

Supplementary Information
for
**The aza-Morita-Baylis-Hillman Reaction of Electronically
and Sterically Deactivated Substrates**

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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. CDCl₃ was refluxed for at least one hour over CaH₂ and subsequently distilled. ¹H and ¹³C 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); ¹³C chemical shifts are reported in ppm (δ) relative to CDCl₃ (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. All kinetic measurements with reaction times longer than 24 h were mechanically shaken; for each reaction the rotation speed was set at 480 turns/minute. Analytical TLC were carried out using aluminium sheets silica gel Si 60 F254.

1. Conduction and evaluation of kinetic measurements

1.1 Experimental procedures for the kinetic measurements

General procedure of benchmark reactions of MVK **2a** with 10 % / 5 % catalyst:

0.5 mL from 5.0 mL of stock solution I (**1a** (220 mg, 0.75 mmol), MVK **2a** (63 mg, 0.90 mmol) and trimethoxybenzene (27 mg)) and 0.1 mL from 2 mL of stock solution II (0.15 mmol / 0.075 mmol of catalyst) were mixed in a NMR-tube and sealed.

General procedure of benchmark reactions of **2b** and **2c** with 25% catalyst:

0.5 mL from 5.0 mL of stock solution I (**1a** (441 mg, 1.50 mmol), **2b** / **2c** (6.0 mmol) and trimethoxybenzene (67.2 mg)) and 0.1 mL from 2 mL of stock solution II (0.375 mmol of catalyst) were mixed in a NMR-tube and flame-sealed.

General procedure of benchmark reactions of **2d** with 25 % catalyst:

0.5 mL from 5.0 mL of stock solution I (**1a** (220 mg, 0.75 mmol), **2d** (252 mg, 3.0 mmol) and trimethoxybenzene (67.2 mg)) and 0.1 mL from 2 mL of stock solution II (0.1875 mmol of catalyst) were mixed in a NMR-tube and flame-sealed.

1.2 Details of the kinetic evaluation

Different models based on possible mechanisms were tested for the simulation in Copasi 4.7¹⁵ and the one with the least RMS deviation respectively best statistical spread was chosen. Following models were tested based on a selected number of catalysts and concentrations. The root mean square deviations were listed in Table S1. For equilibrium reactions '=' and for non reversible reactions '-->' was used. Model A and B were derived from Guy Lloyd Jones.¹¹

A)

MVK + Cat = Intermediate

Intermediate + Imine --> Product + Cat

Intermediate + Imine + Product --> 2 Product

B)

MVK + Cat + Imine = Intermediate

Intermediate --> Product + Cat

Intermediate + Product --> 2 Product

C)

MVK + Catalyst + Imine = Intermediate

Intermediate --> Product + Cat

Cat + Intermediate --> Product + 2 Cat

D)

MVK + Cat = Intermediate

Intermediate + Imine --> Product + Cat

Intermediate + Product = Intermediate+H⁺ + P-H⁺

E)

MVK + Cat = Intermediate

Intermediate + Imine = Intermediate2

Intermediate2 --> Product + Cat

F)

MVK + Cat = Intermediate

Intermediate + Imine --> Product + Cat

Table S1 Root mean square deviations of the tested models for simulation using different catalysts with varying concentration.

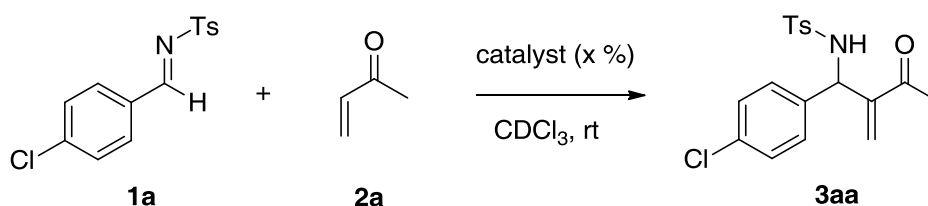
	A	B	C	D	E	F
4k 10%	0.001112	0.001110	0.001253	0.001040	0.001153	0.000925
4k 5%	0.000781	0.000812	0.001076	0.000946	0.000775	0.000775
4d 10%	0.001650	0.001654	0.000980	0.000641	0.001480	0.001480
4f 10%	0.001409	0.001408	0.000921	0.000499	0.001511	0.001510
5a 10%	0.000455	0.000507	0.001076	0.000455	0.000468	0.000455
5a 5%	0.000564	0.000724	0.001037	0.000566	0.000567	0.000581
5a 2.5%	0.001009	0.001262	0.001333	0.000769	0.001157	0.000933
5f 10%	0.001429	0.001789	0.002065	0.001389	0.001440	0.001880
5f 5%	0.001003	0.001199	0.001660	0.000832	0.001025	0.001012
5f 2.5%	0.001306	0.001373	0.001277	0.000933	0.001380	0.001368
average	1.07E-03	1.18E-03	1.27E-03	8.07E-04	1.10E-03	1.09E-03

According to Table S1 model D was used due to the least averaged root mean square deviation.

2. Data of kinetic runs

The used data was normalized. All time specifications are in minutes if not stated different. For every measurement the experimental data and the simulated curve together with the deviations are depicted. The resulting halflife times correspond to 50% conversion and are given with standard deviations if more than one measurement was done.

2.1 Kinetic data for reactions of tosylimine (**1a**) and MVK (**2a**).



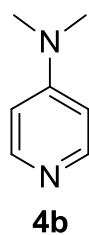
2.1.1 25 mol% catalyst

The following kinetic runs were performed with $c(\text{imine}) = 0.25 \text{ M}$ and $c(\text{MVK}) = 1.00 \text{ M}$.

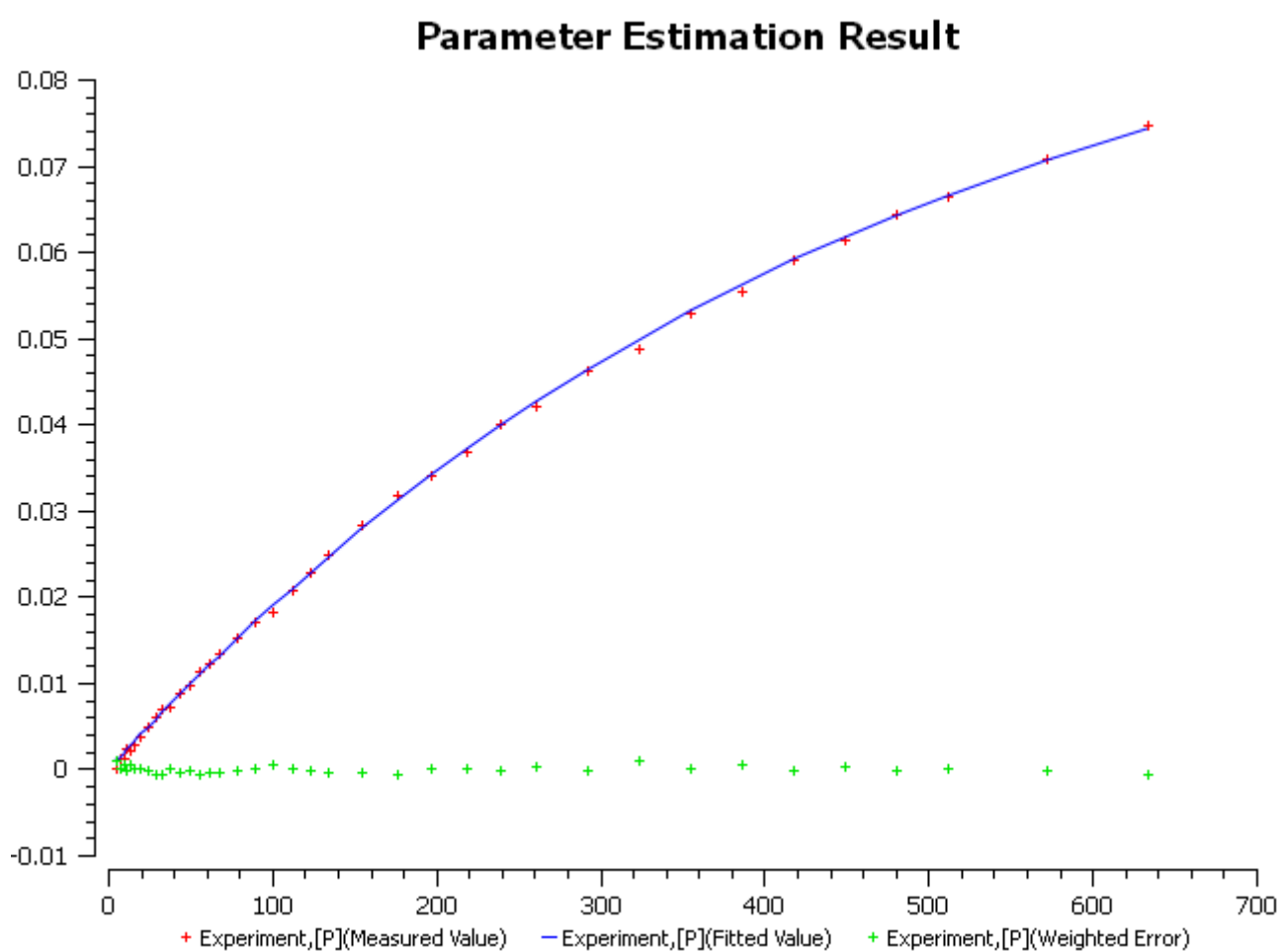
The kinetic measurement of **4k**, **5f** and **5g** are not displayed due to the short reaction times and consequential few data points.

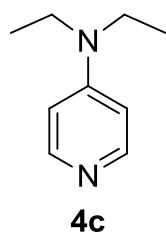
2.1.2 10 mol% catalyst

The following kinetic runs were performed with $c(\text{imine}) = 0.125 \text{ M}$ and $c(\text{MVK}) = 0.15 \text{ M}$.

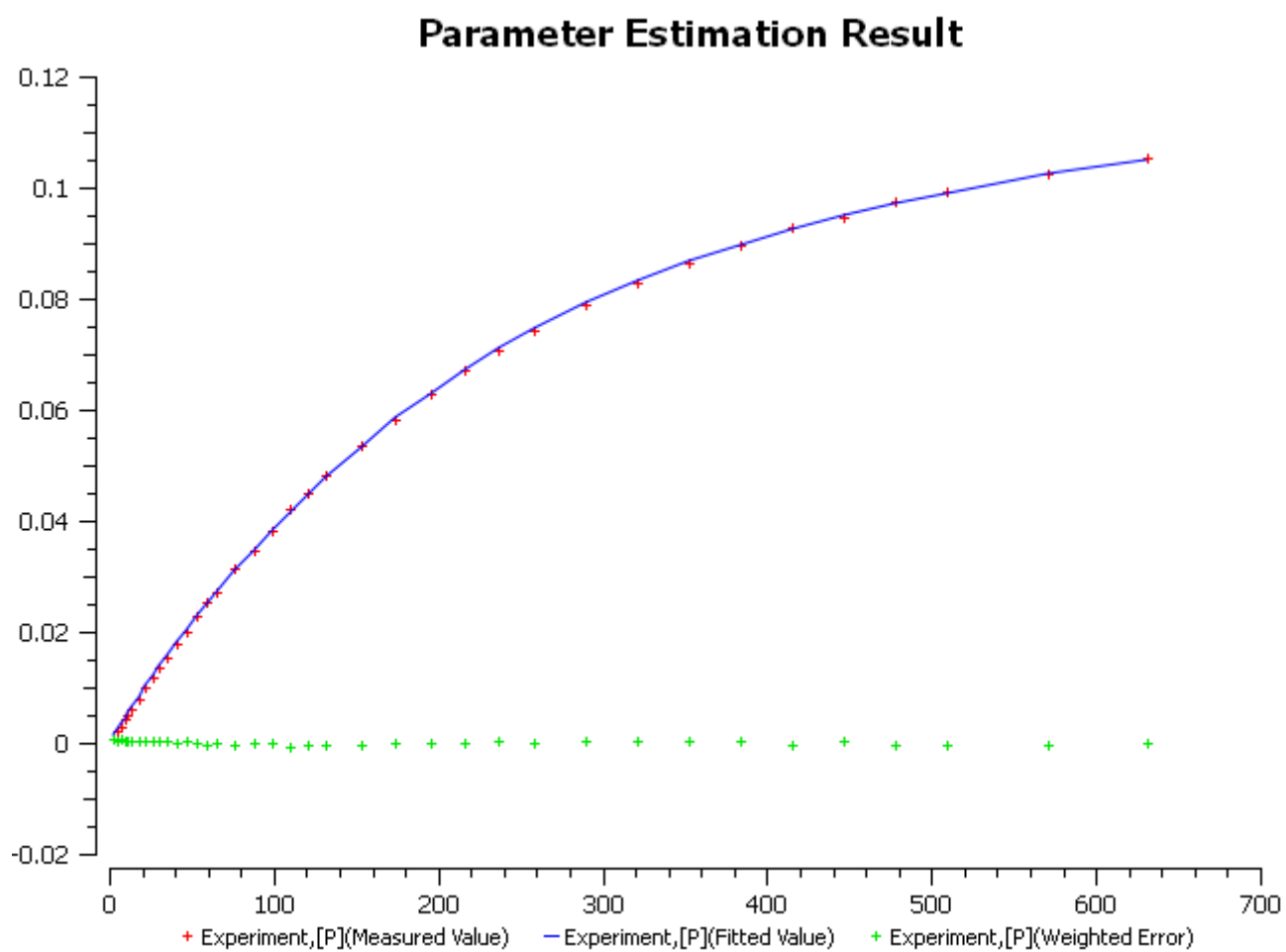


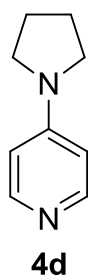
1) 458.6





1) 192.7



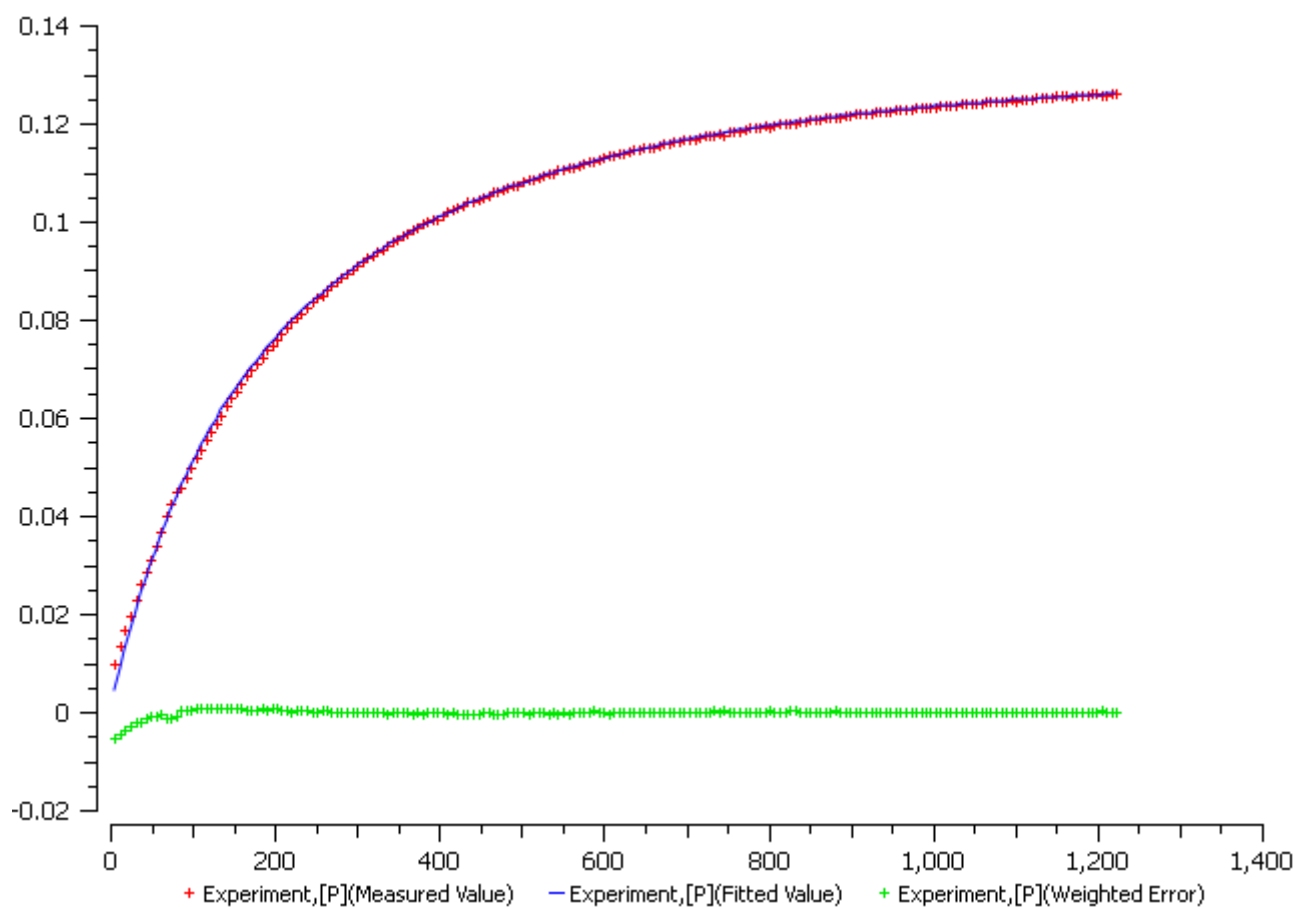


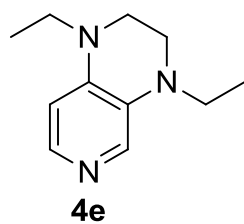
1) 138.6

2) 153.9

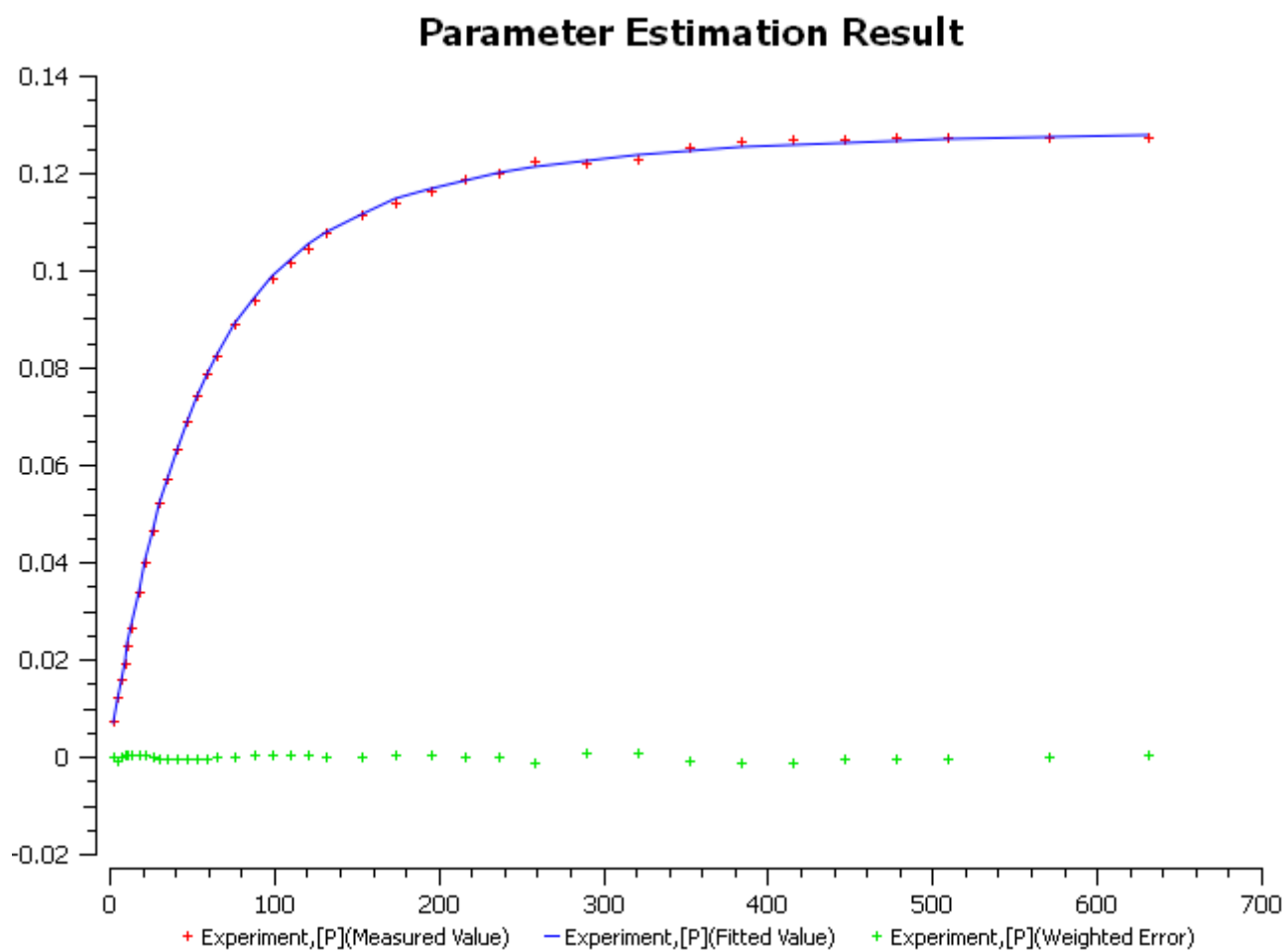
$$= 146.3 \pm 7.7$$

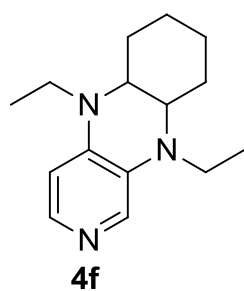
Parameter Estimation Result





1) 40.6





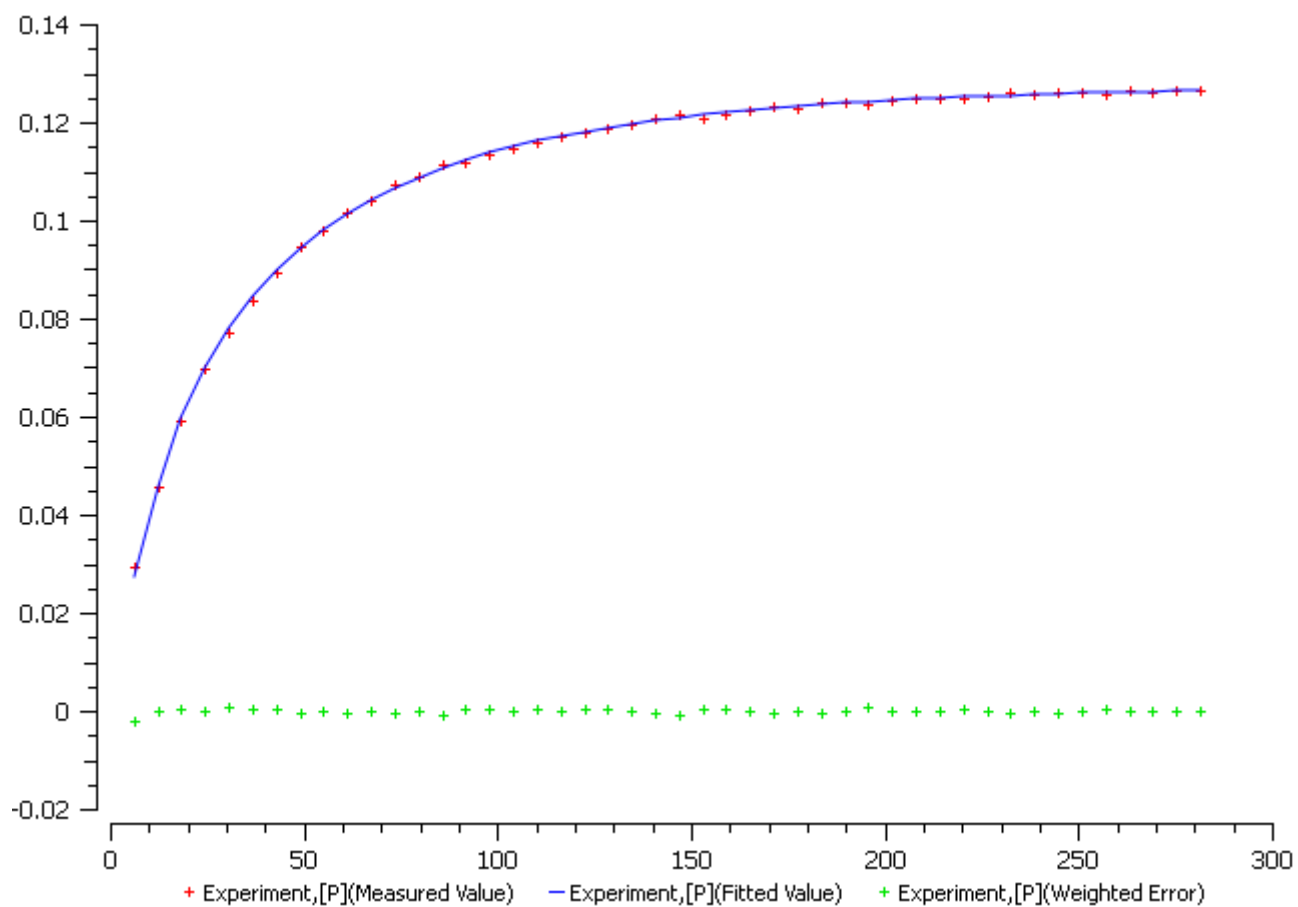
1) 20.2

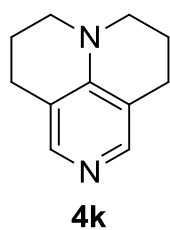
2) 22.1

3) 26.3

$$= 22.9 \pm 2.6$$

Parameter Estimation Result



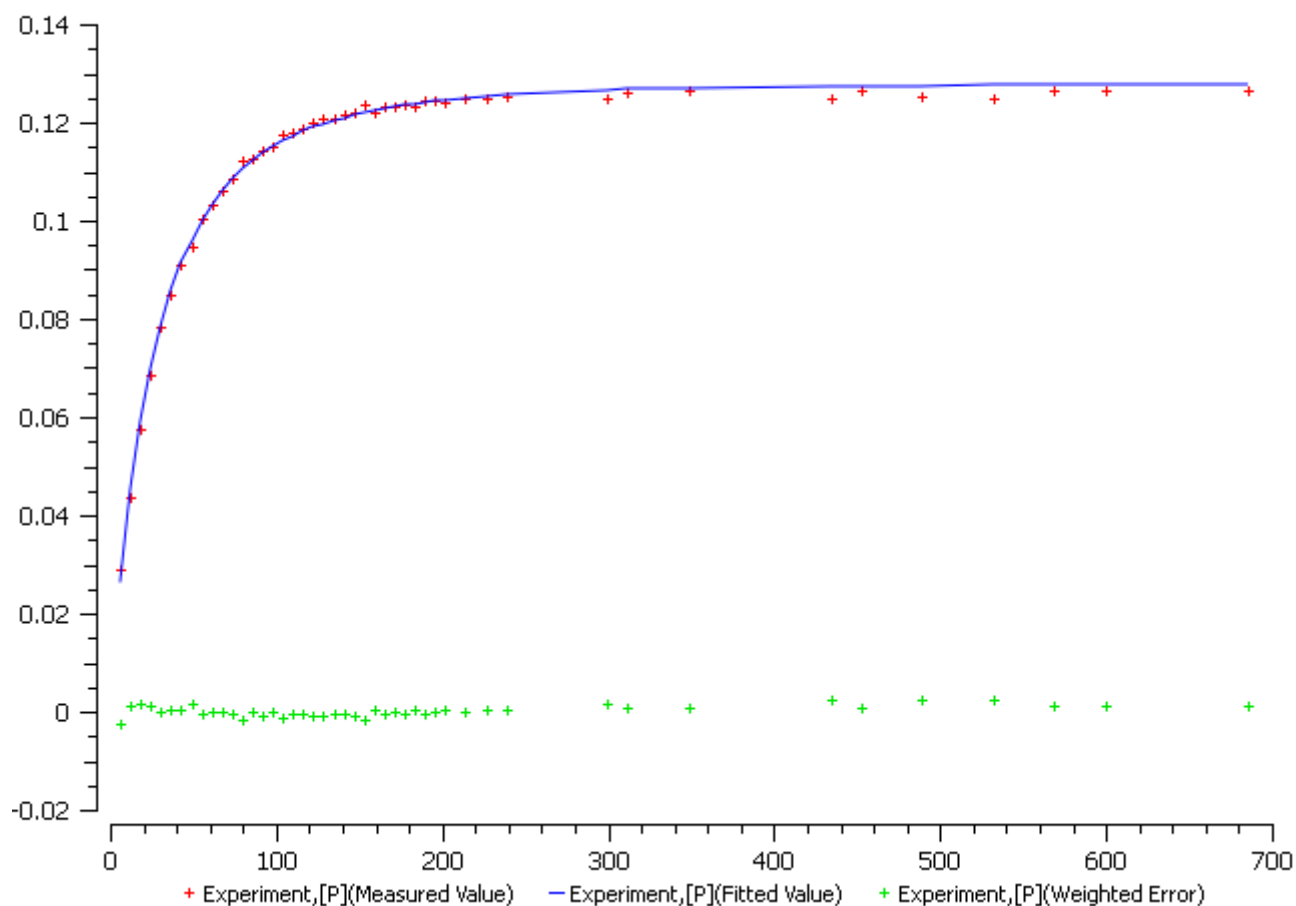


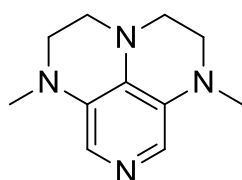
1) 20.3

2) 20.4

$$= 20.3 \pm 0.1$$

Parameter Estimation Result





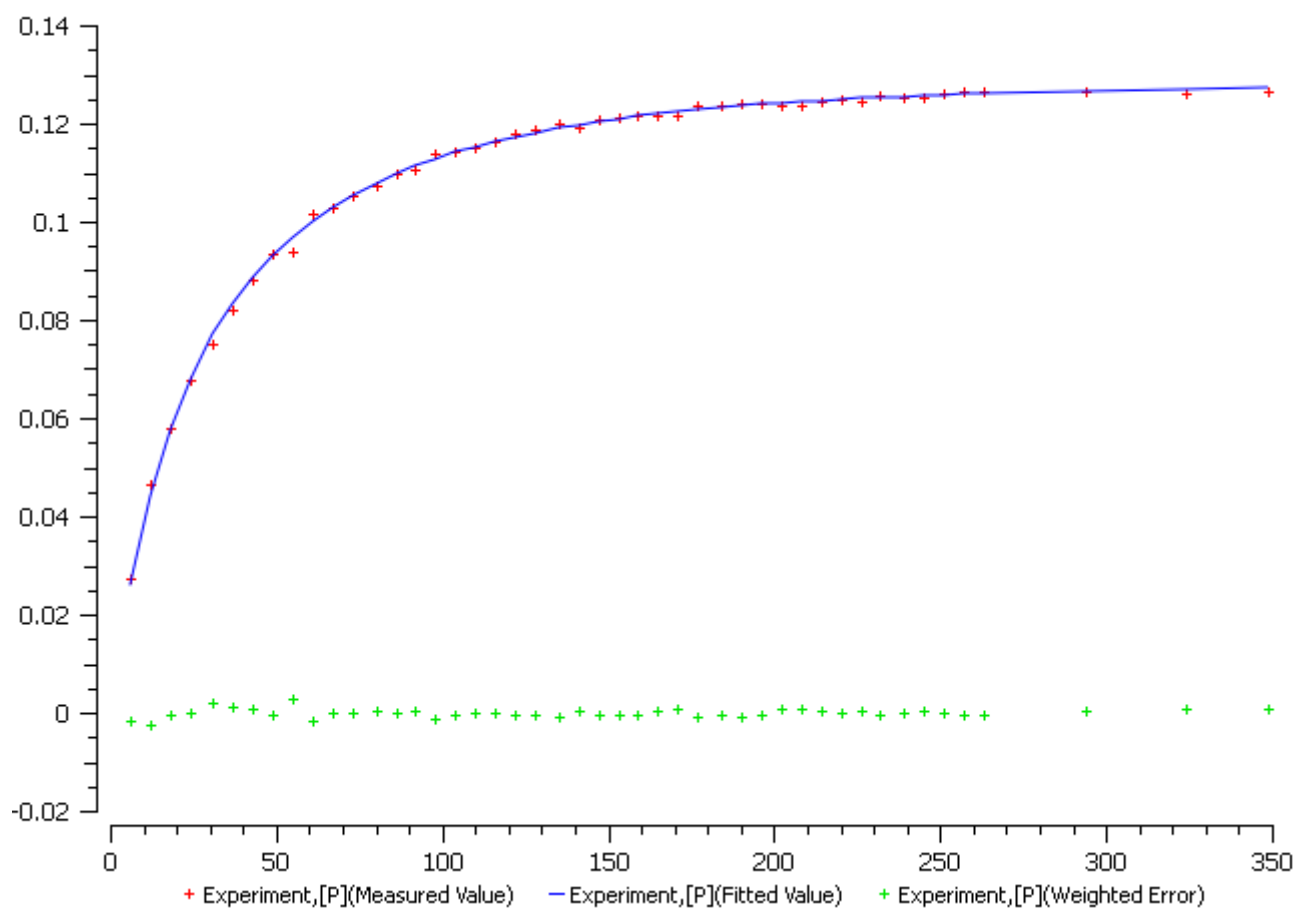
4I

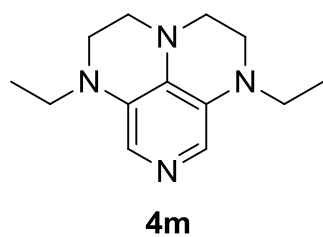
1) 21.0

2) 29.0

$$= 25.0 \pm 4.0$$

Parameter Estimation Result



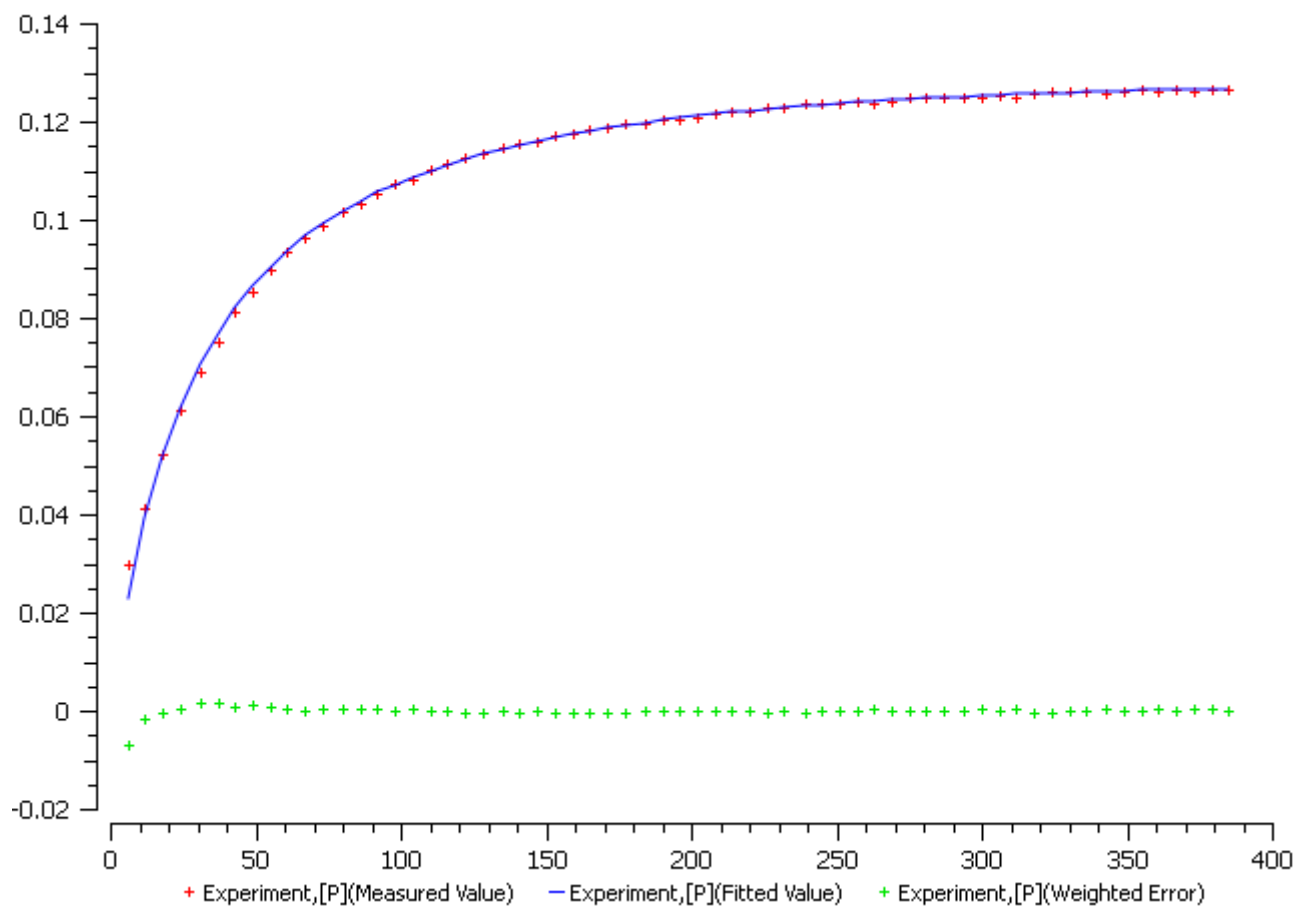


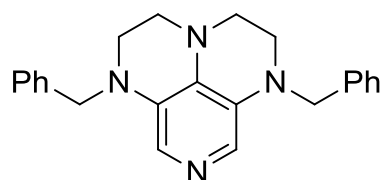
1) 24.7

2) 27.5

$$= 26.1 \pm 1.4$$

Parameter Estimation Result





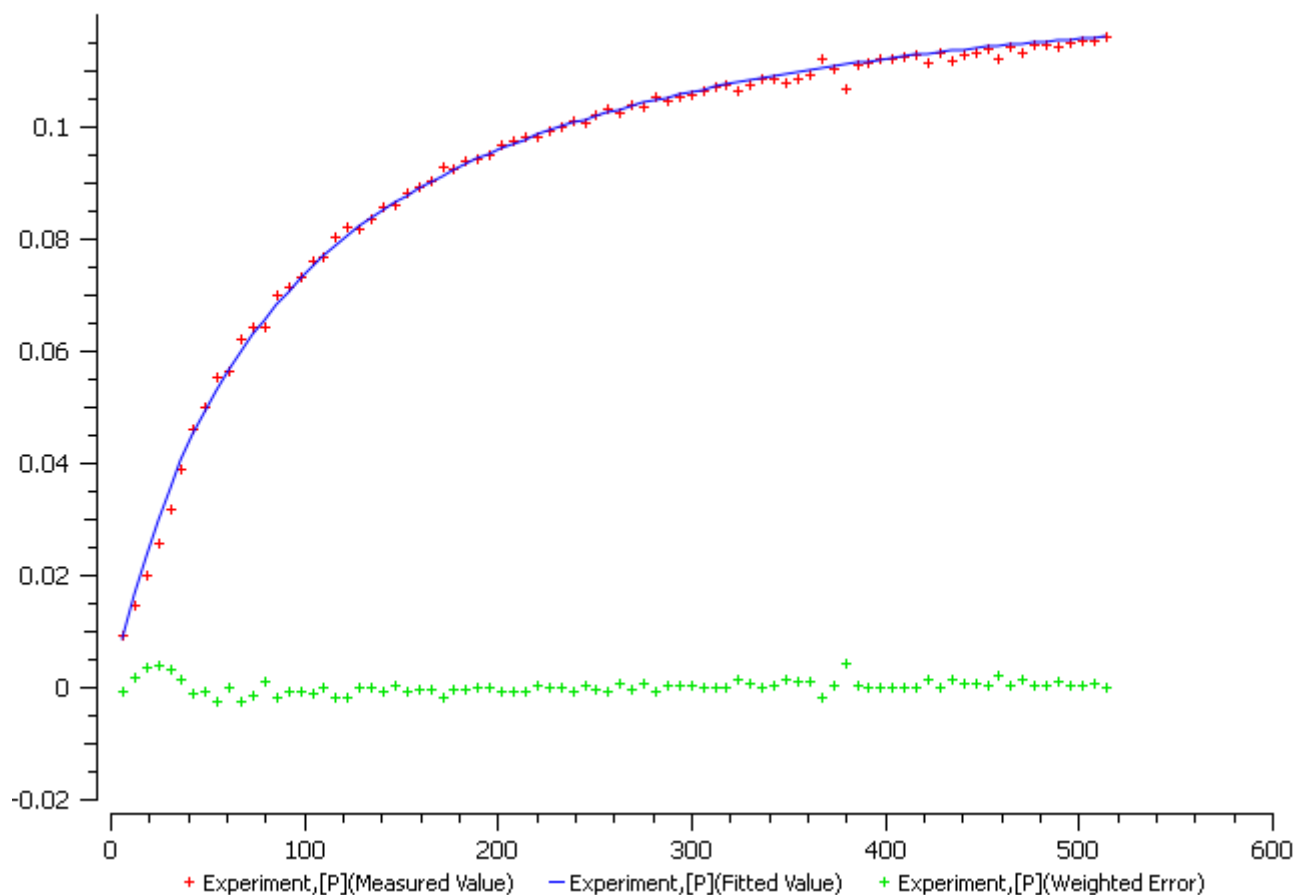
4m

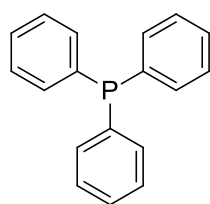
1) 72.6

2) 71.8

$= 72.2 \pm 0.4$

Parameter Estimation Result





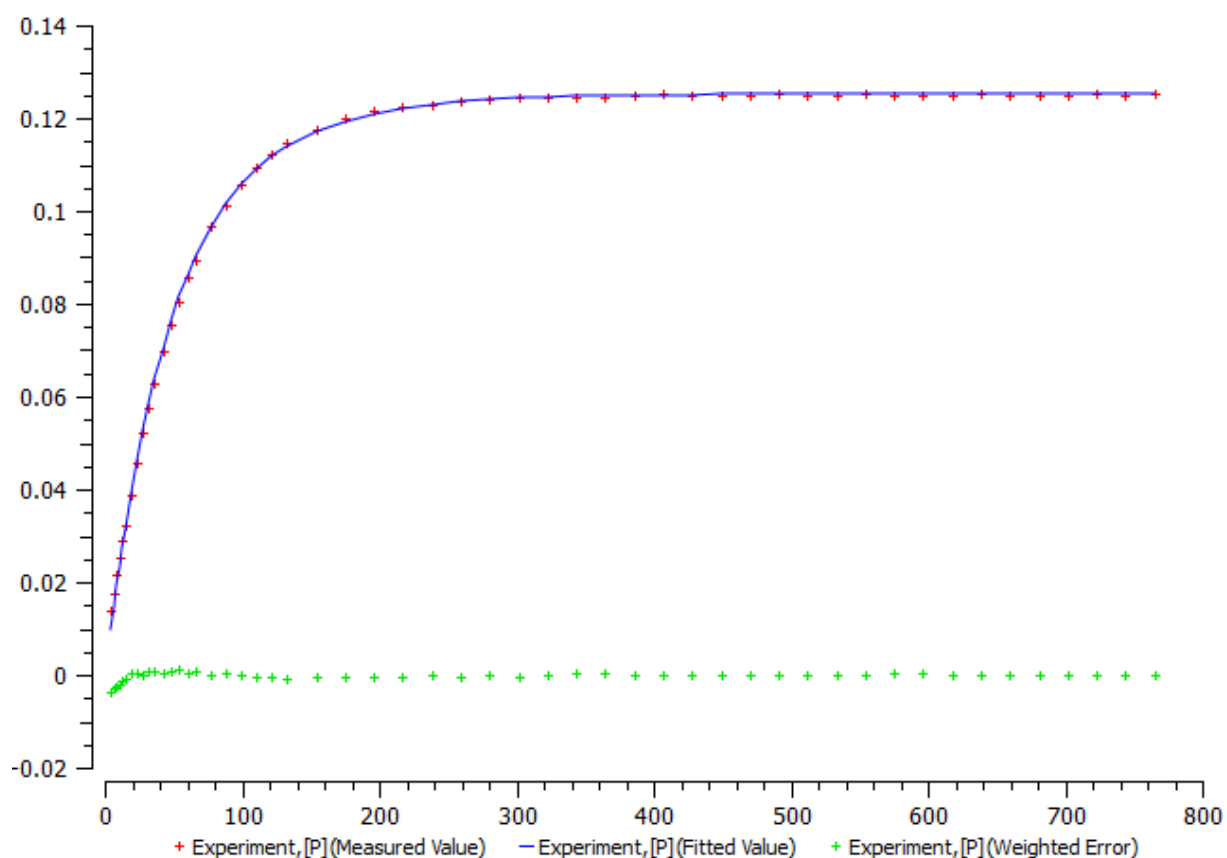
5a

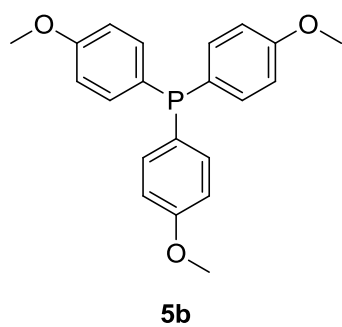
1) 35.1

2) 35.3

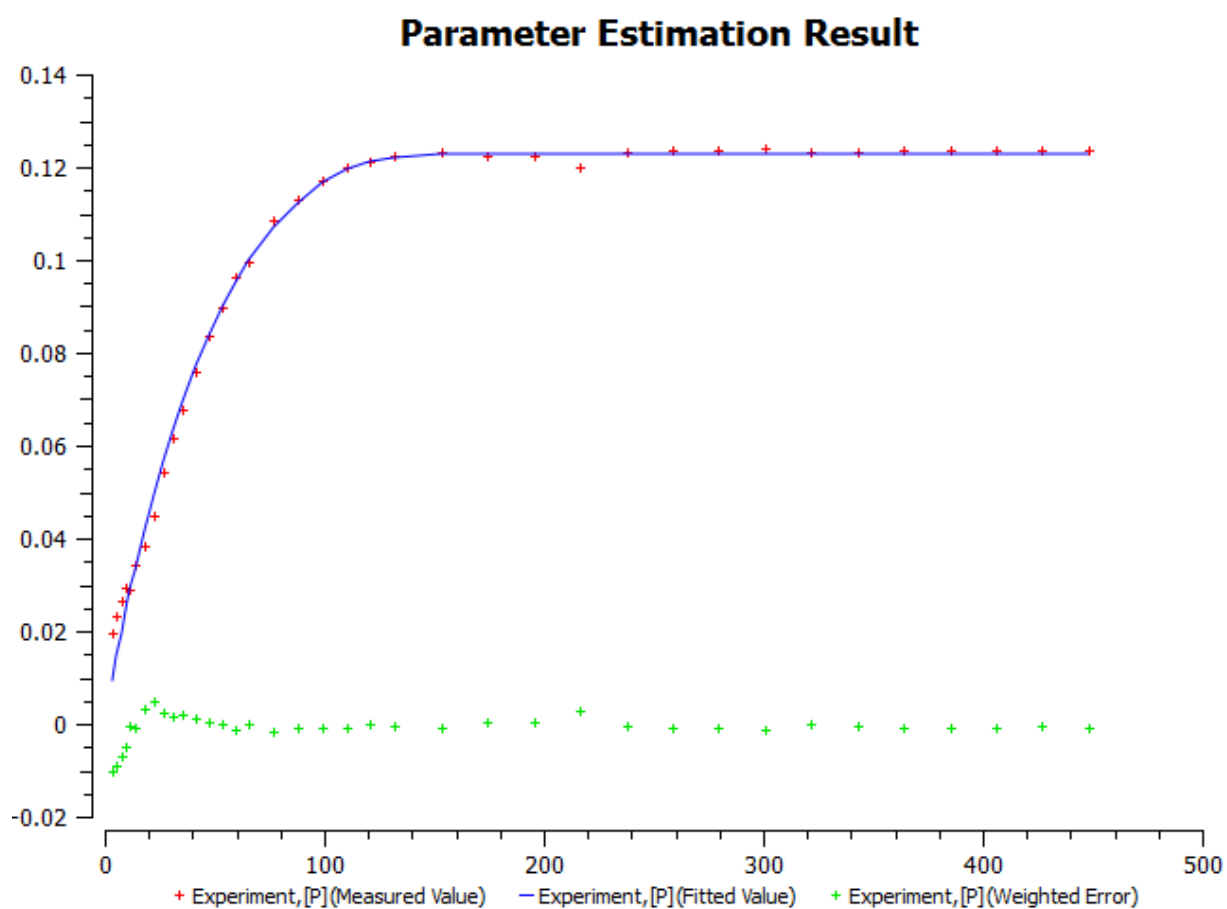
$$= 35.2 \pm 0.1$$

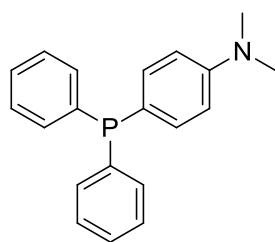
Parameter Estimation Result





$$\begin{aligned} &1) \ 30.5 \\ &2) \ 34.0 \\ &= 32.3 \pm 1.8 \end{aligned}$$





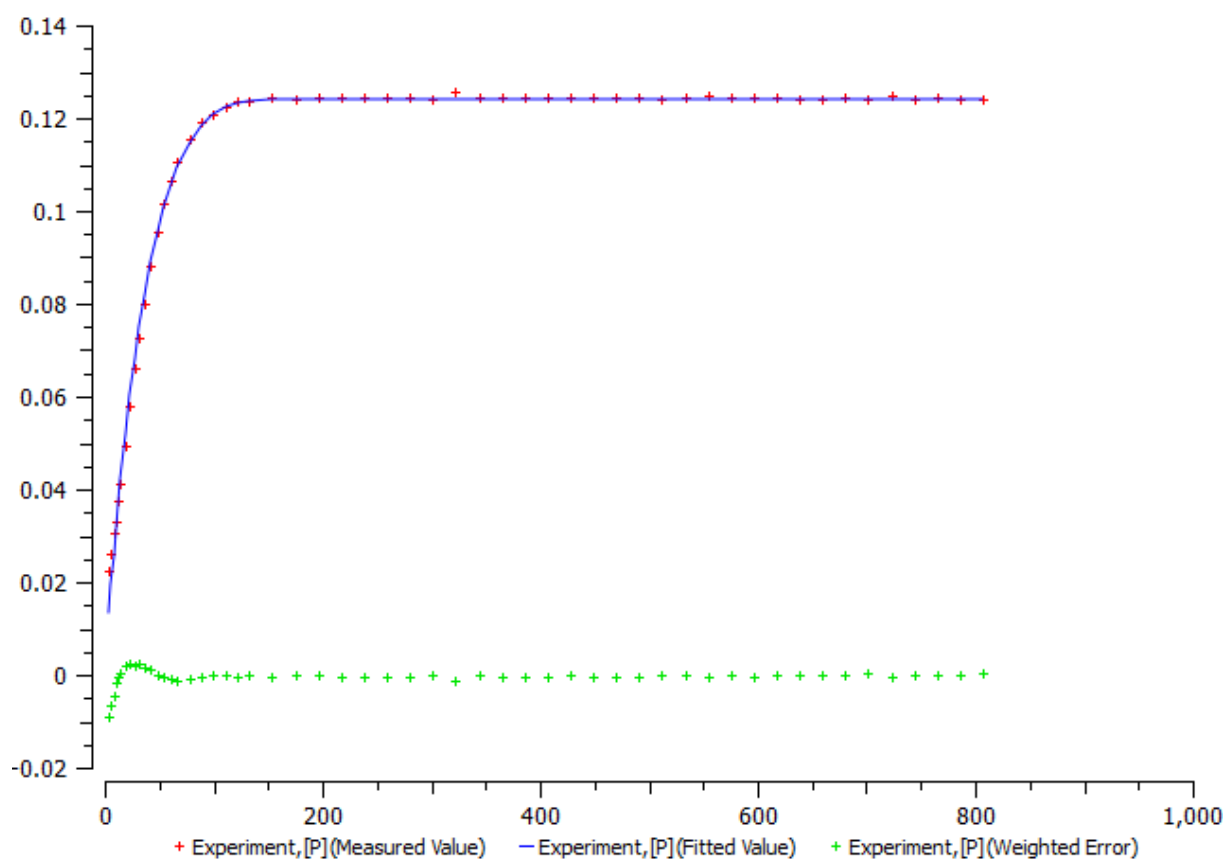
5c

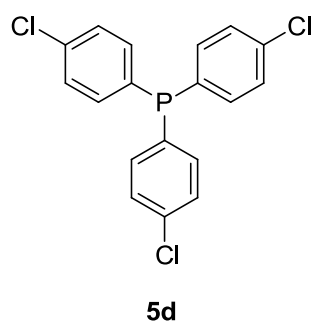
1) 24.2

2) 25.8

$$= 25.0 \pm 0.8$$

Parameter Estimation Result





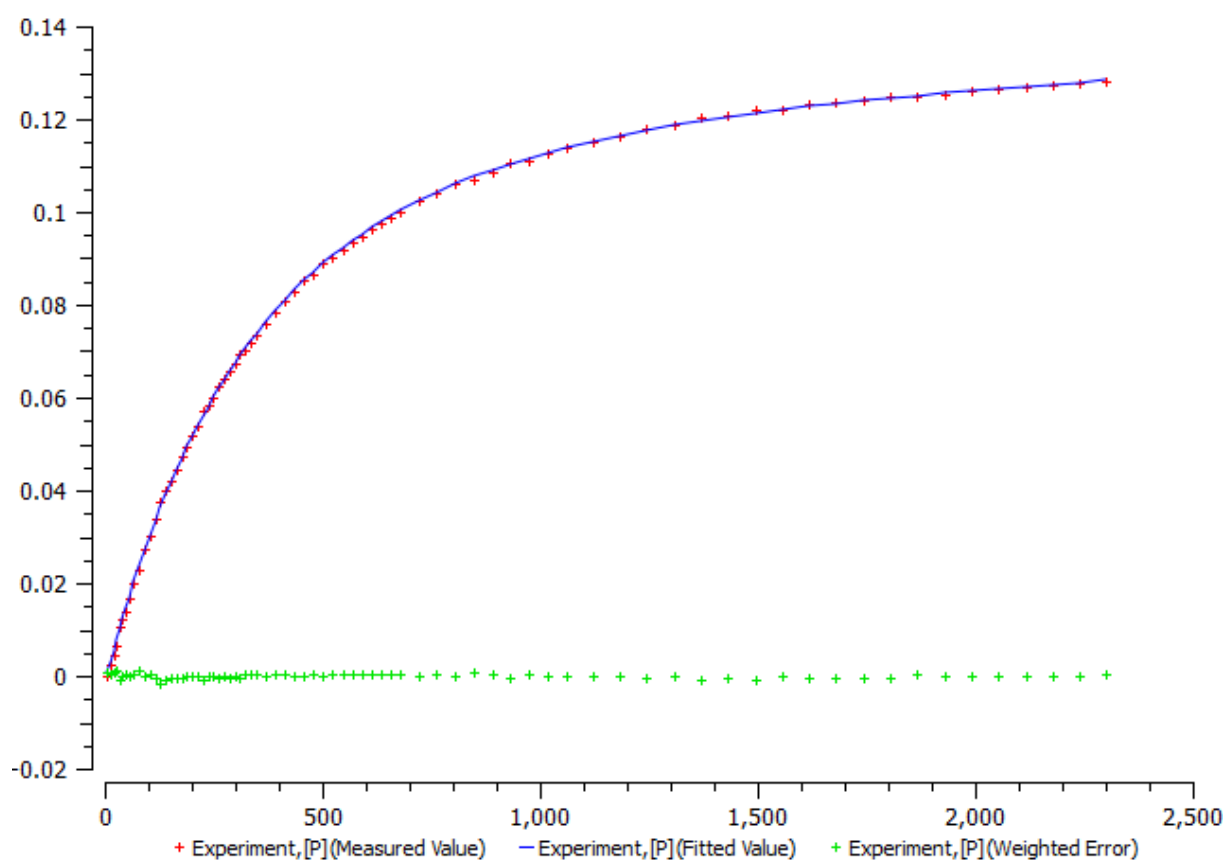
20 mol%!

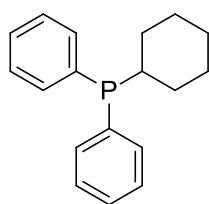
1) 276.2

2) 264.9

$= 270.6 \pm 5.7$

Parameter Estimation Result





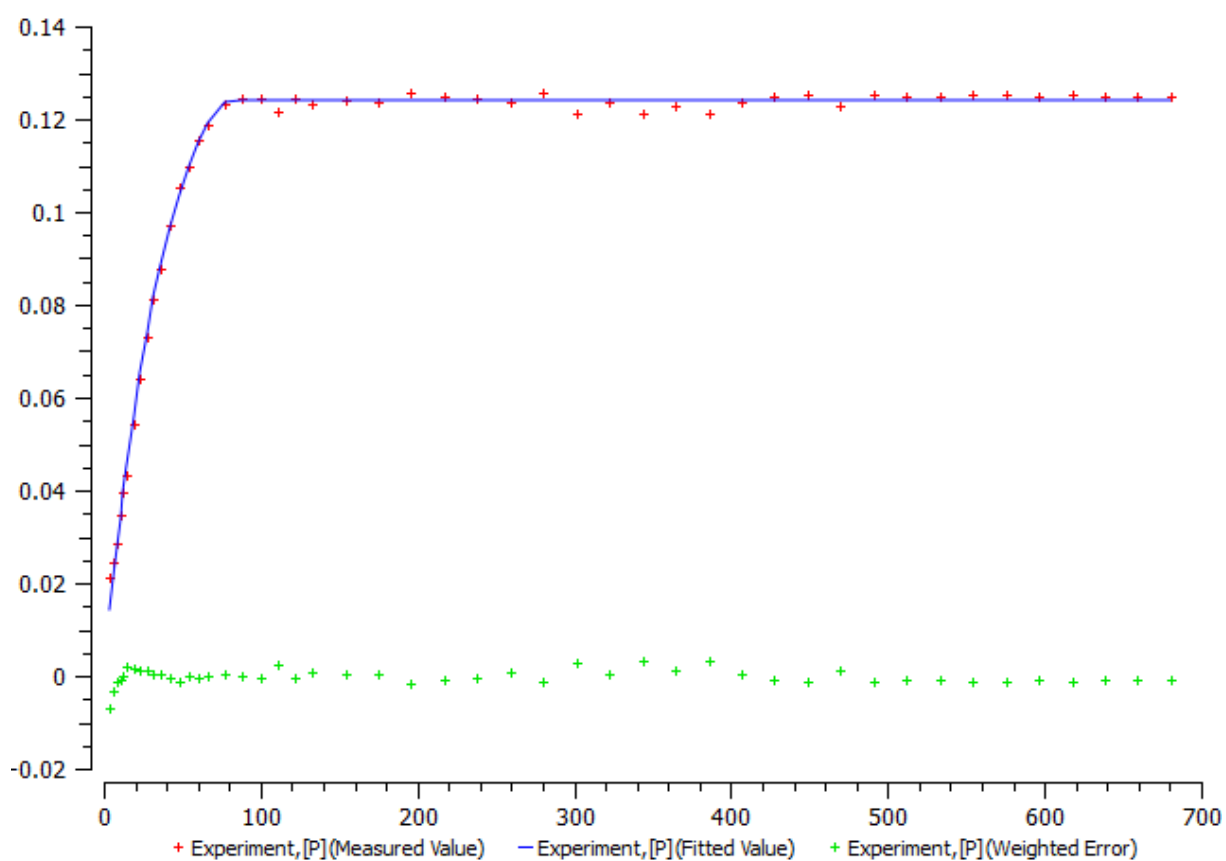
5e

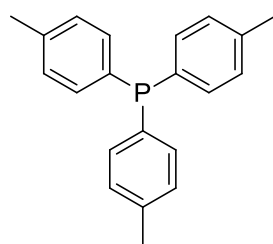
1) 22.0

2) 21.8

$$= 21.9 \pm 0.1$$

Parameter Estimation Result





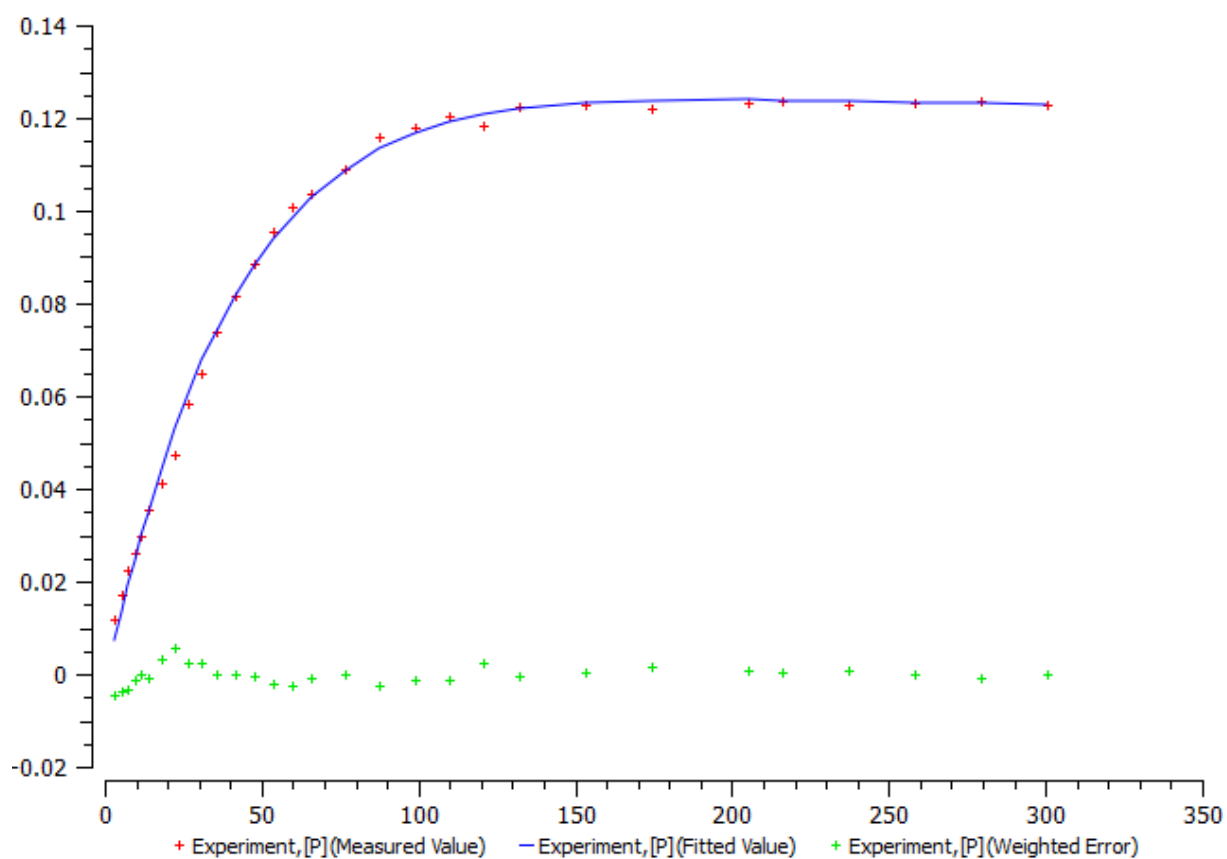
5f

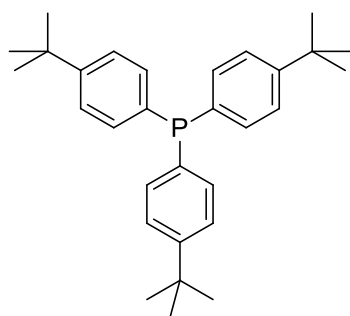
1) 27.8

2) 25.5

$$= 26.7 \pm 1.2$$

Parameter Estimation Result





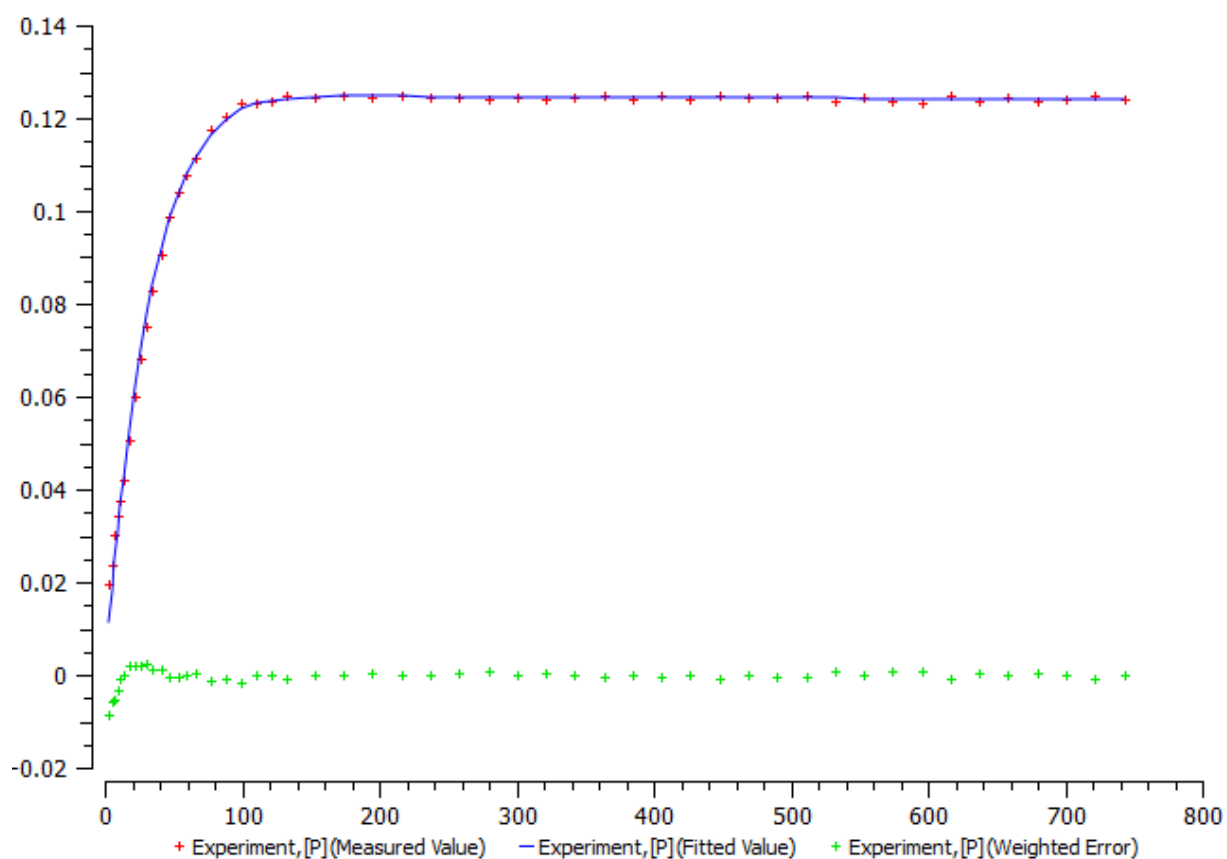
5g

1) 22.1

2) 22.4

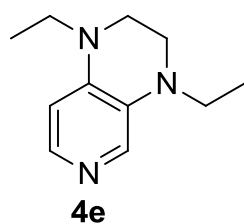
$$= 22.3 \pm 0.2$$

Parameter Estimation Result

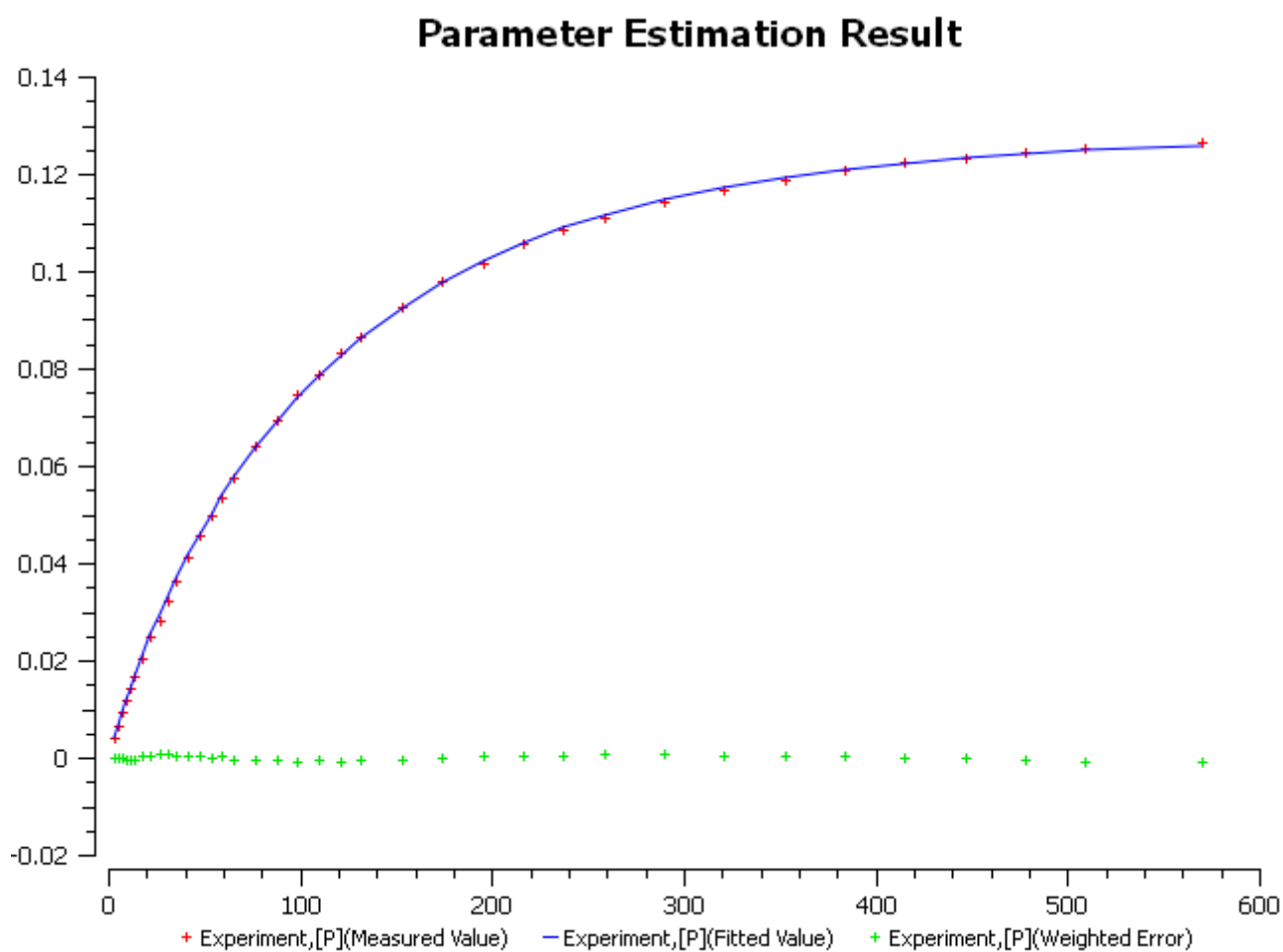


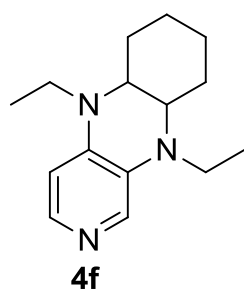
2.1.3 5 mol% catalyst

The following kinetic runs were performed with $c(\text{imine}) = 0.125 \text{ M}$ and $c(\text{MVK}) = 0.15 \text{ M}$.



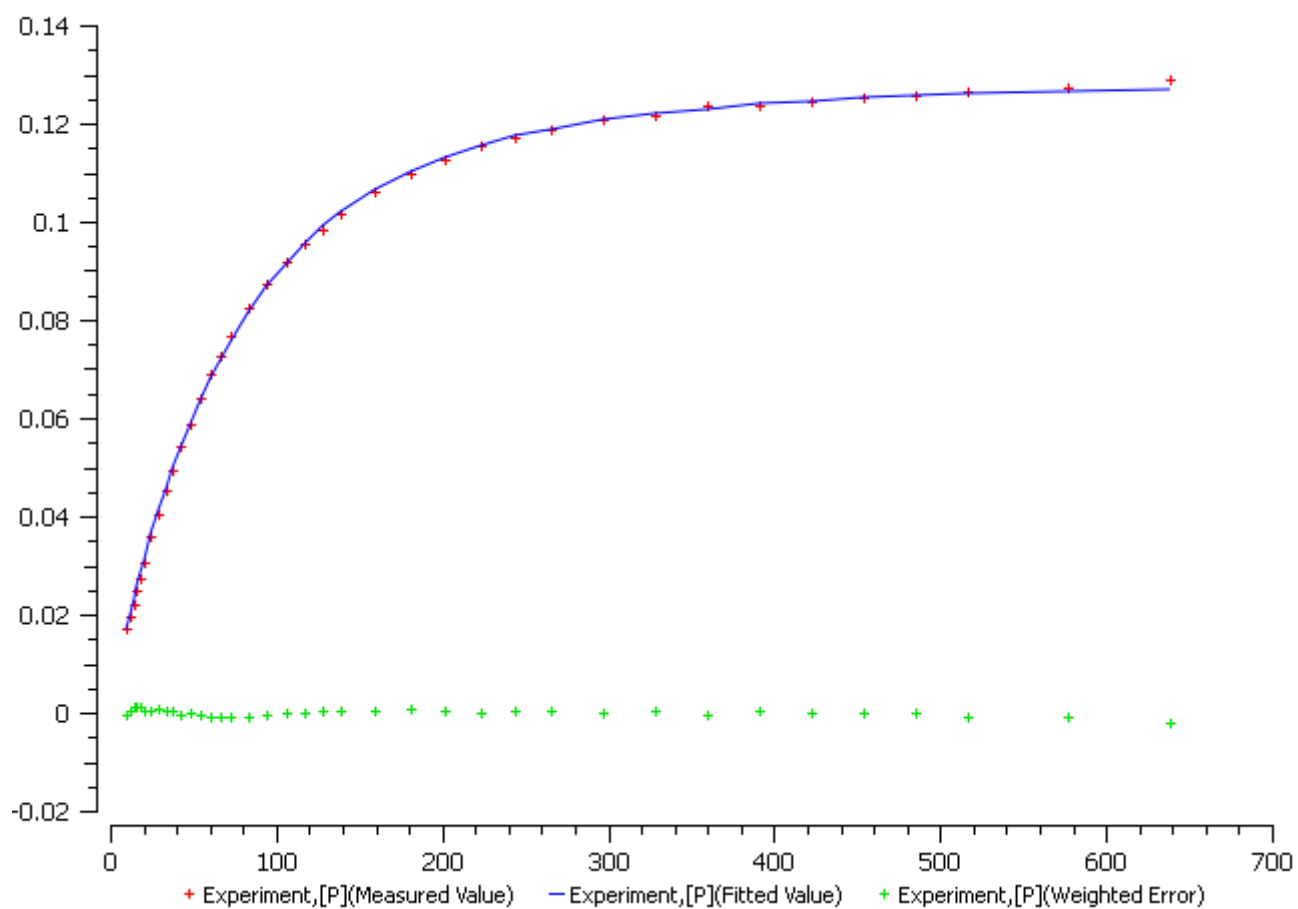
1) 74.6

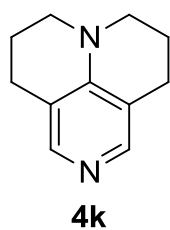




1) 52.3

Parameter Estimation Result



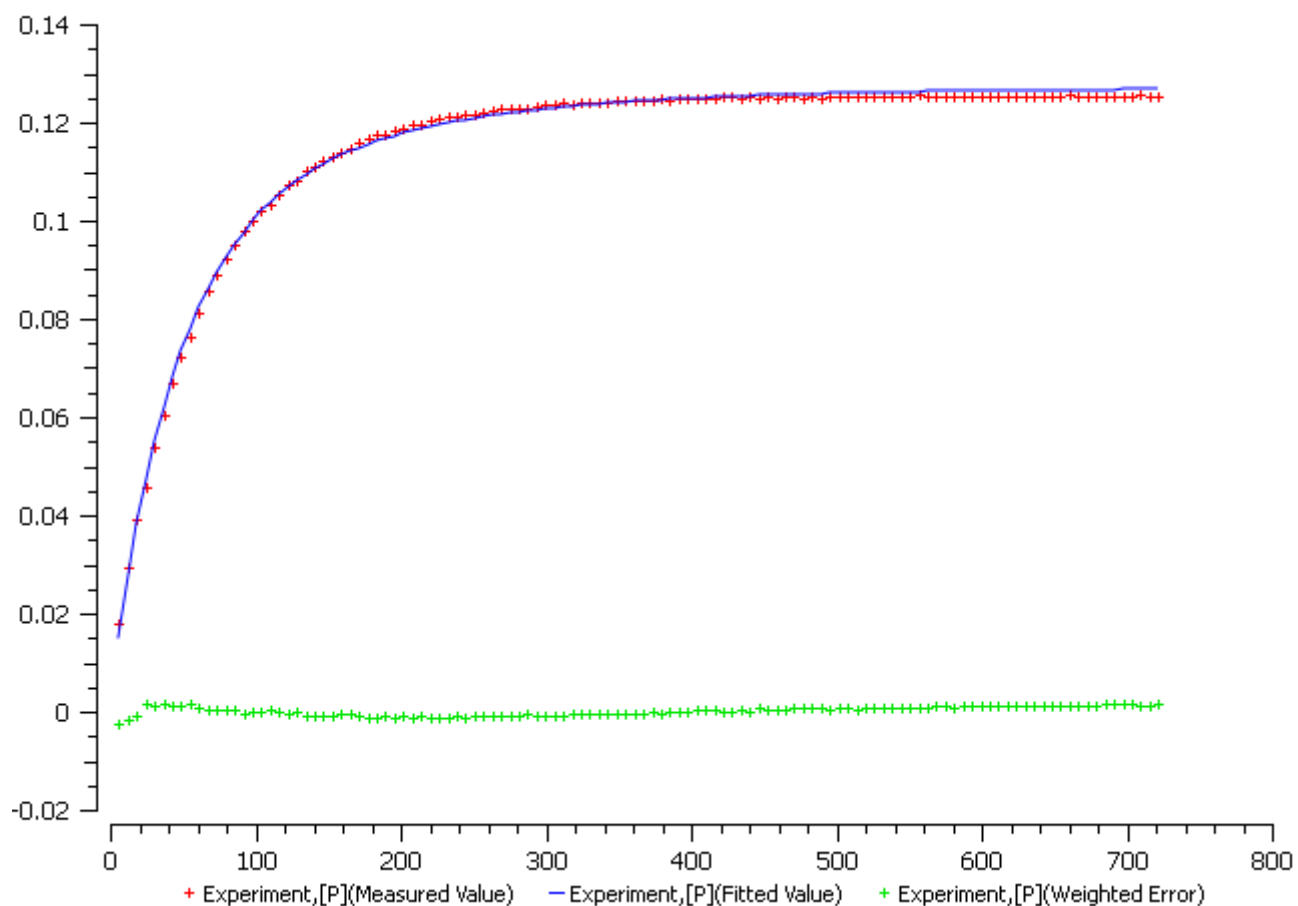


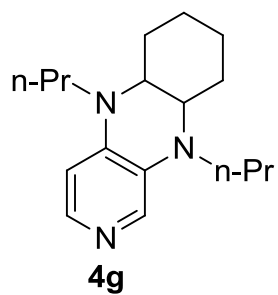
1) 37.1

2) 43.6

$$= 40.4 \pm 3.2$$

Parameter Estimation Result



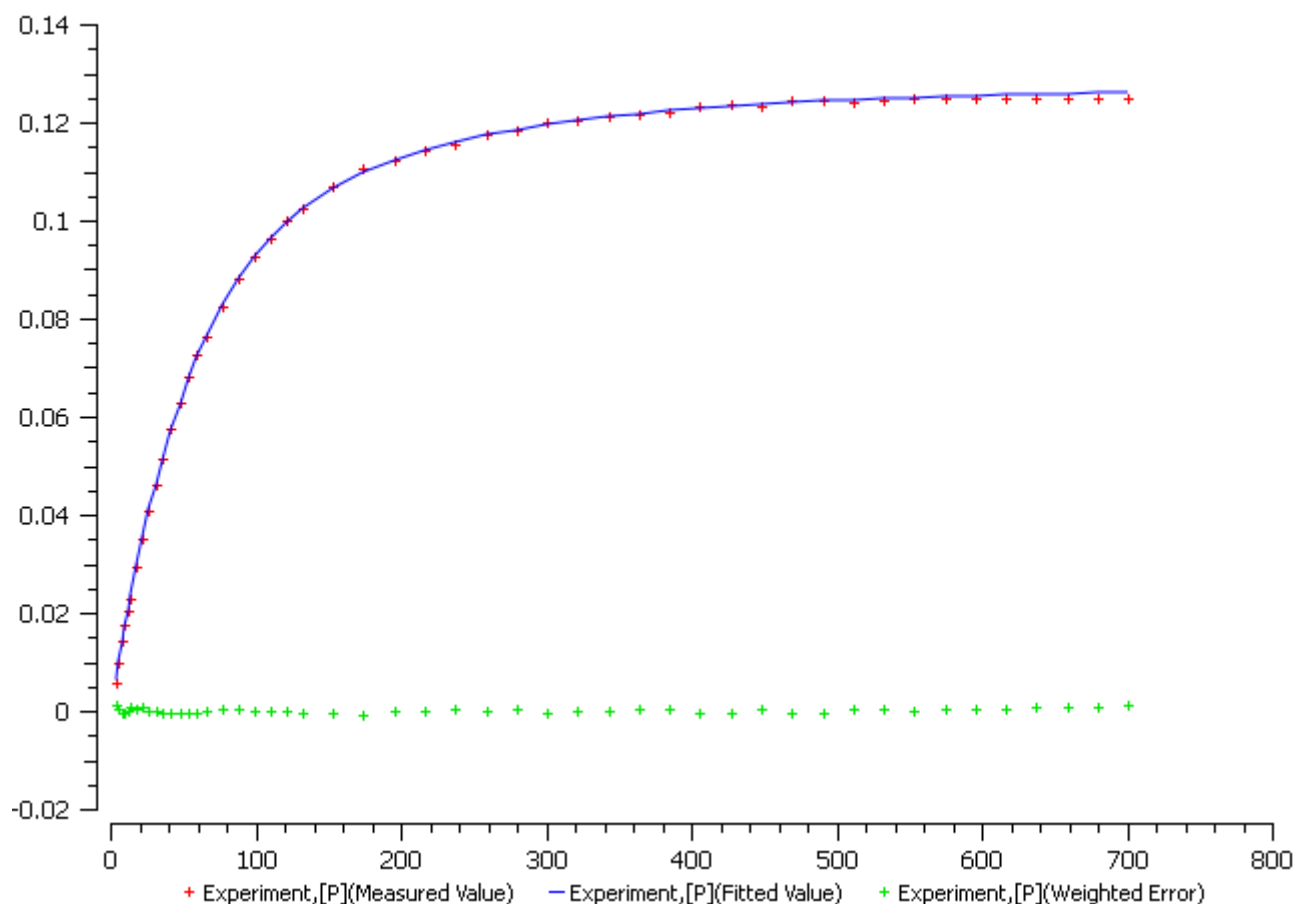


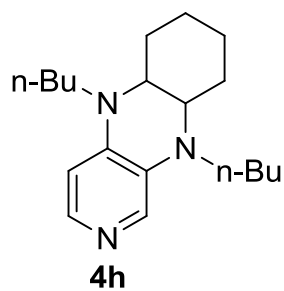
1) 47.6

2) 50.9

$= 49.2 \pm 1.7$

Parameter Estimation Result



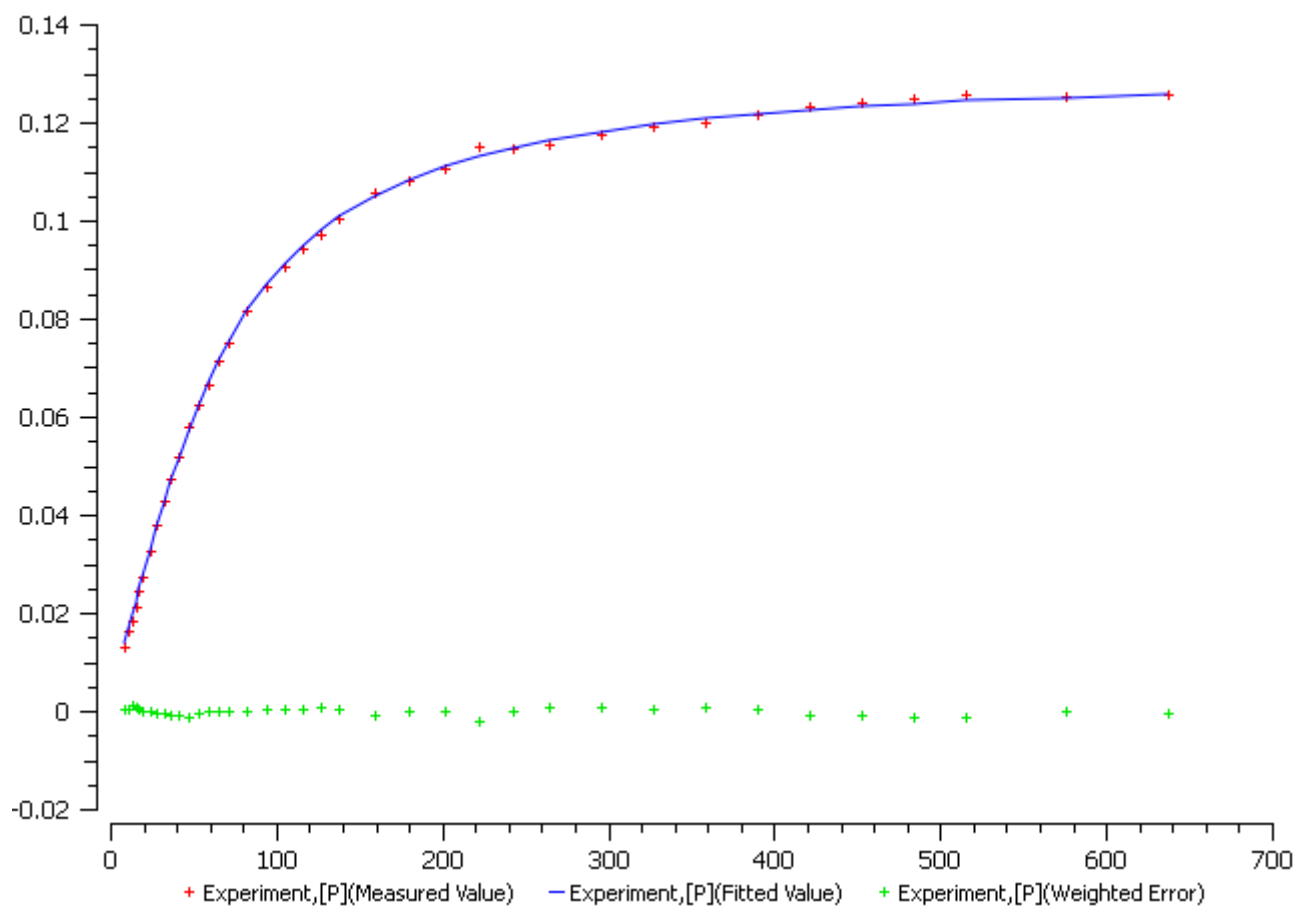


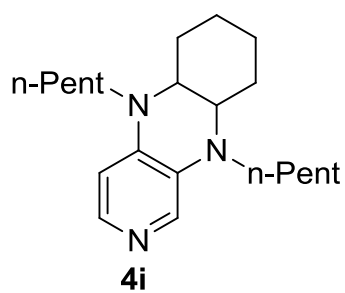
1) 53.7

2) 51.2

$$= 52.5 \pm 1.3$$

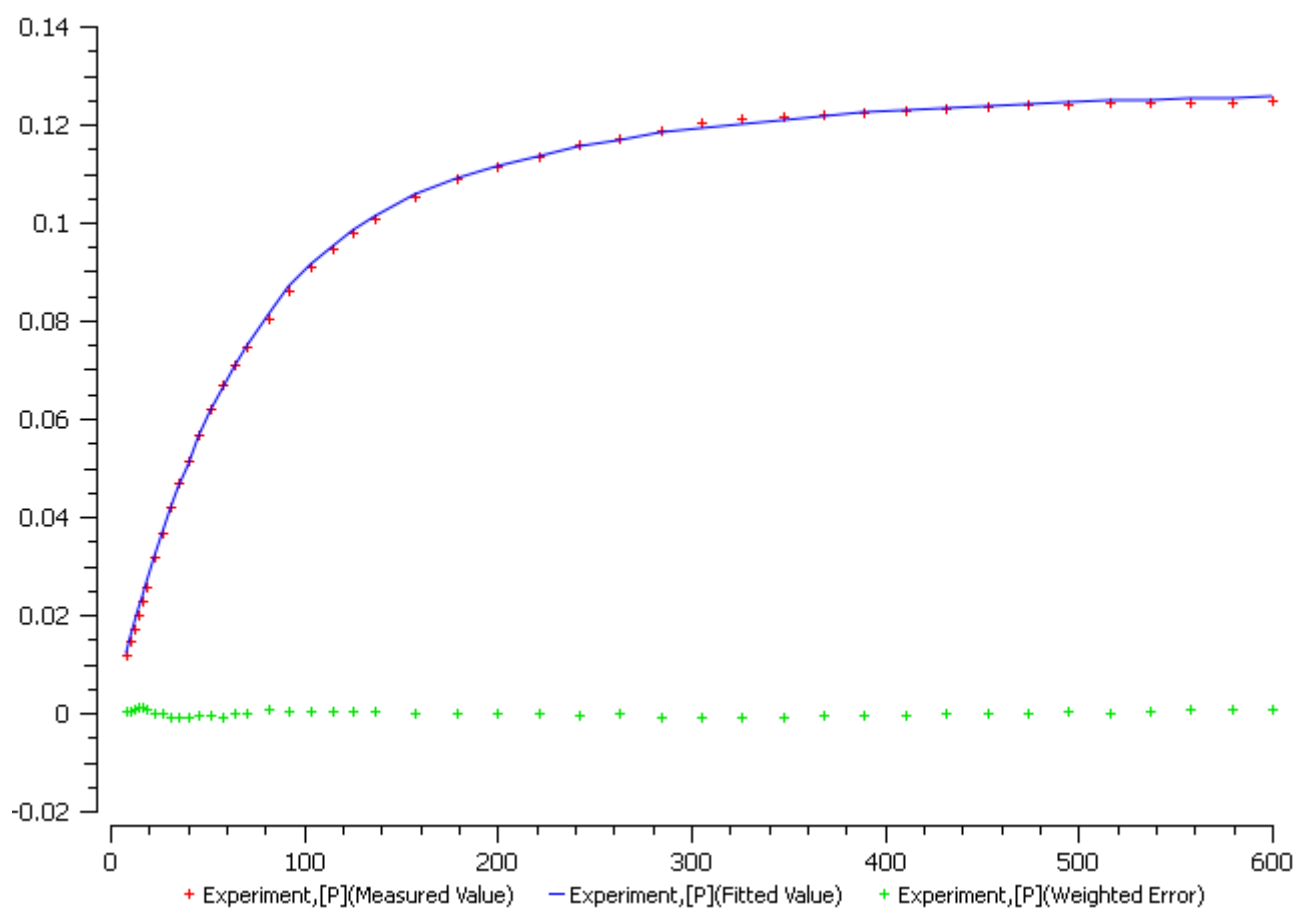
Parameter Estimation Result

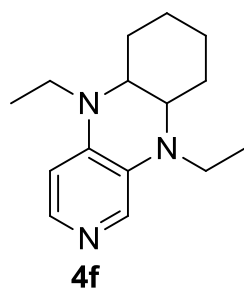




1) 53.3

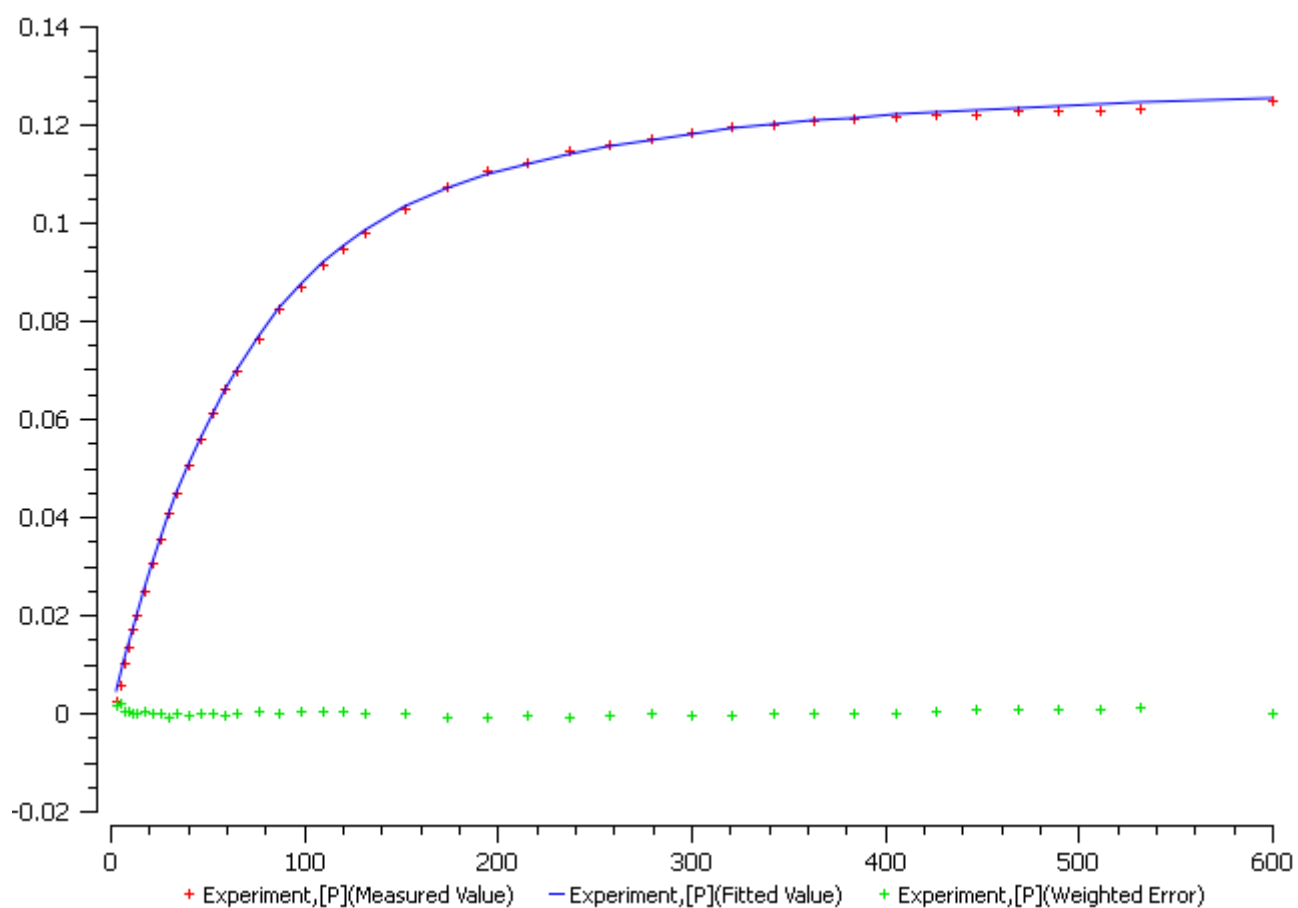
Parameter Estimation Result

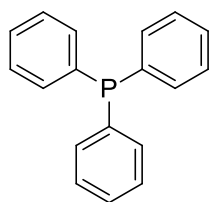




1) 54.8

Parameter Estimation Result

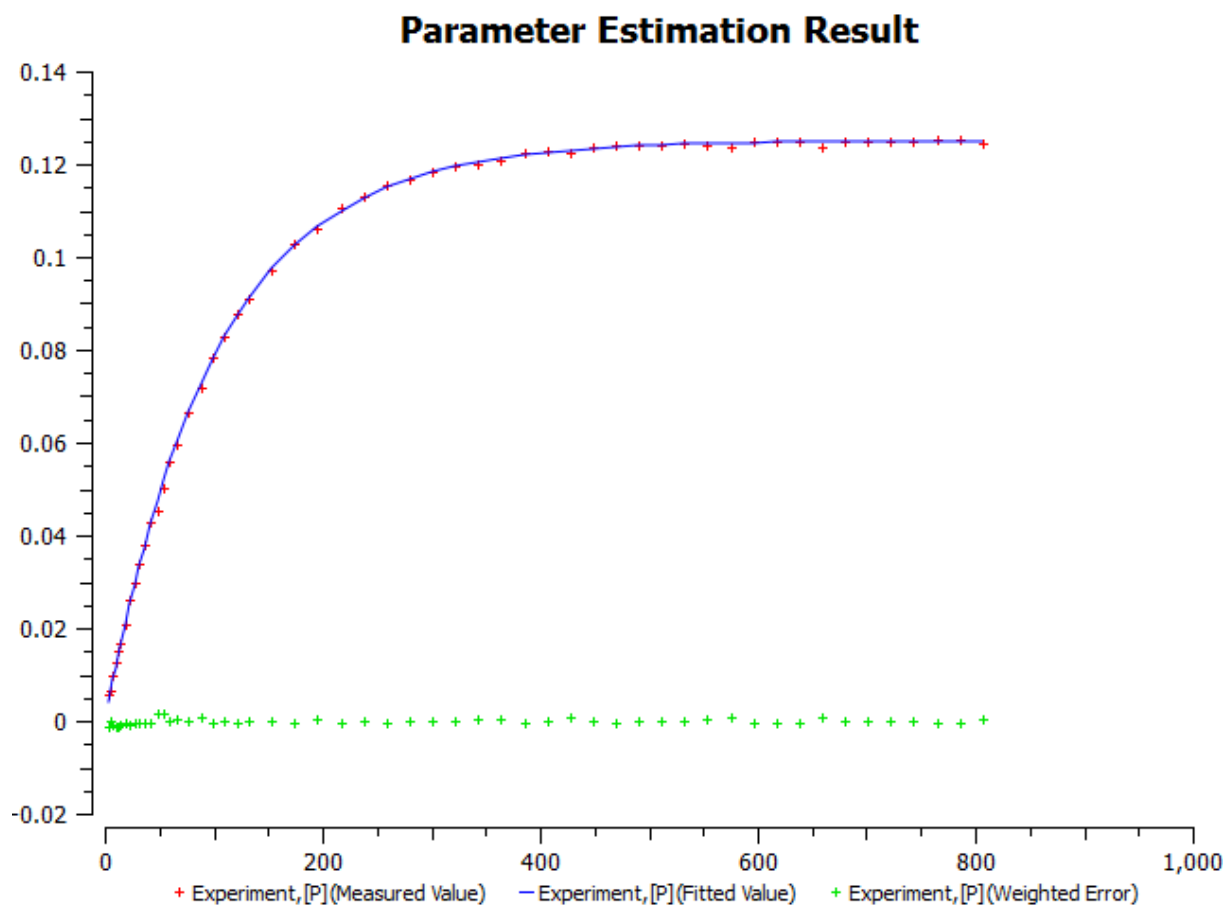


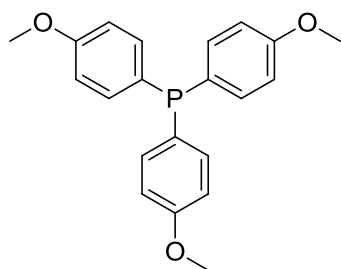


5a

- 1) 70.1
- 2) 68.0
- 3) 70.2

$$= 69.4 \pm 1.0$$





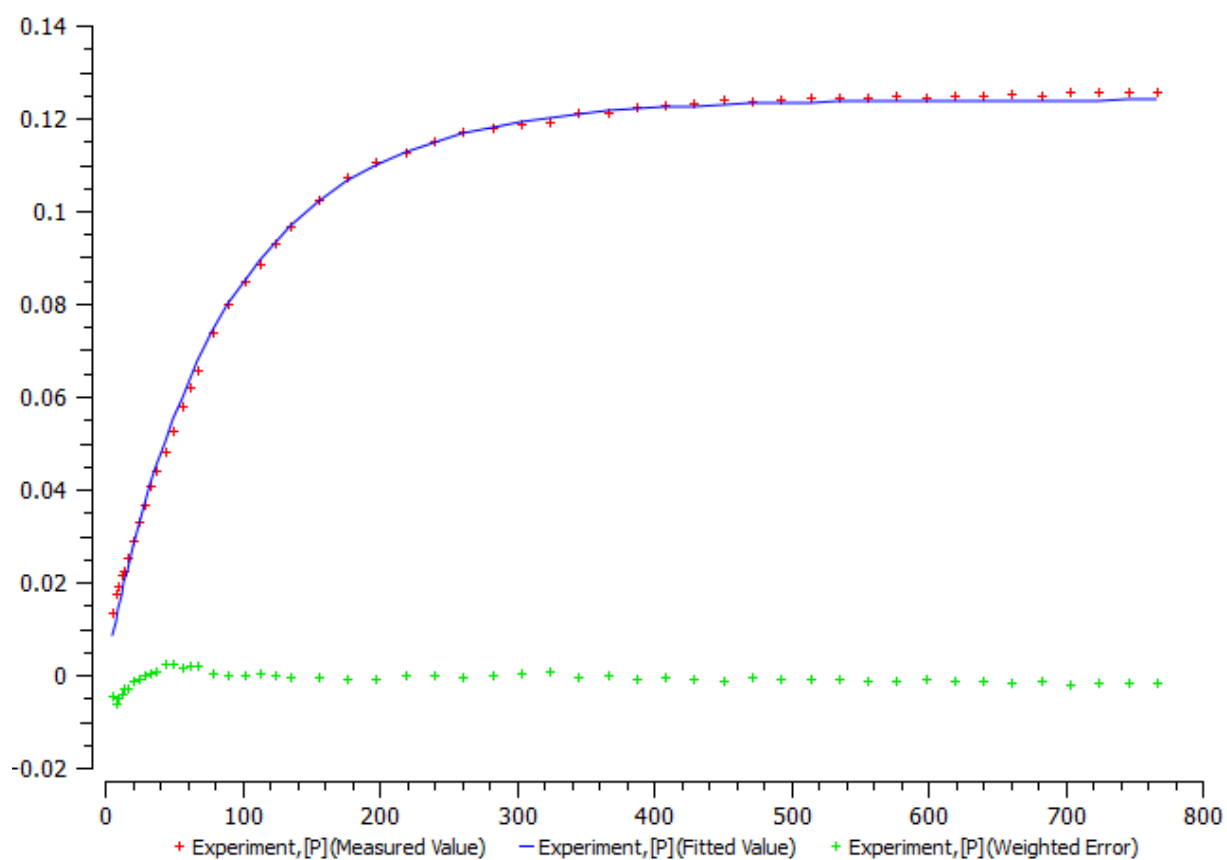
5b

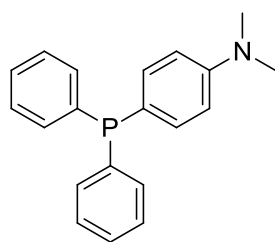
1) 60.1

2) 59.1

$$= 59.6 \pm 0.5$$

Parameter Estimation Result



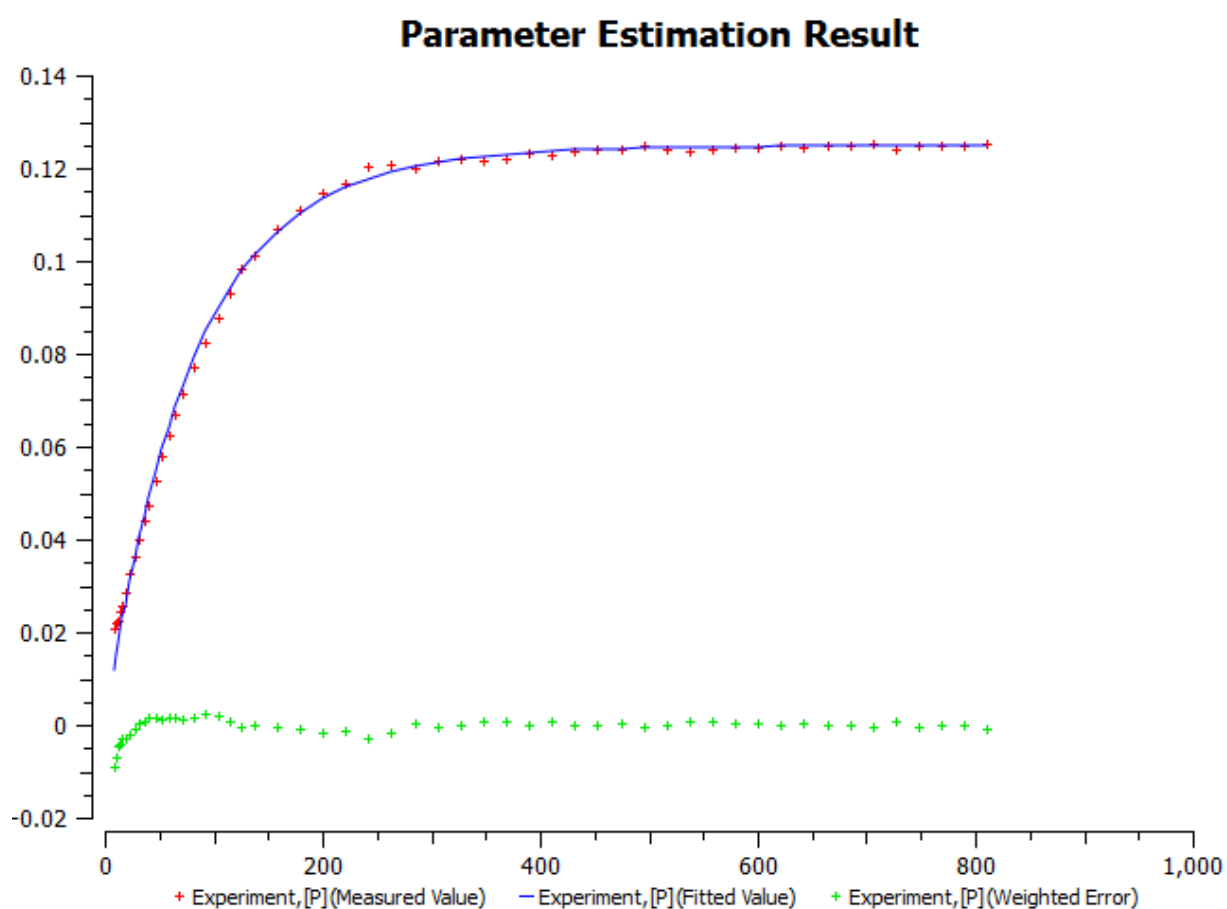


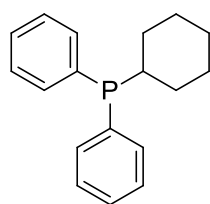
5c

1) 56.1

2) 52.4

$$= 54.3 \pm 1.9$$





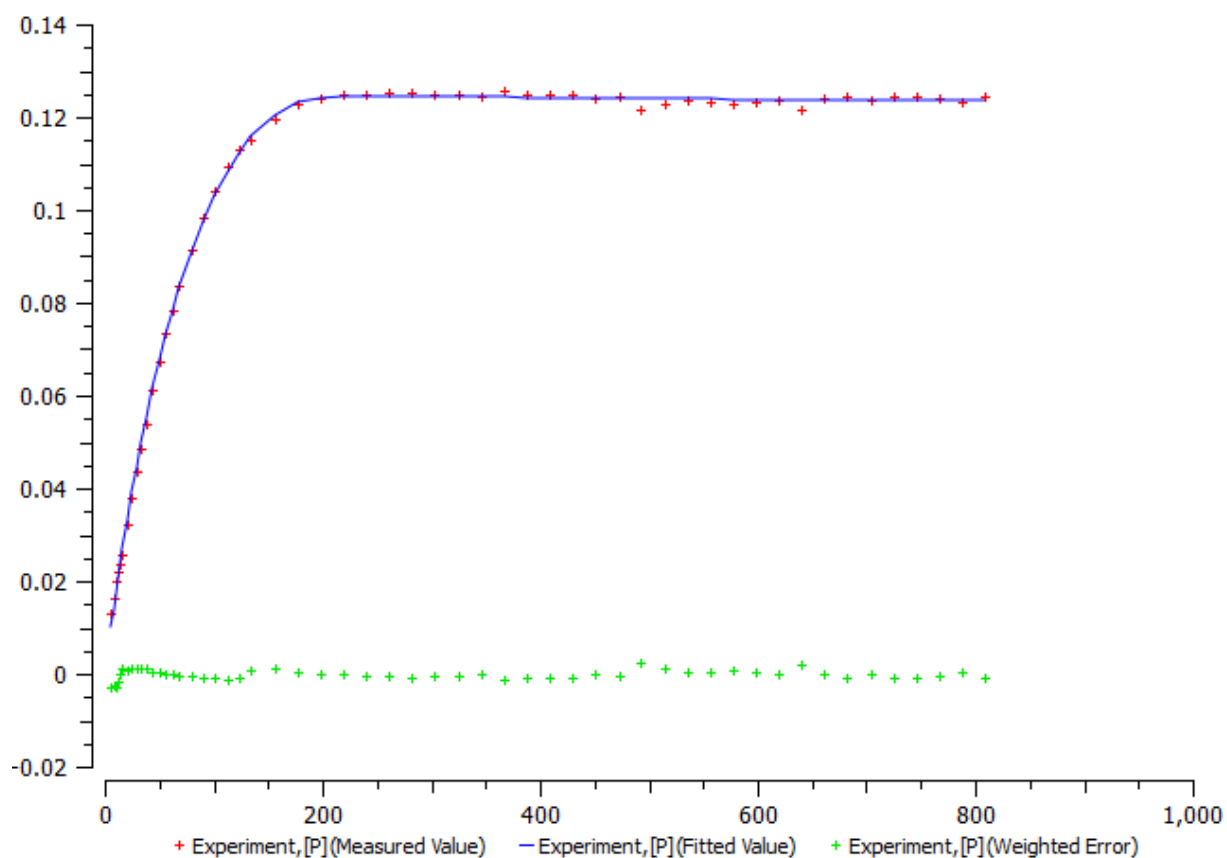
5e

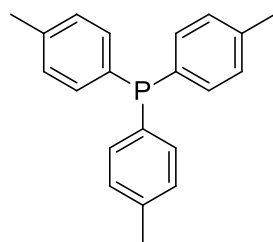
1) 44.9

2) 45.0

$$= 45.0 \pm 0.1$$

Parameter Estimation Result





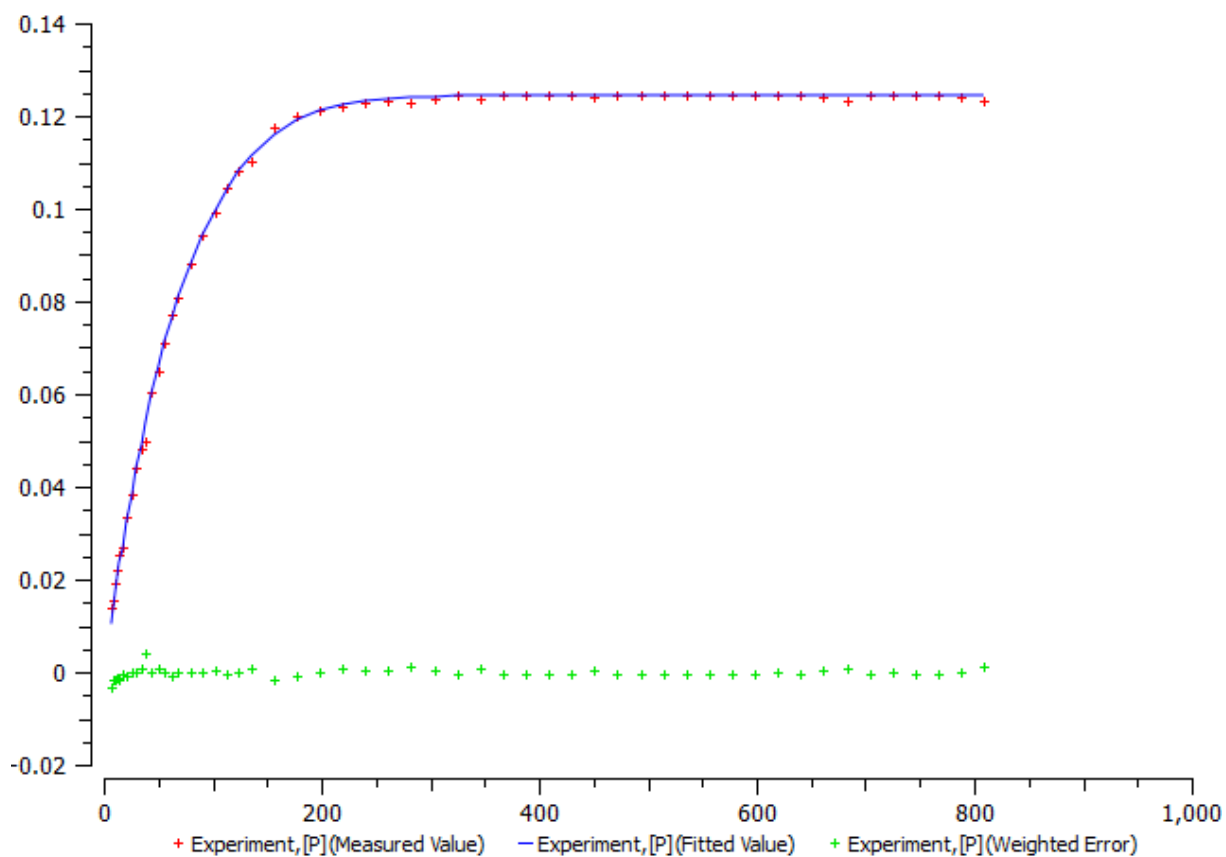
5f

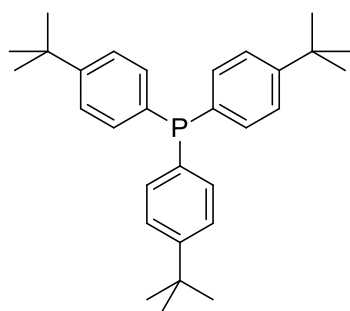
1) 46.7

2) 46.8

$$= 46.8 \pm 0.1$$

Parameter Estimation Result





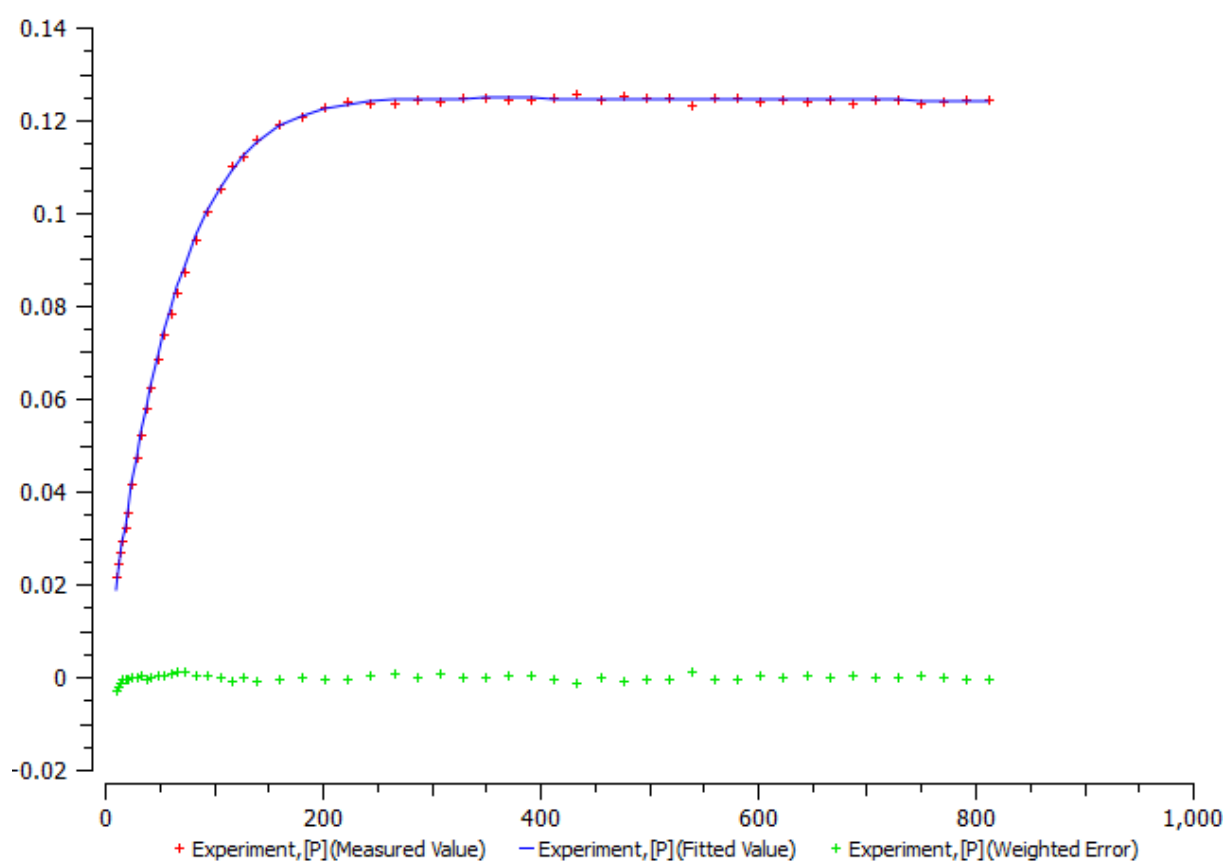
5g

1) 40.7

2) 42.0

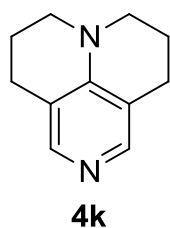
$$= 41.4 \pm 0.7$$

Parameter Estimation Result



2.1.4 2.5 mol% catalyst

The following kinetic runs were performed with $c(\text{imine}) = 0.125 \text{ M}$ and $c(\text{MVK}) = 0.15 \text{ M}$.

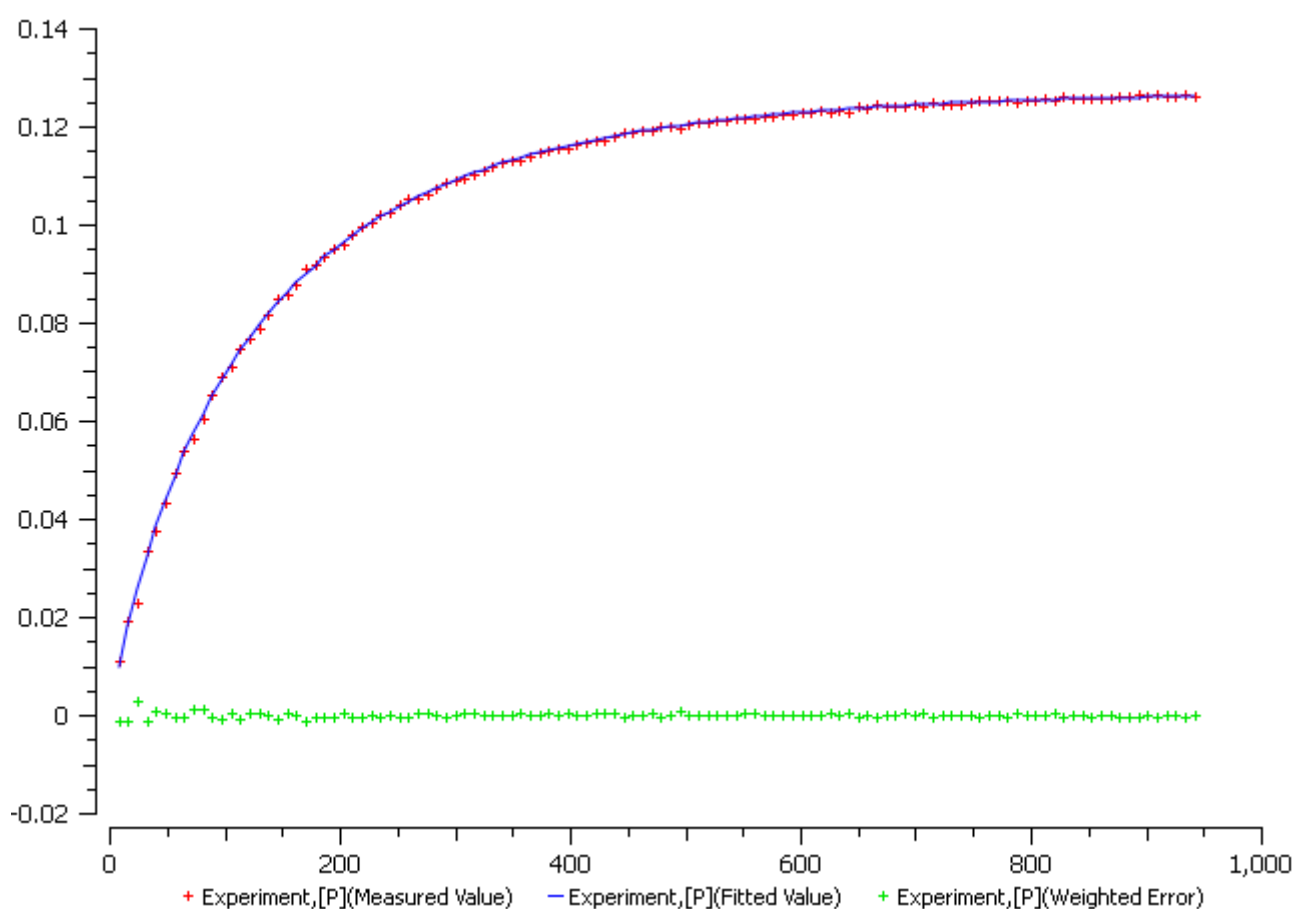


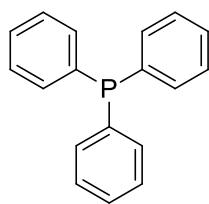
1) 83.59

2) 69.9

$$= 76.8 \pm 6.9$$

Parameter Estimation Result



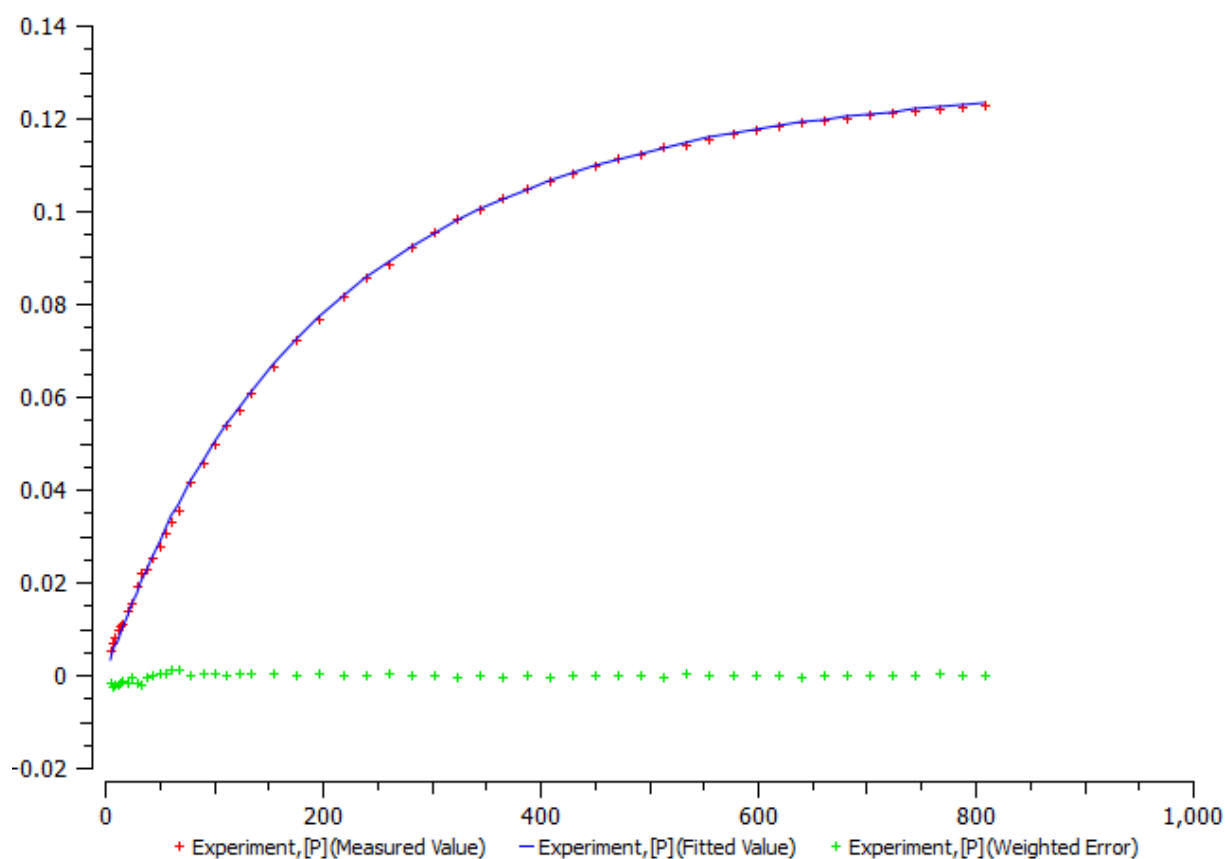


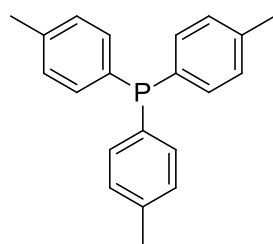
5a

- 1) 147.1
- 2) 139.4
- 3) 152.3

$$= 146.3 \pm 5.3$$

Parameter Estimation Result





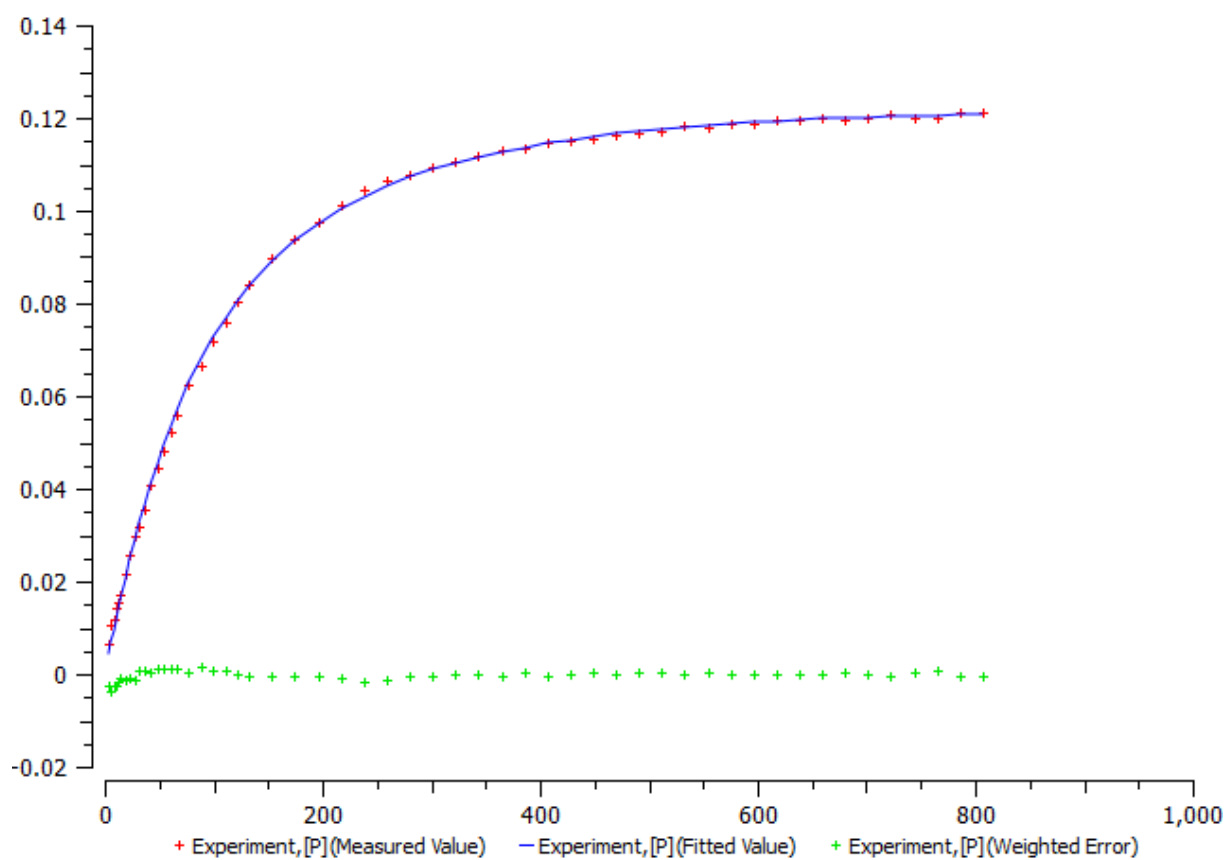
5f

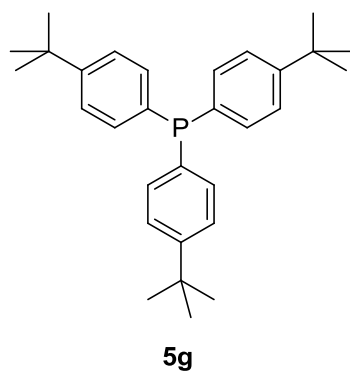
1) 74.8

2) 76.8

$= 75.8 \pm 1.0$

Parameter Estimation Result

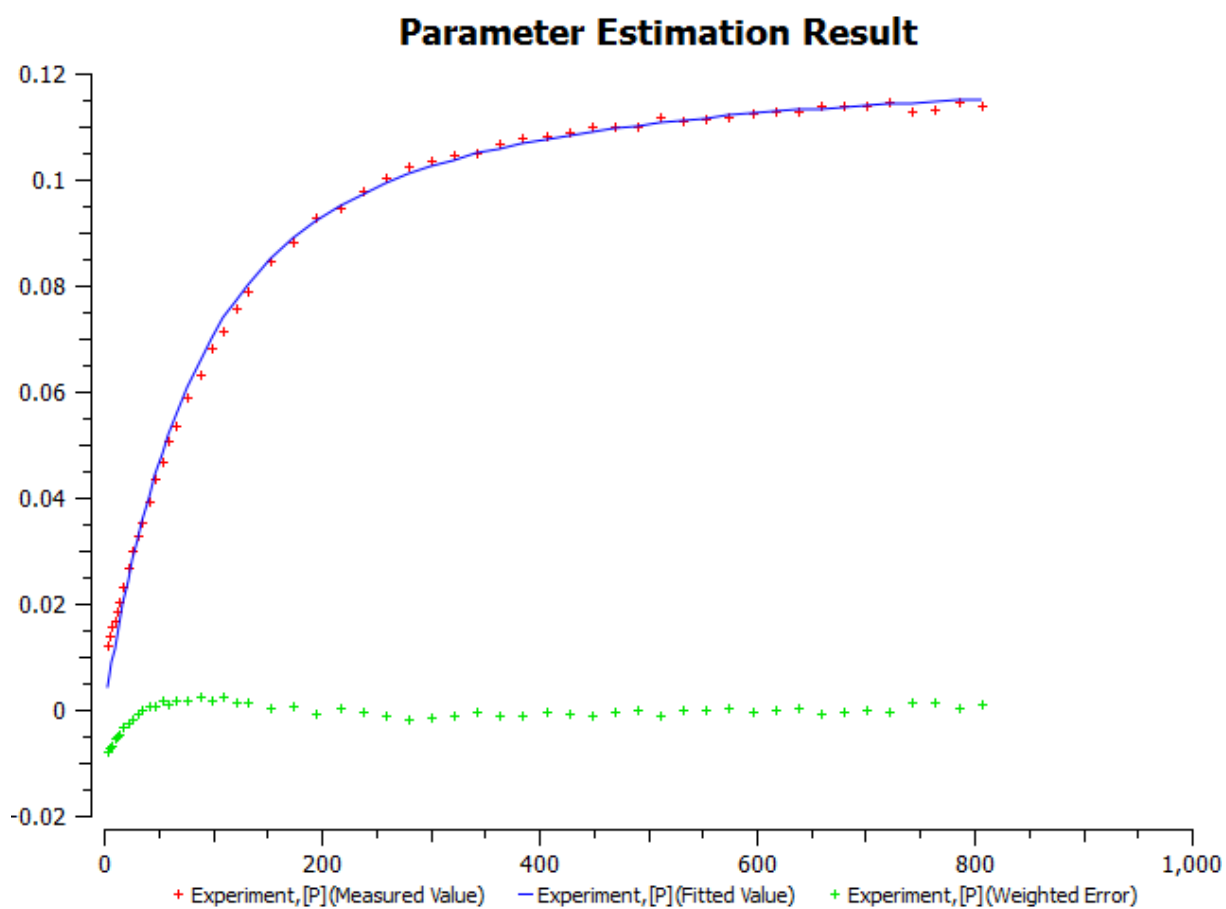




1) 80.6

2) 79.9

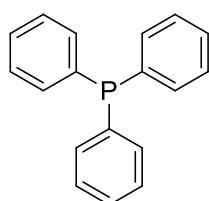
$$= 75.8 \pm 0.4$$



2.1.5 1.25 mol% catalyst

The following kinetic runs were performed with $c(\text{imine}) = 0.125 \text{ M}$ and $c(\text{MVK}) = 0.15 \text{ M}$.

Catalyst	Time [h]	Conversion ^{a,c} [%]	$t_{1/2}$ ^c [min]
5g	> 20	55 – 57%	315
5f	> 20	59 – 63%	273
5a	32	95	337

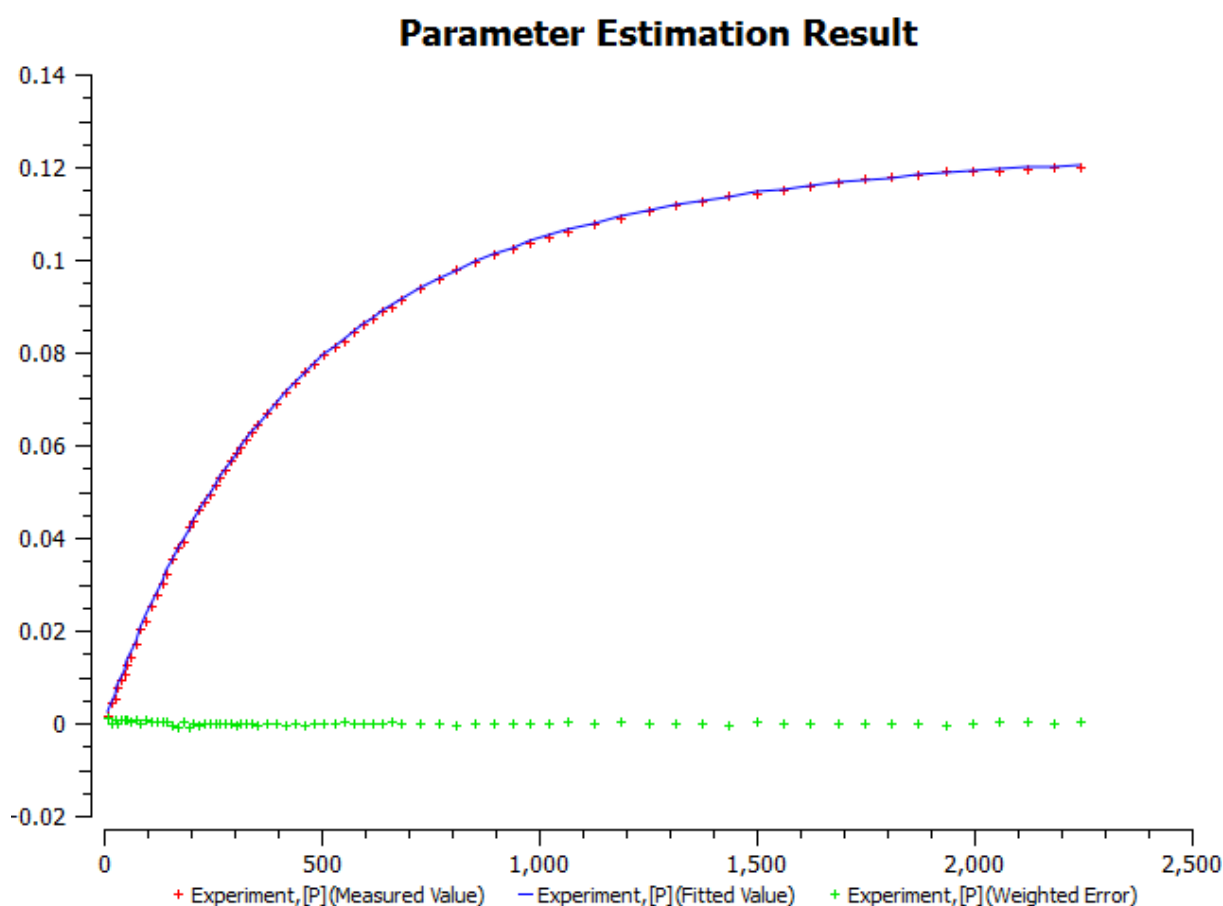


5a

1) 338.0

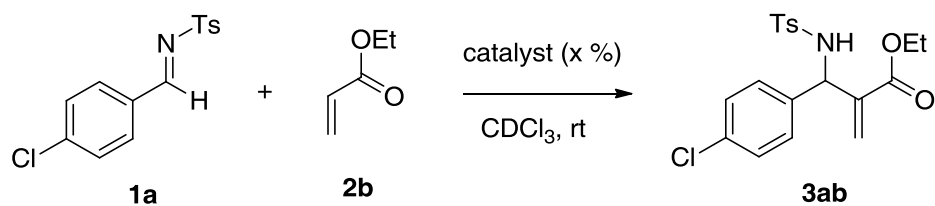
2) 335.4

$$= 336.7 \pm 1.3$$



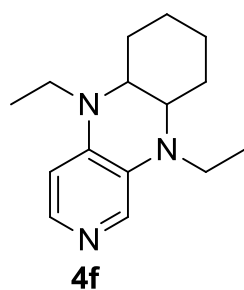
The kinetic measurement of **5f** and **5g** are not displayed due to the low conversion.

2.2 Kinetic data for reactions of tosylimine (**1a**) and ethyl acrylate (**2b**).



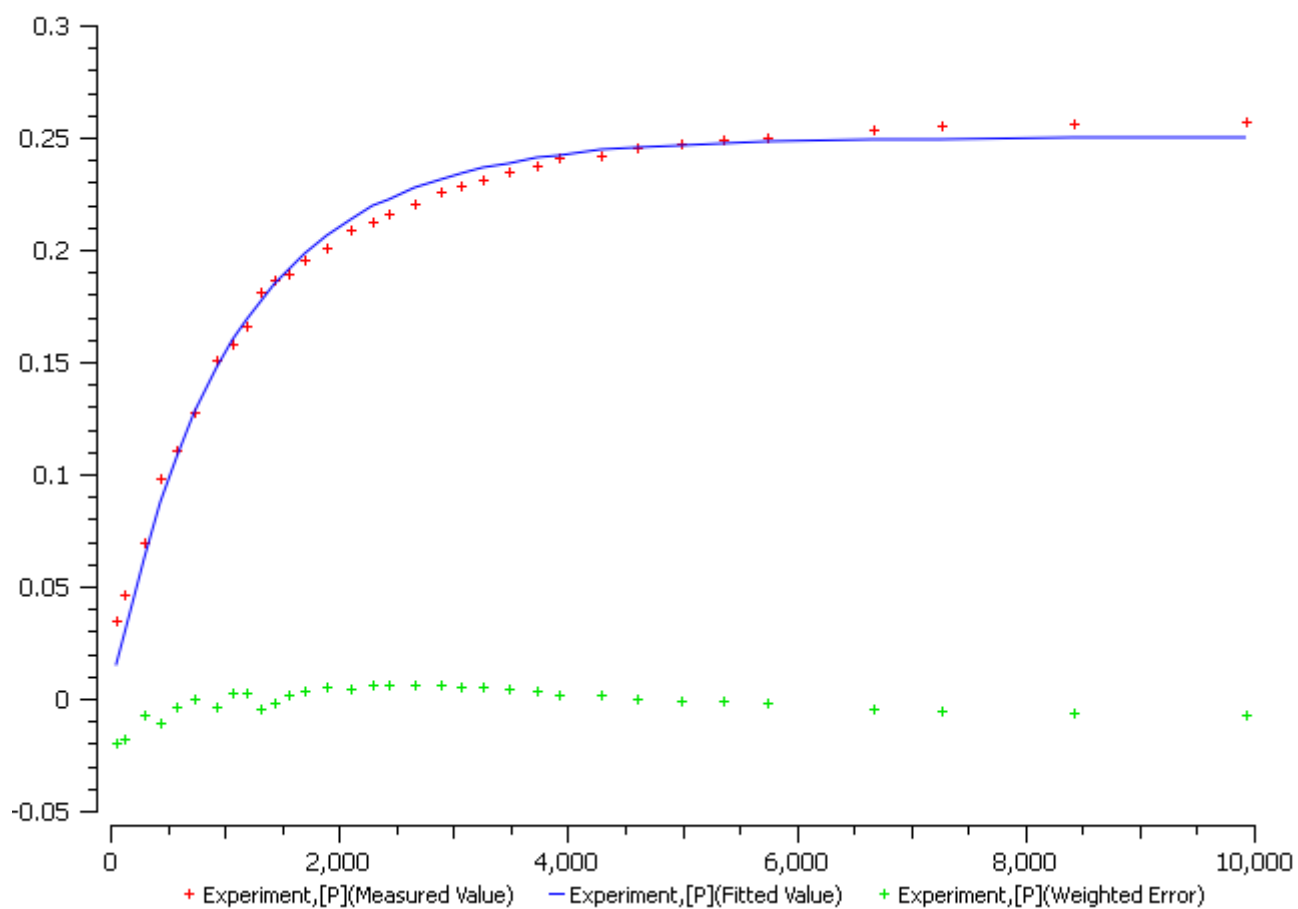
2.2.1 25 mol% catalyst

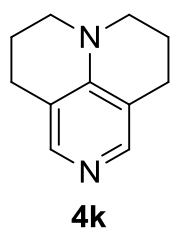
The following kinetic runs were performed with $c(\text{imine}) = 0.25 \text{ M}$ and $c(\text{ethyl acrylate}) = 1.00 \text{ M}$.



1) 715.4
2) 729.8
3) 797.0
= 747.4 ± 35.6

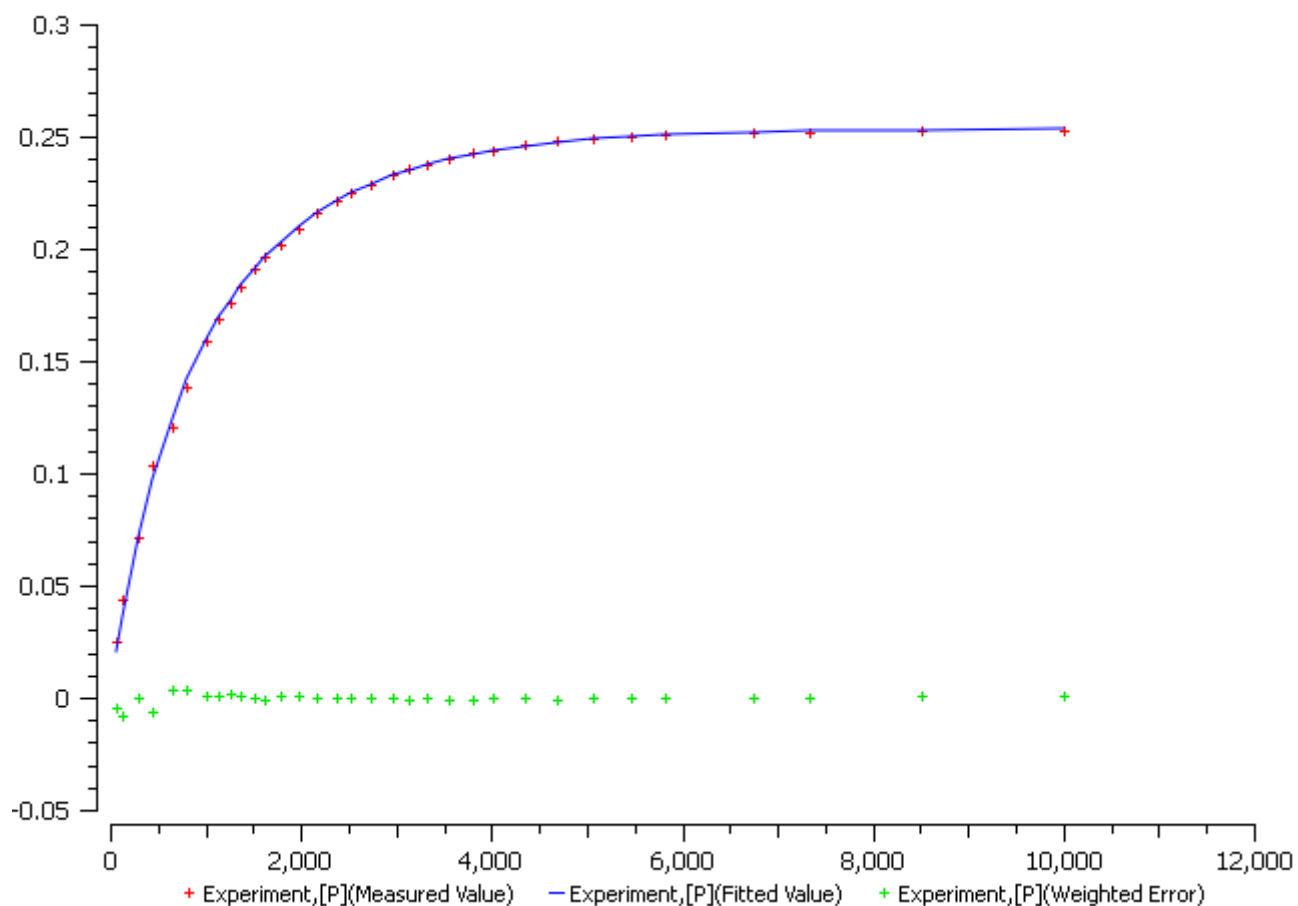
Parameter Estimation Result

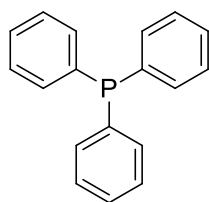




1) 655.4
 2) 568.3
 = 611.9 ± 43.6

Parameter Estimation Result



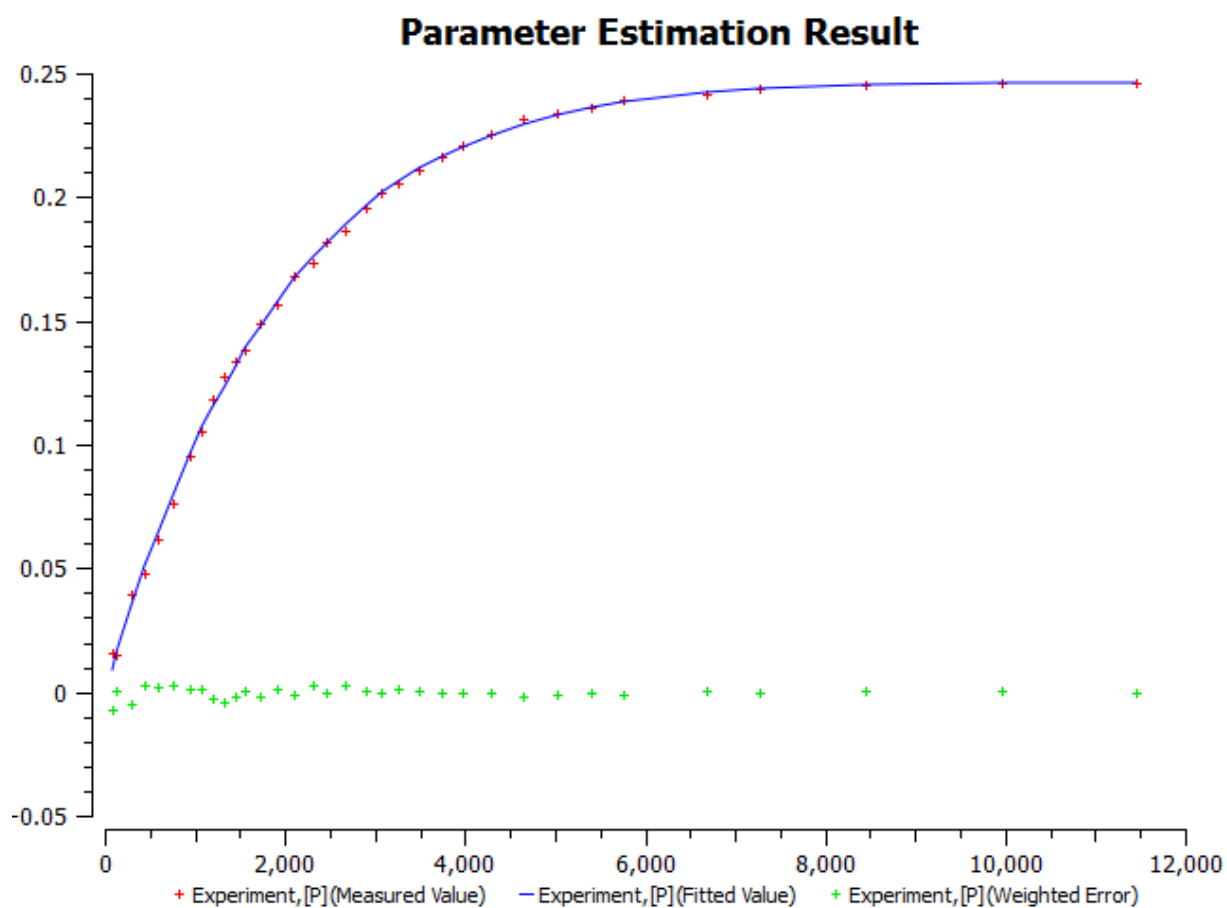


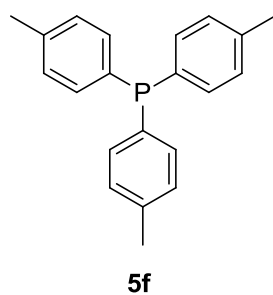
5a

1) 1342

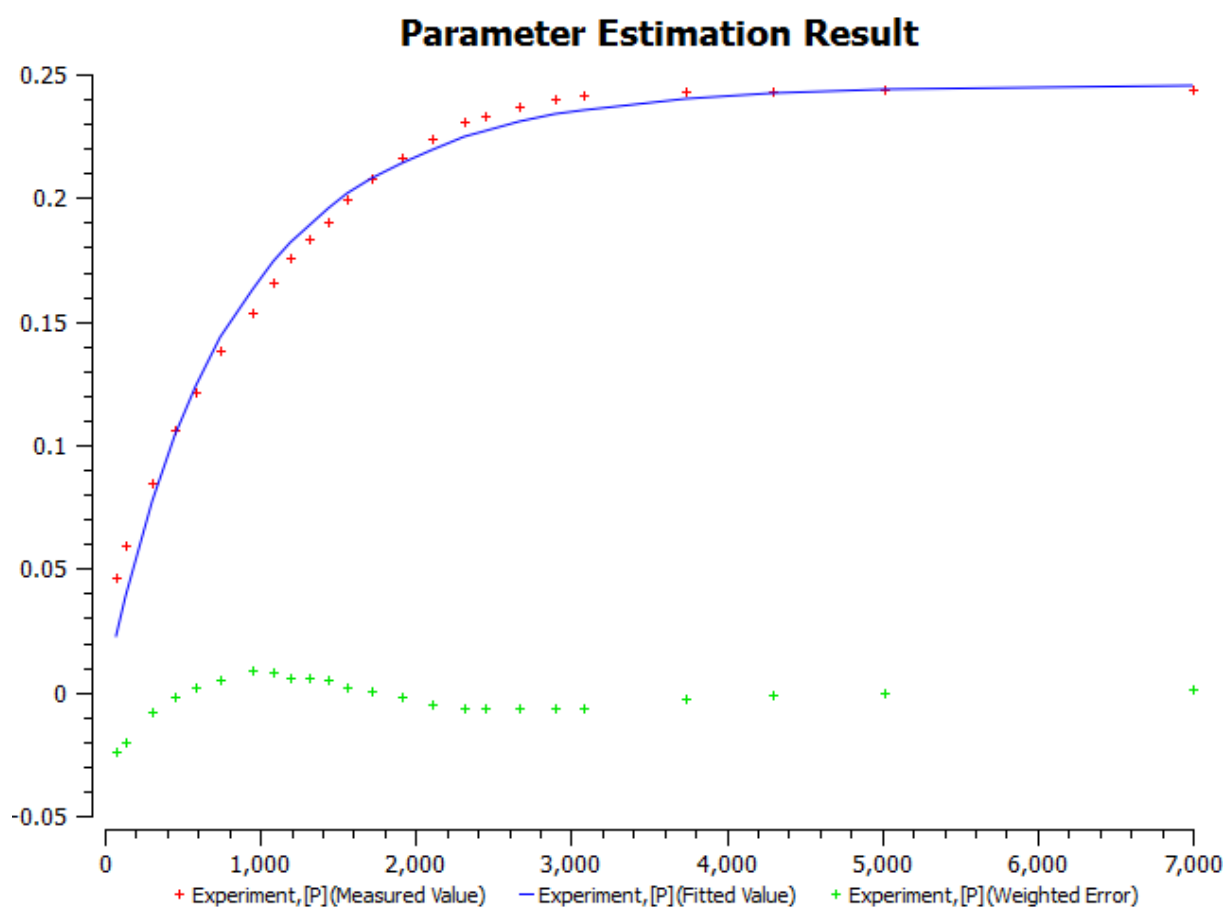
2) 1425

$$= 1384 \pm 42$$





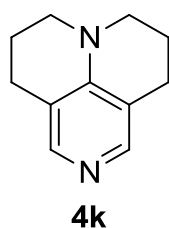
1) 595



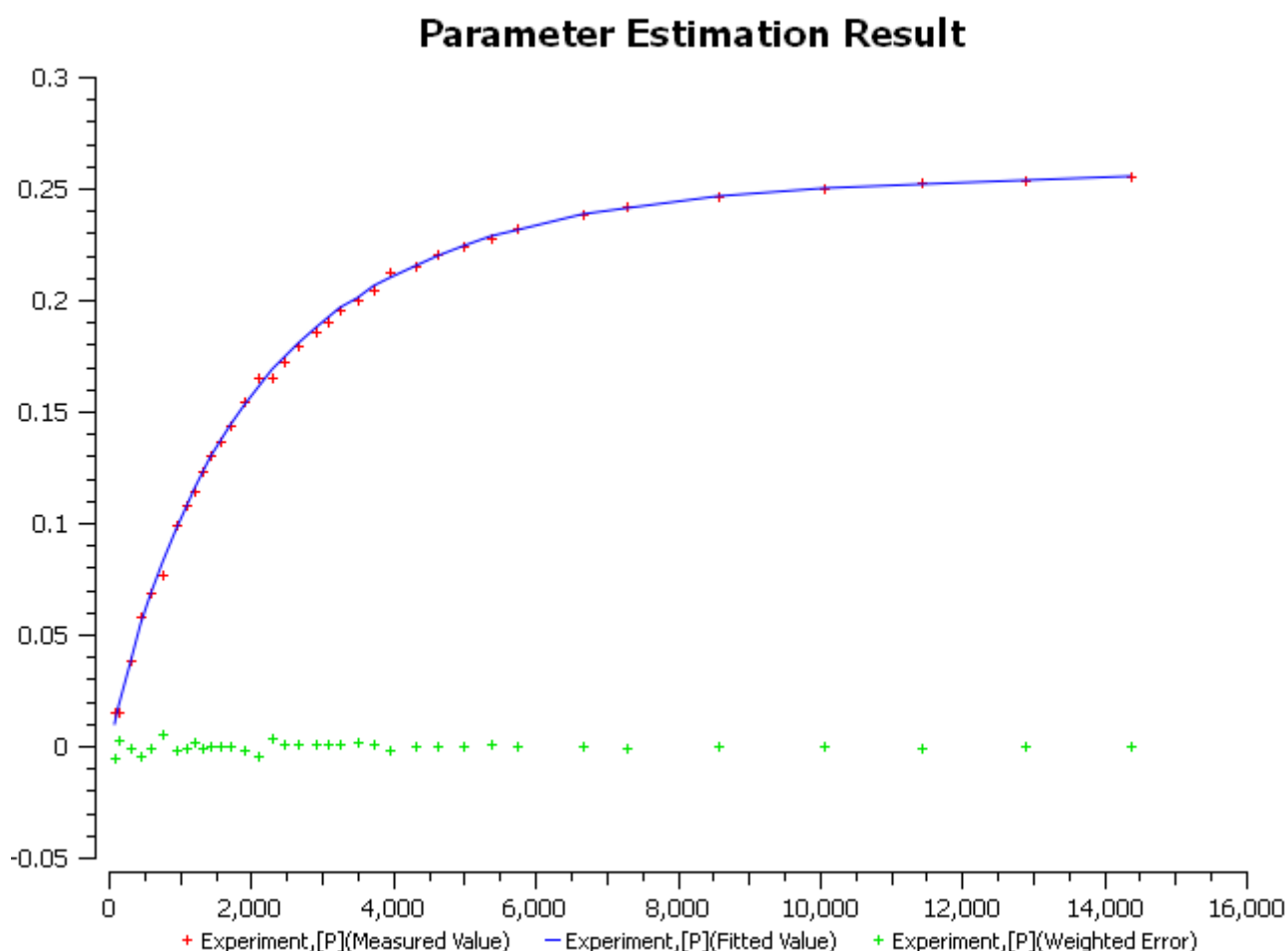
2.2.2 12.5 mol% catalyst

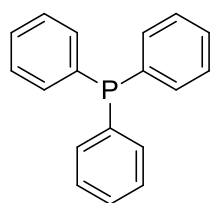
The measurements with 12.5 mol% catalyst loading were done in addition to the measurements with 25 mol%, but not discussed in the manuscript. The following kinetic runs were performed with $c(\text{imine}) = 0.25 \text{ M}$ and $c(\text{ethyl acrylat}) = 1.00 \text{ M}$.

Catalyst	Time [d]	Conversion ^{a,b} [%]	$t_{1/2}$ ^c [min]
5a	14	99	3113
4k	6	99	1355



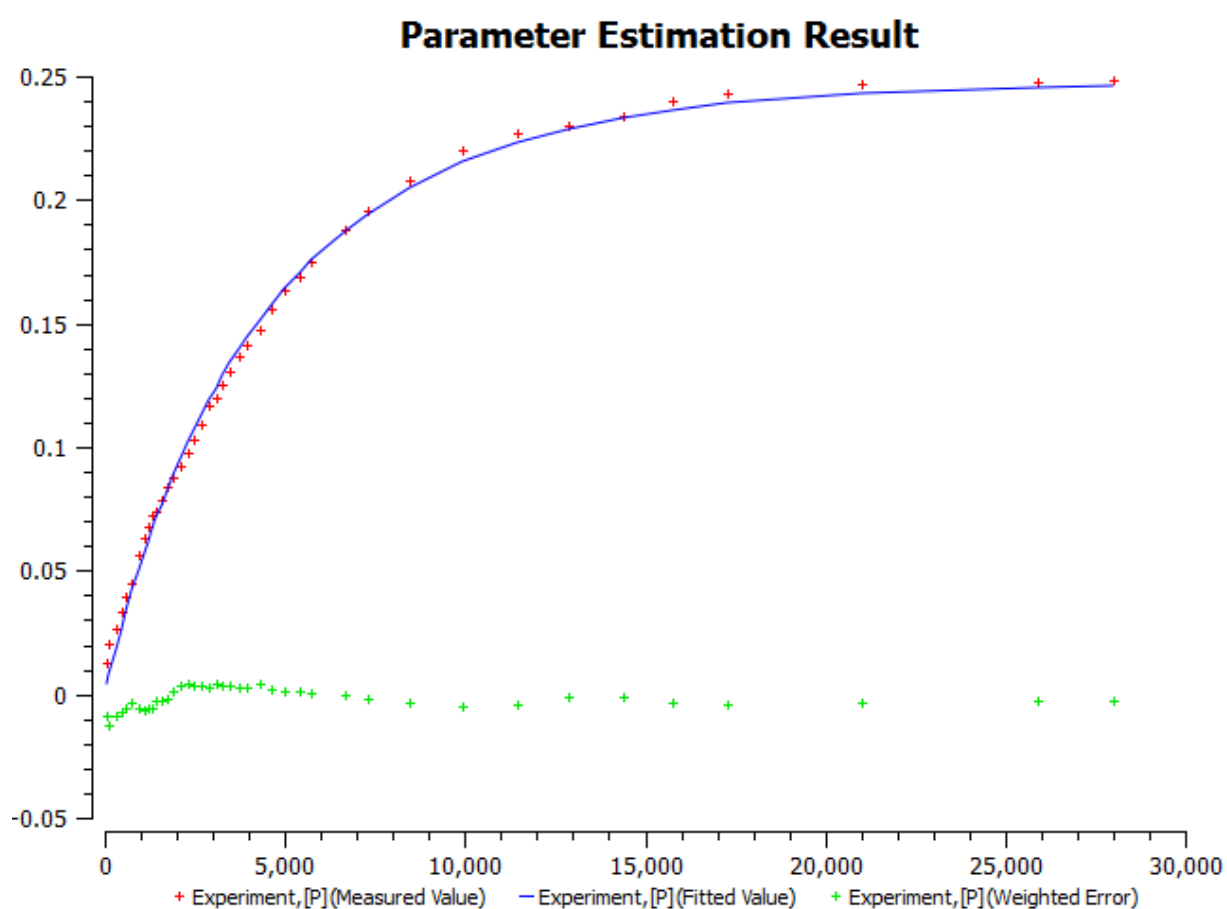
1) 1355



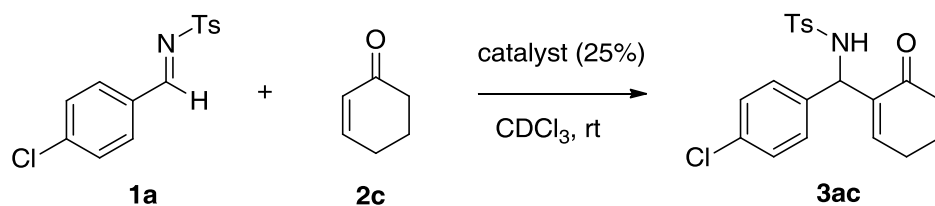


5a

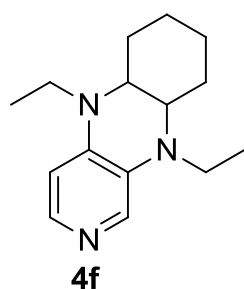
1) 3113



2.3 Kinetic data for reactions of tosylimine (**1a**) and cyclohexenone (**2c**).

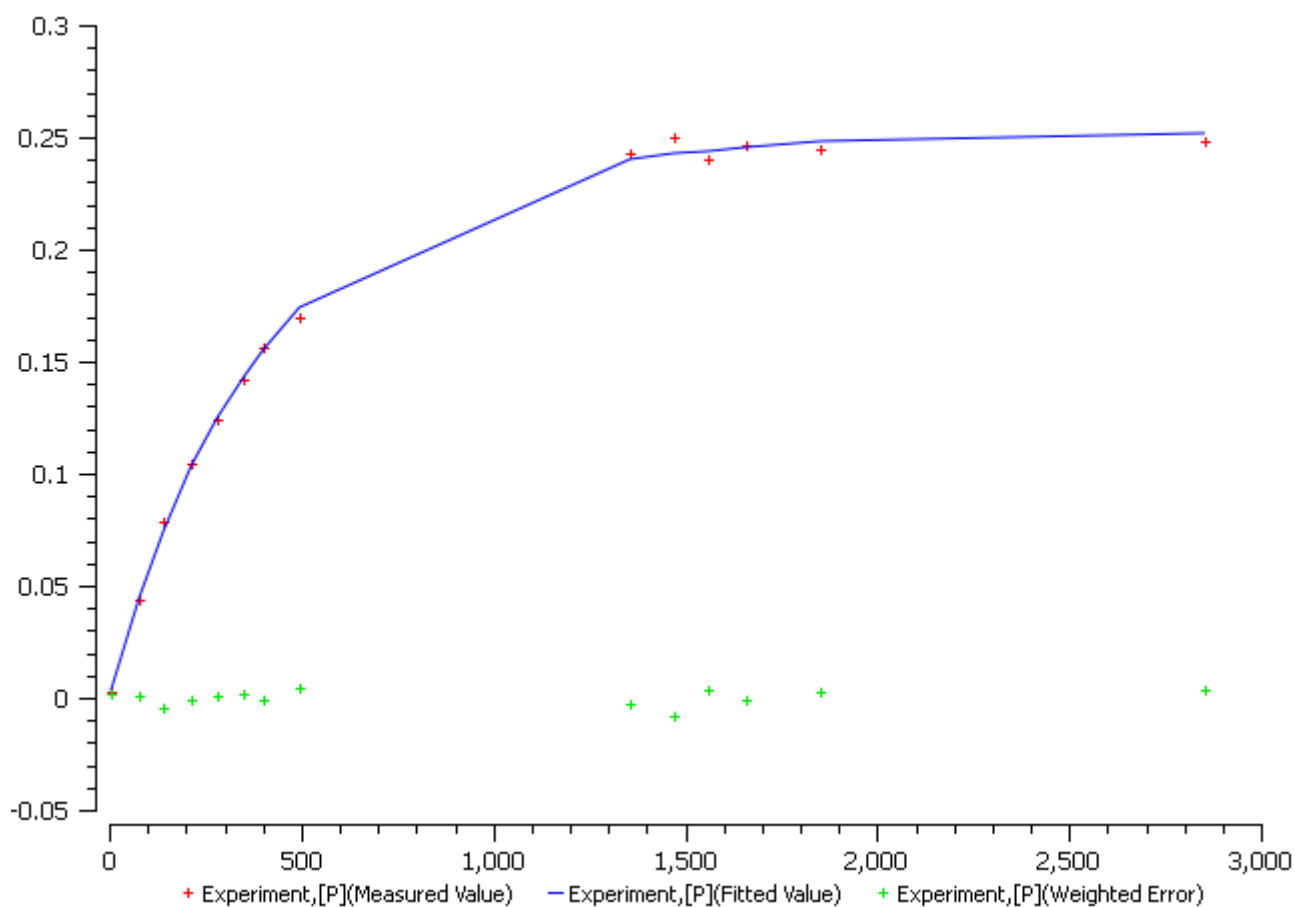


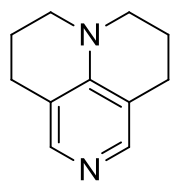
The following kinetic runs were performed with $c(\text{imine}) = 0.25 \text{ M}$ and $c(\text{cyclohexenone}) = 1.00 \text{ M}$.



- 1) 281.5
 - 2) 247.3
- = 264.4 ± 17.1

Parameter Estimation Result

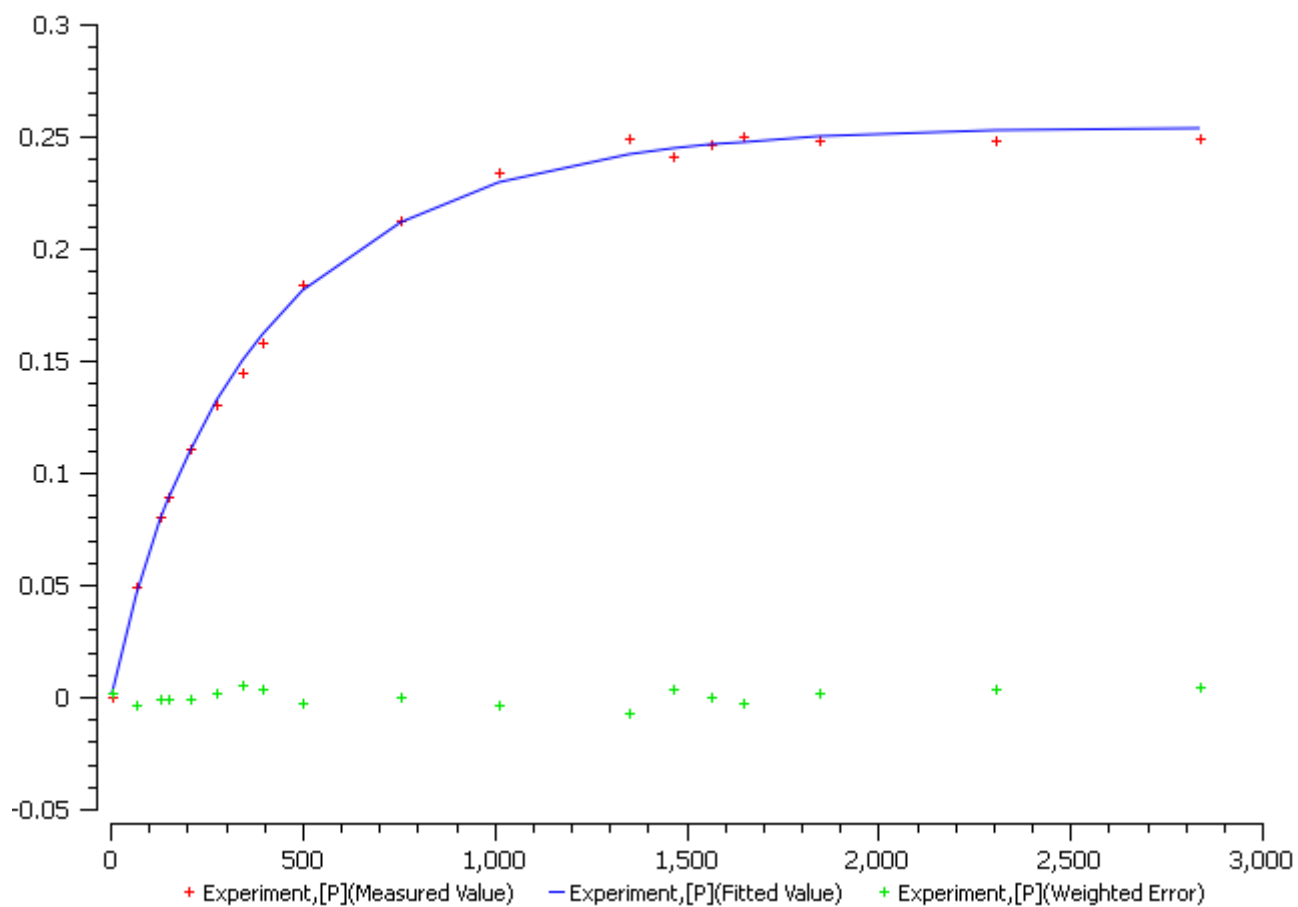


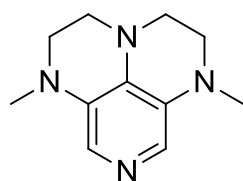


4k

3) 253.9
4) 230.6
= 242.3 ± 11.7

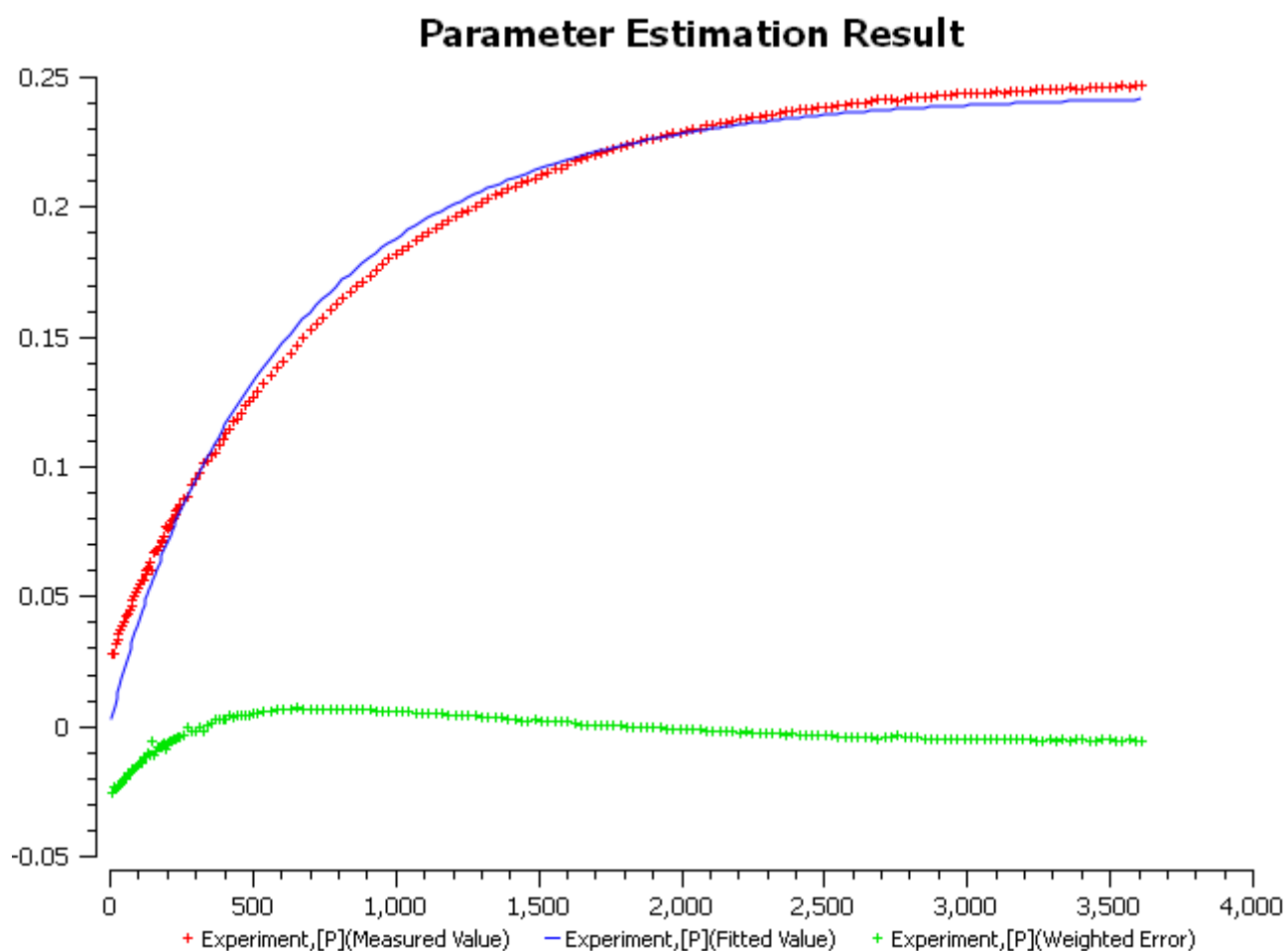
Parameter Estimation Result

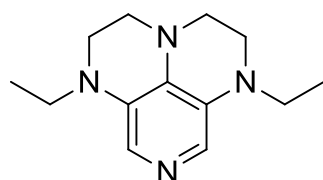




4I

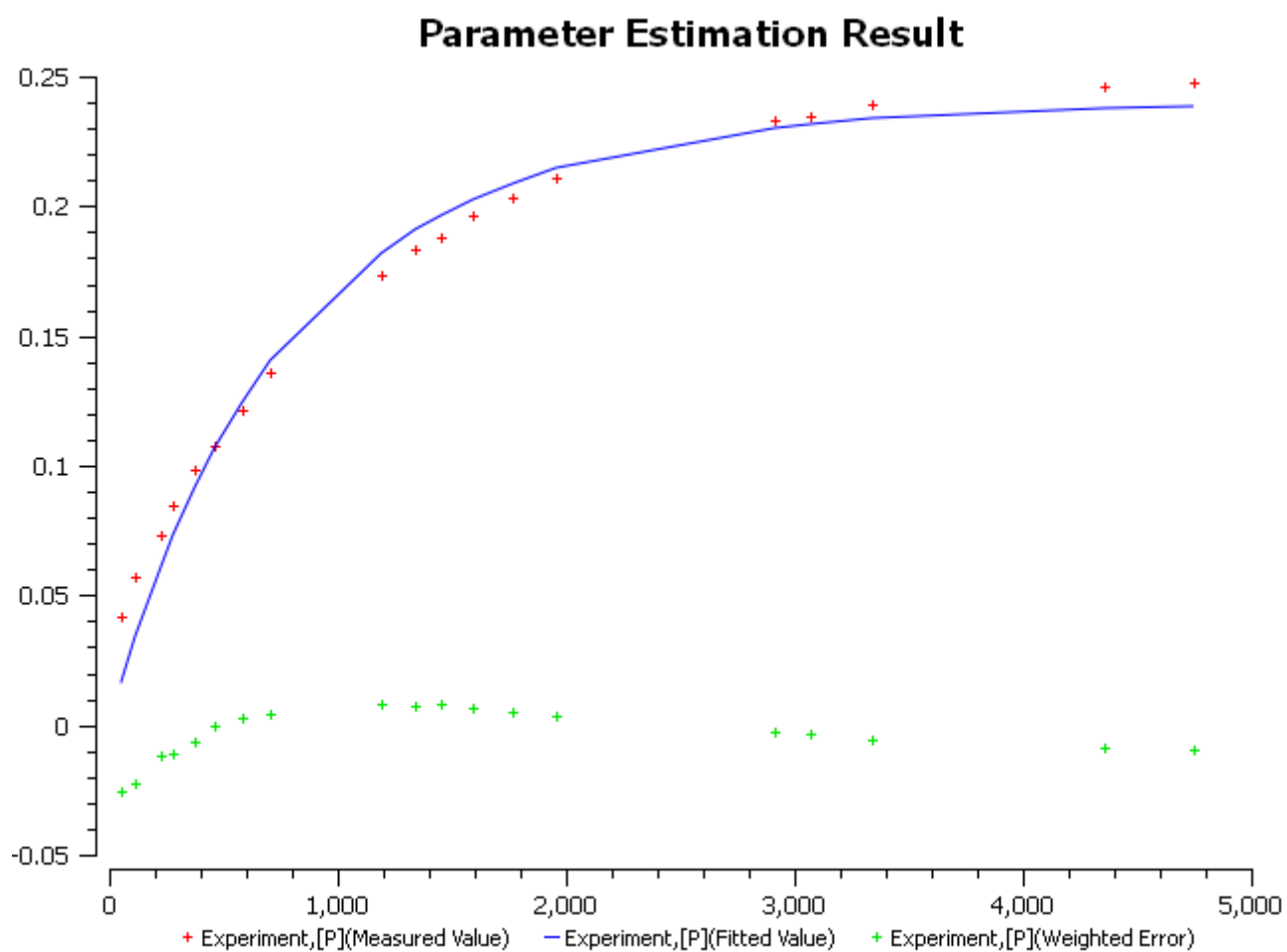
1) 456.6

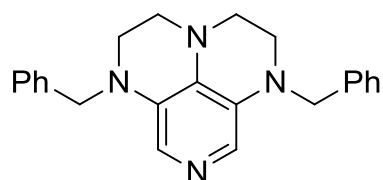




4I

1) 581.1

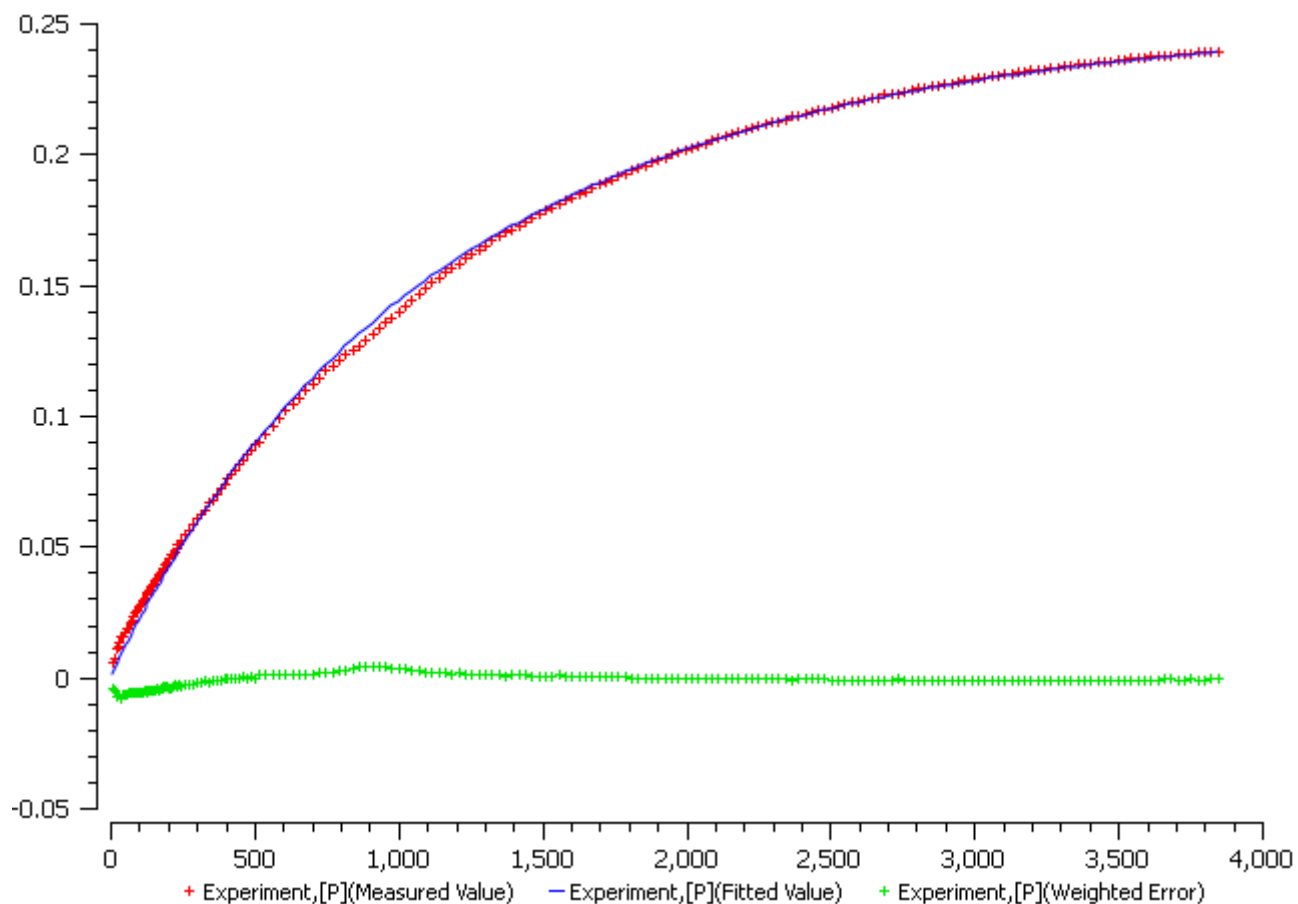




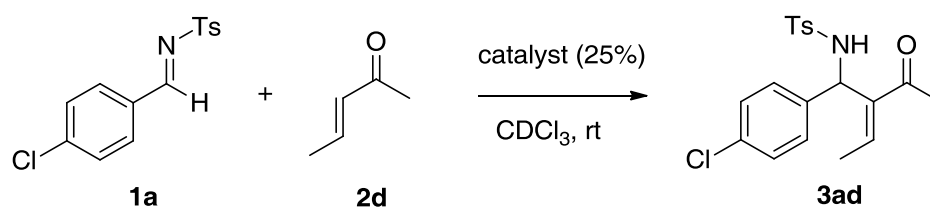
4m

1) 802.2
2) 713.6
= 757.9 ± 44.3

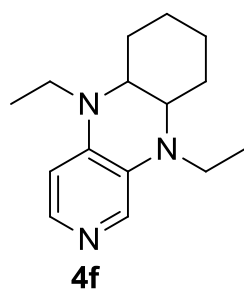
Parameter Estimation Result



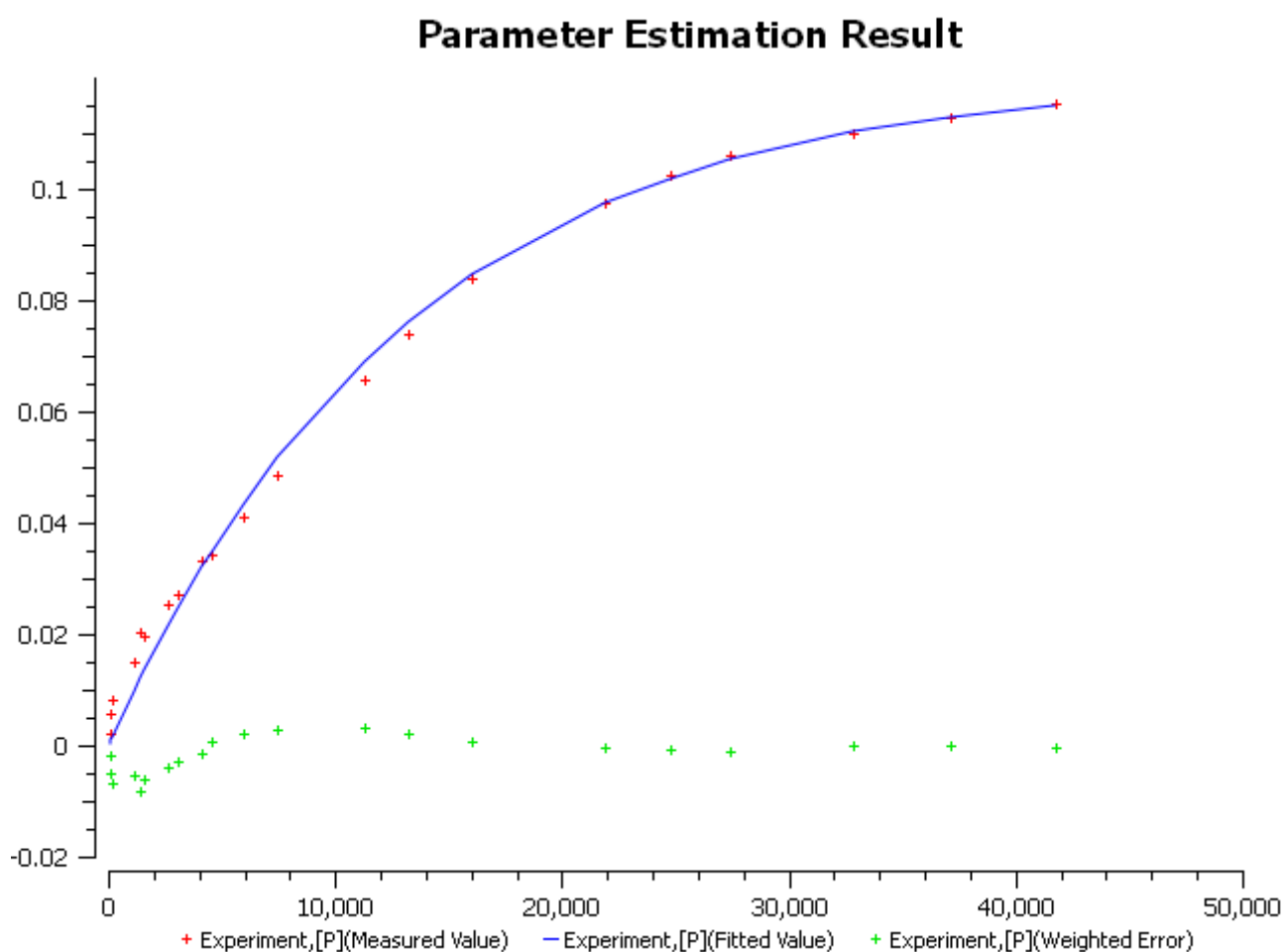
2.4 Kinetic data for reactions of tosylimine (**1a**) and trans-3-penten-2-one (**2d**).

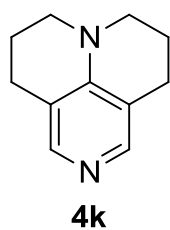


The following kinetic runs were performed with $c(\text{imine}) = 0.125 \text{ M}$ and $c(\text{trans-3-penten-2-one}) = 0.50 \text{ M}$.

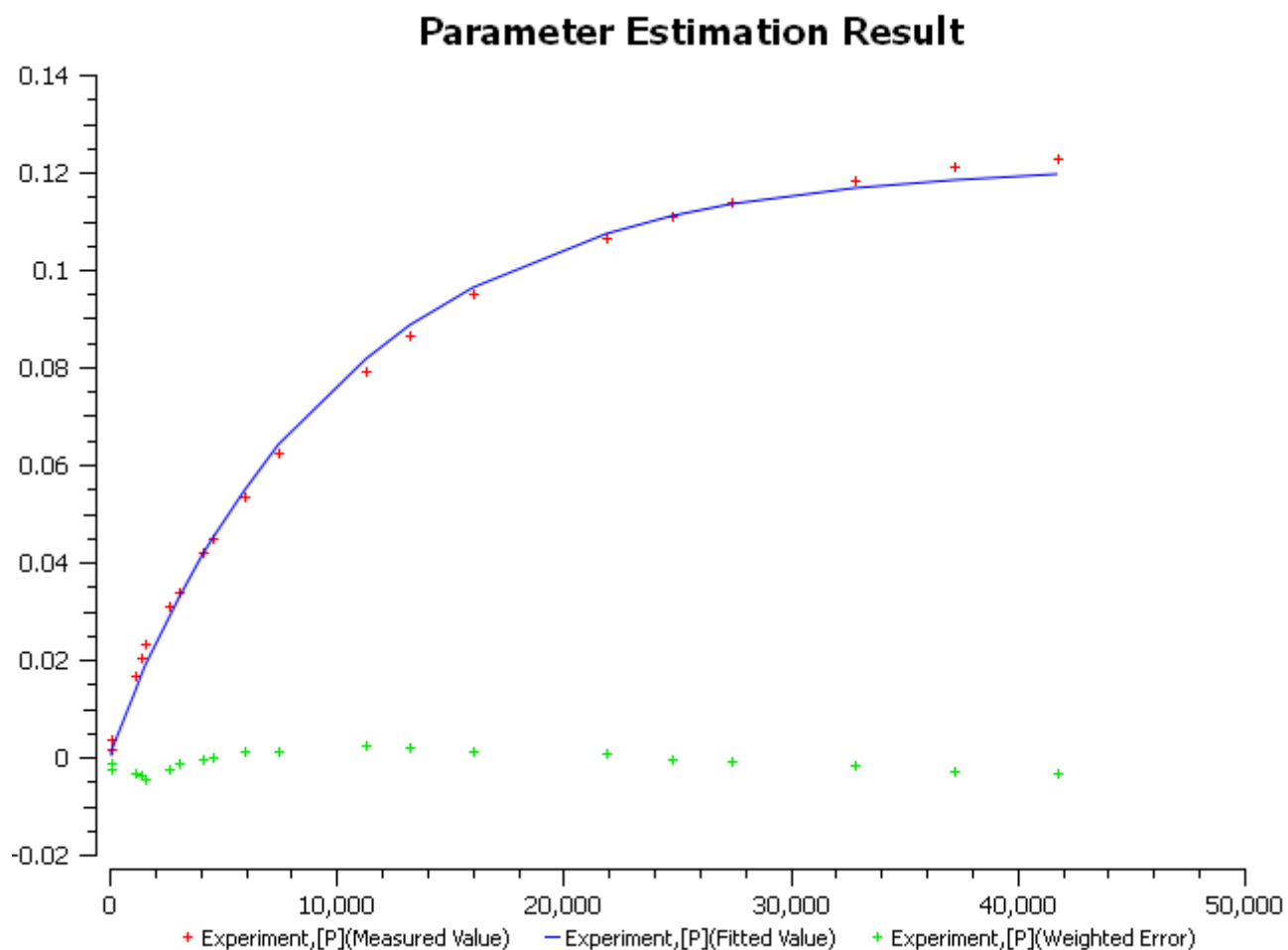


1) 164 h





1) 120 h



3. Synthetical data

Table S2 Results for the azaMBH reaction with MVK (**2a**) using 5 mol% catalyst **4f** and selected tosylimines as shown in Scheme 7. The σ -Parameters are given in the last column.

Entry	Ar	Tosyl-imine	Time [h]	Yield [%] ^{a,c}	Conv. [%] ^{b,c}	Prod.	σ -Parameter
1	<i>p</i> -NO ₂ -C ₆ H ₄	1c	1.5	90	99	3ca	0.778
2	<i>p</i> -NC-C ₆ H ₄	1b	1.5	94	99	3ba	0.660
3	<i>p</i> -Br-C ₆ H ₄	1e	14	86	93	3ea	0.232
4	<i>p</i> -Cl-C ₆ H ₄	1a	10	92	99	3aa	0.227
5	C ₆ H ₅	1f	15	73	99	3fa	0.000
6	<i>p</i> -Me-C ₆ H ₄	1g	20	80	89	3ga	-0.170
7	<i>p</i> -MeO-C ₆ H ₄	1h	48	74	85	3ha	-0.268

^a Isolated yield; ^b Determined by ¹H NMR; ^c 0.125 M imine, 1.2 equ. MVK.

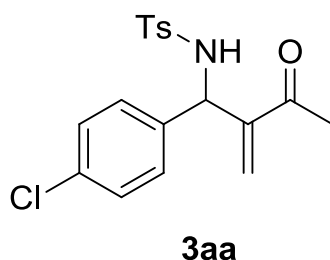
Table S3 Results for the azaMBH reaction with cyclohexenone (**2c**) using 25 mol% catalyst **4f** and selected tosylimines as shown in Scheme 8. The σ -Parameters are given in the last column.

Entry	Ar	Tosyl-imine	Time [h]	Yield [%] ^{a,c}	Conv. [%] ^{b,c}	Prod.	σ -Parameter
1	<i>p</i> -NO ₂ -C ₆ H ₄	1c	24	85	99	3cc	0.778
2	<i>p</i> -NC-C ₆ H ₄	1b	24	88	99	3bc	0.660
3	<i>p</i> -Br-C ₆ H ₄	1e	60	90	99	3ec	0.232
4	<i>p</i> -Cl-C ₆ H ₄	1a	30	98	99	3ac	0.227
5	C ₆ H ₅	1f	60	83	95	3fc	0.000
6	<i>p</i> -MeO-C ₆ H ₄	1h	120	69	90	3hc	-0.268
7	<i>o</i> -Cl-C ₆ H ₄	1d	48	84	95	3dc	-
8	<i>trans</i> -Ph-CH=CH	1i	54	87	96	3ic	-

^a Isolated yield; ^b Determined by ¹H NMR; ^c 0.25 M imine, 4.0 equ. ketone **2c**.

3.1 Synthetical data for the reaction of MVK (**2a**) with different tosylimines

Methyl vinyl ketone (**2a**, 1.2 eq), tosylimine (**1b-i**, 1.0 eq) and **4f** (5 mol%) as a catalyst were mixed in chloroform. The reaction was monitored by ¹H NMR until the disappearance of the tosylimine was observed. The reaction mixture was directly subjected to silica gel column chromatography and eluted with ethyl acetate / isohexane = 1 / 4 to give the corresponding azaMBH product.



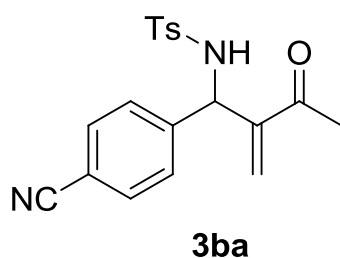
^1H NMR (200 MHz, CDCl_3): δ = 2.12 (3H, s, Me), 2.40 (3H, s, Me), 5.21 (1H, d, J = 8 Hz, NH), 5.72 (1H, d, J = 8.4 Hz, CH), 6.04 (1H, s), 6.08 (1H, s), 7.03 (2H, d, J = 8.7 Hz, Ar), 7.19 (4H, m, Ar), 7.62 (2H, d, J = 8.0 Hz, Ar).

^{13}C NMR (CDCl_3 , 75 MHz): δ = 21.49, 26.28, 58.58, 127.23, 127.79, 128.54, 128.60, 129.53, 133.49, 137.42, 137.43, 143.51, 146.11, 198.80.

MS (EI): m/e 363, 210, 209, 208, 173, 172, 171, 166, 155 (MePhSO_2^+), 151, 149, 130, 115, 91 (MePh^+), 65, 43.

HRMS (ESI) $[\text{M}-\text{H}]^+$ calc. for $\text{C}_{18}\text{H}_{19}\text{ClNO}_3\text{S}^+$: requires 364.0769, found: 364.0768.

IR [cm^{-1}]: $\tilde{\nu}$ = 3261 (NH), 1673 (C=O), 1631, 1594, 1491, 1401, 1325, 1280, 1162, 1090, 1053, 1014, 961, 935, 837, 813, 719, 708, 671.

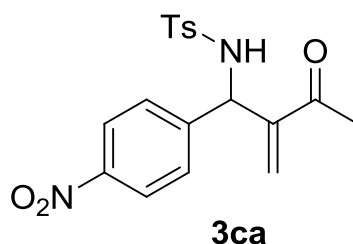


^1H NMR (200 MHz, CDCl_3): δ = 2.14 (3H, s, Me), 2.40 (3H, s, Me), 5.26 (1H, d, J = 9.2 Hz), 5.83 (1H, d, J = 8.7 Hz), 6.04 (1H, s), 6.10 (1H, s), 7.25 (4H, m, Ar), 7.49 (2H, d, J = 6.7 Hz, Ar), 7.63 (2H, d, J = 7.2 Hz, Ar).

^{13}C NMR (CDCl_3 , 75 MHz): δ = 21.51, 26.18, 59.14, 111.47, 118.40, 126.82, 126.98, 127.18, 129.60, 132.23, 137.42, 143.72, 144.21, 145.43, 198.75.

MS (EI): m/e 354, 312, 289, 285, 269, 253, 252, 245, 225, 199, 157, 155 (MePhSO_2^+), 140, 129, 92, 91 (MePh^+), 65, 43.

IR [cm^{-1}]: $\tilde{\nu}$ = 3268 (NH), 2229, 1674 (C=O), 1424, 1328, 1157, 1092, 1067, 914, 814, 729, 665.



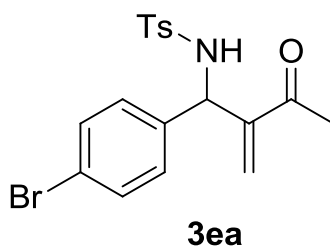
^1H NMR (200 MHz, CDCl_3): δ = 2.15 (3H, s, Me), 2.42 (3H, s, Me), 5.32 (1H, d, J = 9.4 Hz), 5.91 (1H, d, J = 9.4 Hz), 6.08 (1H, s), 6.13 (1H, s), 7.30 (4H, m, Ar), 7.64 (2H, d, J = 8.3 Hz, Ar), 8.06 (2H, d, J = 8.7 Hz).

^{13}C NMR (CDCl_3 , 75 MHz): δ = 21.48, 26.11, 58.48, 123.57, 126.35, 127.17, 127.36, 129.62, 129.68, 137.29, 143.82, 145.57, 146.28, 198.62.

MS (EI): m/e 374, 359, 305, 219, 155 (MePhSO_2^+), 130, 91 (MePh^+), 65, 43.

HRMS (ESI) $[\text{M}-\text{H}]^+$ calc. for $\text{C}_{18}\text{H}_{17}\text{O}_5\text{N}_2\text{S}$: requires 373.0864, found 373.0867.

IR [cm^{-1}]: $\tilde{\nu}$ = 3242 (NH), 2920, 1655, 1598, 1514, 1451, 1342, 1300, 1239, 1183, 1157, 1094, 1066, 1019, 965, 926, 874, 852, 811, 739, 706, 666.

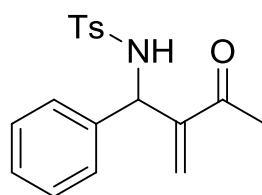


^1H NMR (200 MHz, CDCl_3): δ = 2.13 (3H, s, Me), 2.41 (3H, s, Me), 5.24 (1H, d, J = 9.1 Hz), 6.00 (1H, s), 6.05 (1H, s), 6.08 (1H, s), 7.21 (2H, d, J = 7.8 Hz), 7.30 (4H, m, Ar), 7.61 (2H, J = 7.8 Hz).

^{13}C NMR (CDCl_3 , 75 MHz): δ = 21.56, 26.28, 58.18, 121.55, 127.22, 128.30, 128.56, 129.56, 131.51, 137.35, 138.05, 143.56, 146.13, 198.74.

MS (EI): m/e 351, 340, 339, 338, 255, 254, 252, 155 (MePhSO_2^+), 130, 92, 91 (MePh^+), 65, 43.

IR [cm^{-1}]: $\tilde{\nu}$ = 3277 (NH), 1673 (C=O), 1597, 1486, 1425, 1365, 1325, 1156, 1093, 1069, 1009, 951, 919, 848, 811, 663.



3fa

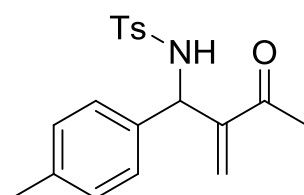
^1H NMR (200 MHz, CDCl_3): δ = 2.17 (3H, s, Me), 2.42 (3H, s, Me), 5.29 (1H, d, J = 8.6 Hz), 5.66 (1H, d, J = 8.6 Hz), 6.09 (1H, s), 6.11 (1H, s), 7.11 (2H, m, Ar), 7.21-7.27 (5H, m, Ar), 7.67 (2H, d, J = 8.1 Hz, Ar).

^{13}C NMR (CDCl_3 , 75 MHz): δ = 21.50, 26.33, 58.97, 126.40, 127.31, 127.63, 128.18, 128.52, 129.50, 137.55, 138.89, 143.34, 146.51, 198.82.

MS (EI): m/e 327, 317, 316, 315, 300, 298, 296, 277, 260, 175, 174, 171, 155, 132, 130, 116, 115, 92, 91, 89, 65, 43.

HRMS (ESI) $[\text{M}-\text{H}]^+$ calc. for $\text{C}_{18}\text{H}_{20}\text{NO}_3\text{S}^+$ req. 330.1158, found 330.1157.

IR [cm^{-1}]: $\tilde{\nu}$ = 3357 (NH), 3262, 1598 (C=O), 1526, 150, 1385, 1300, 1154, 1096, 1019, 902, 813, 729, 704.



3ga

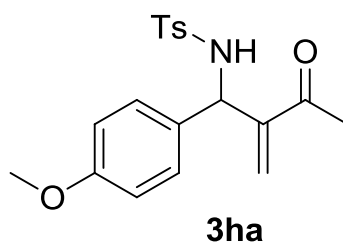
^1H NMR (200 MHz, CDCl_3): δ = 2.15 (3H, s, Me), 2.26 (3H, s, Me), 2.41 (3H, s, Me), 5.26 (1H, d, J = 8.4 Hz), 5.73 (1H, d, J = 8.4 Hz), 6.09 (2H, d, J = 1.0 Hz), 6.86-7.03 (4H, m, Ar), 7.24 (2H, m, Ar), 7.63 (2H, d, J = 8.0 Hz, Ar).

^{13}C NMR (CDCl_3 , 75 MHz): δ = 21.01, 21.54, 26.36, 58.46, 126.39, 127.32, 128.01, 129.21, 129.51, 135.97, 137.37, 137.48, 143.32, 146.64, 198.86.

MS (EI): m/e 344, 343, 342, 275, 274, 273, 188, 155, 118, 91, 65, 43.

HRMS (ESI) $[\text{M}-\text{H}]^+$ calc. for $\text{C}_{19}\text{H}_{20}\text{O}_3\text{NS}$: requires 342.1169, found 342.1172.

IR [cm^{-1}]: $\tilde{\nu}$ = 3278 (NH), 1675, 1598 (C=O), 1514, 1425, 1366, 1326, 1157, 1094, 1060, 1021, 951, 914, 815, 729, 666.



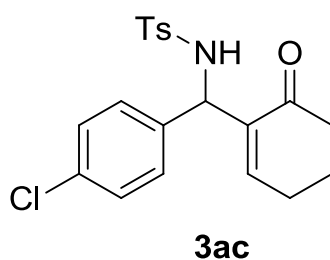
^1H NMR (200 MHz, CDCl_3): δ = 2.16 (3H, s, Me), 2.42 (3H, s, Me), 3.74 (3H, s, Me), 5.24 (1H, d, J = 8.4 Hz, NH), 5.60 (1H, d, J = 8.4 Hz, CH), 6.09 (2H, m), 6.72 (2H, d, J = 8.2 Hz, Ar), 6.99 (2H, d, J = 8.8 Hz, Ar), 7.25 (2H, d, J = 8.0 Hz, Ar), 7.65 (2H, d, J = 8.2 Hz, Ar).

^{13}C NMR (CDCl_3 , 75 MHz): δ = 21.50, 26.36, 55.23, 58.26, 113.90, 127.31, 127.71, 127.73, 129.50, 131.02, 137.51, 143.31, 146.78, 159.03, 198.85.

MS (EI): m/e 360, 359, 358, 332, 322, 321, 316, 306, 290, 205, 204, 155, 134, 109, 91, 65, 43.
IR [cm^{-1}]: $\tilde{\nu}$ = 3282 (NH), 1669, 1611 (C=O), 1512, 1443, 1324, 1304, 1272, 1257, 1235, 1179, 1159, 1094, 1068, 1031, 961, 834, 815, 783, 725, 664.

3.2 Synthetical data for the reaction of cyclohexenone (2b) with different tosylimines

Cyclohexenone (**2b**, 4.0 eq), tosylimine (**1b-i**, 1.0 eq) and **4f** (25 mol%) as a catalyst were mixed in chloroform. The reaction was monitored by ^1H NMR until the disappearance of the tosylimine was observed. The reaction mixture was directly subjected to silica gel column chromatography and eluted with ethyl acetate / isohexane = 1 / 4 to give the corresponding azaMBH product.



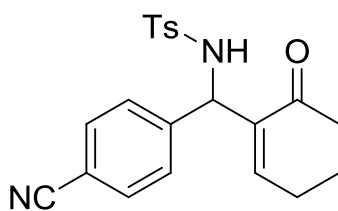
^1H NMR (CDCl_3 , 200 MHz): δ = 1.62-1.74 (1H, m), 1.77-1.90 (1H, m), 2.03-2.17 (2H, m, CH_2), 2.20-2.35 (2H, m, CH_2), 2.40 (3H, s, Me), 5.05 (1H, d, J = 9.4 Hz), 5.96 (1H, d, J = 9.6 Hz), 6.80 (1H, t, J = 4.4 Hz), 7.09-7.25 (6H, m, Ar), 7.61 (2H, d, J = 7.6 Hz, Ar).

^{13}C NMR (CDCl_3 , 75 MHz): δ = 21.46, 21.96, 25.81, 38.36, 59.16, 127.29, 127.68, 128.48, 129.44, 133.28, 136.61, 137.81, 137.89, 143.30, 149.25, 198.89.

MS (EI): m/e 237, 236, 235, 234, 220, 218, 171, 155, 149, 127, 125, 92, 91, 89, 65.

HRMS (ESI) $[\text{M}-\text{H}]^+$ calc. for $\text{C}_{20}\text{H}_{19}\text{O}_3\text{NClS}$: requires 388.0780, found 388.0785.

IR [cm^{-1}]: $\tilde{\nu}$ = 3262, 2917, 1730, 1649, 1493, 1453, 1338, 1302, 1157, 1090, 1050, 1017, 924, 815, 759, 664.



3bc

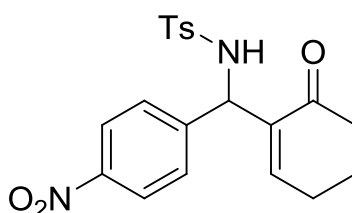
^1H NMR (CDCl_3 , 300 MHz): δ = 1.64-1.74 (1H, m, CH_2), 1.76-1.79 (1H, m, CH_2), 2.05-2.17 (2H, m, CH_2), 2.22-2.30 (2H, m, CH_2), 2.41 (3H, s, Me), 5.09 (1H, s), 6.02 (1H, s), 6.81 (1H, t, J = 3.0 Hz), 7.25 (2H, d, J = 9.0 Hz, Ar), 7.34 (2H, d, J = 9.0 Hz, Ar), 7.51 (2H, d, J = 6.0 Hz, Ar), 7.63 (2H, d, J = 6.0 Hz, Ar).

^{13}C NMR (CDCl_3 , 75 MHz): δ = 21.49, 21.87, 25.84, 38.24, 59.50, 111.27, 118.53, 126.98, 127.23, 129.52, 132.14, 136.07, 137.69, 143.52, 144.64, 150.09, 151.07.

MS (EI): m/e 331, 281, 253, 207, 155 (MePhSO_2^+), 91 (MePh^+).

HRMS (ESI) $[\text{M}-\text{H}]^+$ calc. for $\text{C}_{21}\text{H}_{19}\text{N}_2\text{O}_3\text{S}$: requires 379.1116, found: 379.1123.

IR [cm^{-1}]: $\tilde{\nu}$ = 3265 (NH), 3300, 2954, 2924, 2225, 1662 (C=O), 1606, 1598, 1501, 1495, 1423, 1396, 1330, 1305, 1287, 1248, 1160, 1094, 1079, 1043, 1018, 980, 927, 906, 876, 865, 826, 811, 733, 706.



3cc

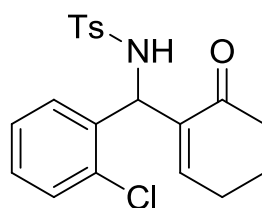
^1H NMR (CDCl_3 , 200 MHz): δ = 1.63-1.70 (1H, m), 1.79-1.87 (1H, m), 2.04-2.13 (2H, m, CH_2), 2.20-2.36 (2H, m, CH_2), 2.40 (3H, s, Me), 5.14 (1H, d, J = 9.4 Hz), 6.09 (1H, d, J = 9.4 Hz), 6.83 (1H, t, J = 4.2 Hz), 7.25 (2H, d, J = 6.8 Hz, Ar), 7.39 (2H, d, J = 8.8 Hz, Ar), 7.63 (2H, d, J = 8.4 Hz, Ar), 8.05 (2H, d, J = 7.0 Hz, Ar).

^{13}C NMR (CDCl_3 , 75 MHz): δ = 21.47, 21.87, 25.85, 38.21, 59.23, 123.52, 127.17, 127.23, 129.55, 136.10, 137.63, 143.61, 146.65, 147.10, 150.20, 198.77.

MS (EI): m/e 400, 398, 378, 350, 316, 305, 246, 245, 229, 199, 155, 115, 91, 65.

HRMS (ESI) $[\text{M}-\text{H}]^+$ calc. for $\text{C}_{20}\text{H}_{19}\text{O}_5\text{N}_2\text{S}$: requires 399.1020, found 399.1024.

IR [cm^{-1}]: $\tilde{\nu}$ = 3242, 2917, 2849, 1730, 1649, 1598, 1516, 1469, 1457, 1344, 1179, 1159, 1094, 1046, 967, 852, 813, 719, 664.



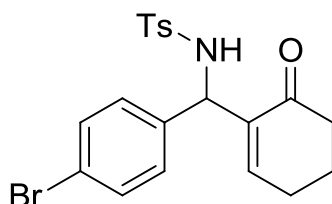
3dc

^1H NMR (CDCl_3 , 300 MHz): δ = 1.75-1.83 (2H, m, CH_2), 2.16-2.30 (4H, m, CH_2), 2.36 (1H, s, Me), 5.53 (1H, d, J = 6.0 Hz), 6.13 (1H, d, J = 6.0 Hz), 7.02-7.33 (6H, m), 7.42-7.44 (1H, m, Ar), 7.62 (2H, d, J = 6.0 Hz, Ar).

^{13}C NMR (CDCl_3 , 75 MHz): δ = 21.44, 21.51, 25.83, 38.47, 56.24, 126.44, 126.71, 127.23, 128.52, 129.21, 129.31, 129.48, 129.68, 132.42, 135.77, 136.38, 143.13, 150.14, 199.0.

HRMS (ESI) $[\text{M}+\text{Na}]^+$ calc. for $\text{C}_{20}\text{H}_{20}\text{ClNNaO}_3\text{S}$: requires 412.0750, found: 412.0743.

IR [cm^{-1}]: $\tilde{\nu}$ = 3260 (NH), 2953, 2922, 2854, 1675, 1594, 1575, 1494, 1472, 1438, 1379, 1328, 1306, 1286, 1258, 1154, 1136, 1088, 1078, 1037, 980, 952, 913, 854, 815, 756, 744, 715, 705, 699, 608.



3ec

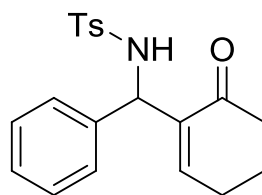
^1H NMR (CDCl_3 , 300 MHz): δ = 1.61-1.74 (1H, m, CH_2), 1.78-1.88 (1H, m, CH_2), 2.07-2.10 (2H, m, CH_2), 2.20-2.28 (2H, m, CH_2), 2.41 (3H, s, Me), 5.03 (1H, d, J = 6.9 Hz), 5.99 (1H, d, J = 6.9 Hz), 6.80 (1H, t, J = 3.3 Hz), 7.06 (2H, d, J = 6.3 Hz, Ar), 7.23 (2H, d, J = 6.3 Hz, Ar), 7.33 (2H, d, J = 6.3 Hz, Ar), 7.61 (2H, d, J = 6.3 Hz, Ar).

^{13}C NMR (CDCl_3 , 75 MHz): δ = 21.48, 21.93, 25.80, 38.33, 59.15, 121.372, 127.26, 128.02, 129.44, 131.40, 136.49, 137.72, 138.38, 143.31, 149.33, 198.87.

MS (EI): m/e 334, 281, 207, 183 ($\text{MePhSO}_2\text{NHCH}_2^+$), 171 ($\text{MePhSO}_2\text{NH}_2^+$), 155 (MePhSO_2^+), 91 (MePh^+).

HRMS (ESI) $[\text{M}]^+$ calc. for $\text{C}_{20}\text{H}_{24}\text{O}_3\text{N}_2\text{BrS}$: requires 451.0691, found: 451.0687.

IR [cm^{-1}]: $\tilde{\nu}$ = 3356 (NH), 3259, 3187, 2925, 2865, 1668 (C=O), 1597, 1527, 1486, 1454, 1423, 1387, 1335, 1303, 1286, 1158, 1092, 1078, 1051, 1007, 980, 957, 933, 917, 905, 814, 797, 736, 708, 688, 660, 633.



3fc

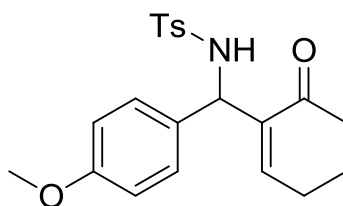
^1H NMR (CDCl_3 , 200 MHz): δ = 1.61-1.69 (1H, m), 1.77-1.85 (1H, m), 2.02-2.13 (2H, m, CH_2), 2.20-2.32 (2H, m, CH_2), 2.39 (3H, s, Me), 5.11 (1H, d, J = 9.2 Hz), 5.98 (1H, d, J = 9.4 Hz), 6.79 (1H, t, J = 4.2 Hz), 7.15-7.22 (6H, m, Ar), 7.62 (2H, d, J = 8.6 Hz, Ar)

^{13}C NMR (CDCl_3 , 150 MHz): δ = 21.46, 21.98, 25.79, 38.38, 59.40, 126.27, 127.34, 128.35, 129.40, 129.66, 136.83, 137.88, 139.34, 143.13, 148.95, 198.90.

MS (EI): m/e 355, 354, 323, 317, 316, 308, 201, 200, 171, 155, 115, 91, 65.

HRMS (ESI) $[\text{M}-\text{H}]^+$ calc. for $\text{C}_{20}\text{H}_{20}\text{O}_3\text{NS}$: requires 354.1169, found 354.1173.

IR [cm^{-1}]: $\tilde{\nu}$ = 3258, 2921, 1671, 1657, 1598, 1493, 1451, 1419, 1326, 1308, 1159, 1094, 1052, 975, 902, 813, 698, 970.



3hc

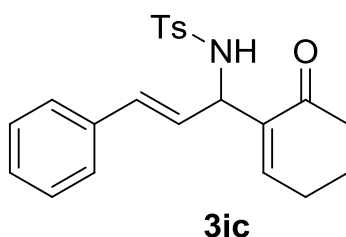
^1H NMR (CDCl_3 , 600 MHz): δ = 1.62-1.69 (1H, m), 1.78-1.85 (1H, m), 2.03-2.13 (2H, m, CH_2), 2.21-2.32 (2H, m, CH_2), 2.40 (3H, s, Me), 3.74 (3H, s, Me), 5.06 (1H, d, J = 9.2 Hz), 5.89 (1H, d, J = 9.4 Hz), 6.72-6.78 (2H, m), 6.82 (1H, s), 7.06 (2H, d, J = 6.8 Hz), 7.22 (2H, d, J = 8.6 Hz, Ar), 7.62 (2H, d, J = 8.2 Hz, Ar).

^{13}C NMR (CDCl_3 , 150 MHz): δ = 21.46, 22.02, 25.78, 38.42, 55.22, 58.92, 113.73, 127.35, 127.53, 129.38, 131.49, 136.98, 137.87, 143.08, 148.61, 158.85, 198.96.

MS (EI): m/e 385, 320, 231, 230, 214, 186, 171, 155, 122, 91, 77, 65, 55.

HRMS (ESI) $[\text{M}-\text{H}]^+$ calc. for $\text{C}_{21}\text{H}_{22}\text{O}_4\text{NS}$: requires 384.1275, found 384.1279.

IR [cm^{-1}]: $\tilde{\nu}$ = 3155, 2921, 1671, 1609, 1510, 1437, 1326, 1241, 1159, 1094, 1078, 1054, 1033, 826, 815, 739, 715, 666.



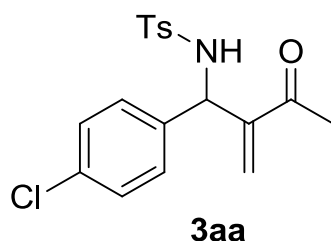
^1H NMR (CDCl_3 , 300 MHz): δ = 1.66-1.78 (1H, m), 1.79-1.93 (1H, m), 2.08-2.22 (2H, m, CH_2), 2.23-2.33 (2H, m, CH_2), 2.35 (3H, s, Me), 4.64 (1H, t, J = 6.0 Hz), 5.85 (1H, d, J = 9.0 Hz), 6.08 (1H, dd, J = 9.0 Hz, J = 6.0 Hz), 6.33 (1H, d, J = 18 Hz), 6.79 (1H, t, J = 6.0 Hz), 7.19-7.28 (6H, m, Ar), 7.69 (2H, d, J = 9.0 Hz, Ar).

^{13}C NMR (CDCl_3 , 75 MHz): δ = 21.40, 22.03, 25.77, 38.37, 59.19, 126.45, 126.48, 127.38, 127.80, 128.40, 129.41, 131.53, 136.15, 143.13, 148.53, 199.11.

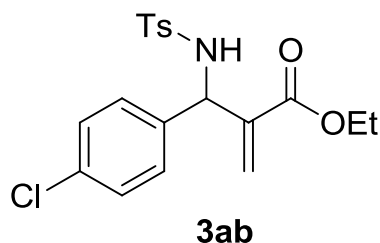
HRMS (ESI) ($\text{M}+\text{Na}$) $^+$ calc. for $\text{C}_{22}\text{H}_{23}\text{NNaO}_3\text{S}$: requires 404.1296, found: 404.1291.

IR [cm^{-1}]: $\tilde{\nu}$ = 3288 (NH), 3026, 2955, 2924, 2867, 1732, 1660, 1596, 1493, 1447, 1426, 1385, 1326, 1304, 1250, 1213, 1160, 1151, 1090, 1028, 974, 914, 883, 841, 815, 757, 747, 698, 632.

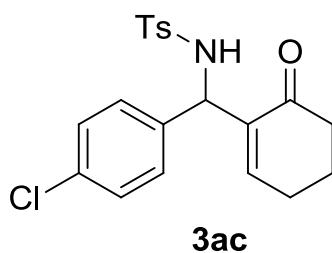
3.3 Analytic data of the products in the kinetic runs (3a – 3d)



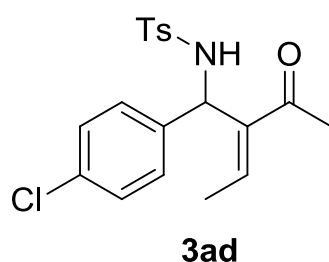
^1H NMR (200 MHz, CDCl_3): δ = 2.15 (3H, s, Me), 2.41 (3H, s, Me), 5.22 (1H, d, J = 8Hz, NH), 5.72 (1H, d, J = 8.4 Hz, CH), 6.05 (1H, s), 6.09 (1H, s), 7.01 (2H, d, J = 8.7Hz, Ar), 7.15 (4H, m, Ar), 7.62 (2H, d, J = 8.0Hz, Ar).



^1H NMR (200 MHz, CDCl_3): δ = 1.13 (3H, t, J =7.1Hz), 2.34 (3H, s), 4.00 (2H, q, J =7.2Hz), 5.29 (1H, d, J =9.2Hz), 5.77 (1H, s), 6.15 (1H, d, J =9.2Hz), 6.17 (1H, s), 7.04 – 7.18 (6H, m), 7.60 (2H, d, J =8.3Hz).



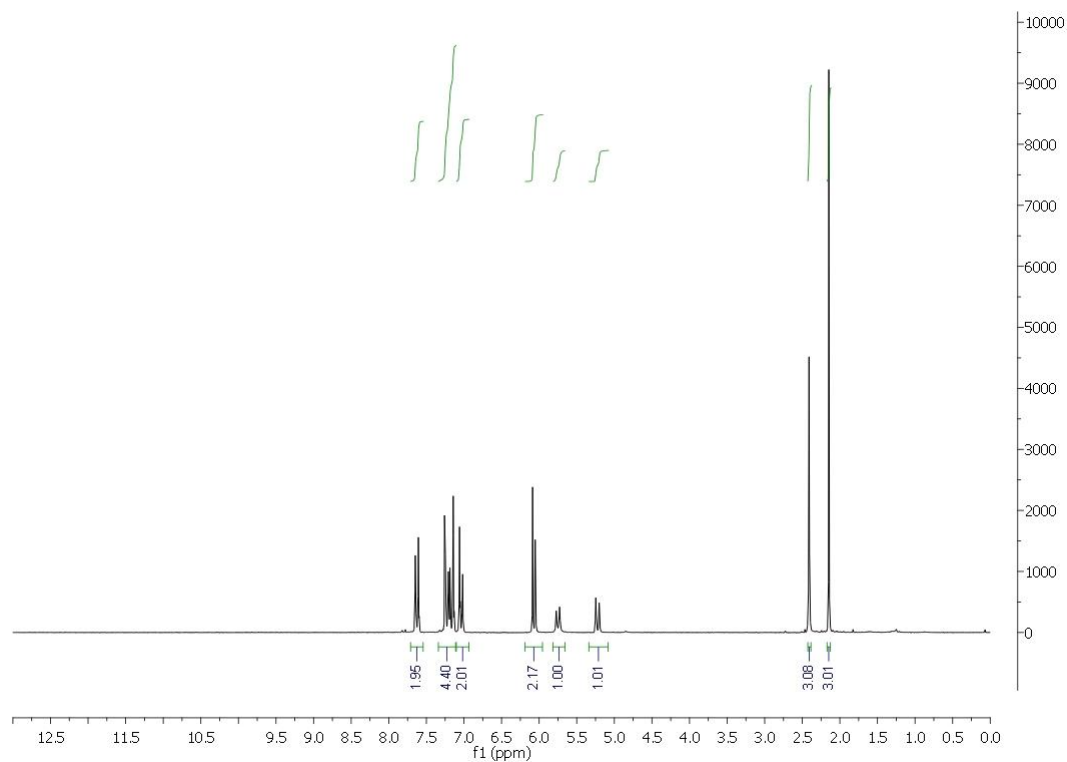
^1H NMR (CDCl_3 , 200 MHz): δ = 1.55-1.96 (2H, m, CH_2), 2.00-2.34 (4H, m, CH_2), 2.41 (3H, s, Me), 5.05 (1H, d, J = 9.4 Hz), 5.96 (1H, d, J = 9.6 Hz), 6.80 (1H, t, J = 4.4 Hz), 7.09-7.27 (6H, m, Ar), 7.61 (2H, d, J = 7.6 Hz, Ar).



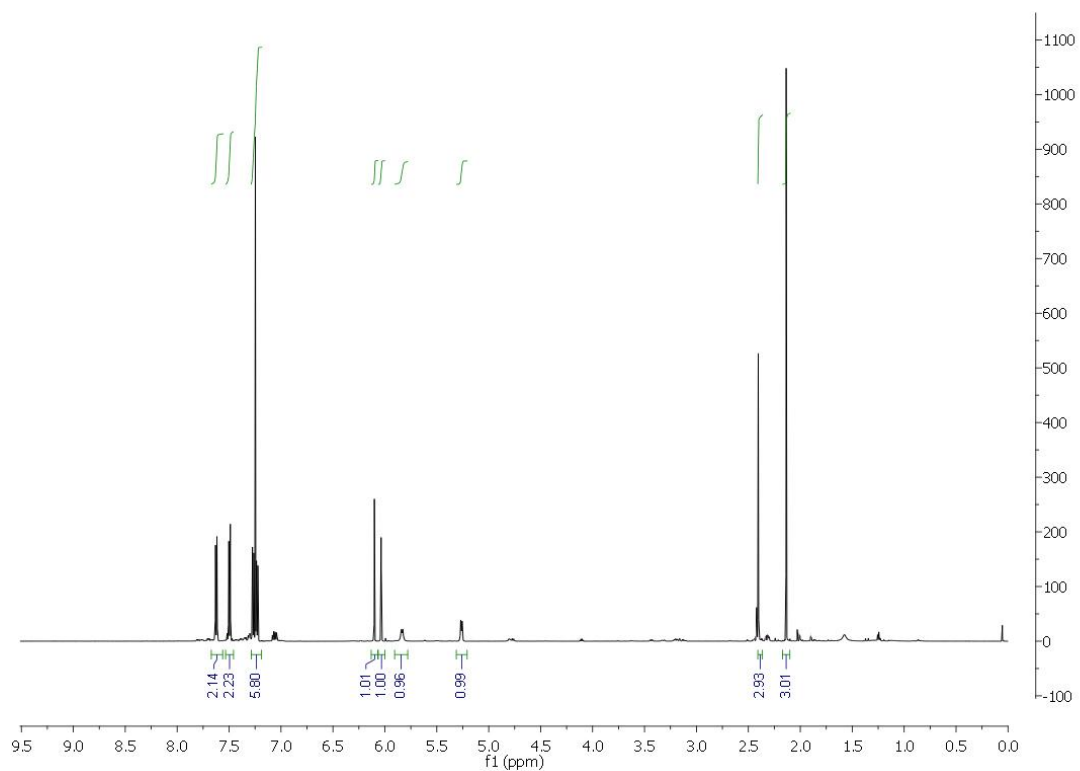
^1H NMR (300 MHz, CDCl_3): δ = 1.91 (3H, d, J = 9.4 Hz, CH_3), 2.02 (3H, s, CH_3), 2.39 (3H, s, CH_3), 5.47 (1H, d, J = 10.3 Hz), 6.39 (1H, d, J = 10.4 Hz, NH), 6.74 (1H, q, J = 7.1 Hz), 7.02-7.33 (6H, m, Ar), 7.62 (2H, d, J = 8.4 Hz, Ar). ^{13}C NMR (75 MHz, CDCl_3): δ = 14.79, 21.46, 25.93, 53.32, 126.40, 126.94, 127.31, 128.46, 129.37, 129.65, 133.05, 137.68, 138.14, 139.94, 142.80, 143.27, 199.65. MS (EI): m/e 91, 155, 222, 223, 224, 225, 296, 297, 298, 334, 344, 346. HRMS (ESI) $[\text{M}-\text{H}]^+$ calc. for $\text{C}_{19}\text{H}_{20}\text{NO}_3\text{SCl}$: requires 378.0925, found: 378.0927. IR [cm^{-1}]: $\tilde{\nu}$ = 3331 (NH), 2954, 1975, 1659, 1598, 1548, 1492, 1415, 1334, 1291, 1162, 1092, 1014, 903, 723, 670.

3.4 ^1H NMR spectra of the synthesized products

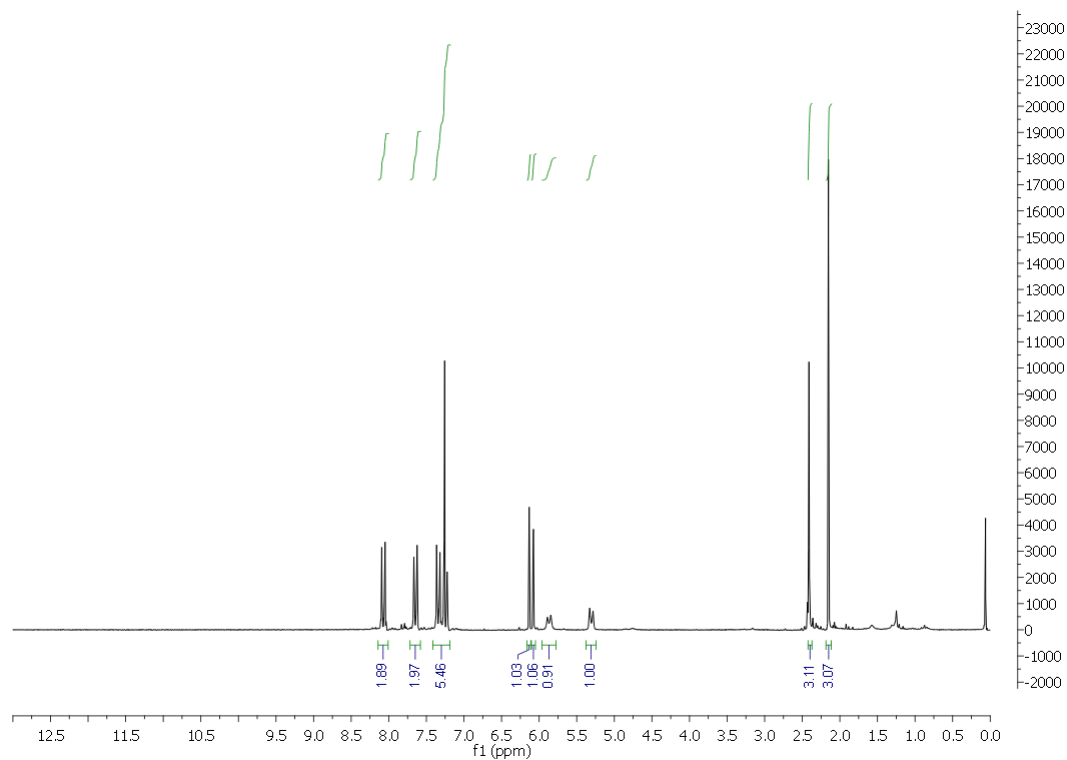
3aa



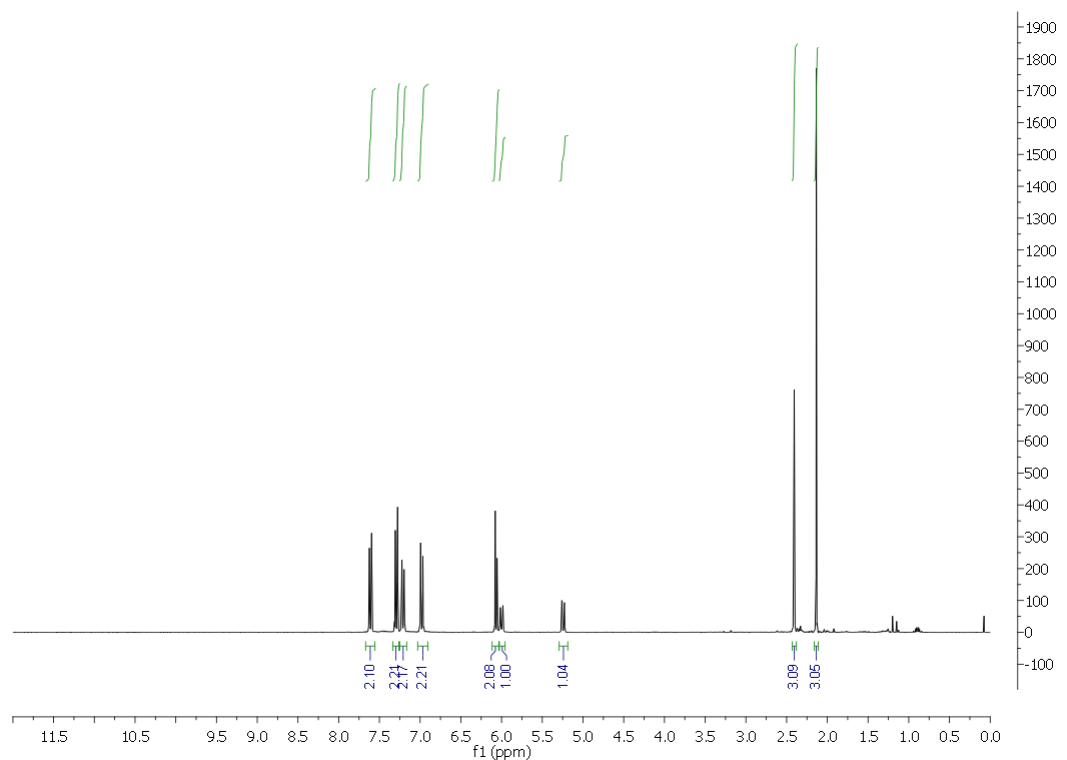
3ba



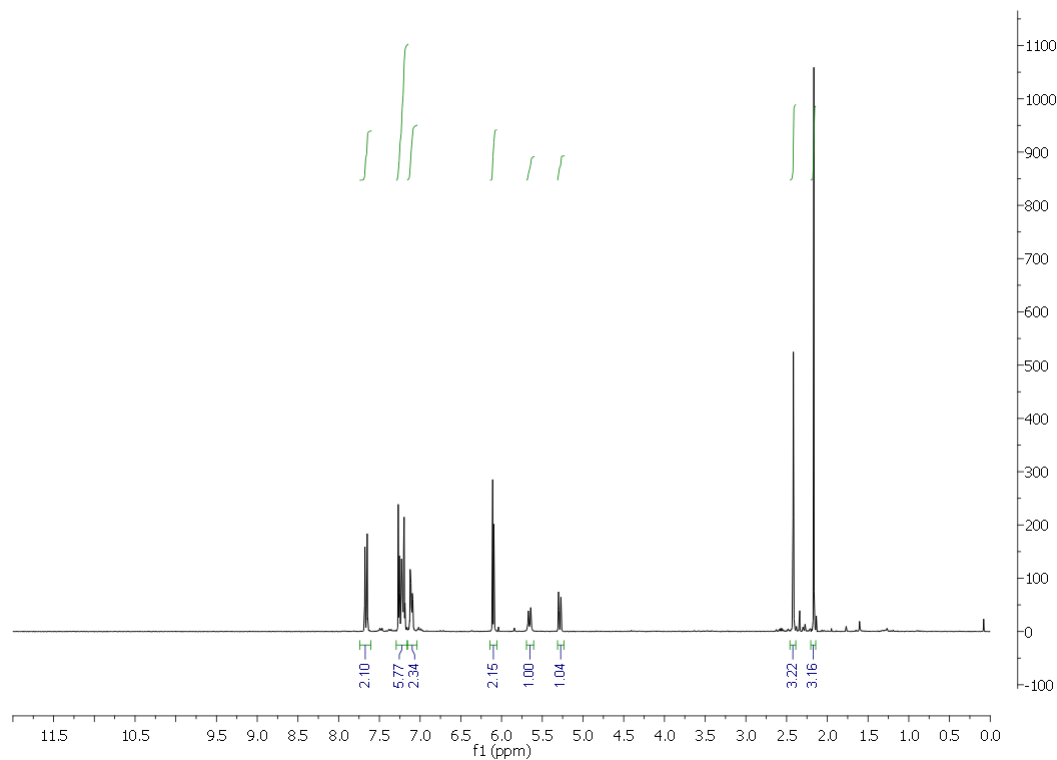
3ca



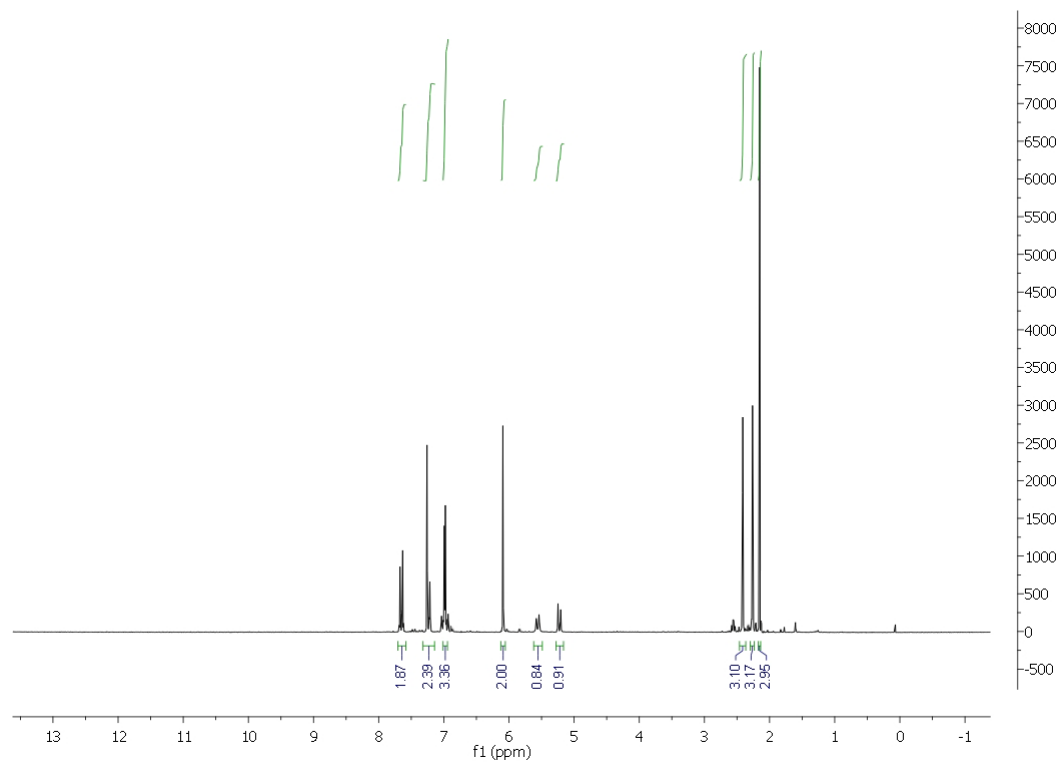
3ea



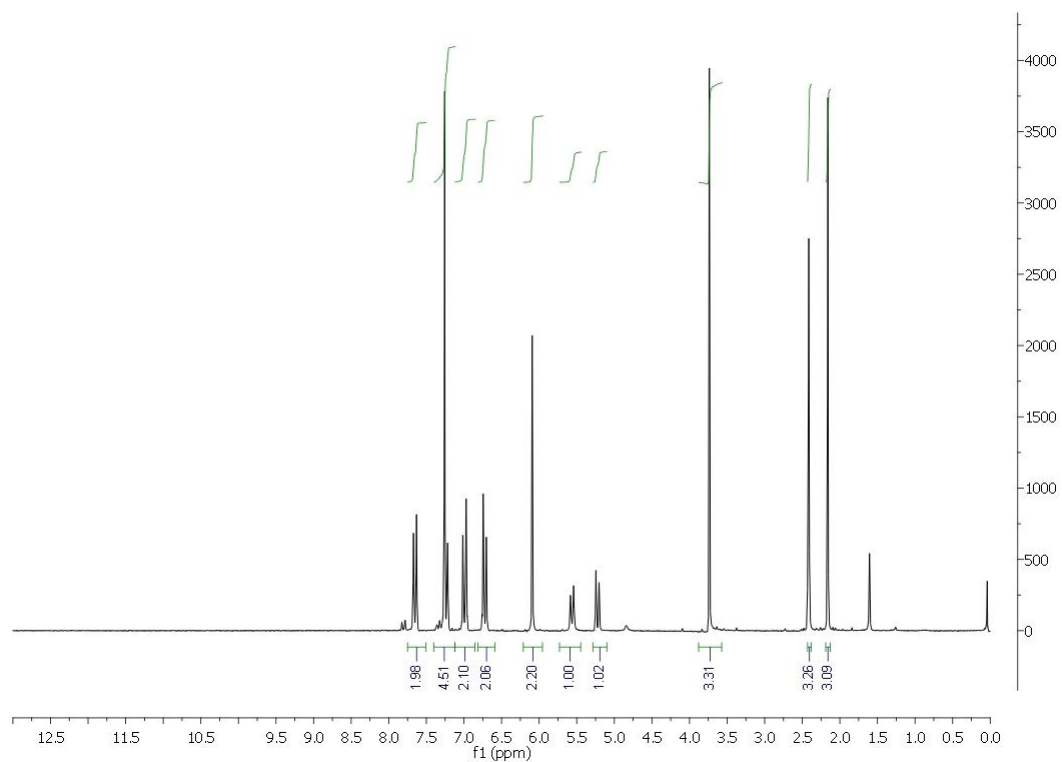
3fa



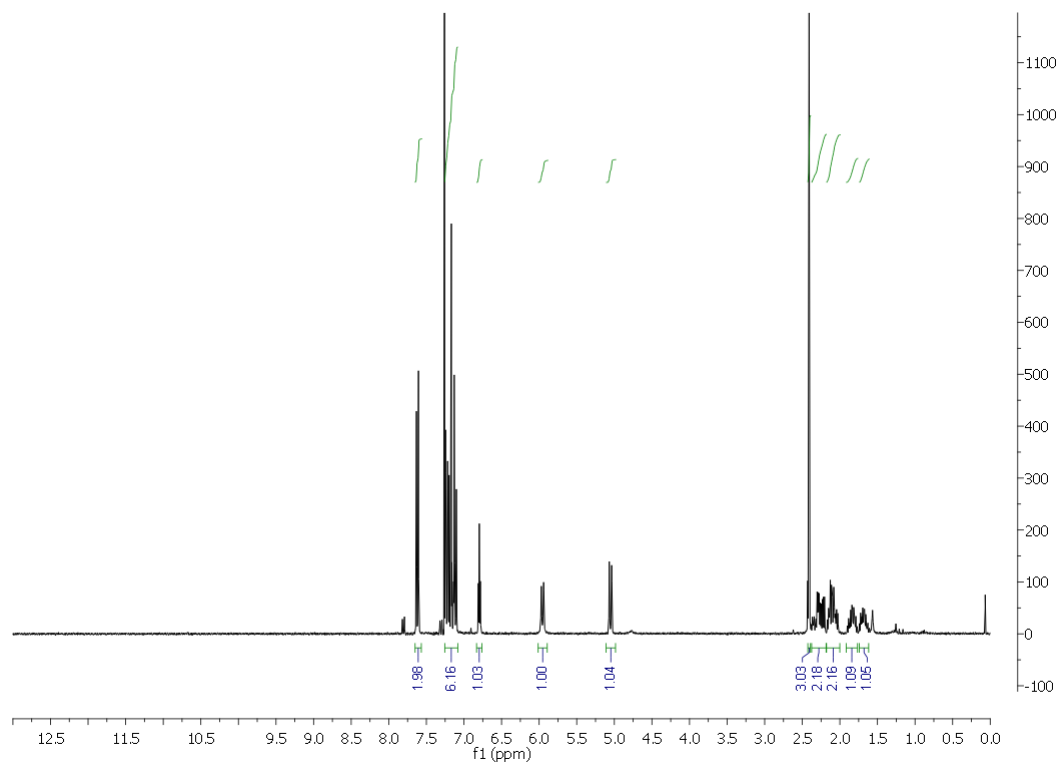
3ga



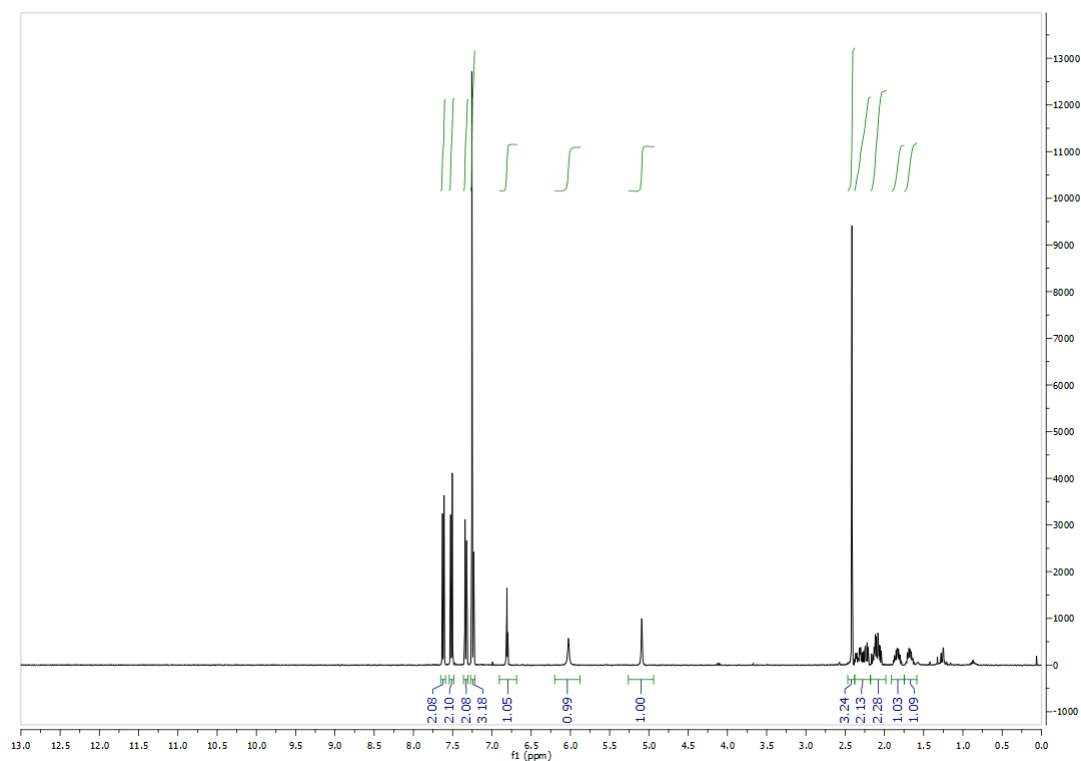
3ha



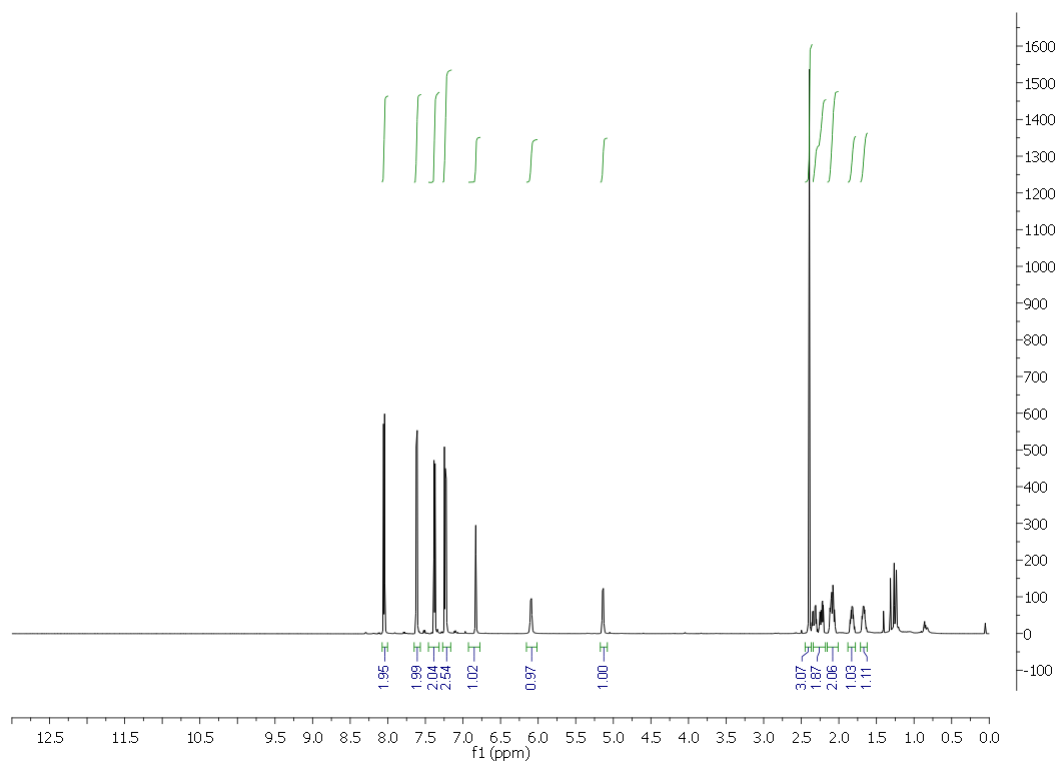
3ac



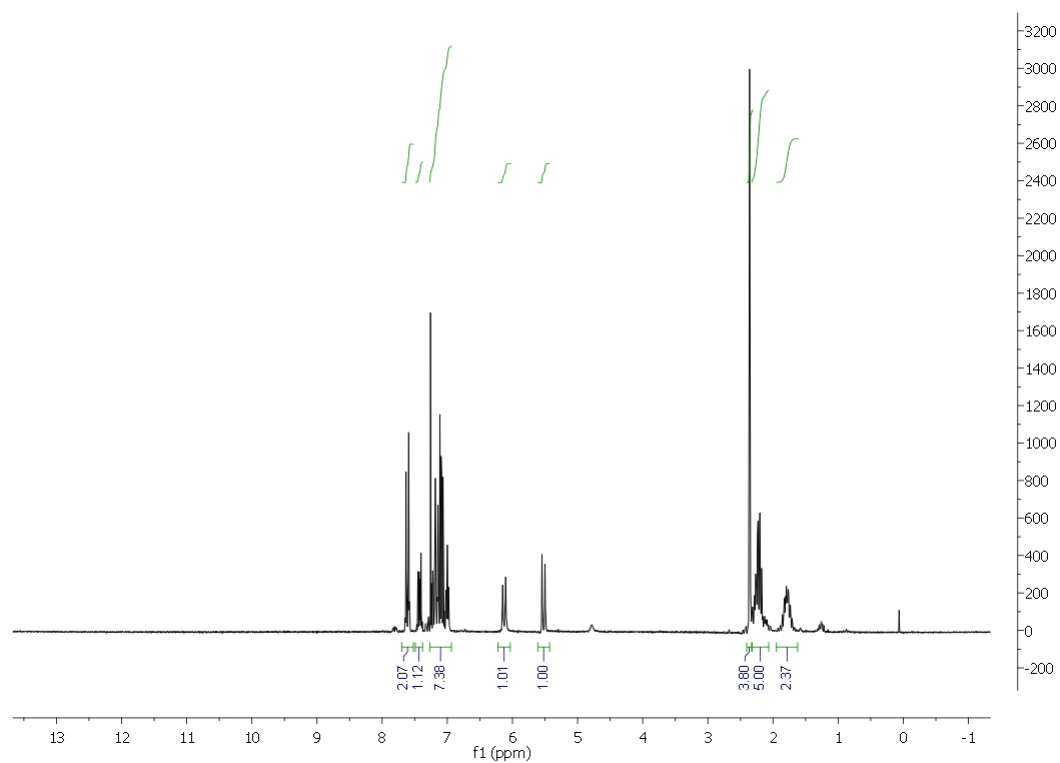
3bc



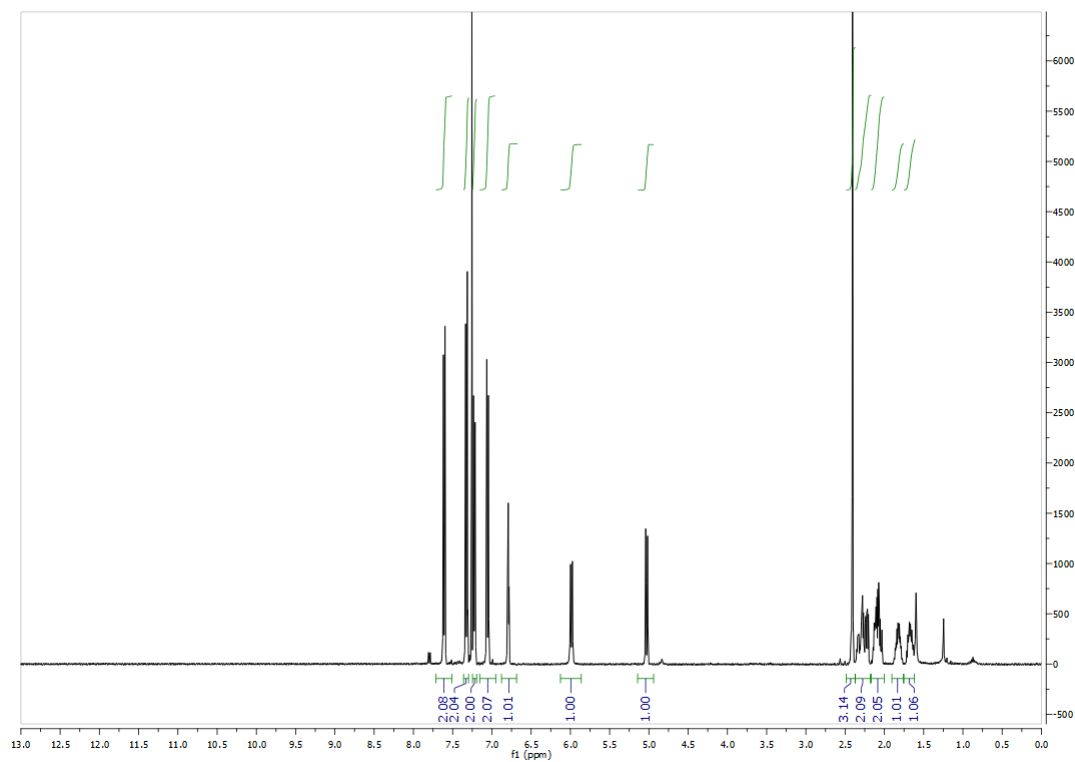
3cc



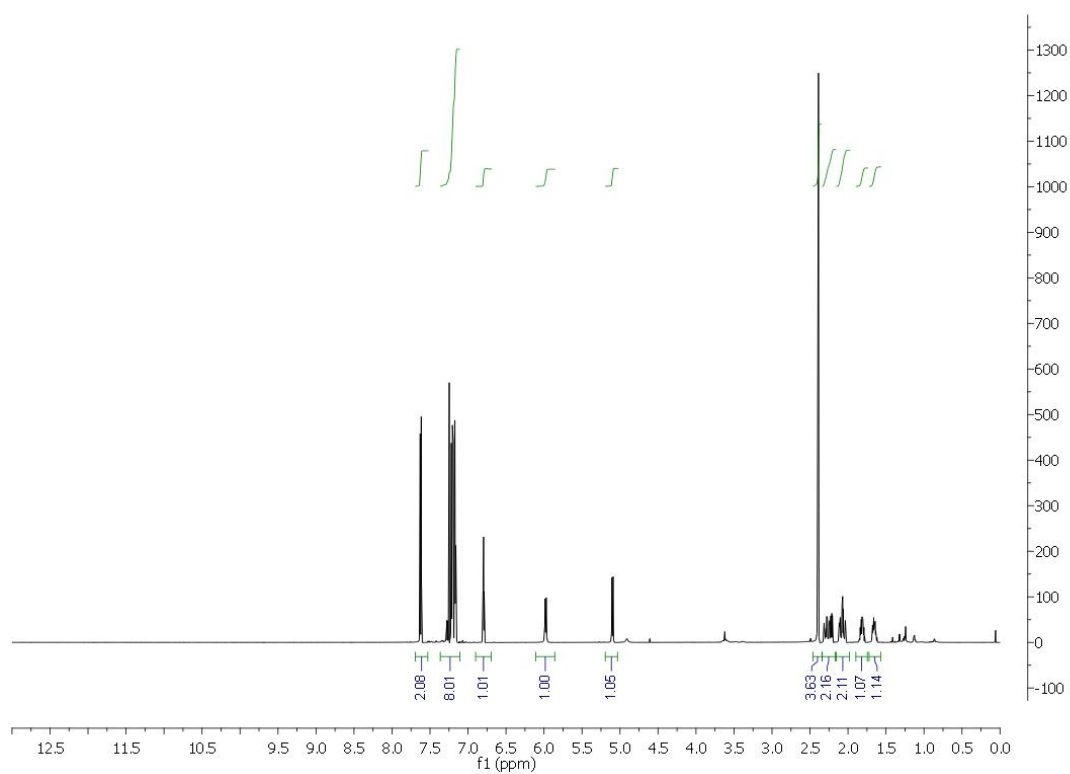
3dc



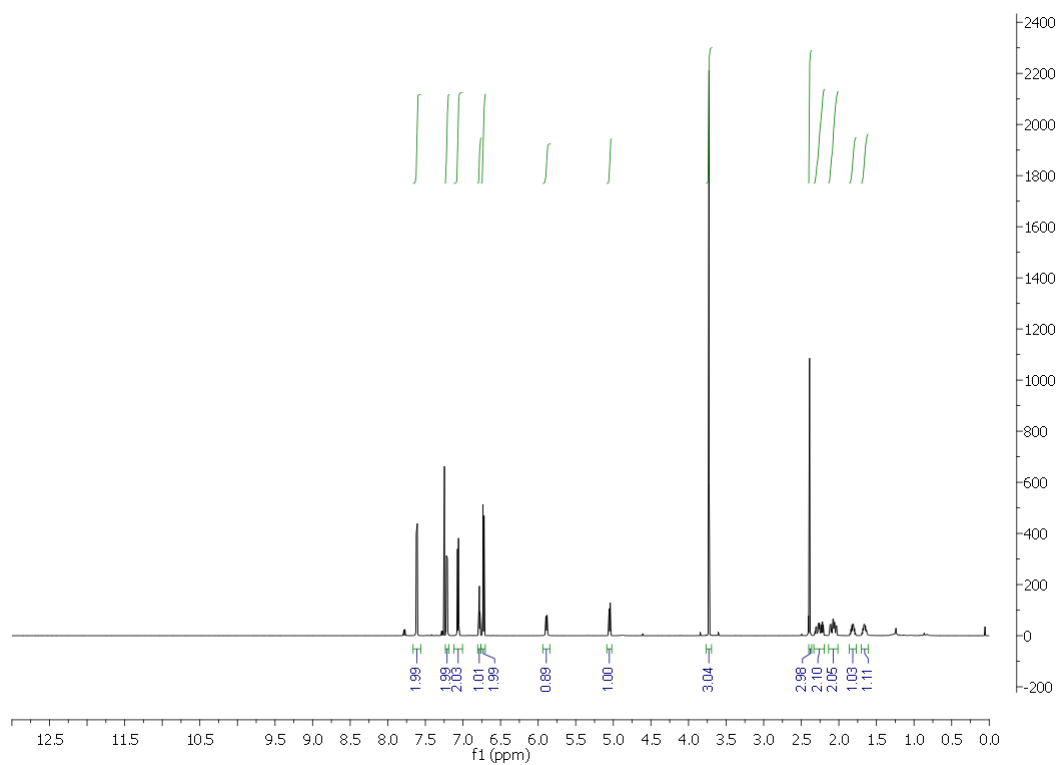
3ec



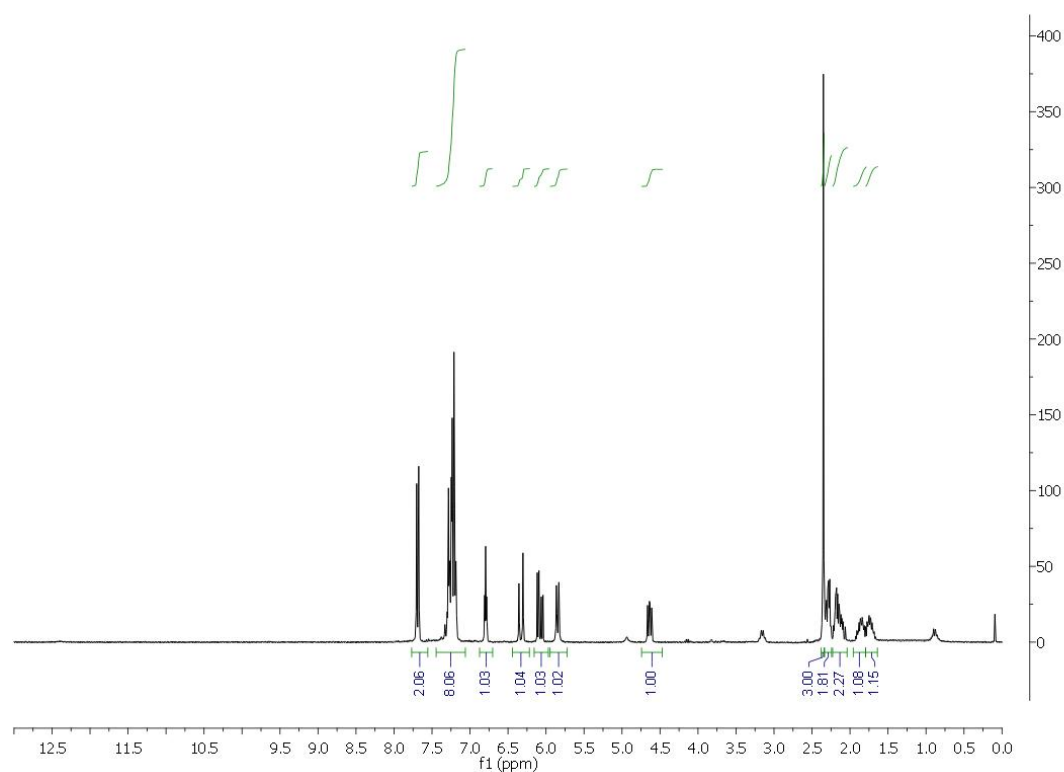
3fc



3hc



3ic



3.5 X-ray analysis of 3ad

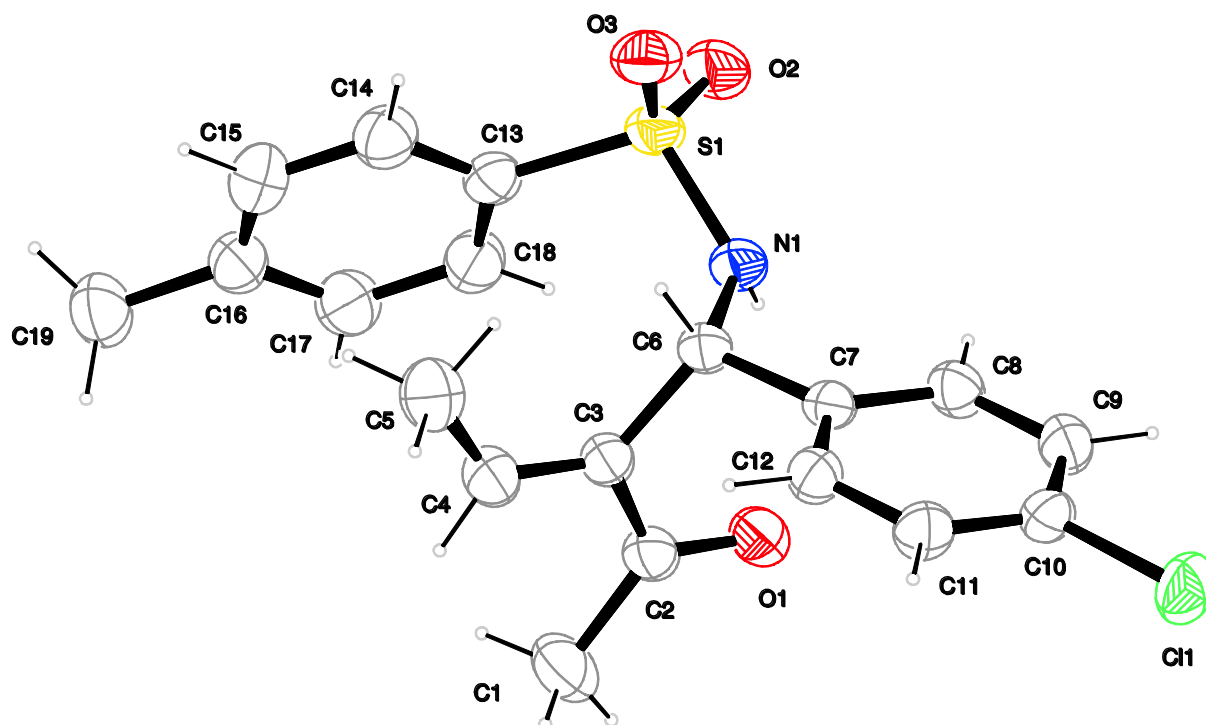


Table S2. Data of the x-ray analysis of 3ad.

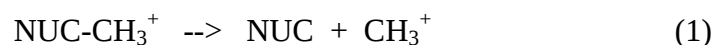
net formula	C ₁₉ H ₂₀ ClNO ₃ S
<i>M_r</i> /g mol ⁻¹	377.886
crystal size/mm	0.33 × 0.29 × 0.27
<i>T</i> /K	173(2)
radiation	MoKα
diffractometer	'KappaCCD'
crystal system	monoclinic
space group	<i>P</i> 2 ₁ / <i>n</i>
<i>a</i> /Å	11.6299(2)
<i>b</i> /Å	12.5750(3)
<i>c</i> /Å	13.4433(2)
α/°	90
β/°	103.9646(13)
γ/°	90
<i>V</i> /Å ³	1907.92(6)
<i>Z</i>	4
calc. density/g cm ⁻³	1.31558(4)
μ/mm ⁻¹	0.327
absorption correction	none
refls. measured	14916
<i>R</i> _{int}	0.0289
mean σ(<i>I</i>)/ <i>I</i>	0.0245
θ range	3.24–27.42
observed refls.	3626
<i>x</i> , <i>y</i> (weighting scheme)	0.0456, 0.6132
hydrogen refinement	mixed
refls in refinement	4332
parameters	233
restraints	0
<i>R</i> (<i>F</i> _{obs})	0.0353
<i>R</i> _w (<i>F</i> ²)	0.0973
<i>S</i>	1.051
shift/error _{max}	0.001
max electron density/e Å ⁻³	0.305
min electron density/e Å ⁻³	–0.296

C-bound H: constr., N-bound H: refall.

4. Computational methods and data

4.1 MCA values

Methyl cation affinities of pyridine and phosphane bases have been calculated as the reaction enthalpy at 298.15 K and 1 atm pressure for the methyl cation detachment reaction shown in eqn. (1). This is in analogy to the mass spectrometric definition of proton affinities.



The geometries of all species in eqn. (1) have been optimized at the B98/6-31G(d) level of theory. The conformational space of flexible pyridines and phosphanes and the corresponding cations has been searched using the MM3* force field and the systematic search routine implemented in MACROMODEL 9.7.¹⁶ All stationary points located at force field level have then been reoptimized at B98/6-31G(d) level as described before. Thermochemical corrections to 298.15 K have been calculated for all minima from unscaled vibrational frequencies obtained at this same level. The thermochemical corrections have been combined with single point energies calculated at the MP2(FC)/6-31+G(2d,p)//B98/6-31G(d) level to yield enthalpies H_{298} at 298.15 K. In conformationally flexible systems enthalpies have been calculated as Boltzmann-averaged values over all available conformers. This procedure has recently been found to reproduce G3 methyl cation affinity values of selected small and medium sized organocatalysts within 4.0 kJ mol⁻¹.¹⁴ All quantum mechanical calculations have been performed with Gaussian 03.¹⁶

Table S3 Total energies and enthalpies (in Hartree) as calculated at the B98/6-31G(d) and MP2(FC)/6-31+G(2d,p)// B98/6-31G(d) level of theory for all systems. If more than one conformer exist at 298.15 K, the single values of each conformer are denoted as well as the Boltzmann-averaged values for H_{298} at MP2(FC)/6-31+G(2d,p)//B98/6-31G(d) level of theory. Only conformers are included with a Boltzmann-weighting of at least 1 % up to a maximum to ten conformations per system.

	B98/6-31G(d)		MP2(FC)/6-31+G(2d,p)// B98/6-31G(d)	
system	E_{tot}	H_{298}	E_{tot}	H_{298}
CH_3^+				-39.316929
CH_3^+	-39.462922	-39.427481	-39.352370	-39.316929
4a				-344.154707
4a_1	-345.194968	-345.003513	-344.346163	-344.154707
4a-Me⁺				-383.685759
4a-Me⁺_1	-384.879826	-384.643824	-383.921760	-383.685759
4b				-381.007963
4b_1	-382.100964	-381.928966	-381.179961	-381.007963
4b-Me⁺				-420.546252
4b-Me⁺_1	-421.801455	-421.585450	-420.762257	-420.546252
4c				-459.337226
4c_1	-460.699626	-460.467717	-459.569493	-459.337583
4c_2	-460.698872	-460.467017	-459.568777	-459.336921
4c_3	-460.695706	-460.463514	-459.566589	-459.334396
4c_4	-460.695601	-460.463698	-459.566199	-459.334296
4c_5	-460.688598	-460.457621	-459.563361	-459.332384
4c-Me⁺				-498.878535
4c-Me⁺_1	-500.402853	-500.126900	-499.155074	-498.879121
4c-Me⁺_2	-500.401457	-500.125500	-499.153700	-498.877743
4c-Me⁺_3	-500.401457	-500.125499	-499.153699	-498.877741
4c-Me⁺_4	-500.401452	-500.125503	-499.153680	-498.877730

4c-Me⁺_5	-500.398591	-500.122432	-499.150782	-498.874623
4d				458.174353
4d_1	-459.498999	-459.289442	-458.383909	-458.174353
4d-Me⁺				-497.716038
4d-Me⁺_1	-499.203048	-498.949398	-497.969688	-497.716038
4e				-591.693361
4e_1	-593.418065	-593.130882	-591.981253	-591.694070
4e_2	-593.417089	-593.130032	-591.980205	-591.693148
4e_3	-593.416648	-593.129503	-591.979900	-591.692755
4e_4	-593.415838	-593.128722	-591.978867	-591.691751
4e_5	-593.415488	-593.128356	-591.979018	-591.691886
4e_6	-593.415277	-593.127873	-591.978972	-591.691568
4e_7	-593.414082	-593.126927	-591.977705	-591.690550
4e-Me⁺				-631.242261
4e-Me⁺_1	-633.129214	-632.797785	-631.574118	-631.242689
4e-Me⁺_2	-633.129077	-632.797925	-631.573803	-631.242651
4e-Me⁺_3	-633.128021	-632.796615	-631.572771	-631.241365
4e-Me⁺_4	-633.127946	-632.796535	-631.572692	-631.241281
4e-Me⁺_5	-633.127843	-632.796281	-631.572934	-631.241371
4e-Me⁺_6	-633.126370	-632.794816	-631.571168	-631.239614
4e-Me⁺_7	-633.125330	-632.793715	-631.570008	-631.238393
4f				-747.191944
4f_1	-749.405682	-749.021776	-747.576377	-747.192470
4f_2	-749.407023	-749.022449	-747.576974	-747.192400
4f_3	-749.404877	-749.020263	-747.576944	-747.192329
4f_4	-749.405930	-749.021754	-747.576291	-747.192115
4f_5	-749.406234	-749.021772	-747.576561	-747.192098
4f_6	-749.404995	-749.020441	-747.576374	-747.191820
4f_7	-749.404598	-749.020095	-747.576157	-747.191654
4f_8	-749.404606	-749.020080	-747.576166	-747.191641

4f_9	-749.404830	-749.020098	-747.576215	-747.191483
4f_10	-749.406393	-749.021713	-747.576140	-747.191460
4f-Me⁺				-786.743479
4f-Me⁺_1	-789.121780	-788.692940	-787.173377	-786.744537
4f-Me⁺_2	-789.120016	-788.691557	-787.171915	-786.743456
4f-Me⁺_3	-789.120407	-788.691692	-787.172037	-786.743323
4f-Me⁺_4	-789.120407	-788.691688	-787.172038	-786.743319
4f-Me⁺_5	-789.119194	-788.690414	-787.171900	-786.743119
4f-Me⁺_6	-789.118810	-788.690096	-787.171405	-786.742691
4f-Me⁺_7	-789.118811	-788.690086	-787.171398	-786.742672
4f-Me⁺_8	-789.119475	-788.691090	-787.170972	-786.742587
4f-Me⁺_9	-789.119294	-788.690807	-787.170819	-786.742332
4f-Me⁺_10	-789.118385	-788.689728	-787.170896	-786.742240
4k				-535.355098
4k_1	-536.905604	-536.658613	-535.602351	-535.355360
4k_2	-536.904889	-536.657992	-535.601147	-535.354250
4k-Me⁺				-574.901592
4k-Me⁺_1	-576.614364	-576.323195	-575.192993	-574.901824
4k-Me⁺_2	-576.613741	-576.322527	-575.192298	-574.901084
4l				-645.721376
4l_1	-647.539246	-647.256369	-646.004511	-645.721634
4l_2	-647.537517	-647.254755	-646.002984	-645.720222
4l-Me⁺				-685.273939
4l-Me⁺_1	-687.253802	-686.926838	-685.601105	-685.274140
4l-Me⁺_2	-687.253201	-686.926208	-685.600563	-685.273570
4m				-724.049255
4m_1	-726.136622	-725.794008	-724.392585	-724.049971
4m_2	-726.135261	-725.792675	-724.391022	-724.048436
4m_3	-726.134093	-725.791344	-724.390368	-724.047619
4m_4	-726.133773	-725.791105	-724.389136	-724.046468

4m_5	-726.133843	-725.791423	-724.389524	-724.047104
4m_6	-726.132311	-725.789756	-724.388635	-724.046080
4m_7	-726.132623	-725.790069	-724.388834	-724.046280
4m_8	-726.132578	-725.790061	-724.388529	-724.046012
4m_9	-726.131575	-725.788592	-724.388232	-724.045249
4m_10	-726.130711	-725.787685	-724.387694	-724.044668
4m-Me⁺				-763.602939
4m-Me⁺_1	-765.851994	-765.465346	-763.990563	-763.603916
4m-Me⁺_2	-765.850785	-765.463869	-763.989319	-763.602403
4m-Me⁺_3	-765.850315	-765.463344	-763.989001	-763.602030
4m-Me⁺_4	-765.849640	-765.463028	-763.988190	-763.601579
4m-Me⁺_5	-765.850795	-765.463913	-763.989104	-763.602221
4m-Me⁺_6	-765.849161	-765.462332	-763.987775	-763.600947
4m-Me⁺_7	-765.849609	-765.462936	-763.988073	-763.601401
4m-Me⁺_8	-765.849628	-765.462808	-763.988274	-763.601454
4m-Me⁺_9	-765.848774	-765.461441	-763.987533	-763.600200
4m-Me⁺_10	-765.848364	-765.461579	-763.986967	-763.600182
4n				-1106.348047
4n_1	-1109.447043	-1108.993196	-1106.802424	-1106.348577
4n_2	-1109.447132	-1108.993055	-1106.802354	-1106.348278
4n_3	-1109.447628	-1108.993564	-1106.802303	-1106.348239
4n_4	-1109.447585	-1108.993563	-1106.802088	-1106.348066
4n_5	-1109.447026	-1108.992980	-1106.801891	-1106.347844
4n_6	-1109.446406	-1108.992420	-1106.801637	-1106.347651
4n_7	-1109.447786	-1108.993676	-1106.802326	-1106.348216
4n_8	-1109.444983	-1108.991221	-1106.800827	-1106.347065
4n_9	-1109.448248	-1108.994131	-1106.802136	-1106.348019
4n_10	-1109.446099	-1108.991892	-1106.800767	-1106.346560
4n-Me⁺				-1145.907501
4n-Me⁺_1	-1149.167468	-1148.669290	-1146.406434	-1145.908256

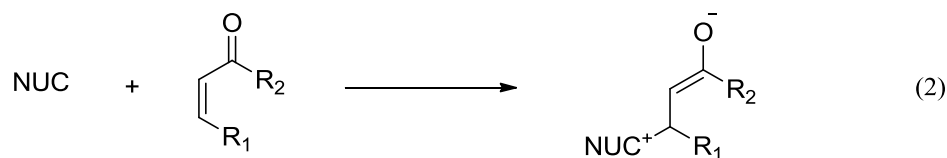
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4n-Me⁺_4	-1149.166725	-1148.668311	-1146.404532	-1145.906118
4n-Me⁺_5	-1149.166180	-1148.667997	-114.640404	-1145.905857
4n-Me⁺_6	-1149.165179	-1148.666903	-1146.403228	-1145.904953
4n-Me⁺_7	-1149.165420	-1148.667213	-1146.403135	-1145.904928
4n-Me⁺_8	-1149.165655	-1148.667434	-1146.402799	-1145.904578
4n-Me⁺_9	-1149.165740	-1148.667407	-1146.402253	-1145.903920
4n-Me⁺_10	-1149.166086	-1148.667599	-1146.402329	-1145.903842
5a				-1033.516761
5a_1	-1035.959965	-1035.669422	-1033.807304	-1033.516761
5a-Me⁺				-1073.069353
5a-Me⁺_1	-1075.664367	-1075.331813	-1073.401907	-1073.069353
5b				-1376.142423
5b_1	-1379.403368	-1379.006497	-1376.539446	-1376.142574
5b_2	-1379.403378	-1379.006406	-1376.539530	-1376.142557
5b_3	-1379.403408	-1379.006460	-1376.539468	-1376.142520
5b_4	-1379.403386	-1379.006524	-1376.539360	-1376.142497
5b_5	-1379.403502	-1379.006618	-1376.539348	-1376.142464
5b_6	-1379.403409	-1379.006481	-1376.539381	-1376.142453
5b_7	-1379.403429	-1379.006643	-1376.539162	-1376.142376
5b_8	-1379.403371	-1379.006555	-1376.539186	-1376.142370
5b_9	-1379.403382	-1379.006546	-1376.539186	-1376.142350
5b_10	-1379.403416	-1379.006513	-1376.539173	-1376.142270
5b-Me⁺				-1415.707295
5b-Me⁺_1	-1419.122130	-1418.683158	-1416.146484	-1415.707512
5b-Me⁺_2	-1419.122205	-1418.683155	-1416.146511	-1415.707461
5b-Me⁺_3	-1419.121974	-1418.682914	-1416.146302	-1415.707242
5b-Me⁺_4	-1419.121735	-1418.682791	-1416.146082	-1415.707138
5b-Me⁺_5	-1419.121543	-1418.682512	-1416.145847	-1415.706816

5c				-1167.026662
5c_1	-1169.875117	-1169.506790	-1167.395027	-1167.026700
5c_2	-1169.875052	-1169.506757	-1167.394914	-1167.026619
5c-Me⁺				-1206.589817
5c-Me⁺_1	-1209.591454	-1209.180837	-1207.000435	-1206.589817
5d				-2410.678523
5d_1	-2414.583096	-2414.317826	-2410.943810	-2410.678540
5d_2	-2414.583097	-2414.317830	-2410.943772	-2410.678505
5d-Me⁺				-2450.218827
5d-Me⁺_1	-2454.272737	-2453.965773	-2450.525791	-2450.218827
5e				-1037.018000
5e_1	-1039.588309	-1039.226223	-1037.380450	-1037.018364
5e_2	-1039.587282	-1039.225103	-1037.379820	-1037.017641
5e_3	-1039.585366	-1039.223294	-1037.378189	-1037.016118
5e-Me⁺				-1076.574948
5e-Me⁺_1	-1079.295052	-1078.890870	-1076.979439	-1076.575256
5e-Me⁺_2	-1079.294427	-1078.890161	-1076.978010	-1076.573744
5e-Me⁺_3	-1079.292320	-1078.888110	-1076.975735	-1076.571526
5f				-1151.020539
5f_1	-1153.86536	-1153.48674	-1151.39917	-1151.020539
5f-Me⁺				-1190.580046
5f-Me⁺_1	-1193.577178	-1193.156631	-1191.000593	-1190.580046
5g				-1503.500853
5g_1	-1507.53191	-1506.88647	-1504.14647	-1503.501025
5g_2	-1507.53199	-1506.88639	-1504.14652	-1503.500915
5g_3	-1507.53203	-1506.88637	-1504.14654	-1503.500881
5g_4	-1507.53198	-1506.88633	-1504.14651	-1503.500857
5g_5	-1507.53204	-1506.88632	-1504.14655	-1503.500832
5g_6	-1507.53196	-1506.88616	-1504.14652	-1503.500716
5g_7	-1507.53200	-1506.88616	-1504.14648	-1503.500648

5g-Me⁺				-1543.063023
5g-Me⁺_1	-1547.24649	-1546.55898	-1543.75067	-1543.063167
5g-Me⁺_2	-1547.24642	-1546.55893	-1543.75063	-1543.063144
5g-Me⁺_3	-1547.24663	-1546.55895	-1543.75077	-1543.063085
5g-Me⁺_4	-1547.24653	-1546.55894	-1543.75065	-1543.063062
5g-Me⁺_5	-1547.24653	-1546.55886	-1543.75067	-1543.063000
5g-Me⁺_6	-1547.24638	-1546.55867	-1543.75050	-1543.062789
5h				-1151.023123
5h_1	-1153.86154	-1153.48264	-1151.40213	-1151.023231
5h_2	-1153.85706	-1153.47789	-1151.39925	-1151.020076
5h-Me⁺				-1190.572649
5h-Me⁺_1	-1193.56149	-1193.14013	-1190.99428	-1190.572912
5h-Me⁺_2	-1193.55958	-1193.13810	-1190.99324	-1190.571761
5i				-2519.319540
5i_1	-2523.894841	-2523.713559	-2519.500822	-2519.319540
5i-Me⁺				-2558.824665
5i-Me⁺_1	-2563.554775	-2563.331554	-2559.047886	-2558.824665

4.2 Initial addition step of 5a and 4f to the Michael-acceptors (2a, 2b and 2c)

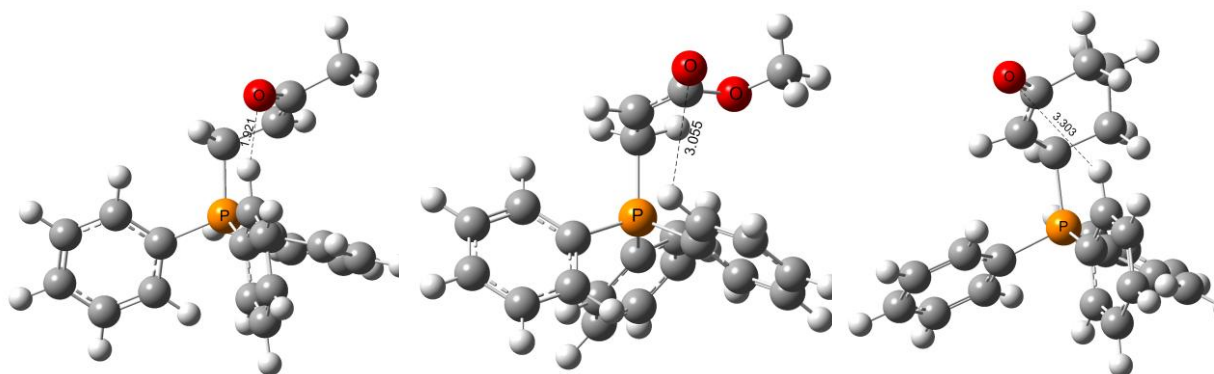
Enthalpies / free energies of the addition step of **4f** and **5a** to different Michael-acceptors (**2a**, **2b** and **2c**) have been calculated as the reaction enthalpy / free energy at 298.15 K and 1 atm pressure like shown in eqn. (2).



The geometries of all species in eqn. (2) have been optimized at the mPW1k/6-31+G(d) level of theory. The conformational space of **5a** and **4f** and the corresponding zwitterionic species has been searched using the MM3* force field and the systematic search routine implemented in MACROMODEL 9.7.^[16] All stationary points located at force field level have then been reoptimized at mPW1k/6-31+G(d) level as described before. Thermochemical corrections to 298.15 K have been calculated for all minima from unscaled vibrational frequencies obtained at this same level. The thermochemical corrections have been combined with single point energies calculated at the MP2(FC)/6-31+G(2d,p)//mPW1k/6-31+G(d) level to yield enthalpies H_{298} / G_{298} at 298.15 K. In conformationally flexible systems enthalpies have been calculated as Boltzmann-averaged values over all available conformers. PCM calculations were performed with RHF/6-31G(d) using UAHF radii and chloroform as the solvent. Combination of the gas phase free energies with the solvation energies yield, after correcting for the solution standard state of 1 mol/l, the free energies in solution at 298.15 K.¹⁷⁻¹⁹ All quantum mechanical calculations have been performed with Gaussian 03.¹⁵

The energetic best conformations of the adducts are depicted in Figure S1. The correlation between the reaction rates and the free energies are displayed in Figure S2.

5a



4f

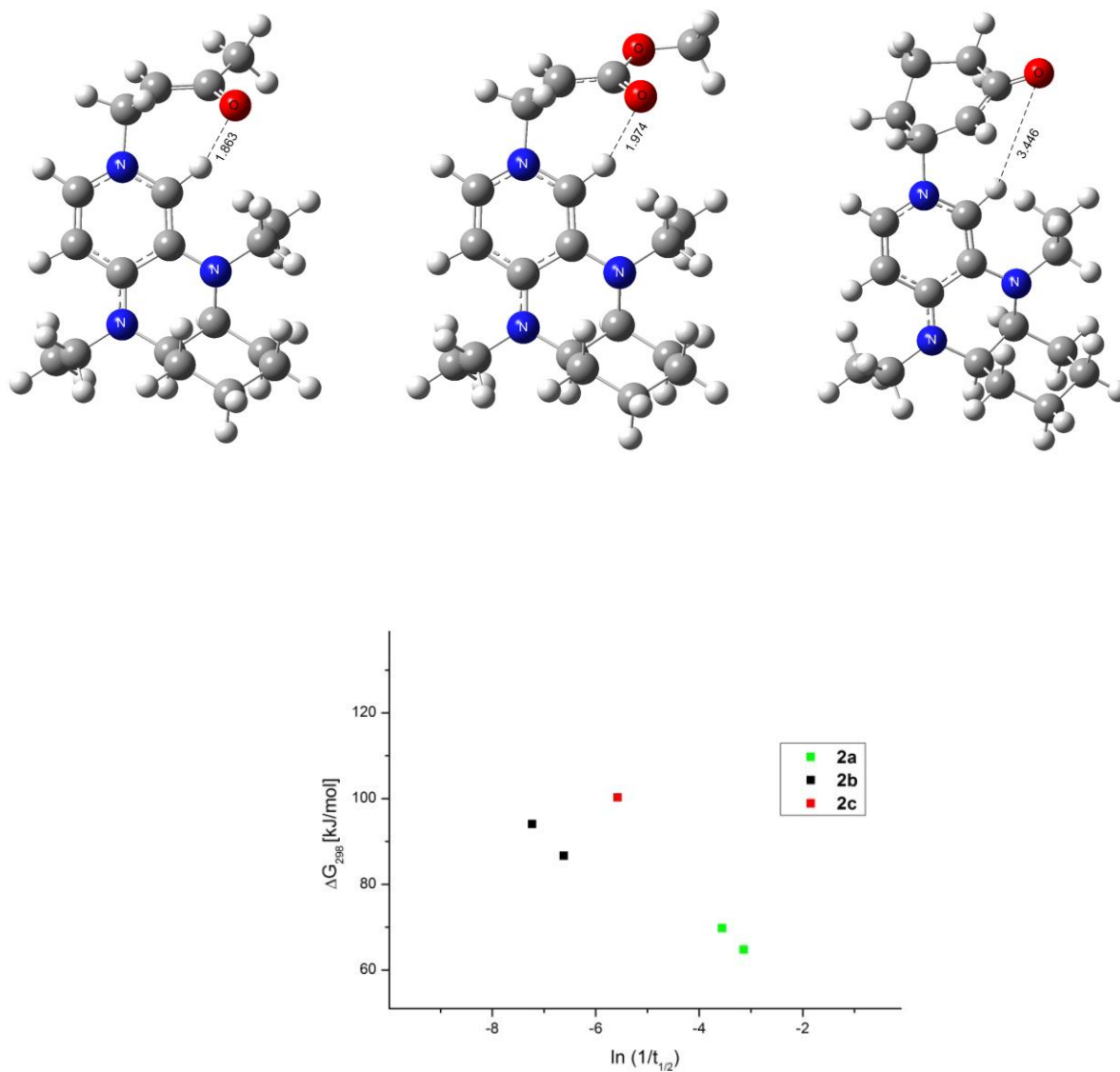


Fig. 7 Plot of free energies vs. reaction rates for different Michael acceptors.

Table S4 Enthalpies, free energies without or with PCM solvation model of the addition of **5a** and **4f** to the Michael-acceptors (**2a**, **2b**, **2c**).

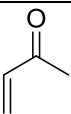
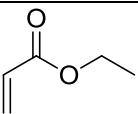
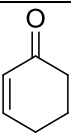
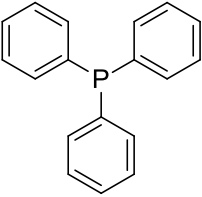
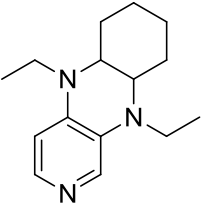
		 2a	 2b	 2c
 5a	H ₂₉₈ [kJ/mol]	+23.9	+50.3	+82.7
	G ₂₉₈ [kJ/mol]	+81.9	+106.8	+139.9
	G _{298,CHCl3} [kJ/mol]	+61.9	+86.2	+113.8
 4f	H ₂₉₈ [kJ/mol]	+12.8	+40.5	+60.7
	G ₂₉₈ [kJ/mol]	+70.3	+95.2	+113.9
	G _{298,CHCl3} [kJ/mol]	+56.9	+78.8	+92.4

Table S5 Total energies, enthalpies and free energies (in Hartree) as calculated at the mPW1k/6-31+G(d) and MP2(FC)/6-31+G(2d,p)// mPW1k/6-31+G(d) level of theory for all systems. If more than one conformer exist at 298.15 K, the single values of each conformer are denoted as well as the Boltzmann-averaged values for H₂₉₈ at MP2(FC)/6-31+G(2d,p)//mPW1k/6-31+G(d) level of theory. For every system a maximum of 10 conformers are included.

	mPW1k/6-31+G(d)		MP2(FC)/6-31+G(2d,p)// mPW1k/6-31+G(d)	
system	E _{tot}	H ₂₉₈	G ₂₉₈	G _{298,CHCl3}
5a			-1033.568131	-1033.565374
5a_1	-1033.805540	-1033.506480	-1033.568131	-1033.565374
4f			-747.239924	-747.243616
4f_1	-747.576237	-747.180888	-747.240774	-747.244328
4f_2	-747.575744	-747.180467	-747.239662	-747.243360
2a			-230.542448	-230.543906
2a_1	-230.606397	-230.507158	-230.542589	-230.544310
2a_2	-230.605751	-230.506640	-230.542340	-230.543695
2b			-305.613642	-305.614462
2b_1	-305.682590	-305.576236	-305.613895	-305.614708
2b_2	-305.681653	-305.575258	-305.612964	-305.613856
2b_3	-305.667879	-305.561711	-305.600247	-305.604104
2b_4	-305.662507	-305.556425	-305.595291	-305.599434
2c			-307.711115	-307.716708
2c_1	-307.813098	-307.674404	-307.711115	-307.716708
5a*2a			-1264.079422	-1264.082890
5a*2a_1	-1264.404815	-1264.004430	-1264.079680	-1264.083154
5a*2a_2	-1264.404793	-1264.004283	-1264.078674	-1264.081814
5a*2a_3	-1264.391293	-1263.991325	-1264.067730	-1264.076192
5a*2a_4	-1264.389128	-1263.988845	-1264.065834	-1264.073116
5a*2b			-1339.141078	-1339.143971
5a*2b_1	-1339.467080	-1339.060242	-1339.139373	-1339.144377
5a*2b_2	-1339.470621	-1339.063517	-1339.141415	-1339.143901
5a*2b_3	-1339.470264	-1339.063181	-1339.140879	-1339.143795
5a*2b_4	-1339.465007	-1339.057932	-1339.136098	-1339.141867
5a*2b_5	-1339.464749	-1339.057654	-1339.134864	-1339.140378
5a*2b_6	-1339.463818	-1339.056751	-1339.134661	-1339.140191
5a*2c			-1341.225978	-1341.235747
5a*2c_1	-1341.588874	-1341.149366	-1341.225978	-1341.235747
4f*2a			-977.756227	-977.763563
4f*2a_1	-978.181725	-977.683257	-977.756636	-977.764047
4f*2a_2	-978.180971	-977.682502	-977.756038	-977.763416
4f*2a_3	-978.178939	-977.680804	-977.754319	-977.762510
4f*2a_4	-978.178764	-977.680510	-977.754090	-977.761628
4f*2a_5	-978.172688	-977.674222	-977.747852	-977.759422
4f*2a_6	-978.172993	-977.674444	-977.747848	-977.758812
4f*2a_7	-978.171366	-977.672989	-977.746462	-977.757968
4f*2a_8	-978.171491	-977.673243	-977.746718	-977.757953

4f*2a_9	-978.166473	-977.669194	-977.745261	-977.756496
4f*2a_10	-978.165121	-977.667628	-977.744339	-977.756435
4f*2b			-1052.817885	-1052.825463
4f*2b_1	-1053.246864	-1052.741815	-1052.818432	-1052.826352
4f*2b_2	-1053.246078	-1052.741080	-1052.817974	-1052.825798
4f*2b_3	-1053.244315	-1052.739584	-1052.816306	-1052.825007
4f*2b_4	-1053.242605	-1052.738150	-1052.815397	-1052.824736
4f*2b_5	-1053.241669	-1052.737363	-1052.815413	-1052.824719
4f*2b_6	-1053.240567	-1052.736544	-1052.814237	-1052.824181
4f*2b_7	-1053.244028	-1052.739206	-1052.815886	-1052.823823
4f*2b_8	-1053.239942	-1052.735868	-1052.813780	-1052.823134
4f*2b_9	-1053.236992	-1052.732622	-1052.810563	-1052.823073
4f*2b_10	-1053.238859	-1052.733921	-1052.811009	-1052.822770
4f*2c			-1054.908250	-1054.922702
4f*2c_1	-1055.368669	-1054.832124	-1054.908215	-1054.922844
4f*2c_2	-1055.366930	-1054.830536	-1054.906427	-1054.921375
4f*2c_3	-1055.364135	-1054.827469	-1054.903211	-1054.921139
4f*2c_4	-1055.362519	-1054.826120	-1054.901800	-1054.919664
4f*2c_5	-1055.368862	-1054.832421	-1054.908757	-1054.923338
4f*2c_6	-1055.364162	-1054.827528	-1054.903843	-1054.921500
4f*2c_7	-1055.366851	-1054.830493	-1054.906424	-1054.921452
4f*2c_8	-1055.362763	-1054.826397	-1054.902445	-1054.920325

4.3 Archive entries of all structures

4.3.1 Structures of all systems: B98/6-31G(d)

4a

see: Y. Wei, G. N. Sastry, H. Zipse, *J. Am. Chem. Soc.* **2008**, *130*, 3473 - 3477.

4a_Me⁺

see: Y. Wei, G. N. Sastry, H. Zipse, *J. Am. Chem. Soc.* **2008**, *130*, 3473 - 3477.

4b

see: Y. Wei, G. N. Sastry, H. Zipse, *J. Am. Chem. Soc.* **2008**, *130*, 3473 - 3477.

4b_Me⁺

see: Y. Wei, G. N. Sastry, H. Zipse, *J. Am. Chem. Soc.* **2008**, *130*, 3473 - 3477.

4c

4c_1

```
1\1\GINC-YIN\SP\RMP2-FC\6-31+G(2d,p)\C9H14N2\RAMAN\01-Jun-2010\0\#P M
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\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)]\
\@
```

4c_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)]\@

4c_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)]\@

4c_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)]\@

4c_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)]
\@

4c-Me⁺

4c-Me⁺_1

1\1\GINC-AZAZEL\SP\RMP2-FC\6-31+G(2d,p)\C10H17N2(1+)\RAMAN\01-Sep-2011
\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geo
m=check\\sp of d2ap4.mca mp2-5 on 2p 900 MB\\1,1\C,0,-0.3339014697,0.0
022653176,0.0057967717\C,0,-1.1039072631,-1.1423164897,0.4017346261\C,
0,-2.4726391918,-1.1035737657,0.3966725139\C,0,-2.4741908609,1.1137318
999,-0.3603570338\C,0,-1.1055165842,1.1490576057,-0.3807737444\H,0,-0.
6300406292,-2.068609749,0.699690733\H,0,-3.0666687451,-1.9639931389,0.
686218951\H,0,-3.0694087937,1.9750061082,-0.6448820971\H,0,-0.6326627,
2.0767813201,-0.6758061856\N,0,1.0086289637,0.0012630857,0.0003275121\
C,0,1.795808716,-1.1527285965,0.4820821853\H,0,2.7396285128,-0.7478075
174,0.8616759173\H,0,1.2888949151,-1.5964779128,1.3451492222\C,0,1.793
7515529,1.1541161735,-0.4875527319\H,0,1.2795788194,1.6002283655,-1.34
50503431\H,0,2.7328035837,0.7473885206,-0.8769720531\C,0,2.0755807329,
2.1950492464,0.6034894151\H,0,2.6252178934,1.7503875747,1.4409532476\H
,0,2.6865202187,3.0055481786,0.1905481899\H,0,1.150175618,2.6303343574
,0.9980389675\C,0,2.0643019152,-2.1958457542,-0.61021351\H,0,1.1339166
527,-2.6294010073,-0.9948168333\H,0,2.6066034582,-1.7536204603,-1.4537
209548\H,0,2.677359295,-3.0072501535,-0.2022208787\N,0,-3.1687330054,0
.0069394808,0.0250481917\C,0,-4.6430125908,-0.010103936,-0.0219667241\

H,0,-4.9852867802,-0.343353947,-1.006980189\H,0,-5.0188925751,-0.68757
22955,0.7475451658\H,0,-5.0200751083,0.994941929,0.1785014289\\Version
=AM64L-G03RevD.01\State=1-A\HF=-497.3358558\MP2=-499.1550739\RMSE=3.81
5e-09\Thermal=0.\PG=C01 [X(C10H17N2)]\\@

4c-Me⁺_2

1\1\GINC-CALYPSO\SP\RMP2-FC\6-31+G(2d,p)\C10H17N2(1+)\RAMAN\01-Sep-201
1\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read ge
om=check\\sp of d2ap5.mca mp2-5 on 2p 900 MB\\1,1\C,0,0.3476258336,-0.
0000428656,-0.2387990678\C,0,1.1078591545,-1.2100820893,-0.1052890445\
C,0,2.4618078733,-1.1711430236,0.097781728\C,0,2.4619719944,1.17082778
75,0.0975452236\C,0,1.1080279834,1.2099152357,-0.1055274928\H,0,0.6395
663803,-2.1838914912,-0.1616289117\H,0,3.0483264399,-2.0787414013,0.19
39874768\H,0,3.0486199152,2.0783634976,0.1935534886\H,0,0.6398685642,2
.1837769075,-0.1620935178\N,0,-0.9743000447,0.0000446986,-0.4853307838
\C,0,-1.733829326,-1.2648417247,-0.5992974943\H,0,-2.6285554364,-1.040
1055662,-1.1862967383\H,0,-1.1483449292,-1.9702898636,-1.1997416581\C,
0,-1.7336331151,1.2650528532,-0.599256049\H,0,-2.6285221763,1.04041440
48,-1.1860414917\H,0,-1.1481466417,1.9703444349,-1.1998886515\C,0,-2.1
298038065,1.8824680012,0.749439347\H,0,-1.2554406547,2.1038001919,1.37
21777099\H,0,-2.6694068247,2.8203136511,0.5750072264\H,0,-2.7880878656
,1.214231905,1.3141495664\C,0,-2.1303740111,-1.8820620129,0.749375359\
H,0,-2.7886799986,-1.2136755158,1.3138823323\H,0,-2.6700778922,-2.8198
471803,0.5749298633\H,0,-1.2561638863,-2.1034513956,1.3723095578\N,0,3
.1507265098,-0.0001963803,0.1925884392\C,0,4.6001168973,-0.0002704997,
0.4679029599\H,0,5.0502787839,0.8877052896,0.019316126\H,0,4.779495517
9,-0.0001663155,1.5478439593\H,0,5.0501506715,-0.8884084632,0.01950881
75\\Version=AM64L-G03RevD.01\State=1-A\HF=-497.3337119\MP2=-499.153699
6\RMSE=4.747e-09\Thermal=0.\PG=C01 [X(C10H17N2)]\\@

4c-Me⁺_3

1\1\GINC-YANG\SP\RMP2-FC\6-31+G(2d,p)\C10H17N2(1+)\RAMAN\01-Sep-2011\0
\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geom=
check\\sp of d2ap2.mca mp2-5 on 2p 900 MB\\1,1\C,0,0.4448318843,-0.093
3656494,-0.1066173442\C,0,1.2564251139,1.0730933833,-0.3125305648\C,0,
2.6213115934,1.0043091982,-0.2287584286\C,0,2.5430777743,-1.2788838967
,0.2845129027\C,0,1.1744106562,-1.2867105336,0.2161412632\H,0,0.821226
7806,2.0380257144,-0.5364150517\H,0,3.2452461643,1.8777930113,-0.38618
87201\H,0,3.1045664605,-2.1755891494,0.524603516\H,0,0.6720943441,-2.2
238326094,0.4141520309\N,0,-0.8966791491,-0.0789338977,-0.2105161142\C
,0,-1.6202708019,1.1843586469,-0.4617526345\H,0,-1.0695171884,1.753229
8233,-1.2174457454\H,0,-2.5739111539,0.9292861958,-0.9244229246\C,0,-1
.652970553,-1.3259872992,0.0885360057\H,0,-1.4703505998,-1.594884853,1
.1385499172\H,0,-1.2325058722,-2.1242151383,-0.5356739177\C,0,-3.15958
70996,-1.266129956,-0.1624819014\H,0,-3.3990787525,-1.0788674156,-1.21
46720999\H,0,-3.5745217691,-2.246159407,0.0977405836\H,0,-3.6648925857
, -0.5217421523,0.4615787445\C,0,-1.8493246762,2.0151184592,0.808493286
4\H,0,-2.4516437835,1.461925196,1.5379151383\H,0,-0.9043110472,2.29134
28259,1.2906106188\H,0,-2.3857142551,2.9365927746,0.5549224917\N,0,3.2
766713902,-0.1552110003,0.0590772424\C,0,4.7454972452,-0.1699944084,0.
195847124\H,0,5.0325244174,0.1259374665,1.2099534377\H,0,5.1139847757,

-1.1764676496,-0.0116902301\H,0,5.181134197,0.5217401404,-0.5285066261
\Version=AM64L-G03RevD.01\State=1-A\HF=-497.3304163\MP2=-499.1507818\
RMSD=4.864e-09\Thermal=0.\PG=C01 [X(C10H17N2)]\@

4c-Me⁺_4

1\1\GINC-AZAZEL\SP\RMP2-FC\6-31+G(2d,p)\C10H17N2(1+)\RAMAN\01-Sep-2011
\0\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geo
m=check\sp of d2ap12.mca mp2-5 on 2p 900 MB\1,1\C,0,0.3391904341,-0.
0132237238,0.2862683392\C,0,1.0480277848,-1.2157748501,-0.0473070102\C
,0,2.3902607787,-1.1887840875,-0.3189072596\C,0,2.4732733997,1.1317048
401,-0.0135692155\C,0,1.1338795217,1.1818693465,0.2682097864\H,0,0.547
4292976,-2.1735162742,-0.101063972\H,0,2.9384119279,-2.0923446489,-0.5
639120654\H,0,3.0859640755,2.026973509,-0.0219148959\H,0,0.7023053493,
2.1536831183,0.4683875562\N,0,-0.9681470222,-0.0078170753,0.600914292\
C,0,-1.6758956786,1.252244607,0.9188820727\H,0,-2.5470119792,0.9779645
077,1.5202124102\H,0,-1.0362277518,1.8561363702,1.5723971022\C,0,-1.76
54942027,-1.2543587891,0.5890103632\H,0,-2.6207103035,-1.0843068492,1.
2488269133\H,0,-1.1758481341,-2.049959591,1.0583482847\C,0,-2.25175920
15,-1.6747873124,-0.8052638574\H,0,-1.4187760719,-1.8349588071,-1.4993
54627\H,0,-2.8140155023,-2.6122242086,-0.7263778407\H,0,-2.914533839,-
0.9191717773,-1.2394465762\C,0,-2.1185296406,2.0517702603,-0.314830143
8\H,0,-2.614245361,2.9740667267,0.0088745998\H,0,-1.2699900881,2.32696
02537,-0.9516458507\H,0,-2.8287229324,1.4825252305,-0.9233660127\N,0,3
.1132732697,-0.0348050459,-0.3043637885\C,0,4.568584822,-0.0544257299,
-0.5446101624\H,0,5.1042575666,-0.1852007671,0.4010910519\H,0,4.809881
1459,-0.8767844383,-1.2212575799\H,0,4.8686207057,0.8861979758,-1.0112
383337\Version=AM64L-G03RevD.01\State=1-A\HF=-497.3337028\MP2=-499.15
36798\RMSD=4.748e-09\Thermal=0.\PG=C01 [X(C10H17N2)]\@

4c-Me⁺_5

1\1\GINC-YANG\SP\RMP2-FC\6-31+G(2d,p)\C10H17N2(1+)\RAMAN\01-Sep-2011\0
\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geom=
check\sp of d2ap10.mca mp2-5 on 2p 900 MB\1,1\C,0,-0.3601063254,0.02
0856022,-0.3962210925\C,0,-1.1404685519,1.2188000729,-0.2701844499\C,0
, -2.5079839188,1.164882545,-0.2157988202\C,0,-2.4883281569,-1.17251857
14,-0.3613966562\C,0,-1.120193825,-1.1963995535,-0.4205730528\H,0,-0.6
771169267,2.1950940011,-0.2158996678\H,0,-3.1090882567,2.0636169351,-0
.1268337038\H,0,-3.0742984416,-2.0852412154,-0.3852994687\H,0,-0.64050
39296,-2.1639893397,-0.4873553929\N,0,0.9805451768,0.0385104957,-0.499
2258086\C,0,1.7371741922,1.3093616866,-0.4524405374\H,0,2.6914336067,1
.1233098691,-0.9528269495\H,0,1.2133907607,2.0499321181,-1.0674210915\
C,0,1.7584100034,-1.215499592,-0.6093502076\H,0,2.708969928,-0.9529446
626,-1.0816952311\H,0,1.2465806512,-1.8828607327,-1.31195487\C,0,2.013
400116,-1.9154589806,0.7331123219\H,0,1.0794137662,-2.1769105193,1.243
614269\H,0,2.5764842431,-2.839576843,0.5596352073\H,0,2.6018859147,-1.
2827206581,1.4054956515\C,0,1.982028454,1.8418522622,0.9665904282\H,0,
1.0444180324,2.0224782307,1.5046962778\H,0,2.5817814529,1.1406559865,1
.5559918023\H,0,2.5294227487,2.7896066794,0.9093581283\N,0,-3.19312113
25,-0.010923695,-0.2679036942\C,0,-4.6635035471,-0.031179062,-0.149173
1103\H,0,-5.0563261927,-0.8856529106,-0.7041651817\H,0,-4.9564760322,-
0.1072742322,0.9028980056\H,0,-5.07048662,0.8860755039,-0.5796993651\

Version=AM64L-G03RevD.01\State=1-A\HF=-497.3337114\MP2=-499.1536991\RM
SD=4.714e-09\Thermal=0.\PG=C01 [X(C10H17N2)]\@

4d

see: Y. Wei, G. N. Sastry, H. Zipse, *J. Am. Chem. Soc.* **2008**, *130*, 3473 - 3477.

4d_Me⁺

see: Y. Wei, G. N. Sastry, H. Zipse, *J. Am. Chem. Soc.* **2008**, *130*, 3473 - 3477.

4e

4e_1

1\1\GINC-CALYPSO\SP\RMP2-FC\6-31+G(2d,p)\C11H17N3\RAMAN\24-Oct-2011\0\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=
read\opt of cat81et7 b98/6-31G(d) on 4p 900 MB\0,1\C,0,-1.2541390147
,0.0294042914,0.8810025329\C,0,-0.5399591715,-1.2966797262,0.619729938
1\N,0,0.8789971733,-1.1380758963,0.8886173738\C,0,1.4986834817,-0.0239
127787,0.2998649794\C,0,0.708274021,1.1070697001,-0.0847401455\N,0,-0.
676810458,1.0679880838,0.04184771\C,0,1.3973699856,2.2131584353,-0.609
6962049\C,0,2.7860535249,2.1709553688,-0.7502910621\N,0,3.5349783195,1
.1224851163,-0.4067770575\C,0,2.8850614287,0.0611486677,0.096747727\C,
0,-1.4906651213,2.2553684924,-0.1901726424\C,0,-1.4873218478,3.2772512
442,0.9611905158\C,0,1.632138916,-2.3630489378,1.1331284602\C,0,1.9325
380061,-3.2157054492,-0.1141585489\H,0,-1.1865186965,0.271963577,1.954
8852556\H,0,-0.9371618193,-2.0637366162,1.2965905122\H,0,1.0460085372,
-2.9559372729,1.8485540035\H,0,2.56402404,-2.0996730844,1.6475831549\H
,0,1.0054689292,-3.5500504137,-0.5961530554\H,0,2.5136951945,-2.652053
459,-0.8526038337\H,0,2.5068382615,-4.1080587977,0.1655023863\H,0,-2.5
165043503,1.9077090257,-0.3711530111\H,0,-1.1609094616,2.7291923328,-1
.122420335\H,0,-1.8765690086,2.8307147453,1.8843261686\H,0,-0.47418941
89,3.6429457774,1.1633615207\H,0,-2.120185891,4.1376177856,0.709069612
\H,0,0.8659631514,3.1119213366,-0.9042172284\H,0,3.5191940523,-0.78250
57548,0.359452835\H,0,3.3131174366,3.032875839,-1.159299591\H,0,-0.746
0551688,-1.620204022,-0.4158375583\H,0,-2.3171047214,-0.0689528204,0.6
247984983\Version=AM64L-G03RevD.01\State=1-A\HF=-589.827159\MP2=-591.
9812532\RMSD=7.365e-09\Thermal=0.\PG=C01 [X(C11H17N3)]\@

4e_2

1\1\GINC-EDDY\SP\RMP2-FC\6-31+G(2d,p)\C11H17N3\RAMAN\24-Oct-2011\0\#P
MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=rea
d\opt of cat81et14 b98/6-31G(d) on 4p 900 MB\0,1\C,0,1.0820258971,-0
.3321071115,-1.3505315505\C,0,0.1106164012,-1.3651158601,-0.7823780493
\N,0,-1.2526241143,-0.8821553901,-0.9400639054\C,0,-1.4907523244,0.398
9909959,-0.4089104832\C,0,-0.404371834,1.3273175016,-0.316176384\N,0,0
.868114902,0.9615089173,-0.7223302972\C,0,-0.7019625746,2.6007368323,0
.2003553793\C,0,-2.0120041066,2.9169553366,0.5658630253\N,0,-3.0371536
241,2.0693139279,0.4704643323\C,0,-2.755449873,0.8416933916,0.00310432
96\C,0,1.9606617038,1.9257521995,-0.7913920809\C,0,2.7468009939,2.0541
774737,0.5231611246\C,0,-2.2996595016,-1.8988313734,-0.899234756\C,0,-
2.5730411975,-2.5200140176,0.4840618668\H,0,0.9563102827,-0.2743528281
, -2.4448860688\H,0,0.2148254492,-2.303452921,-1.3408412136\H,0,-1.9993

000826,-2.6886277351,-1.6012905672\H,0,-3.218153781,-1.4612383474,-1.3
079172006\H,0,-2.8623293504,-1.7566075175,1.2146936818\H,0,-3.38551268
53,-3.2544458537,0.4153329454\H,0,-1.685211042,-3.0376507666,0.8680766
975\H,0,1.5694777923,2.9035154539,-1.1023635573\H,0,2.6349556114,1.600
951019,-1.5943007342\H,0,2.0957797323,2.3822708759,1.3413336955\H,0,3.
1853309827,1.0899582359,0.8085212818\H,0,3.5607076125,2.7827147384,0.4
155541626\H,0,0.0744846776,3.3491516291,0.320431175\H,0,-3.6055124587,
0.1653832644,-0.0526412277\H,0,-2.2363496328,3.9088155221,0.9584841825
\H,0,0.3699444533,-1.5690063194,0.2720434952\H,0,2.1119948109,-0.65596
26534,-1.1474160192\\Version=AM64L-G03RevD.01\State=1-A\HF=-589.826711
9\MP2=-591.9802049\RMSD=7.793e-09\Thermal=0.\PG=C01 [X(C11H17N3)]\@

4e_3

1\1\GINC-AZAZEL\SP\RMP2-FC\6-31+G(2d,p)\C11H17N3\RAMAN\24-Oct-2011\0\\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=r
ead\\opt of cat81et4 b98/6-31G(d) on 4p 900 MB\\0,1\C,0,-1.2452489789,
-0.0272256103,0.7991701765\C,0,-0.681174277,-1.3307457978,0.2358944119
\N,0,0.7671792844,-1.3261062097,0.3566258134\C,0,1.4233769436,-0.15988
11366,-0.0644837571\C,0,0.6993843176,1.0715324167,-0.169793252\N,0,-0.
6678411255,1.1035093455,0.0894750978\C,0,1.4272958536,2.2025537194,-0.
5740599375\C,0,2.7890373513,2.0928684041,-0.8644579587\N,0,3.478171492
1,0.9556355219,-0.7683506244\C,0,2.7919932308,-0.1300354736,-0.3765744
605\C,0,-1.3901121703,2.3682390315,0.1661976659\C,0,-1.1718310896,3.16
09962701,1.4679390358\C,0,1.4461998084,-2.6187125162,0.2762114725\C,0,
2.2945352858,-2.9311166394,1.5188528728\H,0,-1.0487372307,0.0132374034
,1.8839775953\H,0,-1.0786011785,-2.1720840189,0.8163085445\H,0,2.06149
95101,-2.674984397,-0.6353813789\H,0,0.6724527924,-3.3883166022,0.1683
879216\H,0,3.0682608499,-2.1722747083,1.6779842458\H,0,1.6628554157,-2
.9590234147,2.4146302546\H,0,2.7873276957,-3.9059354558,1.4102556093\H
,0,-2.4565500187,2.1332607609,0.0512990662\H,0,-1.1175545055,2.9795071
535,-0.7024558519\H,0,-1.5067091709,2.5863328595,2.3401665526\H,0,-0.1
12714822,3.4042719673,1.6088517533\H,0,-1.7406539539,4.0991187389,1.44
29480516\H,0,0.9465346667,3.1710468188,-0.6631308487\H,0,3.3806194378,
-1.0408712575,-0.2986786936\H,0,3.3454844009,2.9744155116,-1.182542422
7\H,0,-2.332998136,-0.0066407389,0.653502558\H,0,-1.0166166792,-1.4511
454961,-0.8102703534\\Version=AM64L-G03RevD.01\State=1-A\HF=-589.82604
55\MP2=-591.9799004\RMSD=6.702e-09\Thermal=0.\PG=C01 [X(C11H17N3)]\@

4e_4

1\1\GINC-CALYPSO\SP\RMP2-FC\6-31+G(2d,p)\C11H17N3\RAMAN\24-Oct-2011\0\\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=r
ead\\opt of cat81et6 b98/6-31G(d) on 4p 900 MB\\0,1\C,0,1.0809520752,
-0.4292758502,-1.1993050074\C,0,0.288858187,-1.4165325955,-0.344825865
8\N,0,-1.1296524062,-1.0951519697,-0.4279515094\C,0,-1.4340009401,0.22
82742594,-0.0526366128\C,0,-0.4522875505,1.2500258315,-0.2596511059\N,
0,0.7749605607,0.9394816296,-0.8162318902\C,0,-0.8040403841,2.55450617
8,0.1309431338\C,0,-2.0681736408,2.8033524027,0.6692360516\N,0,-2.9970
926752,1.8653467159,0.8578334185\C,0,-2.6603948735,0.612573972,0.50544
23737\C,0,1.7505082792,1.9644194963,-1.1665439944\C,0,2.6948655219,2.3
346602813,-0.0108766746\C,0,-2.0697397201,-2.1661568514,-0.0947170133\
C,0,-3.2097165754,-2.2963813424,-1.1159921739\H,0,0.8557114688,-0.6046

724465,-2.2643987611\H,0,0.4469397978,-2.427512707,-0.7361832023\H,0,-
2.4737685103,-2.0367248925,0.9234958001\H,0,-1.5007036328,-3.103081374
9,-0.0806765247\H,0,-3.7910220352,-1.3718817606,-1.1960852137\H,0,-2.8
048728968,-2.5250966878,-2.1086226474\H,0,-3.891831438,-3.1044921903,-
0.8222968395\H,0,1.2265967322,2.855547821,-1.5350401842\H,0,2.33456895
58,1.5843324239,-2.0150327365\H,0,3.2575868057,1.4560160011,0.32822250
9\H,0,3.4147039088,3.0988952676,-0.330967029\H,0,2.133229588,2.7254030
901,0.8450468204\H,0,-0.1035944722,3.3765917592,0.0257249399\H,0,-3.43
37375822,-0.1335017782,0.671550719\H,0,-2.335657883,3.8178519013,0.965
2705971\H,0,0.6648595727,-1.3910809205,0.6947979924\H,0,2.1555675328,-
0.6072211935,-1.0503549095\\Version=AM64L-G03RevD.01\State=1-A\HF=-589
.8259476\MP2=-591.978867\RMSD=4.195e-09\Thermal=0.\PG=C01 [X(C11H17N3)
J]\@

4e_5

1\1\GINC-EDDY\SP\RMP2-FC\6-31+G(2d,p)\C11H17N3\RAMAN\24-Oct-2011\0\#P
MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=rea
d\opt of cat81et13 b98/6-31G(d) on 4p 900 MB\0,1\C,0,0.1670226765,-1
.3436960899,-0.3123787009\C,0,1.0525433135,-0.4040675839,-1.1279282885
\H,0,0.9282293306,-0.6264226483,-2.2003138689\H,0,0.3452153439,-2.3656
199483,-0.656021454\N,0,-1.230896292,-0.9859561423,-0.5323642307\N,0,0
.7331913471,0.987033793,-0.8484025523\C,0,-0.4941315449,1.3348891181,-
0.3196258769\C,0,-0.8201826631,2.6513474627,0.0533089097\C,0,-1.508828
9352,0.3419202716,-0.1363241229\C,0,-2.088313255,2.9339623143,0.564251
6197\H,0,-0.0979012186,3.4552002847,-0.0451564044\C,0,-2.7263905341,0.
7544682289,0.4191410226\N,0,-3.039388306,2.0188002017,0.7545728912\H,0
,-2.3381961407,3.9578697772,0.8432393147\H,0,-3.5117737653,0.025627993
4,0.6029349525\C,0,1.7519932647,1.9767181013,-1.1728585919\C,0,2.68179
82365,2.3182840456,0.0036316391\H,0,1.2653651452,2.8831473629,-1.55346
02043\H,0,2.3428424079,1.5759055782,-2.0075780945\H,0,3.438176944,3.05
15771839,-0.3041873193\H,0,2.1161682154,2.7369298041,0.8437402802\H,0,
3.2036303815,1.4220335336,0.3619352598\C,0,-2.2386956298,-2.0023864371
,-0.2301781952\C,0,-1.9736771326,-3.3522398735,-0.9069875379\H,0,-3.19
47694211,-1.6211623493,-0.6062877712\H,0,-2.360269065,-2.1472260144,0.
8606716562\H,0,-2.8603978754,-3.9878434695,-0.7984132539\H,0,-1.778182
5217,-3.2171597114,-1.9776119425\H,0,-1.1315054302,-3.8953930803,-0.46
31298431\H,0,0.4438685583,-1.2911087165,0.7570962396\H,0,2.1058972956,
-0.5883623504,-0.8689090918\\Version=AM64L-G03RevD.01\State=1-A\HF=-58
9.8262303\MP2=-591.9790183\RMSD=2.697e-09\Thermal=0.\PG=C01 [X(C11H17N
3)]\@

4e_6

1\1\GINC-AZAZEL\SP\RMP2-FC\6-31+G(2d,p)\C11H17N3\RAMAN\24-Oct-2011\0\#P
MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=r
ead\opt of cat81et18 b98/6-31G(d) on 4p 900 MB\0,1\C,0,-3.5966728336
,0.7160375004,-0.6216831111\C,0,-2.4812012372,1.466218646,-0.240134365
6\C,0,-1.2655790785,0.8261325311,0.0503112254\C,0,-1.2307465718,-0.597
2660704,-0.1099667103\C,0,-2.4268881945,-1.2310174419,-0.4861766306\N,
0,-3.5890878544,-0.6110397166,-0.7430121105\N,0,-0.0291971872,-1.29688
42172,0.0662707561\C,0,1.032694779,-0.6084099183,0.7771698764\C,0,1.14
09576469,0.8313586951,0.276761455\N,0,-0.1295857552,1.5118252549,0.492

1020733\C,0,-0.0166902396,-2.7537706036,0.1351249466\C,0,-0.5608352447
,-3.3518626622,1.4458230853\C,0,-0.1528216478,2.9750917497,0.468060600
3\C,0,1.0410448091,3.6356701903,1.1654114294\H,0,0.8780765301,-0.59608
47897,1.870693831\H,0,1.9224361902,1.3403479272,0.8471036858\H,0,-1.06
15151111,3.2931823517,0.9922249608\H,0,-0.2325910464,3.3544933557,-0.5
677604915\H,0,0.8525330819,4.7130031558,1.2409211588\H,0,1.1726535693,
3.2431474038,2.1811500898\H,0,1.979772519,3.5076446293,0.6148957205\H,
0,1.0264526678,-3.0666021307,-0.0071383035\H,0,-0.5722790227,-3.150321
4486,-0.723292234\H,0,0.0331551639,-3.0207707143,2.3065837052\H,0,-1.6
007814004,-3.0517208287,1.6161567336\H,0,-0.5211741415,-4.4479531569,1
.4099781365\H,0,-2.4519796473,-2.3131339235,-0.5912017499\H,0,-4.53769
54992,1.2206284423,-0.8400256695\H,0,-2.5743421426,2.5445616257,-0.179
8887032\H,0,1.9772165677,-1.1322439432,0.5792288961\H,0,1.4385823908,0
.8322332666,-0.7867570065\\Version=AM64L-G03RevD.01\State=1-A\HF=-589.
8245429\MP2=-591.9789718\RMSD=7.462e-09\Thermal=0.PG=C01 [X(C11H17N3)
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4e_7

1\1\GINC-CALYPSO\SP\RMP2-FC\6-31+G(2d,p)\C11H17N3\RAMAN\24-Oct-2011\0\
\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=
read\\opt of cat81et15 b98/6-31G(d) on 4p 900 MB\\0,1\C,0,3.0800721867
,-1.9326045051,0.6347704984\C,0,2.7968157737,-0.5962631579,0.335338398
3\C,0,1.5289164668,-0.2360907494,-0.1437346773\C,0,0.5616868285,-1.283
3749076,-0.2722190597\C,0,0.966624946,-2.5808297681,0.0880483737\N,0,2
.1902338438,-2.918311012,0.5222840932\N,0,-0.7287518489,-1.0053744651,
-0.7202904271\C,0,-1.0447691926,0.3369398292,-1.1692745155\C,0,-0.2428
024205,1.368265071,-0.3791090819\N,0,1.1804076378,1.0721155704,-0.5081
865169\C,0,-1.6414265613,-2.070122864,-1.1227799832\C,0,-2.5431990679,
-2.5691504331,0.0177515359\C,0,2.1346801631,2.1416650832,-0.2126306278
\C,0,1.780165347,3.4889363792,-0.8514531567\H,0,-0.838382954,0.4697862
951,-2.2462783843\H,0,-0.4471211065,2.3568538873,-0.7975152369\H,0,3.1
03260188,1.8261926954,-0.6165991295\H,0,2.2698041722,2.2702898386,0.87
78789628\H,0,1.5774174789,3.3732120048,-1.9231004347\H,0,0.915565582,3
.9699447404,-0.3804702282\H,0,2.631388386,4.1704496106,-0.7380757503\H
,0,-1.0692332157,-2.9041822314,-1.5517646708\H,0,-2.2656551395,-1.6798
99761,-1.93791314\H,0,-3.2150006786,-3.3598946234,-0.3407271604\H,0,-1
.9484313678,-2.9717761461,0.8453703812\H,0,-3.1570066603,-1.7500687964
,0.4125176271\H,0,0.2551620506,-3.4015135206,0.0272490055\H,0,4.071141
3276,-2.2080035077,0.9946369091\H,0,3.5716425358,0.1479481412,0.482370
7942\H,0,-0.5696199905,1.3701560016,0.6763486195\H,0,-2.1168776706,0.5
207184608,-1.0107722177\\Version=AM64L-G03RevD.01\State=1-A\HF=-589.82
35517\MP2=-591.9777046\RMSD=6.661e-09\Thermal=0.PG=C01 [X(C11H17N3)]\
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4e-Me⁺

4e-Me⁺_1

1\1\GINC-EDDY\SP\RMP2-FC\6-31+G(2d,p)\C12H20N3(1+)\RAMAN\25-Oct-2011\0\
\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geom=
check\\sp of cat81et7.mca mp2-5 on 2p 900 MB\\1,1\C,0,-0.7404970248,-1
.986631002,0.1088414646\C,0,0.7412510273,-1.9522717444,-0.2522111809\N
,0,1.3611565644,-0.7695955677,0.3370464434\C,0,0.7114462452,0.43033846

32,0.1574269217\C,0,-0.7145387548,0.4381175093,-0.1382923316\N,0,-1.38
63370649,-0.7287489069,-0.2782935122\C,0,-1.3355849587,1.702422799,-0.
2670667968\C,0,-0.6213037541,2.8737418628,-0.1206239559\N,0,0.69865617
74,2.8505420409,0.1472417004\C,0,1.3551931142,1.6565017231,0.267362615
2\C,0,-2.8307692352,-0.7767420676,-0.5596568245\C,0,-3.7091251402,-0.6
691068973,0.6950784482\C,0,2.7989740066,-0.8324885407,0.6192943104\C,0
,3.7055615701,-0.6892170498,-0.6144286147\H,0,-0.8630654657,-2.1658537
924,1.1858244931\H,0,1.2322690697,-2.839416784,0.1605296734\H,0,2.9794
073132,-1.7997834017,1.1027304415\H,0,3.0322835739,-0.0711797371,1.373
7881153\H,0,3.5289723917,-1.500277084,-1.3301266799\H,0,3.5438734336,0
.2612896264,-1.1364931547\H,0,4.7575056562,-0.7357723106,-0.3103274284
\H,0,-3.0168422908,-1.7277051071,-1.0706899229\H,0,-3.0706590459,0.009
8861017,-1.2828157647\H,0,-3.5086775412,-1.4917204365,1.3908140318\H,0
, -3.5432544028,0.2752670282,1.2261996634\H,0,-4.7661299579,-0.71996930
77,0.4103860724\H,0,-2.3981498803,1.7840919531,-0.4546889658\H,0,2.417
917228,1.7335940744,0.4523928226\H,0,-1.0891957696,3.8476804803,-0.203
6247621\H,0,0.862313148,-1.9752378381,-1.3461799234\H,0,-1.2324494483,
-2.8021674448,-0.4311259229\C,0,1.468476857,4.0972386981,0.3059531366\
H,0,1.8990059195,4.1396522357,1.3107515424\H,0,2.2661701276,4.13521173
81,-0.4417660889\H,0,0.8016430919,4.9487063461,0.1630978837\\Version=A
M64L-G03RevD.01\State=1-A\HF=-629.2729568\MP2=-631.5741176\RMSD=5.988e
-09\Thermal=0.\PG=C01 [X(C12H20N3)]\\@

4e-Me⁺_2

1\1\GINC-EDDY\SP\RMP2-FC\6-31+G(2d,p)\C12H20N3(1+)\RAMAN\25-Oct-2011\0
\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geom=
check\\sp of cat81et14.mca mp2-5 on 2p 900 MB\\1,1\C,0,0.7629246565,-1
.94761832,-0.5238084133\C,0,-0.6169364755,-1.9473856408,0.123646189\N,
0,-1.3734715482,-0.7853136411,-0.3355604128\C,0,-0.7447625177,0.434088
3277,-0.2054512806\C,0,0.7100947296,0.4801101346,-0.1950797169\N,0,1.4
27947622,-0.6548706992,-0.3341735853\C,0,1.309946806,1.7548684541,-0.0
537182266\C,0,0.547723727,2.9026426816,0.0060545709\N,0,-0.7979317628,
2.8465532527,-0.0414503723\C,0,-1.4323577882,1.6361413447,-0.121396180
1\C,0,2.899913806,-0.660952584,-0.3997513743\C,0,3.5640261628,-0.72873
0783,0.9817413154\C,0,-2.8360090307,-0.8973002893,-0.3487200325\C,0,-3
.5061847739,-0.840324701,1.0343235897\H,0,0.6825836971,-2.1685375788,-
1.5970820596\H,0,-1.1547998544,-2.8510271812,-0.1793244875\H,0,-3.0697
139293,-1.8517712474,-0.8349417136\H,0,-3.2295349134,-0.1176288407,-1.
012261895\H,0,-3.2901392647,0.0966765105,1.5610007135\H,0,-4.593267823
5,-0.9242592778,0.9229535459\H,0,-3.1718628234,-1.6681582332,1.6702287
32\H,0,3.2360687556,0.2164992413,-0.9627533893\H,0,3.1814958676,-1.532
8179601,-1.000097381\H,0,3.3051636771,0.1399295381,1.5977408075\H,0,3.
2583506238,-1.6321091077,1.522380778\H,0,4.653601803,-0.7556072434,0.8
679160961\H,0,2.385696731,1.8626656807,-0.0050428012\H,0,-2.5130519037
,1.6815368167,-0.1186187519\H,0,0.9952893921,3.8860082543,0.0910044906
\H,0,-0.5200280893,-1.9630437491,1.2206273771\H,0,1.3841688895,-2.7226
749404,-0.0608018449\C,0,-1.6168352727,4.0707771986,0.0032964981\H,0,-
2.1769169576,4.1752241669,-0.9308305044\H,0,-2.3103182638,4.0194383558
,0.8477622295\H,0,-0.9617764441,4.9339865597,0.1297356998\\Version=AM6
4L-G03RevD.01\State=1-A\HF=-629.2734791\MP2=-631.5738033\RMSD=7.170e-0
9\Thermal=0.\PG=C01 [X(C12H20N3)]\\@

4e-Me⁺_3

1\1\GINC-CALYPSO\SP\RMP2-FC\6-31+G(2d,p)\C12H20N3(1+)\RAMAN\25-Oct-2011\0\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geom=check\sp of cat81et4.mca mp2-5 on 2p 900 MB\1,1\C,0,-0.7003370543,-1.9814161718,-0.0270928176\C,0,0.6743595687,-1.9442950739,-0.6852052879\N,0,1.4094463927,-0.7630600038,-0.2432009799\C,0,0.7304353423,0.4301813221,-0.1797577018\C,0,-0.7254137411,0.4426967886,-0.2016893215\N,0,-1.4117431841,-0.7228469263,-0.2651218219\C,0,-1.3579251073,1.7063883224,-0.1658626394\C,0,-0.6280779293,2.8752052493,-0.0887524488\N,0,0.717476495,2.8472439859,-0.0411490333\C,0,1.3843643216,1.6541322796,-0.0914456822\C,0,-2.8826894488,-0.7722537357,-0.2815680677\C,0,-3.5220602221,-0.7106236165,1.1134032272\C,0,2.87697178,-0.8022791708,-0.3099363284\C,0,3.5498114069,-0.7128570275,1.0672212299\H,0,-0.5993244462,-2.1685029014,1.0511234376\H,0,1.2349628492,-2.8342152275,-0.3823998792\H,0,3.2393554904,-0.0112300828,-0.9832472678\H,0,3.1483894066,-1.7476756064,-0.7900466546\H,0,3.2955060248,0.2146546536,1.5932649173\H,0,3.242504761,-1.551836467,1.701189202\H,0,4.6392617073,-0.7503273263,0.9527715294\H,0,-3.1566478006,-1.7074454864,-0.7820252601\H,0,-3.2496892893,0.0356940975,-0.9233553805\H,0,-3.1995087821,-1.5532172616,1.7355342804\H,0,-3.2650984703,0.2179572477,1.6359674996\H,0,-4.6129207762,-0.7598545028,1.0209932073\H,0,-2.4369747665,1.7882655447,-0.1734149726\H,0,2.4625065035,1.7284456776,-0.0558248031\H,0,-1.1020171303,3.8488035469,-0.046841505\H,0,-1.2909840573,-2.7948852911,-0.4600061152\H,0,0.5683922855,-1.964319428,-1.781274744\C,0,1.5030067625,4.0882665963,0.081238534\H,0,2.0227384777,4.1040739154,1.0440377397\H,0,2.2301176317,4.143557211,-0.7339106178\H,0,0.8296413783,4.9443339089,0.0191335061\Vers ion=AM64L-G03RevD.01\State=1-A\HF=-629.271548\MP2=-631.572771\RMSE=6.340e-09\Thermal=0.\PG=C01 [X(C12H20N3)]\@

4e-Me⁺_4

1\1\GINC-EDDY\SP\RMP2-FC\6-31+G(2d,p)\C12H20N3(1+)\RAMAN\25-Oct-2011\0\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geom=check\sp of cat81et6.mca mp2-5 on 2p 900 MB\1,1\C,0,-0.74610274,-1.9632727109,0.3370742894\C,0,0.4805664457,-1.9601684323,-0.5668703058\N,0,1.3492150507,-0.8364771424,-0.222843975\C,0,0.7414365149,0.396997136,-0.1348361043\C,0,-0.6894081929,0.4728631532,0.12171404\N,0,-1.4032829699,-0.6535901942,0.3321943087\C,0,-1.2689831879,1.7643160078,0.1483154443\C,0,-0.4975009683,2.8990144593,0.0102276864\N,0,0.8344573866,2.8143512441,-0.1747358023\C,0,1.4400502264,1.5898349215,-0.2622046907\C,0,-2.8401840972,-0.637207985,0.6574252459\C,0,-3.7375287901,-0.6239552078,-0.5870397989\C,0,2.7815521381,-0.9474971917,-0.5354099592\C,0,3.6815800268,-0.7591973748,0.6938474124\H,0,-0.4647424851,-2.2330973449,1.3644581359\H,0,1.0348451402,-2.8897189628,-0.4093641644\H,0,3.0484639445,-0.2420304611,-1.3378484951\H,0,2.9400937926,-1.9466768554,-0.9523407224\H,0,3.5400964001,0.2193983351,1.1667086236\H,0,3.4694959044,-1.527032181,1.4455377858\H,0,4.7342436389,-0.8451034978,0.4007748312\H,0,-3.0498567104,0.2160169983,1.3116050878\H,0,-3.0342525195,-1.5333729632,1.2566880492\H,0,-3.5518874562,-1.5029117848,-1.2152384219\H,0,-4.7907032019,-0.6404046769,-0.284780897\H,0,-3.5698718794,0.2711362582,-1.1967729142\H,0,-2.3339876265,1.8941596533,0.2897757782\H,0,2.50840558

4,1.6167175932,-0.4272413356\H,0,-0.9254512328,3.8938792629,0.05023046
53\H,0,0.1725721007,-1.9221623348,-1.6243186013\H,0,-1.4632795643,-2.7
072184545,-0.0274458105\C,0,1.6690453793,4.0232400883,-0.2902610101\H,
0,2.3767348888,4.0650859044,0.5432215129\H,0,2.2137587691,4.0053299345
,-1.2387387554\H,0,1.0264831505,4.9044492259,-0.2626783328\\Version=AM
64L-G03RevD.01\State=1-A\HF=-629.2723483\MP2=-631.5726924\RMSD=3.791e-
09\Thermal=0.\PG=C01 [X(C12H20N3)]\@

4e-Me⁺_5

1\1\GINC-CALYPSO\SP\RMP2-FC\6-31+G(2d,p)\C12H20N3(1+)\RAMAN\25-Oct-201
1\0\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read ge
om=check\sp of cat81et13.mca mp2-5 on 2p 900 MB\1,1\C,0,-1.014408929
8,-1.6024461311,0.4745318988\C,0,0.2336352293,-1.9868383531,-0.3112182
276\H,0,-0.032732536,-2.2527401255,-1.3432548967\H,0,-1.7697750388,-2.
3737457968,0.3183871684\N,0,-1.5229106844,-0.3227757704,-0.0215401689\
N,0,1.2090959055,-0.892862349,-0.3223464042\C,0,0.814459104,0.38620139
05,-0.161500124\C,0,1.7218748681,1.4741956222,-0.1565418582\C,0,-0.596
2493834,0.7036060817,-0.0015926528\C,0,1.2786802558,2.7738685031,-0.03
7200137\H,0,2.7874177739,1.3113609031,-0.2541987413\C,0,-0.9494671445,
2.0362301893,0.1471138681\N,0,-0.0324068915,3.0527104728,0.1051969564\
H,0,1.9602034343,3.6165769842,-0.0507393851\H,0,-1.9735150538,2.348707
7816,0.2978031331\C,0,2.6131920462,-1.2694130344,-0.5611914241\C,0,3.4
16938904,-1.4533035767,0.7329339224\H,0,3.0751561706,-0.523091088,-1.2
166115745\H,0,2.5916528546,-2.2040520976,-1.1321064857\H,0,4.442408485
7,-1.755054807,0.4918463066\H,0,3.4604737713,-0.5267718388,1.316588093
6\H,0,2.9751307854,-2.2328755063,1.3643925147\C,0,-2.943597931,0.00930
55253,0.167729291\C,0,-3.8990658012,-1.1533271858,-0.1123806556\H,0,-3
.1728296664,0.8158595392,-0.5400379984\H,0,-3.1176542837,0.4037609871,
1.1845508541\H,0,-4.9238577502,-0.7667564015,-0.1219081581\H,0,-3.6997
021022,-1.6031571774,-1.0917553139\H,0,-3.8570620706,-1.9327754811,0.6
557554487\H,0,-0.7908081425,-1.5577581588,1.5531000241\H,0,0.703927887
6,-2.8597636647,0.1565133498\C,0,-0.5116707056,4.4410230549,0.22357905
25\H,0,-1.1424605585,4.6895047563,-0.6352679971\H,0,-1.0835835334,4.55
49209965,1.1491048045\H,0,0.3465128011,5.1142087961,0.2482106264\\Vers
ion=AM64L-G03RevD.01\State=1-A\HF=-629.2731153\MP2=-631.5729337\RMSD=4
.243e-09\Thermal=0.\PG=C01 [X(C12H20N3)]\@

4e-Me⁺_6

1\1\GINC-EDDY\SP\RMP2-FC\6-31+G(2d,p)\C12H20N3(1+)\RAMAN\25-Oct-2011\0
\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geom=
check\sp of cat81et18.mca mp2-5 on 2p 900 MB\1,1\C,0,-0.1509000948,3
.0448718181,0.0590299708\C,0,0.8515885786,2.095433777,0.0667614511\C,0
,0.5631761406,0.715022493,-0.0420600014\C,0,-0.8389212725,0.3436580813
,-0.1733889272\C,0,-1.78338231,1.3630417487,-0.1471039599\N,0,-1.44323
40065,2.6841872497,-0.0490868873\N,0,-1.1799196503,-0.9776973021,-0.33
82811762\C,0,-0.1987243708,-1.971559246,0.081916528\C,0,1.1809511696,-
1.5978078826,-0.4505176449\N,0,1.5304967909,-0.2353240869,-0.035903374
1\C,0,-2.576763262,-1.4092931894,-0.4495243524\C,0,-3.3206887802,-1.53
65077699,0.8901229835\C,0,2.9505213653,0.172962013,0.0562044263\C,0,3.
9402685371,-0.9726906764,0.2713461848\H,0,-0.1628832751,-2.0719131669,
1.1777117215\H,0,1.9166631558,-2.2921864082,-0.0420610052\H,0,3.033935

7749,0.8633820107,0.9039279542\H,0,3.222040426,0.7305286064,-0.8534834
713\H,0,4.9358811744,-0.5346219147,0.4007820047\H,0,3.7125414979,-1.54
7046514,1.1766062407\H,0,3.9938093989,-1.6538264064,-0.5844129006\H,0,
-2.5634408109,-2.3789003604,-0.9608359345\H,0,-3.0953962717,-0.7199315
71,-1.1271684826\H,0,-2.8460303989,-2.2847380975,1.5351337272\H,0,-3.3
472850342,-0.5874072031,1.4385557758\H,0,-4.3541237721,-1.8555749516,0
.7127077751\H,0,-2.8450000557,1.1649719521,-0.2027186842\H,0,0.0599693
616,4.1055103791,0.1287975754\H,0,1.8720818528,2.4479620517,0.13070204
27\H,0,-0.4906005315,-2.940611879,-0.3359409357\H,0,1.2000250529,-1.68
17644867,-1.5466307231\C,0,-2.5202795994,3.6903553256,-0.0531575148\H,
0,-3.0840198248,3.6219323281,-0.9880818703\H,0,-3.1879271549,3.5188213
091,0.7964024335\H,0,-2.0799704509,4.6849543993,0.0304104604\\Version=
AM64L-G03RevD.01\State=1-A\HF=-629.2694234\MP2=-631.5711676\RMSD=2.576
e-09\Thermal=0.\PG=C01 [X(C12H20N3)]\\@

4e-Me⁺_7

1\1\GINC-CALYPSO\SP\RMP2-FC\6-31+G(2d,p)\C12H20N3(1+)\RAMAN\26-Oct-201
1\0\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read ge
om=check\\sp of cat81et15.mca mp2-5 on 2p 900 MB\\1,1\C,0,0.0296691235
,3.0452257904,0.0432299113\C,0,-0.9349728923,2.056723681,0.0755469391\
C,0,-0.5926903883,0.688384294,-0.0051729838\C,0,0.8206244559,0.3662849
285,-0.1434699586\C,0,1.7249639139,1.424307376,-0.1536139219\N,0,1.333
9979605,2.7312495812,-0.0589147743\N,0,1.2224167384,-0.9395554469,-0.2
584826537\C,0,0.208144956,-1.9595930489,-0.4985662314\C,0,-1.048641180
2,-1.665474605,0.3123717409\N,0,-1.5182680001,-0.3037972189,0.03976969
3\C,0,2.626642374,-1.2972138241,-0.4979822821\C,0,3.4599301303,-1.3840
854592,0.7887612363\C,0,-2.9473858947,0.0400938206,0.2082873998\C,0,-3
.9164421281,-1.1268538866,0.0130213455\H,0,-0.0428975108,-2.0271305892
, -1.5686065845\H,0,-1.8249450649,-2.3748149339,0.0232244019\H,0,-3.181
9195425,0.808783042,-0.5372100481\H,0,-3.0979914081,0.4864823203,1.203
6989603\H,0,-3.7865524618,-1.6056390289,-0.9643144328\H,0,-3.834170701
4,-1.8839311282,0.7998726174\H,0,-4.9357853122,-0.7278877015,0.0529120
736\H,0,3.0701761705,-0.5887677318,-1.212423326\H,0,2.6260345955,-2.26
77090839,-1.0047283196\H,0,4.4946416537,-1.6525544822,0.5464431056\H,0
,3.4739279061,-0.4336409999,1.3349145691\H,0,3.0560562218,-2.150036152
7,1.4601560607\H,0,2.7917894178,1.2689677888,-0.2360091694\H,0,-0.2199
049079,4.0971320843,0.116091818\H,0,-1.9649859271,2.3669790876,0.18878
28949\H,0,-0.8490447803,-1.7945412197,1.3863619745\H,0,0.6097615659,-2
.9283506417,-0.1832496895\C,0,2.3729323797,3.7769117004,-0.0643161093\
H,0,3.021015739,3.6570630139,0.8089537025\H,0,2.9661550084,3.700007318
5,-0.9800635878\H,0,1.8939887196,4.7563426757,-0.0275609415\\Version=A
M64L-G03RevD.01\State=1-A\HF=-629.2680104\MP2=-631.5700081\RMSD=8.146e
-09\Thermal=0.\PG=C01 [X(C12H20N3)]\\@

4f

4f_1

1\1\GINC-AZAZEL\SP\RMP2-FC\6-31+G(2d,p)\C15H23N3\EVGENY\27-Feb-2008\0\
\#P MP2/6-31+G(2d,p) scf=tight int=finegrid\\Single point of cat1_1 MP
2/6-31+G(2d,p)\\0,1\C,1,1.39454857\C,2,1.40726329,1,120.06648515\C,3
,1.43204262,2,117.07551457,1,-0.97027423,0\C,4,1.40426177,3,116.861884
28,2,0.28332482,0\N,1,1.3335031,2,123.76816059,3,0.6758559,0\N,4,1.413

74771,3,119.89764318,2,178.8163346,0\C,7,1.47186845,4,114.68657158,3,2
5.42624603,0\C,8,1.54629719,7,108.34560017,4,-52.48835821,0\N,3,1.3820
7371,2,122.53854186,1,179.14217575,0\C,9,1.54550405,8,111.73751379,7,-
68.63862175,0\C,11,1.5387461,9,111.67666761,8,-56.89741253,0\C,12,1.53
834345,11,110.87243318,9,55.20754655,0\C,13,1.53898982,12,110.76801653
,11,-54.0144621,0\C,7,1.46445957,4,117.65009058,3,170.06714944,0\C,15,
1.54013311,7,115.46085922,4,-74.01769279,0\C,10,1.45835197,3,121.90650
144,2,0.58679491,0\C,17,1.53785492,10,113.36107061,3,81.46946372,0\H,8
,1.10572224,7,110.40237588,4,64.8441838,0\H,9,1.10102724,8,106.4579474
2,7,172.8164881,0\H,11,1.09894707,9,109.17762082,8,-179.3740317,0\H,11
,1.09765891,9,108.27495397,8,64.28843043,0\H,12,1.09818077,11,110.0548
4655,9,177.72433044,0\H,12,1.10188896,11,109.5226831,9,-65.46809992,0\
H,13,1.09847611,12,110.39727717,11,-175.53039996,0\H,13,1.09887667,12,
109.16030357,11,67.21390191,0\H,14,1.09679728,13,111.15974951,12,-178.
27292166,0\H,14,1.10039845,13,108.88702951,12,-62.35786772,0\H,17,1.09
893399,10,109.97100909,3,-42.69435116,0\H,17,1.09663476,10,107.2954702
9,3,-157.46277063,0\H,18,1.09562199,17,111.07089109,10,-59.2029716,0\H
,18,1.09690057,17,110.57182652,10,60.57459835,0\H,18,1.09764959,17,110
.53484189,10,-179.52161546,0\H,15,1.09417728,7,107.99681128,4,162.9649
7786,0\H,15,1.09517373,7,107.76488551,4,49.79737652,0\H,16,1.09747106,
15,111.14352053,7,-62.53515806,0\H,16,1.09556146,15,111.41670697,7,57.
85418922,0\H,16,1.09748648,15,110.22933792,7,178.01682937,0\H,5,1.0867
1835,4,119.81530486,3,-179.17280373,0\H,1,1.09009268,6,116.52800469,5,
-179.41388857,0\H,2,1.08492215,1,119.13012133,6,-179.4992021,0\\Versio
n=AM64L-G03RevD.01\State=1-A\HF=-744.8165435\MP2=-747.5769739\RMSE=9.6
27e-09\Thermal=0.\PG=C01 [X(C15H23N3)]\@

4f_2

1\1\GINC-MAX\SP\RMP2-FC\6-31+G(2d,p)\C15H23N3\EVGENY\28-Feb-2008\0\#P
MP2/6-31+G(2D,P) SCF=TIGHT INT=FINEGRID\\Single point of cat1_2 MP2/6
-31+G(2d,p)\0,1\C\C,1,1.39596276\C,2,1.40555418,1,119.94466885\C,3,1.
42789662,2,117.15837568,1,-1.05631966,0\C,4,1.40448307,3,117.03113778,
2,2.68797736,0\N,1,1.33416857,2,123.72947235,3,-1.0250577,0\N,4,1.4105
705,3,121.55921357,2,-177.89372884,0\C,7,1.46955922,4,117.78914873,3,5
.25365339,0\C,8,1.54266188,7,110.44974292,4,-33.39090727,0\N,3,1.38954
933,2,123.41040256,1,179.81143447,0\C,9,1.54701031,8,112.80842011,7,-7
1.02912309,0\C,11,1.53770863,9,111.72719082,8,-55.15088894,0\C,12,1.53
696558,11,110.59426416,9,55.25939127,0\C,13,1.53852449,12,110.90070493
,11,-55.4262519,0\C,7,1.47306487,4,116.72469568,3,148.55724236,0\C,15,
1.53591837,7,114.4894124,4,103.91566426,0\C,10,1.46154928,3,120.568212
57,2,-4.03607408,0\C,17,1.53662862,10,112.81605133,3,83.20735505,0\H,8
,1.10619568,7,109.63815759,4,84.3183693,0\H,9,1.09937135,8,105.8500908
9,7,170.46977028,0\H,11,1.0990754,9,108.87736956,8,-177.54066601,0\H,1
1,1.09830478,9,108.8291431,8,66.22227096,0\H,12,1.09820277,11,110.0093
4304,9,177.67809042,0\H,12,1.10196457,11,109.61495409,9,-65.46770173,0\
\H,13,1.09842744,12,110.4961218,11,-177.15357995,0\H,13,1.09840733,12,
109.14455155,11,65.32892336,0\H,14,1.09709565,13,110.55918032,12,-179.
46643015,0\H,14,1.1010572,13,109.27691208,12,-63.25422207,0\H,17,1.101
2891,10,110.75690068,3,-41.17051304,0\H,17,1.09629779,10,107.26591342,
3,-156.56246952,0\H,18,1.09762274,17,110.41649147,10,-179.65431653,0\H
,18,1.09548094,17,111.40405752,10,-59.34987208,0\H,18,1.09630152,17,11

0.36013679,10,60.40058288,0\H,15,1.09797013,7,108.80358631,4,-19.15778
941,0\H,15,1.09885908,7,108.31679618,4,-133.76367116,0\H,16,1.09602328
,15,111.39451059,7,62.37489283,0\H,16,1.09808209,15,110.09611731,7,-17
7.68211105,0\H,16,1.09600853,15,111.23039325,7,-57.79442665,0\H,5,1.08
817411,4,119.37344563,3,177.09595722,0\H,1,1.08995624,6,116.52220588,5
, -179.49255998,0\H,2,1.08494723,1,119.22643642,6,179.45070511,0\Version=x86-Linux-G03RevB.03\State=1-A\HF=-744.8164305\MP2=-747.5762908\RMS
D=7.135e-09\PG=C01 [X(C15H23N3)]\@

4f_3

1\1\GINC-MAX\SP\RMP2-FC\6-31+G(2d,p)\C15H23N3\EVGENY\29-Feb-2008\0\#P
MP2/6-31+G(2D,P) SCF=TIGHT INT=FINEGRID\Single point of cat1_4 MP2/6
-31+G(2d,p)\0,1\C\C,1,1.54469776\C,2,1.54564688,1,108.61957118\C,3,1.
5469969,2,111.6413388,1,55.78036581,0\C,4,1.53903414,3,111.67224233,2,
-56.55023666,0\C,5,1.53833156,4,111.1435683,3,54.82740057,0\N,3,1.4544
5027,2,109.51467639,1,-177.53113916,0\C,7,1.39529406,3,117.66312792,2,
-44.66728466,0\C,8,1.43178819,7,120.05997757,3,16.99168207,0\N,9,1.401
73098,8,120.49719111,7,-2.68943517,0\C,9,1.40529903,8,116.34251855,7,1
78.81674248,0\C,11,1.39691574,9,120.49666212,8,0.73150548,0\N,12,1.332
9669,11,123.7333309,9,-0.9403148,0\C,13,1.34128645,12,116.40754102,11,
0.47002488,0\C,10,1.46403817,9,118.26158255,8,168.94669613,0\C,15,1.53
915295,10,114.85861229,9,-76.0141288,0\C,7,1.45951546,3,117.96213919,2
,155.3831165,0\C,17,1.53758606,7,113.19827406,3,-116.86377424,0\H,2,1.
10419754,1,108.14861009,6,-172.58322872,0\H,3,1.10048495,2,106.2624371
6,1,-62.39133899,0\H,4,1.09891854,3,109.08262399,2,-178.77858381,0\H,4
,1.09797154,3,108.60418797,2,64.91305739,0\H,5,1.09819561,4,110.080806
23,3,177.49036037,0\H,5,1.10182621,4,109.42420222,3,-65.78996516,0\H,6
,1.09839246,5,110.39085968,4,-175.40042288,0\H,6,1.09912129,5,109.2889
0654,4,67.30517031,0\H,1,1.09689333,6,111.29250424,5,-177.95248266,0\H
,1,1.10031446,6,108.96476609,5,-61.99410454,0\H,17,1.10063225,7,110.58
798614,3,118.69361175,0\H,17,1.09684808,7,107.27566355,3,3.58789425,0\H
,18,1.09543902,17,111.38652433,7,-59.28841787,0\H,18,1.09663382,17,11
0.39788627,7,60.51941877,0\H,18,1.09772286,17,110.44207822,7,-179.5819
1096,0\H,15,1.09361839,10,108.16881842,9,161.03241619,0\H,15,1.0948544
,10,108.03876556,9,47.71920329,0\H,16,1.09729893,15,111.08680493,10,-6
2.10528614,0\H,16,1.09578766,15,111.23408909,10,58.15767746,0\H,16,1.0
9743839,15,110.31701618,10,178.36628125,0\H,11,1.08408254,9,121.171649
23,8,-178.90181207,0\H,14,1.08738934,13,115.04668459,12,-179.34839449,
0\H,12,1.08988105,11,119.62923311,9,179.5974885,0\Version=x86-Linux-G
03RevB.03\State=1-A\HF=-744.8152691\MP2=-747.5765605\RMSD=7.123e-09\PG
=C01 [X(C15H23N3)]\@

4f_4

1\1\GINC-MORITZ\SP\RMP2-FC\6-31+G(2d,p)\C15H23N3\EVGENY\29-Feb-2008\0\
\#P MP2/6-31+G(2D,P) SCF=TIGHT INT=FINEGRID\Single point of cat1_6 MP
2/6-31+G(2d,p)\0,1\C\C,1,1.54793367\C,2,1.54368007,1,109.39006872\C,3
,1.54770417,2,112.96123561,1,52.08098008,0\C,4,1.53751057,3,111.863181
25,2,-54.70695802,0\C,5,1.53663352,4,110.51526904,3,55.38225626,0\N,3,
1.46048939,2,109.1172123,1,179.13240667,0\C,7,1.40218689,3,114.7462165
8,2,-55.2579669,0\C,8,1.42831093,7,118.97340925,3,28.82249764,0\N,9,1.
39738189,8,121.35665831,7,-0.97915363,0\C,9,1.4049773,8,116.69630035,7

,179.25308055,0\C,11,1.39672722,9,120.16787292,8,-1.11675243,0\N,12,1.
33358911,11,123.76817617,9,0.35684962,0\C,13,1.34258806,12,116.4930288
5,11,0.62016767,0\C,10,1.47067214,9,117.6284227,8,151.90328521,0\C,15,
1.53636516,10,114.74547489,9,100.6263589,0\C,7,1.46228861,3,117.283503
27,2,155.93514591,0\C,17,1.53638778,7,112.72225875,3,-129.96252052,0\H
,2,1.10476996,1,108.02909988,6,-169.53971978,0\H,3,1.09951482,2,105.66
442991,1,-66.18834065,0\H,4,1.09896248,3,108.74528838,2,-177.05869087,
0\H,4,1.09848058,3,108.98898016,2,66.81965077,0\H,5,1.09823507,4,110.0
901634,3,177.78499026,0\H,5,1.10192262,4,109.65080575,3,-65.28379144,0
\H,6,1.09846996,5,110.55318566,4,-177.32255232,0\H,6,1.09869151,5,109.
10291925,4,65.27018529,0\H,1,1.09712772,6,110.63250622,5,-179.13441664
,0\H,1,1.10094931,6,109.1277161,5,-63.07812798,0\H,17,1.10234559,7,111
.25510317,3,105.36427046,0\H,17,1.0965782,7,107.13601033,3,-10.2055470
5,0\H,18,1.09521214,17,111.57813093,7,-59.36739414,0\H,18,1.09622979,1
7,110.25322143,7,60.44592255,0\H,18,1.09763323,17,110.35414888,7,-179.
63861195,0\H,15,1.09782619,10,108.60587108,9,-22.50206679,0\H,15,1.098
22501,10,108.06479791,9,-136.90957443,0\H,16,1.09560326,15,111.4447921
2,10,63.01041353,0\H,16,1.09802832,15,110.0608767,10,-177.07109327,0\H
,16,1.09600564,15,111.22850736,10,-57.17499494,0\H,11,1.08517317,9,120
.74901982,8,178.18566044,0\H,14,1.08748423,13,115.00136111,12,-179.578
62076,0\H,12,1.08994932,11,119.69780021,9,-179.84827519,0\\Version=x86
-Linux-G03RevB.03\State=1-A\HF=-744.8160863\MP2=-747.5763769\RMSD=6.85
3e-09\PG=C01 [X(C15H23N3)]\@

4f_5

1\1\GINC-HAENSEL\SP\RMP2-FC\6-31+G(2d,p)\C15H23N3\EVGENY\29-Feb-2008\0
\#P MP2/6-31+G(2D,P) SCF=TIGHT INT=FINEGRID\\Single point of cat1_7 M
P2/6-31+G(2d,p)\0,1\C\C,1,1.54386819\C,2,1.54998899,1,108.91134081\C,
3,1.5484667,2,111.19163129,1,55.86323096,0\C,4,1.53950594,3,111.704762
03,2,-56.56213248,0\C,5,1.53812703,4,111.30542958,3,55.04058369,0\N,3,
1.45308043,2,109.22046994,1,-177.19376272,0\C,7,1.39344518,3,117.93113
765,2,-44.75940525,0\C,8,1.43180797,7,119.94747693,3,16.8404551,0\N,9,
1.4015284,8,120.46219727,7,-2.52253616,0\C,9,1.40581706,8,116.30324174
,7,178.36447787,0\C,11,1.39671132,9,120.48532044,8,0.29012015,0\N,12,1
.33342355,11,123.77026114,9,-0.34645416,0\C,13,1.3406549,12,116.388068
59,11,0.56803362,0\C,10,1.46422354,9,118.25380846,8,169.26199925,0\C,1
5,1.53918735,10,114.87399964,9,-76.21696438,0\C,7,1.45514341,3,119.796
37647,2,142.50840595,0\C,17,1.54159112,7,116.22296054,3,88.09704195,0\H
H,2,1.10428305,1,108.16843155,6,-172.73824898,0\H,3,1.10040067,2,106.6
0957909,1,-62.12624673,0\H,4,1.0971867,3,109.2008502,2,-178.70877613,0
\H,4,1.09800662,3,108.70806803,2,64.90198411,0\H,5,1.09825353,4,110.00
546232,3,177.76224613,0\H,5,1.10191394,4,109.35630518,3,-65.60820788,0
\H,6,1.09847135,5,110.38587465,4,-175.32168545,0\H,6,1.0991043,5,109.2
4545876,4,67.46490506,0\H,1,1.09703526,6,111.30207683,5,-178.20829893,
0\H,1,1.10036925,6,108.93442015,5,-62.23301612,0\H,17,1.09911662,7,107
.13512909,3,-34.12131674,0\H,17,1.09831761,7,108.11772187,3,-148.21283
094,0\H,18,1.09606129,17,111.3192391,7,-64.82492265,0\H,18,1.09558182,
17,111.38048091,7,55.70318623,0\H,18,1.09802531,17,109.97874153,7,175.
66438573,0\H,15,1.0936306,10,108.13874761,9,160.86720783,0\H,15,1.0948
7443,10,108.04184529,9,47.5105757,0\H,16,1.09730442,15,111.10992994,10
, -62.06887911,0\H,16,1.09576554,15,111.22951884,10,58.19785956,0\H,16,

1.09747528,15,110.30144863,10,178.40790968,0\H,11,1.08415171,9,121.186
50991,8,-178.68975107,0\H,14,1.08771198,13,115.13249178,12,179.1426779
4,0\H,12,1.08985365,11,119.61560622,9,179.96936201,0\Version=x86-Linu
x-G03RevB.03\State=1-A\HF=-744.8137329\MP2=-747.5755215\RMSD=5.927e-09
\PG=C01 [X(C15H23N3)]\@

4f_6

1\1\GINC-HAENSEL\SP\RMP2-FC\6-31+G(2d,p)\C15H23N3\EVGENY\07-Mar-2008\0
\#P MP2/6-31+G(2D,P) SCF=TIGHT INT=FINEGRID\Single point of cat1_9 M
P2/6-31+G(2d,p)\0,1\C\C,1,1.39560163\C,2,1.4056507,1,119.87984868\C,3
,1.42783489,2,117.27283861,1,-1.00404468,0\C,4,1.40464388,3,116.954013
09,2,3.0324227,0\N,1,1.33461131,2,123.70437756,3,-1.50657921,0\N,4,1.4
1171488,3,121.50156816,2,-176.72413917,0\C,7,1.47083134,4,117.81737611
,3,5.59119548,0\C,8,1.54627573,7,110.05305186,4,-34.26362866,0\N,3,1.3
8556019,2,123.53619171,1,-179.5862066,0\C,9,1.54878168,8,112.09677928,
7,-70.57907852,0\C,11,1.53814413,9,111.73103931,8,-55.51875014,0\C,12,
1.53612695,11,110.8167244,9,55.68804822,0\C,13,1.53808485,12,110.80456
474,11,-55.24151126,0\C,7,1.47386683,4,116.46682584,3,148.43120422,0\C
,15,1.53575542,7,114.46950849,4,103.69794557,0\C,10,1.45617506,3,121.8
7883889,2,8.08544065,0\C,17,1.54149481,10,116.5092147,3,-84.12719597,0
\H,8,1.10632424,7,109.73797246,4,83.27299187,0\H,9,1.09940674,8,106.39
637728,7,171.0387557,0\H,11,1.09700296,9,109.1349279,8,-177.8147026,0\
H,11,1.09825735,9,108.86139495,8,65.8492189,0\H,12,1.09826806,11,109.9
1030234,9,178.18890023,0\H,12,1.10198817,11,109.52618433,9,-65.0814381
7,0\H,13,1.09846104,12,110.54127282,11,-176.95877227,0\H,13,1.09826636
,12,109.16414517,11,65.46589382,0\H,14,1.09723417,13,110.52800761,12,-
179.73139462,0\H,14,1.10114988,13,109.31526641,12,-63.56250805,0\H,17,
1.09899341,10,107.16748338,3,153.25045154,0\H,17,1.09756243,10,107.621
51936,3,39.36109697,0\H,18,1.09593817,17,111.52643275,10,-66.40214033,
0\H,18,1.09575939,17,111.3607209,10,54.28929293,0\H,18,1.09791293,17,1
09.86206701,10,174.22596638,0\H,15,1.09793438,7,108.79872582,4,-19.369
95253,0\H,15,1.09851311,7,108.36084833,4,-133.98300593,0\H,16,1.095983
69,15,111.23425311,7,-57.54051454,0\H,16,1.09584559,15,111.34283599,7,
62.63921138,0\H,16,1.09808409,15,110.10068051,7,-177.43557801,0\H,5,1.
08827785,4,119.41907239,3,177.2062333,0\H,1,1.08995633,6,116.5059904,5
, -179.51044009,0\H,2,1.08541573,1,119.42014729,6,178.05433201,0\Versi
on=x86-Linux-G03RevB.03\State=1-A\HF=-744.8144672\MP2=-747.5746646\RMS
D=7.380e-09\PG=C01 [X(C15H23N3)]\@

4f_7

1\1\GINC-HAENSEL\SP\RMP2-FC\6-31+G(2d,p)\C15H23N3\EVGENY\07-Mar-2008\0
\#P MP2/6-31+G(2D,P) SCF=TIGHT INT=FINEGRID\SP of cat1_10 with g03d1
2-processor run, 1800MB RAM\0,1\C\C,1,1.54521487\C,2,1.54636916,1,10
8.39627667\C,3,1.54687106,2,111.89379538,1,56.0853273,0\C,4,1.53942729
,3,111.66829187,2,-55.83236982,0\C,1,1.53880892,2,112.90700567,3,-57.2
3928083,0\N,3,1.45895474,2,108.75537166,1,-176.81377903,0\C,7,1.404470
46,3,114.85110087,2,-53.39484901,0\C,8,1.43181404,7,119.63500602,3,27.
25519608,0\N,9,1.39751839,8,120.84730718,7,-6.09556399,0\C,9,1.4064492
,8,116.28725392,7,175.50451058,0\C,11,1.39644512,9,120.39899238,8,1.98
951415,0\N,12,1.33252831,11,123.90459493,9,0.1504058,0\C,13,1.34278404
,12,116.25455685,11,-0.7352155,0\C,10,1.46362712,9,118.56667515,8,167.

36982817,0\C,15,1.53883122,10,114.5525144,9,-75.84308088,0\C,7,1.46280
804,3,118.80516274,2,158.9548592,0\C,17,1.53233854,7,114.15541278,3,-4
1.907717,0\H,2,1.10357151,1,108.28743469,6,-173.23447793,0\H,3,1.09627
283,2,105.59371157,1,-61.77793971,0\H,4,1.09916504,3,109.12118076,2,-1
77.80009683,0\H,4,1.09795982,3,108.96836078,2,65.87387139,0\H,5,1.0983
0125,4,110.03901433,3,176.72935606,0\H,5,1.10186778,4,109.33909794,3,-
66.65625268,0\H,6,1.09840387,1,109.71132589,2,178.71088543,0\H,6,1.099
2314,1,109.79521234,2,-64.05294329,0\H,1,1.09679744,6,111.38240477,5,-
177.14383034,0\H,1,1.10044029,6,109.05044534,5,-61.17342864,0\H,17,1.0
9689759,7,106.94416098,3,-161.00583417,0\H,17,1.10630823,7,111.7039325
,3,82.92316334,0\H,18,1.0967989,17,111.10163135,7,-52.09850292,0\H,18,
1.09624494,17,112.87578115,7,70.22543874,0\H,18,1.09639441,17,108.7788
3996,7,-170.89026356,0\H,15,1.09315728,10,108.15114944,9,161.34989886,
0\H,15,1.09502572,10,108.31362685,9,47.85083769,0\H,16,1.09750811,15,1
10.38783979,10,178.63539619,0\H,16,1.09721788,15,111.0934344,10,-61.73
338695,0\H,16,1.09584898,15,111.0540707,10,58.46779491,0\H,11,1.083999
44,9,121.21171104,8,-177.86921278,0\H,14,1.08668643,13,114.78490517,12
,179.27884827,0\H,12,1.09006548,11,119.5222892,9,179.91268758,0\\Versi
on=x86-Linux-G03RevB.03\State=1-A\HF=-744.8146043\MP2=-747.5763742\RMS
D=7.112e-09\PG=C01 [X(C15H23N3)]\@

4f_8

1\1\GINC-HAENSEL\SP\RMP2-FC\6-31+G(2d,p)\C15H23N3\EVGENY\08-Mar-2008\0
\\#P MP2/6-31+G(2D,P) SCF=TIGHT INT=FINEGRID\\SP of cat1_12 with g03d1
2-processor run, 1800MB RAM\\0,1\C\C,1,1.39561849\C,2,1.40561788,1,12
0.18618729\C,3,1.43219862,2,117.09892162,1,2.3038227,0\C,4,1.4062184,3
,116.72170142,2,-3.12976545,0\N,1,1.33254387,2,123.5829141,3,-0.352447
86,0\N,4,1.4101229,3,120.63259311,2,175.11023261,0\C,7,1.46950666,4,11
6.27678748,3,19.01073959,0\C,8,1.54621566,7,108.79969597,4,-45.0597211
2,0\N,3,1.39303749,2,122.73602993,1,-176.67848454,0\C,9,1.54589383,8,1
11.82775346,7,-67.20166266,0\C,11,1.53903232,9,111.4658783,8,-56.65445
06,0\C,12,1.53879355,11,111.28835132,9,54.36784577,0\C,13,1.53935104,1
2,110.70925023,11,-53.80829565,0\C,7,1.46412352,4,118.02216621,3,166.9
0803061,0\C,15,1.53958428,7,115.0143361,4,-74.12200322,0\C,10,1.464013
45,3,118.43291416,2,-6.51486951,0\C,17,1.53208745,10,114.39720748,3,17
0.56332823,0\H,8,1.10489112,7,110.6701842,4,72.48452381,0\H,9,1.096300
09,8,105.75091947,7,174.74605856,0\H,11,1.0992182,9,109.30549045,8,-17
8.69662395,0\H,11,1.09783422,9,108.75861377,8,64.7763436,0\H,12,1.0982
3273,11,110.06405231,9,177.11783598,0\H,12,1.10194071,11,109.346598,9,
-66.21448557,0\H,13,1.09842524,12,110.31048867,11,-175.36597509,0\H,13
,1.0989649,12,109.36716842,11,67.25165661,0\H,14,1.09671936,13,111.270
60931,12,-177.73541258,0\H,14,1.10048832,13,109.1138691,12,-61.7012998
7,0\H,17,1.09674243,10,107.12016018,3,51.33957206,0\H,17,1.10544993,10
,111.26829229,3,-64.74955043,0\H,18,1.09664891,17,111.21942992,10,-53.
20624173,0\H,18,1.09599644,17,112.87417948,10,69.21671968,0\H,18,1.096
36408,17,108.63617661,10,-171.90833772,0\H,15,1.09371345,7,108.0067018
5,4,162.94171909,0\H,15,1.09498069,7,108.17221229,4,49.69608382,0\H,16
,1.09744444,15,110.35336252,7,178.11612142,0\H,16,1.09739865,15,111.12
79037,7,-62.30585141,0\H,16,1.0957389,15,111.16999591,7,57.99107693,0\
H,5,1.0864225,4,119.85158869,3,-177.65607814,0\H,1,1.08999241,6,116.62
115343,5,179.23752602,0\H,2,1.08408293,1,118.8523108,6,179.32419018,0\

\\Version=x86-Linux-G03RevB.03\\State=1-A\\HF=-744.8142582\\MP2=-747.57619
77\\RMSD=7.155e-09\\PG=C01 [X(C15H23N3)]\\@

4f_9

1\\1\\GINC-HAENSEL\\SP\\RMP2-FC\\6-31+G(2d,p)\\C15H23N3\\EVGENY\\08-Mar-2008\\0
\\#P MP2/6-31+G(2D,P) SCF=TIGHT INT=FINEGRID\\SP of cat1_13 with g03d1
2-processor run, 1800MB RAM\\0,1\\C\\C,1,1.39450823\\C,2,1.40745288,1,12
0.06371034\\C,3,1.43212224,2,117.03495151,1,-1.21383216,0\\C,4,1.4040344
9,3,116.90485403,2,0.58031438,0\\N,1,1.33358318,2,123.79545205,3,0.7080
0833,0\\N,4,1.41412536,3,119.82500898,2,179.15925792,0\\C,7,1.4720958,4,
114.48649707,3,25.98786248,0\\C,8,1.54636846,7,108.30133479,4,-53.17616
511,0\\N,3,1.38169667,2,122.56732778,1,178.75571064,0\\C,9,1.54540347,8,
111.73783999,7,-68.77604606,0\\C,11,1.53866645,9,111.6701467,8,-56.9201
7793,0\\C,12,1.53841045,11,110.86601286,9,55.27157663,0\\C,13,1.53894492
,12,110.78060387,11,-54.0056304,0\\C,7,1.46462078,4,117.6153138,3,170.2
8276166,0\\C,15,1.54021201,7,115.52605408,4,-73.88235253,0\\C,10,1.45810
637,3,122.01371396,2,1.40624689,0\\C,17,1.53793261,10,113.39489015,3,81
.702768,0\\H,8,1.10579707,7,110.35755964,4,64.11321567,0\\H,9,1.10117316
,8,106.46010726,7,172.68371353,0\\H,11,1.09888731,9,109.1864611,8,-179.
42058226,0\\H,11,1.09763134,9,108.24461843,8,64.25710815,0\\H,12,1.09816
639,11,110.05930374,9,177.78547791,0\\H,12,1.10189075,11,109.53018397,9
, -65.40918672,0\\H,13,1.09847389,12,110.39804546,11,-175.52119076,0\\H,1
3,1.0988813,12,109.14917612,11,67.25464675,0\\H,14,1.09672695,13,111.15
261573,12,-178.37007161,0\\H,14,1.1003759,13,108.86962787,12,-62.469269
61,0\\H,17,1.09853189,10,109.87972086,3,-42.43843544,0\\H,17,1.09670002,
10,107.30765046,3,-157.13437916,0\\H,18,1.09762417,17,110.55252041,10,-
179.6863881,0\\H,18,1.09564082,17,111.0580186,10,-59.35638252,0\\H,18,1.
09699672,17,110.5996254,10,60.4298313,0\\H,15,1.09418845,7,107.96949531
,4,163.08293699,0\\H,15,1.09520092,7,107.72986955,4,49.93546204,0\\H,16,
1.09747542,15,110.19846957,7,177.9406274,0\\H,16,1.0974357,15,111.17354
971,7,-62.6240893,0\\H,16,1.09550351,15,111.44262808,7,57.79361064,0\\H,
5,1.08672831,4,119.80157464,3,-179.3438034,0\\H,1,1.09011958,6,116.5200
0488,5,-179.30324938,0\\H,2,1.08494685,1,119.09506398,6,-179.52094865,0
\\Version=x86-Linux-G03RevB.03\\State=1-A\\HF=-744.8165639\\MP2=-747.5769
435\\RMSD=9.561e-09\\PG=C01 [X(C15H23N3)]\\@

4f_10

1\\1\\GINC-HAENSEL\\SP\\RMP2-FC\\6-31+G(2d,p)\\C15H23N3\\EVGENY\\08-Mar-2008\\0
\\#P MP2/6-31+G(2D,P) SCF=TIGHT INT=FINEGRID\\SP of cat1_14 with g03d1
2-processor run, 1800MB RAM\\0,1\\C\\C,1,1.54800083\\C,2,1.5479882,1,109
.80365938\\C,3,1.54972379,2,112.20459804,1,52.36321329,0\\C,4,1.53795366
,3,111.95297872,2,-54.85716097,0\\C,5,1.53595111,4,110.766664,3,55.7331
6574,0\\N,3,1.45565084,2,108.79232174,1,179.09420532,0\\C,7,1.39505214,3
,115.95392124,2,-54.55049149,0\\C,8,1.42782379,7,118.67716892,3,27.5837
088,0\\N,9,1.39906777,8,121.27946569,7,-0.15367572,0\\C,9,1.40512885,8,1
16.57038838,7,179.27478492,0\\C,11,1.39722767,9,120.15412128,8,-1.82533
575,0\\N,12,1.3341935,11,123.81733882,9,0.61786983,0\\C,13,1.34179459,12
,116.46589311,11,1.06528513,0\\C,10,1.47143099,9,117.22297618,8,151.567
33892,0\\C,15,1.53626061,10,114.7389283,9,100.53209932,0\\C,7,1.45454849
,3,120.19620343,2,140.80866834,0\\C,17,1.54210964,7,116.84278292,3,78.9
5224302,0\\H,2,1.10500444,1,107.97930708,6,-169.93850902,0\\H,3,1.099538

7,2,106.27572151,1,-65.91792013,0\H,4,1.0969614,3,108.99834229,2,-177.
24596468,0\H,4,1.09852133,3,108.92284297,2,66.63119577,0\H,5,1.0983109
4,4,109.96498627,3,178.21741222,0\H,5,1.10194159,4,109.57608739,3,-65.
00217608,0\H,6,1.09849364,5,110.58797164,4,-177.17707877,0\H,6,1.09851
834,5,109.15015744,4,65.33087716,0\H,1,1.09740196,6,110.59241778,5,-17
9.46735681,0\H,1,1.10103622,6,109.19605111,5,-63.39340666,0\H,17,1.099
79644,7,107.20582518,3,-43.62594021,0\H,17,1.0977017,7,107.46725601,3,
-157.51718797,0\H,18,1.09575255,17,111.48903348,7,54.85153711,0\H,18,1
.09799706,17,109.8680645,7,174.81197464,0\H,18,1.09623166,17,111.44946
549,7,-65.90448153,0\H,15,1.09781816,10,108.58466995,9,-22.56606216,0\
H,15,1.09784704,10,108.11769444,9,-136.99922565,0\H,16,1.0960033,15,11
1.22704106,10,-56.83631361,0\H,16,1.09554484,15,111.41954234,10,63.365
4351,0\H,16,1.09800002,15,110.05580089,10,-176.72769486,0\H,11,1.08529
03,9,120.81279995,8,178.28326585,0\H,14,1.08841241,13,115.33528919,12,
179.36233023,0\H,12,1.08988906,11,119.66612158,9,-179.60268354,0\\Vers
ion=x86-Linux-G03RevB.03\State=1-A\HF=-744.8137774\MP2=-747.5743643\RM
SD=6.919e-09\PG=C01 [X(C15H23N3)]\@

4f-Me⁺

4f-Me⁺_1

1\1\GINC-EDDY\SP\RMP2-FC\6-31+G(2d,p)\C16H26N3(1+)\RAMAN\06-Aug-2011\0
\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geom=
check\\sp of cat11_1.mca mp2-5 on 2p 900 MB\\1,1\C,0,3.5583861294,0.82
57649773,-0.6577534457\C,0,2.8402078358,-0.3164233271,-0.3797513001\C,
0,1.4362600595,-0.2783207889,-0.1875183622\C,0,0.7950662533,1.02857836
4,-0.2318302473\C,0,1.6025335414,2.1263981172,-0.4993969358\N,0,2.9483
366623,2.0250602972,-0.730919903\N,0,-0.5701111003,1.1300362122,-0.030
864497\C,0,-1.1749083392,0.0358902972,0.7641096446\C,0,-0.7630808133,-
1.3079440256,0.1316843711\N,0,0.7014301553,-1.3887721348,0.0201102668\
C,0,-1.4542576332,-1.5605119239,-1.225545936\C,0,-2.9857902615,-1.5075
202595,-1.0842934597\C,0,-3.4345311963,-0.168892497,-0.4762697449\C,0,
-2.7143293917,0.0950483021,0.8582236062\C,0,-1.184270947,2.4651138572,
0.0112846813\C,0,-0.9809403102,3.2365843214,1.3264884873\C,0,1.3038740
696,-2.7297805618,0.1119273249\C,0,1.8567640172,-3.0415131588,1.509524
0338\H,0,-0.7688402533,0.0693851468,1.7890271875\H,0,-1.061577843,-2.0
943972579,0.8386752512\H,0,-1.1372288735,-2.5346004018,-1.6205947943\H
,0,-1.1154121694,-0.7974638164,-1.9390628961\H,0,-3.4511970008,-1.6595
787182,-2.0655131432\H,0,-3.3253741733,-2.3352578749,-0.4434957425\H,0
, -4.5181803265,-0.171265224,-0.3066949128\H,0,-3.2295289349,0.64007664
53,-1.1917968918\H,0,-3.0374756822,1.0400575318,1.3096866506\H,0,-3.00
20420037,-0.6848682667,1.5779298069\H,0,2.0774575294,-2.8338410028,-0.
6572049891\H,0,0.5178611304,-3.4446268689,-0.1513279375\H,0,2.64845019
54,-2.3406603074,1.7976480953\H,0,1.0639021818,-2.9873722952,2.2646109
274\H,0,2.2735047715,-4.0548973423,1.5269820472\H,0,-2.2515572226,2.34
30836192,-0.1842666204\H,0,-0.8014725026,3.0342952809,-0.8440481104\H,
0,-1.4439179501,2.7100582799,2.1691232096\H,0,0.0790229611,3.380052284
,1.5663730157\H,0,-1.4493292875,4.2250026614,1.2530816551\H,0,1.213139
6914,3.133918516,-0.5370887145\H,0,4.628490128,0.8069518274,-0.8285441
627\H,0,3.3825356828,-1.2514110818,-0.3293730424\C,0,3.7059714687,3.25
33226192,-1.0255880368\H,0,3.3093293554,3.723316745,-1.9303473653\H,0,
3.6284446691,3.9475563979,-0.1832626968\H,0,4.7544417071,2.9968081354,

-1.1841408738\\Version=AM64L-G03RevD.01\\State=1-A\\HF=-784.2660631\\MP2=-787.1733766\\RMSD=6.915e-09\\Thermal=0.\\PG=C01 [X(C16H26N3)]\\@

4f-Me⁺_2

1\\1\\GINC-GOLEM\\SP\\RMP2-FC\\6-31+G(2d,p)\\C16H26N3(1+)\\RAMAN\\06-Aug-2011\\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geom=check\\sp of cat11_4.mca mp2-5 on 2p 900 MB\\1,1\\C,0,-3.1419522996,0.1726058116,0.6401351826\\C,0,-1.608790225,0.036940178,0.7508371744\\C,0,-1.1758349241,-1.3049482626,0.1277793367\\C,0,-1.6886210804,-1.4734684475,-1.3196143952\\C,0,-3.2199952392,-1.3399266209,-1.3911351977\\C,0,-3.6835086218,-0.0022154671,-0.7906565658\\N,0,0.2758432906,-1.4573393511,0.2383598463\\C,0,1.0724768953,-0.373577542,-0.0161628364\\C,0,0.4891728306,0.9589938199,-0.0944050511\\N,0,-0.8437640028,1.1378411988,0.1048679215\\C,0,1.3758887401,2.0207382946,-0.3896448137\\C,0,2.7284633076,1.810773542,-0.57315946\\N,0,3.2546313504,0.5768174839,-0.4691526164\\C,0,2.4476827177,-0.4931723708,-0.200464841\\C,0,-1.4113532439,2.498798932,0.10156673\\C,0,-1.2573450967,3.2379214536,1.4390490512\\C,0,0.8256196968,-2.8146104763,0.3332373002\\C,0,1.436584227,-3.1259710579,1.7076528743\\H,0,-1.3394753125,0.0211847426,1.8178051731\\H,0,-1.6193898343,-2.0889374589,0.7559425122\\H,0,-1.369192997,-2.4521582731,-1.7013901935\\H,0,-1.2158209093,-0.7130517216,-1.9572689187\\H,0,-3.5523560047,-1.4290113123,-2.4323521903\\H,0,-3.6868068083,-2.1704589751,-0.8402210811\\H,0,-4.7789038288,0.0485766868,-0.7699697888\\H,0,-3.3433299653,0.8219540412,-1.4344605815\\H,0,-3.4858735838,1.1095959323,1.0930315819\\H,0,-3.5546555131,-0.6238933488,1.2757576441\\H,0,1.5552034004,-2.9799638173,-0.4729254433\\H,0,0.0011651567,-3.5061636228,0.1324950626\\H,0,2.2526540773,-2.4391523274,1.9603692804\\H,0,0.6770703474,-3.0470859509,2.493553868\\H,0,1.8354360058,-4.146918908,1.7180074385\\H,0,-2.4657676243,2.4167055113,-0.1652710307\\H,0,-0.9488781963,3.0579983145,-0.7173196326\\H,0,-1.7830838262,2.7120813942,2.2446246515\\H,0,-0.2054558831,3.338038266,1.7302932922\\H,0,-1.686785493,4.2430956692,1.3582082742\\H,0,1.0242440094,3.0412965968,-0.4540242113\\H,0,2.9549507794,-1.4460109135,-0.139560272\\H,0,3.4134437461,2.622823537,-0.786658265\\C,0,4.7009733956,0.3462109847,-0.6281940841\\H,0,5.1215806808,-0.0262096121,0.3108187481\\H,0,4.8710216682,-0.3831790401,-1.4254467599\\H,0,5.1852649609,1.2870526403,-0.8934876447\\Version=AM64L-G03RevD.01\\State=1-A\\HF=-784.2629437\\MP2=-787.1719149\\RMSD=3.603e-09\\Thermal=0.\\PG=C01 [X(C16H26N3)]\\@

4f-Me⁺_3

1\\1\\GINC-EDDY\\SP\\RHF\\6-31G(d)\\C16H26N3(1+)\\RAMAN\\06-Aug-2011\\0\\#P RHF/6-31G(d) scf=tight int=finegrid SCRF=(PCM,Read,Solvent=Chloroform) geom=check guess=read\\PCM of cat11_11.mca b98/6-31G(d) structures on 2p 512 MB\\1,1\\C,0,3.5175411963,1.0391705177,-0.3394588982\\C,0,2.8551404265,-0.0934948118,0.0810427507\\C,0,1.4414141799,-0.1360318983,0.1691099444\\C,0,0.7193014329,1.0856883364,-0.1581708525\\C,0,1.4727075647,2.1838879902,-0.5561383131\\N,0,2.8364956522,2.15461874,-0.666011523\\N,0,-0.6604616056,1.1159668872,-0.0763437965\\C,0,-1.2709981497,0.1146773428,0.827046832\\C,0,-0.6996395356,-1.274483853,0.4719353978\\N,0,0.7712075371,-1.2453944456,0.5473558417\\C,0,-1.2110711194,-1.7879251029,-0.892062041\\C,0,-2.7492174331,-1.8329828741,-0.9291826182\\C,0,-3.3521773197,-0.4607484971,-0.5910750854\\C,0,-2.8119552116,0.0552344099,0.7544411063

\C,0,-1.3575498276,2.3912140196,-0.2992300047\C,0,-1.3186737801,3.3672
129529,0.8890196555\C,0,1.4775216807,-2.4705745044,0.9656657643\C,0,2.
0056088677,-3.34851749,-0.1806088069\H,0,-0.984865119,0.343691578,1.86
69584348\H,0,-1.0333752104,-1.9631357004,1.2590195266\H,0,-0.800432854
9,-2.7862054781,-1.0834742444\H,0,-0.83482634,-1.1257468313,-1.6835855
432\H,0,-3.0825272975,-2.1663181806,-1.9193380827\H,0,-3.1116640693,-2
.5809424967,-0.2078036716\H,0,-4.4457790812,-0.5268632885,-0.539042884
5\H,0,-3.1176185409,0.2487863792,-1.3973513839\H,0,-3.248852507,1.0248
071772,1.0199620042\H,0,-3.1249060676,-0.6331592349,1.552670901\H,0,0.
7706590642,-3.0430014288,1.5748424578\H,0,2.2944848909,-2.179712358,1.
637733558\H,0,2.6785430808,-2.7976933818,-0.8465782837\H,0,2.561841193
8,-4.1937955684,0.241054167\H,0,1.1890975595,-3.7526031169,-0.78685180
4\H,0,-2.3931552668,2.1611039992,-0.5571124019\H,0,-0.9347479364,2.848
6368845,-1.2013196335\H,0,-0.2940532331,3.6159383426,1.1891538707\H,0,
-1.8305320975,4.2990801523,0.622030632\H,0,-1.8280245653,2.9456002335,
1.7634666545\H,0,1.0223001032,3.1361012856,-0.7972594725\H,0,4.5966468
46,1.0758325721,-0.4326339627\H,0,3.451516188,-0.9649790948,0.31508263
96\C,0,3.5308224633,3.3636759275,-1.1416116506\H,0,3.2356395719,3.5791
899063,-2.1730402404\H,0,3.2760983977,4.2113344304,-0.4987054257\H,0,4
.6080739818,3.1956373713,-1.1021208638\\Version=AM64L-G03RevD.01\\State
=1-A\\HF=-784.2365216\\RMSD=3.571e-09\\Thermal=0.\\Dipole=2.3166798,1.1712
607,-0.0637123\\PG=C01 [X(C16H26N3)]\\@

4f-Me⁺_4

1\\1\\GINC-NAUTILUS\\SP\\RMP2-FC\\6-31+G(2d,p)\\C16H26N3(1+)\\RAMAN\\06-Aug-20
11\\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read g
eom=check\\sp of cat11_16.mca mp2-5 on 2p 900 MB\\1,1\\C,0,3.5154107139
,1.0471552707,-0.3393447116\C,0,2.8554851394,-0.087125206,0.0806944748
\C,0,1.4418430197,-0.1328815156,0.1683927758\C,0,0.7170612324,1.087370
5568,-0.1584134462\C,0,1.4680831703,2.1873505227,-0.5560018707\N,0,2.8
319470068,2.1611738918,-0.6656899311\N,0,-0.6627848576,1.1145716907,-0
.0766245574\C,0,-1.2711472898,0.111479519,0.8262762942\C,0,-0.69670264
52,-1.2762256407,0.470498377\N,0,0.7740802867,-1.2439337815,0.54597156
36\C,0,-1.2069578559,-1.790099033,-0.893776821\C,0,-2.744996863,-1.838
565915,-0.9309452651\C,0,-3.3510354102,-0.4678558545,-0.5921424358\C,0
, -2.8119640261,0.0486491364,0.7536354531\C,0,-1.362680189,2.3884252354
, -0.2987993405\C,0,-1.3259872949,3.3638370479,0.889983759\C,0,1.483068
181,-2.4678850613,0.9633307715\C,0,2.0134098327,-3.343543253,-0.183637
8404\H,0,-0.9855484227,0.3406256067,1.8663051973\H,0,-1.0289263462,-1.
9660271041,1.2572136103\H,0,-0.794081603,-2.7873588796,-1.0857079828\H
,0,-0.8321866384,-1.1266557226,-1.6849364673\H,0,-3.0775474732,-2.1721
535287,-1.9212725563\H,0,-3.1057896259,-2.5876887294,-0.209943335\H,0,
-4.444485048,-0.5364644949,-0.5401387377\H,0,-3.1180747767,0.242627760
2,-1.3980441131\H,0,-3.2510160425,1.0171095718,1.0196649166\H,0,-3.123
3862111,-0.6408367985,1.5515238983\H,0,0.7773374114,-3.042487364,1.571
7683971\H,0,2.2991872206,-2.175833256,1.6359159549\H,0,2.6852742694,-2
.7905975033,-0.8489254792\H,0,2.5714280602,-4.1879750224,0.2373640842\H
,0,1.1979377592,-3.7488719392,-0.7904560847\H,0,-2.397767824,2.156163
8412,-0.5568118811\H,0,-0.9409269037,2.8472804893,-1.2006548865\H,0,-0
.3019317343,3.6147382792,1.1902249355\H,0,-1.8399762767,4.2946896647,0
.6235375952\H,0,-1.834354313,2.940586438,1.7642139649\H,0,1.0155837309

,3.138621346,-0.7969240494\H,0,4.5944558548,1.0862993779,-0.4322716822
\H,0,3.4537516481,-0.9573141753,0.3147721458\C,0,3.5236372392,3.371574
5743,-1.1416822303\H,0,3.2303911649,3.5844020726,-2.1742123346\H,0,3.2
646013238,4.2194786228,-0.5008788938\H,0,4.6013082057,3.2070506023,-1.
0991263656\\Version=AM64L-G03RevD.01\State=1-A\HF=-784.2637399\MP2=-78
7.1720379\RMSD=4.591e-09\Thermal=0.\PG=C01 [X(C16H26N3)]\@

4f-Me⁺_5

1\1\GINC-GOLEM\SP\RMP2-FC\6-31+G(2d,p)\C16H26N3(1+)\RAMAN\06-Aug-2011\
0\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geom
=check\sp of cat11_10.mca mp2-5 on 2p 900 MB\1,1\C,0,2.4931525882,-1
.1994432235,0.5531867035\C,0,1.1082116324,-0.5531949059,0.7725947057\C
,0,1.1359158815,0.8846611206,0.2147091687\C,0,1.5909854122,0.940715594
9,-1.2602116148\C,0,2.9648695328,0.2734231852,-1.4516711557\C,0,2.9623
069973,-1.1670172242,-0.9125134729\N,0,-0.1692786937,1.5139691791,0.44
19091387\C,0,-1.2646445087,0.7985766852,0.0130851999\C,0,-1.1869264779
, -0.6517323669,-0.084861004\N,0,-0.0197343068,-1.2998881177,0.15298060
39\C,0,-2.3832804461,-1.3238124815,-0.4380698423\C,0,-3.5459333249,-0.
6373765736,-0.7211604907\N,0,-3.586498316,0.707183395,-0.67017362\C,0,
-2.4660467635,1.4119896179,-0.3240524048\C,0,0.0205159081,-2.773861068
2,0.1438662481\C,0,-0.4117589418,-3.4076527026,1.4741675024\C,0,-0.271
538425,2.9795812378,0.5210194006\C,0,0.911579826,3.6596631756,1.213839
3263\H,0,0.9178955262,-0.4934858385,1.8542160139\H,0,1.8623511281,1.42
27604915,0.8307419863\H,0,1.6275479507,1.9888524276,-1.5862205753\H,0,
0.8419043906,0.4386583642,-1.8893882651\H,0,3.239205982,0.2852709128,-
2.5134206879\H,0,3.7323613673,0.8586381383,-0.9229746353\H,0,3.9673151
732,-1.6008937074,-0.980286543\H,0,2.3079832834,-1.7915130831,-1.53855
93338\H,0,2.5271375297,-2.212440136,0.9703522166\H,0,3.1934814522,-0.6
132469572,1.1654422529\H,0,-1.1780760355,3.2027379585,1.0989618463\H,0
, -0.411859743,3.4129724459,-0.4846659115\H,0,1.0946482676,3.2318468662
,2.2061357628\H,0,1.8343555598,3.6071005853,0.6261454794\H,0,0.6712281
77,4.7203003179,1.3449995747\H,0,1.0384075194,-3.0756682104,-0.1050373
57\H,0,-0.5982216944,-3.1280207821,-0.6859504456\H,0,-0.3658269886,-4.
4999265649,1.3965202062\H,0,0.2507265519,-3.1009453403,2.2919387091\H,
0,-1.4363073127,-3.1267424681,1.7443930689\H,0,-2.4279825323,-2.403550
2545,-0.4756248687\H,0,-2.5818477566,2.4866499805,-0.330769151\H,0,-4.
4646090559,-1.1478495564,-0.9857694053\C,0,-4.8184851909,1.4500200877,
-0.9864969418\H,0,-5.1346545904,2.0299184539,-0.1143488153\H,0,-4.6370
406793,2.1210232837,-1.8314849548\H,0,-5.6041785435,0.741555468,-1.253
0242085\\Version=AM64L-G03RevD.01\State=1-A\HF=-784.2631313\MP2=-787.1
718999\RMSD=5.547e-09\Thermal=0.\PG=C01 [X(C16H26N3)]\@

4f-Me⁺_6

1\1\GINC-NAUTILUS\SP\RMP2-FC\6-31+G(2d,p)\C16H26N3(1+)\RAMAN\06-Aug-20
11\0\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read g
eom=check\sp of cat11_12.mca mp2-5 on 2p 900 MB\1,1\C,0,-3.636438924
,0.7680376766,-0.5800162597\C,0,-2.4989296423,1.4853764186,-0.27474853
05\C,0,-1.2593078677,0.8439008146,-0.0344055806\C,0,-1.2288293119,-0.6
07810088,-0.1515134298\C,0,-2.4311444517,-1.2481505659,-0.4330228266\N
,0,-3.6016561731,-0.5753768046,-0.657003698\N,0,-0.0406211929,-1.29342
63121,0.0028189226\C,0,1.0280771804,-0.5947469041,0.749808492\C,0,1.15

79079757,0.8421451111,0.2038350084\N,0,-0.1393616125,1.5288559126,0.29
15279871\C,0,1.7414503866,0.8827128138,-1.2251286563\C,0,3.1113817664,
0.183508428,-1.2832199338\C,0,3.0204849228,-1.2567911392,-0.7515504261
\C,0,2.4082804012,-1.2807506163,0.6604252041\C,0,-0.0551049603,-2.7632
83387,-0.0109612312\C,0,-0.512157779,-3.4144058759,1.305177355\C,0,-0.
1936625944,3.0028325388,0.4134413621\C,0,1.0329124582,3.644680958,1.06
46159107\H,0,0.7437709757,-0.5297839673,1.8128078166\H,0,1.8404675444,
1.3611018158,0.8828246435\H,0,1.8288020207,1.9273637596,-1.5521924984\H,
0,1.038974841,0.3888459953,-1.9105275047\H,0,3.4855987768,0.18982041
58,-2.3140593044\H,0,3.8383935624,0.7504477037,-0.6821298424\H,0,4.016
6612695,-1.7149127399,-0.721859091\H,0,2.4155762077,-1.8619756422,-1.4
419865007\H,0,2.3627094571,-2.2987426739,1.0640307843\H,0,3.0662674166
,-0.7267468917,1.3453412412\H,0,-1.0687852231,3.2422213537,1.028800896
8\H,0,-0.3600319127,3.4445064064,-0.581169801\H,0,1.2241719578,3.23847
36135,2.0642992867\H,0,1.9389657954,3.5465756997,0.4575162606\H,0,0.83
09048207,4.7156610061,1.1757301561\H,0,0.9513492315,-3.1028868959,-0.2
634571339\H,0,-0.6819464889,-3.0843924628,-0.8510666255\H,0,-0.5240188
773,-4.5052473045,1.1976369283\H,0,0.1721774112,-3.1670480402,2.125222
3712\H,0,-1.5169766357,-3.0900007568,1.5999239237\H,0,-2.513870492,-2.
3240454676,-0.4880663234\H,0,-4.5876876884,1.2487258135,-0.7761283453\H,
0,-2.5807104337,2.5634859207,-0.2510219503\C,0,-4.8129335698,-1.3552
6151,-0.9654362362\H,0,-4.649140503,-1.9487271096,-1.8697398012\H,0,-5
.0506484847,-2.0161702688,-0.1263141646\H,0,-5.6457827805,-0.670166541
6,-1.1305845956\\Version=AM64L-G03RevD.01\State=1-A\HF=-784.2621732\MP
2=-787.1714051\RMSD=6.313e-09\Thermal=0.\PG=C01 [X(C16H26N3)]\\@

4f-Me⁺_7

1\1\GINC-GOLEM\SP\RMP2-FC\6-31+G(2d,p)\C16H26N3(1+)\RAMAN\06-Aug-2011\
0\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geom
=check\\sp of cat11_18.mca mp2-5 on 2p 900 MB\\1,1\C,0,-3.6388411307,0
.7601145657,-0.5762398564\C,0,-2.5028436538,1.4799432206,-0.2711990354
\C,0,-1.2612279104,0.8412616436,-0.0336904149\C,0,-1.2276474809,-0.610
3971009,-0.1510291918\C,0,-2.4285442056,-1.253229736,-0.4326687736\N,0
,-3.6008976341,-0.5830672626,-0.6550565593\N,0,-0.0379724057,-1.293537
0066,0.0034642812\C,0,1.029395599,-0.5921575135,0.7499252796\C,0,1.156
3390177,0.8445606274,0.2028768114\N,0,-0.1422844949,1.5287432241,0.290
1569549\C,0,1.7395101024,0.8851910805,-1.2262392001\C,0,3.1106564119,0
.1883063308,-1.2843529107\C,0,3.0226566293,-1.2516758704,-0.7513322578
\C,0,2.4109187782,-1.2755008414,0.660858588\C,0,-0.0500064589,-2.76348
20801,-0.0082445927\C,0,-0.5072837986,-3.4133335729,1.3084220018\C,0,-
0.20017046,3.0024838814,0.4141486165\C,0,1.0279040062,3.6472406925,1.0
59474718\H,0,0.7449411281,-0.5270705129,1.8128810984\H,0,1.8379090878,
1.3655910892,0.8812751955\H,0,1.8250543231,1.9298014175,-1.5538980952\H,
0,1.0376828874,0.389815141,-1.9111904989\H,0,3.4842754003,0.19432141
47,-2.3154113352\H,0,3.8370047253,0.7571002927,-0.6842119823\H,0,4.019
7029026,-1.7079026825,-0.7215744462\H,0,2.4186667136,-1.858590891,-1.4
410353821\H,0,2.3675306509,-2.2931520993,1.0655859612\H,0,3.0679991703
,-0.7194282784,1.344979034\H,0,-1.0728976826,3.2387887914,1.0341563964
\H,0,-0.372855412,3.4445486782,-0.579192563\H,0,0.8241991273,4.7179210
674,1.1704431833\H,0,1.2242975335,3.2424767435,2.0587414911\H,0,1.9315
154708,3.5503369284,0.4485606419\H,0,0.9572235953,-3.1017815575,-0.259

3519859\H,0,-0.6755293888,-3.0868449184,-0.8484603816\H,0,0.1760139904
,-3.1638603105,2.1286934581\H,0,-1.5127922868,-3.0897973136,1.60175482
5\H,0,-0.5176219511,-4.5043544211,1.2025132424\H,0,-2.508645971,-2.329
2740163,-0.4890919891\H,0,-4.5914625509,1.2388059533,-0.7706575718\H,0
,-2.5874936046,2.5577652232,-0.2450229659\C,0,-4.809060518,-1.36535020
18,-0.9693086081\H,0,-4.650887356,-1.935529763,-1.8895119885\H,0,-5.03
16744156,-2.0481498628,-0.1438408631\H,0,-5.6494182003,-0.6835950139,-
1.1078408793\\Version=AM64L-G03RevD.01\State=1-A\HF=-784.2621746\MP2=-
787.1713979\RMSD=6.278e-09\Thermal=0.\PG=C01 [X(C16H26N3)]\\@

4f-Me⁺_8

1\1\GINC-EDDY\SP\RMP2-FC\6-31+G(2d,p)\C16H26N3(1+)\RAMAN\06-Aug-2011\0
\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geom=
check\\sp of cat11_7.mca mp2-5 on 2p 900 MB\\1,1\C,0,-2.827816599,-0.1
403043195,0.6706426757\C,0,-1.3001047233,-0.0006189563,0.83430719\C,0,
-0.6179451641,-1.3242745913,0.4213336288\C,0,-1.0244632052,-1.76312833
14,-1.0042366824\C,0,-2.5529984729,-1.8914655196,-1.1366830989\C,0,-3.
2591227739,-0.5851574309,-0.7380570515\N,0,0.8282680143,-1.1984483293,
0.6101531862\C,0,1.440358987,-0.0664354855,0.1396680783\C,0,0.64580228
21,1.1222682013,-0.1395053543\N,0,-0.6998536156,1.1117036222,0.0479232
497\C,0,1.3537344735,2.2596953862,-0.5964160866\C,0,2.7246731595,2.248
1434187,-0.7577589985\N,0,3.4435192098,1.1429139576,-0.4855425082\C,0,
2.8155748048,0.0055908634,-0.0609490945\C,0,-1.4766059171,2.3504208791
,-0.1458100028\C,0,-1.4586946448,3.2858454242,1.0719841577\C,0,1.59420
72636,-2.3334378005,1.1332448519\C,0,2.0780995799,-3.3585098022,0.0928
267443\H,0,-1.078638942,0.1786140843,1.897014745\H,0,-0.9578375254,-2.
0854429141,1.1352567549\H,0,-0.5404276661,-2.7180865174,-1.2397294611\H,
0,-0.6469536858,-1.0280156499,-1.7289564023\H,0,-2.812871562,-2.1691
026171,-2.1653389448\H,0,-2.9082651449,-2.7095746349,-0.4920145718\H,0
,-4.3476015753,-0.7183936267,-0.7580472951\H,0,-3.0248895987,0.1950272
941,-1.4769105817\H,0,-3.3425349577,0.7749529601,0.9852407443\H,0,-3.1
341728456,-0.9074984525,1.3963034192\H,0,0.9535875996,-2.8341231523,1.
8691666902\H,0,2.4452504384,-1.9292794667,1.6978345561\H,0,1.236416702
2,-3.871383359,-0.3838566375\H,0,2.6783229592,-2.8944222427,-0.6985349
435\H,0,2.6953353542,-4.1182036636,0.5869681434\H,0,-2.5011106354,2.06
59380652,-0.3876744979\H,0,-1.0974868639,2.853539182,-1.0404023542\H,0
,-1.9081394116,2.803356243,1.9477166706\H,0,-0.4392892113,3.5885245777
,-1.3375798571\H,0,-2.0380464965,4.1900203409,0.8527123557\H,0,0.844477
6525,3.192023052,-0.7982497388\H,0,3.4644007473,-0.8441021637,0.101817
1519\H,0,3.2718909373,3.1220126468,-1.0911473799\C,0,4.9077986249,1.12
33305717,-0.6459818092\H,0,5.3814873258,0.9117972703,0.3172137159\H,0,
5.188629637,0.3561162085,-1.3736162616\H,0,5.2405799354,2.0981726375,-
1.0052624594\\Version=AM64L-G03RevD.01\State=1-A\HF=-784.261843\MP2=-7
87.1709719\RMSD=4.218e-09\Thermal=0.\PG=C01 [X(C16H26N3)]\\@

4f-Me⁺_9

1\1\GINC-NAUTILUS\SP\RMP2-FC\6-31+G(2d,p)\C16H26N3(1+)\RAMAN\06-Aug-20
11\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read g
eom=check\\sp of cat11_2.mca mp2-5 on 2p 900 MB\\1,1\C,0,3.05104076,1.
9465748214,-0.6993821724\C,0,2.778256533,0.620350911,-0.4420103866\C,0
,-1.4651862531,0.182441821,-0.1407504756\C,0,0.4387484239,1.2033325973,

-0.0022645241\C,0,0.7993483683,2.5116650204,-0.3071799653\N,0,2.072903
3188,2.8720700338,-0.6567576678\N,0,-0.8358617043,0.883211068,0.429348
8537\C,0,-1.0717863237,-0.4881572985,0.9344007155\C,0,-0.2686556834,-1
.5027789423,0.0980644209\N,0,1.1480411009,-1.1159369721,0.0350611588\C
,0,-0.8416737462,-1.723744277,-1.3200841671\C,0,-2.3155221429,-2.15741
39724,-1.2680331976\C,0,-3.1462199419,-1.1309638045,-0.4850165567\C,0,
-2.5626453133,-0.905900133,0.9207771619\C,0,-1.6449932781,1.9698099089
,1.0198415629\C,0,-2.6141068574,2.6466419544,0.0410545744\C,0,2.148842
4161,-2.193557974,-0.0458780202\C,0,2.9109224637,-2.3971952187,1.27043
19287\H,0,-0.709117523,-0.5468193739,1.9749539351\H,0,-0.308749218,-2.
4501979032,0.6506611409\H,0,-0.2323749125,-2.4764596399,-1.8376004209\
H,0,-0.7484867255,-0.7887285816,-1.8899427613\H,0,-2.7027890117,-2.272
5473839,-2.2875645995\H,0,-2.3951158572,-3.1443319827,-0.7876889822\H,
0,-4.185429087,-1.4692436857,-0.3916208859\H,0,-3.1691735545,-0.184307
7162,-1.0416232296\H,0,-3.1709130993,-0.1882826422,1.4823480396\H,0,-2
.6203846284,-1.8458404986,1.489223884\H,0,2.8347338492,-1.9943318827,-
0.8779278083\H,0,1.6070674622,-3.1064831456,-0.3122821224\H,0,3.628869
905,-3.2179085489,1.1608577677\H,0,3.463029621,-1.4967947677,1.5629195
893\H,0,2.222007626,-2.6524205815,2.0838220238\H,0,-0.9630187683,2.71
08419597,1.4603081619\H,0,-2.2048748751,1.5532008209,1.8617604982\H,0,
-3.3789037527,1.9455639739,-0.3075106234\H,0,-3.1212822788,3.480759226
1,0.5405168647\H,0,-2.0998049466,3.0411855869,-0.8434234204\H,0,0.0860
932749,3.3238399893,-0.2892800025\H,0,4.0460978818,2.2929314232,-0.953
1076431\H,0,3.6009321966,-0.0812066594,-0.4855318428\C,0,2.3414758828,
4.2842668262,-0.9781850244\H,0,1.7765601025,4.575038926,-1.8690816782\
H,0,2.0519433453,4.9161732782,-0.1334393459\H,0,3.4079348486,4.4099384
494,-1.1709551177\Version=AM64L-G03RevD.01\State=1-A\HF=-784.2634384\
MP2=-787.170819\RMSD=6.886e-09\Thermal=0.\PG=C01 [X(C16H26N3)]\@

4f-Me⁺_10

1\1\GINC-GOLEM\SP\RMP2-FC\6-31+G(2d,p)\C16H26N3(1+)\RAMAN\06-Aug-2011\
0\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geom
=check\sp of cat11_13.mca mp2-5 on 2p 900 MB\1,1\C,0,0.4770590598,-1
.6335357499,1.3094078102\C,0,0.1473825935,-1.4522552857,-0.1896736478\
C,0,1.1097282686,-0.502127383,-0.9320767826\C,0,2.573798824,-0.9062307
688,-0.6308304533\C,0,2.8937135628,-1.073467249,0.8648511475\C,0,1.933
576404,-2.0753839459,1.5220439636\H,0,0.93499126,-0.6242430769,-2.0118
174781\H,0,0.2611999372,-2.4181805386,-0.6907129391\H,0,0.2988464786,-
0.6868714456,1.8402808212\H,0,-0.2160968442,-2.3706865682,1.7366820406
\H,0,2.7316587872,-1.8682534459,-1.1397953645\H,0,3.2713653099,-0.2067
270217,-1.1051718455\H,0,3.9330015195,-1.4069813765,0.9737218187\H,0,2
.8154905632,-0.1064652439,1.3812859216\H,0,2.0855504078,-3.0743150621,
1.0859817193\H,0,2.1431306004,-2.165677506,2.5947401976\N,0,-1.2367157
398,-1.0099088742,-0.4120423841\N,0,0.8071559901,0.9141337327,-0.60320
13456\C,0,-0.4232121667,1.2763459812,-0.1699977488\C,0,-0.7536687028,2
.6170814633,0.1465510803\C,0,-1.4879315435,0.2959446603,-0.0462863908\
C,0,-2.0258438317,2.9706886387,0.5459174071\H,0,-0.0116143227,3.402280
4988,0.0882384956\C,0,-2.7319034031,0.731845174,0.3903248965\N,0,-2.99
93587807,2.0470721314,0.6619711615\H,0,-2.2895025064,3.9946738586,0.78
40540074\H,0,-3.5668742188,0.057428139,0.5208041165\C,0,1.7309108743,1
.9482642272,-1.1204615879\C,0,2.6882202509,2.5485442382,-0.0818811125\

H,0,1.1268991709,2.7360618316,-1.5856366331\H,0,2.2993356083,1.4883847
171,-1.9351027917\H,0,3.2650908002,3.3566618433,-0.5467955071\H,0,2.15
10757922,2.9654995227,0.7776440434\H,0,3.3953103634,1.8034469411,0.294
4229474\C,0,-2.3315706153,-1.9874944195,-0.3076349135\C,0,-2.016978009
1,-3.3488935023,-0.9320478471\H,0,-3.1884607123,-1.556616214,-0.841682
5091\H,0,-2.6372239907,-2.1218257715,0.7449531582\H,0,-2.9366899195,-3
.9435940498,-0.9502966679\H,0,-1.6644329598,-3.2418659067,-1.964228912
9\H,0,-1.2765714755,-3.9168037147,-0.3584791104\C,0,-4.359030647,2.416
6124406,1.0916101947\H,0,-5.0762551469,2.1607109779,0.3060271404\H,0,-
4.6127441138,1.8835342503,2.012746054\H,0,-4.3956153965,3.4911456522,1
.2767196499\\Version=AM64L-G03RevD.01\State=1-A\HF=-784.2630676\MP2=-7
87.1708964\RMSD=4.322e-09\Thermal=0.\PG=C01 [X(C16H26N3)]\\@#

4k

4k_1

1\1\GINC-MAX\SP\RMP2-FC\6-31+G(2d,p)\C11H14N2\EVGENY\15-Feb-2008\0\#P
MP2/6-31+G(2D,P) SCF=TIGHT INT=FINEGRID\\Single point of TCAP_b MP2/6
-31+G(2d,p)\0,1\N\N,1,4.22838464\C,1,1.45833541,2,119.82538393\C,3,1.
53235649,1,110.8184192,2,-38.79482405,0\C,4,1.53518041,3,109.84066001,
1,58.66282302,0\C,5,1.51730756,4,110.85178382,3,-49.07547597,0\C,2,1.3
397217,1,57.78757745,3,10.22770154,0\C,2,1.33972114,1,57.78753233,3,-1
68.28074803,0\C,8,1.39498999,2,125.51368698,1,1.3383167,0\C,9,1.517306
48,8,121.31667756,2,179.03829492,0\C,10,1.53518066,9,110.85183757,8,15
7.54361965,0\C,1,1.45833495,3,116.79020006,4,162.50447596,0\C,1,1.3884
336,12,119.49611478,11,40.66769462,0\H,4,1.09712233,3,109.53793908,1,-
179.37028482,0\H,12,1.10630849,1,111.12932786,13,-81.76265034,0\H,12,1
.09778683,1,107.66353296,13,161.35931988,0\H,10,1.10151954,9,109.87569
298,8,-81.80805505,0\H,8,1.09219833,2,115.79603958,1,-178.60948466,0\H
,7,1.09219777,2,115.79604838,1,178.60950633,0\H,3,1.1063085,1,111.1292
7602,13,81.7632637,0\H,5,1.09796751,4,110.5887283,3,-171.4482674,0\H,1
0,1.09796761,9,110.07360705,8,34.87148912,0\H,3,1.09778665,1,107.66348
281,13,-161.35874594,0\H,5,1.10151911,4,109.08592713,3,72.03991039,0\H
,4,1.09805413,3,108.84105851,1,-61.90628135,0\H,11,1.09805315,10,110.0
6868343,9,-70.74876351,0\H,11,1.09712299,10,110.84369116,9,170.2607098
,0\\Version=x86-Linux-G03RevB.03\State=1-A\HF=-533.6584082\MP2=-535.60
23514\RMSD=4.054e-09\PG=C01 [X(C11H14N2)]\\@

4k_2

1\1\GINC-MORITZ\SP\RMP2-FC\6-31+G(2d,p)\C11H14N2\EVGENY\10-Feb-2008\0\
\#P MP2/6-31+G(2D,P) SCF=TIGHT INT=FINEGRID\\Single point of TCAP_a MP
2/6-31+G(2d,p)\0,1\C\C,1,1.39394362\C,2,1.41803967,1,117.92362667\C,3
,1.41803967,2,117.62105248,1,-0.90278082,0\C,4,1.39394362,3,117.923626
67,2,-0.90278082,0\N,5,1.34047829,4,125.47588944,3,2.01012991,0\N,3,1.
37981,2,121.18947376,1,179.09721918,0\C,7,1.46034883,3,122.00703337,2,
174.2732277,0\C,8,1.53272525,7,112.30374561,3,-20.97506505,0\C,4,1.512
55838,3,119.56228125,2,-179.83386588,0\C,2,1.51255838,1,122.50500531,6
, -179.09234592,0\C,11,1.53665415,2,109.48180812,1,-148.11583343,0\C,7,
1.46034883,3,122.00703337,2,-5.7267723,0\H,5,1.09224862,4,118.68197372
,3,-178.42651834,0\H,1,1.09224862,6,115.84081606,5,179.3777194,0\H,8,1
.10007119,7,108.02020576,3,-142.11414333,0\H,8,1.10459071,7,109.996452
2,3,101.73535421,0\H,13,1.10007119,7,108.02020576,3,-142.11414333,0\H,

13,1.10459071,7,109.9964522,3,101.73535421,0\H,9,1.09708393,8,108.9688
3649,7,173.69891932,0\H,12,1.09708393,11,111.31058214,2,-176.24547748,
0\H,12,1.09833486,11,109.50616592,2,64.95079062,0\H,9,1.09833486,8,109
.39872922,7,-68.95783146,0\H,10,1.1019031,4,110.58088519,3,-89.4527374
,0\H,10,1.09765021,4,110.2695343,3,152.96221038,0\H,11,1.1019031,2,110
.58088519,1,91.66717183,0\H,11,1.09765021,2,110.2695343,1,-25.91788039
,0\Version=x86-Linux-G03RevB.03\State=1-A\HF=-533.6569335\MP2=-535.60
11468\RMDS=7.050e-09\PG=C02 [C2(N1C1N1),X(C10H14)]\@

4k-Me⁺

4k-Me⁺_1

1\1\GINC-STEAK\SP\RMP2-FC\6-31+G(2d,p)\C12H17N2(1+)\RAMAN\13-Oct-2011\
0\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geom
=check\sp of TCAP1.mca mp2-5 on 2p 900 MB\1,1\C,0,-2.9926895797,-1.1
746782008,0.0017996958\C,0,-1.6213320467,-1.2299769711,-0.0259095567\C
,0,-0.8790187957,-0.0002624287,0.0029234331\C,0,-1.6207464558,1.229425
3798,0.0443227169\C,0,-2.992417968,1.1743992996,0.0380932426\N,0,-3.68
18280733,-0.0001298754,0.0286559873\N,0,0.4672779555,-0.0004373708,-0.
0048121705\C,0,1.2578714865,1.2421256571,-0.0766431407\C,0,0.455518767
3,2.4076934667,-0.6552699572\C,0,-0.8798679986,2.5482406475,0.09054577
84\C,0,-0.8815255465,-2.5493873946,-0.074447836\C,0,0.463303332,-2.406
2797956,0.6535603579\C,0,1.258251211,-1.2431535111,0.0599418678\H,0,-3
.5946982954,2.0774420509,0.0536051146\H,0,-3.5952930953,-2.0776431475,
-0.006466222\H,0,1.0471317542,3.3248048196,-0.5652363637\H,0,1.0534999
721,-3.3238932077,0.5594954492\H,0,0.2936137167,-2.232263913,1.723813
7238\H,0,0.2719524587,2.2380055437,-1.7239345885\H,0,-0.6890779526,2.8
277123748,1.1374668711\H,0,-1.4922067347,3.3462669705,-0.3447129193\H,
0,-0.7040853504,-2.8338904126,-1.1223735305\H,0,-1.488801251,-3.344918
1145,0.3722409036\H,0,1.6275328041,1.48204408,0.9313023138\H,0,2.13192
7991,1.0325728941,-0.7046671723\H,0,2.14099728,-1.0320021487,0.6751091
911\H,0,1.6138025072,-1.486627553,-0.9522156275\C,0,-5.1551269941,-0.0
000700926,-0.0247521043\H,0,-5.4963524203,0.0073716993,-1.065100191\H,
0,-5.5329817442,-0.8920167562,0.479540874\H,0,-5.5336983338,0.88393910
89,0.4926502894\Version=AM64L-G03RevD.01\State=1-A\HF=-573.1040818\MP
2=-575.1929934\RMDS=2.500e-09\Thermal=0.\PG=C01 [X(C12H17N2)]\@

4k-Me⁺_2

1\1\GINC-STEAK\SP\RMP2-FC\6-31+G(2d,p)\C12H17N2(1+)\RAMAN\13-Oct-2011\
0\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geom
=check\sp of TCAP2.mca mp2-5 on 2p 900 MB\1,1\N,0,0.5087247139,0.028
5526545,-0.1061378104\N,0,-3.6363021308,-0.2216159938,0.0262122061\C,0
,1.2045870325,1.3268541361,-0.1719910042\C,0,0.3548611629,2.3930788032
, -0.8651099845\C,0,-1.0139428181,2.49874663,-0.1804320062\C,0,-1.65544
53709,1.1289091221,-0.0988574624\C,0,-3.0214172472,0.9883127052,-0.077
5746265\C,0,-2.8744738105,-1.3464203696,0.1112530291\C,0,-1.5014869289
, -1.3173479752,0.0989893603\C,0,-0.6935541289,-2.5918578075,0.23128796
8\C,0,0.6582547279,-2.4274825584,-0.4752282138\C,0,1.3615187869,-1.166
6223044,0.0296809327\C,0,-0.836193329,-0.0505811102,-0.0380301437\H,0,
0.881535843,3.3522296781,-0.8217231234\H,0,-0.5275723964,-2.8096982479
,1.2967293678\H,0,-3.4185150226,-2.282058211,0.1955015152\H,0,-3.67858
17169,1.8502244603,-0.1387099391\H,0,-1.6690065357,3.1938550327,-0.718

3066541\H,0,-1.251476157,-3.4402177741,-0.18175112\H,0,-0.8871299882,2
.9032895317,0.834670185\H,0,0.2297368815,2.1327590745,-1.92378505\H,0,
0.5123530744,-2.3576316637,-1.5606079022\H,0,1.2998388037,-3.294145267
6,-0.2841674333\H,0,2.1380557776,1.1675298912,-0.7217959025\H,0,1.4738
090821,1.6434338866,0.8470049942\H,0,1.6577987174,-1.2799695102,1.0834
491937\H,0,2.2733621052,-0.9823403297,-0.547913229\C,0,-5.1066849165,-
0.3181533986,-0.0226522216\H,0,-5.5406808079,0.5830964108,0.4154745213
\H,0,-5.444727186,-0.4239289972,-1.0587085663\H,0,-5.4294846075,-1.183
8004978,0.55960564\\Version=AM64L-G03RevD.01\State=1-A\HF=-573.1033436
\MP2=-575.1922976\RMSD=2.814e-09\Thermal=0.\PG=C01 [X(C12H17N2)]\@

4l

4l_1

1\1\GINC-EDDY\SP\RMP2-FC\6-31+G(2d,p)\C11H16N4\RAMAN\16-Feb-2010\0\#P
MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=rea
d\opt of Me1 b98/6-31G(d) on 4p 900 MB\0,1\N,0,-0.0000242036,1.62990
46451,-0.0406521973\N,0,-0.0000081651,-2.5530452623,-0.5553028068\C,0,
1.2370766142,2.3477483108,-0.2815018655\C,0,2.4074634397,1.5412400271,
0.283624607\C,0,1.2177370797,-0.4697750395,-0.3593491482\C,0,1.1449735
763,-1.8684817207,-0.4890743703\C,0,-1.1449960968,-1.8684950287,-0.489
0374768\C,0,-1.2177741307,-0.4697881565,-0.3593107523\C,0,-2.407499960
2,1.5412174304,0.2836994877\C,0,-1.2371390314,2.3477354451,-0.28146639
46\C,0,-0.0000206271,0.2479792909,-0.2631000972\H,0,3.3472031053,2.059
0439248,0.0557107103\H,0,-1.4079665685,2.5358642099,-1.3564869348\H,0,
-1.1768232517,3.3206117119,0.2252493463\H,0,-2.0541445422,-2.462315748
3,-0.5407652014\H,0,2.054129436,-2.4622891916,-0.5408342017\H,0,1.4078
692712,2.5358819338,-1.3565270366\H,0,1.1767668078,3.3206226656,0.2252
184982\H,0,2.312967667,1.4791227339,1.3833772575\H,0,-2.3129701148,1.4
791040271,1.3834494503\H,0,-3.3472517803,2.0590114514,0.0558129005\N,0
,-2.4382057746,0.2308814744,-0.3476169617\N,0,2.4381618804,0.230905277
3,-0.3476962409\C,0,3.6669150906,-0.5239149078,-0.1784793031\H,0,3.780
1051558,-1.2552745889,-0.9865839379\H,0,4.5127075004,0.1694108688,-0.2
364827604\C,0,-3.6669516309,-0.523942663,-0.1783663894\H,0,-3.78016523
65,-1.2552987966,-0.9864703161\H,0,-4.5127471517,0.1693817969,-0.23634
27331\H,0,-3.7208728207,-1.0620757176,0.7851235795\H,0,3.7208654423,-1
.0620447238,0.785010749\\Version=AM64L-G03RevD.01\State=1-A\HF=-643.68
4728\MP2=-646.0045107\RMSD=3.767e-09\Thermal=0.\PG=C01 [X(C11H16N4)]\@

4l_2

1\1\GINC-EDDY\SP\RMP2-FC\6-31+G(2d,p)\C11H16N4\RAMAN\16-Feb-2010\0\#P
MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=rea
d\opt of Me10 b98/6-31G(d) on 4p 900 MB\0,1\C,0,-1.1631763534,-1.859
3155393,-0.3053774225\C,0,-1.2196616174,-0.4647508117,-0.1568941146\C,
0,0.0003437997,0.2557160348,-0.1850864351\C,0,1.2059472133,-0.47264315
99,-0.3414946333\C,0,1.1216108033,-1.8701663026,-0.4402241398\N,0,-0.0
27702867,-2.55416917,-0.4338472603\N,0,0.014120209,1.6344766952,-0.062
9573986\C,0,1.26595596,2.3663758713,-0.0477037293\C,0,2.4101652627,1.4
602495325,0.4110984672\C,0,-2.3839845146,1.5934029832,-0.5571653479\C,
0,-1.223045581,2.3824679869,0.0514194442\H,0,2.0252833664,-2.466746787
2,-0.5411093292\H,0,-2.0787270437,-2.446250038,-0.3092573587\H,0,1.175

9843197,3.2134312518,0.6488673119\H,0,1.4980927259,2.7764988632,-1.044
7684906\H,0,-1.114776385,3.33627808,-0.4864650818\H,0,-1.4492544149,2.
6165212109,1.1051083516\H,0,3.3613929693,1.9860767692,0.2685678609\H,0
, -3.3249037923,2.1049386363,-0.3233983954\H,0,-2.2781291495,1.56495549
93,-1.6578637966\H,0,2.3020492369,1.2418516607,1.4900579124\N,0,-2.419
2439416,0.2571613112,0.0248654148\N,0,2.4198782195,0.2460590688,-0.395
7836991\C,0,3.6568592093,-0.5150767622,-0.3534956535\H,0,4.4984194807,
0.1793515317,-0.4506807575\H,0,3.6975697917,-1.2109219497,-1.198567769
3\C,0,-3.6709124489,-0.4601382255,-0.1486149383\H,0,-4.4988300949,0.22
30297497,0.0698792554\H,0,-3.8093275884,-0.8642191386,-1.1681888406\H,
0,-3.7272246419,-1.2925131292,0.561205429\H,0,3.7859396569,-1.09446283
29,0.5789296248\\Version=AM64L-G03RevD.01\State=1-A\HF=-643.6831945\MP
2=-646.002984\RMSD=8.364e-09\Thermal=0.\PG=C01 [X(C11H16N4)]\\

4l-Me⁺

4l-Me⁺_1

1\1\GINC-YANG\SP\RMP2-FC\6-31+G(2d,p)\C12H19N4(1+)\RAMAN\22-Jul-2011\0
\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geom=
check\\sp of Me1.mc mp2-5 on 2p 900 MB\\1,1\N,0,0.0000016851,-1.418950
749,-0.0862201701\N,0,-0.0000043565,2.7270195497,-0.0301007848\C,0,-1.
2514947117,-2.15183672,-0.2612705491\C,0,-2.3998675415,-1.3912966755,0
.4000303665\C,0,-1.2326315399,0.6703308606,-0.0527125231\C,0,-1.181523
5269,2.06236966,-0.0228618858\C,0,1.1815167842,2.0623730987,-0.0228624
618\C,0,1.2326288593,0.6703344611,-0.0527131288\C,0,2.3998711024,-1.39
12897461,0.4000290141\C,0,1.2515001164,-2.1518330513,-0.2612713467\C,0
, -0.000000297,-0.05930548,-0.0605484783\H,0,-3.3448558855,-1.878622282
9,0.1420239126\H,0,1.4633009307,-2.3026115707,-1.3295285337\H,0,1.1389
147307,-3.1368394966,0.2068353205\H,0,2.0716024071,2.6754857412,-0.000
5510902\H,0,-2.0716109668,2.6754796334,-0.0005500843\H,0,-1.4632956912
, -2.302615983,-1.3295275967\H,0,-1.1389061873,-3.1368427821,0.20683617
46\H,0,-2.2906020434,-1.4194527362,1.4965415074\H,0,2.2906063146,-1.41
94462589,1.4965402118\H,0,3.3448607233,-1.8786125581,0.1420219561\N,0,
2.4303813612,-0.0235786037,-0.108987086\N,0,-2.4303820759,-0.023585689
, -0.1089858991\C,0,-3.6863488683,0.705616831,-0.0012829854\H,0,-3.7520
270856,1.4640372258,-0.7901907571\H,0,-4.5110170325,0.0040216834,-0.14
97560725\C,0,3.6863461071,0.7056275515,-0.0012849353\H,0,3.7520216479,
1.4640481175,-0.790192766\H,0,4.5110162164,0.0040347897,-0.1497584863\
H,0,3.8161942567,1.1943418643,0.9785048975\H,0,-3.8161978696,1.1943307
383,0.9785069398\C,0,-0.0000061611,4.1987127079,0.0592021548\H,0,-0.00
00014458,4.5123927057,1.1082016871\H,0,0.8881397763,4.5883909131,-0.44
2328474\H,0,-0.8881583128,4.58838814,-0.4423195378\\Version=AM64L-G03R
evD.01\State=1-A\HF=-683.1307077\MP2=-685.6011045\RMSD=5.862e-09\Therm
al=0.\PG=C01 [X(C12H19N4)]\\@

4l-Me⁺_1

1\1\GINC-YANG\SP\RMP2-FC\6-31+G(2d,p)\C12H19N4(1+)\RAMAN\22-Jul-2011\0
\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geom=
check\\sp of Me10.mc mp2-5 on 2p 900 MB\\1,1\C,0,-1.1807234645,2.05974
60069,-0.0557434603\C,0,-1.2304582281,0.6694879323,-0.0739200669\C,0,0

.000089681,-0.0610280481,-0.0004593858\C,0,1.2308995951,0.670481732,0.
0578587141\C,0,1.1812666358,2.0602266256,0.0138875309\N,0,0.0003211503
,2.7267391591,-0.0297412156\N,0,0.0002103926,-1.4158890986,0.008237352
7\C,0,1.2493076015,-2.1706497855,0.1033085125\C,0,2.4116452857,-1.3581
151387,-0.4633198602\C,0,-2.4130664785,-1.3517787305,0.4693674214\C,0,
-1.2483129801,-2.1723131684,-0.0805243556\H,0,2.0723937582,2.672540773
4,0.0182600145\H,0,-2.0719318312,2.6718154187,-0.0663951002\H,0,1.1353
440067,-3.0974778276,-0.471594649\H,0,1.4452619187,-2.4383319992,1.150
8335399\H,0,-1.1364404543,-3.0905059225,0.5085201518\H,0,-1.4400599947
, -2.4555366936,-1.1247447497\H,0,3.3507489285,-1.8634972701,-0.2192286
739\H,0,-3.3510902555,-1.8607499517,0.2285548178\H,0,-2.3394852794,-1.
2763010776,1.5670222671\H,0,2.333296555,-1.2982370312,-1.5615955024\N,
0,-2.4233275078,-0.034491991,-0.1639872026\N,0,2.4242800132,-0.0319376
506,0.1512861752\C,0,3.6822593182,0.7015788252,0.1108413779\H,0,4.5014
477384,-0.0009705933,0.284242097\H,0,3.7084294542,1.4451753544,0.91550
38214\C,0,-3.6817389515,0.6990329545,-0.1384584348\H,0,-4.4997890364,-
0.0058557757,-0.3077753691\H,0,-3.8598543912,1.2173167829,0.8187614508
\H,0,-3.7040855036,1.4330532717,-0.9519752093\H,0,3.8552232169,1.20857
99598,-0.8533487951\C,0,-0.0008105336,4.1993729581,0.0335581227\H,0,-0
.8788899784,4.5808721924,-0.4914679847\H,0,-0.0198726612,4.531878931,1
.0766460202\H,0,0.8969676499,4.5805003559,-0.4577635529\\Version=AM64L
-G03RevD.01\State=1-A\HF=-683.1310748\MP2=-685.6005632\RMSE=6.942e-09\
Thermal=0.PG=C01 [X(C12H19N4)]\@

4m

4m_1

1\1\GINC-NAUTILUS\SP\RMP2-FC\6-31+G(2d,p)\C13H20N4\RAMAN\05-Feb-2011\0
\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess
=read\\opt of Et1 b98/6-31G(d) on 4p 900 MB\0,1\N,0,-0.0378756496,0.0
685634239,0.0312688985\N,0,0.0799913408,-0.1445825009,4.2424901297\C,0
,1.2362327626,0.0357680777,-0.6632709442\C,0,2.2125878918,0.9778254573
,0.0399662337\C,0,1.2048093148,0.2610048612,2.1369816926\C,0,1.1670282
604,0.1869103602,3.5430213767\C,0,-1.04438487,-0.4103444832,3.57470673
51\C,0,-1.1518347934,-0.3755221271,2.1707512708\C,0,-2.4390348385,-0.2
782309028,0.1067122597\C,0,-1.1404755633,-0.6057669557,-0.6293094539\C
,0,0.0067828126,-0.0225599116,1.4331181582\H,0,3.1908582068,0.92623432
54,-0.4550892603\H,0,-1.0013633621,-1.7016607894,-0.6603810513\H,0,-1.
1969793888,-0.2429308337,-1.6644013662\H,0,-1.9054021319,-0.6663431625
,4.1867543033\H,0,2.0558745876,0.4034645508,4.1299940023\H,0,1.6667581
672,-0.9814486886,-0.6981842992\H,0,1.0748615288,0.3699648287,-1.69696
4554\H,0,1.8421062019,2.0139937038,-0.0532919167\H,0,-2.6430139536,0.8
029352623,0.0114168548\H,0,-3.2712557265,-0.8185603808,-0.3625478065\N
,0,-2.3345446825,-0.7120085332,1.4904432525\N,0,2.3774350403,0.5607962
042,1.4229617804\C,0,3.5463324809,1.0910442612,2.1170192816\H,0,3.7734
951513,0.438954862,2.9687185448\H,0,4.3941098575,0.993996254,1.4254607
873\C,0,-3.59254202,-0.8368619884,2.2192421479\H,0,-3.4380068811,-1.50
85587915,3.0719664632\H,0,-4.2944399492,-1.3522651531,1.5498556431\C,0
,3.4262944355,2.5539691963,2.5838187274\C,0,-4.2124752287,0.491147989,
2.6932249637\H,0,-3.5327080654,1.0255869026,3.3662692784\H,0,-4.436106
3023,1.1483584185,1.8436864447\H,0,-5.150936216,0.3032899039,3.2302890
589\H,0,4.345837143,2.8676602907,3.0942059943\H,0,3.266055649,3.228291

1282,1.733366148\H,0,2.5882373669,2.6786053042,3.2786737488\\Version=A
M64L-G03RevD.01\State=1-A\HF=-721.7619251\MP2=-724.3925845\RMSD=9.054e
-09\Thermal=0.\PG=C01 [X(C13H20N4)]\@

4m_2

1\1\GINC-NAUTILUS\SP\RMP2-FC\6-31+G(2d,p)\C13H20N4\RAMAN\05-Feb-2011\0
\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess
=read\\opt of Et2 b98/6-31G(d) on 4p 900 MB\\0,1\N,0,-0.0281542284,0.0
394582013,0.0900226478\N,0,0.1155362875,0.0195398907,4.3073274848\C,0,
1.2462108448,-0.0290931027,-0.6038144669\C,0,2.2229182345,0.9506869042
,0.0453052755\C,0,1.226651281,0.3381941468,2.1801003162\C,0,1.19441057
68,0.3355599079,3.5889113752\C,0,-1.0085698826,-0.2911320321,3.6587175
05\C,0,-1.1274319775,-0.3018452468,2.254608302\C,0,-2.423589883,-0.359
4290203,0.1826149745\C,0,-1.111808867,-0.7167042958,-0.5132858631\C,0,
0.0277745661,0.0166754235,1.4966384611\H,0,3.1990968196,0.8757691381,-
0.4509082166\H,0,-0.9444203247,-1.8076026388,-0.4483367619\H,0,-1.1720
894813,-0.4472490582,-1.5759199149\H,0,-1.8579167543,-0.5524100217,4.2
847830767\H,0,2.0824108297,0.591587548,4.1610960335\H,0,1.678409929,-1
.0461141022,-0.5825004531\H,0,1.0829911723,0.2471749247,-1.6541933453\
H,0,1.8497775624,1.9799175875,-0.0995634847\H,0,-2.6647393195,0.699664
4445,-0.0200276973\H,0,-3.2306774899,-0.9732301726,-0.2373164859\N,0,-
2.3216113454,-0.6365923226,1.6050580511\N,0,2.3948106234,0.6061354569,
1.4473157418\C,0,3.5668376704,1.1699013825,2.1082676542\H,0,3.79053895
98,0.5673466482,2.9964755989\H,0,4.4137988472,1.0284458403,1.423189669
6\C,0,-3.5731715555,-0.7255790595,2.3535581369\H,0,-4.3849796282,-0.43
3111039,1.6753338318\C,0,3.4545893897,2.658236642,2.4889226767\H,0,-3.
5781463024,0.0121105021,3.1690918414\C,0,-3.8522484553,-2.1333818726,2
.903053813\H,0,-3.0550142488,-2.4593710229,3.5801178981\H,0,-4.8012349
243,-2.1498541205,3.4548131649\H,0,-3.9157913666,-2.8605972974,2.08439
79278\H,0,4.3757937664,2.9966743457,2.98019988\H,0,3.2977938192,3.2822
639676,1.6002747191\H,0,2.6173157706,2.8280921827,3.1752023071\\Versio
n=AM64L-G03RevD.01\State=1-A\HF=-721.7609406\MP2=-724.3910218\RMSD=7.6
52e-09\Thermal=0.\PG=C01 [X(C13H20N4)]\@

4m_3

1\1\GINC-NAUTILUS\SP\RMP2-FC\6-31+G(2d,p)\C13H20N4\RAMAN\05-Feb-2011\0
\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess
=read\\opt of Et3 b98/6-31G(d) on 4p 900 MB\\0,1\N,0,-0.0066581107,0.0
654301635,-0.00133604\N,0,-0.0568766337,-0.0608558703,4.2084951795\C,0
,1.2838144898,0.0229042509,-0.6608627504\C,0,2.2498493504,0.9546637745
,0.0716054492\C,0,1.1548538403,0.2753135028,2.1393469845\C,0,1.0599629
195,0.2397402887,3.5431946325\C,0,-1.1538610091,-0.3484502586,3.502727
9351\C,0,-1.2005870199,-0.3711155754,2.095999115\C,0,-2.4248213175,-0.
1921750504,0.0233252411\C,0,-1.1268687244,-0.509797663,-0.7186984811\C
,0,-0.0172732299,-0.0197118031,1.3964594972\H,0,3.2447422908,0.8832718
73,-0.3866538089\H,0,-1.0331772855,-1.6048906629,-0.8308466969\H,0,-1.
155828976,-0.0696104089,-1.7253680631\H,0,-2.0391806387,-0.5712515425,
4.0908859845\H,0,1.9250516637,0.4710364851,4.1596369659\H,0,1.70482508
21,-0.9981698546,-0.6890158938\H,0,1.1534797615,0.3626180099,-1.697171
4959\H,0,1.90059834,1.9961291713,-0.0425225164\H,0,-2.5917171047,0.900
8333774,0.0256225946\H,0,-3.254104132,-0.6584814274,-0.5151950249\N,0,

-2.3515788868,-0.7465542752,1.3685240032\N,0,2.3569880599,0.5456142356
,1.4623150302\C,0,3.5135898299,1.0539527374,2.1914796907\H,0,3.6839514
235,0.413572041,3.0650570745\H,0,4.3851273627,0.9152260725,1.537257838
2\C,0,-3.6040225344,-0.8849051074,2.1126113523\C,0,3.4231200768,2.5298
492252,2.6227107542\H,0,-3.9272016659,0.0817994271,2.543868267\H,0,-3.
4054331925,-1.5552961111,2.9561189143\C,0,-4.7502722366,-1.4937422741,
1.2972299366\H,0,-4.4340284664,-2.4242382581,0.8100490137\H,0,-5.58017
35436,-1.7297416947,1.9737362657\H,0,-5.1398290917,-0.8122830079,0.532
4140181\H,0,4.3294656177,2.8239951516,3.1672150835\H,0,3.3242722696,3.
1904372728,1.7523508255\H,0,2.5600085654,2.6982638772,3.2765058857\\Ve
rsion=AM64L-G03RevD.01\State=1-A\HF=-721.75996\MP2=-724.3903675\RMSD=4
.831e-09\Thermal=0.\PG=C01 [X(C13H20N4)]\\@

4m_4

1\1\GINC-AZAZEL\SP\RMP2-FC\6-31+G(2d,p)\C13H20N4\RAMAN\05-Feb-2011\0\\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=r
ead\\opt of Et11 b98/6-31G(d) on 4p 900 MB\\0,1\C,0,-0.0180571176,0.01
22363609,-0.0543636437\C,0,-0.0096322159,0.037152108,1.3507745271\C,0,
1.2500629885,0.0007475823,2.0040082415\C,0,2.4231603382,-0.0647736192,
1.2075672747\C,0,2.2642653912,-0.0957650303,-0.1884996996\N,0,1.082027
2959,-0.0555070124,-0.8094643236\N,0,1.3327363802,0.0286588114,3.38919
60656\C,0,2.6240649114,0.081454047,4.0455610364\C,0,3.677487164,-0.629
9681189,3.1932299562\C,0,-1.0202144088,0.6846345089,3.4471998336\C,0,0
.1288406128,0.0056088397,4.1961906844\H,0,3.1340865454,-0.1518072832,-
0.8384652139\H,0,-0.9591768419,0.0445349702,-0.5979176942\H,0,2.547437
5511,-0.4216479316,5.0194032625\H,0,2.9408439374,1.1221840512,4.228004
8746\H,0,0.3196807543,0.5474449491,5.1328660872\H,0,-0.1615533686,-1.0
261028747,4.4569447631\H,0,4.6689656723,-0.4729537959,3.6356718887\H,0
, -1.9516840884,0.5479761252,4.0103272875\H,0,-0.8194444894,1.769317639
8,3.3843685169\H,0,3.4732851701,-1.7158206189,3.1984815468\N,0,-1.1777
254413,0.0692576343,2.1378476601\N,0,3.6768193328,-0.0682410899,1.8506
525413\C,0,4.8936709844,-0.2820865724,1.0726597873\H,0,5.7325179224,0.
0461054631,1.7021084569\H,0,4.872571856,0.3976532543,0.2128489997\C,0,
-2.4793953484,0.2523877817,1.5024877882\H,0,-3.2360033771,-0.049515798
5,2.2400420696\C,0,5.1415631957,-1.728714604,0.6034517662\H,0,-2.55797
19489,-0.4615324198,0.6742889036\C,0,-2.7872739673,1.6790646618,1.0084
144097\H,0,-2.0434908198,2.0170006616,0.2783397491\H,0,-3.7753994825,1
.7101818414,0.5318110045\H,0,-2.7945523938,2.3934727844,1.8410792298\H
,0,5.2493007894,-2.4089974631,1.4574766753\H,0,4.3159927123,-2.0928355
421,-0.0180553402\H,0,6.0655033742,-1.7827307606,0.0136087623\\Version
=AM64L-G03RevD.01\State=1-A\HF=-721.7584012\MP2=-724.3891364\RMSD=7.54
8e-09\Thermal=0.\PG=C01 [X(C13H20N4)]\\@

4m_5

1\1\GINC-CALYPSO\SP\RMP2-FC\6-31+G(2d,p)\C13H20N4\RAMAN\05-Feb-2011\0\\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=
read\\opt of Et12 b98/6-31G(d) on 4p 900 MB\\0,1\C,0,-0.0731836996,0.1
78015277,0.0364186206\C,0,-0.0397346949,0.0805760817,1.4370016397\C,0,
1.2294772482,0.0016265646,2.0647900473\C,0,2.3891501709,-0.0271677766,
1.2467790194\C,0,2.2048945794,0.0400801907,-0.1441989159\N,0,1.0141917
307,0.1516074927,-0.7409143027\N,0,1.3319357466,-0.0637523634,3.445903

2292\C,0,2.6336461922,-0.0574080402,4.0824751224\C,0,3.6627461151,-0.7
309720274,3.1747068756\C,0,-0.971285627,0.7919355051,3.5121336106\C,0,
0.1644185471,0.123706527,4.2889641462\H,0,3.0625892193,0.0164013608,-0
.8124201678\H,0,-1.0194641792,0.2791369156,-0.488277442\H,0,2.56597864
44,-0.6122536312,5.0295556087\H,0,2.9634490931,0.9694192596,4.31802336
76\H,0,0.4365729239,0.7615489621,5.1443026359\H,0,-0.1843058773,-0.841
2835315,4.6906159603\H,0,4.6618667433,-0.6148826974,3.6123335126\H,0,-
1.875530867,0.7535147141,4.1247180739\H,0,-0.7281911585,1.8556811845,3
.3313839094\H,0,3.4429982298,-1.8121765908,3.1176214668\N,0,-1.1892237
055,0.0676694587,2.262853327\N,0,3.6528201809,-0.0886221713,1.86816331
63\C,0,4.8532335384,-0.2784450937,1.0596384428\H,0,5.7074923552,-0.005
4130115,1.6946379637\H,0,4.8344325129,0.4525364817,0.2428855915\C,0,-2
.4848427972,0.2517589153,1.6090919853\C,0,5.0654420218,-1.6984964829,0
.5002703725\H,0,-2.5096755675,-0.4382621658,0.758664455\H,0,-2.5956413
545,1.2725349004,1.1947758096\C,0,-3.6788952016,-0.0758731362,2.513426
5753\H,0,-3.8349387474,0.667553667,3.3038000513\H,0,-4.5931257195,-0.0
992592143,1.908384543\H,0,-3.5505975343,-1.059746357,2.9805060258\H,0,
5.1679524893,-2.4318440285,1.3099039295\H,0,4.226159602,-2.0077846574,
-0.1324468241\H,0,5.9818010562,-1.735259371,-0.1025881614\\Version=AM6
4L-G03RevD.01\State=1-A\HF=-721.7583983\MP2=-724.3886347\RMSE=3.636e-0
9\Thermal=0.\PG=C01 [X(C13H20N4)]\\@

4m_6

1\1\GINC-CALYPSO\SP\RMP2-FC\6-31+G(2d,p)\C13H20N4\RAMAN\05-Feb-2011\0\
\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=
read\\opt of Et5 b98/6-31G(d) on 4p 900 MB\\0,1\N,0,0.0050577397,-0.02
99987464,0.1183221033\N,0,-0.0366531526,0.1665442634,4.335088008\C,0,1
.3152208322,-0.1961522154,-0.4891965122\C,0,2.2834950236,0.8183615969,
0.1153282382\C,0,1.1645250551,0.3765912871,2.2434986028\C,0,1.07815328
17,0.426875802,3.6497905809\C,0,-1.1390275378,-0.1536276773,3.65502971
07\C,0,-1.1957982016,-0.2416870354,2.2490993817\C,0,-2.3971640613,-0.4
04532072,0.1267051114\C,0,-1.059296836,-0.815571967,-0.4843639035\C,0,
-0.0058953222,0.0237157241,1.527385032\H,0,3.2828907563,0.6556474005,-
0.3082378921\H,0,-0.9066075074,-1.9012395954,-0.3406759752\H,0,-1.0688
178742,-0.6153922115,-1.5638245208\H,0,-2.0195071625,-0.3667672378,4.2
557026687\H,0,1.9528051243,0.6731331875,4.2463134859\H,0,1.7135825178,
-1.2174346423,-0.3445042663\H,0,1.221313355,-0.0196410766,-1.568730752
5\H,0,1.9613450794,1.8379737727,-0.1633040503\H,0,-2.6158444569,0.6427
363028,-0.1497847597\H,0,-3.1913714954,-1.0346102131,-0.2938307996\N,0
, -2.3652380002,-0.5968114949,1.566532403\N,0,2.3547539637,0.639818076,
1.5554780298\C,0,3.4902840803,1.2508814733,2.2424865777\H,0,4.03442492
72,1.8567894774,1.506728528\C,0,-3.6513497182,-0.6199047615,2.25960335
1\H,0,-4.4261369072,-0.3607242932,1.5267720066\H,0,3.1335490779,1.9531
550287,3.0099101185\C,0,4.4493576831,0.222057804,2.8621696524\H,0,-3.6
817061597,0.1687818799,3.0254463907\C,0,-3.979305955,-1.9856313497,2.8
837246945\H,0,-3.2176351091,-2.2803746976,3.6139963701\H,0,-4.95107442
23,-1.9522609914,3.3935153608\H,0,-4.0215046124,-2.7620567291,2.110122
3207\H,0,5.2832551664,0.7281281774,3.365998125\H,0,3.9344016402,-0.407
0212288,3.5966178946\H,0,4.8618352392,-0.4352352295,2.0869798633\\Vers
ion=AM64L-G03RevD.01\State=1-A\HF=-721.7599615\MP2=-724.3895241\RMSE=8
.119e-09\Thermal=0.\PG=C01 [X(C13H20N4)]\\@

4m_7

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1\1\GINC-YANG\SP\RMP2-FC\6-31+G(2d,p)\C13H20N4\RAMAN\05-Feb-2011\0\#P
MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=rea
d\opt of Et8 b98/6-31G(d) on 4p 900 MB\0,1\N,0,-0.0317088355,0.02390
65197,0.0383368134\N,0,0.1280312473,0.1622518654,4.2466729681\C,0,1.22
26318586,0.0245792875,-0.6891644903\C,0,2.1995442165,0.9909056493,-0.0
198418862\C,0,1.2469497097,0.3568442183,2.1075502165\C,0,1.2103012445,
0.4342344249,3.5133762103\C,0,-0.9950480284,-0.1796579329,3.612543926\
C,0,-1.1157917775,-0.2541302593,2.2115439495\C,0,-2.4268131056,-0.3591
72694,0.151110776\C,0,-1.1218089888,-0.7287923303,-0.5531192243\C,0,0.
0394403034,0.0316878005,1.4394036759\H,0,3.1460805521,0.9591545361,-0.
5660785318\H,0,-0.9599689699,-1.820064602,-0.4857994649\H,0,-1.1888262
077,-0.4629455296,-1.6163584715\H,0,-1.8448454132,-0.4070876061,4.2511
455453\H,0,2.0925560164,0.722680854,4.0768866515\H,0,1.6810148889,-0.9
799194639,-0.7329215462\H,0,1.024494098,0.3493505441,-1.720228509\H,0,
1.8030644278,2.0210521316,-0.0842315432\H,0,-2.6667558715,0.6977278594
,-0.0642385015\H,0,-3.2393905326,-0.9764485303,-0.2523471595\N,0,-2.31
06926357,-0.6180530556,1.5759869669\N,0,2.4235442634,0.5661083902,1.35
5628923\C,0,3.5828019164,1.1215560231,2.0547934044\C,0,-3.5540778737,-
0.7087323848,2.3382624064\H,0,3.3836136,2.1484754716,2.416380533\H,0,-
3.5830409407,0.0718066325,3.1132340334\H,0,3.7504808076,0.5019600325,2
.9425181263\C,0,4.8746532557,1.1067396258,1.2298943118\H,0,-4.37882494
56,-0.4838110536,1.6506178434\C,0,-3.7799789898,-2.0941941141,2.963978
6269\H,0,-2.9639262958,-2.3598529791,3.6448864777\H,0,-4.7204683098,-2
.1116092145,3.5300509967\H,0,-3.8308734197,-2.8635960624,2.184102758\H
,0,5.7165805109,1.3600166347,1.8849644052\H,0,5.0589843042,0.110599214
2,0.8092353009\H,0,4.8696780361,1.837043941,0.4126727322\Version=AM64
L-G03RevD.01\State=1-A\HF=-721.7588564\MP2=-724.3888337\RMSD=4.155e-09
\Thermal=0.\PG=C01 [X(C13H20N4)]\@
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4m_8

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1\1\GINC-YANG\SP\RMP2-FC\6-31+G(2d,p)\C13H20N4\RAMAN\05-Feb-2011\0\#P
MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=rea
d\opt of Et13 b98/6-31G(d) on 4p 900 MB\0,1\C,0,0.0035921796,0.10195
46792,0.047014313\C,0,0.0003140248,0.0592965404,1.4502057792\C,0,1.254
3545048,0.0044329316,2.110122399\C,0,2.4337290377,-0.0340699285,1.3235
084462\C,0,2.2859036452,-0.0454157923,-0.0724864854\N,0,1.1091042412,0
.0359757081,-0.7030008977\N,0,1.3256513428,-0.0113094452,3.4909554783\
C,0,2.5923699502,-0.1891796931,4.1722145794\C,0,3.6221563151,-0.825419
7898,3.2379596271\C,0,-0.9835159205,0.8064581638,3.4940341381\C,0,0.13
61318629,0.1504984986,4.3028647063\H,0,3.157619477,-0.110764745,-0.718
490868\H,0,-0.929930799,0.1806928194,-0.5041750826\H,0,2.4417684167,-0
.8450537276,5.0442845505\H,0,2.9786032544,0.7747690913,4.5436952759\H,
0,0.3767211687,0.787040932,5.1690641465\H,0,-0.2112081807,-0.821735623
7,4.6907771984\H,0,4.5970569227,-0.7978632002,3.731026349\H,0,-1.90246
13935,0.7670534438,4.0842071006\H,0,-0.741622513,1.870136985,3.3114095
021\H,0,3.3617709392,-1.8850890843,3.0575401879\N,0,-1.1699171293,0.06
9100784,2.2470523588\N,0,3.6797332732,-0.060173326,1.9951812218\C,0,4.
8763251536,-0.2256178358,1.1696964306\H,0,4.8098738097,0.5157183288,0.
3657359632\C,0,-2.4448083289,0.2525378271,1.5530359027\H,0,-2.46293259
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74,-0.4705201317,0.7301167556\H,0,-2.5222981544,1.2578380074,1.0956614
617\C,0,-3.6686671074,-0.0119893333,2.4378676848\H,0,4.905982002,-1.22
02753127,0.6842902154\C,0,6.1848690656,0.0214154789,1.9296502871\H,0,-
3.8359210634,0.7740162414,3.1832490321\H,0,-4.5653397982,-0.0546658782
,1.8082633417\H,0,-3.5688772304,-0.9720291829,2.9584592711\H,0,7.01199
95431,0.0799613526,1.2122678188\H,0,6.1394553845,0.9694053049,2.479140
622\H,0,6.4275819162,-0.7807285684,2.636007878\\Version=AM64L-G03RevD.
01\State=1-A\HF=-721.7578364\MP2=-724.3876941\RMSE=7.967e-09\Thermal=0
\PG=C01 [X(C13H20N4)]\@

4m_9

1\1\GINC-NAUTILUS\SP\RMP2-FC\6-31+G(2d,p)\C13H20N4\RAMAN\05-Feb-2011\0
\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess
=read\\opt of Et10 b98/6-31G(d) on 4p 900 MB\\0,1\C,0,0.0135750201,0.1
901315875,-0.0646195597\C,0,0.0039183643,0.073908994,1.3353949125\C,0,
1.253436102,-0.0117113385,2.0014238079\C,0,2.4384137451,0.0080160523,1
.2202177562\C,0,2.298568624,0.1118374542,-0.1739361225\N,0,1.125019172
4,0.206484125,-0.8065181609\N,0,1.315516577,-0.1190310424,3.3832302933
\C,0,2.5964649242,-0.1055653349,4.060627719\C,0,3.6688523464,-0.727088
8419,3.1646931804\C,0,-1.0063420583,0.6689372333,3.4244272883\C,0,0.11
00083009,-0.0458355603,4.1883076584\H,0,3.1781922933,0.1261545552,-0.8
1312077\H,0,-0.9200098106,0.2649081438,-0.616185508\H,0,2.5127684381,-
0.6924411348,4.9865585663\H,0,2.8965011801,0.9196535502,4.3384439829\H
,0,0.3287767601,0.5133602425,5.1103252434\H,0,-0.2310054828,-1.0524966
263,4.4802378502\H,0,4.6512440139,-0.6017354413,3.6364547047\H,0,-1.94
09327103,0.5687327766,3.9871634926\H,0,-0.768824819,1.7463480822,3.347
7014468\H,0,3.4770582371,-1.81079795,3.0674160304\N,0,-1.1720154213,0.
0479664413,2.1157483999\N,0,3.6827054562,-0.0443474652,1.8794797048\C,
0,4.9116471159,-0.1752053986,1.1026369926\H,0,5.7390306375,0.100187468
3,1.7712883568\H,0,4.8950773014,0.5810428157,0.3091054092\C,0,-2.46364
18732,0.2385743934,1.4550118365\H,0,-3.1768300512,0.5515854124,2.22653
32826\H,0,-2.4219925919,1.0618678424,0.7213215217\C,0,5.1800060442,-1.
5699415,0.5052532192\C,0,-2.984986483,-1.0463942397,0.7945915931\H,0,-
3.1234052087,-1.829695715,1.5487239849\H,0,-3.9489631961,-0.8572669834
,0.3051114006\H,0,-2.2879963445,-1.4257922049,0.0402962186\H,0,5.27824
61694,-2.3263793658,1.293862986\H,0,4.3689242077,-1.8803747007,-0.1627
062877\H,0,6.1146968164,-1.5623520807,-0.0698442129\\Version=AM64L-G03
RevD.01\State=1-A\HF=-721.7580374\MP2=-724.3885291\RMSE=2.828e-09\Ther
mal=0.\PG=C01 [X(C13H20N4)]\@

4m_10

1\1\GINC-NAUTILUS\SP\RMP2-FC\6-31+G(2d,p)\C13H20N4\RAMAN\05-Feb-2011\0
\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess
=read\\opt of Et7 b98/6-31G(d) on 4p 900 MB\\0,1\N,0,-0.0085318091,0.0
402013704,-0.0507235684\N,0,-0.0204535565,0.060387058,4.155434719\C,0,
1.2572100094,0.102188831,-0.7501160752\C,0,2.2166764585,1.0173969951,0
.0116785688\C,0,1.1872034284,0.2835199033,2.0673224989\C,0,1.095857743
3,0.3226784233,3.4704801968\C,0,-1.1204773948,-0.2559660991,3.46697266
26\C,0,-1.1768679469,-0.3336753733,2.0635805559\C,0,-2.4275962355,-0.1
9525327,0.0042857735\C,0,-1.1409037768,-0.5240747687,-0.753877338\C,0,
0.003329746,-0.0136605592,1.3429194768\H,0,3.1801609775,1.0144999708,-

0.5045287362\H,0,-1.0570974887,-1.6191252775,-0.8708515588\H,0,-1.1793
704387,-0.0815588928,-1.7593425973\H,0,-2.0045856327,-0.4500432092,4.0
675837198\H,0,1.9602141913,0.5851076362,4.0738592139\H,0,1.7198016219,
-0.8939411391,-0.8666397763\H,0,1.0773715663,0.5079294913,-1.755748463
7\H,0,1.8271480192,2.0522298322,0.0003644774\H,0,-2.593657701,0.897924
9231,-0.0068036261\H,0,-3.2651292282,-0.6684665886,-0.5147414804\N,0,-
2.3343668268,-0.7298732934,1.3561161738\N,0,2.3927298422,0.5042487715,
1.3635778743\C,0,3.5372302065,0.9983928802,2.1297069178\C,0,-3.5766221
223,-0.8586820795,2.1185015771\H,0,3.3440869955,2.0076364436,2.5412025
229\H,0,-3.902489238,0.1158881796,2.5298735236\H,0,-3.3618215923,-1.50
64510779,2.9757098805\C,0,-4.7275713381,-1.4964789345,1.3319569899\H,0
,3.6638161999,0.3276811683,2.9868329139\C,0,4.8554069798,1.0048912517,
1.347084008\H,0,-4.4078357596,-2.4345003716,0.8617411395\H,0,-5.546724
465,-1.7248702045,2.023983089\H,0,-5.1329201859,-0.8361202269,0.556872
0511\H,0,5.6796594516,1.205315442,2.0417154816\H,0,5.0361605048,0.0306
119949,0.8766341908\H,0,4.8887157557,1.7797235827,0.5727037496\\Versio
n=AM64L-G03RevD.01\State=1-A\HF=-721.7580516\MP2=-724.3882324\RMSD=4.1
73e-09\Thermal=0.\PG=C01 [X(C13H20N4)]\@

4m-Me⁺

4m-Me⁺_1

1\1\GINC-NAUTILUS\SP\RMP2-FC\6-31+G(2d,p)\C14H23N4(1+)\RAMAN\26-Jul-20
11\0\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read g
eom=check\sp of Et1.mc mp2-5 on 2p 900 MB\1,1\N,0,-0.0000071454,1.57
98967313,-0.0779654291\N,0,0.0000121166,-2.5402245718,-0.5428257819\C,
0,1.2479933155,2.3266492619,-0.2035660775\C,0,2.3978180111,1.512685455
4,0.3865687089\C,0,1.2356057672,-0.5015891182,-0.2762525637\C,0,1.1817
602204,-1.8860308823,-0.4410334077\C,0,-1.181740761,-1.8860473167,-0.4
40985677\C,0,-1.2355987896,-0.5016060991,-0.2762029908\C,0,-2.39781334
4,1.5126535817,0.3866612049\C,0,-1.2480228658,2.3266312381,-0.20352173
03\C,0,0.0000000021,0.221640683,-0.2017930497\H,0,3.3444583642,2.01877
0826,0.1719456009\H,0,-1.4543393641,2.5642253828,-1.2574379819\H,0,-1.
1375906937,3.2704350032,0.3435391326\H,0,-2.0689049496,-2.5001519016,-
0.5007353676\H,0,2.0689301925,-2.5001235557,-0.500820609\H,0,1.4542657
451,2.5642515908,-1.257489109\H,0,1.1375690478,3.2704488405,0.34350372
13\H,0,2.2875391652,1.4498432384,1.4806480668\H,0,-2.2874906261,1.4498
172398,1.4807364671\H,0,-3.3444693106,2.0187247303,0.1720734284\N,0,-2
.4301906083,0.1948606833,-0.2366760991\N,0,2.4301895931,0.1948951413,-
0.2367751362\C,0,3.7218561542,-0.4948208978,-0.2859092276\H,0,3.675062
8459,-1.2558418036,-1.0745465832\H,0,4.4568196696,0.24390332,-0.627461
0061\C,0,-3.7218496859,-0.4948717258,-0.2857676463\H,0,-3.6750731122,-
1.2558909773,-1.0744076282\H,0,-4.4568348243,0.2438432072,-0.627293103
5\C,0,4.1826316837,-1.1070083343,1.0476501471\C,0,-4.1825713561,-1.107
0673344,1.0478065843\H,0,-3.4719597581,-1.8516060667,1.4261535829\H,0,
-4.3001489105,-0.3340866284,1.81607703\H,0,-5.1534524319,-1.5990084254
,0.9174907567\H,0,5.1535146393,-1.5989369966,0.9173014529\H,0,4.300225
9705,-0.3340250526,1.815915447\H,0,3.4720429444,-1.85155581,1.42602281
05\C,0,0.0000221968,-4.010108874,-0.6566708997\H,0,0.0000788209,-4.464
9244462,0.3392562126\H,0,-0.8881557949,-4.3272629676,-1.2068774521\H,0
,0.8881497861,-4.3272437791,-1.2069704176\\Version=AM64L-G03RevD.01\St

ate=1-A\HF=-761.2087645\MP2=-763.9905634\RMSD=4.840e-09\Thermal=0.\PG=C01 [X(C14H23N4)]\@

4m-Me⁺_2

1\1\GINC-GOLEM\SP\RMP2-FC\6-31+G(2d,p)\C14H23N4(1+)\RAMAN\26-Jul-2011\0\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geom
=check\sp of Et2.mc mp2-5 on 2p 900 MB\1,1\N,0,0.0068146489,1.5681846716,-0.0596163239\N,0,-0.044574118,-2.5763762256,-0.1199259312\C,0,1.2258849101,2.2825479098,-0.4254766128\C,0,2.4426577343,1.5262338919,0.1039880386\C,0,1.2124692803,-0.535837069,-0.1975508695\C,0,1.1410077489,-1.929756923,-0.2163581055\C,0,-1.2066773599,-1.903517323,0.0581069947\C,0,-1.2391865348,-0.5086660824,0.1166837582\C,0,-2.3174368598,1.5879428303,0.6937747284\C,0,-1.2541108753,2.2979167843,-0.1406323797\C,0,-0.0051250196,0.2033959621,-0.0452011232\H,0,3.3537434401,1.9962236382,-0.2799454097\H,0,-1.5871607893,2.3846686004,-1.1857004972\H,0,-1.0899554118,3.3088160542,0.249889217\H,0,-2.0967455863,-2.5108439899,0.1373959468\H,0,2.0147234749,-2.5565888481,-0.3224034415\H,0,1.2975604613,2.3981110255,-1.5171127478\H,0,1.1827715644,3.2827667092,0.0216278838\H,0,2.4685150984,1.584808807,1.2035559063\H,0,-2.0772936095,1.6832145234,1.7648729116\H,0,-3.2839566794,2.0705650221,0.5195477283\N,0,-2.4174705615,0.1910640059,0.2875618225\N,0,2.403020274,0.1476565122,-0.3704913411\C,0,3.681680328,-0.5585394741,-0.4883788555\H,0,3.5497755388,-1.3951565302,-1.1855516757\H,0,4.3753522788,0.1331628572,-0.9809728398\C,0,-3.6900846311,-0.5064865462,0.510739237\H,0,-4.3471268174,0.1895794815,1.0418348618\C,0,4.28360637,-1.037536638,0.8433294327\H,0,-3.5388654446,-1.3532545665,1.1971314547\C,0,-4.3690032459,-0.9614109081,-0.7892143893\H,0,-3.7372773623,-1.6462451896,-1.3669191697\H,0,-5.3090734601,-1.4770366934,-0.5606005387\H,0,-4.5960998108,-0.099587996,-1.4264040801\H,0,5.2325396362,-1.5547853177,0.6600577392\H,0,4.4872507011,-0.1917108393,1.5100592082\H,0,3.6156224828,-1.7286560799,1.3711721228\C,0,-0.0634805045,-4.0505972876,-0.1124060303\H,0,0.0069232666,-4.4225792784,0.9148630408\H,0,-0.9924519672,-4.3995147751,-0.5682519075\H,0,0.779020331,-4.4231650059,-0.6982004639\Version=AM64L-G03RevD.01\Stat
e=1-A\HF=-761.207415\MP2=-763.9893187\RMSD=2.898e-09\Thermal=0.\PG=C01 [X(C14H23N4)]\@

4m-Me⁺_3

1\1\GINC-AZAZEL\SP\RMP2-FC\6-31+G(2d,p)\C14H23N4(1+)\RAMAN\26-Jul-2011\0\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geo
m=check\sp of Et3.mc mp2-5 on 2p 900 MB\1,1\N,0,-0.0702771567,1.479710289,-0.0810077171\N,0,0.2300932039,-2.650983491,-0.1990722817\C,0,1.0986605412,2.3087638952,-0.3588716296\C,0,2.3542232353,1.6351287301,0.1923736688\C,0,1.3117973194,-0.5094486133,-0.2140194229\C,0,1.3584218524,-1.9023078313,-0.2477818221\C,0,-0.9927741434,-2.0793711297,-0.076923601\C,0,-1.148431675,-0.6942435604,-0.048982316\C,0,-2.4070168404,1.2402079085,0.6113591097\C,0,-1.3793107188,2.1253423544,-0.0901449192\C,0,0.0279670508,0.1230000457,-0.1074718478\H,0,3.2363997713,2.1915317687,-0.140208151\H,0,-1.7009675506,2.3301030515,-1.1214743265\H,0,-1.2911049245,3.0836258918,0.4363642385\H,0,-1.8261606812,-2.7633569175,-0.0105021431\H,0,2.2862654072,-2.4525506426,-0.313784259\H,0,1.2031164005,2.4790828618,-1.4401434534\H,0,0.9510707426,3.2803447082,0.126968144

7\H,0,2.3359863736,1.6552573143,1.2934842294\H,0,-2.1933884655,1.19317
50371,1.6919870591\H,0,-3.3931901775,1.6881932752,0.4812760357\N,0,-2.
395921048,-0.0852140393,-0.0030619199\N,0,2.4453295338,0.2764295723,-0.
.3288921461\C,0,3.7815863028,-0.3172172385,-0.4221686153\H,0,3.7384162
637,-1.1485631886,-1.1365683014\H,0,4.4274391494,0.4396239025,-0.88325
91202\C,0,-3.5890339131,-0.937799832,0.1032589068\C,0,4.3867211354,-0.
7692449986,0.9176788694\H,0,-3.5997270229,-1.4765776857,1.067661575\H,
0,-3.5110349208,-1.6911984548,-0.6907835226\C,0,-4.9114877403,-0.19043
50654,-0.0865513316\H,0,-4.9058432789,0.3999033493,-1.0101323534\H,0,-
5.7188669506,-0.9267811114,-0.1630470657\H,0,-5.1537119326,0.465409353
7,0.7563941432\H,0,5.3803410882,-1.2015460085,0.7521356596\H,0,4.50129
89476,0.0777178933,1.6040891514\H,0,3.7658516653,-1.5236025813,1.41560
70191\C,0,0.342090146,-4.1205780994,-0.17190849\H,0,0.4282030067,-4.47
3458183,0.8610202624\H,0,-0.5440849793,-4.5564622184,-0.6377568855\H,0
,1.2241489133,-4.423689732,-0.7395907706\\Version=AM64L-G03RevD.01\\Sta
te=1-A\\HF=-761.2078791\\MP2=-763.9890013\\RMSD=4.007e-09\\Thermal=0.\\PG=C
01 [X(C14H23N4)]\\@

4m-Me⁺_4

1\1\GINC-AZAZEL\SP\RMP2-FC\6-31+G(2d,p)\C14H23N4(1+)\RAMAN\26-Jul-2011
\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geo
m=check\\sp of Et11.mc mp2-5 on 2p 900 MB\\1,1\C,0,-1.1729442681,-1.91
99974205,0.1402266579\C,0,-1.2231340964,-0.5280733615,0.1799338737\C,0
, -0.0005843113,0.2016015042,0.0025865724\C,0,1.220779151,-0.526176136,
-0.1889979572\C,0,1.1695159359,-1.9185183153,-0.1720636741\N,0,-0.0022
142671,-2.5831195298,-0.023783864\N,0,-0.0004894473,1.5601189547,0.010
2091128\C,0,1.2183147141,2.3128791947,-0.2789028822\C,0,2.4475533943,1
.5225528596,0.164623006\C,0,-2.4477284615,1.5253513911,-0.1559014945\C
,0,-1.2203884694,2.3094357199,0.3036223368\H,0,2.0524228632,-2.5337668
213,-0.2707831593\H,0,-2.0556111126,-2.536520835,0.2337625821\H,0,1.17
49627031,3.2613601625,0.2686636549\H,0,1.2763518604,2.5386224473,-1.35
29722616\H,0,-1.1742832917,3.2649446429,-0.2312811183\H,0,-1.283246671
4,2.5211153071,1.3802598891\H,0,3.3482904177,2.0189894009,-0.210475244
2\H,0,-3.350198576,2.0173524985,0.220874541\H,0,-2.4972334548,1.523769
3536,-1.2564678509\H,0,2.502628977,1.5072442867,1.264816035\N,0,-2.400
011289,0.1723133726,0.3893649009\N,0,2.3966873119,0.176434843,-0.39713
92686\C,0,3.6763332136,-0.5165385867,-0.5736897314\H,0,4.3411160917,0.
1853218498,-1.0916516481\H,0,3.5185625822,-1.3486767585,-1.2706463871\
C,0,-3.6809160344,-0.5221768805,0.5508110031\H,0,-4.3479985541,0.17350
74783,1.0741428581\C,0,4.3460558443,-1.0009392741,0.7237617981\H,0,-3.
527324131,-1.363007561,1.2381091113\C,0,-4.3439821507,-0.9894291738,-0
.7562991831\H,0,-3.7039042904,-1.6766518881,-1.3222994746\H,0,-5.28397
6014,-1.5069828419,-0.5322770791\H,0,-4.579882795,-0.1390300973,-1.406
4589939\H,0,4.5864620473,-0.1592824043,1.3836079645\H,0,3.7085632789,-
1.6949816127,1.2843696241\H,0,5.2843269559,-1.5163821281,0.4879560011\
C,0,0.0055684742,-4.0555162698,0.0409013548\H,0,0.8301886183,-4.437515
0304,-0.5642080195\H,0,0.1230225526,-4.3867169335,1.0779388554\H,0,-0.
9344655212,-4.4376076676,-0.3629127414\\Version=AM64L-G03RevD.01\\State
=1-A\\HF=-761.2081096\\MP2=-763.9891036\\RMSD=5.966e-09\\Thermal=0.\\PG=C01
[X(C14H23N4)]\\@

4m-Me⁺_5

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1\1\GINC-AZAZEL\SP\RMP2-FC\6-31+G(2d,p)\C14H23N4(1+)\RAMAN\26-Jul-2011
\0\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geo
m=check\sp of Et12.mc mp2-5 on 2p 900 MB\1,1\C,0,-0.9787712019,-2.07
32758757,-0.2177022715\C,0,-1.13694136,-0.6972119677,-0.0767447115\C,0
,0.0333297754,0.1300285857,-0.1253578935\C,0,1.321260899,-0.4934861866
,-0.2424867321\C,0,1.3753175496,-1.8824771091,-0.3174959188\N,0,0.2492
4822,-2.6383851149,-0.3259146384\N,0,-0.0744251105,1.4800641112,-0.063
3298658\C,0,1.1028374813,2.3388503638,-0.1739575395\C,0,2.3396297264,1
.6122001233,0.3479237516\C,0,-2.4819067186,1.2377706239,-0.5029761017\
C,0,-1.3784319039,2.1285990589,0.0617226907\H,0,2.3075879822,-2.426386
8493,-0.3749763609\H,0,-1.814734169,-2.7569704893,-0.2505110932\H,0,0.
9256385719,3.2418215506,0.4224757187\H,0,1.2501314279,2.6420070242,-1.
2201352643\H,0,-1.3475721874,3.0720334348,-0.4968735918\H,0,-1.5799952
341,2.3611078179,1.1165540584\H,0,3.2308689758,2.1975630422,0.10029403
\H,0,-3.4459328454,1.6756071762,-0.2394751069\H,0,-2.4143388368,1.1984
948205,-1.6031045114\H,0,2.2864540494,1.5243044791,1.4449375692\N,0,-2
.3800825158,-0.0953094837,0.0915953838\N,0,2.4510394424,0.3079829496,-
0.29908783\C,0,3.7929673818,-0.276998445,-0.3781984645\H,0,4.448862612
2,0.5037276047,-0.7818279776\H,0,3.7739037671,-1.0716453194,-1.1339530
148\C,0,-3.5737585865,-0.9531265336,0.0993361993\C,0,4.3620180396,-0.7
929842712,0.9547691718\H,0,-3.371017434,-1.7660595496,0.8074318133\H,0
,-3.7367133173,-1.4127038578,-0.8923534033\C,0,-4.847817786,-0.2375198
255,0.5568548061\H,0,-5.2278455608,0.4724329068,-0.1855040526\H,0,-5.6
318459112,-0.9858976788,0.7155944685\H,0,-4.685602768,0.2884352524,1.5
047262161\H,0,4.4594431493,0.0200617283,1.6835343692\H,0,3.7293276479,
-1.569457393,1.4009702012\H,0,5.3598217973,-1.2175856224,0.794728673\C
,0,0.3664154749,-4.1067959298,-0.3694520875\H,0,1.2558716946,-4.379666
4003,-0.94108576\H,0,0.4408566972,-4.5103405355,0.6457802923\H,0,-0.51
27836061,-4.522250476,-0.8664317214\Version=AM64L-G03RevD.01\State=1-
A\HF=-761.2080763\MP2=-763.9882741\RMSD=2.202e-09\Thermal=0.PG=C01 [X
(C14H23N4)]\@
```

4m-Me⁺_6

```
1\1\GINC-NAUTILUS\SP\RMP2-FC\6-31+G(2d,p)\C14H23N4(1+)\RAMAN\26-Jul-20
11\0\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read g
eom=check\sp of Et5.mc mp2-5 on 2p 900 MB\1,1\N,0,-0.0000978503,1.57
55617516,0.0525187943\N,0,0.0001150456,-2.5519744395,-0.3275232144\C,0
,-1.249504824,2.2602847865,0.3665378423\C,0,-2.3964874117,1.6221182107
,-0.4136095146\C,0,-1.2357032091,-0.5000494388,-0.1955457094\C,0,-1.18
19397651,-1.892452211,-0.2963936882\C,0,1.1821003177,-1.8923264723,-0.
2964213414\C,0,1.2357192893,-0.4999167717,-0.1955830504\C,0,2.39628326
79,1.622380929,-0.4136293943\C,0,1.2492413363,2.2604028357,0.366549343
5\C,0,-0.0000294631,0.2189863266,-0.1038643207\H,0,-3.3408623665,2.058
9887875,-0.0746826421\H,0,1.4563372373,2.2205816878,1.4466089447\H,0,1
.1446909045,3.312627455,0.0780646394\H,0,2.0688789991,-2.5084209925,-0
.3311200664\H,0,-2.0686535914,-2.5086413097,-0.3310751002\H,0,-1.45658
7799,2.2204778795,1.4466003723\H,0,-1.145064628,3.3125109285,0.0780174
248\H,0,-2.285566058,1.841661658,-1.4875956967\H,0,2.2853335142,1.8419
55605,-1.4876061229\H,0,3.3406168521,2.0593335787,-0.0746916063\N,0,2.
4335053304,0.1865669455,-0.1602527083\N,0,-2.4335612734,0.1863099757,-
```

0.160173435\C,0,-3.7138144717,-0.5124609601,-0.3289054898\H,0,-4.42945
84665,0.2199518437,-0.7161236161\C,0,3.7138292244,-0.51206404,-0.32902
4576\H,0,4.4293760363,0.2204202297,-0.7162876964\H,0,-3.6210332575,-1.
2794216719,-1.1125750393\C,0,-4.2530917817,-1.1166513956,0.9756155599\
H,0,3.6210976536,-1.2790479021,-1.1126763742\C,0,4.2532256119,-1.11617
54872,0.9754838412\H,0,3.5581765992,-1.8433573388,1.4112585751\H,0,5.2
050839553,-1.6263468522,0.7868996801\H,0,4.4257560216,-0.3316779672,1.
7205844605\H,0,-5.2049013318,-1.6269246561,0.7870609517\H,0,-3.5579471
703,-1.8437633844,1.4113539767\H,0,-4.4256788788,-0.3321832043,1.72073
37338\C,0,0.0001899484,-4.0262289638,-0.3212526602\H,0,0.8883990143,-4
.387574318,-0.8435072927\H,0,0.0001655751,-4.3970527567,0.7088713064\H
,0,-0.8879378969,-4.3876653907,-0.8435834009\\Version=AM64L-G03RevD.01
\State=1-A\HF=-761.2062128\MP2=-763.9881901\RMSE=7.012e-09\Thermal=0.\
PG=C01 [X(C14H23N4)]\@

4m-Me⁺_7

1\1\GINC-GOLEM\SP\RMP2-FC\6-31+G(2d,p)\C14H23N4(1+)\RAMAN\26-Jul-2011\
0\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geom
=check\sp of Et8.mc mp2-5 on 2p 900 MB\1,1\N,0,-0.0732272051,1.48593
94677,0.0419411567\N,0,0.2720915554,-2.6315720353,-0.2558477936\C,0,-1
.3760866982,2.1034050651,0.2675243722\C,0,-2.4727798201,1.2681247371,-
0.3893205728\C,0,-1.1295833623,-0.6960395728,-0.0583399345\C,0,-0.9611
696585,-2.0748616409,-0.1817378418\C,0,1.3928863357,-1.8702748434,-0.2
617624415\C,0,1.3310886719,-0.4792318379,-0.1781043237\C,0,2.294552410
3,1.7187669124,-0.5206937262\C,0,1.1172237391,2.3015218085,0.258239150
4\C,0,0.0386367103,0.1338203266,-0.0626842437\H,0,-3.4398434929,1.6833
945051,-0.1022118886\H,0,1.3595670016,2.3562760386,1.3296236779\H,0,0.
9047813698,3.3169826059,-0.0953381846\H,0,2.327391471,-2.4090175836,-0
.3244617722\H,0,-1.7909218371,-2.7657885972,-0.2096202347\H,0,-1.57471
53327,2.205093284,1.3442853247\H,0,-1.3586181878,3.1078653347,-0.17276
40882\H,0,-2.3883093448,1.3260616144,-1.4870470917\H,0,2.1339055999,1.
8598399663,-1.6017141416\H,0,3.2048762069,2.2572430582,-0.2406908682\N
,0,2.4657941013,0.3108569473,-0.1799193001\N,0,-2.3792976248,-0.108353
3927,0.0914981756\C,0,-3.5694685538,-0.9702896042,0.0428127878\C,0,3.7
994553919,-0.283340355,-0.3371202961\H,0,-3.6820707204,-1.4251931359,-
0.957578715\H,0,3.7817997522,-1.0519091883,-1.1253363955\H,0,-3.398930
7,-1.7868092228,0.7558177224\C,0,-4.8691721128,-0.2658034714,0.4402248
507\H,0,4.4580836351,0.5070376144,-0.7104039096\C,0,4.3699604649,-0.84
56414114,0.9730365201\H,0,3.7309232228,-1.6267804628,1.4007296389\H,0,
5.3614569774,-1.277799437,0.7943735547\H,0,4.470270087,-0.050590651,1.
7199384576\H,0,-5.656938312,-1.0202355364,0.5409450309\H,0,-4.76549648
5,0.2436113234,1.4052844743\H,0,-5.2083676886,0.4555543914,-0.31088975
39\C,0,0.3992783413,-4.0999719436,-0.2658776472\H,0,1.2991166761,-4.37
94003752,-0.8177174052\H,0,0.4614347326,-4.4792471567,0.7593875197\H,0
, -0.4697522978,-4.5320090155,-0.7664116745\\Version=AM64L-G03RevD.01\St
ate=1-A\HF=-761.2066096\MP2=-763.9877751\RMSE=4.799e-09\Thermal=0.\PG
=C01 [X(C14H23N4)]\@

4m-Me⁺_8

1\1\GINC-NAUTILUS\SP\RMP2-FC\6-31+G(2d,p)\C14H23N4(1+)\RAMAN\26-Jul-20
11\0\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read g

```
eom=check\sp of Et13.mc mp2-5 on 2p 900 MB\1,1\C,0,-1.1820198446,2.0
80542708,0.0150622553\C,0,-1.2359950536,0.6905979569,-0.0080659376\C,0
,-0.0000521724,-0.0377149122,0.0008201462\C,0,1.2356577343,0.690970506
7,-0.0052926682\C,0,1.1811568354,2.0803780163,-0.0547420037\N,0,-0.000
6965982,2.7467181424,-0.0290393251\N,0,0.0001422221,-1.3910752214,0.00
9449873\C,0,1.2490927752,-2.1492984734,-0.0157670045\C,0,2.3698788351,
-1.3200003341,-0.6363809587\C,0,-2.3721299467,-1.3118806181,0.64496831
39\C,0,-1.2485450555,-2.1494516186,0.0407784661\H,0,2.0673901234,2.696
2228294,-0.1105617237\H,0,-2.0683219712,2.6968824131,0.0642219086\H,0,
1.0879299166,-3.0556642667,-0.6127825535\H,0,1.52071497,-2.4547461656,
1.0042720404\H,0,-1.0893763372,-3.0470723398,0.6514220807\H,0,-1.51602
54591,-2.469699547,-0.9758176212\H,0,3.3125409648,-1.8476872542,-0.484
1651862\H,0,-3.3139683859,-1.8419803352,0.4960890447\H,0,-2.2170704228
,-1.1913298737,1.7302596435\H,0,2.2101470978,-1.2144164553,-1.72253759
31\N,0,-2.4326032517,-0.0193453164,-0.0386646063\N,0,2.4325567066,-0.0
181708462,0.0292573909\C,0,3.6901232174,0.7412232894,-0.0261207101\H,0
,3.6171187886,1.5236754112,0.7393527884\C,0,-3.6906224405,0.7403283148
,0.0026040379\H,0,-3.6149373377,1.5133804058,-0.7721029935\H,0,-3.8081
594212,1.2565480043,0.9726065431\C,0,-4.9342727012,-0.1028162456,-0.29
26877053\H,0,3.8036631296,1.2455199119,-1.0028637611\C,0,4.9351317803,
-0.0980067775,0.2745046257\H,0,-5.1903201119,-0.7847262224,0.525117553
4\H,0,-5.788499911,0.5691529522,-0.4291666685\H,0,-4.8083371186,-0.681
4390301,-1.2149971332\H,0,5.7897068731,0.5757526232,0.3994875074\H,0,4
.8129809748,-0.6654725533,1.2042325105\H,0,5.1880809775,-0.789707429,-
0.5360022303\C,0,0.0013595285,4.2189370497,0.0349473993\H,0,-0.9010421
037,4.6010523389,-0.4467377248\H,0,0.0331217639,4.551773241,1.07770317
58\H,0,0.8741909002,4.6005122702,-0.4991602363\Version=AM64L-G03RevD.
01\State=1-A\HF=-761.2079158\MP2=-763.9873541\RMSD=2.204e-09\Thermal=0
.PG=C01 [X(C14H23N4)]\@
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4m-Me⁺_9

```
1\1\GINC-NAUTILUS\SP\RMP2-FC\6-31+G(2d,p)\C14H23N4(1+)\RAMAN\26-Jul-20
11\0\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read g
eom=check\sp of Et10.mc mp2-5 on 2p 900 MB\1,1\C,0,-1.2141723856,-1.
8594079605,-0.4083082478\C,0,-1.2523006456,-0.4798460107,-0.2169062567
\C,0,-0.0087380041,0.2326730246,-0.1595619871\C,0,1.2184302951,-0.5007
514138,-0.2837846851\C,0,1.1487808517,-1.8829710532,-0.4396437809\N,0,
-0.0405868218,-2.5296230902,-0.511266995\N,0,0.0076430049,1.5811657229
,-0.0020129397\C,0,1.262027282,2.330053759,-0.0347520256\C,0,2.4127027
463,1.4580070692,0.461873015\C,0,-2.3916188596,1.6220282136,-0.5184398
359\C,0,-1.2338059213,2.3300285089,0.1803202842\H,0,2.0296508329,-2.50
5720799,-0.5049332055\H,0,-2.1090220668,-2.4609692699,-0.4792766108\H,
0,1.1569404117,3.2058008277,0.6163332017\H,0,1.4634257866,2.6833966427
,-1.0558590646\H,0,-1.1006972981,3.3277990439,-0.2539162273\H,0,-1.448
6150164,2.4479671973,1.2516859037\H,0,3.360629782,1.9707475661,0.26971
48001\H,0,-3.3277596657,2.1074112716,-0.2281004362\H,0,-2.2836329823,1
.7159963361,-1.6116578008\H,0,2.3237070751,1.3073317713,1.5496089873\N
,0,-2.4421207082,0.2232949499,-0.0986402025\N,0,2.4183299854,0.1922013
055,-0.2646350456\C,0,3.7024545154,-0.5069045016,-0.3705153739\H,0,4.4
318373602,0.234146948,-0.7195089421\H,0,3.6198657691,-1.2475162848,-1.
1753493408\C,0,-3.7297741927,-0.4764566563,-0.2044704646\H,0,-4.482976
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0259,0.2811764955,-0.4411292122\H,0,-3.7245392328,-1.1703756741,-1.060
9478079\C,0,4.2070159882,-1.1560621829,0.9296081878\C,0,-4.1320931097,
-1.195399493,1.0909428874\H,0,-4.226078717,-0.4769531442,1.9122467198\
H,0,-5.0989245309,-1.6937394683,0.9548432512\H,0,-3.4006390853,-1.9536
964779,1.3930786317\H,0,4.3715565071,-0.4036508657,1.7096173652\H,0,3.
5018404067,-1.8979959354,1.3227361659\H,0,5.1632689084,-1.6598570193,0
.7469134968\C,0,-0.0572155407,-4.0000190408,-0.6097214425\H,0,-0.05565
82883,-4.4450129199,0.3907082263\H,0,-0.9526368887,-4.3136283334,-1.15
0471001\H,0,0.8233106989,-4.3330224989,-1.1628821921\\Version=AM64L-G0
3RevD.01\State=1-A\HF=-761.207327\MP2=-763.988073\RMSD=2.186e-09\Therm
al=0.\PG=C01 [X(C14H23N4)]\@

4m-Me⁺_10

1\1\GINC-GOLEM\SP\RMP2-FC\6-31+G(2d,p)\C14H23N4(1+)\RAMAN\26-Jul-2011\
0\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geom
=check\sp of Et7.mc mp2-5 on 2p 900 MB\1,1\N,0,0.0000221066,-1.39690
03756,-0.0160445243\N,0,-0.0000310105,2.7434253703,0.0947261883\C,0,-1
.2511722709,-2.1361563547,-0.1532148358\C,0,-2.3963950542,-1.357624191
4,0.4909263492\C,0,-1.2360749459,0.6886849135,0.0185298215\C,0,-1.1819
796134,2.0790856164,0.0831294197\C,0,1.1819370752,2.0791177079,0.08313
43754\C,0,1.2360775526,0.6887147725,0.0185248726\C,0,2.3964346922,-1.3
57578526,0.4909277746\C,0,1.2512296607,-2.1361335189,-0.1532152904\C,0
,0.0000091068,-0.0397572901,0.014113502\H,0,-3.3318991676,-1.869465477
9,0.2610275711\H,0,1.4721124225,-2.3240557926,-1.2136000533\H,0,1.1320
381177,-3.1048879853,0.3469862278\H,0,2.0683063067,2.6954735609,0.1254
786564\H,0,-2.0683752534,2.6954076947,0.1254611767\H,0,-1.4720509652,-
2.324083974,-1.2135993706\H,0,-1.1319605239,-3.1049085188,0.3469868472
\H,0,-2.2762189255,-1.3429003979,1.5868378853\H,0,2.2762627024,-1.3428
515606,1.5868396297\H,0,3.3319586657,-1.8693888068,0.2610261855\N,0,2.
4344132903,-0.0090927006,-0.0697336301\N,0,-2.4343994068,-0.0091308358
, -0.0697257948\C,0,-3.6916506667,0.7514666903,-0.0262960632\C,0,3.6916
850528,0.7514625318,-0.0263339614\H,0,-3.8266926371,1.2291483091,0.960
7433238\H,0,3.8267302242,1.229192292,0.9606817115\H,0,3.5996405339,1.5
547866745,-0.7680907852\C,0,4.9331612419,-0.0728569371,-0.3775727359\H
,0,-3.5995364791,1.5548384725,-0.7679943544\C,0,-4.9331847177,-0.07272
91159,-0.3776301861\H,0,4.7986470515,-0.6083942361,-1.3244419894\H,0,5
.7824541921,0.6090617506,-0.493970381\H,0,5.2022177625,-0.7904721193,0
.4046785731\H,0,-5.7823998349,0.6092769289,-0.4940835998\H,0,-4.798658
5723,-0.6082704094,-1.3244955586\H,0,-5.2023793999,-0.7903190142,0.404
5953411\C,0,-0.0000483162,4.2110788765,0.2303966269\H,0,0.0000026792,4
.4923771372,1.2886581561\H,0,0.8879957535,4.6167793705,-0.2585525314\H
,0,-0.8881575199,4.6167498591,-0.2584577795\\Version=AM64L-G03RevD.01\
State=1-A\HF=-761.2071688\MP2=-763.9875328\RMSD=4.346e-09\Thermal=0.\P
G=C01 [X(C14H23N4)]\@

4n

4n_1

1\1\GINC-NODE24\SP\RMP2-FC\6-31+G(2d,p)\C23H24N4\ZIP08\15-Jan-2011\0\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=r
ead\sp of sdmap5 MP2-5/6-31+G(2d,p)\0,1\N,0,0.0444501612,-0.16957143
68,0.2353654663\N,0,-0.0449319479,0.1764476428,4.437963688\C,0,1.35210

55234,-0.2900358437,-0.3827083488\C,0,2.2940748058,0.7413380556,0.2361
938598\C,0,1.1828689688,0.2917866601,2.356878657\C,0,1.0795706385,0.40
53134351,3.7554021834\C,0,-1.1369211505,-0.1780311628,3.7562893583\C,0
,-1.1719994311,-0.3279706661,2.3578206731\C,0,-2.3621261413,-0.4841336
356,0.2380517566\C,0,-1.0349360609,-0.9182995018,-0.381741665\C,0,0.02
1776346,-0.0812791727,1.6368647539\H,0,3.2920308137,0.6306445807,-0.20
48491687\H,0,-0.9102712739,-2.0100358359,-0.2598946811\H,0,-1.03955782
96,-0.6977491293,-1.4574052148\H,0,-2.0240081834,-0.3793335853,4.35087
09268\H,0,1.9512691518,0.666896075,4.3492787235\H,0,1.7811288257,-1.30
16701515,-0.2610074619\H,0,1.246742421,-0.0959748569,-1.4583269158\H,0
,1.9257889343,1.7550840635,-0.0035995024\H,0,-2.5407878416,0.579512273
4,-0.0018513718\H,0,-3.1766168101,-1.0718641488,-0.2022509202\N,0,-2.3
364137853,-0.731835634,1.6734897803\N,0,2.3947238271,0.5133099378,1.67
15937358\C,0,3.4679903872,1.2217252449,2.3594577319\H,0,4.1126855157,1
.6541834268,1.5820821561\C,0,-3.6188494975,-0.6433813001,2.3622881582\
H,0,-4.3934774459,-0.5844091936,1.5854806018\H,0,3.0720572807,2.074891
6526,2.9361040198\C,0,4.3338954093,0.3525229034,3.269182861\C,0,4.4576
272916,-1.0271733323,3.0633257359\C,0,5.0690604881,0.952818519,4.30203
91261\C,0,5.303722543,-1.7918869794,3.8721458821\H,0,3.8726061214,-1.4
955934898,2.2756752573\C,0,5.9194282535,0.1913155113,5.1083332528\H,0,
4.9725524251,2.0236625025,4.4792955915\C,0,6.0398649079,-1.1856081989,
4.8946793829\H,0,5.3842829467,-2.864144032,3.7057559765\H,0,6.48015853
81,0.671451282,5.9075216135\H,0,6.6957258117,-1.7817249254,5.525284914
3\H,0,-3.6937370115,0.2942533587,2.9388369956\C,0,-3.9440629473,-1.826
0711344,3.2724462668\C,0,-4.87884432,-1.6652829676,4.3058622257\C,0,-3
.3726603292,-3.0879434225,3.0664764621\C,0,-5.2436219492,-2.7465940667
,5.1125988866\H,0,-5.3219123699,-0.6856500536,4.4832058915\C,0,-3.7321
371094,-4.1699460265,3.8757371154\H,0,-2.6333387839,-3.2078128199,2.27
83805814\C,0,-4.6707203521,-4.0044336241,4.8988304041\H,0,-5.967563971
, -2.6045671019,5.9122158009\H,0,-3.2744850561,-5.1429553782,3.70924941
74\H,0,-4.9477270828,-4.8460669372,5.5297762463\\Version=AM64L-G03RevD
.01\\State=1-A\\HF=-1102.8091183\\MP2=-1106.8024241\\RMSD=5.640e-09\\Therma
l=0.\\PG=C01 [X(C23H24N4)]\\@

4n_2

1\\1\\GINC-NODE25\\SP\\RMP2-FC\\6-31+G(2d,p)\\C23H24N4\\ZIP08\\15-Jan-2011\\0\\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=r
ead\\sp of sdmap4 MP2-5/6-31+G(2d,p)\\0,1\\N,0,0.1727448841,0.374190433
9,0.295339641\\N,0,-0.1611740852,-0.114964207,4.4716634559\C,0,1.503926
7933,0.2849055601,-0.2760815675\C,0,2.4826245092,1.0633356943,0.601330
104\C,0,1.2080117454,0.27660745,2.5173978805\C,0,1.0255589164,0.110784
388,3.9027960554\C,0,-1.2343677668,-0.1994889287,3.683213298\C,0,-1.18
90451873,-0.0917034722,2.2796579509\C,0,-2.2484052679,0.2601135543,0.1
047449812\C,0,-0.9113211584,-0.1369423657,-0.5240446824\C,0,0.06890173
06,0.1764418654,1.6817661637\H,0,3.4937537564,0.9658791098,0.188351413
1\H,0,-0.8685397797,-1.2358769487,-0.6333178101\H,0,-0.824439815,0.305
0194296,-1.5257305627\H,0,-2.1838018166,-0.3491712319,4.1922990118\H,0
,1.8772533614,0.1479784663,4.5764473502\H,0,1.8477083115,-0.7613985555
, -0.3712451003\H,0,1.4789505832,0.7238238858,-1.2824390472\H,0,2.21014
45126,2.1339936126,0.5860476567\H,0,-2.3650408503,1.3559131547,0.06406
50733\H,0,-3.0693070636,-0.1819140035,-0.4735489943\N,0,-2.3160700125,

-0.2546553168,1.4612528535\N,0,2.4766567716,0.5088293212,1.9486036894\
C,0,3.5680180064,0.9274806122,2.8206742546\H,0,4.305600373,1.434949001
5,2.1841720659\C,0,-3.6337779434,-0.522174298,2.004753677\H,0,-3.51988
5752,-1.1774608655,2.8778375285\H,0,-4.1818673716,-1.1159124423,1.2580
948681\H,0,3.2255137021,1.6801915194,3.5510872119\C,0,4.2745848864,-0.
2091119737,3.5566639448\C,0,4.2903286478,-1.5130176142,3.0454335136\C,
0,4.9744347874,0.0632323417,4.741352553\C,0,4.9958711669,-2.5245573934
,3.7037008498\H,0,3.7319829161,-1.7292078059,2.1378912342\C,0,5.684691
6662,-0.9453270638,5.3984000742\H,0,4.960316123,1.0712119386,5.1550490
538\C,0,5.6979878861,-2.2441801584,4.8800755348\H,0,4.993500731,-3.534
5547948,3.2989398856\H,0,6.2194228743,-0.7184040636,6.3182758341\H,0,6
.2443932893,-3.0323572949,5.3932705513\C,0,-4.4881251603,0.6943493006,
2.3717464829\C,0,-5.8863885896,0.5724225933,2.3806145517\C,0,-3.918171
4661,1.9285625518,2.714716596\C,0,-6.6983915418,1.6528399961,2.7343663
692\H,0,-6.3438791817,-0.3779365433,2.1061324032\C,0,-4.7295861212,3.0
134134213,3.0637913747\H,0,-2.8371608874,2.0423521488,2.714031916\C,0,
-6.1206867689,2.8799409062,3.0770319921\H,0,-7.7804658256,1.5390627385
,2.7351570203\H,0,-4.2707472653,3.9638786804,3.3279096366\H,0,-6.75006
61833,3.7244578223,3.3487057112\\Version=AM64L-G03RevD.01\State=1-A\HF
=-1102.8079512\MP2=-1106.8023543\RMSD=2.471e-09\Thermal=0.\PG=C01 [X(C
23H24N4)]\@

4n_3

1\1\GINC-NODE25\SP\RMP2-FC\6-31+G(2d,p)\C23H24N4\ZIP08\14-Jan-2011\0\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=r
ead\sp of sdmap6 MP2-5/6-31+G(2d,p)\0,1\N,0,0.0372009575,0.018033852
1,0.0430925389\N,0,-0.4432825894,0.4009068494,4.2091257339\C,0,1.37753
49483,-0.1702947615,-0.4738179196\C,0,2.3405940154,0.7496289619,0.2767
083498\C,0,0.995136174,0.3599232471,2.2651848459\C,0,0.7633599657,0.49
36288353,3.6455143057\C,0,-1.4892788239,0.1455990094,3.4181385559\C,0,
-1.3958068596,-0.0571581608,2.0299824123\C,0,-2.3830994972,0.016656324
7,-0.1726705184\C,0,-1.0639527354,-0.4940390074,-0.749639922\C,0,-0.11
87646527,0.0940651786,1.429607561\H,0,3.3626153946,0.5693581357,-0.077
2706451\H,0,-1.0823522471,-1.597951458,-0.7754052744\H,0,-0.9428354832
, -0.1357180565,-1.7816504674\H,0,-2.4509759127,0.0986858456,3.92201193
96\H,0,1.591687892,0.6721694697,4.3256814456\H,0,1.7183798495,-1.21733
59321,-0.3812721863\H,0,1.3765814912,0.0888563902,-1.541098182\H,0,2.0
828979638,1.8007993055,0.0542992298\H,0,-2.4286300632,1.1169894774,-0.
2649015221\H,0,-3.2160136082,-0.4069672336,-0.741302444\N,0,-2.4915557
088,-0.4209278128,1.2144639903\N,0,2.2852673133,0.454172564,1.70219733
22\C,0,3.364896433,1.0036734912,2.5138736908\H,0,4.1426481044,1.343649
8227,1.8166836582\C,0,-3.8337877361,-0.3941960795,1.7916041957\H,0,3.0
342302392,1.9017821411,3.0634828622\C,0,3.999061383,0.0149449566,3.489
9656134\C,0,3.9888950864,-1.3636350538,3.2420349259\C,0,4.6586539548,0
.4937061973,4.6314559178\C,0,4.6291261015,-2.2464952138,4.1165586902\H
,0,3.461146572,-1.736898885,2.3678209084\C,0,5.3036912926,-0.386727543
,5.5046183294\H,0,4.6641129194,1.5629821816,4.8412154478\C,0,5.2912611
073,-1.761525087,5.2487896752\H,0,4.6069401799,-3.3155326763,3.9150986
079\H,0,5.8075541706,0.0002356089,6.3878152461\H,0,5.7867522813,-2.449
2583269,5.9304656108\H,0,-4.20342751,0.638352691,1.9361726611\H,0,-3.7
72922499,-0.8506420475,2.7858388915\C,0,-4.8403144089,-1.1901930227,0.

9754543537\C,0,-4.5973300614,-2.5407161673,0.6741847068\C,0,-6.0405849
77,-0.6082181079,0.5483095077\C,0,-5.5367015925,-3.2897823695,-0.03689
63018\H,0,-3.6625182809,-2.9945746936,0.9972394903\C,0,-6.9867067155,-
1.3582264316,-0.1601888572\H,0,-6.2378808604,0.438789404,0.7735883851\
C,0,-6.736588276,-2.7005953364,-0.4546884918\H,0,-5.3365332614,-4.3352
991086,-0.2617679197\H,0,-7.9146603238,-0.8913582997,-0.483243548\H,0,
-7.4693598204,-3.2855151841,-1.0061573615\\Version=AM64L-G03RevD.01\St
ate=1-A\HF=-1102.8089779\MP2=-1106.8023029\RMSD=4.568e-09\Thermal=0.\P
G=C01 [X(C23H24N4)]\\@

4n_4

1\1\GINC-NODE14\SP\RMP2-FC\6-31+G(2d,p)\C23H24N4\ZIP08\15-Jan-2011\0\\
#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid geom=check guess=r
ead\\sp of sdmap9 MP2-5/6-31+G(2d,p)\\0,1\N,0,0.1207068889,1.550250043
5,0.3307229613\N,0,-0.5839392513,-2.2597185341,-1.3229709153\C,0,1.485
4863118,1.9575295229,0.6061408191\C,0,2.2946811164,0.7484308743,1.0706
072468\C,0,0.9516056427,-0.6509432779,-0.3649700635\C,0,0.630827271,-1
.9183757533,-0.8836779126\C,0,-1.5563342307,-1.3487609213,-1.255555334
2\C,0,-1.3798486163,-0.0459538058,-0.7522227615\C,0,-2.2579158979,2.03
5623499,0.1781413501\C,0,-0.8403106008,2.6033290331,0.0673490766\C,0,-
0.0937335864,0.3032946192,-0.2638214468\H,0,3.3347496918,1.0478400979,
1.2285968818\H,0,-0.7008911806,3.0537408743,-0.9318072954\H,0,-0.69700
95053,3.3949917696,0.8152361261\H,0,-2.535902837,-1.6777288751,-1.5955
480659\H,0,1.3820280255,-2.7011955527,-0.9408971992\H,0,1.9736946819,2
.4020406304,-0.2791711841\H,0,1.4654999287,2.720885017,1.3968109006\H,
0,1.8939088859,0.3776041641,2.0313930141\H,0,-2.4624379405,1.754938063
6,1.2247983674\H,0,-2.9840548351,2.8073532158,-0.105508131\N,0,-2.4009
330435,0.9147649058,-0.7337578355\N,0,2.2543279256,-0.274026006,0.0308
956157\C,0,3.2910452357,-1.3018108166,0.1019832888\C,0,-3.7233252216,0
.6502084223,-1.2666165089\H,0,3.15158323,-1.9722214832,0.9706052971\H,
0,3.2000646306,-1.9232716024,-0.7956885851\C,0,4.6953258024,-0.7185267
51,0.1239795454\C,0,5.6022770377,-1.0631011297,1.1342458243\C,0,5.1170
527992,0.1477166604,-0.898559765\C,0,6.9083679205,-0.5593830316,1.1249
374419\H,0,5.2852408374,-1.7317331276,1.9332050658\C,0,6.4173873563,0.
6557806671,-0.9076166895\H,0,4.4135045167,0.4233686616,-1.6817015962\C
,0,7.3184768604,0.3016683059,0.1043802643\H,0,7.600748482,-0.837632608
6,1.9165154083\H,0,6.7313328592,1.3243993544,-1.7064275252\H,0,8.33233
64122,0.695609405,0.0955415655\H,0,-4.1197576794,1.601954341,-1.651156
728\H,0,-3.6153959978,-0.0015377644,-2.1432245434\C,0,-4.7511306664,0.
0585052506,-0.2986080296\C,0,-6.1174405993,0.2845453714,-0.5263542995\
C,0,-4.3721993407,-0.7190875776,0.8049128444\C,0,-7.0854609098,-0.2623
876112,0.3196570121\H,0,-6.4262958375,0.8961745773,-1.3738730851\C,0,-
5.3396088243,-1.2633506021,1.6563780659\H,0,-3.3182102686,-0.903697627
5,0.9968626237\C,0,-6.698261874,-1.0393650768,1.4164578295\H,0,-8.1400
145338,-0.0759532718,0.1272015478\H,0,-5.0283579926,-1.8652400301,2.50
75582611\H,0,-7.449279127,-1.4630963198,2.0794433074\\Version=AM64L-G0
3RevD.01\State=1-A\HF=-1102.8079358\MP2=-1106.8020882\RMSD=7.203e-09\T
hermal=0.\PG=C01 [X(C23H24N4)]\\@

4n_5

1\1\GINC-NODE25\SP\RMP2-FC\6-31+G(2d,p)\C23H24N4\ZIP08\16-Jan-2011\0\\

```
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ead\\sp of sdmap1 MP2-5/6-31+G(2d,p)\\0,1\\N,0,-0.000404771,-2.10022066
48,-0.8474074468\\N,0,0.0052501718,0.6712479986,2.3345904334\\C,0,1.2283
338032,-2.8320664688,-1.1005795619\\C,0,2.4180072651,-1.8737164369,-1.0
136837439\\C,0,1.2210521473,-0.7348223225,0.7848828969\\C,0,1.1500176128
,0.2136730672,1.8240168399\\C,0,-1.1414261895,0.2157494288,1.8264101511
\\C,0,-1.2164729766,-0.7326597329,0.7874682196\\C,0,-2.418406987,-1.8670
161839,-1.0102257179\\C,0,-1.231391436,-2.8282880871,-1.1005246074\\C,0,
0.0012942978,-1.2082916116,0.238027491\\H,0,3.35058451,-2.4385977663,-1
.134287302\\H,0,-1.3772463953,-3.6584140653,-0.385692372\\H,0,-1.1753205
513,-3.258850152,-2.1094773761\\H,0,-2.0483278823,0.6436989468,2.247040
9544\\H,0,2.058628087,0.6397495423,2.2428621624\\H,0,1.3727949293,-3.661
1884063,-0.3842858456\\H,0,1.1699655307,-3.2644058423,-2.1086068669\\H,0
,2.363970019,-1.1417075379,-1.8366618975\\H,0,-2.3634621121,-1.13337278
36,-1.8316852558\\H,0,-3.352541655,-2.4292510373,-1.1309499294\\N,0,-2.4
292498648,-1.2354083807,0.2975126099\\N,0,2.4320470066,-1.2393072661,0.
2925912835\\C,0,3.7157648794,-0.8263148182,0.8248131952\\H,0,3.608130274
3,-0.6822302558,1.9078278035\\H,0,4.4083370974,-1.6730064188,0.70570588
87\\C,0,-3.7118288387,-0.8214642958,0.8320599045\\H,0,-3.6014241666,-0.6
736544061,1.9142664943\\H,0,-4.4037164039,-1.6693637464,0.7178390609\\C,
0,4.357542911,0.4135187884,0.1964242034\\C,0,3.6013191168,1.387611575,-
0.4694570657\\C,0,5.7456279634,0.593305538,0.3025539227\\C,0,4.220191283
7,2.5194906033,-1.0115762211\\H,0,2.5250343082,1.264598647,-0.559901234
\\C,0,6.364807062,1.7250558325,-0.2331754303\\H,0,6.3473373124,-0.161191
2952,0.8089842183\\C,0,5.6016870656,2.6938807354,-0.8938337417\\H,0,3.61
83615689,3.2667254603,-1.524472498\\H,0,7.442027556,1.8473143665,-0.141
0442378\\H,0,6.0811574148,3.5746018628,-1.3151709624\\C,0,-4.3573295328,
0.4148299378,0.2005139411\\C,0,-5.7471706093,0.5857732555,0.2979633242\\
C,0,-3.6030894153,1.3947336184,-0.4593145949\\C,0,-6.3702026421,1.71433
05602,-0.2401337335\\H,0,-6.3473188434,-0.1732795021,0.7994056041\\C,0,-
4.2257784535,2.5233425572,-1.0038266494\\H,0,-2.5254795035,1.2789739426
,-0.5432512936\\C,0,-5.6090968502,2.6888344453,-0.8946164062\\H,0,-7.448
7601111,1.8295627077,-0.1548092048\\H,0,-3.6254903375,3.275079535,-1.51
19385374\\H,0,-6.091447307,3.5670864819,-1.3178252282\\Version=AM64L-G0
3RevD.01\\State=1-A\\HF=-1102.8068354\\MP2=-1106.8018905\\RMSD=5.478e-09\\T
hermal=0.\\PG=C01 [X(C23H24N4)]\\@
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4n_6

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1\\GINC-NODE24\\SP\\RMP2-FC\\6-31+G(2d,p)\\C23H24N4\\ZIP08\\16-Jan-2011\\0\\
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ead\\sp of sdmap17 MP2-5/6-31+G(2d,p)\\0,1\\C,0,-0.334490852,0.12841863
08,0.0242748607\\C,0,-0.2163103807,0.1402377872,1.4219118181\\C,0,1.0871
521704,0.0920167686,1.9783223961\\C,0,2.1912088617,-0.0110487013,1.0952
285265\\C,0,1.9280981737,-0.0452671894,-0.2831160746\\N,0,0.7031304931,0
.0295213166,-0.8137497471\\N,0,1.2684973323,0.1231605718,3.3504082511\\C
,0,2.6018803506,0.0615552835,3.9128910368\\C,0,3.5405135623,-0.68658619
88,2.9670150348\\C,0,-1.0071822394,1.0344646911,3.489250367\\C,0,0.16557
32725,0.4170792555,4.2503103887\\H,0,2.7476922968,-0.1009811902,-0.9944
413402\\H,0,-1.3113163679,0.2001118836,-0.4482476668\\H,0,2.5575760264,-
0.4714410525,4.8745165204\\H,0,3.0023289568,1.0712568314,4.1094525909\\H
,0,0.5084235159,1.1250543987,5.0214411567\\H,0,-0.1696710215,-0.4981274
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649,4.7643274737\H,0,4.5635034806,-0.6181750523,3.3534304551\H,0,-1.88
35831625,1.0626743571,4.1429725847\H,0,-0.7633697585,2.0719701272,3.19
56214982\H,0,3.2579730885,-1.754974247,2.9371901756\N,0,-1.3062449196,
0.2048313662,2.3226533587\N,0,3.4949616043,-0.0682123077,1.6448603718\
C,0,4.5990536489,-0.4100102215,0.7528074867\C,0,-2.6459935386,0.361213
3805,1.7599453392\H,0,4.3575656262,-1.283665504,0.1209611999\H,0,-2.80
10727945,1.3654155112,1.3218996351\H,0,5.4357041135,-0.7187347795,1.39
42335811\C,0,5.0758840224,0.7402256457,-0.1290984714\C,0,4.9972508912,
2.0701880517,0.3051993891\C,0,5.6634884177,0.4669343751,-1.372697858\C
,0,5.4974989925,3.1058869697,-0.4887032963\H,0,4.5272943788,2.28459675
04,1.2617498222\C,0,6.1693189296,1.5009315891,-2.1660544824\H,0,5.7211
837905,-0.562284722,-1.7256914863\C,0,6.0875969506,2.8252753913,-1.725
4329614\H,0,5.4234746106,4.1346532605,-0.1421363123\H,0,6.6180696343,1
.2722587609,-3.1303540881\H,0,6.4741635697,3.6324285268,-2.3437099648\
H,0,-2.7361638642,-0.3591403047,0.9377592915\C,0,-3.7421094553,0.06970
0264,2.7723199337\C,0,-4.7879577523,0.9786448843,2.9783089265\C,0,-3.7
437740357,-1.1382389802,3.489628615\C,0,-5.8217995387,0.6886574385,3.8
763265068\H,0,-4.7947212365,1.9201189081,2.4309578294\C,0,-4.770940298
5,-1.4277893843,4.389975443\H,0,-2.9285484452,-1.8430122321,3.33911889
75\C,0,-5.8152830404,-0.5153333231,4.5847534009\H,0,-6.6268621254,1.40
5401681,4.0234547217\H,0,-4.7605890249,-2.3679040353,4.9376117849\H,0,
-6.6162913735,-0.7427895371,5.2846491065\\Version=AM64L-G03RevD.01\Sta
te=1-A\HF=-1102.8083713\MP2=-1106.801637\RMSE=7.091e-09\Thermal=0.\PG=
C01 [X(C23H24N4)]\@

4n_7

1\1\GINC-NODE14\SP\RMP2-FC\6-31+G(2d,p)\C23H24N4\ZIP08\14-Jan-2011\0\\
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ead\\sp of sdmap13 MP2-5/6-31+G(2d,p)\0,1\C,0,0.017386998,0.146871182
4,0.1146322971\C,0,0.0127081892,0.1379105602,1.517696404\C,0,1.2580739
283,0.0028970539,2.1826366501\C,0,2.4285209004,-0.1488585216,1.3962945
702\C,0,2.2794205684,-0.1900912793,0.0017471213\N,0,1.1127417596,-0.02
95797185,-0.6326292477\N,0,1.3293200531,0.0188237994,3.5627453811\C,0,
2.5733469133,-0.2642513151,4.2545934053\C,0,3.5462393366,-0.9963769685
,3.3321689207\C,0,-0.9007849611,1.0310265499,3.5383616819\C,0,0.162779
8898,0.3191467264,4.3722987007\H,0,3.1423666358,-0.3473316002,-0.64103
4579\H,0,-0.9073421191,0.2902963806,-0.4393308647\H,0,2.3596875156,-0.
8950339704,5.1321326872\H,0,3.0396489563,0.6657388986,4.6201519931\H,0
,0.4648764881,0.969660751,5.2084691885\H,0,-0.2622901349,-0.6016647492
,4.8051666399\H,0,4.5280776982,-1.0455183405,3.8115394542\H,0,-1.82811
28238,1.0923200719,4.1150103635\H,0,-0.5716228146,2.0603296089,3.30580
82259\H,0,3.19609278,-2.0303557405,3.1584488226\N,0,-1.1464140294,0.25
89427487,2.3205034395\N,0,3.6642769017,-0.2527746206,2.0780759207\C,0,
4.8612031956,-0.531728552,1.287805435\H,0,4.8322375133,0.1286017502,0.
412646122\C,0,-2.4186658273,0.5210669189,1.651441566\H,0,-2.4791694478
, -0.1592787372,0.7933962243\H,0,-2.4742495308,1.5494114009,1.246978501
7\C,0,-3.6152697202,0.2581439439,2.5523221348\C,0,-4.6315112156,1.2120
100807,2.6930775066\C,0,-3.7388665216,-0.9678688018,3.2269117856\C,0,-
5.7551913258,0.9482518524,3.4850649446\H,0,-4.5442291831,2.1677325967,
2.1782962626\C,0,-4.8558427814,-1.2313017127,4.0221302971\H,0,-2.94690
37081,-1.7072919227,3.1273176403\C,0,-5.8696072067,-0.2739273958,4.151

9524863\H,0,-6.5358199061,1.6995965797,3.5829124543\H,0,-4.9391793401,
-2.1855387733,4.5381714235\H,0,-6.7406322746,-0.4804844807,4.769906977
9\H,0,4.8760780649,-1.5691801882,0.9035608948\C,0,6.1438872494,-0.2495
438869,2.0544051522\C,0,7.1704623627,-1.2010177783,2.111474806\C,0,6.3
347374969,0.9914485105,2.6844618754\C,0,8.3694138572,-0.9204092623,2.7
772390405\H,0,7.0318535771,-2.1681707582,1.6304068636\C,0,7.5273551541
,1.2718115947,3.3541392443\H,0,5.5357726764,1.7292454718,2.6501027248\
C,0,8.5503411751,0.316578936,3.4006792105\H,0,9.1569420426,-1.67015154
29,2.8112909125\H,0,7.6621749153,2.2375130741,3.8368979651\H,0,9.48012
47815,0.536285303,3.9207272712\\Version=AM64L-G03RevD.01\State=1-A\HF=
-1102.8096753\MP2=-1106.8023259\RMSD=9.847e-09\Thermal=0.\PG=C01 [X(C2
3H24N4)]\@

4n_8

1\1\GINC-NODE10\SP\RMP2-FC\6-31+G(2d,p)\C23H24N4\ZIP08\16-Jan-2011\0\\
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ead\\sp of sdmap16 MP2-5/6-31+G(2d,p)\0,1\C,0,-0.0143714092,-0.043455
0862,-0.2813157285\C,0,-0.0154683725,-0.0205918459,1.1214811815\C,0,1.
2358956046,-0.0017774489,1.7872179739\C,0,2.4144417772,-0.0057693027,0
.9994436571\C,0,2.2728839418,-0.0273712416,-0.3962270473\N,0,1.0946893
927,-0.046458348,-1.0280206857\N,0,1.3050955328,0.0190212989,3.1704894
396\C,0,2.5849439403,-0.0194917414,3.8495641087\C,0,3.6434420059,-0.66
27182083,2.9536111868\C,0,-1.0428365688,0.7039418292,3.1654092844\C,0,
0.0999388547,0.0882585043,3.9728650866\H,0,3.1518407497,-0.0036925077,
-1.0349011673\H,0,-0.9527832101,-0.0858642761,-0.8277633445\H,0,2.4835
270194,-0.6141975856,4.7698256037\H,0,2.9127908691,0.9928657749,4.1408
88626\H,0,0.2939574518,0.7149919431,4.8563157095\H,0,-0.1978350025,-0.
9114958537,4.3318493975\H,0,4.6245946486,-0.5543856768,3.428905147\H,0
, -1.9715518062,0.6154321509,3.7398041146\H,0,-0.8423022863,1.779087593
,3.0040032173\H,0,3.4314710599,-1.7427956856,2.8502739323\N,0,-1.19467
67956,-0.0205098093,1.90669066\N,0,3.6664860042,0.0178254451,1.6619099
594\C,0,4.8679393331,-0.1932648373,0.8606878677\C,0,-2.4708069131,0.16
54656545,1.2234203536\H,0,4.7621202474,-1.0611354562,0.1849178349\H,0,
-3.2009777797,0.4451551563,1.9950521505\H,0,-2.4354607537,1.0109454114
,0.51275983\C,0,-2.9875383362,-1.0797663623,0.5090762647\C,0,-2.676983
7866,-2.3649832332,0.9729747637\C,0,-3.8397528744,-0.9453000808,-0.596
384647\C,0,-3.2093992013,-3.4935750282,0.343640294\H,0,-2.0028865518,-
2.4683730675,1.8196588549\C,0,-4.378084917,-2.0727358624,-1.2235419004
\H,0,-4.0801008606,0.0485843852,-0.9728093318\C,0,-4.0638061104,-3.351
8992465,-0.754573562\H,0,-2.9537298386,-4.485893714,0.7095704859\H,0,-
5.0344659977,-1.9514951119,-2.0826164219\H,0,-4.4755018052,-4.23103275
15,-1.2453084366\H,0,5.6718903675,-0.4498615455,1.5639624192\C,0,5.309
7376314,1.0268998349,0.0581956738\C,0,5.0460428117,2.3272741578,0.5086
214899\C,0,6.047296321,0.8544818506,-1.1219246633\C,0,5.5119288449,3.4
335099799,-0.2072645727\H,0,4.4598551328,2.4598721745,1.4145795201\C,0
,6.5192658487,1.9595871449,-1.836201836\H,0,6.2497310702,-0.1517102199
, -1.4878148787\C,0,6.2523649465,3.2541066684,-1.3801659845\H,0,5.29328
96504,4.4378171756,0.1498476445\H,0,7.0865639064,1.8088533387,-2.75216
87553\H,0,6.6121694194,4.1157868782,-1.9380539129\\Version=AM64L-G03Re
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al=0.\PG=C01 [X(C23H24N4)]\@

4n_9

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ead\sp of sdmap7 MP2-5/6-31+G(2d,p)\0,1\N,0,-0.0970547806,0.36831080
62,-0.1552306194\N,0,-0.1153365154,0.4370699518,4.0500611153\C,0,1.153
1376645,0.5017372747,-0.8758296673\C,0,2.1083207494,1.39806966,-0.0878
37657\C,0,1.0950374388,0.631705943,1.9614548574\C,0,1.001366285,0.6914
767277,3.3621466464\C,0,-1.2122604,0.1078412772,3.362065356\C,0,-1.264
184943,0.0096863775,1.9613706349\C,0,-2.5234650211,0.1768675728,-0.087
9999041\C,0,-1.2504701691,-0.1319836563,-0.8759161297\C,0,-0.086764693
1,0.3291012461,1.2344966907\H,0,3.0762826731,1.4308970819,-0.596356387
9\H,0,-1.187842349,-1.2192606833,-1.0556164723\H,0,-1.289114709,0.3663
856856,-1.8551602417\H,0,-2.0989218436,-0.0759629988,3.9632123603\H,0,
1.863342389,0.9687167731,3.9633637296\H,0,1.6347337593,-0.4750778901,-
1.055506645\H,0,0.9411100303,0.9543842317,-1.8550839146\H,0,1.70634576
39,2.4266226179,-0.0464285841\H,0,-2.6808713217,1.2699039091,-0.046585
7679\H,0,-3.3817483229,-0.2718144549,-0.5965797473\N,0,-2.4071763518,-
0.4081177562,1.2430572383\N,0,2.2954895135,0.8317655668,1.2432179601\C
,0,3.4825039966,1.2759431932,1.9688530275\C,0,-3.6589295667,-0.6069206
074,1.9686231591\H,0,3.4204153183,2.3422310713,2.2567611824\H,0,-4.130
6327068,0.35137086,2.25652794\H,0,-3.417778768,-1.1328549575,2.8994099
294\C,0,-4.6558626967,-1.4572264263,1.1960198099\C,0,-4.2806184665,-2.
7191514581,0.7058239614\C,0,-5.9716219393,-1.0197123074,0.9981857404\C
,0,-5.203665543,-3.5233919177,0.0346134217\H,0,-3.2571179395,-3.059365
2191,0.8502953785\C,0,-6.90077372,-1.8262963831,0.3305014148\H,0,-6.27
24049246,-0.0416127847,1.3708482662\C,0,-6.5186153444,-3.0797682438,-0
.1533801234\H,0,-4.8999782394,-4.4992676852,-0.338487425\H,0,-7.919077
1895,-1.471780703,0.1862324644\H,0,-7.2380260067,-3.7077214023,-0.6742
431824\H,0,3.5319511241,0.6994747782,2.8996409129\C,0,4.7691212729,1.0
276837616,1.1963306074\C,0,5.6980646788,2.0570900147,0.9984255222\C,0,
5.0649719586,-0.2552552155,0.7063357573\C,0,6.9041821944,1.813465029,0
.3308714934\H,0,5.4773986354,3.0563776601,1.3709264546\C,0,6.264621136
2,-0.4998492111,0.0352484746\H,0,4.3423107245,-1.0559048442,0.85087284
91\C,0,7.1898489862,0.5344729942,-0.152814337\H,0,7.6152695888,2.62399
65487,0.1865447274\H,0,6.4816604773,-1.4986314842,-0.3377016348\H,0,8.
1253999866,0.3428487799,-0.6735825817\Version=AM64L-G03RevD.01\State=
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1 [X(C23H24N4)]\@
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4n_10

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1\1\GINC-NODE14\SP\RMP2-FC\6-31+G(2d,p)\C23H24N4\ZIP08\16-Jan-2011\0\\
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ead\sp of sdmap12 MP2-5/6-31+G(2d,p)\0,1\C,0,-0.0567129204,0.7038017
771,0.1346603414\C,0,-0.0826752074,0.3800174145,1.5003473395\C,0,1.137
4111001,0.0077431482,2.1203060589\C,0,2.3034949143,-0.070907842,1.3147
273917\C,0,2.1737751599,0.2254620066,-0.0529482234\N,0,1.0355623061,0.
6187902072,-0.631872327\N,0,1.1827834881,-0.2964867845,3.4723911049\C,
0,2.4538070218,-0.5661590282,4.1166780208\C,0,3.4151792762,-1.23407857
52,3.1317323309\C,0,-0.9620721474,0.8923271958,3.6609300291\C,0,0.0325
255292,-0.0552298117,4.3306093648\H,0,3.0335424656,0.1396792025,-0.714
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3942508\H,0,-0.9582443168,1.0398435638,-0.3715622553\H,0,2.2797456697,
-1.2388526104,4.9688342033\H,0,2.9107249787,0.3593051643,4.5088001065\
H,0,0.3770193788,0.3945760197,5.2744120251\H,0,-0.4717501616,-1.002950
5352,4.5770425506\H,0,4.4092275255,-1.306063769,3.5887919999\H,0,-1.89
23605088,0.9017311819,4.236087551\H,0,-0.5545046941,1.9198009248,3.647
615911\H,0,3.073752249,-2.2608332852,2.91634068\N,0,-1.2420196348,0.41
15077547,2.3092336232\N,0,3.518086595,-0.4222658433,1.929211201\C,0,4.
7576614319,-0.5152814137,1.1781062495\H,0,5.5780634443,-0.2732072269,1
.8701525217\H,0,4.7577814403,0.2843578693,0.4263613851\C,0,-2.48783875
71,0.8860191898,1.7117437871\C,0,5.0737664934,-1.8595418121,0.51665641
63\C,0,4.0680668573,-2.7290547366,0.0688067911\C,0,6.4145301467,-2.234
9958794,0.3393193111\C,0,4.3983268801,-3.9411323578,-0.5465094105\H,0,
3.023356613,-2.4575249723,0.1965037253\C,0,6.7467608331,-3.4418506425,
-0.2815807939\H,0,7.207086102,-1.5755485986,0.6923680842\C,0,5.7369848
615,-4.3012355976,-0.7262380603\H,0,3.6052137312,-4.6031053771,-0.8876
720319\H,0,7.7922845807,-3.7142572189,-0.4102095149\H,0,5.9917073873,-
5.2441078442,-1.2049854176\H,0,-2.5777123861,0.4084202136,0.7285783523
\H,0,-2.479006355,1.9783131591,1.5360289268\C,0,-3.7082530023,0.509346
2803,2.5374299431\C,0,-4.6685993709,1.4701721762,2.8791763027\C,0,-3.9
111808005,-0.8223827811,2.9359361653\C,0,-5.8146015642,1.1116916623,3.
598743842\H,0,-4.5199789013,2.5064485528,2.5789729313\C,0,-5.050650051
7,-1.1816811575,3.6584843024\H,0,-3.1633409005,-1.5700551037,2.6796965
762\C,0,-6.0079713667,-0.2151244195,3.9906618818\H,0,-6.5508392965,1.8
70369612,3.8553699104\H,0,-5.1956089452,-2.2171377957,3.9595311292\H,0
,-6.8964969312,-0.49605002,4.5517064638\\Version=AM64L-G03RevD.01\\Stat
e=1-A\\HF=-1102.8065336\\MP2=-1106.8007666\\RMSD=6.762e-09\\Thermal=0.\\PG=
C01 [X(C23H24N4)]\\@

4n-Me⁺

4n_Me⁺_1

1\\1\\GINC-AZAZEL\\SP\\RMP2-FC\\6-31+G(2d,p)\\C24H27N4(1+)\\RAMAN\\14-Oct-2011
\\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geo
m=check\\sp of sdmap5.mc mp2-5 on 2p 900 MB\\1,1\\N,0,-0.0000158851,2.5
329524289,0.4752074254\\N,0,0.0000768728,-1.0701077792,-1.5693677619\C,
0,-1.2519440578,3.0806081517,0.9861886821\C,0,-2.3885730207,2.76262718
06,0.0178550338\C,0,-1.2333420378,0.7265632865,-0.5767570978\C,0,-1.18
24074186,-0.4859273774,-1.260650074\C,0,1.1825307529,-0.4858879798,-1.
2606098121\C,0,1.2333971987,0.7266075354,-0.5767245805\C,0,2.388552948
7,2.7627011719,0.0179372051\C,0,1.2518799058,3.0806437228,0.9862324821
\C,0,0.0000119527,1.3546280762,-0.2087405486\H,0,-3.3364653209,3.07270
62464,0.4676050362\H,0,1.477164962,2.6736187646,1.983041002\H,0,1.1374
981336,4.1669828529,1.0800984632\H,0,2.0725769759,-1.0373681875,-1.529
069388\H,0,-2.0724225279,-1.0374386798,-1.529145381\H,0,-1.4772505495,
2.6735799042,1.9829910416\H,0,-1.1375980134,4.1669509687,1.0800540723\
H,0,-2.2528166323,3.3298434524,-0.9176156603\H,0,2.2528109619,3.329923
1912,-0.9175320029\H,0,3.336421371,3.0728029598,0.4677214994\N,0,2.439
1418528,1.3220611643,-0.220783427\N,0,-2.4391165566,1.3219837241,-0.22
08486942\C,0,-3.69520297,0.7824554655,-0.7514624527\H,0,-4.4669615751,
1.5292506661,-0.5291278539\C,0,3.6952442619,0.7825615603,-0.751385737\
H,0,4.4670067656,1.5293336791,-0.5289867859\H,0,-3.6526124261,0.703481
4056,-1.8517930531\C,0,-4.1132795673,-0.5570769993,-0.1539195124\C,0,-

3.8697218734,-0.8638601867,1.1923711619\C,0,-4.8057973125,-1.481302675
8,-0.9506336542\C,0,-4.3121395862,-2.0748607909,1.7317813761\H,0,-3.32
99197102,-0.1535066368,1.8146187807\C,0,-5.2539535319,-2.6907337209,-0
.4094206202\H,0,-5.0078345908,-1.2506473026,-1.9963509397\C,0,-5.00615
00148,-2.9905207102,0.9333445565\H,0,-4.1190101074,-2.3019285594,2.777
581371\H,0,-5.7952845912,-3.395315695,-1.0361241396\H,0,-5.3526627441,
-3.9302961817,1.3558613777\H,0,3.6526826672,0.7036510301,-1.8517214398
\C,0,4.1132681504,-0.557022248,-0.1539234007\C,0,4.8057896673,-1.48120
82971,-0.9506798377\C,0,3.86964631,-0.8638996392,1.192334087\C,0,5.253
895478,-2.6906896803,-0.4095380315\H,0,5.0078708498,-1.2504823936,-1.9
963730797\C,0,4.3120130202,-2.0749507039,1.7316725617\H,0,3.3298340036
,-0.1535801268,1.814611891\C,0,5.0060328429,-2.9905685993,0.9331956717
\H,0,5.7952312971,-3.3952401442,-1.0362728642\H,0,4.1188351418,-2.3020
915223,2.777447758\H,0,5.3525046237,-3.9303842607,1.3556566517\C,0,0.0
001090518,-2.4100947921,-2.1844938481\H,0,0.8895400193,-2.5182637463,-
2.8084781774\H,0,0.0001030747,-3.1788499254,-1.4051174714\H,0,-0.88929
23319,-2.5182884771,-2.8085160708\\Version=AM64L-G03RevD.01\\State=1-A\\
HF=-1142.2603259\\MP2=-1146.4064345\\RMSD=3.723e-09\\Thermal=0.\\PG=C01 [X
(C24H27N4)]\\@

4n_Me⁺_2

1\\GINC-YIN\\SP\\RMP2-FC\\6-31+G(2d,p)\\C24H27N4(1+)\\RAMAN\\15-Oct-2011\\0\\
\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geom=c
heck\\sp of sdmap16.mc mp2-5 on 2p 900 MB\\1,1\C,0,-1.0852454862,-1.05
27653621,-0.4608751981\C,0,-1.1417242663,0.336392866,-0.4592895353\C,0
,0.0010004614,1.0670915461,0.0039539077\C,0,1.1474105399,0.3377922673,
0.4594497915\C,0,1.0970964484,-1.0513725317,0.4489864452\N,0,0.0087755
601,-1.7154193409,-0.0114779606\N,0,-0.0006768423,2.4240230931,0.00658
43516\C,0,1.1649565951,3.1791430255,0.4595806186\C,0,1.9774413181,2.35
91462139,1.4570823999\C,0,-1.9729945305,2.3606649104,-1.4514643501\C,0
, -1.1671862546,3.1778086632,-0.4463070085\H,0,1.9292114927,-1.66269217
39,0.7678630174\H,0,-1.9163240644,-1.6656310466,-0.7802297408\H,0,0.81
31292549,4.0989623744,0.9424988605\H,0,1.7879064757,3.4618086661,-0.40
09677929\H,0,-0.8167281827,4.1015291832,-0.9226734039\H,0,-1.794280080
1,3.4534205363,0.4135096066\H,0,2.9228731965,2.8739047253,1.6515904609
\H,0,-2.9192568088,2.8734258927,-1.6471110494\H,0,-1.4225485837,2.2873
752814,-2.404304129\H,0,1.4311720472,2.2792790316,2.4118215897\N,0,-2.
2649231083,1.0407279443,-0.8909402189\N,0,2.2711913778,1.043091498,0.8
885861558\C,0,3.3881062661,0.3092671127,1.4944254033\C,0,-3.3777906272
,0.3069259413,-1.5036576558\H,0,3.0431546718,-0.3064943063,2.344091282
1\H,0,-4.0439723577,1.06649504,-1.9304070263\H,0,-3.0276896563,-0.3068
69652,-2.3526598059\C,0,-4.1714359852,-0.5583548461,-0.5314394445\C,0,
-4.4072465631,-0.1431684111,0.7870991409\C,0,-4.7288050997,-1.76603106
04,-0.9773627689\C,0,-5.1871773581,-0.9241653447,1.6441435778\H,0,-3.9
763454742,0.7913004919,1.1391415768\C,0,-5.5149035411,-2.5447355541,-0
.1215725281\H,0,-4.5598638662,-2.094316776,-2.0026686624\C,0,-5.743994
0153,-2.1256652149,1.1921737423\H,0,-5.365339715,-0.5919674025,2.66417
65322\H,0,-5.9468650881,-3.4752566732,-0.4818154885\H,0,-6.3540200053,
-2.7294848268,1.8593449733\H,0,4.0556378897,1.0689013508,1.9189506354\
C,0,4.1773222806,-0.5535016637,0.516427647\C,0,4.4158579905,-0.1298295
038,-0.7989237717\C,0,4.7263536569,-1.7684563912,0.9529444545\C,0,5.19

02433364,-0.9095792784,-1.662060815\H,0,3.9910374354,0.8100624538,-1.1438731994\C,0,5.5067243992,-2.5462025576,0.0909171596\H,0,4.5554943888,-2.103239806,1.9758444059\C,0,5.7385252385,-2.1185566759,-1.2195798705\H,0,5.3705493713,-0.570827703,-2.6795436836\H,0,5.9323772653,-3.4823971484,0.4439322842\H,0,6.3440606092,-2.7214824918,-1.8916228667\C,0,-0.0155354621,-3.1880641948,0.0482538443\H,0,-0.4423612326,-3.5182490831,1.000892859\H,0,-0.6200738598,-3.5706637949,-0.7766920828\H,0,1.0036973776,-3.5664288739,-0.0525067763\\Version=AM64L-G03RevD.01\State=1-A\HF=-1142.2607\MP2=-1146.4058374\RMSD=3.025e-09\Thermal=0.\PG=C01 [X(C24H27N4)]\@

4n_Me⁺_3

1\1\GINC-EDDY\SP\RMP2-FC\6-31+G(2d,p)\C24H27N4(1+)\RAMAN\14-Oct-2011\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geom=check\\sp of sdmap4.mc mp2-5 on 2p 900 MB\\1,1\N,0,0.0089951045,2.4119118546,0.1375462843\N,0,0.0688761807,-1.7213971017,-0.1675440703\C,0,1.2304991093,3.1341527523,0.4762648705\C,0,2.0608149811,2.3139541623,1.4607325887\C,0,1.1844776039,0.3072810007,0.4462947948\C,0,1.1599305591,-1.0804380285,0.3152607346\C,0,-1.0563015862,-1.0499015971,-0.5097171901\C,0,-1.1260849652,0.3393118535,-0.4128200668\C,0,-2.394310237,2.4079408615,-0.2980745502\C,0,-1.0752475887,3.158558759,-0.4919031287\C,0,0.0249967804,1.0496740222,0.0586327812\H,0,3.0231393165,2.8111906202,1.6140005661\H,0,-0.8773886801,3.3064217669,-1.5640574273\H,0,-1.1326698591,4.1443535022,-0.016049375\H,0,-1.8957686999,-1.6494889954,-0.8333449264\H,0,2.017511992,-1.6984559086,0.5403189534\H,0,1.8197829992,3.349568879,-0.4275810199\H,0,0.9481655811,4.0897627045,0.934099586\H,0,1.5448497147,2.2615968516,2.4335251596\H,0,-2.6808114652,2.4410965892,0.7645731275\H,0,-3.1820013172,2.9048005286,-0.8723353129\N,0,-2.2570899114,1.041608215,-0.7838080848\N,0,2.3089919442,0.9858458681,0.9037991978\C,0,3.4333636784,0.2285657873,1.4629492208\H,0,4.0818792403,0.9630058212,1.9555938655\C,0,-3.3836626058,0.3715812973,-1.4274898812\H,0,-3.0049105438,-0.1862590368,-2.2972029509\H,0,-4.0238778844,1.1647403934,-1.8342166591\H,0,3.087550195,-0.4561914017,2.2567551148\C,0,4.25075545,-0.5444597611,0.4331512893\C,0,4.4724384053,-0.0332250089,-0.8534955332\C,0,4.8419333712,-1.7643458798,0.7946202807\C,0,5.2728676063,-0.7305840049,-1.7623090943\H,0,4.0136866478,0.9100007333,-1.1414124304\C,0,5.6480007967,-2.4596683638,-0.1128034504\H,0,4.6830749658,-2.167788789,1.7943663474\C,0,5.86377134,-1.944294361,-1.3942581552\H,0,5.4396270625,-0.32389207,-2.7569605411\H,0,6.1057622471,-3.400792363,0.1821400462\H,0,6.4893330122,-2.4833825158,-2.1012885333\C,0,-4.2188848838,-0.5636739544,-0.5524118313\C,0,-4.8896964718,-1.6394847417,-1.1550472905\C,0,-4.3656177553,-0.359702562,0.8267905698\C,0,-5.7014081125,-2.487820498,-0.3961696901\H,0,-4.7857977794,-1.8100114948,-2.2262466381\C,0,-5.1722106136,-1.2113510689,1.5879262043\H,0,-3.8475060676,0.4632717324,1.3140174467\C,0,-5.843806956,-2.2757258061,0.9786873071\H,0,-6.2194413664,-3.3133125709,-0.878266507\H,0,-5.2782367466,-1.0405679865,2.6565870781\H,0,-6.4734145327,-2.9349386465,1.5708905792\C,0,0.1268601016,-3.1795320734,-0.3778513534\H,0,0.4995753926,-3.3974342819,-1.3838653977\H,0,0.7932625359,-3.6225816246,0.3648075512\H,0,-0.8736551861,-3.5990406495,-0.2543217056\\Version=AM64L-G03RevD.01\State=1-A\HF=-1142.2583885\MP2=-1146.4048479\RMSD=4.123e-09\Thermal=0.\PG=C01 [X(C24H27N

4)J\\@

4n_Me⁺_4

1\\1\\GINC-CALYPSO\\SP\\RMP2-FC\\6-31+G(2d,p)\\C24H27N4(1+)\\RAMAN\\14-Oct-2011\\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geom=check\\sp of sdmap6.mc mp2-5 on 2p 900 MB\\1,1\\N,0,0.2438891655,1.8385470346,0.1212013337\\N,0,-0.9209529321,-1.7627253333,-1.5638457553\\C,0,-0.7598052787,2.7818049049,0.6030094528\\C,0,-2.0070351648,2.7117115035,-0.2753875544\\C,0,-1.5212569894,0.3854727395,-0.6889534985\\C,0,-1.8627647513,-0.839964646,-1.2564412223\\C,0,0.3980192479,-1.5264348442,-1.3485612794\\C,0,0.8365766909,-0.34508448,-0.7565219751\\C,0,2.557561776,1.3054299366,-0.4731389831\\C,0,1.6425581432,2.0856406732,0.4660003732\\C,0,-0.1389480751,0.6564668843,-0.4299548213\\H,0,-2.792645916,3.3272102187,0.1728522439\\H,0,1.8395370963,1.7977805265,1.5084683443\\H,0,1.832493926,3.1613697497,0.3666750718\\H,0,1.0729174596,-2.3122681943,-1.6564275386\\H,0,-2.8890527167,-1.1261522259,-1.4377922895\\H,0,-1.0196221057,2.5684145518,1.650025844\\H,0,-0.3315573912,3.7899641011,0.5579549995\\H,0,-1.7836599514,3.1186742233,-1.2753289298\\H,0,2.5050924454,1.7244574622,-1.4914189431\\H,0,3.5884412327,1.3870935856,-0.1224076434\\N,0,2.1684727818,-0.1032354724,-0.4499342946\\N,0,-2.4809915731,1.3313268682,-0.3421342584\\C,0,-3.8764935768,1.1276964759,-0.7440425512\\H,0,-4.3904359826,2.0773040493,-0.5523295819\\C,0,3.1849392589,-1.1101686939,-0.794516447\\H,0,-3.9506260881,0.9532025531,-1.8317084514\\C,0,-4.5957481196,0.0131059903,0.008349081\\C,0,-4.338210931,-0.2349512118,1.3641220838\\C,0,-5.5764615294,-0.7438045956,-0.6502529917\\C,0,-5.0506883447,-1.2230636437,2.0488865005\\H,0,-3.5767648065,0.3456738738,1.879973056\\C,0,-6.2942760073,-1.7285494054,0.0365642145\\H,0,-5.7909267743,-0.5546755623,-1.7018346589\\C,0,-6.031201043,-1.9711566766,1.3879531153\\H,0,-4.8439313044,-1.4059956061,3.1007116307\\H,0,-7.0567137248,-2.3030550415,-0.4838892169\\H,0,-6.5870900831,-2.7366278517,1.9235174685\\H,0,3.3541439601,-1.1455707449,-1.884632841\\H,0,2.7823114788,-2.0853322616,-0.4922239464\\C,0,4.5010311651,-0.8884647139,-0.0725628985\\C,0,4.5640020628,-0.992912577,1.3270677806\\C,0,5.6700372171,-0.6011189272,-0.7896702362\\C,0,5.7761459177,-0.8098944027,1.9949992506\\H,0,3.6607515067,-1.2210486911,1.8905850384\\C,0,6.8866024055,-0.4225786443,-0.1213536586\\H,0,5.6327558867,-0.5226174553,-1.8751049876\\C,0,6.9406000191,-0.5252682086,1.2709089611\\H,0,5.8161722666,-0.8977375888,3.0780291753\\H,0,7.7878732821,-0.2046046062,-0.6888255098\\H,0,7.8851705771,-0.3882850758,1.7913326755\\C,0,-1.3402012541,-3.0769706411,-2.0823578456\\H,0,-1.4673664343,-3.7836111716,-1.255822445\\H,0,-2.2846124202,-2.9663181938,-2.6185678525\\H,0,-0.5811338401,-3.4496715874,-2.7737220883\\Version=AM64L-G03RevD.01\\State=1-A\\HF=-1142.2593405\\MP2=-1146.4045322\\RMSD=7.654e-09\\Thermal=0.\\PG=C01 [X(C24H27N4)]\\@

4n_Me⁺_5

1\\1\\GINC-EDDY\\SP\\RMP2-FC\\6-31+G(2d,p)\\C24H27N4(1+)\\RAMAN\\15-Oct-2011\\0\\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geom=check\\sp of sdmap17.mc mp2-5 on 2p 900 MB\\1,1\\C,0,0.3686990999,-1.8263402225,-0.6947507459\\C,0,0.8175292381,-0.586127726,-0.2560228202\\C,0,-0.1348779406,0.4815975377,-0.1368133979\\C,0,-1.4882257311,0.2465995782,-0.5429889394\\C,0,-1.8277367128,-1.0142232456,-1.0229316367\\N,0,-0.

9192889272,-2.0185251444,-1.079392403\N,0,0.2469372874,1.6922473679,0.3368907174\C,0,-0.7114805723,2.7884973138,0.4544291805\C,0,-1.8364450127,2.6242294351,-0.5624519345\C,0,2.3071235531,0.6376559244,1.1629378483\C,0,1.6199238881,1.9432885058,0.7775233674\H,0,-2.8343612492,-1.2644740748,-1.3273102156\H,0,1.0118329124,-2.6933983392,-0.7497093478\H,0,-0.1811085311,3.730008251,0.2661068512\H,0,-1.1189087338,2.8240082753,1.474773876\H,0,1.5836499368,2.6137185799,1.6453797839\H,0,2.1813485417,2.4464518253,-0.021734269\H,0,-2.6171310122,3.3600806092,-0.348852239\H,0,3.3739523125,0.8218177071,1.3073720202\H,0,1.8926996232,0.2519714363,2.1092127951\H,0,-1.4557420831,2.8171924722,-1.5793576899\N,0,2.1428059246,-0.3276443853,0.0745258499\N,0,-2.414241565,1.2845110915,-0.4452096592\C,0,-3.7527244012,1.1039239106,-1.0180374031\C,0,3.1338881688,-1.4102502954,-0.0288621415\H,0,-3.6911587945,0.8061022068,-2.0799410129\H,0,2.9908591103,-2.1598064356,0.7689944161\H,0,-4.2251837684,2.093638941,-1.0053771293\C,0,-4.6376365303,0.1234096055,-0.2568708026\C,0,-4.5833921253,0.0244874018,1.1408145449\C,0,-5.568679817,-0.655035007,-0.9608896972\C,0,-5.446295925,-0.8389487657,1.8212444002\H,0,-3.8628600127,0.6237737558,1.6926422337\C,0,-6.4369828364,-1.5142387597,-0.2794477974\H,0,-5.6262011157,-0.5799827885,-2.0465431438\C,0,-6.3760940159,-1.6090258415,1.1139654847\H,0,-5.3968789463,-0.9064916589,2.905490546\H,0,-7.1586803263,-2.1063313687,-0.8369532645\H,0,-7.0496176316,-2.2762866092,1.6458712594\H,0,2.9563326134,-1.9128313544,-0.988365503\C,0,4.5617939055,-0.8963767256,-0.007524562\C,0,5.4499505518,-1.2959699816,0.9996687993\C,0,5.0145345918,-0.0300633759,-1.0165878233\C,0,6.7736632116,-0.8415323237,0.999477838\H,0,5.1097763785,-1.9700059274,1.7843153366\C,0,6.333253405,0.4279148545,-1.0145146775\H,0,4.3302988509,0.2817900165,-1.8038674783\C,0,7.2159810795,0.0214746706,-0.0061018006\H,0,7.4549742532,-1.1620557921,1.7836438689\H,0,6.6763152648,1.0942526907,-1.8022984757\H,0,8.2442062577,0.3744411189,-0.0081422436\C,0,-1.3606601817,-3.367358339,-1.4759493653\H,0,-1.6937228898,-3.9285560678,-0.596743008\H,0,-2.183858397,-3.2801834623,-2.1878856292\H,0,-0.530905854,-3.8903280656,-1.9561239412\\Version=AM64L-G03RevD.01\State=1-A\HF=-1142.260045\MP2=-1146.4040395\RMSD=7.766e-09\Thermal=0.\PG=C01 [X(C24H27N4)]\@

4n_Me⁺_6

1\1\GINC-NAUTILUS\SP\RMP2-FC\6-31+G(2d,p)\C24H27N4(1+)\RAMAN\15-Oct-2011\0\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read g eom=check\sp of sdmap10.mc mp2-5 on 2p 900 MB\1,1\C,0,1.2581643439,-0.289585319,1.3625378341\C,0,1.2865529429,0.8180397197,0.5193664189\C,0,0.042671163,1.3882659167,0.0991532068\C,0,-1.1787091245,0.7791459168,0.5381206436\C,0,-1.106164107,-0.3422864381,1.3595250329\N,0,0.0875284047,-0.8448025331,1.7595004333\N,0,0.0141940806,2.4893410036,-0.6970974877\C,0,-1.2481618159,3.1540396075,-1.0123730038\C,0,-2.383991463,2.1317311671,-1.0710540779\C,0,2.3966831169,2.8234143479,-0.2131229327\C,0,1.2548341838,3.0804074079,-1.1932598885\H,0,-1.9875671596,-0.8802850299,1.6815018094\H,0,2.1586881644,-0.777438786,1.7079386413\H,0,-1.1447078139,3.6444103317,-1.9871637608\H,0,-1.4687303926,3.9258999685,-0.2610659704\H,0,1.104275912,4.1606919362,-1.3012968622\H,0,1.5009072284,2.6679841218,-2.1818589762\H,0,-3.3406743179,2.65757432,-1.1439271288\H,0,3.3378510786,3.137167036,-0.6742430684\H,0,2.2478590178,3.4233498

837,0.7002803687\H,0,-2.2723158193,1.5119722694,-1.9745034145\N,0,2.47
98134008,1.3934798403,0.0853243225\N,0,-2.3864820694,1.3285068786,0.14
53602303\C,0,-3.6473347683,0.8555189075,0.7081042864\H,0,-4.4040436856
,1.6058931211,0.4444916906\H,0,-3.5630043311,0.8858746628,1.8045797866
\C,0,3.7490097001,0.9225885955,0.6506245883\H,0,4.512686582,1.63734196
89,0.3207044545\H,0,3.7341078261,0.9758097308,1.7537487559\C,0,-4.1311
457231,-0.5307749994,0.2778892024\C,0,-3.7365560076,-1.1251324507,-0.9
285023928\C,0,-5.031775071,-1.2158301352,1.1092777374\C,0,-4.238312537
4,-2.3768785603,-1.3005806111\H,0,-3.0318373261,-0.6169861962,-1.58257
5012\C,0,-5.5389888113,-2.4631017251,0.735422438\H,0,-5.3465514862,-0.
7670078567,2.0508919126\C,0,-5.1425343821,-3.0474392414,-0.4720788687\
H,0,-3.9241929885,-2.8252937527,-2.2401311636\H,0,-6.2404279605,-2.978
1461604,1.3872586434\H,0,-5.5348293123,-4.0182351631,-0.7641162968\C,0
,4.1565980031,-0.4774628021,0.2059244802\C,0,3.8960648196,-0.934181011
9,-1.0940207104\C,0,4.8584695159,-1.3069884816,1.0934031016\C,0,4.3303
204209,-2.1996177018,-1.4978493193\H,0,3.3502224227,-0.2967577548,-1.7
85927248\C,0,5.2987270605,-2.5710589079,0.6873451295\H,0,5.0747377878,
-0.9594583504,2.1033848168\C,0,5.0335212035,-3.0206148706,-0.609450631
8\H,0,4.1242129929,-2.5431780353,-2.5088277272\H,0,5.8477085506,-3.201
0927077,1.3829970944\H,0,5.3740376805,-4.0029528707,-0.9270355875\C,0,
0.1126291612,-2.0820811192,2.5606122784\H,0,0.1075696149,-2.9556780327
,1.9008771631\H,0,1.014240494,-2.0920360261,3.1762323145\H,0,-0.763963
7401,-2.1059429699,3.2112057845\\Version=AM64L-G03RevD.01\\State=1-A\\HF
=-1142.2576057\\MP2=-1146.4032282\\RMSD=3.604e-09\\Thermal=0.\\PG=C01 [X(C
24H27N4)]\\@

4n_Me⁺_7

1\1\GINC-YIN\SP\RMP2-FC\6-31+G(2d,p)\C24H27N4(1+)\RAMAN\14-Oct-2011\0\
\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geom=c
heck\\sp of sdmap1.mc mp2-5 on 2p 900 MB\\1,1\N,0,0.0002880174,-2.4419
984041,-0.8699780289\N,0,0.000970119,0.6711875214,1.870170335\C,0,1.24
80589001,-3.1474221459,-1.1468383306\C,0,2.4046185783,-2.1471303183,-1
.1978625667\C,0,1.2324235842,-0.8369649606,0.4753737089\C,0,1.18356079
18,0.1969279157,1.4115187488\C,0,-1.1818558241,0.1967154903,1.41234859
34\C,0,-1.2311727238,-0.837216648,0.4762755495\C,0,-2.4043332842,-2.14
75264387,-1.1961679564\C,0,-1.2475530261,-3.1476083119,-1.1460605227\C
,0,0.0005069808,-1.3927817272,0.0065189136\H,0,3.3499708933,-2.6911361
003,-1.2836096096\H,0,-1.4424398963,-3.9120906703,-0.3787831259\H,0,-1
.1471792872,-3.6533217022,-2.1137220821\H,0,-2.0730640749,0.6790904193
,1.7896750905\H,0,2.0749408215,0.6794579117,1.7882371372\H,0,1.4436137
954,-3.9117774972,-0.3796040309\H,0,1.1471108255,-3.6532667789,-2.1143
703095\H,0,2.3001268276,-1.5114627234,-2.0907636849\H,0,-2.3006240772,
-1.5117498008,-2.0890807509\H,0,-3.3496492039,-2.6916949963,-1.2812770
148\N,0,-2.4288207639,-1.3629986524,0.0310271129\N,0,2.4298571274,-1.3
624633242,0.0292268178\C,0,3.7012607389,-0.950821336,0.6171712385\H,0,
3.6351678691,-1.074931066,1.7086030296\H,0,4.4497531931,-1.6773939747,
0.276157948\C,0,-3.6998546528,-0.9515670891,0.6198615362\H,0,-3.632800
9851,-1.0753241102,1.7112750727\H,0,-4.4484169195,-1.6784869519,0.2797
306636\C,0,4.1793160422,0.4662841483,0.2984393271\C,0,3.8463950485,1.1
128551645,-0.9000095712\C,0,5.0084465948,1.1263182704,1.2188752909\C,0
,4.3382228668,2.3924654176,-1.1757218853\H,0,3.198498497,0.6213664345,

-1.6223958195\C,0,5.5058317499,2.4030597479,0.9415643527\H,0,5.2762714
514,0.6354659708,2.1541207511\C,0,5.1707828064,3.0397311424,-0.2575680
411\H,0,4.0732232205,2.8818949319,-2.1099270436\H,0,6.1517552181,2.899
2498678,1.6618303441\H,0,5.5552855008,4.0330177692,-0.4747889717\C,0,-
4.1786505216,0.4652892383,0.3010839089\C,0,-5.0087932439,1.1245360431,
1.2211817559\C,0,-3.8454387422,1.112371416,-0.8969937182\C,0,-5.506902
589,2.4009801582,0.9438605333\H,0,-5.2768133524,0.6332941493,2.1561645
494\C,0,-4.3379995648,2.3917098537,-1.1727131283\H,0,-3.1967315218,0.6
21517594,-1.6190801276\C,0,-5.1715798721,3.0381680974,-0.2549324486\H,
0,-6.153601469,2.8965561715,1.6638529239\H,0,-4.0727530154,2.881544391
8,-2.1066359987\H,0,-5.5566513371,4.0312341674,-0.4721537887\C,0,0.001
1914547,1.8128746371,2.803555262\H,0,0.0008195766,2.7534610921,2.24361
43847\H,0,-0.8879279848,1.7592688325,3.4348311821\H,0,0.8908557522,1.7
595318924,3.4340839341\\Version=AM64L-G03RevD.01\State=1-A\HF=-1142.25
628\MP2=-1146.403135\RMSD=9.836e-09\Thermal=0.PG=C01 [X(C24H27N4)]\@

4n_Me⁺_8

1\1\GINC-NAUTILUS\SP\RMP2-FC\6-31+G(2d,p)\C24H27N4(1+)\RAMAN\14-Oct-20
11\0\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read g
eom=check\sp of sdmap9.mc mp2-5 on 2p 900 MB\1,1\N,0,0.2573567454,1.
6882670504,0.3093020633\N,0,-0.8163542793,-2.0400330189,-1.1484637574\
C,0,1.6476007222,1.9878728316,0.6461395414\C,0,2.3633511185,0.71504123
99,1.0884691943\C,0,0.878883667,-0.5870228853,-0.2736623297\C,0,0.4640
517835,-1.8278716067,-0.7525858122\C,0,-1.759130267,-1.0741445398,-1.0
415680694\C,0,-1.4471150051,0.1917955125,-0.5468050108\C,0,-2.10302820
27,2.3223741684,0.4149916493\C,0,-0.6709617799,2.806762419,0.177988810
7\C,0,-0.095646375,0.4574899665,-0.1530546029\H,0,3.4289395267,0.92343
33123,1.2045908639\H,0,-0.5859429447,3.2659898969,-0.8177705983\H,0,-0
.4036718387,3.5621762908,0.9258284618\H,0,-2.765180443,-1.3507459605,-
1.3257340781\H,0,1.1306703606,-2.6737014663,-0.8414155052\H,0,2.167111
4803,2.4298115915,-0.2162218052\H,0,1.6503840427,2.7235497553,1.460251
0707\H,0,1.9701648049,0.3742423331,2.0602628203\H,0,-2.229299188,2.058
8479209,1.4765685913\H,0,-2.8024401875,3.1321979326,0.1866511758\N,0,-
2.3917826655,1.1976566215,-0.4646581206\N,0,2.1977498847,-0.3049860578
,0.05419105\C,0,3.2148526379,-1.3634598702,-0.047997707\C,0,-3.7285800
813,1.0250746571,-1.0248114537\H,0,3.090179886,-2.1126679643,0.7528048
718\H,0,3.0485096626,-1.8746956252,-1.0048668084\C,0,4.6318929714,-0.8
204471819,-0.0336754414\C,0,5.5212258342,-1.1731722146,0.9899573907\C,
0,5.0746862979,0.0240984628,-1.0654629422\C,0,6.8359315662,-0.69337744
04,0.9841084916\H,0,5.1887238442,-1.8301879809,1.7920819833\C,0,6.3841
850449,0.5078796465,-1.0689239947\H,0,4.390769221,0.2986491867,-1.8669
275486\C,0,7.2680421827,0.1482352519,-0.0438391702\H,0,7.5183372773,-0
.9778897741,1.7811002343\H,0,6.7194382683,1.1571076063,-1.8741498209\H
,0,8.289371145,0.5206156828,-0.0504187151\H,0,-4.1808944693,2.02450207
69,-1.0607176557\H,0,-3.6258254976,0.7033512772,-2.0721252223\C,0,-4.6
6542626,0.0648658334,-0.2906147923\C,0,-5.7001242405,-0.5542243918,-1.
0095956119\C,0,-4.5474051458,-0.189140682,1.0828160459\C,0,-6.60762293
09,-1.3999437117,-0.3654306102\H,0,-5.8040505432,-0.366332578,-2.07783
84565\C,0,-5.4510891172,-1.0401082449,1.7271577064\H,0,-3.7466680762,0
.273454944,1.6554312033\C,0,-6.4846081937,-1.6453025596,1.0059320663\H
,0,-7.4074702989,-1.8675816683,-0.9344499051\H,0,-5.3488447705,-1.2269

674734,2.7935172199\H,0,-7.1887643841,-2.303627969,1.5083353176\C,0,-1
.2153162906,-3.3857732476,-1.5986268058\H,0,-1.519792956,-3.994566705,
-0.7410851851\H,0,-2.0476454122,-3.2966496771,-2.2994077604\H,0,-0.372
494372,-3.8586099235,-2.1071134664\\Version=AM64L-G03RevD.01\State=1-A
\HF=-1142.2572211\MP2=-1146.4027987\RMSD=3.754e-09\Thermal=0.\PG=C01 [X(C24H27N4)]\@

4n_Me⁺_9

1\1\GINC-NAUTILUS\SP\RMP2-FC\6-31+G(2d,p)\C24H27N4(1+)\RAMAN\14-Oct-20
11\0\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read g
eom=check\sp of sdmap13.mc mp2-5 on 2p 900 MB\1,1\C,0,1.1706462241,2
.4847656699,-0.1703580767\C,0,1.2289744557,1.09588687,-0.1218144618\C,
0,-0.0002373175,0.3657904407,0.0027696172\C,0,-1.2304462639,1.09649075
48,0.1132212648\C,0,-1.1737780303,2.4859036219,0.1371036137\N,0,-0.002
4571219,3.1524745463,-0.0255348723\N,0,0.0001422593,-0.9871151328,0.01
02902524\C,0,-1.2393218551,-1.7477875086,0.1734858317\C,0,-2.296138895
5,-0.9061267934,0.8799855188\C,0,2.2927944915,-0.9151962482,-0.8697255
139\C,0,1.2396393146,-1.7487730319,-0.1482937164\H,0,-2.0507084923,3.1
01957197,0.2785826921\H,0,2.047475137,3.0994738321,-0.3180913658\H,0,-
1.0154455122,-2.6408047748,0.7706330422\H,0,-1.6071711851,-2.075308845
2,-0.8087278844\H,0,1.0140290437,-2.6493559476,-0.7332428991\H,0,1.611
7799925,-2.0634936029,0.8364541366\H,0,-3.2579615796,-1.4209137145,0.8
304668562\H,0,3.2551720703,-1.4287166765,-0.8182089893\H,0,2.022845997
8,-0.7943504466,-1.9321004227\H,0,-2.0310143611,-0.7723787407,1.942045
0671\N,0,2.4185150038,0.3802119603,-0.198645831\N,0,-2.420013785,0.381
0530859,0.1930097345\C,0,-3.6856513602,1.1161334356,0.3490243448\H,0,-
3.6657714981,1.938869358,-0.3772079785\C,0,3.6830428633,1.1143560309,-
0.3675186059\H,0,3.6657490884,1.9442590861,0.3506092114\H,0,3.75613435
6,1.5527865501,-1.3782374171\C,0,4.9011506856,0.2544620136,-0.08627778
27\C,0,5.8395036622,-0.0066734107,-1.0936731273\C,0,5.1110015864,-0.27
21452597,1.1992153976\C,0,6.9737824845,-0.7804627217,-0.8231084778\H,0
,5.6878615292,0.4002605162,-2.0922278627\C,0,6.2395956057,-1.048388919
9,1.4685887122\H,0,4.3883689176,-0.069506771,1.9879049998\C,0,7.173958
4915,-1.3030718989,0.4569583976\H,0,7.6972838583,-0.9727786349,-1.6114
098304\H,0,6.3964156595,-1.4475426848,2.4677664206\H,0,8.0553383982,-1
.9032121303,0.6687565298\H,0,-3.7634692489,1.5644980468,1.3549961595\C
,0,-4.9021834421,0.2529476509,0.0709865467\C,0,-5.8461901724,0.0038016
13,1.076117569\C,0,-5.1052070601,-0.2881989836,-1.2095505212\C,0,-6.97
95058303,-0.7722966148,0.8081271958\H,0,-5.6997772126,0.421998691,2.07
08001522\C,0,-6.2328296268,-1.066771111,-1.4762760474\H,0,-4.378104193
9,-0.0949495225,-1.996486227\C,0,-7.1729743704,-1.3092877177,-0.467011
6145\H,0,-7.7074666805,-0.9551786794,1.5945688467\H,0,-6.3844068391,-1
.4771781589,-2.4717028873\H,0,-8.0536073864,-1.9112000071,-0.676869739
4\C,0,0.0063919021,4.62419465,0.038274785\H,0,0.1439483442,4.957565340
4,1.072290117\H,0,0.8204855068,5.0059009177,-0.5816456408\H,0,-0.94019
65384,5.0065973615,-0.3492640695\\Version=AM64L-G03RevD.01\State=1-A\H
F=-1142.2592223\MP2=-1146.4022527\RMSD=5.331e-09\Thermal=0.\PG=C01 [X(C24H27N4)]\@

4n_Me⁺_10

1\1\GINC-CALYPSO\SP\RMP2-FC\6-31+G(2d,p)\C24H27N4(1+)\RAMAN\14-Oct-201

1\0\#P MP2/6-31+G(2d,p) scf=(direct,tight) int=finegrid guess=read geom=check\sp of sdmap7.mc mp2-5 on 2p 900 MB\1,1\N,0,0.0000029024,-0.8208291701,-0.7040815805\N,0,-0.0000077854,3.1140544309,0.5936697002\C,0,1.2532620502,-1.5577153564,-0.8606091722\C,0,2.3926290029,-0.595876483,-1.1862143515\C,0,1.2354913625,1.1503226642,-0.0170984559\C,0,1.1820839758,2.4816990038,0.3868201347\C,0,-1.1820960658,2.4816921044,0.3868209604\C,0,-1.2354954477,1.1503160004,-0.0170979321\C,0,-2.3926249971,-0.5958889573,-1.1862121802\C,0,-1.2532525693,-1.5577218492,-0.8606084036\C,0,-0.0000002012,0.4619044825,-0.263453678\H,0,3.3401709317,-1.1380610859,-1.1593825741\H,0,-1.4839616987,-2.1183908314,0.0560015178\H,0,-1.1247765088,-2.2774427729,-1.6780594057\H,0,-2.0690759418,3.0756387828,0.5552997414\H,0,2.069059942,3.0756513878,0.5552979868\H,0,1.4839749215,-2.1183826709,0.0560008235\H,0,1.124789204,-2.2774372942,-1.6780597631\H,0,2.26172654,-0.1794237176,-2.1985034521\H,0,-2.2617252096,-0.1794355327,-2.198501338\H,0,-3.3401638064,-1.1380787568,-1.1593802015\N,0,-2.4278157081,0.4560300993,-0.1717898133\N,0,2.4278152899,0.4560421813,-0.1717918347\C,0,3.7034153318,1.1507676774,0.0635326444\C,0,-3.7034170246,1.1507536544,0.0635345939\H,0,3.9135998102,1.8773718341,-0.7405217576\H,0,-3.9136089561,1.8773478881,-0.7405268033\H,0,-3.5894216375,1.7170467792,0.996889241\C,0,-4.8731351232,0.1968675549,0.2177723432\C,0,-4.9079046147,-0.7103994846,1.2899162552\C,0,-5.9409775049,0.2244444357,-0.6890253586\C,0,-5.9922714511,-1.5753451975,1.4481654242\H,0,-4.0840196112,-0.734837717,2.0013698969\C,0,-7.031084267,-0.6383120294,-0.5278155094\H,0,-5.9252030017,0.9263997342,-1.5212915463\C,0,-7.0571029955,-1.5396822879,0.5392253167\H,0,-6.0126605621,-2.2707241982,2.2838199309\H,0,-7.8561525488,-0.6041876287,-1.2348851903\H,0,-7.9038281562,-2.209547675,0.6662931545\H,0,3.5894251984,1.7170487781,0.9968950625\C,0,4.8731364088,0.1968821262,0.217749772\C,0,5.94097266,0.2244734473,-0.6890547391\C,0,4.9079139393,-0.7104006966,1.2898800223\C,0,7.0310819916,-0.6382833444,-0.5278641687\H,0,5.9251915227,0.9264405228,-1.5213108693\C,0,5.9922833641,-1.5753466673,1.4481099709\H,0,4.084033255,-0.7348509499,2.0013382445\C,0,7.0571091546,-1.5396687021,0.5391637082\H,0,7.8561456694,-0.6041474452,-1.2349386699\H,0,6.0126788809,-2.270737804,2.2837542169\H,0,7.9038362853,-2.2095344495,0.6662165385\C,0,-0.0000134572,4.4960035951,1.1043666923\H,0,-0.8880496099,5.0151979836,0.7376969467\H,0,-0.0000401718,4.4935516038,2.1993957062\H,0,0.8880459986,5.0151886236,0.7377407721\\Version=AM64L-G03RevD.01\\State=1-A\\HF=-1142.2583513\\MP2=-1146.4023293\\RMSD=8.258e-10\\Thermal=0.\\PG=C01 [X(C24H27N4)]\\@

5a

5a_1

1\1\GINC-NAUTILUS\SP\RMP2-FC\6-31+G(2d,p)\C18H15P1\CHRISTOPH\15-Jun-20
10\0\#p MP2(FC)/6-31+g(2d,p) scf=tight\pph3sp_24\0,1\PC,1,4.669176
37\C,2,1.39889904,1,58.39835457\C,3,1.39711021,2,120.03404393,1,0.0731
2915,0\C,4,1.4078275,3,120.86573775,2,-0.90074517,0\C,5,1.40613305,4,1
18.52754336,3,1.01520813,0\C,2,1.39811597,1,61.29395672,5,-11.92393355
,0\H,2,1.08782689,1,178.46559567,5,-174.4705313,0\H,3,1.08791198,2,120
.13611998,1,179.40626729,0\H,4,1.08886424,3,119.6438903,2,178.83797575
,0\H,6,1.08715107,5,119.80867374,4,179.24351849,0\H,7,1.08811467,2,120
.05164401,1,-179.56503553,0\C,1,4.66759923,5,102.79294547,4,-161.16960
373,0\C,13,1.39899325,1,58.34285654,5,88.08101099,0\C,14,1.39699231,13
,120.01747891,1,0.16092582,0\C,15,1.40790244,14,120.84580135,13,-0.940
33665,0\C,16,1.40577377,15,118.58358895,14,1.08615587,0\C,13,1.3982075
7,1,61.36936355,16,-9.4420441,0\H,13,1.08783035,1,178.42795474,16,-174
.97501821,0\H,14,1.08790929,13,120.13808228,1,179.49477039,0\H,15,1.08
886588,14,119.66807053,13,178.83597793,0\H,17,1.08732569,16,119.797829
67,15,179.25960058,0\H,18,1.08810966,13,120.05975813,1,-179.64312327,0
\C,1,4.66856397,16,103.01046513,15,-161.85612879,0\C,24,1.39905748,1,5
8.34665971,16,87.0345034,0\C,25,1.39686331,24,120.01994036,1,-0.003546
64,0\C,26,1.40817789,25,120.88422236,24,-0.92025126,0\C,27,1.40580857,
26,118.52755415,25,0.94511419,0\C,24,1.39800658,1,61.33530279,16,-92.6
8200797,0\H,24,1.08781863,1,178.4050661,16,107.46009467,0\H,25,1.08792
536,24,120.14345756,1,179.30720453,0\H,26,1.08888881,25,119.61952007,2
4,178.8662804,0\H,28,1.08719633,27,119.86158696,26,179.37968377,0\H,29
,1.08813364,24,120.05777099,1,-179.49503835,0\Version=AM64L-G03RevD.0
1\State=1-A\HF=-1031.152198\MP2=-1033.8073038\RMSD=3.162e-09\Thermal=0
.PG=C01 [X(C18H15P1)]\@

5a_Me⁺

5a_Me⁺_1

1\1\GINC-CIPCLU04\SP\RMP2-FC\6-31+G(2d,p)\C19H18P1(1+)\C2175\18-Nov-20
10\0\#p MP2(FC)/6-31+G(2d,p) scf=tight\pph3mesp_14\1,1\PC,1,1.8263
4514\H,2,1.09468083,1,110.09519271\H,2,1.09467537,1,109.81417934,3,-12
0.05098936,0\H,2,1.09465709,1,109.81030113,4,-119.81389781,0\C,1,4.604

83596,2,108.65773713,5,58.54188599,0\C,6,1.3979893,1,60.31060999,2,-13
3.99138219,0\C,7,1.39750596,6,120.16250798,1,0.34638876,0\C,8,1.406607
78,7,119.66926518,6,0.00883656,0\C,9,1.40973574,8,120.05344476,7,-0.30
655184,0\C,10,1.39486017,9,119.75441021,8,0.3578895,0\H,6,1.08686592,1
,179.7564295,9,151.81750997,0\H,7,1.08657289,6,120.22442214,1,-179.817
13847,0\H,8,1.08655858,7,119.8478221,6,179.74968497,0\H,10,1.08762418,
9,120.95506978,8,-179.19938879,0\H,11,1.08659261,10,119.7100328,9,179.
80778784,0\C,1,4.60508301,9,110.1771647,8,-16.23460442,0\C,17,1.400660
14,1,59.91828951,9,-68.57193443,0\C,18,1.39469956,17,120.06814151,1,-0
.06315613,0\C,19,1.41016329,18,119.73318545,17,-0.05285141,0\C,20,1.40
624379,19,120.07581639,18,0.28034134,0\C,21,1.39769843,20,119.66412212
,19,-0.2870397,0\H,17,1.08686949,1,179.70569766,9,-82.24936965,0\H,18,
1.08658914,17,120.21835111,1,-179.97769289,0\H,19,1.08787278,18,119.35
747954,17,179.50157312,0\H,21,1.08646294,20,120.48649545,19,179.971730
27,0\H,22,1.08658631,21,119.61988035,20,-179.83927762,0\C,1,4.60462791
,9,110.73737951,8,106.31340037,0\C,28,1.3978858,1,60.26580244,9,-14.31
192615,0\C,29,1.39741046,28,120.16126529,1,0.33207762,0\C,30,1.4065610
8,29,119.68441993,28,0.01943062,0\C,31,1.41004,30,120.0450087,29,-0.20
170608,0\C,32,1.39492119,31,119.7431895,30,0.22272893,0\H,28,1.0868747
2,1,179.77256272,31,157.30357277,0\H,29,1.08656294,28,120.2270055,1,-1
79.81881523,0\H,30,1.08660953,29,119.81233638,28,179.7199043,0\H,32,1.
08764811,31,120.94611096,30,-179.33252035,0\H,33,1.08659108,32,119.709
93263,31,179.82997158,0\\Version=AM64L-G03RevD.01\\State=1-A\\HF=-1070.6
030109\\MP2=-1073.4019066\\RMSD=7.764e-09\\Thermal=0.PG=C01 [X(C19H18P1)
]\\@

5b

5b_1

1\\1\\GINC-CIPCLU03\\SP\\RMP2-FC\\6-31+G(2d,p)\\C21H21O3P1\\C2175\\31-Aug-2010
\\0\\#p MP2(FC)/6-31+G(2d,p) scf=tight\\k6sp_120_2\\0,1\\C\\C,1,1.4021246
1\\C,2,1.40082466,1,119.66808892\\C,3,1.40231074,2,121.61810054,1,-0.253
71352,0\\C,4,1.41126037,3,117.6869434,2,-0.43378246,0\\C,5,1.38997314,4,
121.44996817,3,1.02827823,0\\H,2,1.08569266,1,121.0702342,6,-179.507395
48,0\\H,3,1.08754067,2,118.69132191,1,-179.75792169,0\\H,5,1.08883717,4,
119.47997963,3,-178.75892046,0\\H,6,1.08679056,5,121.39243357,4,179.886
17727,0\\C,3,5.08272855,2,139.27730676,1,-153.40082248,0\\C,11,1.4062579
5,3,67.17765496,2,99.85728461,0\\C,12,1.3898264,11,120.03733118,3,37.24
927687,0\\C,13,1.41136986,12,121.45686691,11,-0.9505674,0\\C,14,1.402078
72,13,117.68493828,12,1.03225058,0\\C,15,1.40107178,14,121.61151792,13,
-0.42151298,0\\H,12,1.0868098,11,118.57314769,3,-143.54310135,0\\H,13,1.
08884778,12,119.05524328,11,178.85500769,0\\H,15,1.0874634,14,119.71572
915,13,179.15243658,0\\H,16,1.08561853,15,119.21922109,14,179.61949561,
0\\C,15,5.07977659,14,95.70785652,13,162.6817052,0\\C,21,1.40163394,15,6
3.53836613,14,86.15800199,0\\C,22,1.40114776,21,119.67208755,15,-38.111
6314,0\\C,23,1.40206075,22,121.62602305,21,-0.18907873,0\\C,24,1.4115812
9,23,117.67998448,22,-0.44793434,0\\C,25,1.38971702,24,121.43767235,23,
1.05697592,0\\H,22,1.08581914,21,121.10621754,15,141.90489215,0\\H,23,1.
08760064,22,118.62491107,21,-179.83062023,0\\H,25,1.08886823,24,119.479
10147,23,-178.69061441,0\\H,26,1.08679152,25,121.42612378,24,179.947481
92,0\\P,24,1.84836361,23,124.92151552,22,-178.85750239,0\\O,1,1.36153232
,2,124.76039238,3,179.97921769,0\\O,21,1.36169663,15,146.24095003,14,-1

60.14200797,0\O,11,1.36163606,3,146.51983715,2,-2.65092644,0\C,32,1.41
557051,1,118.18586516,2,-0.3990078,0\H,35,1.09267961,32,105.92511156,1
, -179.66458664,0\H,35,1.09937325,32,111.5695854,1,-60.84543701,0\H,35,
1.09951972,32,111.5928708,1,61.54174139,0\C,34,1.41552627,11,118.20938
895,3,-93.87805639,0\H,39,1.09269824,34,105.92971658,11,-179.67682022,
0\H,39,1.09938992,34,111.56734668,11,-60.86192476,0\H,39,1.09948689,34
,111.59487025,11,61.52601678,0\C,33,1.41576898,21,118.19059469,15,-96.
09357627,0\H,43,1.09271355,33,105.91857848,21,-178.14977791,0\H,43,1.0
9905628,33,111.60596744,21,-59.32399175,0\H,43,1.09961048,33,111.57715
186,21,63.11573092,0\\Version=AM64L-G03RevD.01\State=1-A\HF=-1372.8201
155\MP2=-1376.5394455\RMSD=8.929e-09\Thermal=0.\PG=C01 [X(C21H21O3P1)]
\\@

5b_2

1\1\GINC-CIPCLU04\SP\RMP2-FC\6-31+G(2d,p)\C21H21O3P1\C2175\30-Aug-2010
\0\#p MP2(FC)/6-31+G(2d,p) scf=tight\\k6sp_117_2\\0,1\C\C,1,1.4056196
9\C,2,1.39175846,1,120.25174153\C,3,1.40941403,2,121.17185103,1,0.2232
2263,0\C,4,1.40385944,3,117.72652983,2,0.53631345,0\C,5,1.39907098,4,1
21.86852366,3,-1.13159116,0\H,2,1.08690207,1,118.46146668,6,179.461760
09,0\H,3,1.0873511,2,119.18425876,1,179.76193899,0\H,5,1.08889465,4,11
9.42788262,3,178.75039047,0\H,6,1.08533075,5,119.42308155,4,-179.78077
438,0\C,4,5.44341009,3,107.96550615,2,-119.29330622,0\C,11,1.40609252,
4,76.77723918,3,-135.00987339,0\C,12,1.39008877,11,120.03359771,4,5.42
513672,0\C,13,1.41124015,12,121.45146892,11,0.87743463,0\C,14,1.402607
01,13,117.67431383,12,-1.06433897,0\C,15,1.40068316,14,121.62894427,13
,0.50716258,0\H,12,1.08672791,11,118.5669811,4,-173.87785201,0\H,13,1.
08877857,12,119.07271033,11,-178.97377774,0\H,15,1.08733211,14,119.696
0863,13,-179.16139819,0\H,16,1.08555039,15,119.27924132,14,-179.693450
01,0\C,3,5.0850445,2,139.7754453,1,151.30828526,0\C,21,1.40638713,3,66
.42044167,2,-98.00399306,0\C,22,1.38967979,21,120.05259073,3,-37.79110
147,0\C,23,1.41178269,22,121.44555413,21,1.00275102,0\C,24,1.40187152,
23,117.66631484,22,-1.19741297,0\C,25,1.40102028,24,121.62776418,23,0.
54175731,0\H,22,1.08671701,21,118.57782704,3,142.95278732,0\H,23,1.088
87104,22,119.02129572,21,-178.82424253,0\H,25,1.0872218,24,119.7132729
7,23,-179.16971724,0\H,26,1.08555101,25,119.24610659,24,-179.71020363,
0\P,14,1.84887445,13,117.54842938,12,-179.71693658,0\O,1,1.36164577,6,
124.73582994,5,179.54201409,0\O,21,1.36167457,3,146.09054374,2,3.45619
2,0\O,11,1.36163785,4,166.3343091,3,68.07431095,0\C,32,1.41571624,1,11
8.24459435,6,-0.27592979,0\H,35,1.09261449,32,105.9073506,1,179.987994
02,0\H,35,1.0992711,32,111.58680519,1,-61.22590257,0\H,35,1.09935872,3
2,111.60053223,1,61.20455485,0\C,34,1.41566901,11,118.19351831,4,-24.8
5427467,0\H,39,1.09262243,34,105.91490552,11,-179.96821469,0\H,39,1.09
940915,34,111.59419326,11,-61.16543658,0\H,39,1.09930658,34,111.570203
18,11,61.21087457,0\C,33,1.41555023,21,118.18035293,3,95.347683,0\H,43
,1.09931146,33,111.55762082,21,60.87347416,0\H,43,1.09261481,33,105.92
663693,21,179.7004731,0\H,43,1.09945359,33,111.5786241,21,-61.48307645
,0\\Version=AM64L-G03RevD.01\State=1-A\HF=-1372.8200915\MP2=-1376.5395
299\RMSD=3.810e-09\Thermal=0.\PG=C01 [X(C21H21O3P1)]\\@

5b_3

1\1\GINC-CIPCLU06\SP\RMP2-FC\6-31+G(2d,p)\C21H21O3P1\C2175\27-Aug-2010

\0\#p MP2(FC)/6-31+G(2d,p) scf=tight\k6sp_91\0,1\C\C,1,1.40607422\C
,2,1.38986147,1,120.03213172\C,3,1.4112848,2,121.44757519,1,-0.9416530
6,0\C,4,1.40234282,3,117.69323216,2,1.02117306,0\C,5,1.40086578,4,121.
61573097,3,-0.4035855,0\H,2,1.08679019,1,118.5652971,6,179.4347214,0\H
,3,1.08883062,2,119.07781963,1,178.88453306,0\H,5,1.08752718,4,119.671
37702,3,179.14322556,0\H,6,1.08569357,5,119.26702754,4,179.620809,0\C,
5,5.08420834,4,95.47025939,3,161.60833576,0\C,11,1.40190988,5,63.85560
058,4,86.36218343,0\C,12,1.40113983,11,119.68341331,5,-37.89828358,0\C
,13,1.4018459,12,121.61242291,11,-0.29118535,0\C,14,1.4116222,13,117.6
893204,12,-0.39237838,0\C,15,1.38974857,14,121.45255039,13,1.03138568,
0\H,12,1.08566916,11,121.08986445,5,142.18361311,0\H,13,1.08741206,12,
118.68340087,11,-179.86416216,0\H,15,1.08888691,14,119.4818652,13,-178
.73644629,0\H,16,1.0868139,15,121.39961595,14,179.89395954,0\C,13,5.07
318122,12,139.50294115,11,-155.74242084,0\C,21,1.40190261,13,64.692196
05,12,-116.9486229,0\C,22,1.40110991,21,119.68813456,13,-37.72368995,0
\C,23,1.4020561,22,121.61491404,21,-0.27952891,0\C,24,1.41159906,23,11
7.66897013,22,-0.45300678,0\C,25,1.38970635,24,121.46385446,23,1.09183
896,0\H,22,1.08570952,21,121.08152452,13,142.34645527,0\H,23,1.0875404
6,22,118.64499732,21,-179.90197882,0\H,25,1.08887911,24,119.49776074,2
3,-178.73432839,0\H,26,1.08681144,25,121.39191609,24,179.82764501,0\P,
4,1.84820041,3,117.45388211,2,179.48979161,0\O,1,1.36148235,6,124.7802
4681,5,-179.98827987,0\O,21,1.36168259,13,146.1682593,12,-1.59532217,0
\O,11,1.36168056,5,146.43327489,4,-159.46964295,0\C,32,1.41555442,1,11
8.19894383,6,-0.44195852,0\H,35,1.09267937,32,105.91799231,1,-179.7396
5344,0\H,35,1.09937712,32,111.56627483,1,-60.926712,0\H,35,1.09951304,
32,111.57985397,1,61.46652895,0\C,34,1.41560353,11,118.1750349,5,-95.1
9101383,0\H,39,1.09267553,34,105.91114234,11,-179.35704985,0\H,39,1.09
935566,34,111.55882517,11,-60.54474124,0\H,39,1.09950528,34,111.612837
17,11,61.85690723,0\C,33,1.4155592,21,118.18627778,13,-96.33817783,0\H
,43,1.09267482,33,105.92213365,21,-179.54833612,0\H,43,1.09934572,33,1
11.56245658,21,-60.72243918,0\H,43,1.09948332,33,111.59332295,21,61.66
527619,0\Version=AM64L-G03RevD.01\State=1-A\HF=-1372.8201353\MP2=-137
6.539468\RMSD=6.271e-09\Thermal=0.\PG=C01 [X(C21H21O3P1)]\@

5b_4

1\1\GINC-CIPCLU10\SP\RMP2-FC\6-31+G(2d,p)\C21H21O3P1\C2175\31-Aug-2010
\0\#p MP2(FC)/6-31+G(2d,p) scf=tight\k6sp_125_2\0,1\C\C,1,1.4020718
5\C,2,1.40098058,1,119.69899375\C,3,1.40216354,2,121.61745968,1,-0.281
64172,0\C,4,1.4114494,3,117.65396975,2,-0.40268001,0\C,5,1.38990422,4,
121.48155936,3,1.04392877,0\H,2,1.08566431,1,121.07069294,6,-179.60083
141,0\H,3,1.08739896,2,118.61565391,1,-179.84029203,0\H,5,1.08888852,4,
119.48678424,3,-178.77538464,0\H,6,1.08679155,5,121.38195482,4,179.84
841276,0\C,3,5.09188105,2,140.0095292,1,-156.79636534,0\C,11,1.4059260
3,3,60.02855779,2,-110.53739183,0\C,12,1.39139381,11,120.23488595,3,-3
8.99303123,0\C,13,1.40993608,12,121.18548952,11,-0.07450001,0\C,14,1.4
0363404,13,117.71347284,12,-0.5625985,0\C,15,1.39921997,14,121.8729128
5,13,1.00733265,0\H,12,1.0869895,11,118.47570402,3,141.2432441,0\H,13,
1.08755094,12,119.1425974,11,-179.52593128,0\H,15,1.08885948,14,119.38
873757,13,-178.74198113,0\H,16,1.08544564,15,119.44281007,14,179.92553
822,0\C,13,5.1055892,12,138.73630482,11,-144.75638001,0\C,21,1.4067375
6,13,66.36795522,12,95.03469928,0\C,22,1.38901669,21,120.05826802,13,3

7.58564018,0\C,23,1.41206678,22,121.45839774,21,-0.9771182,0\C,24,1.40163984,23,117.66608966,22,1.1623893,0\C,21,1.4015934,13,64.20237973,12,-120.99830661,0\H,22,1.08681351,21,118.5088203,13,-143.13894604,0\H,23,1.08889461,22,119.03993129,21,178.91482142,0\H,25,1.08750949,24,119.74712365,23,179.11261672,0\H,26,1.08556818,21,121.112423,13,142.36405517,0\O,14,1.84803927,13,124.80640612,12,-179.19546628,0\O,1,1.36168628,2,124.7921132,3,179.97676252,0\O,21,1.36155988,13,146.28857459,12,-6.27436264,0\O,11,1.36131289,3,145.46657259,2,-17.95199313,0\C,32,1.41564693,1,118.20804825,2,-0.39510573,0\H,35,1.09267635,32,105.91945266,1,-179.67568421,0\H,35,1.09938083,32,111.56239101,1,-60.86226488,0\H,35,1.09946382,32,111.595835,1,61.52528577,0\C,34,1.41577676,11,118.2119742,3,106.88693348,0\H,39,1.09265958,34,105.91541362,11,179.96727139,0\H,39,1.09940129,34,111.59188348,11,-61.2345118,0\H,39,1.09933777,34,111.56425218,11,61.17908741,0\C,33,1.41538662,21,118.17405911,13,-95.49073011,0\H,43,1.0926195,33,105.94417753,21,179.89221743,0\H,43,1.09951835,33,111.61531523,21,61.13686749,0\H,43,1.09964304,33,111.51493371,21,-61.17423501,0\Version=AM64L-G03RevD.01\State=1-A\HF=-1372.8201763\MP2=-1376.5393596\RMSD=8.389e-09\Thermal=0.\PG=C01 [X(C21H21O3P1)]\@

5b_5

1\1\GINC-CIPCLU05\SP\RMP2-FC\6-31+G(2d,p)\C21H21O3P1\C2175\27-Aug-2010
\0\#p MP2(FC)/6-31+G(2d,p) scf=tight\k6sp_15\0,1\C\C,1,1.40269926\C,2,1.39910693,1,119.42797997\C,3,1.40382367,2,121.88564208,1,-0.89804555,0\C,4,1.40966276,3,117.67991151,2,1.08498974,0\C,5,1.39160623,4,121.20253025,3,-0.55213605,0\H,2,1.08554896,1,121.16459852,6,179.42265045,0\H,3,1.08893971,2,118.69598823,1,178.90499688,0\H,5,1.08744238,4,119.71975447,3,178.96309285,0\H,6,1.08698217,5,121.26587673,4,179.73116812,0\C,5,5.09646297,4,94.78803403,3,160.02969643,0\C,11,1.40552253,5,61.46278088,4,90.39639777,0\C,12,1.39172145,11,120.26730067,5,-38.78824507,0\C,13,1.40973229,12,121.19618095,11,-0.14948692,0\C,14,1.40380615,13,117.67145322,12,-0.61139431,0\C,15,1.39893574,14,121.89052144,13,1.14969361,0\H,12,1.08697674,11,118.49086919,5,141.30699397,0\H,13,1.08753127,12,119.04976339,11,-179.67794437,0\H,15,1.08895655,14,119.4472607,13,-178.69553513,0\H,16,1.08547854,15,119.39151991,14,179.78193575,0\C,13,5.08602891,12,139.672141,11,-151.18250678,0\C,21,1.40609206,13,66.7129847,12,98.33954192,0\C,22,1.38984762,21,120.02927592,13,37.60889906,0\C,23,1.4114982,22,121.48957648,21,-0.91470352,0\C,24,1.40221213,23,117.64516304,22,1.11644433,0\C,25,1.40102678,24,121.61228194,23,-0.54760145,0\H,22,1.08679603,21,118.59230088,13,-143.07489036,0\H,23,1.08890381,22,119.00357022,21,178.94581748,0\H,25,1.08747992,24,119.8223952,23,179.06619757,0\H,26,1.08572198,25,119.22644533,24,179.80823461,0\O,1,1.84841827,3,117.39970501,2,179.85465636,0\O,1,1.36159123,2,124.71140193,3,-179.46132264,0\O,21,1.3616866,13,146.21653444,12,-3.59240137,0\O,11,1.36157755,5,145.46236384,4,-174.86113335,0\C,32,1.41563399,1,118.1743393,2,0.07599855,0\H,35,1.09268118,32,105.92590235,1,179.9486192,0\H,35,1.09935174,32,111.57058783,1,61.15116322,0\H,35,1.09938742,32,111.58846346,1,-61.25406892,0\C,34,1.41565306,11,118.16509742,5,103.71473293,0\H,39,1.09265653,34,105.93539693,11,-179.7294289,0\H,39,1.09937519,34,111.55315945,11,-60.9142939,0\H,39,1.09935238,34,111.5582537,11,61.46625213,0\C,33,1.41554736,21,118.14453368,13,-94.27135087,0\H,43,1.09268761,33,105.93023824,21,179.96259337,0\H,43,1.09940263,33,11

1.56492226,21,-61.21766439,0\H,43,1.09942362,33,111.57370154,21,61.153
07791,0\\Version=AM64L-G03RevD.01\State=1-A\HF=-1372.8201528\MP2=-1376
.5393482\RMSD=7.077e-09\Thermal=0.\PG=C01 [X(C21H21O3P1)]\\@

5b_6

1\1\GINC-CIPCLU08\SP\RMP2-FC\6-31+G(2d,p)\C21H21O3P1\C2175\26-Aug-2010
\0\\#p MP2(FC)/6-31+G(2d,p) scf=tight\\k6sp_111\\0,1\C\C,1,1.40215186\
C,2,1.40082878,1,119.68422425\C,3,1.40232199,2,121.62104048,1,0.164303
6,0\C,4,1.41117922,3,117.6662746,2,0.54865225,0\C,5,1.3900938,4,121.46
966983,3,-1.0952587,0\H,2,1.0855381,1,121.07521523,6,179.51603184,0\H,
3,1.08737934,2,118.65421251,1,179.80961461,0\H,5,1.08878147,4,119.5062
3431,3,178.84678521,0\H,6,1.0866705,5,121.34854276,4,-179.79926353,0\C
,4,5.45381121,3,109.58656935,2,-119.82932806,0\C,11,1.40330191,4,76.78
639006,3,-134.16476645,0\C,12,1.39842126,11,119.429238,4,5.17599846,0\
C,13,1.40461687,12,121.87721011,11,0.92125313,0\C,14,1.40894767,13,117
.69314114,12,-1.22449888,0\C,15,1.39234771,14,121.18351598,13,0.638846
74,0\H,12,1.08533182,11,121.09567045,4,-174.05090836,0\H,13,1.08887992
,12,118.72394255,11,-178.84974623,0\H,15,1.0872767,14,119.72224336,13,
-178.86500255,0\H,16,1.08688659,15,121.21704704,14,-179.63716815,0\C,3
,5.08379817,2,139.26289447,1,153.32131316,0\C,21,1.40237857,3,61.99123
071,2,114.28676968,0\C,22,1.40060359,21,119.67570047,3,38.44278096,0\C
,23,1.40268464,22,121.6166838,21,0.17573322,0\C,24,1.41075418,23,117.6
7543445,22,0.48089207,0\C,25,1.39038987,24,121.4684306,23,-1.02600805,
0\H,22,1.08558524,21,121.06095167,3,-141.65248001,0\H,23,1.08741532,22
,118.62692554,21,179.90166764,0\H,25,1.08875541,24,119.49273544,23,178
.81812597,0\H,26,1.08668443,25,121.35179624,24,-179.84184161,0\P,14,1.
8488475,13,117.22721319,12,179.50187527,0\O,1,1.36166402,2,124.7514712
5,3,-179.94905846,0\O,21,1.36180344,3,146.76539212,2,2.81329025,0\O,11
,1.3617484,4,157.93714196,3,58.09453194,0\C,32,1.4152876,1,118.2025213
3,2,0.19798362,0\H,35,1.09263648,32,105.92624343,1,179.83931702,0\H,35
,1.09946432,32,111.61133178,1,-61.36304572,0\H,35,1.09937081,32,111.59
206239,1,61.03617835,0\C,34,1.41537564,11,118.24741678,4,165.13153075,
0\H,39,1.09264281,34,105.92320707,11,179.72901084,0\H,39,1.09935227,34
,111.59416465,11,-61.488893,0\H,39,1.09941019,34,111.61951038,11,60.93
371907,0\C,33,1.41525049,21,118.21765439,3,91.08024026,0\H,43,1.092652
47,33,105.93047936,21,179.5337627,0\H,43,1.09947948,33,111.6227339,21,
-61.67172881,0\H,43,1.09937011,33,111.59806867,21,60.72465857,0\\Versi
on=AM64L-G03RevD.01\State=1-A\HF=-1372.8200478\MP2=-1376.5393812\RMSD=
3.360e-09\Thermal=0.\PG=C01 [X(C21H21O3P1)]\\@

5b_7

1\1\GINC-CIPCLU08\SP\RMP2-FC\6-31+G(2d,p)\C21H21O3P1\C2175\31-Aug-2010
\0\\#p MP2(FC)/6-31+G(2d,p) scf=tight\\k6sp_119_2\\0,1\C\C,1,1.4054904
7\C,2,1.39178442,1,120.2888883\C,3,1.40947977,2,121.18553154,1,0.16493
51,0\C,4,1.40417617,3,117.67065356,2,0.62596924,0\C,5,1.399164,4,121.8
951557,3,-1.19951901,0\H,2,1.08697071,1,118.48571001,6,179.49619252,0\
H,3,1.08751192,2,119.04071485,1,179.66928014,0\H,5,1.08896415,4,119.44
808403,3,178.64041457,0\H,6,1.08545779,5,119.41520122,4,-179.79545345,
0\C,4,5.45672345,3,110.15500988,2,-119.1230699,0\C,11,1.40211033,4,76.
47977146,3,-136.17037347,0\C,12,1.39951504,11,119.4306293,4,6.09607827
,0\C,13,1.40303881,12,121.96448033,11,0.89439113,0\C,14,1.41081106,13,

117.62889085,12,-1.13948595,0\C,15,1.3910991,14,121.17101941,13,0.6555
9295,0\H,12,1.08550965,11,121.21603229,4,-173.31228697,0\H,13,1.089025
38,12,118.58706517,11,-178.99678857,0\H,15,1.08752996,14,119.77173352,
13,-178.96170685,0\H,16,1.08699776,15,121.26900041,14,-179.86644309,0\
C,3,5.07705755,2,139.9142872,1,153.59419563,0\C,21,1.40257252,3,69.048
86877,2,-102.20099422,0\C,22,1.39907848,21,119.44376495,3,-36.73078172
,0\C,23,1.40379922,22,121.89889038,21,0.86364998,0\C,24,1.40970311,23,
117.64926823,22,-1.13688194,0\C,25,1.39162195,24,121.21477874,23,0.637
3066,0\H,22,1.08560551,21,121.15500531,3,143.89529009,0\H,23,1.0889567
3,22,118.66008096,21,-179.02358972,0\H,25,1.08741588,24,119.78736447,2
3,-178.97505946,0\H,26,1.08695779,25,121.23574549,24,-179.85167613,0\P
,4,1.8483469,3,124.99403589,2,179.07121954,0\O,1,1.36160864,6,124.7632
2875,5,179.37258648,0\O,21,1.36149492,3,145.26257228,2,18.99823529,0\O
,11,1.36057754,4,157.97378617,3,58.35884459,0\C,32,1.41563893,1,118.20
761966,6,0.19631929,0\H,35,1.09269823,32,105.9183015,1,179.90831828,0\
H,35,1.09941871,32,111.57685089,1,-61.3076799,0\H,35,1.09936608,32,111
.58737199,1,61.10856869,0\C,34,1.41563171,11,118.19248626,4,163.724186
7,0\H,39,1.09259418,34,105.95282462,11,179.31118272,0\H,39,1.09947757,
34,111.5682843,11,-61.98329547,0\H,39,1.09941113,34,111.60361623,11,60
.37735722,0\C,33,1.41559171,21,118.15137291,3,-103.22314785,0\H,43,1.0
9268537,33,105.92877787,21,179.66407946,0\H,43,1.09934207,33,111.57173
052,21,-61.53794186,0\H,43,1.09937714,33,111.5556209,21,60.85678573,0\
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\RMSD=9.390e-09\Thermal=0.\PG=C01 [X(C21H21O3P1)]\#@

5b_8

1\1\GINC-CIPCLU10\SP\RMP2-FC\6-31+G(2d,p)\C21H21O3P1\C2175\26-Aug-2010
\0\#p MP2(FC)/6-31+G(2d,p) scf=tight\k6sp_121\0,1\C\C,1,1.40271688\
C,2,1.40105796,1,119.73139932\C,3,1.40217739,2,121.55707824,1,-0.19506
113,0\C,4,1.41114307,3,117.69751843,2,-0.48541016,0\C,5,1.38970916,4,1
21.47330332,3,1.0438404,0\H,2,1.08541238,1,121.04399201,6,-179.6393725
3,0\H,3,1.08732645,2,118.65723082,1,-179.80222579,0\H,5,1.08877125,4,1
19.4960288,3,-178.81318424,0\H,6,1.0869582,5,121.34443759,4,179.801477
11,0\C,3,5.0797878,2,140.17367416,1,-159.62931898,0\C,11,1.4024989,3,6
9.34473637,2,105.1656681,0\C,12,1.39954168,11,119.45167715,3,36.391024
22,0\C,13,1.4036352,12,121.84402897,11,-0.84124875,0\C,14,1.40936819,1
3,117.7250913,12,1.08261425,0\C,15,1.39153855,14,121.17590111,13,-0.55
000402,0\H,12,1.08572956,11,121.14248425,3,-144.44196175,0\H,13,1.0890
2906,12,118.73720847,11,178.78711372,0\H,15,1.08761847,14,119.75284669
,13,178.77311008,0\H,16,1.08726024,15,121.2352592,14,179.64475086,0\C,
15,5.09981992,14,94.41446242,13,158.16193137,0\C,21,1.40327607,15,69.8
5397559,14,-51.43781331,0\C,22,1.39964306,21,119.47976088,15,36.213303
13,0\C,23,1.40249165,22,121.88187364,21,-0.8465632,0\C,24,1.4096178,23
,117.66829464,22,1.25525524,0\C,25,1.39087129,24,121.25735667,23,-0.64
521477,0\H,22,1.08498845,21,121.20828391,15,-144.7980698,0\H,23,1.0890
9196,22,118.70899673,21,178.94382467,0\H,25,1.08757077,24,119.5952974,
23,178.8652072,0\H,26,1.08730828,25,121.22196377,24,179.79898986,0\P,1
4,1.84760536,13,117.3822394,12,179.80086977,0\O,1,1.36298081,2,124.749
22964,3,-179.93891173,0\O,21,1.36072624,15,145.3249373,14,-174.0730268
2,0\O,11,1.3614309,3,145.48665089,2,-16.57589851,0\C,32,1.41581455,1,1
18.23990318,2,-0.50641467,0\H,35,1.09292775,32,105.91074084,1,-179.212

62739,0\H,35,1.09955538,32,111.58492949,1,-60.40676173,0\H,35,1.099413
53,32,111.65361329,1,62.07761555,0\C,34,1.41573538,11,118.14537494,3,1
04.66916955,0\H,39,1.09287007,34,105.89832738,11,179.73867778,0\H,39,1
.09945903,34,111.69056689,11,-61.47965515,0\H,39,1.09955702,34,111.516
5059,11,60.99890437,0\C,33,1.41605773,21,118.47587642,15,103.08662509,
0\H,43,1.09286706,33,105.99853303,21,-174.54021437,0\H,43,1.09974057,3
3,111.27759353,21,66.69607838,0\H,43,1.09887947,33,111.7736467,21,-55.
68865054,0\Version=AM64L-G03RevD.01\State=1-A\HF=-1372.8200416\MP2=-1
376.5391863\RMSD=3.473e-09\Thermal=0.\PG=C01 [X(C21H21O3P1)]\@

5b_9

1\1\GINC-CIPCLU03\SP\RMP2-FC\6-31+G(2d,p)\C21H21O3P1\C2175\27-Aug-2010
\0\#p MP2(FC)/6-31+G(2d,p) scf=tight\k6sp_17\0,1\C\C,1,1.4025105\C,
2,1.39920342,1,119.43141152\C,3,1.40372208,2,121.88356663,1,-0.8670376
3,0\C,4,1.40984445,3,117.68913425,2,1.07810452,0\C,5,1.39159813,4,121.
17994738,3,-0.56728163,0\H,2,1.08543396,1,121.16354149,6,179.3896337,0
\H,3,1.08886422,2,118.70462,1,178.92111896,0\H,5,1.08727292,4,119.7534
4446,3,178.87482053,0\H,6,1.08697192,5,121.24458967,4,179.76460038,0\C
,5,5.09374397,4,94.83178066,3,159.89248311,0\C,11,1.40254931,5,68.4160
4177,4,-54.4513135,0\C,12,1.39899143,11,119.46477464,5,36.895946,0\C,1
3,1.40390705,12,121.87768017,11,-0.84144316,0\C,14,1.40954657,13,117.6
6616421,12,1.21783611,0\C,15,1.39201979,14,121.19336176,13,-0.74791758
,0\H,12,1.08553236,11,121.16261276,5,-143.69492651,0\H,13,1.08886707,1
2,118.67642975,11,179.07142572,0\H,15,1.0873625,14,119.78339725,13,178
.82940916,0\H,16,1.08696568,15,121.21376764,14,179.87839065,0\C,15,5.0
7806135,14,95.51926836,13,162.17770372,0\C,21,1.40292307,15,68.1094940
7,14,-56.18565776,0\C,22,1.39893561,21,119.44302722,15,37.16633669,0\C
,23,1.40389295,22,121.90336399,21,-0.95839006,0\C,24,1.40928378,23,117
.66649241,22,1.18875788,0\C,25,1.3920517,24,121.18606268,23,-0.6217892
7,0\H,22,1.08542075,21,121.19671273,15,-143.55116671,0\H,23,1.08893262
,22,118.64444308,21,178.99059806,0\H,25,1.08730798,24,119.78770813,23,
179.00496946,0\H,26,1.08699842,25,121.19018732,24,179.80352979,0\P,4,1
.84903549,3,117.3953648,2,179.84257301,0\O,1,1.36148253,2,124.73993362
,3,-179.41527058,0\O,21,1.36179819,15,145.54023317,14,-176.20241393,0\
O,11,1.36180141,5,145.39333283,4,-174.88033584,0\C,32,1.41560227,1,118
.21970223,2,-0.53118696,0\H,35,1.09275636,32,105.9303371,1,-179.646911
43,0\H,35,1.09928902,32,111.60424942,1,-60.85809144,0\H,35,1.09940206,
32,111.56695957,1,61.58317321,0\C,34,1.41545638,11,118.25463845,5,102.
33610264,0\H,39,1.09277728,34,105.93824411,11,-179.70222795,0\H,39,1.0
9932105,34,111.58513575,11,-60.91954085,0\H,39,1.09933561,34,111.58693
613,11,61.52037775,0\C,33,1.41549227,21,118.24355346,15,102.00385917,0
\H,43,1.09934946,33,111.59599153,21,61.09435601,0\H,43,1.09273824,33,1
05.9304538,21,179.87452746,0\H,43,1.0993898,33,111.58079305,21,-61.349
25329,0\Version=AM64L-G03RevD.01\State=1-A\HF=-1372.8201376\MP2=-1376
.5391858\RMSD=9.286e-09\Thermal=0.\PG=C01 [X(C21H21O3P1)]\@

5b_10

1\1\GINC-CIPCLU07\SP\RMP2-FC\6-31+G(2d,p)\C21H21O3P1\C2175\27-Aug-2010
\0\#p MP2(FC)/6-31+G(2d,p) scf=tight\k6sp_4\0,1\C\C,1,1.4055382\C,2
,1.39164748,1,120.27804062\C,3,1.40974218,2,121.2106295,1,0.14014433,0
\C,4,1.40402032,3,117.63654042,2,0.60355421,0\C,5,1.39883552,4,121.918

01932,3,-1.12824109,0\H,2,1.08691735,1,118.475205,6,179.52339936,0\H,3,1.08736371,2,119.02747183,1,179.66627857,0\H,5,1.08893414,4,119.43533241,3,178.68533457,0\H,6,1.08522343,5,119.40759975,4,-179.79103163,0\C,4,5.45182517,3,108.993163,2,-119.72103972,0\C,11,1.40568822,4,43.46689283,3,34.61496618,0\C,12,1.39152526,11,120.25264492,4,-9.48920342,0\C,13,1.41012348,12,121.20749305,11,0.09660705,0\C,14,1.40386261,13,117.64005261,12,0.68614184,0\C,15,1.398989,14,121.92108721,13,-1.18200174,0\H,12,1.08689191,11,118.48940215,4,170.42687714,0\H,13,1.08751089,12,118.98226696,11,179.58850232,0\H,15,1.08892937,14,119.44054703,13,178.65024431,0\H,16,1.08555164,15,119.45569062,14,-179.80713653,0\C,3,5.08539067,2,139.6346237,1,151.01810798,0\C,21,1.40262546,3,67.77841244,2,-99.24279482,0\C,22,1.39894315,21,119.41862538,3,-37.30738313,0\C,23,1.40414066,22,121.92341957,21,0.93748844,0\C,24,1.40967965,23,117.6406682,22,-1.16281256,0\C,25,1.39167109,24,121.20043414,23,0.5903389,0\H,22,1.08551638,21,121.12550308,3,143.37144161,0\H,23,1.08898023,22,118.646798,21,-178.9926763,0\H,25,1.0873619,24,119.80527293,23,-179.0355812,0\H,26,1.08687994,25,121.24640525,24,-179.80537662,0\P,4,1.8483144,3,125.01815748,2,179.03856226,0\O,1,1.36187538,6,124.73554833,5,179.47871952,0\O,21,1.36138241,3,145.54953307,2,20.2079833,0\O,11,1.36139696,4,157.93794572,3,57.68985288,0\C,32,1.41583607,1,118.26937173,6,0.21943852,0\H,35,1.09261599,32,105.93775338,1,-179.88262229,0\H,35,1.09933945,32,111.59267547,1,-61.07911814,0\H,35,1.09934465,32,111.56010081,1,61.30761923,0\C,34,1.41567479,11,118.11455481,4,162.63483772,0\H,39,1.09938755,34,111.54486106,11,60.7354285,0\H,39,1.0993568,34,111.54106652,11,-61.57358175,0\H,39,1.0926059,34,105.95853125,11,179.59189298,0\C,33,1.41567677,21,118.14355522,3,-101.0719461,0\H,43,1.09939745,33,111.55734115,21,61.21349727,0\H,43,1.09935267,33,111.59140366,21,-61.1436779,0\H,43,1.09260689,33,105.93979186,21,-179.9635042,0\\Version=AM64L-G03RevD.01\\State=1-A\\HF=-1372.82012\\MP2=-1376.5391731\\RMSD=9.344e-09\\Thermal=0.\\PG=C01 [X(C21H21O3P1)]\\@

5b-Me⁺

5b-Me⁺_1

1\1\GINC-CIPCLU02\SP\RMP2-FC\6-31+G(2d,p)\C22H24O3P1(1+)\C2175\04-Sep-2010\0\#p MP2(FC)/6-31+G(2d,p) scf=tight\\k6mesp_62_2\\1,1\C\C,1,1.41283468\C,2,1.38454273,1,120.29909295\C,3,1.41566481,2,120.50888204,1,0.03947431,0\C,4,1.40533313,3,118.88312658,2,0.34973426,0\C,5,1.39526632,4,120.9374786,3,-0.39938427,0\H,2,1.08592443,1,118.42884261,6,179.87952743,0\H,3,1.08770866,2,118.69056278,1,179.60436364,0\H,5,1.0868945,4,120.1735968,3,179.83794537,0\H,6,1.08475725,5,119.23764062,4,-179.95418022,0\C,4,5.5215872,3,95.50177828,2,131.23063908,0\C,11,1.40670165,4,42.75266875,3,-69.39680351,0\C,12,1.39550201,11,119.73542153,4,-4.91559211,0\C,13,1.40519562,12,120.93977889,11,0.0348779,0\C,14,1.41582042,13,118.90200163,12,-0.15818256,0\C,15,1.38442645,14,120.48236623,13,0.10238725,0\H,12,1.0845991,11,121.03414512,4,175.01748308,0\H,13,1.08671903,12,118.87620526,11,179.90845786,0\H,15,1.08790042,14,120.77691682,13,-179.35921987,0\H,16,1.08593863,15,121.24115178,14,179.93545563,0\C,5,5.20653062,4,94.81785545,3,-168.40130705,0\C,21,1.41300265,5,57.55932548,4,75.14773318,0\C,22,1.38432027,21,120.30190696,5,-38.25277045,0\C,23,1.41568341,22,120.49279386,21,-0.02383747,0\C,24,1.40521314,23,118.91528195,22,0.30505798,0\C,25,1.39544741,24,120.9171948,23,-0.33

494287,0\H,22,1.08596205,21,118.43613527,5,141.92504226,0\H,23,1.08780
17,22,118.7671311,21,179.58938225,0\H,25,1.08674851,24,120.16886293,23
, -179.96159756,0\H,26,1.08450394,25,119.22603289,24, -179.70642717,0\O,
1,1.34140539,6,124.92643756,5, -179.93270802,0\O,21,1.34164282,5,146.13
478969,4,163.21200116,0\O,11,1.34130935,4,167.16481216,3, -50.88477484,
0\C,31,1.42672705,1,119.2599967,6,1.83020977,0\H,34,1.09084915,31,105.
53709302,1,177.97281696,0\H,34,1.09712631,31,111.05734825,1,59.3788329
9,0\H,34,1.09735725,31,111.03393622,1, -63.35531511,0\C,33,1.42665913,1
1,119.28179618,4, -14.95490903,0\H,38,1.09721982,33,111.04317038,11,61.
08664533,0\H,38,1.09085035,33,105.52323475,11,179.71870175,0\H,38,1.09
732855,33,111.04377978,11, -61.66275598,0\C,32,1.42670938,21,119.303125
2,5,111.21841691,0\H,42,1.09722951,32,111.03517726,21,61.18460073,0\H,
42,1.09085371,32,105.52105949,21,179.81005588,0\H,42,1.09727579,32,111
.05214527,21, -61.56113357,0\P,4,1.80012588,3,120.29948407,2,179.112202
85,0\C,46,1.82871655,4,108.2583636,3,47.58600026,0\H,47,1.09483212,46,
109.85313788,4,179.45975239,0\H,47,1.09468876,46,109.97230518,4, -60.69
683651,0\H,47,1.09476103,46,110.03346995,4,59.44239353,0\Version=AM64
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09\Thermal=0.\PG=C01 [X(C22H24O3P1)]\@

5b-Me⁺_2

1\1\GINC-CIPCLU10\SP\RMP2-FC\6-31+G(2d,p)\C22H24O3P1(1+)\C2175\02-Sep-
2010\0\#p MP2(FC)/6-31+G(2d,p) scf=tight\k6mesp_43\1,1\C\C,1,1.4068
9461\C,2,1.39528116,1,119.72783207\C,3,1.40527543,2,120.94465964,1,0.0
878775,0\C,4,1.41565266,3,118.90232547,2, -0.24775561,0\C,5,1.38433408,
4,120.49045235,3,0.17449074,0\H,2,1.08451929,1,121.03177272,6,179.9553
6744,0\H,3,1.08684075,2,118.92358493,1,179.75650999,0\H,5,1.08779809,4
,120.75802322,3, -179.40710727,0\H,6,1.08595482,5,121.26672493,4,179.81
896614,0\C,4,5.52247096,3,122.49693142,2, -118.34356904,0\C,11,1.406763
7,4,42.80290733,3,59.62402211,0\C,12,1.39536173,11,119.75270508,4, -5.0
7979172,0\C,13,1.40508109,12,120.92043894,11,0.06637202,0\C,14,1.41583
04,13,118.90795376,12, -0.2577145,0\C,15,1.38431924,14,120.5045242,13,0
.18720138,0\H,12,1.08459308,11,121.0093546,4,174.74661403,0\H,13,1.086
75132,12,118.9164828,11,179.79960743,0\H,15,1.08792454,14,120.73549007
,13, -179.28664627,0\H,16,1.08595954,15,121.28041307,14,179.87081338,0\
C,3,5.20126059,2,142.45027666,1,161.27378916,0\C,21,1.41306328,3,56.91
257562,2, -87.14939628,0\C,22,1.38424389,21,120.29622227,3, -38.40068779
,0\C,23,1.41578956,22,120.51402145,21,0.02252809,0\C,24,1.40530617,23,
118.87804531,22,0.24047729,0\C,25,1.39538579,24,120.94282859,23, -0.287
87729,0\H,22,1.0859669,21,118.43134495,3,141.76316585,0\H,23,1.0877963
9,22,118.70937576,21,179.49948893,0\H,25,1.08681192,24,120.17747252,23
,179.94021872,0\H,26,1.08464646,25,119.2438461,24, -179.79213688,0\O,1,
1.34144319,2,124.93246241,3, -179.88515283,0\O,21,1.34143742,3,145.9719
4197,2,0.07103635,0\O,11,1.34144644,4,167.10390574,3,79.10296211,0\C,3
1,1.42676257,1,119.29615832,2,0.26764775,0\H,34,1.09085396,31,105.5231
8802,1,179.77473473,0\H,34,1.09730323,31,111.04221279,1, -61.57810102,0\
\H,34,1.09720935,31,111.03611212,1,61.13410272,0\C,33,1.42674446,11,11
9.24885024,4, -15.66322318,0\H,38,1.09084996,33,105.52324139,11,179.742
48412,0\H,38,1.09726636,33,111.04212423,11, -61.61076953,0\H,38,1.09723
984,33,111.03030768,11,61.1009187,0\C,32,1.42676178,21,119.27095411,3,
112.32579254,0\H,42,1.09084999,32,105.524499,21,179.78267431,0\H,42,1.

09722069,32,111.0373007,21,61.1399168,0\H,42,1.09731796,32,111.0466027
3,21,-61.57012589,0\H,4,1.799914,3,120.85876962,2,-179.45277215,0\C,46
,1.82861898,4,108.22312935,3,-132.69502572,0\H,47,1.09475145,46,109.87
059844,4,-179.20645963,0\H,47,1.09475937,46,109.9119972,4,-59.33063415
,0\H,47,1.09474619,46,110.0484642,4,60.74016954,0\Version=AM64L-G03Re
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al=0.\PG=C01 [X(C22H24O3P1)]\@

5b-Me⁺_3

1\1\GINC-CIPCLU07\SP\RMP2-FC\6-31+G(2d,p)\C22H24O3P1(1+)\C2175\02-Sep-
2010\0\#p MP2(FC)/6-31+G(2d,p) scf=tight\k6mesp_20\1,1\C\C,1,1.4129
2948\C,2,1.38435225,1,120.29062766\C,3,1.41572623,2,120.51086222,1,0.0
1280243,0\C,4,1.40514074,3,118.88931966,2,-0.24961335,0\C,5,1.39541058
,4,120.9351343,3,0.27465364,0\H,2,1.08596445,1,118.44374538,6,-179.940
08348,0\H,3,1.08786151,2,118.69306373,1,-179.46892165,0\H,5,1.08686476
,4,120.17006178,3,-179.91278573,0\H,6,1.08469937,5,119.24883314,4,179.
81316029,0\C,5,5.19475899,4,95.31430916,3,170.40977414,0\C,11,1.409320
94,5,59.85122532,4,-74.05750699,0\C,12,1.3932575,11,119.67892274,5,38.
03146637,0\C,13,1.40817943,12,120.99941163,11,0.12696896,0\C,14,1.4127
9091,13,118.85863549,12,-0.27633098,0\C,15,1.38636164,14,120.47794553,
13,0.17827265,0\H,12,1.08461372,11,121.01336798,5,-142.17233602,0\H,13
,1.08781228,12,118.25081015,11,-179.60516536,0\H,15,1.08672793,14,120.
23425892,13,179.72286927,0\H,16,1.08592578,15,121.1643348,14,179.70983
999,0\C,15,5.20635343,14,94.43376332,13,165.99662701,0\C,21,1.41317094
,15,57.45426342,14,-73.81347739,0\C,22,1.38415127,21,120.30749708,15,3
8.33004461,0\C,23,1.41573055,22,120.47653547,21,0.04556925,0\C,24,1.40
517737,23,118.91806794,22,-0.31837055,0\C,25,1.39527294,24,120.9340183
5,23,0.33781639,0\H,22,1.0859673,21,118.42983217,15,-141.73256571,0\H,
23,1.08788281,22,118.76221854,21,-179.41323812,0\H,25,1.08673637,24,12
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1134444,0\O,1,1.34155673,6,124.92461431,5,179.88363884,0\O,21,1.341348
44,15,146.03626889,14,-161.80015502,0\O,11,1.34154003,5,147.89759702,4
,177.58883254,0\C,31,1.42661107,1,119.25299281,6,-0.1783913,0\H,34,1.0
9086629,31,105.53056552,1,-179.94473126,0\H,34,1.09726362,31,111.03183
953,1,-61.30810244,0\H,34,1.09728469,31,111.0444714,1,61.39979882,0\C,
33,1.42666895,11,119.37150167,5,88.03660894,0\H,38,1.09086554,33,105.5
1657684,11,179.6259829,0\H,38,1.09734602,33,111.08430346,11,-61.747476
75,0\H,38,1.09723071,33,111.05147691,11,61.00340413,0\C,32,1.4266896,2
1,119.27480109,15,-111.09635966,0\H,42,1.09085162,32,105.52952582,21,-
179.91972579,0\H,42,1.09734586,32,111.04658122,21,61.4358581,0\H,42,1.
09725514,32,111.03916027,21,-61.27416267,0\H,24,1.79993644,23,120.1341
1938,22,-179.41198701,0\C,46,1.82821122,24,108.32428789,23,-50.6910633
5,0\H,47,1.09475079,46,110.01674498,24,61.10622525,0\H,47,1.09466549,4
6,110.05139873,24,-178.60927926,0\H,47,1.09475763,46,109.76410266,24,-
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5b-Me⁺_4

1\1\GINC-CIPCLU05\SP\RMP2-FC\6-31+G(2d,p)\C22H24O3P1(1+)\C2175\02-Sep-
2010\0\#p MP2(FC)/6-31+G(2d,p) scf=tight\k6mesp_19\1,1\C\C,1,1.4092
6688\C,2,1.39327549,1,119.69558028\C,3,1.40804936,2,120.97923196,1,0.1

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,4,120.48659653,3,0.26751208,0\H,2,1.08466691,1,121.00500714,6,179.998
22248,0\H,3,1.08784861,2,118.29181036,1,-179.48593453,0\H,5,1.08675124
,4,120.23509425,3,179.94965542,0\H,6,1.08593774,5,121.17490066,4,179.7
513793,0\C,5,5.20578739,4,94.54038708,3,166.59979,0\C,11,1.4094518,5,5
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,13,-179.99464339,0\H,16,1.08592795,15,121.16900746,14,179.73533852,0\
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076,0\C,23,1.41579531,22,120.48820831,21,0.01907704,0\C,24,1.40502457,
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27374045,0\H,22,1.08595523,21,118.44605369,15,-141.5313175,0\H,23,1.08
79392,22,118.76382527,21,-179.40562327,0\H,25,1.08677824,24,120.159982
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0\O,1,1.34159092,2,124.72411985,3,-179.79977056,0\O,21,1.34145685,15,1
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8390121,0\C,31,1.42667048,1,119.33662741,2,0.50501229,0\H,34,1.0908616
2,31,105.50957373,1,179.70138287,0\H,34,1.09732411,31,111.09674964,1,-
61.68954253,0\H,34,1.09727006,31,111.0580227,1,61.08410652,0\C,33,1.42
664684,11,119.36921664,5,86.29077347,0\H,38,1.09086233,33,105.51247322
,11,179.53678802,0\H,38,1.0973284,33,111.07804041,11,-61.86207798,0\H,
38,1.09725699,33,111.05791095,11,60.91918144,0\C,32,1.42671801,21,119.
2624082,15,-112.93058135,0\H,42,1.09086356,32,105.51833386,21,179.9364
2491,0\H,42,1.09728097,32,111.04684712,21,61.29127267,0\H,42,1.0972908
1,32,111.04028167,21,-61.43029105,0\H,24,1.80006429,23,120.05363417,22
, -179.53285819,0\C,46,1.82856568,24,108.20489271,23,-50.89124297,0\H,4
7,1.09480545,46,109.68597123,24,60.88880151,0\H,47,1.0946869,46,110.08
782992,24,-179.13813539,0\H,47,1.09468192,46,110.06981629,24,-58.86023
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5b-Me⁺_5

1\1\GINC-CIPCLU08\SP\RMP2-FC\6-31+G(2d,p)\C22H24O3P1(1+)\C2175\02-Sep-
2010\0\#p MP2(FC)/6-31+G(2d,p) scf=tight\k6mesp_72\1,1\C\C,1,1.4104
9906\C,2,1.38628303,1,120.37372063\C,3,1.41277847,2,120.49046847,1,-0.
06296446,0\C,4,1.40857924,3,118.8473415,2,-0.25196044,0\C,5,1.39297922
,4,121.00436074,3,0.3238999,0\H,2,1.08593583,1,118.43912517,6,-179.905
01353,0\H,3,1.08673154,2,119.2846003,1,179.66519533,0\H,5,1.08789319,4
,120.70960871,3,-179.22341398,0\H,6,1.08464482,5,119.35342886,4,179.83
131358,0\C,4,5.52152278,3,120.07961857,2,-118.61025293,0\C,11,1.410200
78,4,42.59950605,3,56.46799716,0\C,12,1.3865843,11,120.36242685,4,-5.5
9172284,0\C,13,1.41235634,12,120.48938272,11,-0.05489556,0\C,14,1.4085
775,13,118.87340132,12,-0.17598978,0\C,15,1.39276011,14,120.97466946,1
3,0.23489242,0\H,12,1.08592845,11,118.44979216,4,174.23036515,0\H,13,1
.08677465,12,119.29578584,11,179.67813124,0\H,15,1.08811345,14,120.708
78933,13,-179.20126342,0\H,16,1.08468259,15,119.35675625,14,179.852241
28,0\C,3,5.19025884,2,142.45503819,1,158.13064755,0\C,21,1.41010674,3,

70.80569573,2,126.24194505,0\C,22,1.38661126,21,120.37292966,3,34.1488
5539,0\C,23,1.41252504,22,120.44946468,21,0.02048058,0\C,24,1.4082285,
23,118.89191672,22,-0.40430686,0\C,25,1.39292328,24,120.99302287,23,0.
45180195,0\H,22,1.08596989,21,118.42927989,3,-145.97768269,0\H,23,1.08
665113,22,119.35113279,21,179.7932473,0\H,25,1.08810949,24,120.6975125
7,23,-179.02434465,0\H,26,1.08463603,25,119.33316989,24,179.87911651,0
\O,1,1.34120941,6,124.73016018,5,179.78547333,0\O,21,1.34194127,3,148.
0994742,2,18.32566221,0\O,11,1.34132362,4,157.81222248,3,70.48388276,0
\C,31,1.42624745,1,119.40047765,6,0.14118727,0\H,34,1.09088828,31,105.
53769726,1,179.79904972,0\H,34,1.09740324,31,111.08103868,1,-61.559640
58,0\H,34,1.09739369,31,111.08115955,1,61.16687961,0\C,33,1.42630858,1
1,119.39592734,4,169.34323311,0\H,38,1.09089266,33,105.52879918,11,-17
9.91488184,0\H,38,1.09739087,33,111.07098401,11,-61.28755296,0\H,38,1.
09740023,33,111.105036,11,61.45278775,0\C,32,1.42652958,21,119.3567305
,3,-84.93603553,0\H,42,1.09090278,32,105.53222158,21,179.6978105,0\H,4
2,1.09730256,32,111.07614209,21,61.03405439,0\H,42,1.09741005,32,111.0
7530409,21,-61.69707479,0\P,4,1.79957333,3,120.65214724,2,-178.8614343
1,0\C,46,1.82863278,4,108.46971858,3,-135.33585463,0\H,47,1.09480038,4
6,109.69886451,4,178.72376309,0\H,47,1.09453416,46,110.21213965,4,-61.
28291348,0\H,47,1.09475277,46,109.92612412,4,58.99802935,0\Version=AM
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-09\Thermal=0.\PG=C01 [X(C22H24O3P1)]\@

5c

5c_1

1\1\GINC-CALYPSO\SP\RMP2-FC\6-31+G(2d,p)\C20H20N1P1\CHRISTOPH\09-Aug-2
011\0\#p MP2(FC)/6-31+g(2d,p) scf=tight\pjump_27\0,1\C\C,1,1.399473
73\C,2,1.39663328,1,120.02131141\C,3,1.40854526,2,120.92922162,1,1.015
16314,0\C,4,1.40511607,3,118.46942256,2,-1.19156197,0\C,1,1.39773119,2
,119.63114901,3,-0.19415699,0\H,2,1.08807723,1,120.14309791,6,-179.540
87288,0\H,3,1.08913268,2,119.57902288,1,-178.88770467,0\H,5,1.08712608
,4,119.67756251,3,-179.20982191,0\H,6,1.08831167,1,120.02619031,2,179.
66539546,0\C,4,5.43632051,3,98.95190988,2,124.35973325,0\C,11,1.397780
11,4,42.66056674,3,-80.1955863,0\C,12,1.39950867,11,120.32082215,4,-6.
65249626,0\C,13,1.40583681,12,120.62966894,11,0.23463351,0\C,14,1.4081
1822,13,118.42817376,12,0.41184902,0\C,15,1.39663114,14,120.94384851,1
3,-0.96759521,0\H,12,1.08828826,11,120.05277368,4,173.45370454,0\H,13,
1.08723704,12,119.57425204,11,179.98362253,0\H,15,1.08895647,14,119.44
697609,13,178.86072102,0\H,16,1.0880995,15,119.81650271,14,-179.784284
29,0\C,5,5.10915687,4,96.90060435,3,-169.28251827,0\C,21,1.41668307,5,
69.92392463,4,55.86704256,0\C,22,1.39266769,21,120.85543182,5,-35.5012
1106,0\C,23,1.40655418,22,122.04786647,21,0.33907706,0\C,24,1.40665853
,23,117.01108881,22,-1.18933834,0\C,25,1.39270388,24,121.77393857,23,0
.7322069,0\H,22,1.08485576,21,120.5183708,5,145.15949765,0\H,23,1.0890
6291,22,118.59151069,21,-179.21485952,0\H,25,1.08798432,24,119.6907045
2,23,-178.48849374,0\H,26,1.08499548,25,118.52241885,24,-179.18733378,
0\P,24,1.84095852,23,117.80733873,22,179.95947566,0\N,21,1.38753725,5,
145.3545569,4,172.46988137,0\C,32,1.45351373,21,119.41476263,5,-109.77
801381,0\H,33,1.09787022,32,110.93340433,21,60.79951013,0\H,33,1.09303
625,32,109.04532497,21,179.04280443,0\H,33,1.1029449,32,112.77603309,2
1,-60.62293078,0\C,32,1.45361685,21,119.45400749,5,89.24745534,0\H,37,

1.10292198,32,112.78901674,21,60.64417851,0\H,37,1.09304788,32,109.031
57578,21,-179.01577766,0\H,37,1.09790835,32,110.94032029,21,-60.766219
16,0\H,1,1.08794325,6,120.19768093,5,-179.99440103,0\H,11,1.08792275,4
,162.09523918,3,-61.05816067,0\Version=AM64L-G03RevD.01\State=1-A\HF=
-1164.2433593\MP2=-1167.3950273\RMSD=6.859e-09\Thermal=0.\PG=C01 [X(C2
0H20N1P1)]\@

5c_2

1\1\GINC-PHOBOS\SP\RMP2-FC\6-31+G(2d,p)\C20H20N1P1\CHRISTOPH\10-Aug-20
11\0\#p MP2(FC)/6-31+g(2d,p) scf=tight\pjusp_12\0,1\C\C,1,1.3977704
1\C,2,1.39951106,1,120.31808946\C,3,1.40511605,2,120.62132677,1,0.2434
8743,0\C,4,1.40855486,3,118.46775551,2,0.5431436,0\C,5,1.39668183,4,12
0.91771735,3,-1.17072322,0\H,2,1.08831549,1,120.0311481,6,179.67895452
,0\H,3,1.08711787,2,119.72253766,1,-179.9772036,0\H,5,1.08911908,4,119
.49123867,3,178.73259052,0\H,6,1.08807713,5,119.83243038,4,-179.634802
56,0\C,4,5.43755916,3,115.35282576,2,-116.64951038,0\C,11,1.39927224,4
,77.20965443,3,-126.25677788,0\C,12,1.39655,11,120.04720838,4,3.906814
95,0\C,13,1.40819977,12,120.94094263,11,0.88694812,0\C,14,1.40576482,1
3,118.43916929,12,-0.9534113,0\C,11,1.39772092,4,42.60010141,3,48.4259
4784,0\H,12,1.08808956,11,120.12962553,4,-175.4382063,0\H,13,1.0889534
6,12,119.61182981,11,-178.98520576,0\H,15,1.0872025,14,119.80342838,13
, -179.39317685,0\H,16,1.08829191,11,120.04952459,4,173.81916845,0\C,3,
5.11805538,2,141.34653064,1,163.82081201,0\C,21,1.41674683,3,69.629909
89,2,-109.54521653,0\C,22,1.39265651,21,120.8459665,3,-35.86550718,0\C
,23,1.40649792,22,122.04629275,21,1.12770078,0\C,24,1.4068001,23,117.0
1932454,22,-0.7817926,0\C,25,1.39262177,24,121.78224325,23,0.34962123,
0\H,22,1.08487221,21,120.50026475,3,144.78192639,0\H,23,1.08908246,22,
118.59410607,21,-178.91205187,0\H,25,1.0880232,24,119.69127325,23,-179
.38339811,0\H,26,1.08504233,25,118.53795653,24,179.87537795,0\H,24,1.8
4084357,23,117.85421865,22,179.8702391,0\N,21,1.38676734,3,147.4880549
3,2,7.28908899,0\C,32,1.45321406,21,119.56432476,3,70.42565935,0\H,33,
1.09806693,32,110.99027892,21,60.48287036,0\H,33,1.09298561,32,109.061
29259,21,178.80322593,0\H,33,1.10285308,32,112.72713678,21,-60.9085134
8,0\C,32,1.45335052,21,119.48748529,3,-92.16444484,0\H,37,1.09297502,32
,109.07586114,21,-179.83327045,0\H,37,1.09826725,32,111.05597209,21,-6
1.46384785,0\H,37,1.1027297,32,112.66648485,21,59.91885134,0\H,1,1.087
94023,2,120.19580416,3,179.9960393,0\H,11,1.08792331,4,162.11546667,3,
66.52161075,0\Version=AM64L-G03RevD.01\State=1-A\HF=-1164.2432479\MP2
=-1167.3949138\RMSD=6.846e-09\Thermal=0.\PG=C01 [X(C20H20N1P1)]\@

5c-Me⁺

5c-Me⁺_1

1\1\GINC-PHOBOS\SP\RMP2-FC\6-31+G(2d,p)\C21H23N1P1(1+)\CHRISTOPH\10-Au
g-2011\0\#p MP2(FC)/6-31+g(2d,p) scf=tight\pjumesp_18\1,1\C\C,1,1.3
9758995\C,2,1.39785441,1,120.16222116\C,3,1.40593886,2,119.75105111,1,
0.01245136,0\C,4,1.4094938,3,119.94452715,2,0.30785677,0\C,5,1.3949313
5,4,119.83184859,3,-0.3888374,0\H,2,1.08668802,1,120.22079438,6,179.84
062091,0\H,3,1.08644362,2,119.82241156,1,-179.83079114,0\H,5,1.0877565
9,4,120.75763867,3,179.01105263,0\H,6,1.08670605,5,119.72399417,4,-179
.81522171,0\C,3,5.17472612,2,143.34774361,1,-163.25314383,0\C,11,1.397
66933,3,72.74243205,2,-126.88146794,0\C,12,1.39784892,11,120.13791946,

3,-33.14036331,0\C,13,1.40581582,12,119.77130162,11,-0.00347921,0\C,14
,1.40962534,13,119.95104533,12,0.16650191,0\C,15,1.39504711,14,119.819
59953,13,-0.1742428,0\H,12,1.08669458,11,120.19647196,3,146.99837907,0
\H,13,1.0867317,12,120.06687619,11,-179.69715061,0\H,15,1.08778037,14,
120.85703668,13,179.29670773,0\H,16,1.08673168,15,119.73587686,14,-179
.88154288,0\C,13,5.21726457,12,142.93543228,11,-163.56107392,0\C,21,1.
42695035,13,58.82227677,12,92.74449013,0\C,22,1.38374976,21,121.120403
43,13,38.63872364,0\C,23,1.41447137,22,121.20548245,21,0.12818329,0\C,
24,1.41230445,23,118.07626002,22,-0.38486032,0\C,25,1.38529563,24,121.
17113697,23,0.37241095,0\H,22,1.08376812,21,120.29755557,13,-141.56342
907,0\H,23,1.0881237,22,118.13498892,21,-179.62425704,0\H,25,1.0870479
6,24,120.14052058,23,179.93285218,0\H,26,1.08379344,25,118.52315379,24
,179.62347891,0\P,24,1.78570362,23,120.64401029,22,-178.17206521,0\C,3
1,1.82817419,24,109.40339746,23,-45.09473879,0\H,32,1.09480745,31,109.
91451014,24,61.32572401,0\H,32,1.0946565,31,110.01405887,24,-178.79329
536,0\H,32,1.09456913,31,109.8493449,24,-58.66940962,0\N,21,1.36339104
,13,147.29430794,12,-7.67846264,0\C,36,1.46051189,21,120.26929967,13,-
100.1535912,0\H,37,1.09100135,36,109.05162545,21,-179.89004049,0\H,37,
1.09851625,36,111.43504811,21,-60.70581593,0\H,37,1.09849275,36,111.43
816464,21,60.92870188,0\C,36,1.46074953,21,120.3689824,13,80.14078428,
0\H,41,1.09097227,36,109.02449165,21,179.91812603,0\H,41,1.098549,36,1
11.47971366,21,-60.92575352,0\H,41,1.09852631,36,111.46927747,21,60.75
194495,0\H,1,1.08696343,2,119.9270615,3,179.81238227,0\H,11,1.08697055
,3,147.38384307,2,-7.92178224,0\Version=AM64L-G03RevD.01\State=1-A\HF
=-1203.705071\MP2=-1207.0004346\RMSD=8.695e-09\Thermal=0.\PG=C01 [X(C2
1H23N1P1)]\@

5d

5d_1

1\1\GINC-YANG\SP\RMP2-FC\6-31+G(2d,p)\C18H12Cl3P1\CHRISTOPH\25-Aug-201
0\0\#p MP2(FC)/6-31+g(2d,p) scf=tight\k5sp_2\0,1\C\C,1,1.39681424\C
,2,1.39617418,1,118.90485019\C,3,1.40741106,2,121.32573116,1,0.8877605
7,0\C,4,1.40566653,3,118.34955844,2,-1.07397877,0\C,1,1.39630441,2,121
.21054823,3,-0.11438379,0\H,2,1.08593872,1,120.20227675,6,-179.4428103
4,0\H,3,1.08856694,2,118.98249902,1,-178.87503034,0\H,5,1.0871182,4,12
0.01581685,3,-179.19254098,0\H,6,1.08613593,1,120.09933662,2,179.60803
929,0\C,4,5.42063582,3,104.50835308,2,121.17737159,0\C,11,1.39595366,4
,43.58111921,3,-85.93522181,0\C,12,1.39812434,11,119.15787633,4,-7.497
46214,0\C,13,1.40562193,12,121.06913057,11,0.2472462,0\C,14,1.40771975
,13,118.32044186,12,0.51200359,0\C,15,1.39599832,14,121.32610605,13,-1
.12291046,0\H,12,1.08610548,11,120.11398768,4,172.54098866,0\H,13,1.08
71531,12,118.88433116,11,179.88106688,0\H,15,1.08860362,14,119.7119738
3,13,178.62062847,0\H,16,1.08592869,15,120.88312619,14,-179.76488807,0
\C,5,5.05055424,4,95.65094759,3,-162.3513875,0\C,21,1.3971495,5,67.837
89985,4,57.93396287,0\C,22,1.39594928,21,118.91436477,5,-37.45868224,0
\C,23,1.40776652,22,121.32231361,21,0.92087887,0\C,24,1.40557026,23,11
8.33712509,22,-1.12593531,0\C,21,1.39593991,5,64.25517197,4,-86.896776
99,0\H,22,1.0859622,21,120.17522338,5,143.25094808,0\H,23,1.08860617,2
2,118.98100331,21,-178.80061423,0\H,25,1.08715811,24,120.06177739,23,-
179.07791398,0\H,26,1.08614475,21,120.1226545,5,-141.82539066,0\P,4,1.
85054358,3,116.90000311,2,-179.71875859,0\Cl,1,1.76024844,6,119.396873

54,5,179.93444104,0\Cl,11,1.7603698,4,162.02613308,3,-64.43276597,0\Cl
,21,1.7603272,5,146.08763824,4,168.02506582,0\\Version=AM64L-G03RevD.0
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0.\PG=C01 [X(C18H12Cl3P1)]\\@

5d_2

1\1\GINC-SOLARIS\SP\RMP2-FC\6-31+G(2d,p)\C18H12Cl3P1\CHRISTOPH\25-Aug-
2010\0\\#p MP2(FC)/6-31+g(2d,p) scf=tight\\k5sp_16\\0,1\C\C,1,1.395939
1\C,2,1.3979055,1,119.15214927\C,3,1.40571642,2,121.07134897,1,0.26086
625,0\C,4,1.40769493,3,118.31838051,2,0.48757978,0\C,5,1.39606677,4,12
1.33334622,3,-1.10097561,0\H,2,1.08602514,1,120.10932289,6,179.6578007
8,0\H,3,1.08709453,2,118.89333459,1,179.95521697,0\H,5,1.08855184,4,11
9.70727698,3,178.69946329,0\H,6,1.08587326,5,120.89471149,4,-179.75465
18,0\C,4,5.42311788,3,111.19630793,2,-118.50895529,0\C,11,1.39707647,4
,77.81444027,3,-131.33787397,0\C,12,1.39623706,11,118.90074678,4,4.882
78445,0\C,13,1.40782803,12,121.34605395,11,0.90729085,0\C,14,1.4056197
1,13,118.30772715,12,-1.07689851,0\C,11,1.39608027,4,43.65511726,3,42.
43586003,0\H,12,1.08587357,11,120.18938758,4,-174.46656875,0\H,13,1.08
856759,12,118.95243307,11,-178.91892719,0\H,15,1.08701008,14,120.02124
48,13,-179.27401883,0\H,16,1.08604424,11,120.12116662,4,172.54349209,0
\C,3,5.04643378,2,140.0812365,1,155.80511093,0\C,21,1.39627528,3,64.17
628694,2,114.91945664,0\C,22,1.39801248,21,119.14968268,3,38.13997967,
0\C,23,1.40572686,22,121.07021961,21,0.24713641,0\C,24,1.40761238,23,1
18.31554399,22,0.49795626,0\C,25,1.39624695,24,121.34528592,23,-1.0848
2852,0\H,22,1.08602455,21,120.10323453,3,-141.82060753,0\H,23,1.087003
42,22,118.87833648,21,179.85819054,0\H,25,1.08845469,24,119.70397847,2
3,178.62965638,0\H,26,1.08583684,25,120.88824778,24,-179.79353822,0\P,
14,1.85058365,13,116.90778939,12,-179.54976843,0\Cl,1,1.76059084,2,119
.38951673,3,179.93195124,0\Cl,11,1.7606482,4,162.09590117,3,63.9630816
,0\Cl,21,1.76053428,3,146.13489327,2,9.99220945,0\\Version=AM64L-G03Re
vD.01\State=1-A\HF=-2407.8485236\MP2=-2410.9437721\RMSD=9.646e-09\Ther
mal=0.\PG=C01 [X(C18H12Cl3P1)]\\@

5d-Me⁺

5d-Me_1

1\1\GINC-YIN\SP\RMP2-FC\6-31+G(2d,p)\C19H15Cl3P1(1+)\CHRISTOPH\25-Aug-
2010\0\\#p MP2(FC)/6-31+g(2d,p) scf=tight\\k5mesp_13\\1,1\C\C,1,1.4018
5969\C,2,1.39255632,1,119.34250155\C,3,1.41027561,2,120.28205157,1,0.0
9438319,0\C,4,1.40718604,3,119.63191247,2,-0.22062702,0\C,5,1.39511914
,4,120.240116,3,0.17684494,0\H,2,1.08546322,1,120.06105473,6,179.98518
547,0\H,3,1.08740422,2,118.65136221,1,-179.53415011,0\H,5,1.08642551,4
,120.62146899,3,179.88613482,0\H,6,1.08544714,5,120.52680159,4,179.851
56411,0\C,5,5.17165645,4,95.17455802,3,168.19685292,0\C,11,1.39906535,
5,72.06010002,4,71.48512749,0\C,12,1.3952686,11,119.41061605,5,-33.812
41669,0\C,13,1.40686226,12,120.24003376,11,-0.00438404,0\C,14,1.410554
02,13,119.62584912,12,0.20139102,0\C,15,1.3924747,14,120.28976815,13,-
0.22885029,0\H,12,1.08548598,11,120.08817666,5,146.30135149,0\H,13,1.0
8646353,12,119.14620786,11,-179.82899975,0\H,15,1.08745855,14,121.0703
6663,13,179.24129705,0\H,16,1.0854824,15,120.6264394,14,-179.8953208,0
\C,13,5.17943718,12,143.1313384,11,-162.10556485,0\C,21,1.40189812,13,
59.21981995,12,89.39788323,0\C,22,1.39263968,21,119.32821342,13,37.999

33964,0\C,23,1.41028406,22,120.27174767,21,0.07263063,0\C,24,1.4069918
4,23,119.66097173,22,-0.29258563,0\C,25,1.39511653,24,120.22081225,23,
0.26745977,0\H,22,1.08551086,21,120.06279458,13,-142.1310082,0\H,23,1.
08749102,22,118.65136124,21,-179.62498651,0\H,25,1.08639257,24,120.574
22729,23,179.91231439,0\H,26,1.08545408,25,120.52856487,24,179.7767899
7,0\P,4,1.80623004,3,119.76749698,2,-179.10470148,0\C,31,1.82609906,4,
108.58600341,3,-47.01288217,0\H,32,1.0946674,31,109.9115274,4,-177.570
80838,0\H,32,1.09468038,31,109.96498397,4,62.47409961,0\H,32,1.0947297
3,31,109.94600882,4,-57.62447573,0\Cl,1,1.74095918,6,119.53149065,5,17
9.9021588,0\Cl,11,1.74108216,5,147.16729943,4,-171.50241033,0\Cl,21,1.
74096081,13,147.39542143,12,-7.93448676,0\\Version=AM64L-G03RevD.01\St
ate=1-A\HF=-2447.2845084\MP2=-2450.5257915\RMSE=6.270e-09\Thermal=0.\P
G=C01 [X(C19H15Cl3P1)]\\@

5e

5e_1

1\1\GINC-GOLEM\SP\RMP2-FC\6-31+G(2d,p)\C18H21P1\CHRISTOPH\01-Jun-2010\
0\#p MP2(FC)/6-31+g(2d,p) scf=tight\\x6sp_4\\0,1\P\C,1,4.67695111\C,2
,1.39936064,1,61.21080507\C,3,1.39741489,2,120.22944287,1,0.27644415,0
\C,4,1.40660815,3,120.76418324,2,0.10449305,0\C,5,1.40689694,4,118.357
71317,3,0.45763605,0\C,2,1.39750722,1,58.48233179,5,168.32995648,0\H,2
,1.08790411,1,178.65291203,5,174.66192002,0\H,3,1.08823674,2,120.02054
988,1,-179.8766119,0\H,4,1.0876168,3,119.3804577,2,179.15581487,0\H,6,
1.088715,5,119.32037876,4,178.86281651,0\H,7,1.08803386,2,120.16396872
,1,179.88908764,0\C,1,4.67764545,5,102.13438571,4,-35.58986826,0\C,13,
1.39819308,1,57.96083065,5,-95.8316628,0\C,14,1.39750825,13,120.040972
04,1,-0.46344018,0\C,15,1.40786064,14,121.1697108,13,0.91243715,0\C,16
,1.40772338,15,118.02478059,14,-1.04058266,0\C,13,1.39808389,1,61.6399
5037,16,-0.07244491,0\H,13,1.08780439,1,178.19381746,16,177.32992838,0
\H,14,1.08793955,13,120.13452786,1,-179.86870783,0\H,15,1.08871568,14,
119.61344732,13,-178.8736004,0\H,17,1.08760751,16,120.23298961,15,-179
.3953363,0\H,18,1.08818656,13,120.06387489,1,179.96134202,0\H,1,2.4833
0728,16,87.52204777,15,177.94568651,0\C,1,4.22984992,16,123.55008502,1
5,161.79477757,0\C,25,1.54112877,1,19.34442063,16,164.950444,0\C,26,1.
54674111,25,111.38172643,1,-2.87852087,0\C,27,1.54661916,26,110.152336
22,25,55.8121872,0\C,28,1.54108272,27,111.53769006,26,-55.82833765,0\C
,29,1.53867012,28,111.56695971,27,55.66178197,0\H,25,1.09896282,1,128.
9922496,16,170.37664705,0\H,25,1.10135745,1,101.10242171,16,48.1973111
4,0\H,26,1.10168054,25,109.20372506,1,117.68011783,0\H,26,1.09743396,2
5,109.97147752,1,-125.43954656,0\H,28,1.10136906,27,108.76046864,26,64
.7849892,0\H,28,1.09768909,27,110.55292918,26,-178.56536081,0\H,29,1.0
9894786,28,109.77188977,27,178.31082423,0\H,29,1.10153636,28,109.17622
796,27,-65.20636584,0\H,30,1.09888522,29,110.31835288,28,-177.24119301
,0\H,30,1.10139473,29,109.13872437,28,65.90846938,0\\Version=AM64L-G03
RevD.01\State=1-A\HF=-1034.6567907\MP2=-1037.3804497\RMSE=6.521e-09\Th
ermal=0.\PG=C01 [X(C18H21P1)]\\@

5e_2

1\1\GINC-SOLARIS\SP\RMP2-FC\6-31+G(2d,p)\C18H21P1\CHRISTOPH\01-Jun-201
0\0\#p MP2(FC)/6-31+g(2d,p) scf=tight\\x6sp_42\\0,1\P\C,1,4.67427014\
C,2,1.39956929,1,61.50653735\C,3,1.39738989,2,120.256129,1,0.44132563,

0\C,4,1.40898465,3,120.77666227,2,0.22383022,0\C,5,1.40737115,4,118.21
861881,3,0.41511064,0\C,2,1.39718438,1,58.19533685,5,163.7146163,0\H,2
,1.08788524,1,178.33842213,5,177.45095749,0\H,3,1.08817129,2,120.03928
827,1,-179.45326719,0\H,4,1.08708055,3,119.44518451,2,179.5260511,0\H,
6,1.08859363,5,119.25370825,4,178.6701442,0\H,7,1.08794338,2,120.17148
979,1,179.70647682,0\C,1,4.67516178,5,105.04284245,4,-35.54310892,0\C,
13,1.39861004,1,59.27848038,5,-39.56368945,0\C,14,1.39684788,13,120.34
282327,1,2.57468094,0\C,15,1.40970569,14,121.10559906,13,0.5415571,0\C
,16,1.40837348,15,117.79273436,14,-1.30130773,0\C,13,1.39724231,1,60.0
6796531,16,79.69529212,0\H,13,1.08763636,1,177.75406258,16,-179.320171
74,0\H,14,1.08815331,13,120.11257063,1,-177.33295635,0\H,15,1.08781319
,14,119.19812417,13,-179.77715851,0\H,17,1.08749832,16,120.25677379,15
, -178.66525916,0\H,18,1.0881551,13,120.12019176,1,177.4464501,0\H,1,2.
40636936,16,91.5517804,15,-176.30212384,0\C,1,4.31165593,16,93.5348112
,15,-139.62991844,0\C,25,1.54239771,1,22.34649133,16,55.62246424,0\C,2
6,1.54258927,25,111.36756028,1,1.80080703,0\C,27,1.54749162,26,110.602
46212,25,55.69313982,0\C,28,1.54152927,27,111.41526165,26,-55.23470754
,0\C,25,1.53841024,1,98.57303568,16,-177.12111525,0\H,25,1.10171261,1,
98.3302704,16,-66.0082405,0\H,25,1.09907319,1,132.09879824,16,55.34253
871,0\H,26,1.09948378,25,109.01615303,1,122.01860606,0\H,26,1.09769853
,25,110.03594443,1,-121.10229334,0\H,28,1.09867335,27,110.06992866,26,
-177.66995522,0\H,28,1.10090432,27,109.16352071,26,65.49006935,0\H,29,
1.09895405,28,109.76146378,27,177.76568914,0\H,29,1.10151993,28,109.07
415873,27,-65.79295114,0\H,30,1.09883957,25,110.37052473,1,158.6558668
6,0\H,30,1.10134031,25,109.11080005,1,-84.44196335,0\\Version=AM64L-G0
3RevD.01\State=1-A\HF=-1034.6537009\MP2=-1037.3798197\RMSD=5.988e-09\T
hermal=0.\PG=C01 [X(C18H21P1)]\@

5e_3

1\1\GINC-CALYPSO\SPRMP2-FC\6-31+G(2d,p)\C18H21P1\CHRISTOPH\31-May-201
0\0\\#p MP2(FC)/6-31+g(2d,p) scf=tight\\x6sp_26\\0,1\P\C,1,4.67790838\
C,2,1.39815317,1,61.7618655\C,3,1.39884545,2,120.28751696,1,0.13257917
,0\C,4,1.40752404,3,120.91336272,2,-0.33461294,0\C,5,1.4083125,4,117.9
7180978,3,-0.37193765,0\C,6,1.39721621,5,121.23489131,4,1.0107874,0\H,
2,1.08774204,1,178.05096663,5,-177.78523784,0\H,3,1.08812336,2,120.064
73109,1,-179.98029166,0\H,4,1.08759126,3,118.77792921,2,179.90292584,0
\H,6,1.08878587,5,119.16566615,4,-178.70184378,0\H,7,1.08793075,6,119.
80474183,5,179.68517043,0\C,1,4.67702159,5,103.76344023,4,-85.33783778
,0\C,13,1.39979873,1,61.16100153,5,33.16247055,0\C,14,1.39701674,13,12
0.23269931,1,-0.40929277,0\C,15,1.40692086,14,120.76480285,13,-0.05474
722,0\C,16,1.40665509,15,118.34932088,14,-0.65186586,0\C,13,1.3972206,
1,58.53039558,5,-146.00836189,0\H,13,1.08785752,1,178.6884904,5,-159.8
3583124,0\H,14,1.08814138,13,120.01709193,1,179.73402847,0\H,15,1.0878
7676,14,119.37038633,13,-178.9610952,0\H,17,1.08877804,16,119.32209572
,15,-178.69702509,0\H,18,1.08796649,13,120.17416981,1,-179.74466027,0\
H,1,2.46920454,5,87.30941187,4,-0.98106336,0\C,1,3.4106182,5,104.74480
205,4,68.81102655,0\C,25,1.54094629,1,56.20599516,5,-58.04671906,0\C,2
6,1.55072957,25,113.11650516,1,-36.14727305,0\C,27,1.5507797,26,109.96
702726,25,-52.30759138,0\C,28,1.5408258,27,113.22498917,26,52.25438347
,0\C,25,1.53893281,1,102.4321701,5,-165.68452547,0\H,25,1.09963366,1,6
0.65776118,5,88.99724426,0\H,25,1.0986717,1,147.24242396,5,14.34742039

,0\H,26,1.1022662,25,108.68803109,1,-155.57948569,0\H,26,1.09756062,25
,110.06840454,1,88.19810404,0\H,28,1.09735053,27,110.31625671,26,176.6
5169508,0\H,28,1.10189204,27,107.47337508,26,-67.72469202,0\H,29,1.098
79717,28,109.41066267,27,-176.80055833,0\H,29,1.09986213,28,109.676327
85,27,66.47661871,0\H,30,1.09863673,25,110.25614447,1,-119.5204804,0\H
,30,1.10193025,25,109.22049685,1,123.61751998,0\\Version=AM64L-G03RevD
.01\\State=1-A\\HF=-1034.6526734\\MP2=-1037.3781893\\RMSD=6.398e-09\\Therma
l=0.\\PG=C01 [X(C18H21P1)]\\@

5e-Me⁺

5e-Me⁺_1

1\\1\\GINC-YANG\\SP\\RMP2-FC\\6-31+G(2d,p)\\C19H24P1(1+)\\CHRISTOPH\\02-Jun-20
10\\0\\#p MP2(FC)/6-31+g(2d,p) scf=tight\\x6mesp_1\\1,1\\P\\C,1,1.8265762
8\\H,2,1.09379007,1,112.00725224\\H,2,1.09500838,1,109.31656707,3,-121.5
7733883,0\\H,2,1.09573752,1,108.40624773,4,-118.26796795,0\\C,1,4.609604
57,2,110.21208308,3,60.90791383,0\\C,6,1.39955148,1,59.89524222,2,159.3
942588,0\\C,7,1.39551002,6,120.13720192,1,-1.10297608,0\\C,8,1.41045413,
7,119.9049454,6,-0.01206,0\\C,9,1.40794488,8,119.69373291,7,-0.00708441
,0\\C,10,1.39696631,9,119.91947616,8,-0.0392422,0\\H,6,1.08684303,1,179.
17282519,9,178.36115886,0\\H,7,1.08666124,6,120.2208447,1,179.16325909,
0\\H,8,1.08714807,7,119.57066935,6,-179.08219135,0\\H,10,1.08646899,9,12
0.99091561,8,-179.69334087,0\\H,11,1.08657361,10,119.61144348,9,-179.68
438157,0\\C,1,4.61046755,9,110.72982951,8,45.963131,0\\C,17,1.39890069,1
,59.88164409,9,30.72960059,0\\C,18,1.39620027,17,120.1503861,1,-1.76750
313,0\\C,19,1.40871893,18,119.87375638,17,-0.04105379,0\\C,20,1.40829643
,19,119.7521687,18,0.40538705,0\\C,21,1.39641881,20,119.90071315,19,-0.
52807033,0\\H,17,1.08684411,1,178.59257,9,113.08418104,0\\H,18,1.0866591
2,17,120.21986119,1,178.34825838,0\\H,19,1.08716074,18,119.62719559,17,
-179.599133,0\\H,21,1.08687272,20,121.03464324,19,179.58091856,0\\H,22,1
.08660727,21,119.63430491,20,-179.65961924,0\\C,1,4.21266244,9,101.1279
9207,8,-61.94305637,0\\C,28,1.54226405,1,20.91511842,9,53.4536517,0\\C,2
9,1.5503426,28,110.49777726,1,-1.78579332,0\\C,30,1.55203894,29,111.175
0051,28,-56.23626889,0\\C,31,1.54319916,30,110.44797959,29,55.78854316,
0\\C,32,1.53712206,31,111.90942518,30,-55.30628044,0\\H,28,1.10057436,1,
99.19557836,9,174.41242201,0\\H,28,1.09700532,1,129.83058337,9,53.60069
833,0\\H,29,1.09941026,28,109.18092926,1,-121.62960872,0\\H,29,1.0974889
6,28,110.11906669,1,120.89314629,0\\H,30,1.10219241,29,108.97737263,28,
62.80296263,0\\H,31,1.09757116,30,110.91158399,29,177.04409075,0\\H,31,1
.09982551,30,109.30581488,29,-64.78683799,0\\H,32,1.10041514,31,109.065
61058,30,66.17383777,0\\H,32,1.09699055,31,108.8468317,30,-177.84655994
,0\\H,33,1.10047119,32,109.45959316,31,-65.74480719,0\\H,33,1.09676135,3
2,109.96388868,31,177.4029462,0\\Version=AM64L-G03RevD.01\\State=1-A\\HF
=-1074.1099397\\MP2=-1076.9794388\\RMSD=5.061e-09\\Thermal=0.\\PG=C01 [X(C
19H24P1)]\\@

5e-Me⁺_2

1\\1\\GINC-AZAZEL\\SP\\RMP2-FC\\6-31+G(2d,p)\\C19H24P1(1+)\\CHRISTOPH\\02-Jun-
2010\\0\\#p MP2(FC)/6-31+g(2d,p) scf=tight\\x6mesp_37\\1,1\\P\\C,1,1.8252
9429\\H,2,1.09476558,1,109.98371399\\H,2,1.09460493,1,109.71778626,3,119
.58434374,0\\H,2,1.09430783,1,110.28725379,4,120.73820648,0\\C,1,4.61232
947,2,109.18809835,5,-50.56731416,0\\C,6,1.39817924,1,59.99631471,2,142

.92310394,0\C,7,1.39659876,6,120.16767411,1,-0.786261,0\C,8,1.40747576
,7,119.85242004,6,0.21218647,0\C,9,1.40954338,8,119.79515767,7,-0.3714
741,0\C,10,1.39564768,9,119.86118547,8,0.24551873,0\H,6,1.08694906,1,1
79.52323612,9,-179.96382465,0\H,7,1.08672263,6,120.22813113,1,179.6607
8103,0\H,8,1.08684653,7,119.61839632,6,-178.91051595,0\H,10,1.08718677
,9,120.98245269,8,-179.48564322,0\H,11,1.08673186,10,119.65016187,9,-1
79.73851699,0\C,1,4.61319682,9,109.0028543,8,25.01797122,0\C,17,1.3983
9704,1,59.98824081,9,91.56931117,0\C,18,1.39638338,17,120.15631044,1,0
.5612593,0\C,19,1.40784766,18,119.98565893,17,0.16354556,0\C,20,1.4093
2694,19,119.60829566,18,-0.26787751,0\C,21,1.39629643,20,119.97266853,
19,0.16308649,0\H,17,1.08687638,1,179.60539177,20,-175.37915126,0\H,18
,1.08666348,17,120.24498956,1,-179.49265501,0\H,19,1.08686609,18,119.1
0015535,17,-179.77034373,0\H,21,1.08723972,20,120.94884775,19,179.9213
7403,0\H,22,1.08672181,21,119.64357461,20,179.78666871,0\C,1,4.2140401
4,20,128.39467831,19,-150.75415221,0\C,28,1.54296601,1,21.39715337,20,
-178.32806973,0\C,29,1.55035229,28,110.11139569,1,-3.38339779,0\C,30,1
.55161701,29,111.22664614,28,-56.6318608,0\C,31,1.54265152,30,110.2159
8443,29,56.74814752,0\C,32,1.53772234,31,111.71149797,30,-55.77492986,
0\H,28,1.10031421,1,98.2337749,20,-56.18037248,0\H,28,1.097086,1,130.3
0959994,20,-176.32202875,0\H,29,1.09671875,28,109.93086316,1,118.81639
126,0\H,29,1.10062133,28,108.907522,1,-123.63439446,0\H,30,1.10175147,
29,107.62244592,28,62.59381165,0\H,31,1.10026656,30,109.28465504,29,-6
3.05281338,0\H,31,1.09716008,30,110.88836169,29,178.99524189,0\H,32,1.
10047887,31,109.10426806,30,65.71152968,0\H,32,1.09710066,31,108.94292
951,30,-178.22424036,0\H,33,1.10068543,32,109.39603001,31,-65.94739851
,0\H,33,1.0968785,32,110.01619047,31,177.28671842,0\\Version=AM64L-G03
RevD.01\\State=1-A\\HF=-1074.1090739\\MP2=-1076.9780101\\RMSD=7.533e-09\\Th
ermal=0.\\PG=C01 [X(C19H24P1)]\\@

5e-Me⁺_3

1\\1\\GINC-EDDY\\SP\\RMP2-FC\\6-31+G(2d,p)\\C19H24P1(1+)\\CHRISTOPH\\02-Jun-20
10\\0\\#p MP2(FC)/6-31+g(2d,p) scf=tight\\x6mesp_26\\1,1\\P\C,1,1.827712
95\\H,2,1.09531349,1,111.10254301\\H,2,1.09485947,1,109.48501283,3,-120.
92710539,0\\H,2,1.09468887,1,109.11287994,4,-118.93132318,0\C,1,4.61087
097,2,109.4420002,5,-173.78724437,0\C,6,1.39894787,1,60.08565989,2,150
.84899432,0\C,7,1.3963616,6,120.1539622,1,-1.34569953,0\C,8,1.40877461
,7,119.85228344,6,-0.041635,0\C,9,1.40815983,8,119.77268123,7,0.191311
81,0\C,10,1.39644903,9,119.90722503,8,-0.26665286,0\H,6,1.08685292,1,1
79.02042822,9,-179.38242969,0\H,7,1.08665863,6,120.21632281,1,178.8815
3553,0\H,8,1.08709615,7,119.70400702,6,-179.2239346,0\H,10,1.08714013,
9,121.00451233,8,-179.89690857,0\H,11,1.08661461,10,119.65343555,9,-17
9.55699519,0\C,1,4.61282788,9,109.01120523,8,38.30703891,0\C,17,1.3976
1291,1,61.03161829,9,-135.31324075,0\C,18,1.39727596,17,120.24077365,1
,1.14361454,0\C,19,1.40704856,18,119.91357961,17,0.27604297,0\C,20,1.4
1090079,19,119.58978245,18,-0.34362386,0\C,21,1.39497352,20,120.031965
74,19,0.17151964,0\H,17,1.08683271,1,178.6125355,9,89.83033861,0\H,18,
1.08658674,17,120.22606923,1,-178.89399527,0\H,19,1.08464325,18,119.03
937373,17,-179.85474827,0\H,21,1.08774143,20,120.57588644,19,179.43372
499,0\H,22,1.08662539,21,119.64448122,20,179.87716488,0\C,1,4.23555045
,9,124.45061278,8,-98.49595692,0\C,28,1.54332634,1,22.6703662,9,-171.6
4274156,0\C,29,1.5510583,28,109.9102499,1,-6.62018095,0\C,30,1.5504589

,29,112.38856643,28,-55.31829294,0\C,31,1.54235447,30,110.19836676,29,
55.34054886,0\C,32,1.53789045,31,111.70243878,30,-55.01305547,0\H,28,1
.10038868,1,96.70820884,9,-46.75416336,0\H,28,1.09699809,1,131.5140903
7,9,-166.0507597,0\H,29,1.09830609,28,109.13795486,1,-127.87630919,0\H
,29,1.0974627,28,109.66661716,1,115.30296596,0\H,30,1.10438955,29,107.
40003943,28,62.54398728,0\H,31,1.09855022,30,109.91753604,29,-65.21918
128,0\H,31,1.09739882,30,110.27684161,29,176.96905348,0\H,32,1.1002713
9,31,109.15669333,30,66.40988642,0\H,32,1.09694957,31,108.9653885,30,-
177.480892,0\H,33,1.09671816,32,110.03051569,31,177.87843295,0\H,33,1.
10078265,32,109.46864328,31,-65.31438472,0\Version=AM64L-G03RevD.01\State=1-A\HF=-1074.1070135\MP2=-1076.9757352\RMSD=3.703e-09\Thermal=0.\PG=C01 [X(C19H24P1)]\@

5f

5f_1

1\1\GINC-PHOENIX\SP\RMP2-FC\6-31+G(2d,p)\C21H21P1\CHRISTOPH\23-Jul-201
1\0\#p MP2(FC)/6-31+g(2d,p) scf=tight\tol3sp_4\0,1\PC,1,4.69217448
\C,2,1.40491306,1,57.52241238\C,3,1.39468719,2,121.00797892,1,0.093451
85,0\C,4,1.40811273,3,121.02388549,2,-0.99020948,0\C,5,1.40450676,4,11
8.00705461,3,0.90596381,0\C,6,1.39880419,5,120.72987669,4,-0.31272048,
0\H,3,1.0893539,2,119.50061907,1,179.45032387,0\H,4,1.08904015,3,119.4
6503263,2,178.9425355,0\H,6,1.08731549,5,119.84357027,4,179.39284115,0
\H,7,1.08919918,6,119.36183849,5,179.86966853,0\C,1,4.69164199,5,102.6
6864915,4,-160.87538088,0\C,12,1.40289586,1,60.46866829,5,-92.5456168,
0\C,13,1.3978243,12,121.29063483,1,0.27718083,0\C,14,1.40546193,13,120
.70255346,12,-0.11838416,0\C,15,1.4072017,14,118.01122686,13,-0.450708
27,0\C,16,1.39546052,15,121.03367869,14,1.04042858,0\H,13,1.08931583,1
2,119.39287302,1,-179.91695863,0\H,14,1.08749826,13,119.42544704,12,17
9.94602918,0\H,16,1.08897194,15,119.53879838,14,-178.96719493,0\H,17,1
.0891363,16,119.50976497,15,179.52293488,0\C,1,4.69160088,15,102.95146
983,14,16.24560977,0\C,22,1.40423452,1,57.4997693,15,86.44012092,0\C,2
3,1.39536722,22,121.00422619,1,0.13322531,0\C,24,1.40771102,23,121.037
47667,22,-1.11361021,0\C,25,1.40459787,24,118.00002128,23,1.06355131,0
\C,26,1.39819746,25,120.72554651,24,-0.47225403,0\H,23,1.08918396,22,1
19.49526796,1,179.56586536,0\H,24,1.08903547,23,119.40732785,22,178.98
655698,0\H,26,1.08739337,25,119.86828839,24,179.57626263,0\H,27,1.0893
7074,26,119.30941801,25,-179.92524624,0\C,2,1.51389269,1,177.92273022,
25,121.30162873,0\H,32,1.09752568,2,111.3701103,1,-80.18992784,0\H,32,
1.0989025,2,111.18848052,1,39.1890452,0\H,32,1.09579817,2,111.39889624
,1,159.19197295,0\C,12,1.51390626,1,177.9459789,25,-123.77625455,0\H,3
6,1.09940201,12,111.1182686,1,47.79981104,0\H,36,1.09645605,12,111.432
88677,1,167.39421691,0\H,36,1.0964545,12,111.4252063,1,-71.79688555,0\
C,22,1.51382284,1,177.84744015,25,-148.5613974,0\H,40,1.09663078,22,11
1.42463548,1,-77.69113423,0\H,40,1.09940988,22,111.13692855,1,41.85531
548,0\H,40,1.09629214,22,111.40435246,1,161.51191905,0\Version=AM64L-
G03RevD.01\State=1-A\HF=-1148.2764067\MP2=-1151.3991652\RMSD=6.492e-09
\Thermal=0.\PG=C01 [X(C21H21P1)]\@

5f-Me⁺

5f-Me_1

1\1\GINC-BORIX\SP\RMP2-FC\6-31+G(2d,p)\C22H24P1(1+)\CHRISTOPH\26-Oct-2

011\0\#p MP2(FC)/6-31+g(2d,p) scf=tight\|tol3mesp_cart_1\|1,1\C\C,1,1
.40856535\C,2,1.39163201,1,121.1957706\C,3,1.41068309,2,119.9854014,1,
0.03173749,0\C,4,1.40546738,3,119.37812951,2,0.38773696,0\C,5,1.396387
94,4,119.89523273,3,-0.3495003,0\H,2,1.08781865,1,119.53427885,6,179.6
8601071,0\H,3,1.08790531,2,119.11321014,1,179.50389157,0\H,5,1.0868620
4,4,120.43780977,3,179.8458615,0\H,6,1.08762439,5,119.17730109,4,-179.
89100997,0\C,4,5.53742203,3,94.96808682,2,131.62322351,0\C,11,1.408074
29,4,76.29988969,3,112.790254,0\C,12,1.3918829,11,121.19821776,4,4.120
11596,0\C,13,1.41050672,12,119.97918346,11,-0.15229646,0\C,14,1.405716
4,13,119.36718558,12,0.32438596,0\C,15,1.39606648,14,119.90695832,13,-
0.31495469,0\H,12,1.0878437,11,119.51728488,4,-175.63588846,0\H,13,1.0
879084,12,119.09862561,11,179.59819312,0\H,15,1.08668088,14,120.448065
99,13,-179.85533325,0\H,16,1.08756851,15,119.16935851,14,-179.60338327
,0\C,5,5.2134584,4,95.18836477,3,-168.96281368,0\C,21,1.40872879,5,57.
345652,4,74.94728056,0\C,22,1.39142084,21,121.1860728,5,-38.46490142,0
\C,23,1.41100953,22,119.99205596,21,-0.0243813,0\C,24,1.4053222,23,119
.36056888,22,0.2704971,0\C,25,1.39663307,24,119.90163984,23,-0.2508120
9,0\H,22,1.08775931,21,119.53673907,5,141.63349585,0\H,23,1.08785845,2
2,119.10392596,21,179.4608053,0\H,25,1.08667983,24,120.43699252,23,179
.98277039,0\H,26,1.08759763,25,119.17425762,24,-179.88834624,0\C,11,1.
51069103,4,162.85772976,3,-57.39419577,0\H,31,1.09855735,11,110.535642
51,4,-114.55912868,0\H,31,1.09461967,11,111.54274795,4,5.24108541,0\H,
31,1.09613747,11,111.26668665,4,126.39490584,0\P,4,1.80532207,3,119.85
091249,2,179.39741121,0\C,35,1.82707338,4,108.33598569,3,48.07545285,0
\H,36,1.09463854,35,109.92155746,4,58.27640899,0\H,36,1.09468339,35,10
9.90435354,4,178.27514854,0\H,36,1.09463934,35,109.90915695,4,-61.7264
745,0\C,21,1.51082994,5,147.76317295,4,171.44837405,0\H,40,1.09725388,
21,111.03696813,5,-21.10566079,0\H,40,1.09427752,21,111.53132013,5,99.
65952776,0\H,40,1.09782885,21,110.77964125,5,-140.07115287,0\C,1,1.511
14917,6,121.23675333,5,-178.90656489,0\H,44,1.09877925,1,110.67369276,
6,106.63795022,0\H,44,1.09670342,1,111.16955977,6,-134.29031199,0\H,44
,1.09461757,1,111.52605481,6,-13.35587705,0\|Version=AM64L-G03RevD.01\
State=1-A\HF=-1187.7354701\MP2=-1191.0005934\RMSD=3.971e-09\Thermal=0.
\PG=C01 [X(C22H24P1)]\|@

5g

5g_1

1\1\GINC-PHOBOS\SP\RMP2-FC\6-31+G(2d,p)\C30H39P1\CHRISTOPH\23-Oct-2011
\0\#p MP2(FC)/6-31+g(2d,p) scf=tight\|btol3sp_77_2\|0,1\P\C,1,4.7071
4272\C,2,1.40905443,1,56.92825965\C,3,1.39323402,2,121.58204733,1,0.03
447206,0\C,4,1.40821163,3,121.13673552,2,0.9991844,0\C,5,1.40213414,4,
117.61259924,3,-1.10042832,0\C,6,1.40080662,5,120.98248727,4,0.5111349
,0\H,3,1.0882956,2,119.92827551,1,-179.23688509,0\H,4,1.08914011,3,119
.25722221,2,-178.85937697,0\H,6,1.08749574,5,119.94242313,4,-179.23654
539,0\H,7,1.08628259,6,118.1828569,5,-179.84556425,0\C,1,4.7067025,5,1
04.38118171,4,-85.05443101,0\C,12,1.40406442,1,57.10876371,5,160.86188
38,0\C,13,1.39853322,12,121.36508285,1,-0.32426835,0\C,14,1.40354537,1
3,121.30293403,12,0.77834621,0\C,15,1.40643259,14,117.65328962,13,-1.0
729913,0\C,16,1.39539296,15,120.79292605,14,0.6844537,0\H,13,1.0859229
6,12,120.33806205,1,-179.74563703,0\H,14,1.08906579,13,119.15798258,12
, -179.01994553,0\H,16,1.08771121,15,119.80099261,14,-179.02503264,0\H,

17,1.088353,16,118.37802205,15,-179.96270022,0\C,1,4.70614686,15,104.4
9283434,14,-92.06035434,0\C,22,1.40385939,1,57.14171716,15,161.1040403
8,0\C,23,1.39860422,22,121.38056182,1,-0.0880691,0\C,24,1.40387566,23,
121.27124414,22,0.84598221,0\C,25,1.40613992,24,117.64604539,23,-0.951
83324,0\C,26,1.39530128,25,120.83542955,24,0.48037715,0\H,23,1.0858680
6,22,120.20469428,1,-179.43076927,0\H,24,1.08905613,23,119.184161,22,-
178.88313159,0\H,26,1.08740708,25,119.84439968,24,-179.07893349,0\H,27
,1.08834963,26,118.39072972,25,-179.86908409,0\C,2,1.54167892,1,176.87
121158,25,156.23684041,0\C,32,1.55028097,2,109.35463668,1,-48.06256025
,0\H,33,1.09716857,32,110.83825967,2,-60.78271925,0\H,33,1.09635616,32
,111.77505537,2,59.5167772,0\H,33,1.09836633,32,110.2931159,2,179.4285
768,0\C,32,1.5433274,2,112.37872295,1,-168.18473471,0\H,37,1.09732276,
32,111.82485265,2,61.19056668,0\H,37,1.09720767,32,109.56004483,2,-179
.6469764,0\H,37,1.09744458,32,111.79736325,2,-60.45657429,0\C,32,1.550
3909,2,109.46115428,1,71.70350323,0\H,41,1.09833425,32,110.28031568,2,
-179.61488,0\H,41,1.09633085,32,111.84634872,2,-59.7394827,0\H,41,1.09
730346,32,110.86228145,2,60.62164725,0\C,12,1.54191369,1,179.91759551,
25,89.1529096,0\C,45,1.55054818,12,109.35132132,1,-61.35434575,0\H,46,
1.09726355,45,110.87547879,12,-60.75919485,0\H,46,1.09644253,45,111.80
683489,12,59.60073061,0\H,46,1.09831963,45,110.25451791,12,179.4772863
3,0\C,45,1.55029034,12,109.47461576,1,58.40555747,0\H,50,1.09636266,45
,111.82856206,12,-59.72243649,0\H,50,1.09714452,45,110.83747345,12,60.
61787037,0\H,50,1.09832197,45,110.22525592,12,-179.60895355,0\C,45,1.5
4352425,12,112.37069499,1,178.56334092,0\H,54,1.09722625,45,109.566388
52,12,179.64081556,0\H,54,1.09735762,45,111.79271351,12,-61.18609407,0
\H,54,1.09734246,45,111.806426,12,60.45334369,0\C,22,1.54173272,1,179.
73842828,25,104.41312554,0\C,58,1.55031968,22,109.52294957,1,-34.57866
873,0\H,59,1.09644936,58,111.85746075,22,-60.20768785,0\H,59,1.0971522
6,58,110.881249,22,60.16527558,0\H,59,1.09830533,58,110.22723905,22,17
9.92563604,0\C,58,1.54352371,22,112.3346384,1,85.55426146,0\H,63,1.097
37897,58,111.79027905,22,-60.8635964,0\H,63,1.09737089,58,111.83084368
,22,60.7858419,0\H,63,1.09729973,58,109.59719292,22,179.94907776,0\C,5
8,1.55039952,22,109.35884982,1,-154.39320232,0\H,67,1.09832249,58,110.
26797207,22,179.48964021,0\H,67,1.09733054,58,110.85837806,22,-60.7917
7062,0\H,67,1.09641691,58,111.80725778,22,59.55612604,0\\Version=AM64L
-G03RevD.01\\State=1-A\\HF=-1499.6072887\\MP2=-1504.146465\\RMSD=9.564e-09
\\Thermal=0.\\PG=C01 [X(C30H39P1)]\\@

5g_2

1\1\GINC-PHOBOS\SP\RMP2-FC\6-31+G(2d,p)\C30H39P1\CHRISTOPH\24-Oct-2011
\0\\#p MP2(FC)/6-31+g(2d,p) scf=tight\\tbtol3sp_75_2\\0,1\P\C,1,4.7068
113\C,2,1.40863713,1,57.00643977\C,3,1.39384705,2,121.59114923,1,0.107
53457,0\C,4,1.40776018,3,121.10213432,2,-0.84536627,0\C,5,1.40251124,4
,117.62459559,3,0.96795206,0\C,6,1.40016114,5,121.01484074,4,-0.454303
81,0\H,3,1.08809147,2,119.87674016,1,179.46467977,0\H,4,1.08903813,3,1
19.32934886,2,178.97310628,0\H,6,1.08752479,5,119.87789716,4,179.36182
408,0\H,7,1.08616437,6,118.18785312,5,179.90672076,0\C,1,4.7069663,5,1
02.91726516,4,-161.0774814,0\C,12,1.40889567,1,57.01825163,5,88.011831
61,0\C,13,1.39360809,12,121.61400489,1,0.0644558,0\C,14,1.40781396,13,
121.08521251,12,-0.91523867,0\C,15,1.40227941,14,117.63155839,13,1.044
67852,0\C,16,1.40035322,15,121.02340522,14,-0.50782791,0\H,13,1.087986

23,12,119.84971434,1,179.43481987,0\H,14,1.08906701,13,119.34368706,12,
178.92234256,0\H,16,1.08747993,15,119.82786937,14,179.18389123,0\H,17,
1.08601708,16,118.14043006,15,179.88334212,0\C,1,4.70647691,5,104.601
02867,4,89.54382101,0\C,22,1.40900177,1,56.98709758,5,-166.02733182,0\
C,23,1.39361357,22,121.60617369,1,0.05341829,0\C,24,1.40804356,23,121.
0938371,22,-0.88019587,0\C,25,1.40203328,24,117.63497767,23,0.95691044
0\C,26,1.40045027,25,121.00800582,24,-0.41395201,0\H,23,1.08811789,22,
119.86861259,1,179.37813306,0\H,24,1.08899818,23,119.33614175,22,178.
96324786,0\H,26,1.08758902,25,119.86707828,24,179.28316465,0\H,27,1.08
595156,26,118.13415904,25,179.79222613,0\C,2,1.54171493,1,177.0233684,
25,95.69532053,0\C,32,1.54335193,2,112.30150328,1,173.73151456,0\H,33,
1.09731564,32,111.79930078,2,-60.87137979,0\H,33,1.09737704,32,111.767
92436,2,60.71677399,0\H,33,1.09724223,32,109.59646495,2,179.92392446,0\
C,32,1.55054751,2,109.40279158,1,53.61162343,0\H,37,1.09714511,32,110
.84679818,2,60.71354885,0\H,37,1.09828348,32,110.28392285,2,-179.50955
082,0\H,37,1.09636225,32,111.80315058,2,-59.59969327,0\C,32,1.55039121
,2,109.43033678,1,-66.19347411,0\H,41,1.09826944,32,110.26300882,2,179
.89269891,0\H,41,1.09727478,32,110.86095552,2,-60.35777443,0\H,41,1.09
629963,32,111.83942976,2,59.99193612,0\C,12,1.54192836,1,176.94236827,
25,-158.6919856,0\C,45,1.54347471,12,112.40217399,1,173.78481662,0\H,4
6,1.09729579,45,111.81940012,12,-61.00326829,0\H,46,1.09738001,45,111.
78643324,12,60.6494214,0\H,46,1.09725271,45,109.55590194,12,179.811730
11,0\C,45,1.55052867,12,109.35733897,1,-66.11701318,0\H,50,1.09722137,
45,110.85343037,12,-60.70440907,0\H,50,1.0963752,45,111.78472119,12,59
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049957,12,109.44927413,1,53.62465825,0\H,54,1.09829951,45,110.25771753
,12,-179.42978901,0\H,54,1.09631323,45,111.82687064,12,-59.53346701,0\
H,54,1.09717971,45,110.86066193,12,60.79702686,0\C,22,1.54193831,1,176
.88706784,25,177.5953661,0\C,58,1.55029621,22,109.46082279,1,-68.84865
611,0\H,59,1.09720336,58,110.85827183,22,-60.40701798,0\H,59,1.0962523
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79.84083045,0\C,58,1.55039929,22,109.35633855,1,50.83508197,0\H,63,1.0
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,22,60.5555775,0\H,63,1.09840936,58,110.2858631,22,-179.65781991,0\C,5
8,1.54361784,22,112.46317471,1,171.01021895,0\H,67,1.09730734,58,109.5
8568432,22,179.82901887,0\H,67,1.09723047,58,111.83512278,22,-60.96686
856,0\H,67,1.09735346,58,111.76288508,22,60.66917202,0\Version=AM64L-
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5g_3

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1121908,0\C,4,1.40795059,3,121.09373064,2,0.91164402,0\C,5,1.40227786,
4,117.64253369,3,-1.04055841,0\C,6,1.40037435,5,120.99423955,4,0.47550
478,0\H,3,1.08818599,2,119.87125782,1,-179.44184499,0\H,4,1.08908851,3
,119.31378439,2,-178.91818826,0\H,6,1.08758554,5,119.88800891,4,-179.3
0611964,0\H,7,1.08609368,6,118.15083426,5,-179.88438551,0\C,1,4.706257
02,5,104.54096114,4,-87.84501277,0\C,12,1.40853819,1,57.01691167,5,164
.08972141,0\C,13,1.39381382,12,121.59508884,1,-0.07428602,0\C,14,1.407

61948,13,121.08829866,12,0.83829927,0\C,15,1.40243505,14,117.65240088,
13,-0.97261327,0\C,16,1.40013616,15,120.99806041,14,0.48309776,0\H,13,
1.08813072,12,119.88470936,1,-179.44693732,0\H,14,1.08909039,13,119.32
861585,12,-178.91203587,0\H,16,1.08748714,15,119.85705461,14,-179.2479
7214,0\H,17,1.08614578,16,118.16605931,15,-179.85898773,0\C,1,4.706189
92,5,102.84251158,4,162.68802129,0\C,22,1.40893236,1,56.99842799,5,-87
.31342856,0\C,23,1.39352028,22,121.60150787,1,-0.07220337,0\C,24,1.408
03507,23,121.08858424,22,0.92676801,0\C,25,1.40204353,24,117.64079828,
23,-1.02572587,0\C,26,1.40042004,25,121.0075601,24,0.44368237,0\H,23,1
.08811563,22,119.86241105,1,-179.38159561,0\H,24,1.08909985,23,119.331
82296,22,-178.8823739,0\H,26,1.08746523,25,119.85890836,24,-179.302639
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1,176.95834469,25,158.93007003,0\C,32,1.55031029,2,109.41023386,1,66.4
5259374,0\H,33,1.09638921,32,111.83614277,2,-59.56616192,0\H,33,1.0972
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,-179.4517464,0\C,32,1.55043749,2,109.37326896,1,-53.28866745,0\H,37,1
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438,2,179.52413276,0\H,37,1.09716866,32,110.8556344,2,-60.68510086,0\C
,32,1.54350752,2,112.38692233,1,-173.43745247,0\H,41,1.09728525,32,109
.60247599,2,-179.49046917,0\H,41,1.09739178,32,111.78186902,2,-60.2864
1806,0\H,41,1.09733851,32,111.79963373,2,61.32388676,0\C,12,1.54159971
,1,176.96779553,25,-95.82634996,0\C,45,1.55065891,12,109.41523531,1,-5
3.78605014,0\H,46,1.09723595,45,110.85804979,12,-60.90240876,0\H,46,1
.09642459,45,111.8261634,12,59.40850154,0\H,46,1.09837837,45,110.273461
96,12,179.3221924,0\C,45,1.55037431,12,109.40280569,1,65.95779021,0\H,
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.86158129,12,61.26810227,0\H,50,1.0983175,45,110.26339992,12,-178.9712
5525,0\C,45,1.54348753,12,112.36684121,1,-173.93864605,0\H,54,1.097317
85,45,109.58491779,12,179.99126267,0\H,54,1.09743236,45,111.77380272,1
2,-60.83815486,0\H,54,1.09729778,45,111.82551697,12,60.78648777,0\C,22
,1.54168668,1,176.92070878,25,-175.72307065,0\C,58,1.55044619,22,109.3
9982215,1,-52.20116415,0\H,59,1.09718881,58,110.86485982,22,-60.236858
15,0\H,59,1.09641785,58,111.79138144,22,60.0942122,0\H,59,1.0983427,58
,110.26817632,22,179.97647558,0\C,58,1.55045028,22,109.39403188,1,67.5
358228,0\H,63,1.09629218,58,111.78789966,22,-59.8252608,0\H,63,1.09727
438,58,110.8689351,22,60.52789467,0\H,63,1.09835941,58,110.28211359,22
, -179.69840888,0\C,58,1.54351067,22,112.39961154,1,-172.34395231,0\H,6
7,1.0972466,58,109.55550321,22,-179.57357156,0\H,67,1.09742817,58,111.
81177361,22,-60.39233571,0\H,67,1.09731218,58,111.79022984,22,61.25359
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5g_4

1\1\GINC-PHOBOS\SP\RMP2-FC\6-31+G(2d,p)\C30H39P1\CHRISTOPH\24-Oct-2011
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406\C,2,1.40883846,1,57.01294616\C,3,1.39381893,2,121.58865051,1,-0.02
613368,0\C,4,1.40790232,3,121.08357001,2,0.93378562,0\C,5,1.40206326,4
,117.6506746,3,-1.00076862,0\C,6,1.40014698,5,121.01156851,4,0.4494573
8,0\H,3,1.08819787,2,119.86957557,1,-179.30593128,0\H,4,1.08907777,3,1
19.33564867,2,-178.82754082,0\H,6,1.08756855,5,119.8580036,4,-179.2370
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5,104.76314694,4,-88.51052365,0\C,12,1.40888137,1,56.97420415,5,165.83
715913,0\C,13,1.39335995,12,121.60053429,1,-0.0934039,0\C,14,1.4079747
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1.02967507,0\C,16,1.40058982,15,120.99902438,14,0.46393118,0\H,13,1.08
813684,12,119.86720944,1,-179.41166685,0\H,14,1.08904589,13,119.307592
85,12,-178.90817989,0\H,16,1.08747553,15,119.88470327,14,-179.329385,0
\H,17,1.0861775,16,118.18891617,15,-179.84871738,0\C,1,4.70614662,5,10
2.80264713,4,162.00353681,0\C,22,1.40808927,1,59.91440614,5,90.3087399
3,0\C,23,1.39549466,22,121.85461192,1,-0.34627255,0\C,24,1.40613053,23
,120.79767459,22,0.19669874,0\C,25,1.40401414,24,117.64815509,23,0.517
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79.96866973,0\H,26,1.08909634,25,119.57316323,24,178.79206536,0\H,27,1
.08594505,26,118.34071159,25,-179.64001027,0\C,2,1.54150219,1,176.9005
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32,111.79173646,2,60.87559989,0\H,37,1.09716265,32,109.56758559,2,-179
.94303405,0\H,37,1.09743243,32,111.79708993,2,-60.74594547,0\C,32,1.55
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2,-179.62781691,0\H,41,1.09633895,32,111.78536699,2,-59.74986402,0\H,4
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,111.78541526,12,60.95069099,0\H,46,1.09734717,45,109.61146848,12,-179
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.26692987,12,-179.71341418,0\H,54,1.09634777,45,111.81416852,12,-59.82
286587,0\H,54,1.09729456,45,110.87559225,12,60.5224957,0\C,22,1.541603
34,1,179.74345499,5,167.33251114,0\C,58,1.55033349,22,109.3767977,1,-1
6.60369567,0\H,59,1.09638191,58,111.7384292,22,-59.96904437,0\H,59,1.0
971524,58,110.85016958,22,60.32470527,0\H,59,1.09832957,58,110.2933916
2,22,-179.87452581,0\C,58,1.54362084,22,112.33660651,1,103.54226615,0\
H,63,1.09733243,58,111.82037654,22,-61.11479751,0\H,63,1.09741802,58,1
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784402,0\C,58,1.55046641,22,109.42409306,1,-136.37095795,0\H,67,1.0982
3747,58,110.25981851,22,179.78743265,0\H,67,1.09722634,58,110.86239349
,22,-60.4684173,0\H,67,1.09637431,58,111.84248767,22,59.92858888,0\\Ve
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5g_5

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7435,0\\C,4,1.40799413,3,121.09722958,2,-0.9058479,0\\C,5,1.40212659,4,1
17.6404395,3,1.06186243,0\\C,6,1.4003723,5,121.00098507,4,-0.50300812,0
\\H,3,1.08816768,2,119.87154981,1,179.38003183,0\\H,4,1.08908109,3,119.3

2655163,2,178.92627248,0\H,6,1.08745905,5,119.85056079,4,179.2813381,0
\H,7,1.08606808,6,118.18381679,5,179.85514906,0\C,1,4.7066952,5,104.49
971488,4,87.82944182,0\C,12,1.40325045,1,60.01116554,5,14.27373728,0\C
,13,1.40039553,12,121.64703286,1,0.48054966,0\C,14,1.4023752,13,121.00
107445,12,-0.22221572,0\C,15,1.40795988,14,117.63199679,13,-0.45777064
,0\C,16,1.39355631,15,121.09932208,14,1.01880146,0\H,13,1.08611238,12,
120.17767838,1,-179.58339608,0\H,14,1.08763092,13,119.10895881,12,-179
.91872839,0\H,16,1.08905307,15,119.58329858,14,-178.80084927,0\H,17,1.
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05,4,-162.73661891,0\C,22,1.40815094,1,59.91588446,5,-89.32720008,0\C,
23,1.39547839,22,121.85965978,1,0.40153217,0\C,24,1.40618081,23,120.79
906268,22,-0.15478484,0\C,25,1.40394299,24,117.64295199,23,-0.4630214,
0\C,26,1.39847944,25,121.29766732,24,0.97651535,0\H,23,1.08837224,22,1
19.79720111,1,-179.58350434,0\H,24,1.08750875,23,119.32734206,22,-179.
81750322,0\H,26,1.08908448,25,119.56300892,24,-178.77210787,0\H,27,1.0
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,5,175.37479391,0\C,32,1.54350378,2,112.40905305,1,173.17493653,0\H,33
,1.09728791,32,111.80515107,2,-60.95292332,0\H,33,1.09740189,32,111.81
426369,2,60.70979272,0\H,33,1.09728875,32,109.53945902,2,179.88000698,
0\C,32,1.55023682,2,109.3759812,1,53.01199473,0\H,37,1.09717567,32,110
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2,0\H,37,1.09639248,32,111.76471235,2,-59.79839303,0\C,32,1.55039947,2
,109.38084431,1,-66.69965383,0\H,41,1.09833156,32,110.26440987,2,179.5
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24,12,60.49618074,0\H,46,1.09830395,45,110.23941016,12,-179.72964947,0
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2,179.34340063,0\H,54,1.09728789,45,110.88977483,12,-60.8974452,0\H,54
,1.09640575,45,111.79940694,12,59.44661773,0\C,22,1.54153024,1,179.552
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\H,59,1.09716452,58,110.85865564,22,-60.61387326,0\H,59,1.09637594,58,
111.78754632,22,59.70030806,0\H,59,1.09831373,58,110.26869117,22,179.6
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5693,58,111.83732776,22,-59.78079469,0\H,63,1.09726873,58,110.86987618
,22,60.58694072,0\H,63,1.09829704,58,110.26456076,22,-179.66436609,0\C
,58,1.54350892,22,112.33782437,1,-97.32476987,0\H,67,1.09723294,58,109
.59338881,22,-179.78173997,0\H,67,1.0973601,58,111.80011273,22,-60.567
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9\Thermal=0.\PG=C01 [X(C30H39P1)]\@

5g_6

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5g_7

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5g-Me⁺

5g-Me⁺_1

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5g-Me⁺_2

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,179.81850659,0\H,50,1.09691065,49,111.107826,22,-60.73711532,0\C,49,1
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54,1.09678308,49,109.73333049,22,-179.55502995,0\C,49,1.54339896,22,11
2.34571757,1,171.49959902,0\H,58,1.09600214,49,109.32424874,22,-179.93
002602,0\H,58,1.09740747,49,111.9864065,22,-61.10150926,0\H,58,1.09738
339,49,112.02163251,22,61.1878946,0\C,2,1.53917015,1,178.24583103,25,6
3.56427278,0\C,62,1.55144953,2,109.07781438,1,-53.72945752,0\H,63,1.09
651492,62,112.12385126,2,60.33047201,0\H,63,1.09681887,62,109.8032555,

2,179.86640498,0\H,63,1.09703808,62,111.09442649,2,-60.71354452,0\C,62
,1.5512444,2,109.08262491,1,65.91463584,0\H,67,1.09647604,62,112.17353
924,2,-60.28600534,0\H,67,1.09699158,62,111.09695928,2,60.74548514,0\H
,67,1.09684852,62,109.76510139,2,-179.83944941,0\C,62,1.54317569,2,112
.30126397,1,-173.88909264,0\H,71,1.09600775,62,109.34855148,2,-179.881
59674,0\H,71,1.09742249,62,112.01983181,2,-60.99413528,0\H,71,1.097413
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\HF=-1539.0691056\MP2=-1543.7506323\RMSD=9.169e-09\Thermal=0.\PG=C01 [X(C31H42P1)]\@

5g-Me⁺_3

1\1\GINC-PHOENIX\SP\RMP2-FC\6-31+G(2d,p)\C31H42P1(1+)\CHRISTOPH\19-Oct
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0.35192748,0\C,4,1.40346043,3,120.17477734,2,0.04748706,0\C,5,1.410257
4,4,119.00634728,3,-0.23677003,0\C,6,1.3906222,5,120.02270392,4,0.2431
6464,0\H,3,1.08490224,2,120.20338542,1,-179.78969835,0\H,4,1.08687993,
3,119.41221684,2,179.78324317,0\H,6,1.08803758,5,120.91323315,4,-179.2
6034137,0\H,7,1.08667162,6,118.34375883,5,179.82140641,0\C,1,4.6451705
,5,110.74524507,4,108.20082213,0\C,12,1.40462678,1,58.78806002,5,-13.8
1428242,0\C,13,1.39770518,12,121.68080213,1,0.24836681,0\C,14,1.403582
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, -0.22854239,0\C,16,1.39065266,15,120.01274666,14,0.2680601,0\H,13,1.0
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983,12,179.61879984,0\H,16,1.08808003,15,120.92610712,14,-179.35284134
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110.27486641,4,-14.61516564,0\C,22,1.41206224,1,58.46122354,5,-69.0458
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,23,120.02370398,22,-0.0179774,0\C,25,1.40334053,24,119.02764712,23,0.
26752691,0\C,26,1.39779879,25,120.14544006,24,-0.28639928,0\H,23,1.086
61202,22,119.81870787,1,179.92176844,0\H,24,1.08816036,23,119.06996006
,22,179.44998546,0\H,26,1.08680861,25,120.41682836,24,179.91095402,0\H
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39299364,4,-132.92466582,0\H,32,1.09471791,1,109.89804464,5,178.353130
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109.85028284,5,58.43169294,0\C,12,1.53907419,1,178.34186735,5,164.4357
1926,0\C,36,1.54333724,12,112.29876366,1,-178.50286815,0\H,37,1.097453
58,36,111.98317466,12,-61.07379464,0\H,37,1.09741387,36,112.00199656,1
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,1.55136565,12,109.12099565,1,61.27240434,0\H,41,1.09707099,36,111.101
03147,12,60.7191742,0\H,41,1.09683651,36,109.77872145,12,-179.86178784
,0\H,41,1.09651574,36,112.11029428,12,-60.34154329,0\C,36,1.55142737,1
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.87213201,0\H,45,1.09704308,36,111.10650262,12,-60.69936866,0\H,45,1.0
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49,112.10712132,22,-60.16703614,0\H,54,1.09713496,49,111.12249099,22,6
0.88586014,0\H,54,1.09687723,49,109.77724724,22,-179.69053515,0\C,49,1

.54323671,22,112.32537637,1,-178.22174308,0\H,58,1.09603309,49,109.33588245,22,179.86247544,0\H,58,1.097432,49,112.00378655,22,-61.27410718,0\H,58,1.09743087,49,111.98203352,22,60.97853375,0\C,2,1.53919868,1,178.32837901,5,117.0844555,0\C,62,1.54326345,2,112.31068761,1,172.21494756,0\H,63,1.09741172,62,111.9865429,2,61.24828393,0\H,63,1.09602251,62,109.33555756,2,-179.88855068,0\H,63,1.09744239,62,111.99688679,2,-60.9954584,0\C,62,1.55138542,2,109.10253682,1,-67.59040017,0\H,67,1.09701503,62,111.0991194,2,-60.6906771,0\H,67,1.09642438,62,112.13222964,2,60.34169245,0\H,67,1.09691932,62,109.78179273,2,179.8771231,0\C,62,1.55144803,2,109.09242653,1,52.02329138,0\H,71,1.09691776,62,109.76111128,2,-179.7707624,0\H,71,1.09644693,62,112.11453178,2,-60.26529232,0\H,71,1.09706805,62,111.11816965,2,60.78077824,0\Version=AM64L-G03RevD.01\State=1-A\HF=-1539.0693595\MP2=-1543.7507654\RMSD=6.718e-09\Thermal=0.\PG=C01 [X(C31H42P1)]\@

5g-Me⁺_4

1\1\GINC-PHOBOS\SP\RMP2-FC\6-31+G(2d,p)\C31H42P1(1+)\CHRISTOPH\19-Oct-2011\0\#p MP2(FC)/6-31+g(2d,p) scf=tight\btol3mesp_69\1,1\P\C,1,4.64484598\C,2,1.40471625,1,58.75973494\C,3,1.39765996,2,121.67693308,1,-0.54564718,0\C,4,1.40371385,3,120.16699437,2,0.04906808,0\C,5,1.41015278,4,119.0192833,3,0.25762052,0\C,6,1.39077925,5,120.01205932,4,-0.3698051,0\H,3,1.08483958,2,120.19494993,1,179.63191202,0\H,4,1.08688163,3,119.42443282,2,-179.70657438,0\H,6,1.08783926,5,120.92618261,4,179.25635437,0\H,7,1.08651947,6,118.35379417,5,-179.69386153,0\C,1,4.6458618,5,110.23803408,4,18.39927467,0\C,12,1.40904769,1,58.85681978,5,-112.28889807,0\C,13,1.39340302,12,121.9303347,1,0.00437286,0\C,14,1.40651608,13,119.91792044,12,-0.05352838,0\C,15,1.40686168,14,119.05343082,13,0.35995033,0\C,16,1.39500134,15,120.2249785,14,-0.3397209,0\H,13,1.0866434,12,119.80114361,1,-179.85093236,0\H,14,1.08672968,13,119.6224572,12,-179.85039757,0\H,16,1.08831047,15,120.85848838,14,179.11440565,0\H,17,1.08489496,16,118.20192288,15,-179.94506258,0\C,1,4.64553467,5,110.78115582,4,-104.70953955,0\C,22,1.40444815,1,58.78929529,5,12.06938167,0\C,23,1.39786714,22,121.69512327,1,-0.2251851,0\C,24,1.40324257,23,120.16531002,22,-0.08394176,0\C,25,1.41049412,24,119.01965696,23,0.17780473,0\C,26,1.39062682,25,120.00901557,24,-0.14336654,0\H,23,1.08496059,22,120.24863763,1,179.81116609,0\H,24,1.08680666,23,119.3915531,22,-179.87488552,0\H,26,1.08818246,25,120.91778535,24,179.41388722,0\H,27,1.08671917,26,118.34960563,25,-179.85076804,0\C,1,1.82758497,5,108.52001317,4,136.26700348,0\H,32,1.09474675,1,109.71860751,5,-178.12075946,0\H,32,1.09473683,1,109.85965608,5,-58.34660152,0\H,32,1.09469977,1,110.11750399,5,61.94116987,0\C,12,1.53945746,1,178.72164937,5,-129.8057369,0\C,36,1.55109191,12,109.22265976,1,76.20164297,0\H,37,1.09648188,36,112.16790726,12,-60.3726942,0\H,37,1.0970776,36,111.14070092,12,60.70156607,0\H,37,1.09685635,36,109.758008,12,-179.86608851,0\C,36,1.55144795,12,108.93065725,1,-43.38556837,0\H,41,1.09643424,36,112.00877849,12,60.10437355,0\H,41,1.09690837,36,109.82461546,12,179.67521896,0\H,41,1.09700832,36,111.11229621,12,-60.82762312,0\C,36,1.54344465,12,112.34744649,1,-163.55138579,0\H,45,1.09596801,36,109.35785027,12,-179.84850828,0\H,45,1.09753035,36,111.98236147,12,-60.95935825,0\H,45,1.09745841,36,112.02601846,12,61.28005428,0\C,22,1.53903164,1,178.30853019,5,-169.98398081,0\C,49,1.54317088,22,112.27070169,1,-177.22204389,0\H,

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5g-Me⁺_5

1\1\GINC-PHOBOS\SP\RMP2-FC\6-31+G(2d,p)\C31H42P1(1+)\CHRISTOPH\19-Oct-2011\0\#p MP2(FC)/6-31+g(2d,p) scf=tight\btol3mesp_45\1,1\PC,1,4.64512879\C,2,1.41202404,1,58.39084531\C,3,1.39035453,2,121.80252061,1,0.12144563,0\C,4,1.41056708,3,120.02615246,2,-0.03744344,0\C,5,1.40323995,4,119.04017413,3,-0.27363246,0\C,6,1.39810438,5,120.1275511,4,0.32563734,0\H,3,1.08658784,2,119.81016353,1,179.99384202,0\H,4,1.08815164,3,119.08870233,2,-179.48279557,0\H,6,1.08680146,5,120.41558382,4,-179.97410736,0\H,7,1.08491238,6,118.13593371,5,179.79283371,0\C,1,4.64470465,5,110.55361471,4,-168.80759719,0\C,12,1.4045069,1,58.83253327,5,-109.68461516,0\C,13,1.39779418,12,121.67546982,1,-0.11126478,0\C,14,1.40342278,13,120.14822681,12,0.0185795,0\C,15,1.41049149,14,119.04373074,13,0.27132007,0\C,16,1.39051659,15,119.99879022,14,-0.28583562,0\H,13,1.08479355,12,120.15176097,1,-179.94343809,0\H,14,1.08683054,13,119.4696902,12,-179.63257734,0\H,16,1.0880319,15,120.89762132,14,179.32146128,0\H,17,1.08656012,16,118.42423646,15,-179.80331246,0\C,1,4.6457037,15,110.08854153,14,13.5998443,0\C,22,1.40716906,1,58.54779034,15,71.3309266,0\C,23,1.39513008,22,121.61704742,1,0.33410154,0\C,24,1.40660254,23,120.23367575,22,0.03345481,0\C,25,1.40720207,24,118.99364167,23,-0.26214788,0\C,26,1.39315653,25,119.96457459,24,0.26717859,0\H,23,1.08484239,22,120.16616559,1,-179.80575268,0\H,24,1.08800326,23,118.83717757,22,-179.49862037,0\H,26,1.08677097,25,120.42439858,24,179.93421644,0\H,27,1.08664297,26,118.27106891,25,179.77131566,0\C,1,1.82744303,15,108.24970711,14,132.14710138,0\H,32,1.09464401,1,110.04820061,15,-60.03095845,0\H,32,1.09472873,1,109.76682066,15,59.95413975,0\H,32,1.09468563,1,109.86681876,15,179.79200638,0\C,12,1.53944493,1,178.20636766,15,-135.51878962,0\C,36,1.5432322,12,112.3253778,1,168.61592728,0\H,37,1.0973262,36,111.99074024,12,-61.43197638,0\H,37,1.0973899,36,111.97575944,12,60.85090825,0\H,37,1.09602006,36,109.33228955,12,179.72619067,0\C,36,1.55168304,12,108.94226806,1,48.47599394,0\H,41,1.09695452,36,111.10214963,12,60.84973435,0\H,41,1.09687053,36,109.75789995,12,-179.698

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1.09637503,36,112.18886867,12,60.4312885,0\C,22,1.5395364,1,178.723245
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22,60.67323777,0\H,54,1.09686214,49,109.76783417,22,-179.91583795,0\C,
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,178.13462887,15,-163.677391,0\C,62,1.55147501,2,109.10088166,1,-64.95
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639052,62,112.08296891,2,-60.07493542,0\H,67,1.09693035,62,111.1117341
4,2,60.94325648,0\H,67,1.09676558,62,109.76467446,2,-179.58103103,0\C,
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02,0\H,71,1.09738639,62,112.01616539,2,61.23106284,0\Version=AM64L-GO
3RevD.01\State=1-A\HF=-1539.0691762\MP2=-1543.7506707\RMSD=7.328e-09\T
hermal=0.\PG=C01 [X(C31H42P1)]\@

5g-Me⁺_6

1\1\GINC-PHOBOS\SP\RMP2-FC\6-31+G(2d,p)\C31H42P1(1+)\CHRISTOPH\21-Oct-
2011\0\#p MP2(FC)/6-31+g(2d,p) scf=tight\btol3mesp_35_2\1,1\PC,1,
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1,-0.21515374,0\C,4,1.40740685,3,119.96138339,2,0.02815014,0\C,5,1.406
59904,4,119.00458063,3,0.342158,0\C,6,1.39533688,5,120.22492734,4,-0.4
0981757,0\H,3,1.08666996,2,119.83569866,1,-179.93737852,0\H,4,1.086873
85,3,119.62892911,2,-179.50067328,0\H,6,1.08793863,5,120.9521597,4,179
.27672535,0\H,7,1.08489777,6,118.18460662,5,-179.78727219,0\C,1,4.6457
7552,5,109.99754357,4,16.30789052,0\C,12,1.40754926,1,58.53010071,5,71
.81556347,0\C,13,1.39511488,12,121.60213663,1,0.23887027,0\C,14,1.4064
3407,13,120.22278328,12,0.16194889,0\C,15,1.40713344,14,119.03425272,1
3,-0.39534097,0\C,16,1.3931325,15,119.95859086,14,0.31968948,0\H,13,1.
0847006,12,120.17110436,1,-179.91721284,0\H,14,1.08800138,13,118.85435
927,12,-179.49648666,0\H,16,1.08680285,15,120.4110918,14,179.90850235,
0\H,17,1.08656735,16,118.29549141,15,179.67126817,0\C,1,4.64572752,5,1
11.04924756,4,-106.63001718,0\C,22,1.40714018,1,58.52962422,5,-168.689
59173,0\C,23,1.39491852,22,121.61601921,1,0.02468156,0\C,24,1.4067528,
23,120.21763119,22,0.08188247,0\C,25,1.4067496,24,119.02394074,23,-0.3
222186,0\C,26,1.39324016,25,119.96073943,24,0.31402266,0\H,23,1.085007
03,22,120.14156171,1,179.84991445,0\H,24,1.08816156,23,118.88187879,22
, -179.52341992,0\H,26,1.08677414,25,120.42707564,24,179.99522379,0\H,2
7,1.08658451,26,118.26943748,25,179.73879182,0\C,1,1.82707279,5,108.41
186366,4,134.72717368,0\H,32,1.09464881,1,109.9136514,5,61.50525155,0\H,
32,1.09471338,1,109.74016123,5,-178.65804542,0\H,32,1.09456134,1,110
.01315765,5,-58.58843571,0\C,12,1.53944793,1,178.65438296,5,-118.33871

647,0\C,36,1.55138828,12,109.08307915,1,70.87501401,0\H,37,1.09644473,
36,112.08630539,12,-60.0214921,0\H,37,1.09704913,36,111.11907525,12,61
.00345538,0\H,37,1.09686033,36,109.75885327,12,-179.58847946,0\C,36,1.
55159833,12,109.11591711,1,-48.71664815,0\H,41,1.09638583,36,112.12355
426,12,60.62261805,0\H,41,1.09677642,36,109.75222322,12,-179.83389478,
0\H,41,1.09699439,36,111.12654975,12,-60.38426107,0\C,36,1.54349777,12
,112.36688548,1,-168.87366235,0\H,45,1.09595299,36,109.30904256,12,179
.70225469,0\H,45,1.09736861,36,112.02517647,12,-61.44646168,0\H,45,1.0
9743565,36,111.98794513,12,60.85813296,0\C,22,1.53959332,1,178.6840302
7,5,-6.67560952,0\C,49,1.55141115,22,109.18815178,1,76.28763268,0\H,50
,1.0970585,49,111.11300304,22,60.97130145,0\H,50,1.09676845,49,109.735
10011,22,-179.62376493,0\H,50,1.09622334,49,112.14284532,22,-60.087404
38,0\C,49,1.54344973,22,112.31566404,1,-163.49389885,0\H,54,1.09745655
,49,111.97903082,22,-60.27283438,0\H,54,1.09738337,49,111.99697503,22,
62.01826422,0\H,54,1.09602664,49,109.34469991,22,-179.11193321,0\C,49,
1.55144942,22,109.01789175,1,-43.34844643,0\H,58,1.09690567,49,109.781
83603,22,-179.99606089,0\H,58,1.09700554,49,111.12654635,22,-60.545071
76,0\H,58,1.09645484,49,112.06474567,22,60.44562271,0\C,2,1.53911419,1
,178.58736079,5,50.73185437,0\C,62,1.54353208,2,112.31726774,1,-171.62
363403,0\H,63,1.09736807,62,111.98423698,2,61.52135755,0\H,63,1.095994
65,62,109.33633304,2,-179.64484151,0\H,63,1.09745454,62,112.019384,2,-
60.75764199,0\C,62,1.55142237,2,109.0760492,1,-51.51707085,0\H,67,1.09
696091,62,111.10774024,2,-61.48498559,0\H,67,1.09635728,62,112.0901762
7,2,59.51916596,0\H,67,1.09689535,62,109.76584091,2,179.05754549,0\C,6
2,1.55137454,2,109.15820117,1,68.12219677,0\H,71,1.09680852,62,109.756
77085,2,179.93755749,0\H,71,1.09634363,62,112.09940178,2,-60.52620671,
0\H,71,1.09706544,62,111.13894576,2,60.52375163,0\Version=AM64L-G03Re
vD.01\State=1-A\HF=-1539.0689083\MP2=-1543.7505021\RMSD=7.331e-09\Ther
mal=0.\PG=C01 [X(C31H42P1)]\@

5g-Me⁺_7

1\1\GINC-PHOENIX\SP\RMP2-FC\6-31+G(2d,p)\C31H42P1(1+)\CHRISTOPH\19-Oct
-2011\0\#p MP2(FC)/6-31+g(2d,p) scf=tight\|tbtol3mesp_55\1,1\PC,1,4
.64625345\C,2,1.40695124,1,58.32410706\C,3,1.39419554,2,121.42655263,1
, -0.27992918,0\C,4,1.40648168,3,120.17855018,2,0.12729059,0\C,5,1.4036
4129,4,119.11316382,3,0.13597998,0\C,6,1.39459605,5,119.92685504,4,-0.
22837444,0\H,3,1.08383191,2,120.17959603,1,179.82785754,0\H,4,1.088995
85,3,119.38696361,2,-179.6310341,0\H,6,1.08899691,5,121.14238266,4,179
.38056945,0\H,7,1.08866365,6,118.52436228,5,-179.79586922,0\C,1,4.6388
7213,5,109.57519905,4,14.26868208,0\C,12,1.39555924,1,59.11146734,5,72
.08221257,0\C,13,1.39887801,12,121.21588361,1,0.38128936,0\C,14,1.4056
3894,13,120.24932532,12,0.02301132,0\C,15,1.4095053,14,119.11834546,13
, -0.20870834,0\C,16,1.39314571,15,119.79459211,14,0.15156372,0\H,13,1.
09107761,12,119.83755705,1,-179.65349858,0\H,14,1.08919913,13,118.7754
1555,12,-179.27084339,0\H,16,1.08874922,15,120.87914758,14,-179.984014
75,0\H,17,1.08931229,16,118.77511688,15,179.9277325,0\C,1,4.65052334,1
5,110.08850588,14,-165.35544037,0\C,22,1.40796231,1,58.80686487,15,-11
0.70922328,0\C,23,1.39250171,22,122.41164313,1,-0.11664604,0\C,24,1.40
431903,23,119.38767003,22,-0.07246609,0\C,25,1.40474264,24,119.4672517
6,23,0.35879165,0\C,26,1.39554186,25,120.38174103,24,-0.34637895,0\H,2
3,1.08535472,22,119.39266598,1,179.93465562,0\H,24,1.08546417,23,119.8

9071963,22,-179.83233386,0\H,26,1.09270172,25,120.65834262,24,179.2003
7481,0\H,27,1.08104386,26,117.81312863,25,-179.82127443,0\C,1,1.832131
73,15,108.1772437,14,-47.62321813,0\H,32,1.09810034,1,109.83111393,15,
-58.68228201,0\H,32,1.09790601,1,111.10588635,15,61.75655646,0\H,32,1.
09712731,1,109.37388377,15,-178.11285197,0\C,12,1.52446319,1,179.60602
38,15,84.91637077,0\C,36,1.55407299,12,109.74465493,1,49.76081285,0\H,
37,1.09504903,36,111.90257155,12,-60.38700132,0\H,37,1.09970752,36,111.
.4734789,12,60.64324581,0\H,37,1.09801459,36,110.48607306,12,-179.8392
5863,0\C,36,1.55171105,12,108.94065603,1,-69.91759608,0\H,41,1.0986217
,36,111.62095746,12,60.93238598,0\H,41,1.10029384,36,110.06811527,12,-
179.58896226,0\H,41,1.09946553,36,111.75938821,12,-60.05169942,0\C,36,
1.53709896,12,111.59128788,1,169.73676691,0\H,45,1.09617184,36,109.499
45604,12,179.40844232,0\H,45,1.10141642,36,112.02432366,12,-61.5612809
6,0\H,45,1.09862009,36,112.13889968,12,60.52211451,0\C,22,1.53937744,1
,176.06606943,15,-111.5550953,0\C,49,1.55041392,22,108.94233736,1,60.4
462703,0\H,50,1.09832053,49,111.4807875,22,61.20714495,0\H,50,1.099841
16,49,110.46461949,22,-179.15039411,0\H,50,1.09970749,49,111.95949969,
22,-59.74938138,0\C,49,1.54492538,22,113.3871754,1,-179.33997474,0\H,5
4,1.0993462,49,112.04983887,22,-61.27141786,0\H,54,1.10164435,49,112.7
2608152,22,61.06792827,0\H,54,1.09570898,49,109.3546879,22,-179.996500
23,0\C,49,1.54877766,22,108.36439531,1,-59.15916423,0\H,58,1.09832722,
49,110.49151917,22,179.23451949,0\H,58,1.09981845,49,111.22374073,22,-
61.2379556,0\H,58,1.09725838,49,111.7435708,22,59.64433808,0\C,2,1.531
69491,1,179.288112,15,14.97685202,0\C,62,1.54486864,2,108.71614952,1,5
8.85500534,0\H,63,1.10001081,62,111.00113976,2,60.59872763,0\H,63,1.10
028755,62,110.29739164,2,179.92741566,0\H,63,1.10029115,62,112.1497768
9,2,-60.3923315,0\C,62,1.54696273,2,112.2693357,1,179.02605646,0\H,67,
1.10116056,62,112.44779499,2,-61.01675562,0\H,67,1.10296454,62,112.260
59001,2,61.27434639,0\H,67,1.09729271,62,109.48640141,2,-179.83675357,
0\C,62,1.55228255,2,109.50533284,1,-60.82149535,0\H,71,1.09527229,62,1
10.39681369,2,179.57116455,0\H,71,1.09959248,62,111.26088136,2,-60.968
5687,0\H,71,1.09757705,62,112.34323362,2,60.11009367,0\Version=AM64L-
G03RevD.01\State=1-A\HF=-1539.0649378\MP2=-1543.7479099\RMSD=8.224e-09
\Thermal=0.\PG=C01 [X(C31H42P1)]\@@

5h

5h_1

1\1\GINC-EDDY\SP\RMP2-FC\6-31+G(2d,p)\C21H21P1\CHRISTOPH\16-Oct-2011\0
\#p MP2(FC)/6-31+g(2d,p) scf=tight\otol3sp_4\0,1\P\C,1,4.67071617\C
,2,1.39766614,1,59.04678464\C,3,1.40229374,2,121.63722595,1,-1.2293127
9,0\C,4,1.42032727,3,118.71878411,2,-0.48405216,0\C,5,1.40639789,4,119
.09398991,3,0.22586817,0\C,2,1.39553925,1,60.60318871,5,-69.42610906,0
\H,2,1.08794936,1,178.24538772,5,163.76495264,0\H,3,1.08892059,2,119.5
4591119,1,178.46637257,0\H,6,1.08708277,5,119.40157806,4,-179.7794642,
0\H,7,1.08791265,2,120.48767367,1,-178.63823255,0\C,1,4.67066497,5,103
.57876687,4,81.25170282,0\C,12,1.39586746,1,60.59024707,5,9.64381753,0
\C,13,1.39794544,12,119.61514326,1,1.41941488,0\C,14,1.4063216,13,121.
27801013,12,-0.25505308,0\C,15,1.41976154,14,119.12701216,13,0.1150279
3,0\C,12,1.39744985,1,59.06797138,5,-171.72202417,0\H,12,1.08797689,1,
178.3662417,5,-119.180696,0\H,13,1.0878995,12,120.49046278,1,-178.8097
1289,0\H,14,1.08714424,13,119.45075577,12,179.80855116,0\H,17,1.088886

57,12,119.53667199,1,178.60129192,0\C,1,4.67082252,5,104.83013489,4,-1
69.03986953,0\C,22,1.3957051,1,60.59674258,5,-97.19119509,0\C,23,1.398
00611,22,119.62531015,1,1.51127674,0\C,24,1.40647998,23,121.29335175,2
2,-0.31316819,0\C,25,1.41986365,24,119.0886391,23,0.30478888,0\C,22,1.
39746615,1,59.05114886,25,109.82379531,0\H,22,1.08795953,1,178.2871643
,25,163.52781084,0\H,23,1.08789796,22,120.48268952,1,-178.72848996,0\H
,24,1.0870586,23,119.34337396,22,179.65849607,0\H,27,1.08891585,22,119
.54072462,1,178.53086097,0\C,4,1.51469484,3,119.51625094,2,-179.578359
58,0\H,32,1.09789749,4,111.39393883,3,-127.19584982,0\H,32,1.09578301,
4,110.86155002,3,-6.52445611,0\H,32,1.09846482,4,111.44494003,3,113.55
876653,0\C,16,1.51482247,15,121.7966411,14,179.14562503,0\H,36,1.09580
124,16,110.89045419,15,172.79073855,0\H,36,1.09857411,16,111.35780295,
15,-67.20947208,0\H,36,1.09766228,16,111.45866799,15,52.0125567,0\C,26
,1.51486351,25,121.79207671,24,179.03049666,0\H,40,1.09574449,26,110.8
4936023,25,174.23958797,0\H,40,1.09857698,26,111.39665799,25,-65.73827
039,0\H,40,1.09773076,26,111.43369594,25,53.48361663,0\Version=AM6L-
G03RevD.01\State=1-A\HF=-1148.266021\MP2=-1151.4021269\RMSD=3.304e-09\
Thermal=0.PG=C01 [X(C21H21P1)]\@

5h_2

1\1\GINC-GOLEM\SP\RMP2-FC\6-31+G(2d,p)\C21H21P1\CHRISTOPH\16-Oct-2011\
0\#p MP2(FC)/6-31+g(2d,p) scf=tight\otol3sp_11\0,1\P\C,1,4.67360858
\C,2,1.39690682,1,58.89520937\C,3,1.40345246,2,121.7277935,1,-1.238998
31,0\C,4,1.41967587,3,118.70931859,2,-0.95378312,0\C,5,1.40661989,4,11
8.97605233,3,1.12964278,0\C,2,1.39626324,1,60.64026264,5,-69.33447343,
0\H,2,1.0878557,1,178.1611729,5,162.34362078,0\H,3,1.08894969,2,119.53
447839,1,178.25619826,0\H,6,1.08775555,5,119.33555301,4,-179.82976816,
0\H,7,1.08792293,2,120.49036673,1,-178.57945139,0\C,1,4.66773579,5,109
.55184155,4,69.54548163,0\C,12,1.39502285,1,56.9080723,5,-142.02242094
,0\C,13,1.3964736,12,119.12374961,1,0.01188752,0\C,14,1.40957953,13,12
2.01271547,12,-0.75630221,0\C,15,1.42132446,14,118.7879287,13,0.570082
57,0\C,12,1.39688205,1,62.73396777,5,38.39124323,0\H,12,1.08799767,1,1
77.39093715,5,-135.65704554,0\H,13,1.08756858,12,120.71784144,1,179.63
294442,0\H,14,1.08849276,13,119.40992993,12,179.02977001,0\H,17,1.0889
375,12,119.2833326,1,-179.86114585,0\C,1,4.6699179,5,106.84440591,4,-1
75.25701425,0\C,22,1.39545498,1,60.50123432,5,-105.63169382,0\C,23,1.3
9743691,22,119.67050097,1,2.02298329,0\C,24,1.4066556,23,121.43303913,
22,0.04996239,0\C,25,1.42175529,24,118.88377901,23,-1.44109439,0\C,22,
1.3971088,1,59.03178139,25,102.59151158,0\H,22,1.08787207,1,178.072894
13,25,162.39164695,0\H,23,1.08785387,22,120.50591163,1,-177.98140648,0
\H,24,1.08655041,23,119.12671513,22,-179.13798253,0\H,27,1.08890638,22
,119.54228427,1,177.75991226,0\C,4,1.51489171,3,119.31904925,2,179.502
0156,0\H,32,1.0957339,4,110.78274103,3,-8.24786478,0\H,32,1.09804927,4
,111.74198799,3,112.06965972,0\H,32,1.09839557,4,111.26226877,3,-128.7
0374471,0\C,16,1.51532986,15,123.57471438,14,179.91612865,0\H,36,1.094
84609,16,111.9436006,15,46.08941495,0\H,36,1.09606602,16,110.23583077,
15,166.48606935,0\H,36,1.09694761,16,111.59950948,15,-73.61049716,0\C,
26,1.51498125,25,122.01677932,24,-177.74474419,0\H,40,1.09799386,26,11
1.85623826,25,-67.36824773,0\H,40,1.09818335,26,111.18163204,25,51.942
47318,0\H,40,1.09565302,26,110.73707507,25,172.28478941,0\Version=AM6
4L-G03RevD.01\State=1-A\HF=-1148.2600639\MP2=-1151.3992458\RMSD=5.448e

-09\Thermal=0.\PG=C01 [X(C21H21P1)]\@

5h-Me⁺

5h-Me_1

1\1\GINC-EVGENIX\SP\RMP2-FC\6-31+G(2d,p)\C22H24P1(1+)\CHRISTOPH\17-Oct
-2011\0\#p MP2(FC)/6-31+g(2d,p) scf=tight\otol3mesp_6\1,1\C\C,1,1.3
9697884\C,2,1.40274736,1,122.06474851\C,3,1.42189805,2,117.44317692,1,
0.13378888,0\C,4,1.41012927,3,120.30209333,2,-0.85797987,0\C,5,1.39482
677,4,120.72878299,3,0.93297453,0\H,1,1.0869499,6,120.28144696,5,-179.
99614918,0\H,2,1.08769969,1,119.39575258,6,-179.22461774,0\H,5,1.08612
26,4,119.98760351,3,-179.10519392,0\H,6,1.0863598,5,119.87455981,4,179
.88317562,0\C,4,5.4527073,3,95.97560478,2,-128.99901601,0\C,11,1.39576
076,4,41.00125468,3,68.47761648,0\C,12,1.39486515,11,119.40495939,4,5.
32471603,0\C,13,1.40992389,12,120.7321889,11,-0.22796724,0\C,14,1.4218
5821,13,120.30743763,12,0.9106399,0\C,11,1.39699964,4,79.21076779,3,-1
16.63147658,0\H,11,1.08694846,4,160.84253153,3,54.26595653,0\H,12,1.08
636866,11,120.71953706,4,-174.82939136,0\H,13,1.0860308,12,119.3261362
6,11,179.79258572,0\H,16,1.08767047,11,119.40524829,4,176.84720698,0\C
,5,5.09915943,4,99.61015958,3,172.54824315,0\C,21,1.39574992,5,70.7968
8925,4,68.01692865,0\C,22,1.39481832,21,119.40615949,5,-33.86471336,0\C
,23,1.41006124,22,120.73029256,21,-0.26783625,0\C,24,1.42185907,23,12
0.30210805,22,1.01817984,0\C,21,1.39694283,5,58.7852234,4,-78.18007885
,0\H,21,1.08694096,5,147.46482429,4,-175.45693488,0\H,22,1.08635951,21
,120.7189003,5,145.97022891,0\H,23,1.0860445,22,119.30474095,21,179.75
746367,0\H,26,1.08768187,21,119.4039721,5,-141.82242496,0\C,3,1.516295
32,2,118.42845543,1,-179.79534663,0\H,31,1.09429772,3,110.0383177,2,18
.68781387,0\H,31,1.09617018,3,112.63228937,2,138.28787962,0\H,31,1.097
99743,3,111.55176674,2,-99.84780742,0\C,15,1.51621147,14,124.08445001,
13,179.05617024,0\H,35,1.09621868,15,112.55987853,14,-42.00937126,0\H,
35,1.09790699,15,111.59185515,14,79.81006473,0\H,35,1.09429882,15,110.
06140044,14,-161.60500088,0\C,25,1.51641266,24,124.121461,23,178.91939
629,0\H,39,1.09625183,25,112.60932801,24,-41.61813849,0\H,39,1.0979865
3,25,111.57292721,24,80.23919736,0\H,39,1.09429524,25,110.03976083,24,
-161.21158388,0\H,24,1.82225218,23,117.14539145,22,179.63629231,0\C,43
,1.83745114,24,109.4865603,23,132.27199598,0\H,44,1.0930277,43,109.714
84659,24,88.97835093,0\H,44,1.09304351,43,109.7702752,24,-151.05342792
,0\H,44,1.09299312,43,109.80701507,24,-31.02606178,0\Version=AM64L-G0
3RevD.01\State=1-A\HF=-1187.7115776\MP2=-1190.9942801\RMSD=1.935e-09\T
hermal=0.\PG=C01 [X(C22H24P1)]\@

5h-Me⁺_2

1\1\GINC-EVGENIX\SP\RMP2-FC\6-31+G(2d,p)\C22H24P1(1+)\CHRISTOPH\17-Oct
-2011\0\#p MP2(FC)/6-31+g(2d,p) scf=tight\otol3mesp_1\1,1\C\C,1,1.3
9645519\C,2,1.40370412,1,122.0743977\C,3,1.42078559,2,117.39935155,1,-
0.10779924,0\C,4,1.40947149,3,120.33657744,2,-0.38094222,0\C,5,1.39387
871,4,120.79544965,3,0.64754462,0\H,1,1.08698241,2,119.71094209,3,179.
99088397,0\H,2,1.08766591,1,119.39157898,6,-179.54122898,0\H,5,1.08662
083,4,119.91037924,3,-178.83765341,0\H,6,1.08642528,5,119.92149766,4,1
79.95315084,0\C,4,5.61478593,3,91.95713775,2,-137.62922754,0\C,11,1.39
582269,4,72.36137906,3,-95.24340191,0\C,12,1.39396455,11,119.30993271,
4,-11.92948086,0\C,13,1.41126831,12,120.99975269,11,0.03252929,0\C,14,

1.42228002,13,120.08990162,12,-0.8560195,0\C,11,1.39618366,4,49.118809
82,3,99.18805389,0\H,11,1.08693918,4,163.2276976,3,45.83562815,0\H,12,
1.08635231,11,120.80052403,4,168.14469626,0\H,13,1.08569605,12,118.387
54055,11,-179.53314436,0\H,16,1.08751879,11,119.33495249,4,-164.769918
76,0\C,5,5.21949272,4,97.62065314,3,177.92407558,0\C,21,1.39529891,5,7
4.44680783,4,58.11600175,0\C,22,1.39451351,21,119.40390646,5,-30.28311
124,0\C,23,1.41023296,22,120.89118772,21,0.02229834,0\C,24,1.42277189,
23,120.12439663,22,-0.51006677,0\C,21,1.39666944,5,54.17587728,4,-89.0
614334,0\H,21,1.08695707,5,148.49007512,4,-178.62113275,0\H,22,1.08635
282,21,120.75051111,5,149.78935336,0\H,23,1.08565792,22,119.03426547,2
1,-179.32911016,0\H,26,1.087694,21,119.36505949,5,-143.11723839,0\C,3,
1.51656936,2,118.30108381,1,179.39985834,0\H,31,1.09440391,3,110.09077
42,2,20.21185985,0\H,31,1.09589028,3,112.92778672,2,140.04550364,0\H,3
1,1.09855491,3,111.27895029,2,-98.07738014,0\C,15,1.51597495,14,124.39
570474,13,-178.84130421,0\H,35,1.09574647,15,112.57696715,14,45.850677
47,0\H,35,1.09439041,15,109.8570225,14,165.54613711,0\H,35,1.09685985,
15,111.70794679,14,-75.11074146,0\C,25,1.51700242,24,124.60404669,23,-
177.78884714,0\H,39,1.0950623,25,113.28339553,24,-38.19975318,0\H,39,1
.09852446,25,111.02599843,24,83.76766982,0\H,39,1.09459794,25,110.0609
8457,24,-158.17129406,0\P,4,1.82332936,3,121.95228729,2,-178.71952022,
0\C,43,1.83405296,4,108.9153897,3,-56.4483191,0\H,44,1.09467923,43,109
.80391626,4,-160.65911243,0\H,44,1.09288021,43,109.05492016,4,-41.4176
2175,0\H,44,1.09236585,43,110.62003631,4,78.24007003,0\Version=AM64L-
G03RevD.01\State=1-A\HF=-1187.7087838\MP2=-1190.9932402\RMSD=9.312e-09
\Thermal=0.\PG=C01 [X(C22H24P1)]\@

5i

5i_1

1\1\GINC-EVGENIX\SP\RMP2-FC\6-31+G(2d,p)\C18F15P1\CHRISTOPH\16-Nov-201
1\0\#p MP2(FC)/6-31+g(2d,p) scf=tight\15sp_1\0,1\P\C,1,4.67376517\
C,2,1.39504834,1,57.63099575\C,3,1.39484468,2,119.21498162,1,-2.183598
28,0\C,4,1.40545103,3,122.67705576,2,-0.31262641,0\C,5,1.40325643,4,11
6.31349279,3,-0.39728535,0\C,6,1.3948822,5,122.21768365,4,0.96095455,0
\C,1,4.67567282,5,107.22825441,4,-145.65608072,0\C,8,1.39520551,1,57.5
8782879,5,93.52572961,0\C,9,1.39464816,8,119.21212727,1,-2.05609901,0\
C,10,1.40515482,9,122.715136,8,-0.31701986,0\C,11,1.40310249,10,116.29
600338,9,-0.47675289,0\C,12,1.39521457,11,122.20757142,10,1.12128752,0
\C,1,4.67548265,5,107.46987969,4,97.50916381,0\C,14,1.39525451,1,57.49
447631,5,-157.19778252,0\C,15,1.39449782,14,119.19393929,1,-1.82093969
0\C,16,1.40537188,15,122.751429,14,-0.42985792,0\C,17,1.40266408,16,1
16.26564026,15,-0.33675745,0\C,18,1.39535237,17,122.22033479,16,1.0694
54,0\F,16,1.33687658,15,117.36260465,14,179.98295055,0\F,15,1.33172309
,14,120.11254876,1,178.07741165,0\F,14,1.32805746,1,177.09280548,5,-12
1.37409167,0\F,19,1.3322713,18,120.44262344,17,179.92908484,0\F,18,1.3
3391747,17,121.08166919,16,-178.28724057,0\F,4,1.33631755,3,117.308818
02,2,179.84301284,0\F,6,1.33374652,5,121.02594074,4,-178.29639935,0\F,
7,1.33226951,6,120.48615544,5,179.91223329,0\F,2,1.32787473,1,176.9785
3994,5,-177.70833033,0\F,3,1.33179782,2,120.10905251,1,177.6402134,0\F
,10,1.3366204,9,117.37036678,8,179.92950934,0\F,9,1.33175352,8,120.114
27582,1,177.79997207,0\F,8,1.32803768,1,177.07105543,5,132.47885245,0\
F,13,1.33230307,12,120.4461884,11,179.88944008,0\F,12,1.33396124,11,12

1.09046231,10,-178.27362893,0\\Version=AM64L-G03RevD.01\\State=1-A\\HF=-
2513.8625432\\MP2=-2519.5008217\\RMSD=2.890e-09\\Thermal=0.\\PG=C01 [X(C18
F15P1)]\\@

5i-Me⁺

5i-Me⁺_1

1\\1\\GINC-EVGENIX\\SP\\RMP2-FC\\6-31+G(2d,p)\\C19H3F15P1(1+)\\CHRISTOPH\\17-N
ov-2011\\0\\#p MP2(FC)/6-31+g(2d,p) scf=tight\\f15mesp_1\\1,1\\P\\C,1,1.8
2754442\\H,2,1.09243705,1,109.12889448\\H,2,1.09234649,1,109.03391975,3,
-120.09592272,0\\H,2,1.09260984,1,108.95104513,4,-119.93766212,0\\C,1,4,
63102293,2,106.32555149,4,171.94075406,0\\C,6,1.39816595,1,61.15872011,
2,-131.99986251,0\\C,7,1.39533337,6,119.78735089,1,-1.02841196,0\\C,8,1,
40720531,7,121.42485654,6,0.96537591,0\\C,9,1.40821322,8,117.17812998,7
, -1.95283625,0\\C,10,1.3899474,9,122.35118058,8,1.79484882,0\\C,1,4.6314
9845,9,110.79795,8,-15.1296692,0\\C,12,1.40128066,1,59.02287384,9,-65.7
5133232,0\\C,13,1.38972537,12,119.02079542,1,0.86478654,0\\C,14,1.408579
09,13,122.37704533,12,-0.46622006,0\\C,15,1.40737,14,117.1666382,13,1.4
6445635,0\\C,16,1.39565985,15,121.41215659,14,-1.65646868,0\\C,1,4.63076
473,9,112.15526742,8,111.86871032,0\\C,18,1.39803347,1,61.12557918,9,-1
3.60324892,0\\C,19,1.39542257,18,119.80025786,1,-1.09460295,0\\C,20,1.40
73079,19,121.41142771,18,0.88027959,0\\C,21,1.40858801,20,117.17764053,
19,-1.71735908,0\\C,22,1.38982243,21,122.36145585,20,1.54723715,0\\F,20,
1.33074922,19,117.36352425,18,-178.84963822,0\\F,19,1.32223435,18,120.1
5215564,1,179.28927209,0\\F,18,1.31559002,1,178.7104291,21,172.22978941
,0\\F,23,1.32170082,22,120.64039707,21,-179.9383631,0\\F,22,1.3379433,21
,119.33170591,20,-177.04601428,0\\F,10,1.33800272,9,119.35994601,8,-176
.75558824,0\\F,11,1.32176759,10,120.61941597,9,179.99005732,0\\F,6,1.315
63403,1,178.71325794,21,-99.58815907,0\\F,7,1.32221234,6,120.16492374,1
,179.42618524,0\\F,8,1.33086767,7,117.37772487,6,-178.56476958,0\\F,14,1
.33810776,13,118.29552931,12,178.08954318,0\\F,13,1.32168981,12,120.330
20426,1,-179.67357483,0\\F,12,1.3156104,1,178.66926087,21,138.56847409,
0\\F,17,1.32223262,16,120.03054736,15,-179.49213033,0\\F,16,1.33072192,1
5,121.26403417,14,178.0032282,0\\Version=AM64L-G03RevD.01\\State=1-A\\HF
=-2553.25774\\MP2=-2559.0478864\\RMSD=4.074e-09\\Thermal=0.\\PG=C01 [X(C19
H3F15P1)]\\@

4.3.2 Structures of all systems: mPW1k/6-31+G(d)

5a

5a_1

1\1\GINC-NODE8\SP\RMP2-FC\6-31+G(2d,p)\C18H15P1\ZIP04\12-Dec-2009\0\#
p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\catcycle_smp2-5_013\0
,1P,0,0.,0.,1.23217\C,0,0.,1.647061,0.424534\C,0,-0.794373,2.638688,1
.00047\C,0,0.751074,1.965375,-0.704112\C,0,-0.857227,3.908048,0.448095
\H,0,-1.368223,2.413421,1.889681\C,0,0.699118,3.240111,-1.25009\H,0,1.
381765,1.215657,-1.159774\C,0,-0.107875,4.212332,-0.679462\H,0,-1.4826
7,4.66217,0.90436\H,0,1.289904,3.471685,-2.125151\H,0,-0.148237,5.2042
06,-1.106568\C,0,1.426397,-0.82353,0.424534\C,0,1.326527,-1.633137,-0.
704112\C,0,2.682358,-0.631397,1.00047\C,0,2.456459,-2.22551,-1.25009\H
,0,0.361907,-1.804472,-1.159774\C,0,3.813082,-1.211644,0.448095\H,0,2.
774195,-0.021794,1.889681\C,0,3.701924,-2.012743,-0.679462\H,0,2.36161
5,-2.852932,-2.125151\H,0,4.778893,-1.047055,0.90436\H,0,4.581093,-2.4
73726,-1.106568\C,0,-1.426397,-0.82353,0.424534\C,0,-1.887985,-2.00729
1,1.00047\C,0,-2.077601,-0.332238,-0.704112\C,0,-2.955856,-2.696404,0.
448095\H,0,-1.405972,-2.391626,1.889681\C,0,-3.155577,-1.014601,-1.250
09\H,0,-1.743673,0.588815,-1.159774\C,0,-3.594049,-2.199588,-0.679462\

H,0,-3.296223,-3.615115,0.90436\H,0,-3.65152,-0.618753,-2.125151\H,0,-
4.432856,-2.73048,-1.106568\\Version=AM64L-G03RevD.01\State=1-A\HF=-10
31.1562959\MP2=-1033.8055395\RMSD=3.348e-09\Thermal=0.\PG=C03 [C3(P1),
X(C18H15)]\\@

4f

4f_1

1\1\GINC-NODE19\SP\RMP2-FC\6-31+G(2d,p)\C15H23N3\ZIP04\03-Feb-2011\0\\
#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\\cat11_spmp2-5_seq_1\\0
,1\C,0,3.458714,0.874262,-0.666014\C,0,2.775166,-0.291867,-0.371839\C,
0,1.396824,-0.258994,-0.161927\C,0,0.76105,1.005124,-0.245608\C,0,1.56
919,2.098317,-0.534303\N,0,2.880869,2.057142,-0.752933\N,0,-0.624084,1
.101479,-0.069311\C,0,-1.202872,0.039545,0.736712\C,0,-0.769544,-1.301
489,0.149662\N,0,0.668649,-1.381885,0.11525\C,0,-1.401809,-1.547404,-1
.217248\C,0,-2.919781,-1.488622,-1.150908\C,0,-3.382224,-0.16666,-0.55
8897\C,0,-2.726921,0.074467,0.792401\C,0,-1.1911,2.425209,0.070027\C,0
, -0.933133,3.104611,1.407317\C,0,1.279574,-2.685664,0.188186\C,0,1.927
239,-2.972812,1.532922\H,0,-0.819699,0.087925,1.764992\H,0,-1.1171,-2.
071689,0.844189\H,0,-1.071962,-2.515578,-1.598002\H,0,-1.029674,-0.789
496,-1.907615\H,0,-3.344358,-1.631269,-2.145178\H,0,-3.292339,-2.312,-
0.533709\H,0,-4.467305,-0.157646,-0.446758\H,0,-3.128539,0.641503,-1.2
47226\H,0,-3.079141,1.001746,1.242728\H,0,-3.032366,-0.71759,1.480618\
H,0,2.003664,-2.805393,-0.619714\H,0,0.499262,-3.42111,-0.003564\H,0,2
.696248,-2.239107,1.765915\H,0,1.185724,-2.941203,2.330213\H,0,2.38669
6,-3.961321,1.534764\H,0,-2.261904,2.351811,-0.101614\H,0,-0.81822,3.0
38852,-0.747009\H,0,-1.382814,2.545227,2.227468\H,0,0.131686,3.19598,1
.612503\H,0,-1.365463,4.10506,1.412993\H,0,1.136776,3.085046,-0.595725
\H,0,4.527194,0.842866,-0.834877\H,0,3.323336,-1.217905,-0.309343\\Ver
sion=AM64L-G03RevD.01\State=1-A\HF=-744.8206523\MP2=-747.5762368\RMSD=
8.402e-09\Thermal=0.\PG=C01 [X(C15H23N3)]\\@

4f_2

1\1\GINC-NODE19\SP\RMP2-FC\6-31+G(2d,p)\C15H23N3\ZIP04\03-Feb-2011\0\\
#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\\cat11_perevert_spmp2-5
_seq_6\\0,1\C,0,-2.602434,-0.971245,-0.724789\C,0,-1.146538,-0.553746,
-0.929112\C,0,-0.232364,-1.513424,-0.176151\C,0,-0.625321,-1.681921,1.
290496\C,0,-2.076152,-2.107576,1.440449\C,0,-2.990495,-1.119117,0.7378
74\N,0,1.140222,-1.097363,-0.353725\C,0,1.391662,0.211562,0.04255\C,0,
0.355001,1.166936,-0.059131\N,0,-0.901532,0.815954,-0.509963\C,0,0.664
367,2.470052,0.321038\C,0,1.941088,2.781599,0.759486\N,0,2.916793,1.89
8397,0.854\C,0,2.626507,0.647886,0.507203\C,0,-1.697949,1.839004,-1.16
356\C,0,-2.762478,2.475845,-0.287492\C,0,2.15939,-2.10451,-0.161709\C,
0,3.194242,-2.113952,-1.27315\H,0,-0.908573,-0.651567,-1.995761\H,0,-0
.340821,-2.477961,-0.67671\H,0,0.040028,-2.414069,1.75155\H,0,-0.46313
3,-0.737781,1.813643\H,0,-2.336775,-2.187758,2.496374\H,0,-2.215679,-3
.103704,1.009316\H,0,-4.030927,-1.439256,0.809855\H,0,-2.920719,-0.151
942,1.238271\H,0,-3.270649,-0.276434,-1.232933\H,0,-2.734878,-1.931966
, -1.229774\H,0,2.64497,-1.998784,0.814364\H,0,1.656747,-3.070557,-0.14
2542\H,0,3.695185,-1.153207,-1.368434\H,0,2.720406,-2.335515,-2.227914
\H,0,3.952875,-2.872505,-1.080148\H,0,-1.028532,2.608731,-1.549125\H,0
, -2.16725,1.391492,-2.040989\H,0,-3.510462,1.74953,0.022996\H,0,-3.271

304,3.271297,-0.832666\H,0,-2.328715,2.906314,0.61314\H,0,-0.083324,3.
246456,0.292806\H,0,3.445889,-0.050758,0.586973\H,0,2.176105,3.796674,
1.051503\\Version=AM64L-G03RevD.01\State=1-A\HF=-744.8202663\MP2=-747.
5757444\RMSD=6.022e-09\Thermal=0.\PG=C01 [X(C15H23N3)]\\@

2a

2a_1

1\1\GINC-NODE26\SP\RMP2-FC\6-31+G(2d,p)\C4H6O1\ZIP04\12-Dec-2009\0\\#p
MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\\catcycle_smp2-5_015\\0,
1\C,0,-0.541391,-0.185824,0.\O,0,-1.427627,-1.009005,0.\C,0,0.868525,-
0.637652,0.\C,0,1.923621,0.170024,0.\C,0,-0.843741,1.287552,0.\H,0,-0.
418885,1.770631,-0.879375\H,0,-1.919918,1.425497,0.\H,0,-0.418885,1.77
0631,0.879375\H,0,0.987018,-1.712768,0.\H,0,1.827627,1.24662,0.\H,0,2.
929854,-0.222949,0.\\Version=AM64L-G03RevD.01\State=1-A\HF=-229.83330
06\MP2=-230.6063971\RMSD=6.385e-09\Thermal=0.\PG=CS [SG(C4H4O1),X(H2)]
\\@

2a_2

1\1\GINC-NODE8\SP\RMP2-FC\6-31+G(2d,p)\C4H6O1\ZIP04\12-Dec-2009\0\\#p
MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\\catcycle_smp2-5_014\\0,1
\C,0,0.442115,0.164641,0.\O,0,0.400672,1.372149,0.\C,0,-0.794018,-0.66
1747,0.\C,0,-1.997707,-0.101204,0.\C,0,1.742787,-0.585785,0.\H,0,1.803
78,-1.231863,-0.876733\H,0,2.575452,0.109794,0.\H,0,1.80378,-1.231863,
0.876733\H,0,-0.67807,-1.737937,0.\H,0,-2.093811,0.975476,0.\H,0,-2.90
1654,-0.692001,0.\\Version=AM64L-G03RevD.01\State=1-A\HF=-229.8328687
\MP2=-230.6057514\RMSD=3.063e-09\Thermal=0.\PG=CS [SG(C4H4O1),X(H2)]\\
@

2b

2b_1

1\1\GINC-NODE17\SP\RMP2-FC\6-31+G(2d,p)\C4H6O2\ZIP04\17-Dec-2010\0\\#p
MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\\b_smp2-5_01\\0,1\C,0,0.
,0.118138,0.\O,0,0.492807,1.215661,0.\C,0,-1.446887,-0.174011,0.\C,0,-
2.332429,0.813122,0.\H,0,-1.73681,-1.214226,0.\H,0,-2.004136,1.842651,
0.\H,0,-3.394368,0.618762,0.\O,0,0.715598,-1.00624,0.\C,0,2.121502,-0.
839374,0.\H,0,2.43927,-0.294764,0.884869\H,0,2.536425,-1.840275,0.\H,0
,2.43927,-0.294764,-0.884869\\Version=AM64L-G03RevD.01\State=1-A\HF=-
304.7112118\MP2=-305.6825902\RMSD=6.005e-09\Thermal=0.\PG=CS [SG(C4H4O
2),X(H2)]\\@

2b_2

1\1\GINC-NODE17\SP\RMP2-FC\6-31+G(2d,p)\C4H6O2\ZIP04\17-Dec-2010\0\\#p
MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\\b_smp2-5_03\\0,1\C,0,0.
,0.478861,0.\O,0,-0.611902,1.515517,0.\C,0,1.472886,0.408283,0.\C,0,2.
164389,-0.724124,0.\H,0,1.954898,1.374499,0.\H,0,1.671716,-1.684759,0.
\H,0,3.244503,-0.716398,0.\O,0,-0.588403,-0.716192,0.\C,0,-2.00414,-0.
702015,0.\H,0,-2.307766,-1.742243,0.\H,0,-2.379861,-0.195866,0.884975\
H,0,-2.379861,-0.195866,-0.884975\\Version=AM64L-G03RevD.01\State=1-A'
\HF=-304.7105548\MP2=-305.6816527\RMSD=6.543e-09\Thermal=0.\PG=CS [SG(
C4H4O2),X(H2)]\\@

2b_3

1\1\GINC-NODE28\SP\RMP2-FC\6-31+G(2d,p)\C4H6O2\ZIP04\17-Dec-2010\0\#p
MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\b_smp2-5_02\0,1\C,0,0.
068642,0.521144,0.000028\O,0,0.615609,1.587993,-0.000011\C,0,0.812304,
-0.764333,0.000008\C,0,2.139452,-0.750363,-0.000006\H,0,0.276314,-1.70
0383,0.000007\H,0,2.675729,0.187311,-0.000005\H,0,2.711003,-1.666452,-
0.000018\O,0,-1.269596,0.483955,-0.000001\C,0,-1.990739,-0.727079,-0.0
00007\H,0,-1.786269,-1.315619,-0.892665\H,0,-1.786308,-1.315604,0.8926
71\H,0,-3.036518,-0.441058,-0.000032\Version=AM64L-G03RevD.01\State=1
-A\HF=-304.6954483\MP2=-305.6678791\RMSE=8.766e-09\Thermal=0.\PG=C01 [X(C4H6O2)]\@

2b_4

1\1\GINC-NODE28\SP\RMP2-FC\6-31+G(2d,p)\C4H6O2\ZIP04\17-Dec-2010\0\#p
MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\b_smp2-5_04\0,1\C,0,0.
018717,0.750695,0.009449\O,0,0.13324,1.937149,-0.10684\C,0,1.224172,-0
.065236,0.315547\C,0,1.587364,-1.213427,-0.233952\H,0,1.913039,0.46142
,0.960802\H,0,0.978605,-1.752916,-0.940041\H,0,2.55629,-1.63566,-0.008
447\O,0,-1.185667,0.208869,-0.173382\C,0,-1.519912,-1.121035,0.159836\H,
0,-1.38967,-1.765781,-0.706451\H,0,-0.930991,-1.481752,0.997427\H,0,
-2.5699,-1.099432,0.433211\Version=AM64L-G03RevD.01\State=1-A\HF=-304
.6894173\MP2=-305.662507\RMSE=6.096e-09\Thermal=0.\PG=C01 [X(C4H6O2)]\@

2c

2c_1

1\1\GINC-NODE28\SP\RMP2-FC\6-31+G(2d,p)\C6H8O1\ZIP04\17-Dec-2010\0\#p
MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\c_smp2-5_1\0,1\C,0,-0.
956658,1.311717,0.026338\H,0,-1.465488,2.268067,0.017543\C,0,0.375754,
1.282945,-0.052391\H,0,0.962006,2.185894,-0.146907\C,0,1.131337,0.0220
66,0.018596\C,0,0.327003,-1.228439,0.274035\H,0,0.897,-2.081281,-0.087
885\H,0,0.244629,-1.336201,1.360201\C,0,-1.802544,0.085045,0.131256\H,
0,-2.115841,-0.036604,1.173899\H,0,-2.722048,0.225125,-0.438355\C,0,-1
.059218,-1.152333,-0.34494\H,0,-1.62823,-2.051708,-0.11098\H,0,-0.9650
85,-1.112053,-1.431932\O,0,2.337376,0.001593,-0.081618\Version=AM64L-
G03RevD.01\State=1-A\HF=-306.7554187\MP2=-307.8130978\RMSE=5.849e-09\T
hermal=0.\PG=C01 [X(C6H8O1)]\@

5a*2a

5a*2a_1

1\1\GINC-CALYPSO\SP\RMP2-FC\6-31+G(2d,p)\C22H21O1P1\BORIS\16-Dec-2010\0\#p
MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\int3_2_smp2-5_01\0,1\C,0,-0.84990779,0.12472501,-1.83909153\C,0,-2.09534017,0.86657303,
-1.55\C,0,-3.2959292,0.1731711,-1.57440405\O,0,-3.38963611,-1.07707108
, -1.70626888\C,0,-4.57995305,0.95555955,-1.42922679\H,0,-0.19552647,0.
57472895,-2.59294591\H,0,-1.11531882,-0.88568468,-2.16137962\H,0,-2.06
467474,1.9428429,-1.47709659\H,0,-5.19976156,0.78972709,-2.31012699\H,
0,-4.41599391,2.02537069,-1.30745574\H,0,-5.13790442,0.58031125,-0.571
24341\O,0,0.19883464,-0.0121215,-0.34724221\C,0,-0.5539804,-1.01393691
,0.94072603\C,0,0.09464478,-1.12224057,2.17262179\C,0,-1.72831979,-1.7
1996469,0.69525215\C,0,-0.42758962,-1.93917786,3.15807083\H,0,1.002444

63,-0.56800554,2.36789734\C,0,-2.24122914,-2.53557973,1.69638033\H,0,-
2.26721904,-1.62819808,-0.24833951\C,0,-1.59767901,-2.64922138,2.91715
608\H,0,0.07519106,-2.02223536,4.11067215\H,0,-3.15665037,-3.07736193,
1.50890169\H,0,-2.00610906,-3.28843833,3.68703167\C,0,1.81986827,-0.72
93297,-0.73096143\C,0,2.96236495,-0.4461704,0.01527566\C,0,1.89937729,
-1.63754573,-1.78465043\C,0,4.16403459,-1.06400236,-0.2887123\H,0,2.91
981062,0.26276695,0.82971491\C,0,3.1043456,-2.25221127,-2.08717283\H,0
,1.02282568,-1.87164819,-2.37122628\C,0,4.23622218,-1.96679613,-1.3400
0918\H,0,5.04478904,-0.83923195,0.29512161\H,0,3.1559,-2.95365304,-2.9
0685938\H,0,5.17500622,-2.44630852,-1.57642444\C,0,0.48551451,1.645644
76,0.29311332\C,0,1.46691415,2.45833403,-0.27199879\C,0,-0.36483082,2.
16343084,1.26625526\C,0,1.6083912,3.76970921,0.14907907\H,0,2.12143772
,2.07160248,-1.04034375\C,0,-0.21746723,3.47698522,1.68438742\H,0,-1.1
4293439,1.5450846,1.68800644\C,0,0.76842653,4.27803589,1.13006388\H,0,
2.37178986,4.39474937,-0.29063273\H,0,-0.87982201,3.87444524,2.4392720
2\H,0,0.88002233,5.30157577,1.45761575\\Version=AM64L-G03RevD.01\State
=1-A\HF=-1260.9479688\MP2=-1264.404815\RMSD=5.692e-09\Thermal=0.\PG=C0
1 [X(C22H21O1P1)]\\@

5a*2a_2

1\1\GINC-SOLARIS\SP\RMP2-FC\6-31+G(2d,p)\C22H21O1P1\BORIS\16-Dec-2010\
0\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\\int_spm2-5_001_6-3
1+gd\0,1\p,0,-0.233083,0.013007,-0.308277\C,0,-0.493361,1.702252,0.26
7153\C,0,0.636594,2.461259,0.577583\C,0,-1.761106,2.260508,0.405443\C,
0,0.490512,3.771242,1.002236\H,0,1.620045,2.024772,0.477769\C,0,-1.898
148,3.571134,0.836463\H,0,-2.64271,1.676103,0.187954\C,0,-0.774091,4.3
27523,1.130451\H,0,1.367575,4.356283,1.237377\H,0,-2.884601,3.997857,0
.945272\H,0,-0.883389,5.348525,1.466759\C,0,-1.847014,-0.76864,-0.5359
11\C,0,-2.677786,-0.315936,-1.563231\C,0,-2.232857,-1.875609,0.215585\
C,0,-3.882463,-0.949171,-1.817234\H,0,-2.389369,0.533015,-2.167447\C,0
, -3.439365,-2.507038,-0.044246\H,0,-1.589707,-2.248694,0.998592\C,0,-4
.265371,-2.044877,-1.05669\H,0,-4.518743,-0.590376,-2.612999\H,0,-3.72
9894,-3.365077,0.544118\H,0,-5.203664,-2.540777,-1.258502\C,0,0.65287,
-0.856748,0.986728\C,0,1.687217,-1.733716,0.671179\C,0,0.256659,-0.673
036,2.313651\C,0,2.308767,-2.434282,1.69727\H,0,2.053445,-1.836878,-0.
350294\C,0,0.87897,-1.385092,3.322665\H,0,-0.528335,0.029428,2.558668\
C,0,1.904661,-2.269949,3.011703\H,0,3.122252,-3.102332,1.455396\H,0,0.
572275,-1.243975,4.34893\H,0,2.395495,-2.821245,3.801246\C,0,0.665997,
0.024203,-1.915631\C,0,1.9959,0.656849,-1.873779\C,0,3.118038,-0.15814
, -1.952857\C,0,4.472732,0.497951,-2.086829\H,0,5.111349,0.182992,-1.26
1489\H,0,4.945698,0.152956,-3.005905\H,0,4.42118,1.58588,-2.101746\O,0
,3.084389,-1.416115,-1.926018\H,0,0.768107,-1.028132,-2.19628\H,0,-0.0
44398,0.491401,-2.603718\H,0,2.074379,1.727978,-1.981618\\Version=AM64
L-G03RevD.01\State=1-A\HF=-1260.9481542\MP2=-1264.4047933\RMSD=5.166e-
09\Thermal=0.\PG=C01 [X(C22H21O1P1)]\\@

5a*2a_3

1\1\GINC-NODE6\SP\RMP2-FC\6-31+G(2d,p)\C22H21O1P1\ZIP04\17-Dec-2010\0\
\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\\int1-cis_spm2-5_1\\0
,1\p,0,-0.26482,-0.037936,-0.344705\C,0,-0.616921,1.655812,0.159796\C,
0,-0.624738,1.997904,1.509357\C,0,-0.941234,2.615502,-0.796141\C,0,-0.

956292,3.286623,1.897674\H,0,-0.359683,1.262545,2.255393\C,0,-1.26937,
3.90227,-0.404021\H,0,-0.924898,2.369932,-1.847492\C,0,-1.277986,4.238
119,0.942105\H,0,-0.954305,3.547477,2.945859\H,0,-1.508734,4.644713,-1
.150942\H,0,-1.527929,5.244582,1.24501\C,0,-1.83783,-0.932212,-0.36594
\C,0,-1.867658,-2.186301,-0.979456\C,0,-3.023636,-0.379307,0.11357\C,0
, -3.058732,-2.884523,-1.08692\H,0,-0.95931,-2.6221,-1.373277\C,0,-4.21
4064,-1.080015,-0.000875\H,0,-3.017697,0.596597,0.576481\C,0,-4.233391
, -2.33206,-0.597045\H,0,-3.070095,-3.855951,-1.559212\H,0,-5.128149,-0
.645706,0.377198\H,0,-5.163468,-2.874389,-0.685709\C,0,0.811417,-0.776
58,0.883746\C,0,2.031781,-0.154703,1.160878\C,0,0.483633,-1.9783,1.512
652\C,0,2.925394,-0.759557,2.031935\H,0,2.293276,0.776915,0.682971\C,0
, 1.376171,-2.562285,2.394489\H,0,-0.465662,-2.455722,1.319562\C,0,2.60
1233,-1.958255,2.646363\H,0,3.877295,-0.286496,2.221412\H,0,1.116604,-
3.490759,2.881923\H,0,3.300259,-2.422003,3.327485\C,0,0.604598,0.02846
9,-2.018031\C,0,1.833613,0.80248,-1.897015\C,0,3.120277,0.24354,-1.814
2\C,0,3.283855,-1.263337,-1.995177\H,0,4.34338,-1.494806,-1.935827\H,0
, 2.765038,-1.833201,-1.221456\H,0,2.90951,-1.599208,-2.964155\O,0,4.14
7302,0.910302,-1.61208\H,0,0.765313,-1.014167,-2.290123\H,0,-0.159179,
0.419416,-2.696906\H,0,1.761619,1.879265,-1.827451\\Version=AM64L-G03R
evD.01\State=1-A\HF=-1260.9276522\MP2=-1264.3912932\RMSE=7.839e-09\The
rmal=0.\PG=C01 [X(C22H21O1P1)]\@

5a*2a_4

1\1\GINC-NODE4\SP\RMP2-FC\6-31+G(2d,p)\C22H21O1P1\ZIP04\17-Dec-2010\0\
\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\int1-cis_smp2-5_3\0
,1\P,0,-0.306148,0.022042,-0.366636\C,0,-0.071386,1.615597,0.42431\C,0
, 1.222311,2.131926,0.556864\C,0,-1.163743,2.36573,0.864002\C,0,1.40247
8,3.392215,1.109028\H,0,2.084077,1.572237,0.225249\C,0,-0.969087,3.617
949,1.419575\H,0,-2.165537,1.972195,0.776412\C,0,0.314434,4.134482,1.5
37931\H,0,2.4038,3.786806,1.198151\H,0,-1.82012,4.189816,1.759873\H,0,
0.464295,5.113811,1.969391\C,0,-2.077076,-0.341719,-0.40116\C,0,-2.861
861,0.332749,-1.339325\C,0,-2.669192,-1.302701,0.416862\C,0,-4.215056,
0.058372,-1.447232\H,0,-2.419936,1.081463,-1.98233\C,0,-4.02269,-1.576
674,0.30174\H,0,-2.074692,-1.832521,1.146325\C,0,-4.796877,-0.898176,-
0.628157\H,0,-4.81299,0.588674,-2.173945\H,0,-4.473589,-2.319671,0.943
498\H,0,-5.851505,-1.115357,-0.715562\C,0,0.484181,-1.258413,0.625206\
C,0,0.481251,-2.56613,0.139403\C,0,1.098705,-0.981016,1.841816\C,0,1.0
81657,-3.580511,0.863225\H,0,0.009402,-2.797275,-0.805841\C,0,1.705578
, -1.999532,2.561231\H,0,1.109446,0.027488,2.22702\C,0,1.698318,-3.2965
88,2.074118\H,0,1.077929,-4.589549,0.477956\H,0,2.187931,-1.774864,3.5
01132\H,0,2.176394,-4.087023,2.634263\C,0,0.544124,0.038613,-2.130265\
C,0,1.812678,0.724367,-2.105622\C,0,3.065093,0.172543,-1.776472\C,0,3.
273446,-1.331686,-1.754445\H,0,2.451351,-1.915361,-2.165704\H,0,4.1719
06,-1.545733,-2.330465\H,0,3.459636,-1.665129,-0.733539\O,0,4.055503,0
.873009,-1.508819\H,0,0.577312,-1.0233,-2.370537\H,0,-0.217845,0.50659
2,-2.753694\H,0,1.787217,1.803611,-2.173372\\Version=AM64L-G03RevD.01\
State=1-A\HF=-1260.9243226\MP2=-1264.3891277\RMSE=6.169e-09\Thermal=0.
\PG=C01 [X(C22H21O1P1)]\@

5a*2b

5a*2b_1

1\1\GINC-NODE21\SP\RMP2-FC\6-31+G(2d,p)\C22H21O2P1\ZIP04\17-Dec-2010\0
\\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\zw3_b_smp2-5_05\0,
1\P,0,-0.407677,-0.037138,-0.329012\C,0,-1.094245,1.584608,0.057451\C,
0,-1.296119,1.963128,1.382069\C,0,-1.483951,2.440461,-0.969897\C,0,-1.
884687,3.183648,1.674611\H,0,-0.983043,1.311133,2.184891\C,0,-2.069261
,3.659836,-0.673346\H,0,-1.320425,2.167696,-2.001708\C,0,-2.271151,4.0
31467,0.648091\H,0,-2.033082,3.473636,2.704518\H,0,-2.35957,4.323111,-
1.474779\H,0,-2.722852,4.985861,0.876875\C,0,-1.795066,-1.198769,-0.41
3057\C,0,-1.558766,-2.457921,-0.968333\C,0,-3.089105,-0.854126,-0.0292
11\C,0,-2.596115,-3.364115,-1.112616\H,0,-0.562478,-2.735325,-1.285166
\C,0,-4.124751,-1.763098,-0.179591\H,0,-3.288566,0.122408,0.386926\C,0
, -3.880238,-3.017749,-0.717442\H,0,-2.402085,-4.337498,-1.538972\H,0,-
5.124653,-1.489223,0.124358\H,0,-4.690085,-3.723214,-0.834018\C,0,0.66
0243,-0.522938,1.030445\C,0,1.707794,0.321595,1.403184\C,0,0.475792,-1
.735199,1.693464\C,0,2.576105,-0.068224,2.410594\H,0,1.854079,1.262288
,0.894413\C,0,1.341707,-2.108956,2.707002\H,0,-0.342559,-2.386475,1.42
5182\C,0,2.395875,-1.278858,3.061285\H,0,3.395517,0.581003,2.681508\H,
0,1.192831,-3.048844,3.218372\H,0,3.073798,-1.574515,3.849194\C,0,0.55
148,0.10146,-1.925603\C,0,1.622403,1.079184,-1.753897\C,0,2.951786,0.7
02856,-1.52996\O,0,3.921037,1.432494,-1.34854\H,0,0.932947,-0.898718,-
2.12337\H,0,-0.201291,0.32707,-2.68616\H,0,1.41407,2.134153,-1.827574\
O,0,3.128547,-0.668802,-1.512366\C,0,4.448057,-1.095641,-1.298645\H,0,
4.422059,-2.18179,-1.333269\H,0,5.117195,-0.715608,-2.068057\H,0,4.819
954,-0.765514,-0.33032\\Version=AM64L-G03RevD.01\State=1-A\HF=-1335.80
87975\MP2=-1339.4670805\RMSD=8.755e-09\Thermal=0.PG=C01 [X(C22H21O2P1
)]\@

5a*2b_2

1\1\GINC-NODE11\SP\RMP2-FC\6-31+G(2d,p)\C22H21O2P1\ZIP04\17-Dec-2010\0
\\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\zw3_b_smp2-5_01\0,
1\P,0,-0.446778,0.011948,-0.282486\C,0,-0.773678,1.694463,0.274084\C,0
,0.313704,2.455986,0.707419\C,0,-2.052198,2.246792,0.280804\C,0,0.1167
11,3.763586,1.119863\H,0,1.304454,2.025143,0.708725\C,0,-2.240247,3.55
3552,0.702643\H,0,-2.903186,1.660018,-0.031567\C,0,-1.156727,4.313484,
1.117187\H,0,0.961838,4.350916,1.447764\H,0,-3.234848,3.975236,0.70973
7\H,0,-1.306109,5.332071,1.445403\C,0,-2.020545,-0.77533,-0.691415\C,0
, -2.742893,-0.305187,-1.790973\C,0,-2.469953,-1.907129,-0.01468\C,0,-3
.906067,-0.943248,-2.187302\H,0,-2.402666,0.562451,-2.339225\C,0,-3.63
3988,-2.5429,-0.417152\H,0,-1.910313,-2.293602,0.824064\C,0,-4.354397,
-2.061766,-1.499398\H,0,-4.458866,-0.569578,-3.036809\H,0,-3.97534,-3.
418219,0.11596\H,0,-5.26044,-2.560506,-1.811454\C,0,0.288842,-0.866532
,1.099892\C,0,1.351926,-1.744083,0.905209\C,0,-0.257614,-0.690375,2.37
2862\C,0,1.850576,-2.450793,1.991665\H,0,1.833103,-1.843606,-0.063092\
C,0,0.242625,-1.407864,3.444366\H,0,-1.065556,0.011629,2.527646\C,0,1.
296809,-2.292064,3.251378\H,0,2.686262,-3.118692,1.843202\H,0,-0.18155
9,-1.270913,4.428473\H,0,1.692937,-2.847079,4.089882\C,0,0.653572,0.05
1023,-1.783485\C,0,1.934918,0.721761,-1.562742\C,0,3.086833,-0.055584,
-1.48214\O,0,3.155127,-1.294614,-1.46448\H,0,0.794627,-0.997169,-2.056
336\H,0,0.013664,0.508368,-2.543841\H,0,2.014,1.790996,-1.669783\O,0,4
.236669,0.679146,-1.419046\C,0,5.426802,-0.062666,-1.372196\H,0,5.5315
89,-0.703206,-2.245873\H,0,6.231085,0.667621,-1.350682\H,0,5.472562,-0

.688083,-0.482015\\Version=AM64L-G03RevD.01\\State=1-A\\HF=-1335.8178356
\\MP2=-1339.4706208\\RMSD=3.776e-09\\Thermal=0.\\PG=C01 [X(C22H21O2P1)]\\@

5a*2b_3

1\\1\\GINC-NODE16\\SP\\RMP2-FC\\6-31+G(2d,p)\\C22H21O2P1\\ZIP04\\17-Dec-2010\\0
\\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\\zw3_b_smp2-5_03\\0,
1\\C,0,-0.677639,0.017873,-1.779552\\C,0,-1.938886,0.689482,-1.437936\\C,
0,-3.099358,-0.074189,-1.389155\\O,0,-3.186474,-1.309779,-1.488972\\H,0,
-0.08085,0.489334,-2.567538\\H,0,-0.870889,-1.017118,-2.067364\\H,0,-1.9
92794,1.76509,-1.410421\\P,0,0.44404,-0.003288,-0.315582\\C,0,-0.223301,
-0.978921,1.039731\\C,0,0.414621,-0.930318,2.280034\\C,0,-1.312331,-1.82
3367,0.842843\\C,0,-0.02778,-1.729889,3.318194\\H,0,1.249491,-0.263027,2
.442809\\C,0,-1.747745,-2.618923,1.894174\\H,0,-1.854046,-1.843481,-0.09
8121\\C,0,-1.109662,-2.578661,3.122972\\H,0,0.46752,-1.688717,4.277404\\H
,0,-2.599894,-3.265058,1.742648\\H,0,-1.457193,-3.202605,3.934055\\C,0,2
.093464,-0.654262,-0.702704\\C,0,3.225717,-0.334133,0.044931\\C,0,2.2068
75,-1.551603,-1.762256\\C,0,4.449114,-0.90455,-0.263331\\H,0,3.157251,0.
366209,0.86489\\C,0,3.433908,-2.119409,-2.069679\\H,0,1.339249,-1.81356,
-2.350213\\C,0,4.554379,-1.797287,-1.320821\\H,0,5.32118,-0.651856,0.322
168\\H,0,3.511125,-2.812935,-2.894098\\H,0,5.510201,-2.240301,-1.560184\\
C,0,0.64973,1.692082,0.24665\\C,0,1.644365,2.509664,-0.28743\\C,0,-0.288
92,2.228498,1.125794\\C,0,1.712961,3.844535,0.074578\\H,0,2.364964,2.109
713,-0.986359\\C,0,-0.215058,3.565928,1.482473\\H,0,-1.0791,1.606094,1.5
17776\\C,0,0.785433,4.371735,0.962282\\H,0,2.48771,4.473014,-0.339698\\H,
0,-0.946534,3.977737,2.16204\\H,0,0.840132,5.413671,1.243039\\O,0,-4.233
863,0.663238,-1.203074\\C,0,-5.431507,-0.066637,-1.169601\\H,0,-6.222397
,0.666974,-1.038732\\H,0,-5.588148,-0.61853,-2.094558\\H,0,-5.445148,-0.
774881,-0.3426\\Version=AM64L-G03RevD.01\\State=1-A\\HF=-1335.8170849\\MP
2=-1339.4702639\\RMSD=6.714e-09\\Thermal=0.\\PG=C01 [X(C22H21O2P1)]\\@

5a*2b_4

1\\1\\GINC-NODE2\\SP\\RMP2-FC\\6-31+G(2d,p)\\C22H21O2P1\\ZIP04\\20-Dec-2010\\0\\
\\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\\zw3_b_smp2-5_04_2\\0
,1\\C,0,-0.688232,-0.056626,-1.789512\\C,0,-2.068642,0.332856,-1.450161\\
C,0,-3.043796,-0.661341,-1.511596\\O,0,-2.828371,-1.866017,-1.710053\\H,
0,-0.17764,0.58812,-2.512848\\H,0,-0.679977,-1.07894,-2.172223\\H,0,-2.2
92459,1.377877,-1.325132\\P,0,0.391471,-0.001216,-0.303406\\C,0,-0.04364
6,-1.232002,0.932219\\C,0,0.660664,-1.241448,2.137977\\C,0,-1.019273,-2.
191795,0.677699\\C,0,0.392284,-2.209622,3.087454\\H,0,1.415628,-0.494216
,2.340392\\C,0,-1.278869,-3.157622,1.641976\\H,0,-1.596034,-2.190606,-0.
245248\\C,0,-0.579628,-3.170817,2.83707\\H,0,0.938523,-2.215387,4.019484
\\H,0,-2.041775,-3.896744,1.446573\\H,0,-0.790453,-3.927918,3.578931\\C,0
,2.138375,-0.242928,-0.726271\\C,0,3.177429,0.334532,0.001067\\C,0,2.437
57,-1.08109,-1.79882\\C,0,4.494647,0.073462,-0.338759\\H,0,2.961805,0.99
4689,0.82898\\C,0,3.756848,-1.338053,-2.136929\\H,0,1.644395,-1.538763,-
2.372453\\C,0,4.785308,-0.762269,-1.407465\\H,0,5.294337,0.523936,0.2310
52\\H,0,3.97865,-1.988075,-2.970494\\H,0,5.813416,-0.963202,-1.671585\\C,
0,0.242105,1.636252,0.429877\\C,0,0.931105,2.716067,-0.120306\\C,0,-0.66
0835,1.849062,1.46759\\C,0,0.733287,3.99211,0.379116\\H,0,1.622403,2.564
584,-0.937411\\C,0,-0.853483,3.128997,1.96477\\H,0,-1.214309,1.019041,1.
880346\\C,0,-0.156409,4.197981,1.424516\\H,0,1.271229,4.825171,-0.049139

\H,0,-1.554355,3.289014,2.770864\H,0,-0.309018,5.194234,1.813832\O,0,-
4.357896,-0.33443,-1.326905\C,0,-4.717324,0.99958,-1.13083\H,0,-4.2593
51,1.414885,-0.230559\H,0,-4.446138,1.62134,-1.986067\H,0,-5.7977,1.01
1052,-1.014659\\Version=AM64L-G03RevD.01\State=1-A\HF=-1335.8102018\MP
2=-1339.4650074\RMSD=5.827e-09\Thermal=0.\PG=C01 [X(C22H21O2P1)]\\@

5a*2b_5

1\1\GINC-NODE14\SP\RMP2-FC\6-31+G(2d,p)\C22H21O2P1\ZIP04\17-Dec-2010\0
\\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\\zw3_b_smp2-5_02\\0,
1\P,0,-0.395861,0.023842,-0.26465\C,0,-0.441253,1.687615,0.428809\C,0,
0.750477,2.207239,0.937718\C,0,-1.601818,2.45574,0.464944\C,0,0.775764
,3.490249,1.458224\H,0,1.648266,1.606565,0.917691\C,0,-1.568758,3.7369
6,0.993568\H,0,-2.533629,2.0561,0.093308\C,0,-0.381009,4.255864,1.4859
38\H,0,1.700584,3.889613,1.848211\H,0,-2.47351,4.326483,1.023469\H,0,-
0.358134,5.254232,1.898495\C,0,-2.077209,-0.452665,-0.725172\C,0,-2.69
3874,0.19543,-1.797758\C,0,-2.728154,-1.517287,-0.106694\C,0,-3.94836,
-0.203458,-2.226937\H,0,-2.199735,1.014379,-2.301754\C,0,-3.983198,-1.
913621,-0.541764\H,0,-2.253955,-2.040895,0.709997\C,0,-4.595373,-1.257
698,-1.598225\H,0,-4.417186,0.305367,-3.056465\H,0,-4.479661,-2.740415
, -0.055197\H,0,-5.572373,-1.570677,-1.936644\C,0,0.178498,-1.068841,1.
037876\C,0,1.073539,-2.099074,0.762037\C,0,-0.325509,-0.894333,2.32895
8\C,0,1.447298,-2.957612,1.78786\H,0,1.523422,-2.209703,-0.222056\C,0,
0.047505,-1.763729,3.337599\H,0,-1.0002,-0.077896,2.547591\C,0,0.93381
8,-2.798683,3.064288\H,0,2.15594,-3.745114,1.577997\H,0,-0.343418,-1.6
29141,4.33571\H,0,1.23179,-3.473212,3.854418\C,0,0.680028,0.008616,-1.
772356\C,0,2.08,0.383086,-1.528969\C,0,3.027166,-0.642037,-1.580116\O,
0,2.772445,-1.849132,-1.682129\H,0,0.613628,-1.010078,-2.160913\H,0,0.
144431,0.666843,-2.462499\H,0,2.341973,1.426815,-1.538104\O,0,4.358407
, -0.339196,-1.507505\C,0,4.763961,0.993485,-1.43411\H,0,4.451599,1.561
21,-2.31254\H,0,4.380421,1.486272,-0.537846\H,0,5.849617,0.980777,-1.3
90347\\Version=AM64L-G03RevD.01\State=1-A\HF=-1335.8102789\MP2=-1339.4
647495\RMSD=3.917e-09\Thermal=0.\PG=C01 [X(C22H21O2P1)]\\@

5a*2b_6

1\1\GINC-NODE27\SP\RMP2-FC\6-31+G(2d,p)\C22H21O2P1\ZIP04\17-Dec-2010\0
\\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\\zw3_b_smp2-5_07\\0,
1\P,0,-0.411898,-0.012663,-0.25834\C,0,-0.992529,1.646772,0.12749\C,0,
-0.039636,2.589898,0.518669\C,0,-2.333011,2.014124,0.033522\C,0,-0.430
748,3.891928,0.786015\H,0,0.999121,2.305258,0.600014\C,0,-2.715138,3.3
16685,0.311065\H,0,-3.081517,1.287225,-0.244281\C,0,-1.764497,4.2568,0.
.68125\H,0,0.311314,4.61983,1.079318\H,0,-3.756618,3.594886,0.240541\H
,0,-2.064959,5.272348,0.895474\C,0,-1.840605,-1.0733,-0.562228\C,0,-2.
605305,-0.842486,-1.708912\C,0,-2.128491,-2.178907,0.236131\C,0,-3.652
776,-1.687957,-2.03323\H,0,-2.389063,-0.000175,-2.351407\C,0,-3.176946
, -3.022669,-0.094841\H,0,-1.534239,-2.381606,1.114839\C,0,-3.941825,-2
.778012,-1.225372\H,0,-4.239635,-1.497425,-2.919886\H,0,-3.39441,-3.87
4309,0.533206\H,0,-4.757795,-3.438536,-1.480067\C,0,0.449052,-0.611967
,1.200713\C,0,1.636718,-1.327042,1.081602\C,0,-0.110081,-0.387705,2.45
9212\C,0,2.249154,-1.826585,2.222002\H,0,2.108381,-1.456932,0.117451\C
,0,0.504323,-0.896869,3.59005\H,0,-1.018424,0.19062,2.556349\C,0,1.684
121,-1.618935,3.470151\H,0,3.178594,-2.369029,2.130244\H,0,0.068902,-0

.721992,4.56307\H,0,2.16874,-2.008737,4.353795\C,0,0.691548,0.051977,-
1.776754\C,0,1.802595,0.986208,-1.637804\C,0,3.140633,0.591496,-1.5472
04\O,0,4.136094,1.303619,-1.505795\H,0,1.016794,-0.976482,-1.933078\H,
0,-0.026201,0.28726,-2.569741\H,0,1.626694,2.040002,-1.778921\O,0,3.30
8742,-0.790016,-1.514702\C,0,4.646329,-1.219741,-1.51663\H,0,5.184031,
-0.850135,-0.64556\H,0,4.614415,-2.306631,-1.504285\H,0,5.168332,-0.87
6612,-2.407382\Version=AM64L-G03RevD.01\State=1-A\HF=-1335.808149\MP2
=-1339.4638177\RMSD=7.525e-09\Thermal=0.\PG=C01 [X(C22H21O2P1)]\@

5a*2c

5a*2c_1

1\1\GINC-NODE17\SP\RMP2-FC\6-31+G(2d,p)\C24H23O1P1\ZIP04\17-Dec-2010\0
\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\zw3_c_spm2-5_6\0,1
\P,0,-0.316192,0.003919,-0.128973\C,0,-0.879866,1.664192,-0.556289\C,0
,0.044216,2.705627,-0.450245\C,0,-2.177131,1.935506,-0.984198\C,0,-0.3
24281,3.994307,-0.797704\H,0,1.046698,2.508134,-0.099867\C,0,-2.539843
,3.229782,-1.322174\H,0,-2.912776,1.147591,-1.040529\C,0,-1.613518,4.2
57872,-1.236075\H,0,0.399134,4.792594,-0.721528\H,0,-3.549296,3.433178
, -1.648814\H,0,-1.898327,5.265485,-1.502329\C,0,-1.742855,-1.098904,-0
.054035\C,0,-2.080727,-1.80726,1.097873\C,0,-2.431888,-1.36574,-1.2414
12\C,0,-3.10625,-2.738899,1.069118\H,0,-1.541907,-1.636898,2.017704\C,
0,-3.456078,-2.297084,-1.26348\H,0,-2.167307,-0.852357,-2.155599\C,0,-
3.798684,-2.98262,-0.107084\H,0,-3.361434,-3.277351,1.970221\H,0,-3.98
2336,-2.490818,-2.186759\H,0,-4.597393,-3.709654,-0.125241\C,0,0.39842
6,0.157219,1.519736\C,0,-0.397458,0.688466,2.536159\C,0,1.713964,-0.20
5417,1.790975\C,0,0.108098,0.820861,3.81752\H,0,-1.409223,1.007366,2.3
25289\C,0,2.215505,-0.064832,3.076491\H,0,2.356354,-0.549035,0.997245\
C,0,1.415593,0.440575,4.088556\H,0,-0.513717,1.230937,4.599904\H,0,3.2
41018,-0.337541,3.276736\H,0,1.813821,0.553266,5.086645\C,0,0.883673,-
0.622534,-1.451139\C,0,2.063226,0.244959,-1.530954\C,0,3.382848,-0.195
492,-1.376332\C,0,3.617594,-1.699116,-1.257096\H,0,4.550285,-1.907082,
-1.779219\H,0,3.795405,-1.961474,-0.208435\O,0,4.381982,0.542692,-1.37
2925\H,0,0.22972,-0.55365,-2.333844\H,0,1.9256,1.272313,-1.836657\C,0,
1.17089,-2.101507,-1.155258\H,0,1.265251,-2.277298,-0.081172\H,0,0.334
903,-2.713758,-1.493284\C,0,2.472017,-2.522956,-1.813558\H,0,2.634886,
-3.589579,-1.645662\H,0,2.402823,-2.376719,-2.893196\Version=AM64L-G0
3RevD.01\State=1-A\HF=-1337.835217\MP2=-1341.5888739\RMSD=2.039e-09\Th
ermal=0.\PG=C01 [X(C24H23O1P1)]\@

4f*2a

4f_2a_1

1\1\GINC-NODE12\SP\RMP2-FC\6-31+G(2d,p)\C19H29N3O1\ZIP04\02-Feb-2011\0
\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\cat11_1_b981_spm2-5
_seq_1\0,1\C,0,-3.461867,1.460525,-0.97471\H,0,-3.743603,2.501122,-1.
122954\H,0,-3.530385,0.933972,-1.92713\C,0,-4.262886,0.787499,0.059716
\H,0,-4.803193,1.389396,0.77504\C,0,-4.38146,-0.589792,0.044843\C,0,-5
.341697,-1.246383,1.009077\H,0,-5.845022,-0.533803,1.660751\H,0,-6.092
505,-1.795313,0.440565\H,0,-4.80896,-1.975196,1.62021\O,0,-3.728622,-1
.356351,-0.725591\N,0,-1.978593,1.499242,-0.68749\C,0,-1.302298,2.6301
45,-0.545296\C,0,-1.374242,0.310344,-0.524585\C,0,0.036983,2.614759,-0
.246342\H,0,-1.854119,3.548219,-0.666529\C,0,-0.031689,0.199758,-0.240

167\H,0,-2.061706,-0.529512,-0.636948\C,0,0.72322,1.401793,-0.10192\H,
0,0.543323,3.557058,-0.128019\N,0,0.588703,-1.032873,-0.107136\N,0,2.0
48427,1.34568,0.154809\C,0,1.784367,-1.012206,0.719571\C,0,-0.270117,-
2.206208,-0.027599\C,0,2.722642,0.065528,0.185873\C,0,2.854062,2.53552
3,0.313977\C,0,2.532765,-2.340236,0.746775\H,0,1.524251,-0.745691,1.75
2275\C,0,-0.979716,-2.388201,1.303226\H,0,0.342333,-3.075952,-0.249575
\H,0,-0.999821,-2.153104,-0.830727\C,0,3.301007,-0.304208,-1.17631\H,0
,3.538899,0.156392,0.907301\C,0,2.774641,3.130511,1.709251\H,0,2.5768,
3.272372,-0.440261\H,0,3.882569,2.257555,0.090728\C,0,3.114086,-2.7311
, -0.603169\H,0,1.898982,-3.128429,1.149\H,0,3.348247,-2.224082,1.46493
7\H,0,-0.272083,-2.529486,2.120902\H,0,-1.613298,-1.536068,1.538926\H,
0,-1.625329,-3.262911,1.255962\C,0,4.030059,-1.637513,-1.128167\H,0,3.
971663,0.48855,-1.51232\H,0,2.481733,-0.355273,-1.894428\H,0,1.755251,
3.411775,1.96619\H,0,3.118675,2.41371,2.453364\H,0,3.400981,4.019133,1
.780024\H,0,3.658473,-3.671122,-0.507956\H,0,2.310559,-2.902943,-1.321
185\H,0,4.402723,-1.893115,-2.120221\H,0,4.906622,-1.554029,-0.478745\
\Version=AM64L-G03RevD.01\State=1-A\HF=-974.6193856\MP2=-978.1817253\R
MSD=5.767e-09\Thermal=0.\PG=C01 [X(C19H29N3O1)]\@

4f*2a_2

1\1\GINC-NODE19\SP\RMP2-FC\6-31+G(2d,p)\C19H29N3O1\ZIP04\03-Feb-2011\0
\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\cat11_1_b981_spm2-5
_seq_4\0,1\C,0,-3.534318,1.585121,0.307561\H,0,-3.728051,1.225421,1.3
18728\H,0,-3.821259,2.632769,0.243055\C,0,-4.203992,0.740683,-0.69374\
H,0,-4.641297,1.210596,-1.561942\C,0,-4.322421,-0.619544,-0.479931\C,0
, -5.143517,-1.437275,-1.448995\H,0,-5.566556,-0.842242,-2.256883\H,0,-
4.527231,-2.229651,-1.874201\H,0,-5.954588,-1.921098,-0.904732\O,0,-3.
777903,-1.246342,0.479364\N,0,-2.02648,1.58911,0.205912\C,0,-1.319362,
2.687994,-0.016279\C,0,-1.421957,0.39688,0.339928\C,0,0.047422,2.63175
8,-0.130708\H,0,-1.86691,3.612279,-0.106135\C,0,-0.058295,0.245585,0.2
28675\H,0,-2.127839,-0.414626,0.52555\C,0,0.724427,1.409618,-0.026478\
H,0,0.581202,3.548957,-0.31058\N,0,0.548234,-0.995234,0.331487\N,0,2.0
64859,1.308146,-0.166311\C,0,1.940627,-0.951682,0.744795\C,0,-0.270803
, -2.107557,0.789507\C,0,2.689586,0.002465,-0.181056\C,0,2.90195,2.4588
4,-0.420299\C,0,2.631988,-2.31036,0.709538\H,0,2.019639,-0.554679,1.76
5487\C,0,-0.552237,-2.118405,2.282846\H,0,0.229252,-3.026565,0.496682\
H,0,-1.207217,-2.096744,0.237654\C,0,2.809164,-0.5531,-1.596383\H,0,3.
690612,0.127431,0.239996\C,0,3.257349,3.229911,0.839218\H,0,2.424475,3
.109492,-1.153446\H,0,3.810602,2.095161,-0.896497\C,0,2.763037,-2.8840
32,-0.692909\H,0,2.134335,-3.010057,1.378764\H,0,3.630732,-2.163433,1.
128229\H,0,0.364369,-2.208042,2.866805\H,0,-1.071035,-1.215692,2.59830
6\H,0,-1.195186,-2.961512,2.528549\C,0,3.492589,-1.910963,-1.604547\H,
0,3.356456,0.156352,-2.219451\H,0,1.806274,-0.639966,-2.016216\H,0,2.3
67713,3.597971,1.34658\H,0,3.799705,2.595277,1.538511\H,0,3.888793,4.0
84147,0.597207\H,0,3.293157,-3.83598,-0.649308\H,0,1.775106,-3.092109,
-1.106957\H,0,3.535892,-2.299151,-2.622246\H,0,4.528368,-1.803341,-1.2
68492\Version=AM64L-G03RevD.01\State=1-A\HF=-974.6192535\MP2=-978.180
9709\RMSD=5.973e-09\Thermal=0.\PG=C01 [X(C19H29N3O1)]\@

4f_2a_3

1\1\GINC-CALYPSO\SP\RMP2-FC\6-31+G(2d,p)\C19H29N3O1\BORIS\01-Feb-2011\

0\\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\\cat11_1_b986_smp2-5_1\\0,1\\C,0,3.282012,1.685147,1.023616\\H,0,3.390141,2.751085,1.213885\\H,0,3.346213,1.144258,1.968315\\C,0,4.258081,1.16732,0.054415\\H,0,4.757369,1.859511,-0.606971\\C,0,4.584381,-0.176526,0.07188\\C,0,5.712797,-0.661661,-0.807934\\H,0,6.153219,0.131034,-1.410729\\H,0,6.488384,-1.09843,-0.17868\\H,0,5.35291,-1.453041,-1.465608\\O,0,3.991516,-1.045088,0.778361\\N,0,1.836935,1.514328,0.607827\\C,0,1.004272,2.536823,0.477757\\C,0,1.430206,0.259075,0.358338\\C,0,-0.297107,2.34157,0.079535\\H,0,1.396948,3.516566,0.696582\\C,0,0.144904,-0.018967,-0.053964\\H,0,2.21616,-0.484864,0.497167\\C,0,-0.772677,1.057299,-0.202826\\H,0,-0.938266,3.202646,0.000046\\N,0,-0.266096,-1.294457,-0.365646\\N,0,-2.05082,0.833775,-0.617921\\C,0,-1.67075,-1.542829,-0.140707\\C,0,0.659157,-2.404558,-0.204975\\C,0,-2.493063,-0.523265,-0.921925\\C,0,-2.775697,1.920816,-1.254884\\C,0,-2.028596,-1.597018,1.34316\\H,0,-1.900219,-2.510476,-0.58916\\C,0,1.615013,-2.541387,-1.374227\\H,0,1.219723,-2.31967,0.729038\\H,0,0.054755,-3.306556,-0.122543\\C,0,-3.97979,-0.733805,-0.635901\\H,0,-2.318936,-0.711431,-1.986746\\C,0,-3.694937,2.706099,-0.3362\\H,0,-2.052962,2.590713,-1.721026\\H,0,-3.351448,1.496314,-2.076582\\C,0,-3.513462,-1.829356,1.562769\\H,0,-1.438231,-2.383798,1.814405\\H,0,-1.730642,-0.659424,1.817276\\H,0,2.232457,-1.655172,-1.494897\\H,0,1.065343,-2.712723,-2.29899\\H,0,2.289795,-3.377998,-1.203023\\C,0,-4.321751,-0.762841,0.845273\\H,0,-4.578254,0.01237,-1.157485\\H,0,-4.252208,-1.692957,-1.083538\\H,0,-4.513829,2.09207,0.030695\\H,0,-4.124045,3.551344,-0.873824\\H,0,-3.160599,3.092202,0.529837\\H,0,-3.739426,-1.830773,2.629275\\H,0,-3.793533,-2.816631,1.184078\\H,0,-5.390685,-0.941217,0.967722\\H,0,-4.110345,0.208633,1.29559\\Version=AM64L-G03RevD.01\\State=1-A\\HF=-974.6165457\\MP2=-978.1789388\\RMSD=2.291e-09\\Thermal=0.\\PG=C01 [X(C19H29N3O1)]\\@

4f*2a_4

1\\GINC-NAUTILUS\\SP\\RMP2-FC\\6-31+G(2d,p)\\C19H29N3O1\\BORIS\\01-Feb-2011\\0\\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\\cat11_1_b986_smp2-5_4\\0,1\\C,0,3.38622,1.855755,-0.156387\\H,0,3.746898,1.559175,-1.141798\\H,0,3.513884,2.929958,-0.039109\\C,0,4.039675,1.076044,0.905349\\H,0,4.296334,1.568237,1.831486\\C,0,4.373356,-0.246067,0.677725\\C,0,5.174767,-0.98269,1.725373\\H,0,5.405738,-0.369034,2.594733\\H,0,4.628073,-1.868685,2.048905\\H,0,6.107216,-1.328493,1.279208\\O,0,4.045227,-0.900382,-0.357203\\N,0,1.889895,1.65148,-0.24213\\C,0,1.018479,2.631732,-0.05175\\C,0,1.473415,0.39661,-0.476335\\C,0,-0.334414,2.390693,-0.094842\\H,0,1.421627,3.611217,0.148415\\C,0,0.135856,0.076393,-0.550744\\H,0,2.293386,-0.31361,-0.599972\\C,0,-0.824343,1.106392,-0.353594\\H,0,-1.002703,3.214056,0.090618\\N,0,-0.295359,-1.19834,-0.842898\\N,0,-2.158654,0.840821,-0.424563\\C,0,-1.578063,-1.537996,-0.271376\\C,0,0.685124,-2.265227,-0.979163\\C,0,-2.616495,-0.513633,-0.716535\\C,0,-3.068775,1.928828,-0.74166\\C,0,-1.520114,-1.715252,1.244787\\H,0,-1.887074,-2.48327,-0.720549\\C,0,1.324165,-2.304079,-2.353676\\H,0,1.458449,-2.191445,-0.211106\\H,0,0.155965,-3.200142,-0.801562\\C,0,-3.962206,-0.830856,-0.065236\\H,0,-2.728928,-0.612788,-1.801601\\C,0,-3.729538,2.58495,0.45766\\H,0,-2.52467,2.674563,-1.321589\\H,0,-3.831107,1.536108,-1.413568\\C,0,-2.880508,-2.0501,1.830638\\H,0,-0.794729,-2.495952,1.476525\\H,0,-1.141679,-0.797032,1.698935\\H,0,1.87328,-1.391335,-2.570084\\H,0,0.568375,-2.446,-3.125181\\H,0,2.038516,-3.123721,-2.403965\\C,0,-3.892629,-0.985794,1.445751\\H,0,

-4.706674,-0.086109,-0.344906\H,0,-4.3086,-1.77014,-0.503862\H,0,-4.39
6221,1.897966,0.972962\H,0,-4.317227,3.443943,0.134548\H,0,-2.992802,2
.931123,1.180061\H,0,-2.809732,-2.139049,2.914847\H,0,-3.214659,-3.023
66,1.46011\H,0,-4.881789,-1.236415,1.830777\H,0,-3.605982,-0.038346,1.
905583\\Version=AM64L-G03RevD.01\State=1-A\HF=-974.6167399\MP2=-978.17
87641\RMSD=2.114e-09\Thermal=0.\PG=C01 [X(C19H29N3O1)]\@

4f*2a_5

1\1\GINC-NODE18\SP\RMP2-FC\6-31+G(2d,p)\C19H29N3O1\ZIP04\03-Feb-2011\0
\\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\\cat11_1_b981_smp2-5
_seq_3\\0,1\C,0,3.400305,-1.418166,-0.481088\H,0,3.083061,-2.45844,-0.
526246\H,0,3.845579,-1.136582,-1.435506\C,0,4.316225,-1.135476,0.62962
5\H,0,4.350254,-1.809266,1.47274\C,0,5.159847,-0.041086,0.537505\C,0,6
.2018,0.165328,1.612497\H,0,7.190456,0.155563,1.153653\H,0,6.069665,1.
147845,2.065634\H,0,6.166164,-0.595276,2.391138\O,0,5.115112,0.812445,
-0.393785\N,0,2.108772,-0.623634,-0.437398\C,0,2.199219,0.703125,-0.47
7126\C,0,0.916132,-1.226879,-0.336206\C,0,1.062689,1.469341,-0.411733\
H,0,3.217088,1.089643,-0.553649\C,0,-0.270666,-0.53681,-0.230261\H,0,0
.955442,-2.301358,-0.33238\C,0,-0.201576,0.88792,-0.266891\H,0,1.17778
,2.53831,-0.459494\N,0,-1.499715,-1.169672,-0.066968\N,0,-1.32943,1.62
4861,-0.158017\C,0,-2.64015,-0.394945,-0.533809\C,0,-1.544429,-2.60653
2,-0.242262\C,0,-2.590001,0.978706,0.127466\C,0,-1.307024,3.071689,-0.
188005\C,0,-3.987187,-1.038372,-0.222002\H,0,-2.574528,-0.244427,-1.61
9148\C,0,-1.453224,-3.086332,-1.683622\H,0,-2.464867,-2.968781,0.20646
8\H,0,-0.751367,-3.043345,0.36191\C,0,-2.863661,0.899658,1.626117\H,0,
-3.369223,1.581347,-0.346139\C,0,-1.264028,3.640117,-1.59545\H,0,-0.47
1626,3.440237,0.406911\H,0,-2.206474,3.415082,0.319732\C,0,-4.281448,-
1.130529,1.267621\H,0,-4.073706,-2.010492,-0.705422\H,0,-4.746529,-0.4
11224,-0.695137\H,0,-2.300871,-2.733474,-2.269885\H,0,-0.546596,-2.736
945,-2.174095\H,0,-1.456667,-4.175111,-1.719636\C,0,-4.204099,0.243335
,1.913405\H,0,-2.829512,1.902817,2.053558\H,0,-2.060568,0.328231,2.093
203\H,0,-0.379385,3.306881,-2.134146\H,0,-2.138811,3.328105,-2.164391\
H,0,-1.250958,4.728889,-1.563898\H,0,-5.269008,-1.567798,1.417702\H,0,
-3.565087,-1.796294,1.752586\H,0,-4.358941,0.168791,2.989758\H,0,-5.01
1397,0.87207,1.526464\\Version=AM64L-G03RevD.01\State=1-A\HF=-974.6151
104\MP2=-978.1726884\RMSD=4.042e-09\Thermal=0.\PG=C01 [X(C19H29N3O1)]\
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4a*2a_6

1\1\GINC-NODE19\SP\RMP2-FC\6-31+G(2d,p)\C19H29N3O1\ZIP04\02-Feb-2011\0
\\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\\cat11_1_b981_smp2-5
_seq_2\\0,1\C,0,-3.350841,-1.288922,-1.004331\H,0,-3.725075,-0.870955,
-1.938927\H,0,-3.034679,-2.316537,-1.174215\C,0,-4.341069,-1.150446,0.
06956\H,0,-4.44416,-1.937621,0.80156\C,0,-5.162853,-0.035887,0.07649\C
,0,-6.273306,0.042812,1.098556\H,0,-6.302387,-0.819379,1.763449\H,0,-6
.158327,0.94909,1.693189\H,0,-7.228207,0.120854,0.578841\O,0,-5.0451,0
.936771,-0.722105\N,0,-2.063747,-0.524936,-0.759553\C,0,-2.137113,0.80
1281,-0.678333\C,0,-0.903961,-1.161226,-0.542871\C,0,-1.011087,1.53497
9,-0.401174\H,0,-3.13902,1.211406,-0.815601\C,0,0.27277,-0.505838,-0.2
594\H,0,-0.963365,-2.233462,-0.59641\C,0,0.228941,0.919203,-0.199232\H
,0,-1.114551,2.604424,-0.339413\N,0,1.479172,-1.170878,-0.058701\N,0,1

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.356371,1.62305,0.045288\C,0,2.423366,-0.441679,0.776415\C,0,1.435858,
-2.612846,0.074855\C,0,2.625888,0.943612,0.171664\C,0,1.354799,3.06697
6,0.141979\C,0,3.780501,-1.123746,0.90656\H,0,2.00846,-0.308326,1.7838
3\C,0,0.882494,-3.127045,1.395988\H,0,2.443482,-2.991137,-0.072522\H,0
,0.866005,-3.009733,-0.763497\C,0,3.37657,0.882469,-1.154711\H,0,3.219
746,1.514312,0.890376\C,0,0.91908,3.575381,1.505213\H,0,0.732785,3.487
189,-0.647689\H,0,2.368773,3.401566,-0.069795\C,0,4.547615,-1.197474,-
0.404777\H,0,3.6765,-2.107474,1.361964\H,0,4.357623,-0.532526,1.621407
\H,0,1.511843,-2.823109,2.231642\H,0,-0.122679,-2.758309,1.590818\H,0,
0.845691,-4.215813,1.389655\C,0,4.721185,0.189718,-1.001519\H,0,3.5078
9,1.89364,-1.542668\H,0,2.759242,0.343234,-1.874148\H,0,-0.090547,3.25
0861,1.748353\H,0,1.584857,3.208543,2.285342\H,0,0.939638,4.664251,1.5
28007\H,0,5.518564,-1.663142,-0.233401\H,0,4.016085,-1.830698,-1.11761
\H,0,5.221502,0.130488,-1.968114\H,0,5.369509,0.785614,-0.352404\\Vers
ion=AM64L-G03RevD.01\State=1-A\HF=-974.6153322\MP2=-978.1729927\RMSE=3
.797e-09\Thermal=0.\PG=C01 [X(C19H29N3O1)]\\@
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4f*2a 7

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1\1\G\INC-CALYPSO\SP\RMP2-FC\6-31+G(2d,p)\C19H29N3O1\BORIS\01-Feb-2011\
0\#\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\cat11_1_b986_smp2-
5_3\0,1\C,0,-3.526275,1.179048,-0.337861\H,0,-3.383646,2.254208,-0.24
7186\H,0,-3.985299,0.957291,-1.301488\C,0,-4.305175,0.598297,0.761682\
H,0,-4.39383,1.139743,1.691692\C,0,-4.96461,-0.601077,0.551176\C,0,-5.
886712,-1.123144,1.628499\H,0,-6.89183,-1.218375,1.2177\H,0,-5.568909,
-2.121415,1.929366\H,0,-5.923663,-0.479721,2.506437\O,0,-4.843837,-1.3
02393,-0.493526\N,0,-2.123523,0.615436,-0.470864\C,0,-2.002109,-0.6888
26,-0.701009\C,0,-1.039272,1.387945,-0.31542\C,0,-0.754227,-1.257648,-
0.798894\H,0,-2.948251,-1.22727,-0.782606\C,0,0.242991,0.894947,-0.401
924\H,0,-1.239218,2.429381,-0.134132\C,0,0.407416,-0.495286,-0.657028\
H,0,-0.702367,-2.318955,-0.970907\N,0,1.369668,1.691442,-0.294932\N,0,
1.649966,-1.042818,-0.763279\C,0,2.522548,1.007982,0.253434\C,0,1.2183
99,3.095523,0.020963\C,0,2.834879,-0.208822,-0.609101\C,0,1.80447,-2.2
78819,-1.515271\C,0,2.368085,0.675175,1.73553\H,0,3.374436,1.679356,0.
134149\C,0,0.877039,3.938153,-1.195457\H,0,0.481014,3.24568,0.817396\H
,0,2.168243,3.435564,0.429208\C,0,4.017111,-0.970593,-0.010177\H,0,3.1
30283,0.159307,-1.597802\C,0,1.818413,-3.545545,-0.678729\H,0,1.006911
,-2.330738,-2.255879\H,0,2.729679,-2.201792,-2.085719\C,0,3.581931,-0.
060213,2.277861\H,0,2.199165,1.601042,2.287763\H,0,1.47581,0.061622,1.
875615\H,0,-0.039159,3.608173,-1.680425\H,0,1.67673,3.880138,-1.931292
\H,0,0.747962,4.981258,-0.908874\C,0,3.843028,-1.312574,1.460884\H,0,4
.228104,-1.865781,-0.593788\H,0,4.895543,-0.330542,-0.126906\H,0,2.686
636,-3.586062,-0.025421\H,0,1.848135,-4.418194,-1.330527\H,0,0.930816,
-3.622327,-0.053981\H,0,3.428817,-0.310853,3.327537\H,0,4.458655,0.592
908,2.238034\H,0,4.733286,-1.828663,1.821666\H,0,3.006281,-2.00139,1.5
87155\\Version=AM64L-G03RevD.01\State=1-A\HF=-974.6134525\MP2=-978.171
3658\RMSD=4.446e-09\Thermal=0.\PG=C01 [X(C19H29N3O1)]\@
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4f*2a 8

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1\1\GINC-AZAZEL\SP\RMP2-FC\6-31+G(2d,p)\C19H29N3O1\BORIS\01-Feb-2011\0
\\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\\cat11_1_b986_spmp2-5
_2\\0,1\C,0,-3.427396,0.9638,1.054684\H,0,-3.648909,0.451616,1.991001\
```

H,0,-3.26264,2.020793,1.255015\C,0,-4.468506,0.709119,0.054593\H,0,-4.754671,1.49473,-0.628604\C,0,-5.09389,-0.526405,0.051179\C,0,-6.258859,-0.75062,-0.884608\H,0,-6.486101,0.120404,-1.497657\H,0,-6.04701,-1.599753,-1.534362\H,0,-7.139988,-1.009344,-0.297582\O,0,-4.752027,-1.494782,0.78834\N,0,-2.059706,0.426947,0.670462\C,0,-1.918865,-0.891498,0.563689\C,0,-1.042193,1.250675,0.382075\C,0,-0.71716,-1.424965,0.160648\H,0,-2.823102,-1.463823,0.779028\C,0,0.182083,0.795389,-0.052788\H,0,-1.258965,2.299791,0.481949\C,0,0.368924,-0.610906,-0.16673\H,0,-0.640117,-2.4975,0.107841\N,0,1.217421,1.637942,-0.413659\N,0,1.557165,-1.125551,-0.591999\C,0,2.534963,1.08468,-0.186443\C,0,1.05928,3.067346,-0.255545\C,0,2.658804,-0.236009,-0.937544\C,0,1.562187,-2.446066,-1.204121\C,0,2.881459,0.970401,1.296349\H,0,3.248775,1.76013,-0.660594\C,0,0.288782,3.704248,-1.398425\H,0,0.597022,3.310639,0.707926\H,0,2.058582,3.497496,-0.220468\C,0,4.027208,-0.856417,-0.657738\H,0,2.597671,-0.009353,-2.007739\C,0,1.93037,-3.587291,-0.273822\H,0,0.580461,-2.62413,-1.642291\H,0,2.256271,-2.415155,-2.043697\C,0,4.258297,0.366431,1.510946\H,0,2.820524,1.961567,1.749088\H,0,2.130043,0.353457,1.793719\H,0,-0.703971,3.274868,-1.515871\H,0,0.819983,3.561978,-2.337642\H,0,0.173888,4.774023,-1.226732\C,0,4.350102,-0.984055,0.822515\H,0,4.117577,-1.818996,-1.159487\H,0,4.769352,-0.207998,-1.130879\H,0,2.953993,-3.501046,0.083229\H,0,1.837676,-4.536948,-0.800225\H,0,1.278366,-3.621244,0.596923\H,0,4.462496,0.269211,2.577376\H,0,5.02344,1.036092,1.107193\H,0,5.346452,-1.410955,0.942149\H,0,3.651434,-1.674815,1.297572\\Version=AM64L-G03RevD.01\State=1-A\HF=-974.6133819\MP2=-978.171491\RMSE=3.945e-09\Thermal=0.\PG=C01 [X(C19H29N3O1)]\\@

4f*2a_9

1\1\GINC-CIPCLU04\SP\RMP2-FC\6-31+G(2d,p)\C19H29N3O1\BRYCH\03-Feb-2011
\\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\\cat11_1cis_b981_fr
eq_2\\0,1\C,0,-3.615444,1.342827,-0.967463\H,0,-3.974582,1.947112,-0.138421\H,0,-3.655443,1.914597,-1.891284\C,0,-4.146206,0.021544,-1.05339\H,0,-4.166773,-0.472322,-2.015576\C,0,-4.635629,-0.707419,0.052113\C,0,-4.674774,-0.021509,1.416488\H,0,-5.413293,0.782,1.430093\H,0,-4.959652,-0.760315,2.160083\H,0,-3.714119,0.412715,1.700969\O,0,-5.042076,-1.87399,-0.008895\N,0,-1.988158,1.399606,-0.668757\C,0,-1.341387,2.547431,-0.561957\C,0,-1.351628,0.246171,-0.499878\C,0,0.004089,2.577284,-0.287143\H,0,-1.922536,3.448677,-0.69598\C,0,-0.000705,0.161147,-0.234215\H,0,-2.022458,-0.600456,-0.59523\C,0,0.723533,1.384149,-0.12627\H,0,0.491089,3.533741,-0.200911\N,0,0.657365,-1.050953,-0.093266\N,0,2.053779,1.367298,0.117133\C,0,1.858149,-0.987477,0.724925\C,0,-0.156485,-2.252837,-0.023439\C,0,2.763039,0.107141,0.167259\C,0,2.82888,2.580809,0.248408\C,0,2.641638,-2.294578,0.769608\H,0,1.596361,-0.711363,1.75455\C,0,-0.879981,-2.468362,1.296008\H,0,0.488296,-3.101014,-0.235789\H,0,-0.866652,-2.224493,-0.846298\C,0,3.345789,-0.271739,-1.190424\H,0,3.57972,0.232425,0.883029\C,0,2.741712,3.201001,1.632123\H,0,2.529165,3.295454,-0.518462\H,0,3.863133,2.325429,0.024709\C,0,3.234897,-2.691819,-0.573443\H,0,2.030947,-3.093918,1.185813\H,0,3.453844,-2.14475,1.4851\H,0,-0.176812,-2.590296,2.11987\H,0,-1.542211,-1.640104,1.538236\H,0,-1.494097,-3.365429,1.241121\C,0,4.116215,-1.580402,-1.119569\H,0,3.989606,0.53461,-1.54559\H,0,2.525119,-0.361985,-1.903163\H,0,1.716859,3.461381,1.889385\H,0,3.108094,2.508095,2.388116\H,0,3.34522,4.10663

4,1.681897\H,0,3.80809,-3.612408,-0.460018\H,0,2.438654,-2.903257,-1.2
8916\H,0,4.495743,-1.842839,-2.107133\H,0,4.990176,-1.457829,-0.473016
\Version=AM64L-G03RevD.01\State=1-A\HF=-974.601532\MP2=-978.1664728\R
MSD=2.565e-09\Thermal=0.\PG=C01 [X(C19H29N3O1)]\@

4f*2a_10

1\1\GINC-CIPCLU08\SP\RMP2-FC\6-31+G(2d,p)\C19H29N3O1\BRYCH\03-Feb-2011
\0\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\cat11_1cis_b981_fr
eq_1\0,1\C,0,3.627701,1.574827,-0.145283\H,0,3.779684,2.378672,-0.862
436\H,0,3.862127,1.931306,0.85386\C,0,4.222892,0.328337,-0.524328\H,0,
4.369992,0.135936,-1.57937\C,0,4.632322,-0.695892,0.352685\C,0,4.52254
7,-0.502777,1.860441\H,0,3.930896,0.352876,2.182996\H,0,4.095556,-1.40
575,2.29322\H,0,5.527603,-0.39848,2.26928\O,0,5.101513,-1.778765,-0.02
4976\N,0,1.997303,1.546439,-0.080125\C,0,1.293998,2.653358,0.09241\C,0
,1.38869,0.372627,-0.216732\C,0,-0.077435,2.617409,0.14566\H,0,1.85106
4,3.574714,0.182953\C,0,0.019269,0.221928,-0.157057\H,0,2.097465,-0.42
9423,-0.387003\C,0,-0.76213,1.398026,0.038143\H,0,-0.611432,3.543318,0
.275424\N,0,-0.599552,-1.013914,-0.259547\N,0,-2.109059,1.3137,0.11868
5\C,0,-1.966194,-0.960045,-0.754209\C,0,0.2238,-2.150511,-0.633744\C,0
, -2.753281,0.017968,0.113054\C,0,-2.945962,2.479756,0.293993\C,0,-2.67
8606,-2.308007,-0.742513\H,0,-1.977981,-0.5767,-1.782797\C,0,0.61725,-
2.207507,-2.101042\H,0,-0.314323,-3.053089,-0.35909\H,0,1.109276,-2.14
6582,-0.002679\C,0,-2.966743,-0.517029,1.525153\H,0,-3.72553,0.151346,
-0.368671\C,0,-3.228534,3.21457,-1.004852\H,0,-2.499373,3.148045,1.030
41\H,0,-3.881058,2.139111,0.734901\C,0,-2.909259,-2.860244,0.656062\H,
0,-2.152817,-3.025525,-1.370261\H,0,-3.646364,-2.151642,-1.225198\H,0,
-0.256707,-2.307768,-2.744619\H,0,1.162684,-1.318262,-2.410336\H,0,1.2
64596,-3.064847,-2.277435\C,0,-3.675511,-1.861593,1.507939\H,0,-3.5358
2,0.210615,2.106078\H,0,-1.99233,-0.617016,2.005054\H,0,-2.310266,3.55
8926,-1.476561\H,0,-3.741498,2.564142,-1.711807\H,0,-3.86233,4.081482,
-0.821533\H,0,-3.454378,-3.802221,0.589634\H,0,-1.954901,-3.083168,1.1
36208\H,0,-3.789758,-2.235231,2.525501\H,0,-4.685915,-1.739432,1.10631
1\Version=AM64L-G03RevD.01\State=1-A\HF=-974.6014225\MP2=-978.1651212
\RMSD=2.312e-09\Thermal=0.\PG=C01 [X(C19H29N3O1)]\@

4f*2b

4f*2b_1

1\1\GINC-NODE2\SP\RMP2-FC\6-31+G(2d,p)\C19H29N3O2\ZIP04\04-Feb-2011\0\
\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\cat11_2_b981_spmp2-5_
mpr_1\0,1\C,0,-3.02097,1.966073,-0.970591\H,0,-3.168083,3.040944,-1.0
57804\H,0,-3.112792,1.513333,-1.957908\C,0,-3.905811,1.342459,0.005786
\H,0,-4.372735,1.935812,0.774786\C,0,-4.20409,-0.005747,-0.120625\O,0,
-3.68304,-0.818844,-0.911834\N,0,-1.526278,1.824731,-0.664818\C,0,-0.7
22624,2.863998,-0.505289\C,0,-1.066547,0.573173,-0.513453\C,0,0.604098
,2.688352,-0.197376\H,0,-1.162256,3.842159,-0.618666\C,0,0.251933,0.29
7821,-0.228361\H,0,-1.833624,-0.181793,-0.645112\C,0,1.141952,1.401608
, -0.068636\H,0,1.215993,3.563193,-0.060042\N,0,0.722987,-1.001574,-0.1
14365\N,0,2.449694,1.186235,0.193683\C,0,1.915711,-1.136557,0.706845\C
,0,-0.266215,-2.066978,-0.04906\C,0,2.970811,-0.163658,0.19115\C,0,3.3
88985,2.270744,0.370862\C,0,2.504505,-2.542993,0.701723\H,0,1.691156,-

0.863431,1.74607\C,0,-0.991475,-2.182644,1.281044\H,0,0.240027,-2.9995
13,-0.28235\H,0,-0.982722,-1.920561,-0.852864\C,0,3.496518,-0.566877,-
1.182709\H,0,3.794401,-0.185194,0.909417\C,0,3.376567,2.850992,1.77452
7\H,0,3.202509,3.045661,-0.373027\H,0,4.378424,1.87725,0.14505\C,0,3.0
29987,-2.968706,-0.660539\H,0,1.785782,-3.261361,1.092165\H,0,3.331049
,-2.538409,1.416674\H,0,-0.301657,-2.403515,2.095996\H,0,-1.530489,-1.
270298,1.527341\H,0,-1.722372,-2.987613,1.231318\C,0,4.0638,-1.977253,
-1.169292\H,0,4.254591,0.148948,-1.505176\H,0,2.674249,-0.50448,-1.896
654\H,0,2.395654,3.242414,2.036805\H,0,3.637034,2.089754,2.508407\H,0,
4.099483,3.661889,1.857017\H,0,3.462411,-3.967197,-0.589664\H,0,2.2080
24,-3.030616,-1.375741\H,0,4.398211,-2.25245,-2.169684\H,0,4.948263,-2
.011436,-0.526075\O,0,-5.160985,-0.451586,0.748016\C,0,-5.490334,-1.80
9755,0.647054\H,0,-6.260635,-1.985194,1.393407\H,0,-5.872031,-2.056366
,-0.342098\H,0,-4.631287,-2.448538,0.849091\\Version=AM64L-G03RevD.01\
State=1-A\HF=-1049.4888694\MP2=-1053.246864\RMSD=4.160e-09\Thermal=0\
PG=C01 [X(C19H29N3O2)]\\@

4f*2b_2

1\1\GINC-NODE5\SP\RMP2-FC\6-31+G(2d,p)\C19H29N3O2\ZIP04\04-Feb-2011\0\
\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\\cat11_2_b981_smp2-5_
mpr_4\0,1\C,0,-3.067503,2.121483,0.314287\H,0,-3.265091,1.864621,1.35
5235\H,0,-3.207166,3.19258,0.181116\C,0,-3.856219,1.31999,-0.613263\H,
0,-4.229211,1.754574,-1.526157\C,0,-4.168096,0.010947,-0.281084\O,0,-3
.737542,-0.640732,0.694022\N,0,-1.552186,1.929701,0.193663\C,0,-0.7160
72,2.92196,-0.066836\C,0,-1.099965,0.676525,0.354753\C,0,0.631875,2.69
1642,-0.196773\H,0,-1.144817,3.905306,-0.176875\C,0,0.232019,0.348791,
0.237645\H,0,-1.887238,-0.035424,0.579895\C,0,1.151068,1.398037,-0.063
122\H,0,1.274083,3.528149,-0.412336\N,0,0.681286,-0.954363,0.375576\N,
0,2.465968,1.124488,-0.214107\C,0,2.076031,-1.074224,0.766009\C,0,-0.2
60928,-1.940782,0.880227\C,0,2.92008,-0.24943,-0.201002\C,0,3.435473,2
.152661,-0.519514\C,0,2.590693,-2.509711,0.760656\H,0,2.224079,-0.6610
17,1.772425\C,0,-0.528726,-1.862581,2.37408\H,0,0.120782,-2.924367,0.6
21068\H,0,-1.1924,-1.838149,0.329708\C,0,2.938555,-0.85409,-1.60083\H,
0,3.937313,-0.241221,0.198848\C,0,3.90163,2.919401,0.705989\H,0,3.0314
5,2.830371,-1.272129\H,0,4.285021,1.661667,-0.990703\C,0,2.61569,-3.13
4276,-0.625799\H,0,2.025701,-3.121711,1.46161\H,0,3.609369,-2.477535,1
.154989\H,0,0.378269,-2.032874,2.954821\H,0,-0.939506,-0.896221,2.6583
42\H,0,-1.258784,-2.61876,2.656775\C,0,3.442589,-2.288302,-1.580273\H,
0,3.559094,-0.237854,-2.253536\H,0,1.924784,-0.82305,-2.002021\H,0,3.0
71291,3.410326,1.209852\H,0,4.375662,2.249761,1.422079\H,0,4.626861,3.
681911,0.42396\H,0,3.020767,-4.144763,-0.563566\H,0,1.600034,-3.224849
,-1.014297\H,0,3.41283,-2.707026,-2.586263\H,0,4.490891,-2.305465,-1.2
67361\O,0,-5.0256,-0.599177,-1.152747\C,0,-5.339707,-1.934059,-0.86498
8\H,0,-6.030219,-2.250977,-1.642111\H,0,-4.453714,-2.568245,-0.881379\
H,0,-5.811405,-2.033161,0.110919\\Version=AM64L-G03RevD.01\State=1-A\H
F=-1049.488573\MP2=-1053.2460776\RMSD=5.151e-09\Thermal=0\PG=C01 [X(C
19H29N3O2)]\\@

4f*2b_3

1\1\GINC-CIPCLU03\SP\RMP2-FC\6-31+G(2d,p)\C19H29N3O2\BRYCH\05-Feb-2011
\0\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\\cat11_2_b986_smp2

-5_1\O,1\C,0,2.891789,2.032649,0.976308\H,0,2.914851,3.11506,1.087805
\H,0,2.959266,1.569678,1.960772\C,0,3.903167,1.524845,0.060271\H,0,4.3
5331,2.175731,-0.67122\C,0,4.34085,0.216201,0.205283\O,0,3.85629,-0.65
5496,0.954569\O,0,5.401429,-0.112132,-0.591787\C,0,5.867945,-1.428276,
-0.472356\H,0,6.705579,-1.510282,-1.15992\H,0,6.2,-1.644209,0.541528\H
,0,5.100325,-2.153155,-0.740649\N,0,1.441991,1.741761,0.56051\C,0,0.53
1151,2.692161,0.426883\C,0,1.133024,0.45844,0.325077\C,0,-0.753637,2.3
92926,0.036405\H,0,0.847317,3.701933,0.634971\C,0,-0.128374,0.072404,-
0.072772\H,0,1.962446,-0.225011,0.470071\C,0,-1.128265,1.072711,-0.228
839\H,0,-1.46031,3.200367,-0.050894\N,0,-0.441982,-1.235921,-0.364417\N
,0,-2.387292,0.744441,-0.632417\C,0,-1.822015,-1.588203,-0.124489\C,0
,0.56505,-2.268648,-0.188904\C,0,-2.725384,-0.646655,-0.913831\C,0,-3.
200096,1.762835,-1.277253\C,0,-2.164782,-1.648987,1.362674\H,0,-1.9789
51,-2.577064,-0.55792\C,0,1.527761,-2.349948,-1.358188\H,0,1.115592,-2
.129373,0.744884\H,0,0.03239,-3.21347,-0.093937\C,0,-4.189327,-0.96817
7,-0.613367\H,0,-2.544528,-0.836352,-1.977263\C,0,-4.174419,2.482358,-
0.362029\H,0,-2.535236,2.482476,-1.755187\H,0,-3.743645,1.283594,-2.09
0732\C,0,-3.62506,-1.995567,1.595474\H,0,-1.511074,-2.379709,1.840682\H
,0,-1.939679,-0.683941,1.821712\H,0,2.075768,-1.421605,-1.499018\H,0,
0.991159,-2.574916,-2.278854\H,0,2.261029,-3.134367,-1.179127\C,0,-4.5
18738,-1.005165,0.870398\H,0,-4.847676,-0.277761,-1.139457\H,0,-4.3890
08,-1.951219,-1.047327\H,0,-4.935019,1.807014,0.022352\H,0,-4.67825,3.
279314,-0.908495\H,0,-3.66726,2.926634,0.492371\H,0,-3.844018,-2.00120
4,2.663387\H,0,-3.827842,-3.006663,1.230642\H,0,-5.569645,-1.265115,1.
002424\H,0,-4.381503,-0.014768,1.307949\Version=AM64L-G03RevD.01\Stat
e=1-A\HF=-1049.4862292\MP2=-1053.2443146\RMSD=5.138e-09\Thermal=0.\PG=
C01 [X(C19H29N3O2)]\@

4f*2b_4

1\1\GINC-CIPCLU06\SP\RMP2-FC\6-31+G(2d,p)\C19H29N3O2\BRYCH\07-Feb-2011
\O\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\cat11_2cis_b981_sp
mp2-5_2\O,1\C,0,-3.250458,1.56662,-1.158586\H,0,-3.643173,2.085752,-0
.28823\H,0,-3.265864,2.220915,-2.027767\C,0,-3.843098,0.27889,-1.39074
6\H,0,-3.945097,-0.097932,-2.39582\C,0,-4.388671,-0.500687,-0.358854\O
,0,-4.969629,-1.575245,-0.440059\N,0,-1.685554,1.532455,-0.810959\C,0,
-1.00734,2.651589,-0.613591\C,0,-1.098364,0.350069,-0.658794\C,0,0.320
815,2.620818,-0.270589\H,0,-1.552581,3.576459,-0.731753\C,0,0.23083,0.
207849,-0.321585\H,0,-1.791029,-0.464267,-0.835179\C,0,0.990111,1.3968
22,-0.125268\H,0,0.833862,3.554816,-0.117393\N,0,0.837275,-1.033116,-0
.190155\N,0,2.304651,1.322003,0.182959\C,0,1.986708,-1.04038,0.701107\N
,0,-0.023467,-2.203298,-0.205243\C,0,2.963207,0.034727,0.233556\C,0,3
.113533,2.499554,0.405092\C,0,2.717405,-2.377479,0.751677\H,0,1.672687
,-0.78439,1.721346\C,0,-0.837129,-2.42445,1.059857\H,0,0.601754,-3.069
828,-0.401176\H,0,-0.678172,-2.125594,-1.070059\C,0,3.61193,-0.325899,
-1.098753\H,0,3.739916,0.107294,0.999623\C,0,2.979367,3.064402,1.80871
\H,0,2.877014,3.255912,-0.343487\H,0,4.148157,2.215976,0.220172\C,0,3.
37769,-2.757342,-0.564833\H,0,2.052215,-3.164497,1.103005\H,0,3.487935
,-2.28169,1.520478\H,0,-0.191866,-2.585422,1.923556\H,0,-1.489354,-1.5
81452,1.278044\H,0,-1.469072,-3.303579,0.944762\C,0,4.329184,-1.664172
,-1.022992\H,0,4.304818,0.465226,-1.38999\H,0,2.8328,-0.364108,-1.8611
02\H,0,1.953045,3.353026,2.027123\H,0,3.282221,2.327473,2.551153\H,0,3

.612158,3.943302,1.926933\H,0,3.910409,-3.701273,-0.445754\H,0,2.61963
3,-2.918883,-1.333178\H,0,4.758264,-1.912165,-1.993862\H,0,5.166193,-1
.592836,-0.32202\O,0,-4.186467,0.058394,0.893238\C,0,-4.814137,-0.6159
06,1.951843\H,0,-4.45817,-1.640747,2.039415\H,0,-4.56895,-0.058261,2.8
52377\H,0,-5.894285,-0.644177,1.818395\\Version=AM64L-G03RevD.01\State
=1-A\HF=-1049.4822027\MP2=-1053.2426051\RMSD=6.023e-09\Thermal=0.\PG=C
01 [X(C19H29N3O2)]\\@

4f*2b_5

1\1\GINC-CIPCLU02\SP\RMP2-FC\6-31+G(2d,p)\C19H29N3O2\BRYCH\07-Feb-2011
\0\\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\\cat11_2cis_b981_sp
mp2-5_1\\0,1\C,0,3.314495,1.802332,-0.40674\H,0,3.409932,2.659652,-1.0
69836\H,0,3.59587,2.075645,0.606837\C,0,3.957508,0.61445,-0.894168\H,0
,4.172604,0.506656,-1.945305\C,0,4.405939,-0.408279,-0.043019\O,0,5.00
8429,-1.433272,-0.335517\N,0,1.720337,1.690175,-0.259082\C,0,0.987176,
2.747967,0.048057\C,0,1.153296,0.50054,-0.430363\C,0,-0.372531,2.64372
1,0.20091\H,0,1.511975,3.684606,0.166322\C,0,-0.199464,0.282357,-0.276
458\H,0,1.881608,-0.25117,-0.709913\C,0,-1.011287,1.402992,0.060743\H,
0,-0.932714,3.532514,0.43636\N,0,-0.77107,-0.974188,-0.414042\N,0,-2.3
43022,1.249587,0.24007\C,0,-2.175585,-0.955309,-0.790148\C,0,0.065556,
-2.037926,-0.940302\C,0,-2.927498,-0.073473,0.202764\C,0,-3.20856,2.35
737,0.577237\C,0,-2.824223,-2.334982,-0.809589\H,0,-2.292332,-0.5083,-
1.786134\C,0,0.327703,-1.970329,-2.436502\H,0,-0.404826,-2.984231,-0.6
89274\H,0,1.002444,-2.0324,-0.388599\C,0,-2.99352,-0.705392,1.589241\H
,0,-3.942736,0.04066,-0.186312\C,0,-3.637593,3.172053,-0.630811\H,0,-2
.725918,2.99037,1.322158\H,0,-4.085421,1.94015,1.069088\C,0,-2.903381,
-2.984297,0.56355\H,0,-2.324798,-2.984046,-1.52701\H,0,-3.837006,-2.19
7361,-1.196165\H,0,-0.596844,-2.057916,-3.007139\H,0,0.811621,-1.03826
4,-2.721394\H,0,0.984612,-2.785547,-2.735507\C,0,-3.636951,-2.081766,1
.542076\H,0,-3.545031,-0.046526,2.261899\H,0,-1.978065,-0.7823,1.97989
1\H,0,-2.781192,3.59668,-1.151095\H,0,-4.182571,2.550933,-1.340176\H,0
, -4.289924,3.989726,-0.326223\H,0,-3.407182,-3.947931,0.48249\H,0,-1.9
00093,-3.184675,0.943326\H,0,-3.643711,-2.523705,2.538474\H,0,-4.68337
4,-1.987914,1.236602\O,0,4.066518,-0.184285,1.280463\C,0,4.56041,-1.13
207,2.189594\H,0,4.211796,-0.818774,3.170464\H,0,4.19051,-2.130727,1.9
64446\H,0,5.648538,-1.164106,2.17709\\Version=AM64L-G03RevD.01\State=1
-A\HF=-1049.4819676\MP2=-1053.2416687\RMSD=2.211e-09\Thermal=0.\PG=C01
[X(C19H29N3O2)]\\@

4f*2b_6

1\1\GINC-CIPCLU08\SP\RMP2-FC\6-31+G(2d,p)\C19H29N3O2\BRYCH\07-Feb-2011
\0\\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\\cat11_2cis_b986_sp
mp2-5_2\\0,1\C,0,-3.087707,1.692319,-1.212672\H,0,-3.468876,2.282464,-
0.383595\H,0,-2.95384,2.316681,-2.093579\C,0,-3.819598,0.483234,-1.458
01\H,0,-3.890444,0.085434,-2.457689\C,0,-4.541975,-0.182702,-0.454618\
O,0,-5.252623,-1.173712,-0.558526\O,0,-4.364519,0.387459,0.795443\C,0,
-5.154862,-0.162493,1.816674\H,0,-4.948718,-1.222265,1.954146\H,0,-4.9
03329,0.386016,2.720904\H,0,-6.215842,-0.050178,1.599867\N,0,-1.562113
,1.474704,-0.747791\C,0,-0.747741,2.503856,-0.581805\C,0,-1.151614,0.2
38303,-0.49017\C,0,0.542068,2.322507,-0.142407\H,0,-1.147545,3.48042,-
0.812349\C,0,0.115827,-0.041635,-0.022329\H,0,-1.926683,-0.49674,-0.67

2447\C,0,1.016269,1.040825,0.16224\H,0,1.177748,3.186467,-0.046816\N,0
,0.523356,-1.31661,0.307132\N,0,2.280931,0.82978,0.627336\C,0,1.939922
, -1.550353,0.139279\C,0,-0.376247,-2.432108,0.07516\C,0,2.719255,-0.52
276,0.953403\C,0,2.963771,1.921691,1.302291\C,0,2.359822,-1.600421,-1.
328331\H,0,2.159961,-2.515832,0.597342\C,0,-1.422801,-2.582046,1.16362
1\H,0,-0.852572,-2.354334,-0.906776\H,0,0.238009,-3.330359,0.043128\C,
0,4.218634,-0.72166,0.731436\H,0,2.501063,-0.711249,2.010154\C,0,3.919
894,2.718319,0.432529\H,0,2.212854,2.583675,1.733865\H,0,3.502191,1.50
0293,2.150672\C,0,3.854629,-1.819751,-1.484175\H,0,1.798416,-2.392753,
-1.82526\H,0,2.074554,-0.665213,-1.814713\H,0,-2.047841,-1.697384,1.25
8047\H,0,-0.945449,-2.763019,2.12536\H,0,-2.079009,-3.420679,0.936552\
C,0,4.622369,-0.746025,-0.733844\H,0,4.787154,0.029859,1.278099\H,0,4.
480518,-1.678438,1.190315\H,0,4.762066,2.11363,0.104609\H,0,4.313699,3
.56565,0.993328\H,0,3.425377,3.102583,-0.457653\H,0,4.125394,-1.819765
, -2.540153\H,0,4.126644,-2.804376,-1.09301\H,0,5.697001,-0.914153,-0.8
12421\H,0,4.419941,0.223873,-1.191642\\Version=AM64L-G03RevD.01\State=
1-A\HF=-1049.4799011\MP2=-1053.2405671\RMSD=3.750e-09\Thermal=0.\PG=C0
1 [X(C19H29N3O2)]\\@

4f*2b_7

1\1\GINC-CIPCLU05\SP\RMP2-FC\6-31+G(2d,p)\C19H29N3O2\BRYCH\05-Feb-2011
\0\\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\\cat11_2_b986_smp2
-5_4\\0,1\C,0,-2.970568,2.2221,0.152135\H,0,-3.306944,2.044947,1.17374
3\H,0,-2.994176,3.291347,-0.04956\C,0,-3.716793,1.435222,-0.820762\H,0
, -3.939403,1.840391,-1.794206\C,0,-4.185703,0.182646,-0.455317\O,0,-3.
936047,-0.433881,0.601177\O,0,-4.987319,-0.410096,-1.390135\C,0,-5.463
002,-1.686877,-1.062779\H,0,-6.082289,-1.997069,-1.900297\H,0,-4.64774
2,-2.396902,-0.926641\H,0,-6.056416,-1.67135,-0.150467\N,0,-1.474062,1
.894662,0.22207\C,0,-0.530101,2.785004,-0.037584\C,0,-1.155925,0.62453
1,0.514325\C,0,0.799977,2.434316,-0.013383\H,0,-0.856197,3.783598,-0.2
80994\C,0,0.150768,0.19614,0.584329\H,0,-2.017023,-0.00962,0.700404\C,
0,1.187819,1.129351,0.304522\H,0,1.529161,3.186626,-0.261105\N,0,0.486
119,-1.090897,0.94584\N,0,2.496402,0.755639,0.356374\C,0,1.714203,-1.5
69801,0.352205\C,0,-0.572549,-2.063586,1.165919\C,0,2.850168,-0.616055
,0.705877\C,0,3.505258,1.7761,0.588568\C,0,1.584102,-1.822564,-1.14835
8\H,0,1.959008,-2.512438,0.844096\C,0,-1.19026,-1.959608,2.547053\H,0,
-1.348497,-1.983287,0.400364\H,0,-0.121661,-3.047596,1.048363\C,0,4.13
9541,-1.080866,0.028999\H,0,2.994578,-0.668203,1.790407\C,0,4.184307,2
.308022,-0.660941\H,0,3.044564,2.5957,1.140329\H,0,4.251116,1.354093,1
.261461\C,0,2.889664,-2.302627,-1.758172\H,0,0.788996,-2.550942,-1.312
161\H,0,1.266331,-0.901526,-1.641563\H,0,-1.666299,-0.995974,2.709056\
H,0,-0.433331,-2.10547,3.316451\H,0,-1.9615,-2.71888,2.663674\C,0,3.99
8601,-1.307196,-1.467715\H,0,4.953349,-0.388515,0.241973\H,0,4.423065,
-2.021931,0.507013\H,0,4.768647,1.537495,-1.158169\H,0,4.858424,3.1228
97,-0.397906\H,0,3.460402,2.687021,-1.379834\H,0,2.771408,-2.44396,-2.
832575\H,0,3.155797,-3.279084,-1.342997\H,0,4.948464,-1.656644,-1.8739
13\H,0,3.768833,-0.36424,-1.966804\\Version=AM64L-G03RevD.01\State=1-A
\HF=-1049.4863201\MP2=-1053.2440284\RMSD=4.237e-09\Thermal=0.\PG=C01 [
X(C19H29N3O2)]\\@

4f*2b_8

1\1\GINC-CIPCLU09\SP\RMP2-FC\6-31+G(2d,p)\C19H29N3O2\BRYCH\07-Feb-2011
\0\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\cat11_2cis_b986_sp
mp2-5_1\0,1\C,0,3.209348,1.971014,-0.228879\H,0,3.282026,2.865991,-0.
842962\H,0,3.34288,2.218344,0.820813\C,0,4.019865,0.880316,-0.68646\H,
0,4.357937,0.846748,-1.709839\C,0,4.473592,-0.137155,0.16944\O,0,5.205
872,-1.082033,-0.093221\O,0,3.971786,-0.013813,1.453481\C,0,4.461451,-
0.95131,2.375548\H,0,3.981935,-0.720317,3.32348\H,0,4.22092,-1.969495,
2.074925\H,0,5.542425,-0.876735,2.480812\N,0,1.621315,1.691863,-0.2689
3\C,0,0.754223,2.639722,0.046238\C,0,1.20435,0.472483,-0.588382\C,0,-0.
.598145,2.393483,0.037449\H,0,1.164424,3.602766,0.312684\C,0,-0.13148,
0.130644,-0.631687\H,0,2.026844,-0.189541,-0.833087\C,0,-1.088951,1.12
8325,-0.307585\H,0,-1.266671,3.190917,0.314612\N,0,-0.567536,-1.122425
, -1.008578\N,0,-2.425038,0.855875,-0.340811\C,0,-1.820777,-1.520304,-0.
.406878\C,0,0.409968,-2.164903,-1.265196\C,0,-2.885084,-0.474663,-0.72
2059\C,0,-3.354815,1.95572,-0.540622\C,0,-1.691065,-1.81639,1.085721\H
,0,-2.143445,-2.429977,-0.915808\C,0,1.010587,-2.081332,-2.656022\H,0,
1.197323,-2.160306,-0.506171\H,0,-0.108158,-3.116319,-1.158707\C,0,-4.
197904,-0.858521,-0.039535\H,0,-3.045361,-0.488171,-1.805658\C,0,-3.97
5229,2.513279,0.727887\H,0,-2.839231,2.748637,-1.082856\H,0,-4.139189,
1.606588,-1.211333\C,0,-3.021534,-2.209699,1.703813\H,0,-0.952379,-2.6
07123,1.223133\H,0,-1.298503,-0.933116,1.593827\H,0,1.527723,-1.139424
, -2.82354\H,0,0.233404,-2.178761,-3.412324\H,0,1.736171,-2.880912,-2.7
96829\C,0,-4.05666,-1.128463,1.44983\H,0,-4.960072,-0.102781,-0.22668\
H,0,-4.556194,-1.764917,-0.534179\H,0,-4.608034,1.779095,1.220613\H,0,
-4.590438,3.38076,0.48986\H,0,-3.215344,2.824066,1.442403\H,0,-2.90061
3,-2.382651,2.773288\H,0,-3.365801,-3.154399,1.272896\H,0,-5.024819,-1.
.41655,1.860872\H,0,-3.752651,-0.216313,1.966199\Version=AM64L-G03Rev
D.01\State=1-A\HF=-1049.4799101\MP2=-1053.2399419\RMSD=9.421e-09\Therm
al=0.PG=C01 [X(C19H29N3O2)]\@

4f*2b_9

1\1\GINC-CIPCLU03\SP\RMP2-FC\6-31+G(2d,p)\C19H29N3O2\BRYCH\07-Feb-2011
\0\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\cat11_2cis_b981_sp
mp2-5_6\0,1\C,0,3.190604,-1.42805,-0.672355\H,0,3.195645,-1.887512,0.
312907\H,0,2.929209,-2.162117,-1.432736\C,0,4.367005,-0.668449,-0.9732
87\H,0,4.711538,-0.580109,-1.991173\C,0,5.160441,-0.075641,0.023034\O,
0,6.209949,0.539646,-0.106992\N,0,1.832496,-0.567272,-0.59182\C,0,1.88
5493,0.743148,-0.694159\C,0,0.664112,-1.189044,-0.397956\C,0,0.743935,
1.503932,-0.596886\H,0,2.883161,1.133049,-0.862096\C,0,-0.533636,-0.52
2088,-0.269683\H,0,0.734531,-2.263251,-0.347382\C,0,-0.496949,0.904772
, -0.36325\H,0,0.834029,2.572375,-0.693061\N,0,-1.740996,-1.168999,-0.0
33957\N,0,-1.634619,1.621444,-0.222892\C,0,-2.91495,-0.434582,-0.48307
3\C,0,-1.762469,-2.6132,-0.14295\C,0,-2.870715,0.960772,0.130308\C,0,-
1.647104,3.065714,-0.311119\C,0,-4.235399,-1.09567,-0.102685\H,0,-2.89
1148,-0.319551,-1.574366\C,0,-1.716719,-3.15611,-1.563722\H,0,-2.65680
4,-2.972534,0.35778\H,0,-0.936756,-3.005977,0.447311\C,0,-3.091437,0.9
27109,1.639232\H,0,-3.678344,1.53192,-0.334797\C,0,-1.695512,3.577065,
-1.740237\H,0,-0.788353,3.474486,0.220811\H,0,-2.524161,3.411297,0.233
111\C,0,-4.478931,-1.140607,1.398206\H,0,-4.315089,-2.086164,-0.548353
\H,0,-5.024178,-0.502729,-0.571686\H,0,-2.595673,-2.851562,-2.130713\H
,0,-0.839157,-2.808597,-2.105555\H,0,-1.693331,-4.245102,-1.549861\C,0

, -4.408973, 0.256275, 1.993061\H, 0, -3.061694, 1.94444, 2.031982\H, 0, -2.262597, 0.385574, 2.096882\H, 0, -1.707678, 4.666218, -1.753439\H, 0, -0.834199, 3.241049, -2.313979\H, 0, -2.592438, 3.2224, -2.246165\H, 0, -5.451838, -1.591428, 1.595968\H, 0, -3.733908, -1.774536, 1.882644\H, 0, -4.527647, 0.216938, 3.075826\H, 0, -5.240655, 0.855624, 1.611208\O, 0, 4.621377, -0.223258, 1.289614\C, 0, 5.408873, 0.287959, 2.332282\H, 0, 5.579588, 1.356432, 2.214425\H, 0, 4.855359, 0.09866, 3.248705\H, 0, 6.377802, -0.206449, 2.376948\\Version=AM64L-G03RevD.01\State=1-A\HF=-1049.4805766\MP2=-1053.2369917\RMSD=2.262e-09\Thermal=0.\PG=C01 [X(C19H29N3O2)]\@

4f*2b_10

1\1\GINC-NODE8\SP\RMP2-FC\6-31+G(2d,p)\C19H29N3O2\ZIP04\04-Feb-2011\0\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\\cat11_2_b981_spmp2-5_mpr_3\0, 1\C, 0, 3.016514, -1.646729, -0.448919\H, 0, 2.635079, -2.662644, -0.360407\H, 0, 3.377739, -1.48507, -1.464177\C, 0, 4.019173, -1.315463, 0.548902\H, 0, 4.080959, -1.868818, 1.471644\C, 0, 4.930336, -0.306692, 0.262565\O, 0, 4.912983, 0.454814, -0.722333\N, 0, 1.743789, -0.777785, -0.397351\C, 0, 1.892718, 0.539728, -0.474556\C, 0, 0.52643, -1.320933, -0.279651\C, 0, 0.795017, 1.362029, -0.43095\H, 0, 2.915521, 0.88572, -0.586363\C, 0, -0.62815, -0.57454, -0.189966\H, 0, 0.516451, -2.396268, -0.248205\C, 0, -0.494601, 0.843339, -0.265711\H, 0, 0.958282, 2.422356, -0.515649\N, 0, -1.884908, -1.14404, -0.007992\N, 0, -1.586756, 1.63428, -0.172884\C, 0, -2.983303, -0.333334, -0.513424\C, 0, -1.995142, -2.582951, -0.129203\C, 0, -2.880903, 1.055014, 0.109026\C, 0, -1.499559, 3.076576, -0.25182\C, 0, -4.361873, -0.907922, -0.205876\H, 0, -2.894891, -0.217524, -1.601453\C, 0, -1.924115, -3.123277, -1.550178\H, 0, -2.931611, -2.88559, 0.330613\H, 0, -1.223039, -3.031141, 0.493609\C, 0, -3.183536, 1.033907, 1.604054\H, 0, -3.623573, 1.678569, -0.395577\C, 0, -1.439238, 3.595413, -1.677887\H, 0, -0.644659, 3.425972, 0.326562\H, 0, -2.379213, 3.477299, 0.248602\C, 0, -4.684942, -0.94015, 1.280177\H, 0, -4.482166, -1.890399, -0.660084\H, 0, -5.085533, -0.264322, -0.711664\H, 0, -2.7575, -2.761964, -2.151522\H, 0, -1.004806, -2.830502, -2.053794\H, 0, -1.970499, -4.211635, -1.541545\C, 0, -4.55817, 0.448247, 1.884701\H, 0, -3.109818, 2.046921, 2.002185\H, 0, -2.416136, 0.440194, 2.102428\H, 0, -0.572502, 3.206341, -2.208279\H, 0, -2.329393, 3.302668, -2.23311\H, 0, -1.379388, 4.683069, -1.68341\H, 0, -5.693032, -1.329345, 1.425819\H, 0, -4.006573, -1.619948, 1.798863\H, 0, -4.735937, 0.414956, 2.95956\H, 0, -5.328624, 1.100129, 1.462517\O, 0, 5.918081, -0.162361, 1.195749\C, 0, 6.834444, 0.87035, 0.952563\H, 0, 6.34309, 1.841867, 0.916612\H, 0, 7.538173, 0.844555, 1.780407\H, 0, 7.363622, 0.722064, 0.013\\Version=AM64L-G03RevD.01\State=1-A\HF=-1049.4851654\MP2=-1053.2388591\RMSD=3.487e-09\Thermal=0.\PG=C01 [X(C19H29N3O2)]\@

4f*2c

4f*2c_1

1\1\GINC-NODE12\SP\RMP2-FC\6-31+G(2d,p)\C21H31N3O1\ZIP04\01-Feb-2011\0\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\\cat11_3_b981_spmp2-5_seq_4\0, 1\C, 0, -1.084792, 2.337828, -0.636601\C, 0, 0.262932, 2.467741, -0.412459\C, 0, 1.058005, 1.338406, -0.170558\C, 0, 0.406301, 0.070341, -0.147642\C, 0, -0.953971, 0.050986, -0.36887\N, 0, -1.667044, 1.149478, -0.614335\N, 0, 1.141868, -1.085589, 0.059003\C, 0, 2.374157, -0.890323, 0.806656\C, 0, 3.181442, 0.210279, 0.125023\N, 0, 2.39329, 1.419789, 0.021556\C, 0, 3.718778, -0.23429, -1.23137\C, 0, 4.572361, -1.485983, -1.108299\C, 0, 3.791878, -2.60353, -0.

436338\C,0,3.238872,-2.142592,0.903614\C,0,0.409414,-2.325094,0.251186
\C,0,-0.244035,-2.481524,1.614748\C,0,3.097376,2.682973,0.01255\C,0,3.
017704,3.421848,1.337085\H,0,2.145755,-0.553331,1.826079\H,0,4.022205,
0.437366,0.785521\H,0,4.292268,0.579554,-1.678068\H,0,2.870782,-0.4262
4,-1.890136\H,0,4.917449,-1.799205,-2.093612\H,0,5.468544,-1.263375,-0
.521451\H,0,4.428301,-3.475967,-0.285887\H,0,2.977935,-2.918266,-1.091
716\H,0,2.699376,-2.943573,1.406324\H,0,4.072743,-1.893279,1.564398\H,
0,2.730537,3.305674,-0.803765\H,0,4.137299,2.467712,-0.225826\H,0,3.45
595,2.826917,2.13701\H,0,1.98747,3.639853,1.611571\H,0,3.560792,4.3644
97,1.279874\H,0,1.096847,-3.146894,0.073254\H,0,-0.334033,-2.402918,-0
.538318\H,0,-0.943904,-1.675047,1.824165\H,0,-0.801244,-3.415942,1.654
36\H,0,0.498264,-2.497958,2.412663\H,0,-1.572927,-0.83846,-0.389862\H,
0,-1.722049,3.186305,-0.836715\H,0,0.693878,3.454036,-0.437822\C,0,-3.
248345,0.998747,-0.798933\C,0,-3.603982,-0.347564,-1.195752\C,0,-3.837
563,1.461017,0.534242\C,0,-4.394903,-1.225329,-0.440505\H,0,-3.288991,
-0.689502,-2.174703\H,0,-3.172536,1.14743,1.342696\H,0,-3.878545,2.551
655,0.570712\C,0,-5.200371,0.844502,0.778374\C,0,-5.065807,-0.665908,0
.810661\O,0,-4.620514,-2.41076,-0.730667\H,0,-5.613099,1.224806,1.7156
23\H,0,-5.888981,1.136934,-0.016626\H,0,-6.034792,-1.156361,0.890981\H
,0,-4.490534,-0.972006,1.690345\H,0,-3.400141,1.750724,-1.580177\\Vers
ion=AM64L-G03RevD.01\State=1-A\HF=-1051.5163767\MP2=-1055.3686686\RMSD
=2.452e-09\Thermal=0.\PG=C01 [X(C21H31N3O1)]\\@

4f*2c_2

1\1\GINC-NODE12\SP\RMP2-FC\6-31+G(2d,p)\C21H31N3O1\ZIP04\01-Feb-2011\O
\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\\cat11_3_b986_spmp2-5
_seq_4\0,1\C,0,-3.14211,1.167507,-0.829653\C,0,-3.626876,-0.13143,-1.
241986\C,0,-3.763845,1.719546,0.453287\C,0,-4.568664,-0.897568,-0.5391
37\H,0,-3.28557,-0.524154,-2.19253\H,0,-3.197775,1.345,1.309735\H,0,-3
.678095,2.807906,0.475771\C,0,-5.203515,1.270402,0.606902\C,0,-5.25022
7,-0.244684,0.659635\O,0,-4.915384,-2.050627,-0.838722\H,0,-5.630979,1
.710744,1.510631\H,0,-5.79734,1.629019,-0.235983\H,0,-6.273227,-0.6173
39,0.679198\H,0,-4.77333,-0.601514,1.578221\H,0,-3.138687,1.919775,-1.
625139\N,0,-1.567992,1.129567,-0.524725\C,0,-0.834643,2.229741,-0.5629
28\C,0,-1.021843,-0.036644,-0.186188\C,0,0.501564,2.201937,-0.239515\H
,0,-1.337835,3.136661,-0.863855\C,0,0.304562,-0.161447,0.169231\H,0,-1
.736665,-0.850676,-0.224839\C,0,1.115877,1.006596,0.151915\H,0,1.06460
6,3.11719,-0.309206\N,0,0.85866,-1.358729,0.565809\N,0,2.43109,0.95112
4,0.503493\C,0,2.271394,-1.485955,0.286002\C,0,0.052476,-2.565856,0.51
7743\C,0,3.017867,-0.31787,0.920567\C,0,3.07431,2.164723,0.981668\C,0,
2.566577,-1.649991,-1.203435\H,0,2.62031,-2.37717,0.809891\C,0,-0.8587
48,-2.715392,1.721578\H,0,-0.525706,-2.615089,-0.409143\H,0,0.744126,-
3.405769,0.487933\C,0,4.504693,-0.417912,0.582888\H,0,2.905923,-0.4093
87,2.006343\C,0,3.875804,2.922033,-0.06172\H,0,2.309568,2.813979,1.407
867\H,0,3.72024,1.889348,1.814696\C,0,4.056356,-1.766662,-1.475485\H,0
,2.035847,-2.529432,-1.570285\H,0,2.160831,-0.793313,-1.745639\H,0,-1.
551793,-1.882803,1.816138\H,0,-0.273176,-2.772292,2.637706\H,0,-1.4527
24,-3.623014,1.629239\C,0,4.789153,-0.565925,-0.903748\H,0,5.049048,0.
428908,0.999247\H,0,4.885889,-1.297448,1.107772\H,0,4.734544,2.348168,
-0.401049\H,0,4.243101,3.857527,0.359508\H,0,3.272242,3.158869,-0.936\
H,0,4.235752,-1.851978,-2.547262\H,0,4.44471,-2.682876,-1.021437\H,0,5

.864322,-0.660725,-1.059366\H,0,4.471636,0.332269,-1.436172\\Version=A
M64L-G03RevD.01\State=1-A\HF=-1051.5142747\MP2=-1055.3669303\RMSD=5.30
6e-09\Thermal=0.\PG=C01 [X(C21H31N3O1)]\\@

4f*2c_3

1\1\GINC-NODE2\SP\RMP2-FC\6-31+G(2d,p)\C21H31N3O1\ZIP04\01-Feb-2011\0\
\\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\\cat11_3_b981_smp2-5_
mpr_3\\0,1\C,0,1.665692,1.205855,-0.213763\C,0,0.443114,1.821483,-0.09
4651\C,0,-0.738487,1.073356,-0.078422\C,0,-0.623163,-0.34382,-0.23171\
C,0,0.647284,-0.859698,-0.356866\N,0,1.752867,-0.105198,-0.327773\N,0,
-1.765386,-1.135269,-0.226771\C,0,-2.975232,-0.448253,-0.657055\C,0,-3
.134429,0.814093,0.183164\N,0,-1.954683,1.641844,0.06882\C,0,-3.46802,
0.494166,1.636652\C,0,-4.7274,-0.350348,1.744406\C,0,-4.594926,-1.6202
66,0.920178\C,0,-4.240322,-1.288776,-0.521479\C,0,-1.617604,-2.531658,
-0.583884\C,0,-1.404309,-2.801248,-2.06603\C,0,-2.120557,3.071345,0.22
4917\C,0,-2.117229,3.822774,-1.094671\H,0,-2.87887,-0.140615,-1.706127
\H,0,-3.960431,1.379156,-0.256134\H,0,-3.580762,1.424488,2.195112\H,0,
-2.623078,-0.039107,2.074359\H,0,-4.925839,-0.591204,2.788702\H,0,-5.5
873,0.225455,1.389812\H,0,-5.524147,-2.190092,0.944826\H,0,-3.824428,-
2.25507,1.361506\H,0,-4.175049,-2.188507,-1.131528\H,0,-5.050346,-0.70
0614,-0.959133\H,0,-1.354685,3.458666,0.8964\H,0,-3.068823,3.22823,0.7
35829\H,0,-2.928484,3.481133,-1.736001\H,0,-1.183166,3.68027,-1.634224
\H,0,-2.249174,4.89022,-0.922648\H,0,-2.501779,-3.059393,-0.238448\H,0
,-0.800582,-2.943516,0.005507\H,0,-0.531944,-2.279714,-2.455197\H,0,-1
.262082,-3.867435,-2.237871\H,0,-2.266019,-2.484184,-2.652162\H,0,0.83
2166,-1.912609,-0.490873\H,0,2.622265,1.716057,-0.239889\H,0,0.419989,
2.894838,-0.01647\C,0,3.189895,-0.798345,-0.400204\C,0,4.2006,0.129211
,-0.858591\C,0,3.412625,-1.366775,1.000995\C,0,5.334375,0.509692,-0.12
596\H,0,4.132083,0.492322,-1.877351\H,0,2.997543,-0.670253,1.733392\H,
0,2.867968,-2.306172,1.11975\C,0,4.889308,-1.539129,1.296537\C,0,5.577
205,-0.189922,1.207967\O,0,6.173935,1.344155,-0.496088\H,0,5.016172,-1
.983772,2.286382\H,0,5.334892,-2.228701,0.576644\H,0,6.656311,-0.27925
8,1.322945\H,0,5.231023,0.460023,2.01775\H,0,2.954984,-1.595932,-1.115
276\\Version=AM64L-G03RevD.01\State=1-A\HF=-1051.5147808\MP2=-1055.364
1354\RMSD=2.928e-09\Thermal=0.\PG=C01 [X(C21H31N3O1)]\\@

4f*2c_4

1\1\GINC-NODE10\SP\RMP2-FC\6-31+G(2d,p)\C21H31N3O1\ZIP04\01-Feb-2011\0
\\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\\cat11_3_b986_smp2-5_
_seq_3\\0,1\C,0,-3.248771,0.626686,-0.377645\C,0,-4.163984,-0.399816,-
0.822026\C,0,-3.424824,1.074029,1.072858\C,0,-5.176047,-0.969876,-0.03
4665\H,0,-4.137253,-0.687717,-1.866419\H,0,-2.868386,0.392942,1.721158
\H,0,-2.99449,2.067228,1.219539\C,0,-4.882528,1.034858,1.48625\C,0,-5.
399585,-0.385203,1.357094\O,0,-5.928324,-1.885859,-0.398272\H,0,-4.983
978,1.40132,2.510421\H,0,-5.467791,1.700594,0.84871\H,0,-6.469068,-0.4
44465,1.552914\H,0,-4.912319,-1.029645,2.095425\H,0,-3.176955,1.489228
,-1.050711\N,0,-1.728468,0.13162,-0.460712\C,0,-1.461957,-1.158927,-0.
484491\C,0,-0.736309,1.030219,-0.466346\C,0,-0.161806,-1.611837,-0.513
16\H,0,-2.343108,-1.791312,-0.488607\C,0,0.592545,0.673968,-0.507864\H
,0,-1.055839,2.059654,-0.46628\C,0,0.909407,-0.716768,-0.532301\H,0,0.
004648,-2.675605,-0.518855\N,0,1.622423,1.592191,-0.570504\N,0,2.20339

6,-1.135632,-0.594303\C,0,2.856633,1.139845,0.035909\C,0,1.320261,3.00
5697,-0.486574\C,0,3.289412,-0.163525,-0.624481\C,0,2.482082,-2.454428
,-1.143083\C,0,2.769487,1.045336,1.557251\H,0,3.624085,1.870227,-0.224
486\C,0,0.881432,3.594128,-1.815518\H,0,0.575189,3.20396,0.29152\H,0,2
.229262,3.508101,-0.161346\C,0,4.561511,-0.679251,0.047148\H,0,3.52224
6,0.061682,-1.670953\C,0,2.64953,-3.558354,-0.114567\H,0,1.683705,-2.7
11121,-1.83882\H,0,3.383904,-2.373722,-1.749052\C,0,4.06922,0.550994,2
.168007\H,0,2.504294,2.026004,1.955384\H,0,1.957405,0.368148,1.829665\H,
0,-0.000154,3.097592,-2.215268\H,0,1.675984,3.496223,-2.552689\H,0,0
.64705,4.651781,-1.700885\C,0,4.457602,-0.785415,1.56024\H,0,4.861884,
-1.630906,-0.388976\H,0,5.358069,0.024563,-0.207289\H,0,3.529354,-3.40
0656,0.504508\H,0,2.761576,-4.518151,-0.617913\H,0,1.78772,-3.623692,0
.546594\H,0,3.965695,0.46574,3.249707\H,0,4.864119,1.280471,1.98771\H,
0,5.408881,-1.131031,1.965911\H,0,3.70953,-1.531989,1.831973\\Version=
AM64L-G03RevD.01\State=1-A\HF=-1051.5128563\MP2=-1055.3625191\RMSE=1.8
14e-09\Thermal=0.\PG=C01 [X(C21H31N3O1)]\\@

4f*2c_5

1\1\GINC-CIPCLU04\SP\RMP2-FC\6-31+G(2d,p)\C21H31N3O1\BRYCH\02-Feb-2011
\0\\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\\cat11_3s_b981_smp
2-5_2\\0,1\C,0,1.07297,2.439823,-0.19442\C,0,-0.296571,2.516369,-0.138
151\C,0,-1.075371,1.351155,-0.102722\C,0,-0.388666,0.101842,-0.160323\
C,0,0.986033,0.135571,-0.239475\N,0,1.688357,1.269335,-0.236503\N,0,-1
.102827,-1.085397,-0.126575\C,0,-2.463557,-0.980944,-0.630082\C,0,-3.1
67787,0.147953,0.116453\N,0,-2.423383,1.381736,-0.021743\C,0,-3.417678
,-0.202977,1.579301\C,0,-4.224765,-1.484171,1.713362\C,0,-3.539757,-2.
628884,0.984897\C,0,-3.277509,-2.260017,-0.467024\C,0,-0.371112,-2.315
636,-0.376996\C,0,0.005994,-2.560934,-1.828808\C,0,-3.165518,2.622081,
0.025983\C,0,-3.402907,3.232283,-1.344522\H,0,-2.449904,-0.718702,-1.6
9579\H,0,-4.127942,0.302177,-0.382791\H,0,-3.93005,0.626968,2.068561\H
,0,-2.452411,-0.317981,2.074118\H,0,-4.362332,-1.728427,2.766697\H,0,-
5.224928,-1.333808,1.296109\H,0,-4.153737,-3.528951,1.026701\H,0,-2.60
1155,-2.864948,1.489295\H,0,-2.812162,-3.082406,-1.007719\H,0,-4.23342
,-2.085834,-0.966841\H,0,-2.661006,3.328173,0.685608\H,0,-4.120076,2.4
0481,0.501787\H,0,-2.466104,3.455458,-1.851407\H,0,-3.968504,2.550059,
-1.977445\H,0,-3.969439,4.158434,-1.254936\H,0,-0.973588,-3.13955,-0.0
05568\H,0,0.516965,-2.30955,0.250562\H,0,0.581605,-3.481169,-1.911404\
H,0,-0.87831,-2.65921,-2.45834\H,0,0.62042,-1.758932,-2.231978\H,0,1.6
28862,-0.730645,-0.342513\H,0,1.700749,3.318206,-0.214973\H,0,-0.75502
7,3.490362,-0.12423\C,0,3.274883,1.164752,-0.26843\C,0,3.703093,-0.058
952,-0.918201\C,0,3.706236,1.307267,1.190519\C,0,4.455676,-1.072211,-0
.308901\H,0,3.487065,-0.174814,-1.973955\H,0,3.693865,2.358629,1.48551
1\H,0,2.977728,0.796318,1.825004\C,0,5.063637,0.675146,1.424859\C,0,4.
989715,-0.803804,1.095226\O,0,4.749524,-2.157302,-0.835913\H,0,5.81224
7,1.157564,0.793269\H,0,5.369424,0.833915,2.461499\H,0,4.35187,-1.3172
68,1.821764\H,0,5.967391,-1.279869,1.1538\H,0,3.498448,2.075427,-0.834
609\\Version=AM64L-G03RevD.01\State=1-A\HF=-1051.5168779\MP2=-1055.368
8615\RMSE=1.733e-09\Thermal=0.\PG=C01 [X(C21H31N3O1)]\\@

4f*2c_6

1\1\GINC-CIPCLU10\SP\RMP2-FC\6-31+G(2d,p)\C21H31N3O1\BRYCH\01-Feb-2011

\0\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\cat11_3s_b981_smp
2-5_1\0,1\C,0,-1.631846,1.241083,-0.300475\C,0,-0.416695,1.833316,-0.
053739\C,0,0.754746,1.071244,0.001063\C,0,0.628572,-0.343178,-0.168679
\C,0,-0.635903,-0.837896,-0.395535\N,0,-1.725532,-0.063335,-0.469807\N
,0,1.761807,-1.146377,-0.127466\C,0,2.853176,-0.596108,0.664869\C,0,3.
161481,0.804636,0.147173\N,0,1.971795,1.624923,0.191865\C,0,3.78522,0.
773479,-1.244404\C,0,5.052376,-0.065901,-1.264969\C,0,4.774204,-1.4721
87,-0.759286\C,0,4.129355,-1.428527,0.617612\C,0,1.568283,-2.582221,-0.
.108927\C,0,1.073332,-3.152219,1.21221\C,0,2.147926,3.050485,0.369833\
C,0,1.894587,3.512,1.794209\H,0,2.544127,-0.503392,1.713998\H,0,3.8759
2,1.245898,0.847119\H,0,3.995164,1.793366,-1.569751\H,0,3.053764,0.361
924,-1.940935\H,0,5.462063,-0.096756,-2.27448\H,0,5.813955,0.40297,-0.
635032\H,0,5.697655,-2.04985,-0.710687\H,0,4.11991,-1.984147,-1.467307
\H,0,3.952196,-2.430566,1.005532\H,0,4.826291,-0.96506,1.319812\H,0,1.
514047,3.589161,-0.333807\H,0,3.172015,3.283122,0.08347\H,0,0.878878,3.
.286913,2.113219\H,0,2.578148,3.022135,2.486332\H,0,2.044527,4.58774,1.
.876279\H,0,2.51103,-3.048917,-0.378979\H,0,0.888893,-2.839021,-0.9195
98\H,0,0.130954,-2.705657,1.523414\H,0,0.922197,-4.227422,1.124325\H,0
,1.796721,-2.984186,2.009224\H,0,-0.826924,-1.889196,-0.532765\H,0,-2.
576944,1.766147,-0.386182\H,0,-0.389496,2.901133,0.079819\C,0,-3.16181
5,-0.730835,-0.701586\C,0,-4.123909,0.239107,-1.174852\C,0,-3.500249,-
1.388401,0.636526\C,0,-5.301242,0.598005,-0.501642\H,0,-3.977462,0.660
576,-2.162362\H,0,-2.985247,-2.347378,0.729177\H,0,-3.129376,-0.754173
,1.44528\C,0,-4.997813,-1.546508,0.810106\C,0,-5.652308,-0.179023,0.76
3554\O,0,-6.097908,1.470871,-0.877292\H,0,-5.400306,-2.175533,0.013617
\H,0,-5.206205,-2.053568,1.755157\H,0,-5.353149,0.408931,1.636974\H,0,
-6.738359,-0.250337,0.795811\H,0,-2.877079,-1.480394,-1.448847\Versio
n=AM64L-G03RevD.01\State=1-A\HF=-1051.5145789\MP2=-1055.3641623\RMSD=2
.807e-09\Thermal=0.\PG=C01 [X(C21H31N3O1)]\@

4f*2c_7

1\1\GINC-CIPCLU06\SP\RMP2-FC\6-31+G(2d,p)\C21H31N3O1\BRYCH\01-Feb-2011
\0\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\cat11_3s_b986_smp
2-5_2\0,1\C,0,3.176351,1.34198,-0.291689\C,0,3.815831,0.170785,-0.854
993\C,0,3.460604,1.586294,1.18943\C,0,4.647945,-0.709028,-0.148403\H,0
,3.707069,-0.004443,-1.918957\H,0,3.282431,2.634135,1.440042\H,0,2.757
441,0.998706,1.784844\C,0,4.866915,1.155868,1.556362\C,0,5.024356,-0.3
2776,1.280512\O,0,5.130526,-1.756292,-0.607366\H,0,5.593406,1.720085,0.
.968205\H,0,5.059211,1.384814,2.60701\H,0,4.407368,-0.905509,1.976061\
H,0,6.050502,-0.659418,1.431801\H,0,3.31816,2.257242,-0.87621\N,0,1.58
8567,1.230356,-0.38573\C,0,0.823469,2.308988,-0.416514\C,0,1.044375,0.
014022,-0.400407\C,0,-0.546692,2.20501,-0.471075\H,0,1.330162,3.262316
, -0.397783\C,0,-0.317335,-0.190379,-0.458364\H,0,1.79326,-0.768883,-0.
418891\C,0,-1.166221,0.950655,-0.502302\H,0,-1.127892,3.111376,-0.4863
79\N,0,-0.877565,-1.445994,-0.528452\N,0,-2.518471,0.813467,-0.594068\
C,0,-2.208484,-1.539337,0.027498\C,0,-0.021681,-2.615158,-0.432127\C,0
, -3.111835,-0.518182,-0.654941\C,0,-3.29187,1.903852,-1.166757\C,0,-2.
221199,-1.430452,1.550868\H,0,-2.603526,-2.516257,-0.254802\C,0,0.6596
31,-2.963281,-1.742463\H,0,0.719188,-2.491958,0.363471\H,0,-0.656778,-
3.445333,-0.128137\C,0,-4.50631,-0.569587,-0.031421\H,0,-3.196055,-0.8
09346,-1.707448\C,0,-3.921375,2.845511,-0.156168\H,0,-2.649134,2.46163

4,-1.847869\H,0,-4.067643,1.463808,-1.792316\C,0,-3.630016,-1.509721,2
.11328\H,0,-1.595074,-2.222818,1.963202\H,0,-1.761835,-0.484911,1.8467
19\H,0,1.303473,-2.163156,-2.099485\H,0,-0.081948,-3.171847,-2.511909\
H,0,1.285321,-3.844726,-1.613186\C,0,-4.506767,-0.441695,1.483824\H,0,
-5.154599,0.180078,-0.483778\H,0,-4.937522,-1.535042,-0.307598\H,0,-4.
667279,2.338726,0.451165\H,0,-4.412665,3.669632,-0.672799\H,0,-3.17801
7,3.265574,0.518888\H,0,-3.607132,-1.398807,3.197471\H,0,-4.05404,-2.4
974,1.910704\H,0,-5.529839,-0.515524,1.853961\H,0,-4.136083,0.542487,1
.775789\\Version=AM64L-G03RevD.01\State=1-A\HF=-1051.5144837\MP2=-1055
.366851\RMSD=5.605e-09\Thermal=0.\PG=C01 [X(C21H31N3O1)]\\@

4f*2c_8

1\1\GINC-CIPCLU08\SP\RMP2-FC\6-31+G(2d,p)\C21H31N3O1\BRYCH\31-Jan-2011
\0\\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid\\cat11_3s_b986_smp
2-5_1\\0,1\C,0,-3.192487,0.552385,0.651353\C,0,-3.957383,-0.544793,1.1
98355\C,0,-3.724911,1.134211,-0.657842\C,0,-5.115233,-1.085282,0.61891
4\H,0,-3.670353,-0.930249,2.169568\H,0,-3.36607,2.157281,-0.791319\H,0
, -3.32603,0.551916,-1.491887\C,0,-5.237989,1.065412,-0.71432\C,0,-5.67
6289,-0.383441,-0.614777\O,0,-5.738542,-2.064647,1.054343\H,0,-5.66738
5,1.638517,0.109819\H,0,-5.591824,1.522905,-1.641144\H,0,-5.36256,-0.9
31363,-1.508912\H,0,-6.760034,-0.474284,-0.560893\H,0,-2.964758,1.3453
83,1.372795\N,0,-1.692491,0.102671,0.309366\C,0,-1.431375,-1.169989,0.
085994\C,0,-0.721815,1.019983,0.225155\C,0,-0.163443,-1.581586,-0.2574
54\H,0,-2.285044,-1.825756,0.218596\C,0,0.574031,0.705638,-0.118063\H,
0,-1.033701,2.031994,0.425996\C,0,0.881027,-0.662604,-0.377203\H,0,0.0
05123,-2.634026,-0.409806\N,0,1.57265,1.650189,-0.257348\N,0,2.140854,
-1.040264,-0.728141\C,0,2.900511,1.157442,0.044492\C,0,1.290552,3.0338
87,0.062325\C,0,3.200242,-0.045611,-0.841566\C,0,2.313653,-2.278235,-1
.473546\C,0,3.104647,0.880185,1.532149\H,0,3.603851,1.931848,-0.265175
\C,0,0.59297,3.769185,-1.068083\H,0,0.716675,3.11545,0.991891\H,0,2.24
5588,3.516614,0.260579\C,0,4.576702,-0.608962,-0.489265\H,0,3.230719,0
.31039,-1.877138\C,0,2.67913,-3.490986,-0.636818\H,0,1.397293,-2.47249
7,-2.030419\H,0,3.081727,-2.102882,-2.226204\C,0,4.495517,0.342416,1.8
21538\H,0,2.923249,1.801,2.088763\H,0,2.35705,0.159509,1.869981\H,0,-0
.349124,3.300705,-1.344373\H,0,1.224202,3.785619,-1.954403\H,0,0.38298
6,4.797474,-0.776149\C,0,4.757466,-0.901478,0.991555\H,0,4.790928,-1.4
93035,-1.088241\H,0,5.311186,0.139238,-0.798143\H,0,3.659784,-3.383737
, -0.179644\H,0,2.698087,-4.380656,-1.265524\H,0,1.959148,-3.658682,0.1
6167\H,0,4.598385,0.124384,2.884492\H,0,5.243788,1.104744,1.585976\H,0
,5.766075,-1.276525,1.167427\H,0,4.069148,-1.688948,1.302589\\Version=
AM64L-G03RevD.01\State=1-A\HF=-1051.5129189\MP2=-1055.3627628\RMSD=2.2
31e-09\Thermal=0.\PG=C01 [X(C21H31N3O1)]\\@