,-0.6734691659\C,0,0.0350360303,-0.313
3782684,4.3578176558\H,0,-0.7547283158,-0.803712582,3.7828181826\H,0,0
.3375492833,-1.0270907953,5.133083674\C,0,2.5124241482,-0.078138053,4.
2274136955\H,0,2.2871092601,0.3075114712,5.2266362564\H,0,3.1659693842
,0.6642504015,3.7566431804\C,0,-0.4775699981,0.9827003834,5.0145668\H,
0,-1.2349976504,0.6796316897,5.751238943\H,0,0.3368521972,1.4435886597
,5.5920770739\C,0,3.2058355528,-1.4476602705,4.337988806\H,0,3.4098363
527,-1.8458067847,3.3334374278\H,0,2.5214275154,-2.1606189527,4.819484
791\C,0,4.5154800629,-1.3573896362,5.1416158685\H,0,5.1892365389,-0.62
85129664,4.6644626816\H,0,4.299801388,-0.9643750328,6.1467157437\C,0,-
1.0808089486,2.0200655381,4.0535570626\H,0,-0.340519389,2.3002075258,3
.2881982097\H,0,-1.9351544146,1.5743037938,3.5198220006\C,0,-1.5524975
133,3.2909085071,4.7822590623\H,0,-2.2866074861,3.0136038303,5.5538534
14\H,0,-0.6996812276,3.738135843,5.3156730566\C,0,5.2368155995,-2.7103
378839,5.2668872944\H,0,4.5643540079,-3.4376722234,5.7468735416\H,0,5.
4492206323,-3.1044146493,4.2608357899\C,0,6.5472897095,-2.6200370253,6
.0668317249\H,0,6.33218997,-2.2281603474,7.0730135217\H,0,7.2155292094
,-1.8869206398,5.5884591298\C,0,-2.1714487336,4.337390616,3.8407337838
\H,0,-3.0300129555,3.8915900212,3.3144843233\H,0,-1.4391313096,4.60671
06301,3.0629127364\C,0,-2.6278546005,5.6117601253,4.5702007252\H,0,-3.
358111133,5.3429794304,5.3492656671\H,0,-1.7688482309,6.0570110297,5.0
960712637\C,0,7.2769472178,-3.9677844947,6.1908271026\H,0,6.6096836002
,-4.7008215947,6.6706120521\H,0,7.4906576153,-4.3608022957,5.184308441
8\C,0,-3.2488319021,6.6612542121,3.6331988604\H,0,-2.5204454488,6.9259
158852,2.8516483929\H,0,-4.1106719226,6.2175232777,3.1125206266\C,0,-3
.6936194071,7.9328404556,4.3697520792\H,0,-4.1320849579,8.6606996832,3
.6767061246\H,0,-4.4467676172,7.7045112951,5.1351609527\H,0,-2.8455203
992,8.4170933431,4.8712613487\C,0,8.5885500907,-3.8769046069,6.9886523
618\H,0,8.3742681948,-3.4851836497,7.9942569611\H,0,9.2539930777,-3.14
33444835,6.5091034125\C,0,9.3129564188,-5.2253433945,7.1074066242\H,0,
10.2427295867,-5.1274372001,7.6803381686\H,0,8.6848053963,-5.969502504
7,7.6143696511\H,0,9.5705977061,-5.6256810754,6.1179991183\C,0,0.96899
18366,0.1079064135,-2.1417891336\O,0,-0.1354404162,0.0914476266,-2.611
5441296\C,0,2.2514157164,0.1799216272,-2.9325496873\H,0,2.8853246065,-
0.6968600432,-2.7523475514\H,0,1.9779104231,0.2087401352,-3.9887078324
\H,0,2.8245047841,1.0826848462,-2.688198126\\Version=AM64L-G03RevD.01\
State=1-A\HF=-1078.5500223\MP2=-1082.5343231\RMSD=8.784e-09\Thermal=0.
\PG=C01 [X(C23H41N2O1)]\\@

1h.4.ac

1\1\GINC-NODE15\SP\RMP2-FC\6-31+G(2d,p)\C23H41N2O1(1+)\ZIP08\27-Jul-20
11\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check g
uess=read\\sp of d8ap48.ac2 MP2-5/6-31+G(2d,p)\\1,1\C,0,-0.024165462,0
.0554527804,0.1048107247\C,0,0.0310156393,0.0102116824,1.4667608406\C,
0,1.2939124163,-0.0607624059,2.1585712396\C,0,2.4533688855,-0.06925199
18,1.3050433001\C,0,2.3300892545,-0.0209330616,-0.0505674388\H,0,-0.97
17577897,0.1014219185,-0.4163119357\H,0,-0.9065715975,0.0115853194,2.0
065285223\H,0,3.4542357087,-0.0856850834,1.7143134397\H,0,3.1800672266
,-0.0195629023,-0.7229781201\N,0,1.3684633402,-0.1124879049,3.49270425
24\N,0,1.1058532935,0.037804465,-0.6720691945\C,0,2.6359284552,-0.2940
529828,4.2384089899\H,0,2.4098834245,-1.0029197561,5.0436100961\H,0,3.
3684880188,-0.7871756142,3.5942295886\C,0,0.1568476859,-0.0635588795,4
.3424408832\H,0,-0.5398256642,0.675197077,3.9316162479\H,0,0.475343343
9,0.3282509018,5.3135143407\C,0,3.2059938853,1.0071595377,4.8348974043

\H,0,2.4492226389,1.4708226889,5.4841632738\H,0,4.0306212487,0.7101019
292,5.4982026081\C,0,-0.520319476,-1.4333496981,4.5261510445\H,0,0.208
5935262,-2.1429854207,4.942876917\H,0,-0.8195202318,-1.8368329003,3.54
7915351\C,0,-1.7465434048,-1.340806791,5.4518665207\H,0,-1.4349414326,
-0.9462368931,6.430851044\H,0,-2.4627807195,-0.612343209,5.0404964975\
C,0,3.7130889903,2.0387825886,3.8140300618\H,0,2.9031439151,2.31193256
92,3.1200244592\H,0,4.514426098,1.590859031,3.2051704937\C,0,4.2480015
538,3.3158590091,4.4859557899\H,0,5.05037312,3.0454350113,5.1889806493
\H,0,3.4472085059,3.7668675166,5.0918939829\C,0,-2.4530362351,-2.69314
21036,5.6482347402\H,0,-2.7635708685,-3.0874686845,4.6681165559\H,0,-1
.7371722573,-3.4207914232,6.0601443796\C,0,-3.6784798071,-2.6016050905
,6.5730666266\H,0,-3.3649383318,-2.2112313517,7.5536432191\H,0,-4.3892
451067,-1.8669083733,6.1633494052\C,0,4.7762609811,4.3549103764,3.4829
533279\H,0,5.5856243239,3.906277453,2.8859093124\H,0,3.9761507215,4.61
48401246,2.7715420516\C,0,-4.3946339728,-3.9483850981,6.7667992148\H,0
,-3.6845235145,-4.6831303214,7.1774852914\H,0,-4.7072554188,-4.3396319
561,5.785772253\C,0,5.2919412014,5.637424339,4.1564946946\H,0,6.088297
3318,5.377831455,4.8712697519\H,0,4.4813075561,6.0869394025,4.75104418
25\C,0,-5.6209804989,-3.8566457321,7.6902396837\H,0,-5.3079614008,-3.4
663511948,8.6701847187\H,0,-6.3294567221,-3.1216839585,7.2794222716\C,
0,-6.332006792,-5.2042884351,7.8785981044\H,0,-5.6579279131,-5.9497494
578,8.3204754592\H,0,-7.2006288708,-5.1058022942,8.5404977532\H,0,-6.6
864868316,-5.603262067,6.9190448603\C,0,5.826002241,6.6779124187,3.157
9025022\H,0,6.6406594424,6.2302520851,2.5690867228\H,0,5.0316967745,6.
9325228613,2.4397918059\C,0,6.329344845,7.9583608409,3.8393451994\H,0,
7.1464859545,7.7398462512,4.5391688738\H,0,6.7042701499,8.6792652284,3
.1030938837\H,0,5.5264804419,8.4466398251,4.4070378516\C,0,1.087852587
1,0.0823176538,-2.1456909463\O,0,2.1426928187,0.0640394339,-2.71812939
13\C,0,-0.264017295,0.1473528395,-2.8115039892\H,0,-0.8127191914,1.051
3636822,-2.5202654794\H,0,-0.0921560417,0.1687594328,-3.8890537221\H,0
,-0.8765462626,-0.7286573944,-2.5656133173\\Version=AM64L-G03RevD.01\S
tate=1-A\HF=-1078.5500198\MP2=-1082.5343235\RMSD=4.965e-09\Thermal=0.\
PG=C01 [X(C23H41N2O1)]\\@

1h.5.ac

1\1\GINC-NODE16\SP\RMP2-FC\6-31+G(2d,p)\C23H41N2O1(1+)\ZIP08\28-Jul-20
11\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check g
uess=read\\sp of d8ap78.ac2 MP2-5/6-31+G(2d,p)\\1,1\C,0,0.1727950979,3
.189132791,-0.7489900831\C,0,-0.2528164847,1.9156723402,-0.5099626659\
C,0,0.3705731137,1.1002282565,0.5024525766\C,0,1.455108397,1.732394817
1,1.2075061787\C,0,1.83272296,3.0090347166,0.9197564902\H,0,-0.2988712
054,3.8051302658,-1.5037676359\H,0,-1.0852114644,1.5474842744,-1.09474
33597\H,0,2.0186832563,1.2045000326,1.9646101219\H,0,2.6476012557,3.51
39430076,1.4253601275\N,0,-0.0365515765,-0.1480080957,0.7559688267\N,0
,1.2063414005,3.7564489388,-0.0484952258\C,0,-1.130922087,-0.781441314
,-0.014472178\H,0,-1.0221380453,-0.5206881325,-1.0727903945\H,0,-0.969
095432,-1.8620479748,0.0489992634\C,0,0.502752098,-0.9805989183,1.8565
991\H,0,-0.363246967,-1.484172334,2.3020134388\H,0,0.9124728809,-0.331
9035072,2.6351189802\C,0,-2.5346126568,-0.4299561822,0.5096363475\H,0,
-2.6033658143,-0.7081583318,1.5709776695\H,0,-2.6889266115,0.657906944
1,0.4649826753\C,0,1.5377394735,-2.0280365465,1.4032008638\H,0,1.08939
60458,-2.6712097555,0.632132209\H,0,1.7208036575,-2.6794193356,2.26948
30341\C,0,2.8735684765,-1.4635293911,0.8928085986\H,0,3.3502104772,-0.
8696125853,1.6887662087\H,0,2.6957763331,-0.7780884173,0.0496944814\C,
0,-3.6357328764,-1.1484845385,-0.2906445959\H,0,-3.5509159452,-0.87896
46091,-1.355081709\H,0,-3.4756364702,-2.235914231,-0.2352400741\C,0,3.
8447007411,-2.5693188977,0.4426157893\H,0,4.0198400702,-3.2598074812,1
.2814856185\H,0,3.3696586286,-3.1649323529,-0.3520055616\C,0,-5.052832
0948,-0.8155515708,0.2068349808\H,0,-5.2119122191,0.2726557044,0.15171
24642\H,0,-5.1373881496,-1.0856468619,1.270562922\C,0,-6.1536335579,-1
.5333792956,-0.5921375319\H,0,-5.992101611,-2.621058202,-0.5364035986\

H,0,-6.0648363054,-1.2641611276,-1.6563127728\C,0,5.192058053,-2.02656
30204,-0.0621210429\H,0,5.6726859589,-1.4429354879,0.7386193613\H,0,5.
0145070261,-1.3237164514,-0.8917657822\C,0,-7.5729783589,-1.2038613323
,-0.1011350432\H,0,-7.7343650231,-0.1156574333,-0.1556812884\H,0,-7.66
2536826,-1.4738856905,0.9627496181\C,0,6.151716188,-3.1325973147,-0.53
13524782\H,0,6.3263568986,-3.8376199109,0.2962323362\H,0,5.6713440359,
-3.7145976306,-1.3333527365\C,0,-8.6737607901,-1.9203842972,-0.9011028
728\H,0,-8.5833309936,-1.6499159812,-1.9639092584\H,0,-8.511864587,-3.
0073093787,-0.8463986102\C,0,-10.0883274614,-1.5872431913,-0.405955093
7\H,0,-10.2914603902,-0.5107941923,-0.4805937991\H,0,-10.8492693346,-2
.1121959574,-0.9956225081\H,0,-10.2195755034,-1.8787402673,0.644361469
8\C,0,7.5023079366,-2.5951310995,-1.0334157661\H,0,7.9855886015,-2.020
9413959,-0.2287308542\H,0,7.3269557891,-1.8845766803,-1.8554768862\C,0
,8.4486886675,-3.7060129571,-1.510453292\H,0,9.4019044437,-3.292638467
1,-1.8609505154\H,0,8.6689607574,-4.4137700265,-0.7006548297\H,0,8.005
9340458,-4.2748786786,-2.3384919583\C,0,1.6936085333,5.1294422101,-0.2
753262998\O,0,2.6089326892,5.5158739787,0.3981227409\C,0,0.9949053109,
5.9355711359,-1.3416483871\H,0,-0.0703508854,6.0656291503,-1.115062284
8\H,0,1.4736675693,6.9159083606,-1.3705131751\H,0,1.0882896944,5.46440
49954,-2.3277711107\\Version=AM64L-G03RevD.01\State=1-A\HF=-1078.55002
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