

Supplemental Material

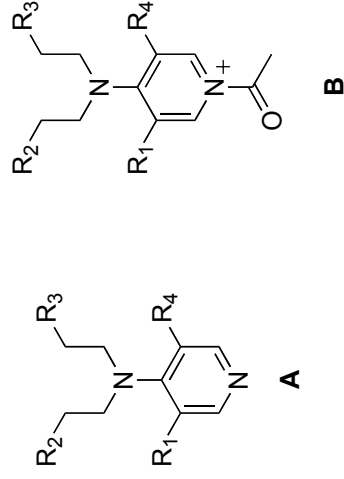
"Stacking Interactions as the Principal Design Element in Acyl-Transfer Catalysts"

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A. Modified OPLS-AA Force Field for 4-Aminopyridines

Two OPLS-AA force fields for calculations on 4-aminopyridines (**A**) and N-acetyl-4-aminopyridinium cations (**B**) have been developed.

Supplemental Scheme 1.



Atom types: The nitrogen connected to the C4 position of the pyridine ring is termed "NN" in both cases. All other atom types are taken from the AMBER atom type

defined in *J. Am. Chem. Soc.* **1995**, 117, 5179

Force field parameters for A and B

In both cases, the charges are calculated either by the CHELPG scheme at RHF/6-31G(d) level or using CMI scheme with AM1 wavefunction. In both cases, RHF/3-21G optimized geometries have been used. Lennard-Jones parameters are taken from comparable compounds described well by the OPLS-AA force field. Bond and angle parameters are chosen from the OPLS-AA force field. For missing bond and angle parameters, the r_{eq} and θ_{eq} are taken from the MP2/6-31G(d) optimized geometries of 4-dimethylaminopyridine (DMAP). The parameters K_r and K_θ are also taken from similar compounds in OPLS-AA force field. Dihedral parameters, so not available from similar atom types, have been selected such as to reproduce the potential energy profile at the B3LYP/6-31G(d) level of theory for conformational isomers of A with $R_1=R_4=H$, $R_2=R_3=Me$.

Supplemental Table 1. List of atom types for A and B.

Atom type	Description	σ , Å	ϵ , kcal mol ⁻¹
CT	Any sp ³ carbon	3.500	0.066
CA	Any aromatic sp ² carbon	3.550	0.070
C	Any carbonyl sp ² carbon	3.750	0.105
NC	Nitrogen in pyridine ring	3.250	0.170
NN	Nitrogen in amino group connected to pyridine ring	3.250	0.170
N	Nitrogen in amide group	3.250	0.170
O	Carbonyl oxygen or in amides	2.960	0.210
OH	Oxygen in hydroxyl group	3.120	0.170
OS	sp ³ oxygen in five-member ring	2.900	0.140
S	S in five-member ring	3.550	0.250
S=	In C=S group	3.550	0.250

HC	hydrogen attached to aliphatic carbon	2.420	0.030
HA	Hydrogen attached to aromatic carbon	2.420	0.030
HO	Alcohol hydrogen	0.000	0.000
H	Amide hydrogen	0.000	0.000

Supplemental Table 2. Bond and Angle parameters for A.

Type	r_{eq} or θ_{eq}	K_r	Source ^a
CA-CA	1.400	469.0	old
CA-NC	1.339	483.0	old
CA-HA	1.080	367.0	old
CA-NN	1.360	529.0	new
CT-NN	1.456	337.0	new
CT-HC	1.090	340.0	old
CT-CT	1.529	268.0	old
CA-CT	1.510	317.0	old
CT-OH	1.410	320.0	old
OH-HO	0.945	553.0	old
C-O	1.212	570.0	old
C-CT	1.500	317.0	new
CT-N	1.335	490.0	old
C-N	1.449	337.0	old
N-H	1.010	434.0	old
CT-OS	1.410	320.0	old
CA-OS	1.364	450.0	new
C-S=	1.640	400.0	old
C-S	1.760	250.0	old
CTS	1.810	220.0	new
CA-CA-CA	120.0	63.0	old
CA-CA-NC	124.0	70.0	old
CA-NC-CA	117.0	70.0	old
HA-CA-CA	120.0	35.0	old
HA-CA-NC	116.0	35.0	old
NN-CA-CA	121.4	70.0	new

NN-CT-CT	102.0	65.0	new
CT-NN-CA	117.6	150.0	new
CT-NN-CT	116.0	30.0	new
CT-NN-CT in five-member ring	110.0	60.0	new
NN-CT-HC	109.5	35.0	new
HC-CT-HC	107.8	33.0	old
HC-CT-CT	110.7	37.5	old
CT-CT-CT	112.7	58.35	old
CT-OH-HO	108.5	55.0	old
OH-CT-CT	109.5	50.0	old
CA-CT-CT	114.0	63.0	old
CT-CA-CA	120.0	63.0	old
C-CT-CT	111.1	63.0	old
CT-C-N	116.6	70.0	old
C-N-H	119.8	35.0	old
N-C-O	122.9	80.0	old
H-N-CT	118.4	38.0	old
CT-CT-N	109.7	80.0	old
HC-CT-N	109.5	35.0	old
CA-C-O	120.4	80.0	new
CA-OS-CT	111.8	100.0	new
N-CT-CA	111.2	80.0	new
CA-CA-OS	109.5	50.0	old
CT-CT-OS	120.0	70.0	new
HC-CT-OS	109.5	35.0	old
N-C-S=	125.0	70.0	new
S-C-S=	125.0	70.0	new
C-S-CT	98.9	62.0	new

S-CT-CT	114.7	50.0	old
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^a old parameters published in the literature.

Supplemental Table 3. Dihedral angle parameters for A.

Dihedral angle	V ₁	V ₂	V ₃	V ₄	Source ^a
HC-CT-CT-HC	0.0	0.0	0.30	0.0	old
HC-CT-CT-CT	0.0	0.0	0.30	0.0	old
CT-CT-CT-CT	6.622	-2.6	-0.4	1.3	new
CA-CA-CA-CA	0.0	7.250	0.0	0.0	old
CA-CA-CA-NC	0.0	7.250	0.0	0.0	old
CA-CA-NC-CA	0.0	7.250	0.0	0.0	old
HA-CA-CA-CA	0.0	7.250	0.0	0.0	old
HA-CA-CA-HA	0.0	7.250	0.0	0.0	old

HA-CA-CA-NC	0.0	7.250	0.0	0.0	0.0	old
CT-CA-CA-CA	0.0	7.250	0.0	0.0	0.0	old
CT-NN-CT-CT	0	1.2	0	0.7	0.7	new
CA-CA-NN-CT	0	3.75	1.0	0	0	new
CA-NN-CT-HC	0	0	0.35	0	0	new
CT-NN-CT-HC	0	0	0.435	0	0	new
CA-NN-CT-CT	0	1.2	0	0.7	0.7	new
CA-N -CT-CT	0	1.2	0	0.7	0.7	new
NN-CT-CT-CT	2.392	-0.674	-0.6	0	0	new
NN-CT-CT-OH	6.28	-5.1	2.03	0	0	new
CT-C -N -H	0.0	4.9	0.0	0.0	0.0	old
CT-C -N -CT	2.3	6.089	0.0	0.0	0.0	old
NN-CT-C -O	0.0	0.0	0.0	0.0	0.0	new
H -N -CT-CT	0.0	0.0	0.0	0.0	0.0	old
H -N -CT-CA	0.0	0.0	0.0	0.0	0.0	old
CT-CT-C -O	0.0	1.166	0.0	0.0	0.0	old
O -C -N -H	0.0	4.90	0.0	0.0	0.0	old
H -N -CT-HC	0.0	0.0	0.0	0.0	0.0	old
N -CT-CT-HC	0.0	0.0	0.464	0.0	0.0	old
HC-CT-CA-CA	0.0	0.0	0.0	0.0	0.0	old
CT-CA-CA-HA	0.0	7.25	0.0	0.0	0.0	old
CA-CA-CA-OS	0.0	7.25	0.0	0.0	0.0	new
CT-CA-CA-OS	0.0	7.25	0.0	0.0	0.0	new
CA-CT-CT-OS	-1.336	0.00	0.00	0.00	0.00	new
CA-OS-CT-CT	0.650	-0.250	0.670	0.0	0.0	new
CT-OS-CA-CA	0.0	3.0	0.0	0.0	0.0	new
CA-CA-C -O	0.0	0.0	0.0	0.0	0.0	new
CA-CA-C -N	0.0	1.1	0.0	0.0	0.0	new
CA-C -N -C	2.30	6.089	0.0	0.0	0.0	new

CA-CA-CA-C	0.0	7.250	0.0	0.0	0.0	new
S=C -N -C	0.0	6.50	0.0	0.0	0.0	new
C -N -CT -CT	-1.396	-0.427	0.0	0.0	0.0	new
CT-CT-S -C	0.925	-0.576	0.677	0.0	0.0	new
HC-CT-S -C	0.0	0.0	0.647	0.0	0.0	new
S=C -S -CT	0.0	6.5	0.0	0.0	0.0	new

^a old parameters published in the literature.

Supplemental Table 4. Bond and Angle parameters for **B**^a.

Type	r_{eq} or θ_{eq}	K_r	Source ^b
CA-CA	1.412	469.0	new
CA-NC	1.369	483.0	new
CA-NN	1.320	483.0	new
CT-NN	1.448	483.0	new
CT-C	1.500	317.0	new
NC-C -CT	116.6	700.0	new
NC-C-O	122.5	80.0	new
O -C -CT	120.4	80.0	old
CT-NN-CT	119.0	60.0	new
CT-NN-CT in five-member ring	108.0	60.0	new
CA-NN-CA	117.6	150.0	new

^a only listing parameters different from **A**. ^b old parameters published in the literature.

Supplemental Table 5. Dihedral angle parameters for **B**^a.

Dihedral angle	V ₁	V ₂	V ₃	V ₄	Source ^b
CA-CA-NN-CT	0.0	4.50	1.0	0.0	new
CA-NC-C-O	0.0	7.5	0.0	0.0	new
CA-NC-C-CT	0.0	14.0	0.0	0.0	new
O -C -CT-HC	0.0	0.0	0.0	0.0	new
NN-CT-CT-OH	7.5	0.0	3.0	0.0	new
NC-C -CT-HC	0.0	0.0	0.0	0.0	new

^a only listing parameters different from **A**. ^b old parameters published in the literature.

Conformational search using the modified OPLS-AA Force Field with BOSS4.6

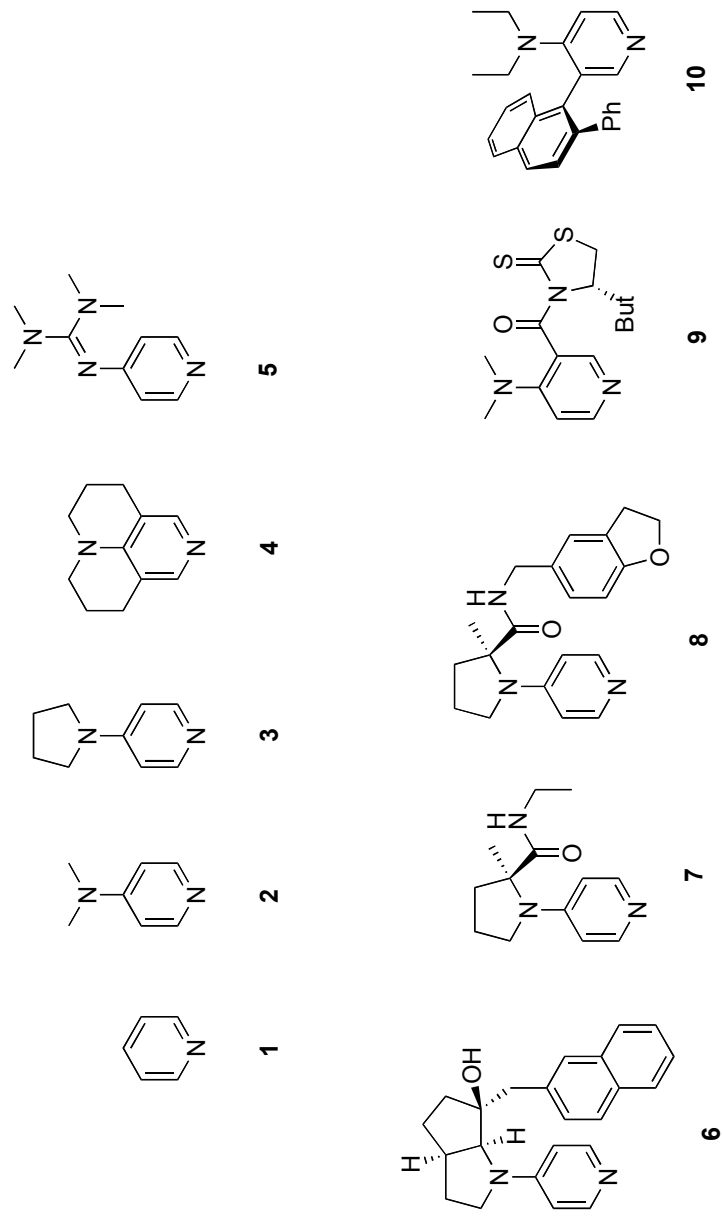
The Z-matrix for the BOSS input file can be converted from **PDB** or **mol** file using the **xPDBZ** or **xMOLZ** scripts included in the BOSS program suit. The atom types and parameters should be described in the parameter file. The correct atom type number for each atom has to be specified manually in the BOSS input file and should correspond to the atom type number in the parameter file. In a first run all charges are set to zero in the parameter file and CM1 charges are calculated using the script **xAMICM1**. The CM1A charges obtained in this first run are then inserted in the parameter file. After that, Monte Carlo conformational searching can be run using the **xCS** script included in the BOSS program suit, and the number of trial structures can be varied by changing the variable “configurations” in the **xCS** script. Monte Carlo conformational searching results are written to the ***.out** file and the Cartesian coordinates of all optimized conformers are summarized in the ***.plt** file using the **mol** format. The utility program **csmol** in the BOSS program suit is used to separate the concatenated ***.plt.mol** file into single structure files.

Literature

- W. L. Jorgensen, D. S. Maxwell, and J. Tirado-Rives, *J. Am. Chem. Soc.* **1996**, *118*, 11225-11236.
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- W. L. Jorgensen and N. A. McDonald, *J. Phys. Chem. B* **1998**, *102*, 8049-8059.
- R. C. Rizzo and W. L. Jorgensen, *J. Am. Chem. Soc.* **1999**, *121*, 4827-4836.

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Supplemental Scheme 2. Compounds described in this manuscript.



Supplemental Table 6. Total Energies and Enthalpies (in Hartree) as Calculated at the RHF/3-21G(*), RHF/MIDI, B3LYP/6-31G(d), and MP2(FC)/6-31G(d) Level of Theory for all Systems. Enthalpies Represent Boltzmann-Averaged Values over all Conformers at 298.15 K.

system	RHF/3-21G(*)		RHF/MIDI		B3LYP/6-31G(d)		MP2(FC)/6-31G(d)	
	E _{tot}	H ₂₉₈	E _{tot}	H ₂₉₈	E _{tot}	H ₂₉₈	E _{tot}	H ₂₉₈
1 (pyridine)								
neutral	-245.312006	-245.210873	-245.239861	-245.138871	-248.2849730	-248.190715	-247.482532	-247.381399
cationic	-396.611964	-396.453100	-396.502142	-396.343739	-401.2995391	-401.151170	-400.047896	-399.889032
2 (DMAP)								
neutral	-377.662675	-377.478683	-377.549433	-377.365951	-382.2573045	-382.085088	-380.995265	-380.811273
cationic	-528.997389	-528.754901	-528.845015	-528.603374	-535.3039587	-535.076979	-533.590978	-533.34849
3 (PPY)								
neutral	-454.150742	-453.926606	-453.994262	-453.771056	-459.6842867	-459.474417	-458.165699	-457.941563
cationic	-605.489443	-605.206794	-605.293543	-605.012166	-612.7351191	-612.470454	-610.766062	-610.483413
4 (TCAP)								
neutral	-530.641930	-530.378134	-530.451331	-530.188070	-537.120287	-536.872902	-535.350370	-535.086379
cationic	-681.985246	-681.662480	-681.753326	-681.431814	-690.176536	-689.874134	-687.955445	-687.632677
5 (hassner)								
neutral	-602.383832	-602.092424	-602.223406	-601.932562	-609.6827138	-609.409084	-607.694519	-607.403111
cationic	-753.730110	-753.379503	-753.527572	-753.177979	-762.742090	-762.413064	-760.299073	-759.948535
6 (Fuji)								
neutral	-1062.779108	-1062.299958	-1062.386677	-1061.906916	-1075.637970	-1075.189326	-1072.172053	-1071.694251
cationic	-1214.126219	-1213.586451	-1213.689635	-1213.151531	-1228.694660	-1228.191998	-1224.783758	-1224.247268
7 (camp. 1)								
neutral	-737.456443	-737.105080	-	-	-	-	-743.917660	-743.566306
cationic	-888.791029	-888.380658	-	-	-	-	-896.515880	-896.106163
8 (camp. 2)								
neutral	-1077.818934	-1077.361609	-	-	-	-	-1087.252421	-1086.795387
cationic	-1229.163093	-1228.646988	-	-	-	-	-1239.859269	-1239.343424

9 (yamada)													
neutral	-1605.228930	-1604.834070	-	-	-	-	-	-	-	-	-	-1616.334113	-1615.940289
cationic	-1756.560014	-1756.106872	-	-	-	-	-	-	-	-	-	-1768.927544	-1768.474493
10 (spivey)													
neutral	-1063.622982	-1063.139172	-	-	-	-	-	-	-	-	-	-1073.1186586	-1072.634876
cationic	-1214.966385	-1214.422984	-	-	-	-	-	-	-	-	-	-1229.7209592	-1225.177906

Supplemental Table 7. Total Energies and Enthalpies (in Hartree) as Calculated at the MP2(FC)/6-31G(d)//RHF/3-21G(*), MP2(FC)/6-31G(d)//RHF/MIDI!, B3LYP/6-311+G(d,p)//B3LYP/6-31G(d), and MP2(FC)/6-311+G(d,p)//MP2(FC)/6-31G(d) Level of Theory for all Systems. Enthalpies Represent Boltzmann-Averaged Values over all Conformers at 298.15 K.

system	MP2(FC)/6-31G(d)// RHF/3-21G(*)		MP2(FC)/6-31G(d)// RHF/MIDI!		B3LYP/6-311+G(d,p)// B3LYP/6-31G(d)		MP2(FC)/6-311+G(d,p)// MP2(FC)/6-31G(d)	
	E _{tot}	H ₂₉₈	E _{tot}	H ₂₉₈	E _{tot}	H ₂₉₈	E _{tot}	H ₂₉₈
1 (pyridine)								
neutral	-247.480304	-247.379171	-247.480857	-247.379867	-248.3511637	-248.2569057	-247.608924	-247.507791
cationic	-400.044798	-399.885934	-400.044747	-399.886344	-401.4019729	-401.2536038	-400.251941	-400.093077
2 (DMAP)								
neutral	-380.991642	-380.807650	-380.993441	-380.809959	-382.3599769	-382.1877604	-381.213684	-381.029692
cationic	-533.586980	-533.344492	-533.587477	-533.345836	-535.4427011	-535.2157214	-533.886472	-533.643984
3 (PPY)								
neutral	-458.162244	-457.938108	-458.163261	-457.940055	-459.8042135	-459.5943438	-458.425954	-458.201818
cationic	-610.761224	-610.478575	-610.761889	-610.480512	-612.8911759	-612.6265108	-611.102583	-610.819934
4 (TCAP)								
neutral	-535.345874	-535.081962	-535.347705	-535.084678	-537.254445	-537.0070597	-535.651626	-535.387643
cationic	-687.950248	-687.627479	-687.951018	-687.629470	-690.347629	-690.0452261	-688.333589	-688.010819
5 (hassner)								
neutral	-607.687554	-607.396146	-607.690260	-607.399416	-609.8458029	-609.5721731	-608.050009	-607.758601
cationic	-760.29153	-759.940989	-760.294290	-759.944809	-762.940980	-762.611971	-760.730507	-760.379970
6 (Fuji)								
neutral	-1072.160959	-1071.682893	-1072.163484	-1071.685718	-1075.915101	-1075.467624	-1072.764316	-1072.286499
cationic	-1224.768436	-1224.231467	-1224.770119	-1224.234057	-1229.007589	-1228.506292	-1225.457641	-1224.921420
7 (camp. 1)								
neutral	-743.911902	-743.560388	-	-	-	-	-744.357643	-744.006246
cationic	-896.508466	-896.098366	-	-	-	-	-897.032430	-896.622801
8 (camp. 2)								
neutral	-1087.238575	-1086.780666	-	-	-	-	-1087.859053	-1087.401980
cationic	-1087.847005	-1239.331018	-	-	-	-	-1240.544747	-1240.029325

9 (yamada)												
neutral	-1616.326463	-1615.932519	-	-	-	-	-	-1616.891340	-	-1616.497581		
cationic	-1768.918946	-1768.465745	-	-	-	-	-	-1769.562782	-	-1769.109634		
10 (spivey)												
neutral	-1073.106046	-1072.621996	-	-	-	-	-1076.892420	-1073.691705	-1076.439019	-1073.208010		
cationic	-1225.707404	-1225.163917	-	-	-	-	-1229.984546	-1226.370998	-1229.475804	-1225.827967		

Supplemental Table 8. Total Energies and Enthalpies (in Hartree) as Calculated at the SCS-MP2(FC)/6-311+G(d,p)//MP2(FC)/6-31G(d) Level of Theory for all Systems. Enthalpies Represent Boltzmann-Averaged Values over all Conformers at 298.15 K.

system	SCS-MP2(FC)/6-311+G(d,p)// MP2(FC)/6-31G(d)	E_{tot}	H_{298}
1 (pyridine)			
neutral	-247.583611	-247.482478	
cationic	-400.215941	-400.057077	
2 (DMAP)			
neutral	-381.181350	-380.997358	
cationic	-533.844447	-533.601959	
3 (PPY)			
neutral	-458.386137	-458.162000	
cationic	-611.053190	-610.770541	
4 (TCAP)			
neutral	-535.602550	-535.338577	
cationic	-688.274568	-687.951801	
5 (hassner)			
neutral	-607.997488	-607.706080	

cationic	-760.668735	-760.318195
6 (Fuji)		
neutral	-535.602550	-1072.168817
cationic	-688.274568	-1224.789477
7 (camp. 1)		
neutral	-744.292015	-743.940629
cationic	-896.957388	-896.547743
8 (camp. 2)		
neutral	-1087.744456	-1087.287380
cationic	-1240.417955	-1239.902269
9 (yamada)		
neutral	-1616.802534	-1616.408729
cationic	-1769.464658	-1769.011525
10 (spivey)		
neutral	-1073.565565	-1073.0818010
cationic	-1226.234859	-1225.6918564

Supplemental Table 9. Total Energies and Enthalpies (in Hartree) as Calculated at the RHF/6-311+G(d,p)//MP2(FC)/6-31G(d) Level of Theory for all Systems. Enthalpies Represent Boltzmann-Averaged Values over all Conformers at 298.15 K.

system	RHF/6-311+G(d,p)// MP2(FC)/6-31G(d)	
	E_{tot}	H_{298}
1 (pyridine)		
neutral	-246.7509029	-246.6497699
cationic	-398.9237915	-398.7649275
2 (DMAP)		
neutral	-379.8691959	-379.6852039
cationic	-532.0743842	-531.8318962
3 (PPY)		
neutral	-456.7987245	-456.5745885
cationic	-609.0083452	-608.7256962
4 (TCAP)		
neutral	-533.731066	-533.4670918
cationic	-685.9458719	-685.6231073
5 (hassner)		
neutral	-605.9001196	-605.6087116
cationic	-758.1184977	-757.7679479
6 (Fuji)		
neutral	-1068.955233	-1068.477411
cationic	-1221.163428	-1220.627081
7 (camp. 1)		
neutral	-741.750892	-741.399740
cationic	-893.958842	-893.549178
8 (camp. 2)		
neutral	-1084.0820908	-1083.624969
cationic	-1236.297955	-1235.782026

9 (yamada)			
neutral	-1613.693426	-1613.299462	
cationic	-1765.896857	-1765.443668	
10 (spivey)			
neutral	-1069.8038777	-1069.3203059	
cationic	-1222.0151850	-1221.4721568	

mp2/6-31G(d) optimized structures of catalysts and acetyl intermediates

1

```
1\INGC-MORITZFOpt\RMP2-FC\6-31G(d)\C5H5N\YIN\30-Jan-2006\0\#P MP2
/6-31G(D) OPT FREQ\pyridine geometry optimization\0,1\C,-1.170991974
5,0.0002199961,-0.6788571108\C,-1.1724301541,0.0001152571,0.7169946331
\C,0.0505968052,-0.0000944822,1.3867423958\C,1.221563651,-0.0002300398
,0.6296637796\C,1.1184077664,-0.0001124457,-0.7623714062\N,-0.05200342
24,0.0001011762,-1.4253512141\H,0.0902097379,-0.0001840066,2.473217818
9\H,-2.108271358,0.0003744272,-1.2326297001\H,-2.1121393509,0.00025643
25,1.2620503633\H,2.1985103006,-0.0003523545,1.1047602485\H,2.01283806
25,-0.0001924457,-1.3829739816\Version=x86-Linux-G03RevB.03\State=1-A
\HF=-246.6934589\MP2=-247.4825323\RMSE=3.962e-09\RMSE=1.007e-04\Dipole
=0.0332064,-0.0000487,0.910208\PG=C01 [X(C5H5N)]\@
```

1-Ac

```
1\INGC-MORITZFOpt\RMP2-FC\6-31G(d)\C7H8NIO1(1+)\YIN\30-Jan-2006\0\
#P MP2/6-31G(D) OPT FREQ\pyacmp, mp2/6-31G(d) optimization calculatio
n\1,1\C,-1.1464075291,-0.0004354277,0.4969330671\C,-1.1428232345,-0.0
005531569,1.8844947457\C,0.0716898773,-0.0002848128,2.5716077894\C,1.2
63748912,0.0000926965,1.8447300627\C,1.2226102778,0.000197236,0.459262
3899\H,0.0891177739,-0.0003705718,3.657805036\H,-2.0606736826,-0.00063
44512,-0.081988481\H,-2.0912723831,-0.0008514033,2.4117628426\H,2.2286
80599,0.0003110417,2.3412132791\H,2.0994141075,0.0004791941,-0.1789488
756\C,0.084844075,0.0000703802,-1.7216375951\C,-1.2322469433,0.0000717
231,-2.42754321\H,-1.0172142309,0.0006119796,-3.4962539221\H,-1.814716
5755,-0.8917144932,-2.1805463648\H,-1.8151799203,0.89132776,-2.1797340
491\N,0.0275518112,-0.0000672539,-0.1824363372\O,1.1825611278,0.000794
9864,-2.2079173253\Version=x86-Linux-G03RevB.03\State=1-A\HF=-398.831
443\MP2=-400.0478965\RMSE=7.257e-09\RMSE=3.832e-05\Dipole=-0.8847377,-
```

0.0005282,1.0144406\PG=C01 [X(C7H8N1O1)]\@

2

1\1\GINC-MAX\FOpt\RMp2-FC\6-31G(d)\C7H10N2\YIN\26-Sep-2005\0\#P MP2/6
-31G(D) OPT\dmopc mp2/6-31G(d) Opt calculation\0,1\C,-0.1553446643,-
0.0976662592,-0.0983406105\C,-0.1563739349,-0.0691085407,1.3105825587\
C,1.0511414162,-0.0065487273,1.9986223526\N,2.2651838416,0.0336739251,
1.4213041808\C,2.2568661319,0.0109588648,0.0766005012\C,1.1123971657,-
0.0506854906,-0.711940284\N,-1.3278079183,-0.2073053189,-0.8348501557\
C,-2.5790092849,0.1093887821,-0.1617925258\C,-1.2690332398,0.128410144
1,-2.2499993533\H,-1.077538493,-0.0870635835,1.8810316424\H,1.04391391
69,0.0170311371,3.0877303206\H,3.234028169,0.0488324485,-0.4034873633\
H,1.2251837532,-0.0536271602,-1.7896922109\H,-0.9550980431,1.167166362
, -2.431366145\H,-2.259901548,-0.0191550995,-2.6820278353\H,-0.58099341
7,-0.5411301351,-2.7707811696\H,-2.7429078883,-0.5725219746,0.67548380
31\H,-3.3980069394,-0.0356808328,-0.8677966076\H,-2.614172513,1.143075
955,0.2133315563\Version=x86-Linux-G03RevB.03\State=1-A\HF=-379.7768
252\MP2=-380.9952652\RMSE=7.830e-09\RMSE=6.183e-06\Dipole=-1.42291,0.1
587677,-0.8911751\PG=CS [SG(C1N2),X(C6H10)]\@

2-Ac

1\1\GINC-MORITZ\FOpt\RMp2-FC\6-31G(d)\C9H13N2O1(1+)\YIN\27-Sep-2005\0\
\#P MP2/6-31G(D) MAXDISK=1GB OPT\dmopc-ac, Opt calculation\1,1\C,-1,
1440191714,-0.0449709912,-0.7638928586\C,-1.1620261365,-0.0498399883,0
.6637900395\C,0.0051841865,-0.0037132627,1.3781320343\C,1.2792973215,0
.0551378619,-0.608172583\C,0.1469477959,0.0106324306,-1.3725883852\N,-
2.2678018337,-0.0897554169,-1.4869882677\C,-2.2055691244,-0.0828843317
, -2.954630156\C,-3.57634388,-0.1459021249,-0.8227231572\H,-2.089549506
4,-0.0899092454,1.2208343484\H,0.0006054094,-0.0070623803,2.4604088042
\H,2.2777666115,0.0978163209,-1.0281545428\H,0.2680598506,0.0191570579
, -2.4484443882\H,-3.6586283478,-1.0467322257,-0.2085140826\H,-4.350885

1365,-0.1756530092,-1.585684428\H,-3.7326422013,0.7413508465,-0.203153
9364\H,-1.7311501213,0.8335150944,-3.3159032802\H,-3.2202081941,-0.124
4047804,-3.3440639234\H,-1.6560449354,-0.9541717011,-3.3210299722\N,1.
2222908038,0.048516288,0.7590571112\C,2.5115989542,0.0993907737,1.4959
290699\C,2.430633843,0.0917332657,2.9928882312\H,3.4536949564,0.132834
2917,3.3659497839\H,1.8792770395,0.9589238691,3.3663119847\H,1.9526434
559,-0.8199929868,3.3613300506\O,3.5264269495,0.143187619,0.8404047834
\\Version=x86-Linux-G03Rev B.03\State=1-A\HF=-531.9475151\MP2=-533.5909
776\RMSD=9.986e-09\RMSE=6.623e-06\Dipole=-1.610906,-0.0666491,0.055661
8\PG=C01 [X(C9HI3N2O1)]\@

3

1\1\GINC-NODE21\FOpt\RMPE2-FC\6-31G(d)\C9HI2N2\ZIP05\30-Jan-2006\0\#p
mp2/6-31g(d) opt\ppymp\0,1\C,0,0,0,0,0,0,1.39027749\C,1.2294677
935,-0.000000001,2.0802650548\C,2.3932331398,-0.0007774727,1.28444880
15\C,2.270516616,-0.0022296064,-0.1004013872\N,1.1033864877,-0.0014919
5,-0.7709542481\H,-0.9494947978,-0.0021688608,-0.5344679372\H,-0.94507
30436,-0.0160592437,1.9235860664\H,3.3816905192,0.0157951481,1.7322393
241\H,3.1691290108,-0.0006628491,-0.7165948309\C,0.1171034947,0.126084
4218,4.306248496\C,2.5339784496,-0.1238107087,4.1995047184\C,0.7286193
294,0.3884885684,5.6820757872\H,-0.4858104166,-0.7952305432,4.30187375
04\H,-0.5263006572,0.9486387377,3.9715493321\C,2.0463026467,-0.3847494
27,5.6242122617\H,3.1341103611,0.7974713362,4.1409669518\H,3.145366145
5,-0.9467438829,3.8101795179\H,0.9267151684,1.4589899655,5.8010750961\H,
0.0744005392,0.071562886,6.4990385511\H,2.7700646287,-0.0670008235,6
.3799084238\H,1.8595332497,-1.4551167956,5.7613506104\N,1.289950733,0.
0007157088,3.4480342389\Version=AM64L-G03RevD.01\State=1-A\HF=-456.69
22857\MP2=-458.1656992\RMSE=2.291e-09\RMSE=3.181e-05\Thermal=0.Dipole
=-0.0879387,0.0010406,1.9886574\PG=C02 [C2(N1C1N1),X(C8H12)]\@

1\GINC-NODE25\Fopt\RMP2-FC\6-31G(d)\C11H15N2O1(1+)\ZIP05\30-Jan-2006
0\#p MP2/6-31G(d) opt\ppyacmp, opt\1,1\C,-0.0045776285,-0.00753922
44,-0.0148762126\C,-0.0024996534,-0.0064761042,1.3533580374\C,1.228131
913,0.000718396,2.0781311883\C,2.4221746429,0.0098620129,1.2936096797\
C,2.3587694391,-0.0144498828,-0.0708331091\H,-0.9305003927,-0.021608932
3,-0.5749936135\H,-0.9577309474,-0.0316356584,1.8640027666\H,3.4009947
43,0.0335323964,1.7575601241\H,3.2362334305,0.0293729921,-0.7070798601
\C,0.0593868351,0.0734031128,4.2685825344\C,2.5039688038,-0.0772688269
4,2068083659\C,0.6445528523,0.3603292523,5.6489672215\H,-0.4727827987
,-0.8854294285,4.2409732504\H,-0.6094357418,0.8629998106,3.9144641979\
C,1.9890537635,-0.3656120951,5.6145346652\H,3.0346097972,0.8812288189,
4.1529780004\H,3.1534693351,-0.866586875,3.817988408\H,0.794540974,1.4
370567308,5.7749460192\H,-0.0122644671,0.013401411,6.4497326636\H,2.68
54200157,-0.0193506968,6.3814407065\H,1.8457204802,-1.4424611328,5.747
0757866\N,1.2605594838,-0.0010185526,3.4083310704\C,1.2007927515,0.007
9802596,-2.2148389923\C,-0.119810835,0.0024405112,-2.9255606861\H,0.09
52758026,0.0086722114,-3.9937911801\H,-0.6989862959,-0.8927791862,-2.6
834625863\H,-0.7112160613,0.8872418451,-2.6750616825\N,1.1595431635,0.
0042070408,-0.7338044902\O,2.2881710161,0.0155887333,-2.7448443146\Ve
rsion=AM64L-G03RevD.01\State=I-A\HF=608.8667261\MP2=-610.7660622\RMSD
=9.992e-09\RMSF=1.256e-05\Thermal=0\Dipole=-0.9096299,-0.0066366,0.55
01874\PG=C01 [X(C11H15N2O1)]\@

4-1

1\GINC-NODE19\Fopt\RMP2-FC\6-31G(d)\C11H14N2\ZIP05\30-Jan-2006\0\#p
MP2/6-31G(d) opt\itcapmp\0,1\N,-0.0006116568,-0.0229399494,-0.000647
503\C,-0.0002178335,-0.0081703852,1.3925742004\C,1.2094546111,0.002962
6903,2.1201572074\C,-1.2075778762,0.0674148618,2.1201571778\N,0.005028
3548,0.1885694038,4.2248459678\C,-1.1324421385,0.1644255196,3.50890573
21\C,1.1395956758,0.1038397544,3.5089057599\H,-2.0566244496,0.23137262
74,4.0857101498\H,2.0660324621,0.1214385782,4.085710198\C,1.2224752861

,-0.4447307768,-0.6683922473\C,-1.2444392517,-0.3789485011,-0.668392226
39\H,-1.4397898414,-1.464716047,-0.6090562636\H,-1.1327100347,-0.12464
49112,-1.7286264721\H,1.1244576641,-0.1848340837,-1.7286264525\H,1.359
6836374,-1.5393662836,-0.6090562809\C,-2.4008152653,0.3938657139,-0.05
10331804\H,-2.1954179401,1.4653673629,-0.148448777\H,-3.3267105635,0.1
812513117,-0.597468809\C,2.5399478181,-0.1207865356,1.4195895772\H,3.2
860140719,0.504129316,1.9244692972\H,2.9007718535,-1.1555761132,1.4938
432845\C,2.4183941,0.2653575443,-0.0510331168\H,3.3316425811,0.0037008
747,-0.5974687322\H,2.2703930164,1.3462828561,-0.1484486844\C,-2.54277
53385,0.0147484859,1.4195895204\H,-2.9582344422,-0.9993408516,1.493843
2458\H,-3.2544772248,0.6785369528,1.9244692109\Version=AM64L-G03RevD.
01\State=1-A\HF=-533.6117067\MP2=-535.3503697\RMSD=5.689e-09\RMSF=2.24
8e-05\Thermal=0.\Dipole=-0.0071063,-0.2664963,-1.6445959\PG=C01 [X(C11
H14N2)]\@

4-2

11\GINC-MORITZ\Fopt\RMP2-FC\6-31G(d)\C11H14N2\YIN\31-Jan-2006\0\#P M
P2\6-31G(D) OPT MAXDISK=1GB\itcap2mp\0,1\N,0.0012150088,-0.0042592186
,-1.2886549425\C,0.0009109974,-0.0057265837,0.0893241278\C,1.210193477
1,-0.0256173763,0.8165998426\C,-1.2065219514,0.0029849139,0.8199431852
\N,0.0053998991,-0.0229576827,2.9272141767\C,-1.1331990142,-0.02699818
54,2.2104382148\C,1.1420811379,-0.0109751389,2.2073483335\H,-2.0584752
004,-0.0470894991,2.7891296682\H,2.069172638,0.0016408163,2.7832891971
\C,1.2213450795,0.1843718807,-2.0613763693\C,-1.2280130853,-0.12944305
11,-2.0577998018\H,-1.0163815086,-0.7566006544,-2.934768495\H,-1.54486
85828,0.856349428,-2.4369135507\H,0.9918208758,0.8526362001,-2.9031442
165\H,1.5486472385,-0.7752292876,-2.4935846385\C,-2.3447095518,-0.7518
10729,-1.2318647843\H,-3.2699686605,-0.7496154213,-1.8188647971\C,2.50
98532806,-0.0332363573,0.06322418884\H,3.312454178,0.3750210402,0.68816
14577\H,2.7994475393,-1.0608822948,-0.197437316\C,2.337868672,0.781804
4202,-1.216645841\H,3.2612356943,0.8031643327,-1.8061956678\H,2.086324

3208,1.816208266,-0.9569252733\C,-2.5116554646,0.0202097163,0.07486333
28\H,-3.3052825475,-0.4155362509,0.6927275725\H,-2.8141345472,1.052492
266,-0.1501140978\H,-2.0952172564,-1.7954216895,-1.0097072534\Version
=x86-Linux-G03RevB.03\State=1-A\HF=-533.6100975\MP2=-535.3489854\RMDS=
7.273e-09\RMSF=6.082e-06\Dipole=-0.0032941,0.0287703,-1.8539349\PG=C01
[X(C11H14N2)]\@

4Ac-1

1\1\GINC-NODE26FOpt\RMF2-FC\6-31G(d)\C13H17N2O1(1+)\ZIP05\31-Jan-2006
\0\#p MP2/6-31G(d) opt maxdisk=1GB\rcap2acmp\1,1\N,0.0002244475,0.0
000877609,-0.0218140118\C,0.0008241632,-0.000118548,1.3183373216\C,1.2
275931353,-0.0082469822,2.0537959633\C,-1.2254543889,0.0076898611,2.05
60716394\N,0.0024425082,0.00052851,4.1130982636\C,-1.1814335436,-0.005
9901718,3.4249764121\C,1.184669852,0.0068458819,3.4250557652\H,-2.0724
023902,-0.0091256754,4.0441573531\H,2.0962676219,0.0101849911,4.010272
5668\C,1.2371568945,0.1217215743,-0.8120333158\C,-1.2386323709,-0.1213
989403,-0.8100344171\H,-1.001390495,-0.7456043297,-1.6782045775\H,-1.5
154571253,0.8743196206,-1.1803722232\H,0.9992578732,0.7471858456,-1.67
90924604\H,1.5134173662,-0.8734457679,-1.184418622\C,-2.3632035946,-0.
7359278843,0.004399153\H,-3.2845028119,-0.7095426847,-0.5851449368\C,2
.5317867282,-0.036037544,1.30689648\H,3.3318969375,0.3913739495,1.9199
551101\H,2.8114531075,-1.075020296,1.0891462434\C,2.3633129518,0.73526
68762,0.0009462361\H,3.2839239053,0.7088147244,-0.5897004085\H,2.13879
091,1.7862409854,0.212510908\C,-2.5304757151,0.0338129888,1.3112477622
\H,-3.3270355137,-0.3945810434,1.9276067294\H,-2.811756472,1.072900785
7,1.0963206201\H,-2.1381483931,-1.7871162217,0.2144448697\C,-0.0726458
293,-0.0002215966,5.5891580544\O,-1.1709027998,-0.0153409024,6.0984165
741\C,1.2307138782,0.0178300505,6.3323453635\H,1.8316608722,-0.8665832
387,6.1042488896\H,1.8123066043,0.9128653343,6.0959562798\H,0.98952647
57,0.0198349334,7.3950425963\Version=AM64L-G03RevD.01\State=1-A\HF=-6
85.7902033\MP2=-687.9554452\RMDS=3.397e-09\RMSF=1.825e-05\Thermal=0\ID

ipole=0.9070696,0.0123228,-0.8533392\PG=C01 [X(C13HI7N2O1)]\@

4A c-2

1\1\GINC-NODE23\Fopt\RMP2-FC\6-31G(d)\C13HI7N2O1(1+)\ZIP05\31-Jan-2006
\0\#p MP2/6-31G(d) opt MaxDisk=1GB\lcapacmp\1,1\C,0.0140705822,-0.0
090948116,0.0008772477\C,0.0080219467,-0.0054316964,1.5057033419\C,1.2
454034791,-0.0025139471,2.2256260381\N,2.4217256339,0.0683116865,1.582
4758465\C,2.4975779435,0.0795098573,0.1113640031\C,1.259493101,0.71355
16481,-0.4989971012\C,1.1858155627,-0.0694138554,3.6551592113\C,2.4562
963053,-0.1397810782,4.4579438785\C,3.5670057218,0.5867803098,3.708878
7001\C,3.7021723937,0.0110380392,2.3096635737\C,-1.1734796726,-0.01280
53549,2.2042766971\N,-1.2089598679,-0.0423542891,3.5703891624\C,-0.036
3609631,-0.0743113229,4.2747835521\C,-2.4671485587,-0.0440759239,4.347
0213988\C,-3.745447885,-0.0103740133,3.5622635203\O,-2.3844328195,-0.0
721481097,5.5544471289\H,-2.1248100968,-0.0018396942,1.686211728\H,-0.
1494956696,-0.1078576763,5.3533634207\H,2.6322691802,-0.9496473596,-0.
2472237036\H,3.3935431037,0.6451139621,-0.1589762991\H,4.4279095993,0.
5830008261,1.72493418\H,4.0471000962,-1.0309291238,2.3426557397\H,1.21
77382224,1.7737460285,-0.22761781\H,1.3291676864,0.6555938678,-1.58942
43712\H,2.2980422354,0.2935875047,5.4505859236\H,2.7360144348,-1.19047
3019,4.6075953377\H,4.5216790056,0.4794193144,4.2326020426\H,3.3452031
381,1.6574169831,3.6457751649\H,0.0169001053,-1.0445177811,-0.36327691
9\H,-0.8964723342,0.4628709171,-0.3826510959\H,-3.8386993571,-0.886546
1451,2.9149859789\H,-4.5611655357,-0.013044645,4.2848327767\H,-3.81335
73345,0.892536491,2.9495769668\Version=AM64L-G03RevD.01\State=I-A\HF=
-685.7893532\MP2=-687.9545275\RMSE=6.291e-09\RMSE=6.098e-06\Thermal=0.
\Dipole=0.2719475,-0.0391215,-1.1851803\PG=C01 [X(C13HI7N2O1)]\@

5

1\1\GINC-NODE24\Fopt\RMP2-FC\6-31G(d)\C10HI6N4\ZIP05\30-Jan-2006\0\#p
mp2/6-31G(d) opt max=1GB\lrsamp\0,1\C,0.0358543028,0.011482438,-0.06

98919899\C,-0.0555441278,-0.0112652677,1.3292207036\C,1.2907237508,0.0
014240192,-0.6724564865\H,-0.8733284341,0.0261928253,-0.6652944691\C,1
.1534299424,0.0113199848,2.0446359401\N,-1.3056310333,0.0757003686,1.9
461368651\C,2.3585541479,0.0062548334,1.3452617108\N,2.4568800791,-0.0
047566898,0.00271773\H,3.3034598837,0.0195242166,1.8878832711\H,1.3746
667709,0.00471167,-1.7585148172\C,-1.5806008805,-0.6799746883,2.971976
409\N,-1.0175048575,-1.910961288,3.282336731\N,-2.5614924024,-0.266884
1177,3.8614102639\C,-0.4299877505,-2.7482650608,2.2529196238\C,-0.6092
206068,-2.223926681,4.6425984039\H,-0.6522091022,-3.7944793675,2.49296
77425\H,-0.8769523569,-2.5058589666,1.2884840364\H,0.658145177,-2.6269
461135,2.1750497352\H,-1.0056130748,-1.468789389,5.320547385\H,-0.9811
281646,-3.2106717249,4.943991594\H,0.4876124621,-2.2329831568,4.717484
9385\C,-3.6090646432,-1.2087256836,4.2457100785\C,-3.042182769,1.09885
93237,3.7060489197\H,-4.4715153721,-1.1302487678,3.5680522224\H,-3.224
7637085,-2.2263306302,4.2051002727\H,-3.9464685441,-0.9913968276,5.263
6746563\H,-2.1948435072,1.7671121485,3.5594986971\H,-3.7149064324,1.20
2317164,2.8446929384\H,-3.5790462696,1.3760417928,4.6179677531\H,1.145
6418107,0.0440868567,3.1320708953\Version=AM64L-G03RevD.01\State=1-A\
HF=-605.7539366\MP2=-607.694519\RMSD=7.052e-09\RMSF=1.201e-05\Thermal=
0.\Dipole=-1.2397082,-0.8637968,1.4118125\PG=CO1 [X(C10H16N4)]\@

5Ac-1

1\INGINC-NODE25\FOpt\RMP2-FC\6-31G(d)\C12H19N4O1(1+)\ZIP05\31-Jan-2006
\0\#p mp2/6-31g(d) opt maxdisk=1GB\hsaac2mp\1,1\C,-0.0143332514,-0.
0029448106,-0.0139344395\C,-0.0320419903,0.0521791744,1.4138539418\C,1
.1597860617,-0.0386812238,-0.7120687706\H,-0.9593948631,-0.0195300929,
-0.547319453\C,1.254713729,0.0920269977,2.0442621924\N,-1.2161144992,0
.1376182992,2.0218013102\C,2.4029732288,0.0617360476,1.3036585949\H,3.
3965054098,0.0979286384,1.7358541977\H,1.1792005167,-0.089919621,-1.79
27423008\C,-1.3378746747,-0.0605962369,3.3538079183\N,-0.8408186941,-1
.1650944069,3.967539503\N,-2.071676852,0.8185198443,4.058945883\C,-0.4

979309477,-2.3637989575,3.2054877976\C,-0.4465855774,-1.1818428106,5.3
77193268\H,-0.7883951075,-3.237029669,3.7951300424\H,-1.0497462101,-2.
3683256018,2.2662135767\H,0.5774315911,-2.4163732323,3.0010806072\H,-0
.4586498525,-0.1682971186,5.7757914099\H,-1.100784326,-1.8219574164,5.
9761974783\H,0.5740195448,-1.5726417653,5.4394186345\C,-2.9456250319,0
.4181696509,5.1656734572\C,-2.3625273425,2.1315864342,3.4784827199\H,-
3.9513633813,0.7903472498,4.9522374068\H,-2.9856288434,-0.6677737626,5
.2319503123\H,-2.6093031141,0.8376774812,6.1175081647\H,-1.5325874336,
2.4510949121,2.8519947008\H,-3.2750767121,2.093555227,2.8756462371\H,-
2.4939807988,2.8417285104,4.2975657879\N,2.3719094254,-0.011314474,-0.
0656718027\C,3.6631479091,-0.0462944747,-0.7709640516\C,3.6143581343,-
0.0980575394,-2.2702081396\O,4.6759694934,-0.0303758736,-0.1055289548\
H,3.1078274558,0.7784086555,-2.6830078488\H,4.6459159087,-0.1126598627
,-2.6207708432\H,3.1045421224,-0.9990519489,-2.62180222352\H,1.34012372
84,0.1769476824,3.1231563478\Version=AM64L-G03RevD.01\State=I-A\HF=-7
57.9368638\MP2=-760.299073\RMSE=8.815e-09\RMSE=8.107e-06\Thermal=0.\Di
pole=-0.6637693,-0.1927122,0.2456167\PG=C01 [X(C12HI9N4O1)]\@

5Ac-2

1\1\GINC-NODE21\FOpt\RMPP2-FC\6-31G(d)\C12HI9N4O1(I+)\ZIP05\31-Jan-2006
\0\#p mp2/6-31g(d) opt maxdisk=1GB\hlsaac lmp\1,1\C,-0.0117136185,-0.
0312171635,-0.0165785427\C,-0.0279122462,0.035154007,1.4107507252\C,1.
159460767,-0.0697610758,-0.71607984\H,-0.9577521428,-0.0539730154,-0.5
480845027\C,1.2586771092,0.0806707439,2.0397661494\N,-1.2106964203,0.1
265236638,2.0208753559\C,2.4076111705,0.0507844799,1.2955421446\H,3.38
44169474,0.097542562,1.7597923795\H,1.2151180471,-0.1303367601,-1.7965
036872\C,-1.3387058622,-0.0721035385,3.3506782299\N,-0.844113617,-1.177
2961557,3.9667562186\N,-2.0766242299,0.8060775532,4.0533587964\C,-0.50
30548202,-2.3773471589,3.2062852339\C,-0.4629675253,-1.1968990601,5.37
95087126\H,-0.8004252868,-3.2497427468,3.7938175092\H,-1.0498030559,-2
.3792593563,2.2640067141\H,0.5729800779,-2.435212865,3.0067286744\H,-0

.477955257,-0.1839517971,5.7796342369\H,-1.1232235004,-1.8371286198,5
.9718436272\H,0.5565014233,-1.5892385525,5.4511217046\C,-2.9619820125,
0.4018353255,5.1497575896\C,-2.367204747,2.1177795299,3.469471784\H,-3
.9663789149,0.7715270645,4.9258498396\H,-3.0001668177,-0.6842748515,5.
2142537687\H,-2.6372536489,0.8209391182,6.105797799\H,-1.5318423908,2.
4412019653,2.8521862812\H,-3.2724347295,2.0755167004,2.8559560166\H,-2
.5113803967,2.8272148161,4.2870031033\N,2.3740223999,-0.0314726287,-0.
0710956663\C,3.5868647049,-0.0733957041,-0.9047467499\C,4.9056114766,-
0.0153459852,-0.189051823\O,3.4484885422,-0.1508425186,-2.1058196581\H
,5.0284867509,-0.8616751259,0.4919509688\H,5.6817566033,-0.0572952706,
-0.9526698413\H,5.0114928941,0.9138795523,0.377151151\H,1.3451809591,0
.1708766071,3.1181831582\Version=AM64L-G03RevD.01\State=1-A\HF=-757.9
356128\MP2=-760.2981328\RMSD=3.744e-09\RMSF=1.614e-05\Thermal=0.\Dipol
e=0.3155491,-0.1124329,1.7846297\PG=C01 [X(C12H19N4O1)]\@

6-1

1\1\GINC-LX64I163\FOpt\RMP2-FC\6-31G(d)\C23H24N2O1\UI271AC\25-Sep-2005
\0\#P MP2/6-31G(D) OPT\fujihf04-m, optimization calculation\0,1\C,2
.0442017607,-0.1691528996,-1.2721780986\C,1.9651850842,-0.1270752204,0
.2935924919\C,3.5547851964,-0.1894460902,-1.5668951515\C,1.4266910506,
1.0822959022,-1.9275044309\O,1.3654704468,-1.2936599414,-1.8091448559\
C,3.3866939596,0.257401386,0.7773670926\N,1.6916844198,-1.4648145112,0
.8739400729\H,1.1981631854,0.5845777727,0.6267880171\C,3.9514968039,-1
.0371212142,1.3791867499\C,4.1626609693,0.6885928868,-0.4749796343\H,3
.3468660403,1.0397044805,1.5438589076\C,2.7300462767,-1.7891091855,1.8
678315923\H,4.4672388136,-1.6209655955,0.6099764147\H,4.6685732616,-0.
8431286225,2.1829311279\H,2.425165954,-1.4469153354,2.869420839\H,2.89
31850754,-2.8705067768,1.9152315447\C,0.3723343744,-1.7878632158,1.246
0102658\C,0.1077677728,-2.7545976324,2.2323654819\C,-0.7420935573,-1.2
015508659,0.6262909395\C,-1.213800831,-3.0529835059,2.5573797344\H,0.9
029322136,-3.2777186107,2.7514138602\N,-2.2896671835,-2.4785017564,1.9

922395294\H,-1.4211780479,-3.7979831631,3.3248336163\C,-2.0209447127,-
1.5676180296,1.038025954\H,-2.8838868811,-1.0952702948,0.5708641842\H,
-0.6306310927,-0.4796561238,-0.1687714904\H,5.2426079411,0.5479439967,
-0.3526017768\H,4.0005066035,1.7494295096,-0.6956008055\H,3.9097338914
,-1.223392914,-1.4801569927\H,3.7758727827,0.1431219895,-2.5866122518\
C,-0.0463492115,1.2419993464,-1.6909643246\H,1.9603244736,1.9720999123
,-1.5702726323\H,1.6231999,1.0003518175,-3.0043937605\C,-0.5303578653,
2.1103500027,-0.7256649038\C,-0.9683884282,0.4630705775,-2.4407181329\
C,-1.9133274685,2.1886978983,-0.4245154595\H,0.1627310302,2.7398509658
,-0.1645781614\C,-2.8309259108,1.3732127889,-1.1636594642\C,-2.4181316
587,3.0480672403,0.5852308646\C,-2.3208889427,0.5240148129,-2.18019065
12\C,-4.2134944276,1.4357995131,-0.8520163786\H,-3.0167401362,-0.08439
1063,-2.7569210558\H,-0.5863562667,-0.2141523059,-3.1998668868\C,-4.67
28607827,2.2747800455,0.1430602298\H,-4.9092837653,0.8138292086,-1.4113
6241777\C,-3.7682919677,3.0856807851,0.8674915194\H,-5.7345301305,2.31
12085713,0.375967646\H,-4.1418584131,3.7433798686,1.6489688651\H,-1.72
10874029,3.6701007041,1.1454046872\H,1.4785218364,-1.9936965447,-1.1129
6358028\\Version=IA64L-G03RevC.02\State=-A\HF=-1068.7034029\MP2=-1072
.1720526\RMMSD=5.578e-09\RMSE=9.020e-06\Dipole=1.6601722,0.6518833,0.29
79258\PG=C01 [X(C23H24N2O1)]\@

6-2

1\1\GINC-LX64I161\FOpt\RMMP2-FC\6-31G(d)\C23H24N2O1\UI271AC\06-Oct-2005
\0\#P MP2/6-31G(D) OPT\fujihf02-m, geometry optimization\0,1\C,0.61
55497981,-0.5676772033,0.5417225445\C,0.5400188034,-0.6055347211,2.089
5716676\C,2.1089962976,-0.4032288749,0.2923431233\C,-0.2452181597,0.50
89329559,-0.1290408088\O,0.2520849942,-1.8656671906,0.0596508166\C,1.7
974228544,-1.4039823716,2.5080697108\N,-0.6121318387,-1.3659919084,2.6
001145239\H,0.556681957,0.4142851954,2.4991666014\C,1.25530157344,-2.8
016712154,2.8203089766\C,2.7813849645,-1.3261526955,1.3208784262\H,2.2
246863268,-0.9678768002,3.4189782323\C,-0.1393525495,-2.5358219842,3.3

715891662\H,1.1890062058,-3.3830004848,1.8972687791\H,1.8747148715,-3.3526513825,3.5331807603\H,-0.1121201528,-2.2967253098,4.4460352827\H,-0.8124397767,-3.3882850429,3.2323156184\C,-1.7453594454,-0.7018336007,3.0785420857\C,-2.6835232774,-1.3671854765,3.8896784019\C,-2.0403915108,0.6351950705,2.7587366856\C,-3.8146825583,-0.6868781886,4.3311637994\H,-2.5490214908,-2.403633767,4.1782727552\N,-4.1002057653,0.5945982923,4.0398947835\H,-4.5384795335,-1.2026189347,4.960855044\C,-3.2005524652,1.2196518772,3.2600438469\H,-3.4234687327,2.2580513964,3.018171407\H,-1.3829899441,1.2286796344,2.1367649746\H,2.9311472973,-2.3214478334,0.8923210148\H,3.7643953449,-0.9525510586,1.6241248436\H,2.3633884158,-0.6414796166,-0.7440902934\H,2.3840098311,0.6452679497,0.4684498188\C,0.0512384913,0.6665659709,-1.5970277333\H,-1.3022953218,0.2512565022,0.0219081226\H,-0.0696811986,1.4706566771,0.3730582167\C,0.7192800652,1.7861758144,-2.0629328079\C,-0.3309600033,-0.3408798223,-2.5230511263\C,1.031437087,1.9486484703,-3.4360064527\H,1.0101308973,2.5732610488,-1.3653523996\C,0.6441812005,0.9260066699,-4.3605463405\C,1.71401957,3.0929126174,-3.9240180578\C,-0.0428654854,-0.2121765938,-3.8650674771\C,0.9533188925,1.0874282372,-5.7352337328\H,-0.3438116946,-0.9912716516,-4.5646248388\H,-0.842749132,-1.225525342,-2.156167019\C,1.6198769009,2.2110686411,-6.1798537407\H,0.6571887932,0.3087285517,-6.4368733785\C,2.0029370741,3.2215795288,-5.2671609772\H,1.8521996797,2.3231389294,-7.2364593095\H,2.5270894719,4.103499565,-5.6284263177\H,2.0081689102,3.8711124383,-3.2207790058\H,-0.5346876621,-2.1026364619,0.5983743281\Version=IA64L-G03RevC.02\State=1-A\HF=-1068.7099511\MP2=-1072.1682026\RMSD=4.256e-09\RMSF=8.433e-06\Dipole=1.166033,-0.5271992,0.321634\PG=C01 [X(C23H24N2O1)]\@

6Ac-1

I1\GINC-LX64I154\FOpt\RMP2-FC\6-31G(d)\C25H27N2O2(1+)\UI271AC\02-Sep-2005\0\#P OPT MP2/6-31G(D) GEOM=CONNECTIVITY\fujiaImp2, geometry optimization\1,1\C,-0.2995223929,-1.218921888,-0.8370892385\C,-0.159609

5909,-1.271309524,0.5805737658\C,0.7930768978,-1.2824570443,-1.6534211
817\H,-1.2686681291,-1.1351784469,-1.3090895581\N,-1.2059592228,-1.232
8805024,1.4115824457\C,1.172161011,-1.421943514,1.0680616956\C,-2.5665
062274,-0.8171949652,1.0584942009\C,-1.17239369,-1.6855681317,2.815049
5482\C,-2.8501981535,0.6957173204,1.2922855728\C,-3.4819498896,-1.5794
697868,2.0634340276\H,-2.7961565195,-1.0811301948,0.0213525481\C,-4.30
44213219,0.6629065888,1.7777656979\C,-2.6464896545,1.63065527,0.097667
3757\O,-2.0010979142,1.0644048954,2.3927381685\C,-4.3158561051,-0.4973
511271,2.7705084258\H,-4.607267442,1.6261966299,2.20671367\H,-4.973731
7299,0.4579381014,0.9324942317\H,-5.3235323824,-0.8480817161,3.0101543
065\H,-3.8369075531,-0.1941148639,3.706266168\C,-2.5253836059,-2.38573
18418,2.9550191909\H,-4.1491666249,-2.2510992076,1.5134310161\H,-2.437
0220081,-3.4146301692,2.5931984582\H,-2.8599961148,-2.4240285651,3.995
8592273\H,-1.0762374976,-0.823014002,3.4789367903\H,-0.3350513123,-2.3
69601842,2.9682071531\C,-1.2806124235,1.651261231,-0.5527041477\H,-2.9
077288667,2.6451016025,0.4364669139\H,-3.3983963908,1.3737044541,-0.66
0374266\C,-0.1040887348,1.7546721298,0.1791876527\C,-1.1981759888,1.61
38326686,-1.9693967764\C,1.1580520962,1.8064380028,-0.4599357159\H,-0.
146325121,1.8133176569,1.2635986379\C,1.2302842319,1.7190927987,-1.889
6334181\C,2.3649490487,1.8774786139,0.2852748412\C,2.498747161,1.77419
13972,-2.5227694876\C,0.0179282242,1.6634790389,-2.6231814401\C,3.6550
146362,1.8498022724,-1.7698008971\H,2.5525319276,1.7310201005,-3.60956
55875\C,3.5871519069,1.9219983391,-0.3567879359\H,4.6207037045,1.91246
35474,-2.2670389943\H,4.5034554,2.015722676,0.2227791328\H,2.309939902
4,1.9589698957,1.3703966633\H,0.0559934948,1.6446563994,-3.7119479952\
H,-2.1170667933,1.5758341165,-2.5539952842\H,-2.3218534079,1.926909425
2,2.7217302815\C,2.2368699877,-1.4462115752,0.2075342566\H,1.381702138
4,-1.4289319824,2.1310899693\N,2.0625137329,-1.3908333572,-1.146329223
9\H,3.253340109,-1.5077845508,0.5731345205\C,3.1739939076,-1.445407079
5,-2.108098917\C,4.5541698052,-1.5697119263,-1.5342174843\O,2.90538556
32,-1.4097238422,-3.2892526679\H,5.2488393009,-1.5761233037,-2.3739513

799\H,4.7809792436,-0.7227814033,-0.8824160368\H,4.6672265975,-2.50027
91004,-0.9706615751\H,0.7270664976,-1.2779902702,-2.734343239\Version
=IA64L-G03RevC.02\State=1-A\HF=-1220.8734918\MP2=-1224.7837577\RMSE=4.
884e-09\RMSE=4.612e-06\Dipole=0.07232249,-1.2768574,1.1445331\PG=C01 [X
(C25H27N2O2)]\@

6Ac-2

1\GINC-LX64I160\FOpt\RMF2-FC\6-31G(d)\C25H27N2O2(1+)\UI271AC\27-Sep-
2005\0\#P MP2/6-31G(D) OPT\fujiachf06-m, opt calculation\1,1\C,-0.8
048138913,0.1952661283,-2.8257764024\C,-0.9971088378,0.4156028362,-1.4
284861263\C,0.4458245062,0.2354055399,-3.3751508859\H,-1.6319405743,-0
.0499006849,-3.4801881934\N,-2.2157851682,0.4291007195,-0.8812666967\C
,0.1808751466,0.6688452205,-0.6675236852\C,-2.4847796109,0.3733127004,
0.5566566585\C,-3.4552510285,0.1851324429,-1.628365732\C,-2.4108615343
,-1.0960807931,1.1045684005\C,-3.9601735981,0.8191030357,0.7054104396\
H,-1.7894739974,1.0300017239,1.0847313973\C,-3.8799258596,-1.517438780
9,1.2670385614\C,-1.6828191538,-1.1548116409,2.4677875589\O,-1.7122185
791,-1.8715726744,0.1297995749\C,-4.601442159,-0.2223071692,1.63108437
77\H,-4.2417563094,-1.9038494863,0.3061333468\H,-4.0029330117,-2.31245
66366,2.0116123803\H,-4.4203140968,0.0359477976,2.6805164705\H,-5.6863
187059,-0.279240688,1.5001166173\C,-4.528977446,0.8086791586,-0.734118
1001\H,-4.0287993421,1.8273983874,1.1247654729\H,-4.7310499359,1.83101
68101,-1.0639672815\H,-5.4697250488,0.253747119,-0.7971970459\H,-3.588
4015525,-0.8948875561,-1.7675596768\H,-3.4095856648,0.6652483771,-2.60
84215012\C,-0.2902422854,-0.5944392951,2.4232351625\H,-1.6631704164,-2
.2090134189,2.778605945\H,-2.2804794537,-0.6230571193,3.2190757978\C,0
.7485356948,-1.3155709441,1.8547589107\C,-0.036304889,0.7261811776,2.8
826141877\C,2.0369749852,-0.7512595875,1.6904636336\H,0.5813471417,-2.
3378988161,1.5203635031\C,2.2593775801,0.6096101603,2.0875798948\C,3.0
927247389,-1.4663521163,1.0661598473\C,3.5390594298,1.1897061168,1.880
9143134\C,1.2055418231,1.312280653,2.7274566214\C,4.5473325984,0.46708

60522,1.2726655172\H,3.7148544646,2.2143134338,2.2055337651\C,4.326786
 6695,-0.8752628303,0.8761525928\H,5.5286365935,0.9153228675,1.13408424
 6\H,5.1381016724,-1.4441729871,0.4268149809\H,2.9280564742,-2.50220793
 2,0.7727924984\H,1.3823722528,2.3255985506,3.0856117001\H,-0.829768030
 8,1.275836852,3.3887971388\H,-1.7751405687,-2.8052571,0.4089214163\C,1
 4101106763,0.7057932459,-1.2679044356\H,0.1436681301,0.8371491237,0.3
 99424002\N,1.5538912291,0.4970324357,-2.6146059305\H,2.3071313957,0.89
 31476285,-0.6899653141\C,2.858349005,0.522268259,-3.2992195274\C,4.048
 9205789,0.8643034463,-2.4556861848\O,2.8826795925,0.2757822452,-4.4854
 249008\H,4.9209658665,0.8370216396,-3.1087982664\H,3.9503664972,1.8644
 47279,-2.024196378\H,4.1770125831,0.1495858485,-1.6385622796\H,0.63963
 42699,0.0592322366,-4.426827335\Version=IA64L-G03RevC.02\State=1-A\HF
 =-1220.8832273\MP2=-1224.7834123\RMSD=6.228e-09\RMSF=1.553e-06\Dipole=
 -0.8418683,0.2851433,-0.7095441\PG=C01 [X(C25H27N2O2)]\@

6Ac-3

1\1\GINC-LX64I162\FOpt\RMP2-FC\6-31G(d)\C25H27N2O2(1+)\UI271AC\26-Sep-
 2005\0\#P MP2/6-31G(D) OPT\fujiachi36-m, opt calculation\1,1\C,0.64
 80431588,-0.7116099724,0.0750255939\C,0.8134137616,-0.707924955,1.4938
 648801\C,1.7291997544,-0.6355678163,-0.7601028337\H,-0.3287889398,-0.7
 867331318,-0.3838314484\N,-0.2223769658,-0.809721624,2.3271660069\C,2.
 1610172249,-0.6345947268,1.9640394793\C,-1.620166954,-0.6015869273,1.9
 328371652\C,-0.1017109355,-0.8250683164,3.7910850871\C,-1.9312003748,0
 9394934922,1.765999195\C,-2.4600883023,-1.0899856772,3.1410972583\H,-
 1.8238877512,-1.1632149352,1.017149382\C,-2.5868401219,1.3295385984,3.
 0924457965\C,-2.9037596744,1.1839643183,0.5840052057\O,-0.7507482783,1
 7118561096,1.6164068917\C,-3.375470257,0.0913105478,3.505839063\H,-1.
 7937690219,1.5562876486,3.8143987694\H,-3.1981479598,2.2316583086,2.99
 03267344\H,-4.3128969917,0.0296919539,2.9420405692\H,-3.6461232648,0.0
 869867213,4.5660575296\C,-1.4238888225,-1.4510129272,4.2291447504\H,-3
 .0464987547,-1.9774053126,2.8840491665\H,-1.305623013,-2.5366936453,4.

2863422571\H,-1.7273113443,-1.1001270615,5.2196803309\H,0.0319691298,0
.1998782244,4.1587585431\H,0.7590242912,-1.4253686344,4.0949508393\C,-
2.3112062461,0.770528625,-0.7328194964\H,-3.1340108535,2.2562932387,0.
5855305703\H,-3.8427336317,0.6470773986,0.7652747993\C,-1.3752438001,1
.5750445238,-1.3726806104\C,-2.598662027,-0.5087091591,-1.2833190251\C
, -0.6619381178,1.1233953882,-2.5128768408\H,-1.2159880451,2.5995780291
,-1.0301616869\C,-0.8993597103,-0.2049629554,-2.9991880078\C,0.3423219
002,1.9136513137,-3.130095949\C,-0.1515819312,-0.6788607246,-4.1091155
171\C,-1.9265460382,-0.9775080187,-2.3952659511\C,0.8226660283,0.11277
78928,-4.686640164\H,-0.3513287257,-1.6771480153,-4.4956641099\C,1.060
4353086,1.4229626499,-4.2037669099\H,1.3812987237,-0.253965179,-5.5447
438277\H,1.808137381,2.0477147865,-4.687531677\H,0.5154241371,2.926843
13,-2.7698884942\H,-2.1648313879,-1.9576871752,-2.8063089747\H,-3.3875
980455,-1.1134057297,-0.837056849\H,-0.4685698856,1.6403831873,0.68297
57216\C,3.2047234384,-0.5534397425,1.0864863629\H,2.3897799812,-0.5931
719738,3.0217685564\N,3.0058521665,-0.5552851165,-0.2700519725\H,4.239
4271584,-0.4746949593,1.3995260007\C,4.1953662669,-0.4545447802,-1.134
0028853\C,3.9505364099,-0.4752220195,-2.6129135395\O,5.279322546,-0.36
66223306,-0.6000819059\H,4.9215246958,-0.375170917,-3.0976627961\H,3.4
879875337,-1.416914052,-2.9220363804\H,3.2977836589,0.3452632176,-2.92
2515481\H,1.602470745,-0.6351899615,-1.8363188154\Version=IA64L-G03Re
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6Ac-4

1\INGINC-LX64I159\Fopt\RMP2-FC\6-31G(d)\C25H27N2O2(1+)\UI271AC\27-Sep-
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833332977\C,0.5385366161,0.2938615948,-3.2896833589\H,-1.5249715145,-0
.0720453993,-3.4503796371\N,-2.1961999444,0.3715806717,-0.8678484108\C

,0.1793913865,0.7367005163,-0.5944346752\C,-2.4990835654,0.274882022,0
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,-1.2054990014,1.0765500458\C,-3.9905938499,0.6683219652,0.6799857533\
H,-1.839507645,0.9390822628,1.1246207591\C,-3.8502881735,-1.6676320553
,1.2216365105\C,-1.666678981,-1.2804392769,2.4403584782\O,-1.671394011
6,-1.9401366404,0.0843909129\C,-4.6105124289,-0.3966179366,1.592092870
4\H,-4.1934242428,-2.0538283322,0.2538014535\H,-3.9579149297,-2.473359
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322747,-0.482131142,1.4528743108\C,-4.5293428048,0.6356275805,-0.77117
95858\H,-4.103364132,1.6737665491,1.0966402141\H,-4.7831634359,1.64689
77696,-1.0992441636\H,-5.4354594298,0.0283739644,-0.8561331193\H,-3.48
08425573,-1.0053144739,-1.8016663569\H,-3.359227266,0.5735288718,-2.61
99770491\C,-0.296427845,-0.6657103809,2.4239172921\H,-1.6106843526,-2.
3429348089,2.7176869118\H,-2.2888934933,-0.7962733948,3.2039806928\C,0
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477680774\C,-2.0283739984,-0.6878251503,1.6658764249\H,0.6402757583,-2.
325051241,1.4317386093\C,2.1959837171,0.6606474623,2.1262339875\C,3.09
17597244,-1.3092285851,-0.9598050362\C,3.4368744182,1.3157495455,1.9092
499884\C,1.1237182436,1.2808935178,2.8184932954\C,4.4476694676,0.68759
5313,1.2082145482\H,3.5716115733,2.3312543737,2.2786661319\C,4.2790564
234,-0.6388925417,0.7431931095\H,5.3898947098,1.2016286674,1.035772536
3\H,5.0880417205,-1.1242141917,0.2026819877\H,2.96645815,-2.334062655,
0.6127893642\H,1.2618764204,2.2819633559,3.2249950255\H,-0.9055339433,
1.1299482757,3.4849158072\H,-1.685048379,-2.8769862185,0.3596687487\C,
1.4205812278,0.8218983896,-1.1597689733\H,0.1037947032,0.9197478689,0.
4686944628\N,1.6136881059,0.6005976585,-2.5006724467\H,2.3131679374,1.
0615291491,-0.592353966\C,2.9892518728,0.6897030007,-3.0130694718\C,3.
1858613708,0.4184296205,-4.4770238754\O,3.8714056604,0.9737003577,-2.2
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5936897745,-4.7420814799\H,2.6345409632,1.1343009977,-5.0926507132\H,0
.7301391416,0.1128801337,-4.3392457165\\Version=IA64L-G03RevC.02\State

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Dipole=-1.2649483,-0.0987311,-2.4862844\PG=C01 [X(C25H27N2O2)]\@

6Ac-5

1\GINC-LX64I165\FOpt\RMP2-FC\6-31G(d)\C25H27N2O2(1+)\UI271AC\26-Jan-
2006\0\#P MP2/6-31G(D) OPT\fujiachf05-m, opt calculation\1,1\C,0.83
93930159,-0.3243537519,0.1061512564\C,0.9606966623,-0.3987872612,1.529
3327293\C,1.945499171,-0.3047734775,-0.692172862\H,-0.1264859323,-0.29
99295245,-0.3824624449\N,-0.1035538585,-0.4956215262,2.3226651408\C,2.
2950216467,-0.4130235707,2.0409512354\C,-1.4833197115,-0.2899144791,1.
8635010463\C,-0.0514559632,-0.6527136359,3.782986042\C,-1.790373147,1.
2422384398,1.6799422184\C,-2.3767067916,-0.7851198573,3.0304267749\H,-
1.6358754826,-0.852230148,0.9381708968\C,-2.3864406468,1.6535607286,3.
0266751339\C,-2.8066240978,1.4405250251,0.5266720487\O,-0.6146518445,2
.011075868,1.4761794638\C,-3.1962547111,0.4428442233,3.4798159804\H,-1
.5575141842,1.8624618387,3.7129298369\H,-2.9742109954,2.5729649417,2.9
429591586\H,-4.1760911724,0.4367700623,2.9906648406\H,-3.3855598845,0.
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3.0389551952,-1.5929257039,2.7041121921\H,-1.2745140504,-2.4071459838,
3.9686149324\H,-1.7231933167,-1.1325386551,5.1063082229\H,0.0515484957
,0.3290618525,4.2608677825\H,0.7995104712,-1.275842892,4.0680425528\C,
-2.2012052014,1.1122698823,-0.8095742553\H,-3.1315715769,2.4879261548,
0.5552101426\H,-3.6907310409,0.81781597,0.7114564122\C,-2.3346162561,-
0.1469072648,-1.3798820474\C,-1.3514656929,2.0608346465,-1.4457720019\
C,-1.6018394391,-0.5236210837,-2.5350087838\H,-3.0316499472,-0.8668493
713,-0.9470930293\C,-0.6711896835,0.4113469293,-3.1013893709\C,-1.6954
350332,-1.8252432294,-3.0933684023\C,0.1001712678,0.0225925537,-4.2281
400894\C,-0.6186747793,1.7243643511,-2.5676469555\C,-0.0099628176,-1.2
534812572,-4.7431748492\H,0.7889616225,0.7394599651,-4.6725161817\C,-0
.925194717,-2.1763603021,-4.1831142\H,0.5859036618,-1.5434560081,-5.60
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2.5348412146,-2.6678742196\H,0.0220240003,2.4652973828,-3.0443713969\H
,-1.3303555021,3.0865997913,-1.0770470802\H,-0.403712279,1.999470675,0
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4.3820898257,-0.3712496917,1.5759138879\C,4.3416624176,-0.2918868894,-
1.1080565352\C,5.7202826911,-0.3529416812,-0.5172720592\O,4.0908290175
,-0.2153498386,-2.2914239889\H,6.4235532898,-0.3369650565,-1.349382194
2\H,5.9145263877,0.5070970685,0.1294729846\H,5.8673820031,-1.269826306
7,0.0596036951\H,1.8872264767,-0.2676247278,-1.7745716138\Version=IA6
4L-G03RevC.02\State=1-A\HF=-1220.8823448\MP2=-1224.7789134\RMSD=9.647e
-09\RMSF=4.570e-06\Dipole=2.0373901,-0.9516162,1.8493686\PG=C01 [X(C25
H27N2O2)]\@

6Ac-6

1\1\GINC-LX64I162\FOpt\RMF2-FC\6-31G(d)\C25H27N2O2(1+)\UI271AC\14-Feb-
2006\0\#P MP2/6-31G(D) OPT=CALCHFFC SCF=TIGHT\fujiachf02-m\1,1\N,-1
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3,-0.3149519249,-1.3406714299\C,1.1528048632,-0.2470560383,-2.76528506
49\C,-0.0462111639,-0.2092388726,-3.4241180316\N,2.3723812144,-0.37650
05947,-0.6876422575\C,2.5327041091,-0.3667942307,0.7881397246\C,4.0502
043508,-0.5698734304,0.9464518574\C,4.4679151997,-1.3711600344,-0.2796
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1338379,0.9801419834\C,3.5890287333,1.6219999708,1.8149390822\C,2.2059
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761\C,0.0066562836,0.3135355078,2.5596081259\C,-1.0022301466,1.1404698
907,2.0879917202\C,-2.2589194853,0.6155242543,1.7005585153\C,-2.491917
6915,-0.7968707704,1.8096846428\C,-1.4820034147,-1.6116350569,2.382792
7913\C,-0.263850275,-1.0691552987,2.7432736647\C,-3.7329609039,-1.3281
977505,1.3683596237\C,-4.6956550603,-0.5026207377,0.8206332506\C,-4.46
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5627545,1.6480291221\H,3.7982160394,1.4687621844,2.8798326593\H,5.6222
767282,0.8957682694,1.3964767073\H,4.6706083924,1.2692935923,-0.035585
9591\H,4.2791178388,-1.0873363297,1.885260823\H,4.2134448383,-2.429047
3774,-0.1585336688\H,5.5391783541,-1.3008982025,-0.491079214\H,4.09690
43196,0.1208087154,-1.8423787744\H,3.3924884175,-1.4726997283,-2.18432
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33\H,-5.2453394443,1.5354457352,0.3096104812\H,-3.1013392986,2.5119886
804,1.0712424434\H,-1.6744639187,-2.6740101791,2.5263998745\H,0.499272
6397,-1.7077191454,3.1876930743\H,2.0346766153,2.2264383241,-0.0540081
626\H,2.0559213763,-0.1784539729,-3.3601703456\H,-0.1320396798,-0.1386
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8481725495,-1.1808709197,-2.2007751728\H,-3.8371932704,0.5830508505,-2
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9\RMSE=3.875e-06\Dipole=1.2987203,-0.4812959,-1.2314765\PG=C01 [X(C25H
27N2O2)]\@

7-1

1\1\GINC-LX6418\FOpt\MP2-FC\6-31G(d)\C13H19N3O1\UI271AC\19-May-2006\0
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2779995541,-2.7695955296\C,0.3922242812,0.2977957513,-1.3642190038\C,1
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82,-1.1056045701,0.1484521092\H,-2.3265645323,0.977971534,-1.993799195
7\H,-2.0366688503,-0.7748553106,-2.0646426051\H,-0.7948452572,2.886746
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603,-2.2152921861,2.4679466842\H,-0.0991064848,-3.3125512746,2.1104516
248\H,-0.2109630724,-2.0859733211,3.3818349045\H,2.147849658,-2.948205
4755,3.1730679752\H,2.1855816046,-2.401938751,1.4849584621\H,2.0347122
193,-1.2171262717,-2.802956842\C,2.8078078482,0.3048657365,-1.432745012
5\H,1.6871077475,0.2880515359,0.3914309954\N,2.8688217398,0.2890435795
,-2.7781988259\H,3.7665388952,0.3114109234,-0.9157889714\H,1.723259068
5,0.2639979794,-4.4967903115\\Version=IA64-Linux-G03RevB.01\State=1-A\
HF=-741.5701462\MP2=-743.9176604\RMSE=8.822e-09\RMSE=6.278e-06\Dipole=
-1.4767659,-0.6050581,-0.3521628\PG=C01 [X(C13H19N3O1)]\@

7-2

1\I\GINC-LX64H61\FOpt\TMP2-FC\6-31G(d)\C13H19N3O1\UI271AC\20-May-2006\
O\#P OPT MP2/6-31G(D)\campb001, optimization\0,1\C,1.5542682443,-0
.3207457865,-1.287566492\C,1.5535586133,-0.316119084,0.1213622051\C,2.
766252704,-0.3652748167,-1.9675592909\H,0.6283573247,-0.2660725054,-1
.8494071965\N,0.3722654862,-0.2246284221,0.8514205405\C,2.812254842,-0
.3257961045,0.7477570413\C,-0.8846855426,-0.8897359899,0.4257496186\C,
0.4167779479,-0.0593339286,2.305721926\C,-1.6730091126,-1.003731457,1.
7531926227\C,-0.6876310888,-2.2746594247,-0.1893608982\C,-1.7067303409
,-0.0089931282,-0.5295223791\C,-1.0583449101,0.056393752,2.6606255339\
H,-1.500155277,-1.9986395183,2.1812532707\H,-2.7476542295,-0.894570623

2,1.5832181473\H,-1.2526031261,-0.1219582149,3.722309288\H,-1.43074056
58,1.053719104,2.4047006053\H,0.8712129498,-0.9273078144,2.8119003588\
H,1.0028169328,0.8288018049,2.5664728277\H,-0.1128780574,-2.9000222747,
0.5005175403\H,-0.1647841108,-2.2408134386,-1.1461673433\H,-1.67024227
93,-2.7210514578,-0.3557793383\N,-1.2917663107,1.2756683073,-0.6522514
766\O,-2.7076980374,-0.4603361675,-1.1004878736\C,-2.0377529926,2.2355
211614,-1.4513618251\H,-0.4627957588,1.543589565,-0.1345859735\C,-3.22
43596202,2.8171618004,-0.6919649196\H,-2.3852964404,1.7138581355,-2.34
70297613\H,-1.342493063,3.0206520847,-1.7624925859\H,-2.8908584289,3.3
326441446,0.2130040553\H,-3.7696580507,3.531963508,-1.3159963606\H,-3.
906076265,2.0119245167,-0.4102634744\C,3.9647313519,-0.3585342353,-0.0
3465773\H,2.9068934617,-0.3254040185,1.8285096526\N,3.977430403,-0.383
8729072,-1.3781289797\H,4.9409788305,-0.3715125304,0.4486584446\H,2.77
02374315,-0.374196052,-3.0566922335\\Version=IA64-Linux-G03RevB.01\Sta
te=1-A\HF=-741.5700654\MP2=-743.9170536\RMSD=6.848e-09\RMSF=2.453e-06\
Dipole=-0.3800887,0.6796577,1.4352816\PG=C01 [X(C13H19N3O1)]\@

7Ac-1

1\1\GINC-LX64161\FOpt\RMP2-FC\6-31G(d)\C15H22N3O2(1+)\UI271AC\20-May-2
006\0\#P MP2/6-31G(D) OPT\campacb015-mp2, mp2_optimization\1,1\C,-1
.9836688019,0.5690799121,-2.4011050175\C,-2.0428303794,0.626970266,-1.
0354310354\C,-0.854321103,0.5788726606,-0.244789685\C,0.3717071627,0.4
76105413,-0.9716194397\C,0.3713422591,0.4088715516,-2.3360535456\N,-0.
7908953369,0.4568766948,-3.0604701872\N,-0.9098034763,0.6317212883,1.0
865324183\C,0.2840694525,0.6472501153,1.9672386572\C,-0.3498749176,0.5
706409275,3.3737379531\C,-1.6535395178,-0.1882497504,3.1603028493\C,-2
.1588980882,0.385124428,1.8423096451\C,1.0841921757,1.9407062137,1.805
8751853\C,1.0491932796,-0.6697141857,1.7141312862\O,0.4454238661,-1.66
73714616,1.3063361552\C,-0.6804961496,0.3766549461,-4.532233144\O,0.42
90225533,0.3043044395,-5.0105844549\N,2.3785082376,-0.6540709499,1.977
9316302\C,3.1521926506,-1.8998717133,1.9730657234\C,2.9653394678,-2.70

09372227,3.2542950138\C,-1.9654207375,0.388847677,-5.3062578653\H,-0.5
499406417,1.5880498632,3.7309541449\H,0.3261544143,0.089970212,4.08724
65823\H,-2.3701155782,-0.0404605673,3.9722763972\H,-1.4625649123,-1.25
7515427,3.0461052013\H,-2.7038027909,1.3268992139,1.9838827938\H,-2.79
02069496,-0.3184994295,1.2943520859\H,0.3988766459,2.7899726142,1.8715
304187\H,1.6293667113,2.0090276096,0.8628766187\H,1.8019167352,2.04385
9708,2.6260118073\H,2.788498629,0.1577225331,2.4230351638\H,4.19957899
21,-1.6279552755,1.8190599504\H,2.81898171,-2.4755303828,1.107571621\H
,1.9152601603,-2.9774167751,3.3720735725\H,3.5595006233,-3.6180816066,
3.2171088576\H,3.2833844172,-2.1246985255,4.1273508945\H,1.3266958201,
0.3960900834,-0.4698239787\H,1.2752663609,0.3019291835,-2.9243091393\H
, -2.5163757649,1.3200918787,-5.1487173877\H,-1.7015753057,0.306591243,
-6.36028988\H,-2.6051547362,-0.4534680036,-5.0298176995\H,-2.880284342
,0.6189754164,-3.005067432\H,-3.0176180422,0.7451859448,-0.5781807101\
\Version=IA64-Linux-G03RevB.01\State=1-A\HF=-893.7420977\MP2=-896.5158
799\RMSD=3.853e-09\RMSF=2.060e-06\Dipole=-1.2147798,1.3817393,-0.42410
22\PG=C01 [X(C15H22N3O2)]\@

7Ae-2

1\1\GINC-LX64117\Fopt\RMP2-FC\6-31G(d)\C15H22N3O2(1+)\UI271AC\20-May-2
006\0\#P MP2/6-31G(D) OPT\campac016-mp2, mp2, optimization\1,1\C,-1
.9995166192,0.5214511624,-2.429556678\C,-2.0706070288,0.5849930907,-1.
0669404017\C,-0.8883583713,0.5600992995,-0.265004227\C,0.3454232341,0.
4749875446,-0.9794852353\C,0.3570856457,0.3978577989,-2.3456277968\N,-
0.798106507,0.4223142748,-3.0789648308\N,-0.9571217745,0.617141695,1.0
656478763\C,0.2250921674,0.6639521912,1.9597236428\C,-0.4239686527,0.5
846343598,3.3593204591\C,-1.7075890979,-0.2047574579,3.1355450781\C,-2
2.100162712,0.3495770461,1.808484273\C,1.0000351062,1.9727417479,1.79
73492613\C,1.023478302,-0.6367512287,1.7270527334\O,0.4545049495,-1.64
65572062,1.3000221134\C,-0.8253406435,0.3467914334,-4.5550751338\O,-1.
9048886684,0.3839717184,-5.1010178709\N,2.3444803862,-0.5932018582,2.0

304151061\C,3.1404308722,-1.8245604596,2.0592217157\C,2.926179909,-2.6
216598876,3.3386811647\C,0.4995240471,0.2279375315,-5.2484655758\H,-0.
6513578144,1.6002111367,3.7052348414\H,0.2535687563,0.1252053432,4.085
2878937\H,-2.4367497732,-0.0686406091,3.9382691372\H,-1.4916772979,-1.
2703263364,3.0302807679\H,-2.7759147787,1.2806345685,1.9376745287\H,-2
.8202382778,-0.3699847142,1.2574172249\H,0.2959183551,2.8076883803,1.8
452967864\H,1.5566017048,2.0433222618,0.8611799787\H,1.7045189996,2.09
92261435,2.6255973636\H,2.7200964669,0.2238087375,2.4960981375\H,4.187
3440253,-1.5345982988,1.9380258663\H,2.8460972784,-2.4114229261,1.1872
209242\H,1.878023431,-2.9168370017,3.4237538746\H,3.5378721981,-3.5279
015744,3.3271422346\H,3.2047389125,-2.0346172141,4.2180324317\H,1.2973
288933,0.4144579598,-0.4691542901\H,1.2858814986,0.3004143094,-2.89228
35899\H,1.0259165237,-0.681547054,-4.9464212797\H,0.2949295774,0.18282
31144,-6.3178026737\H,1.136500569,1.0922622212,-5.0424283159\H,-2.8711
655466,0.5499271789,-3.0731233935\H,-3.0510442783,0.6890344609,-0.6183
591288\\Version=IA64-Linux-G03RevB.01\State=1-A\HF=-893.7420295\MP2=-8
96.5157157\RMMSD=8.407e-09\RMSEF=2.801e-06\Dipole=0.589348,1.2737818,-0.
3493782\PG=C01 [X(C15H22N3O2)]\@

7Ac-3

I\1\GINC-LX64I66\FOpt\RMP2-FC\6-31G(d)\C15H22N3O2(1+)\UI271AC\20-May-2
0060\#P MP2/6-31G(D) OPT\campacb014-mp2, mp2, mp2 optimization\1,1\C,-0
.446034167,-0.3847482973,-2.1374492689\C,-0.3600908372,-0.4574493896,-
0.7760481943\C,0.911221574,-0.5041933457,-0.1248109808\C,2.0502105244,
-0.4949861579,-0.9868497635\C,1.9054890041,-0.4345640255,-2.3459553914
\N,0.6708845758,-0.3750933874,-2.9312809324\N,1.0503941391,-0.55702715
07,1.2001418232\C,-0.084934234,-0.6279094057,2.1534819304\C,0.63100241
06,-0.524269374,3.5179709157\C,1.8811078979,0.2963655399,3.2271804042\
C,2.3308854596,-0.2519824893,1.8787701251\C,-0.83325501,-1.956689417,2
.0375524621\C,-0.925664008,0.6508759876,1.9485964994\O,-0.3959438602,1
.6756823997,1.5050613116\C,0.4674668793,-0.2933895254,-4.3928911853\O,

-0.6713608999,-0.2698321469,-4.8024153703\N,-2.2236815286,0.5858448788
2.3235546623\C,-3.0880039711,1.766628832,2.23745333351\C,-3.608406686
2,1.9896179899,0.8240157785\C,1.7020036201,-0.2431853502,-5.2435403946
\H,0.9019675734,-1.5319076226,3.8558078824\H,-0.022189789,-0.079032244
9,4.2739109059\H,2.6528696396,0.1826894693,3.9927274874\H,1.6323887784
,1.3551989387,3.128506177\H,2.9269939817,-1.1671739518,1.9833506355\H,
2.8932819393,0.4807635903,1.2951271453\H,-1.4943510809,-2.0903468703,2
.8998795308\H,-0.1078748427,-2.7742429066,2.0602705326\H,-1.4292649387
,-2.051796874,1.1278041535\H,-2.6144624368,-0.2827551736,2.6638617237\
H,-2.500733964,2.6257474507,2.5693915221\H,-3.9072185239,1.619405818,2
.945449148\H,-4.1909670308,1.1294061511,0.4830437987\H,-4.2524168648,2
.8727035744,0.7915462609\H,-2.7700876877,2.151877905,0.1428710348\H,3.
0554284923,-0.569682671,-0.5903641926\H,2.7650786621,-0.4406536001,-3.
0034238934\H,2.3034281129,-1.148806326,-5.1263475609\H,1.370957147,-0.
1685572188,-6.2790130343\H,2.3183515237,0.6264113814,-5.0004353265\H,-
1.3881177845,-0.318470668,-2.6691746143\H,-1.2857938688,-0.424584297,-
0.2177233492\\Version=IA64-Linux-G03RevB.01\State=1-A\HF=-893.7416531\
MP2=-896.5156371\RMSE=6.115e-09\RMSE=4.184e-06\Dipole=1.2683425,-1.321
2631,-0.3615027\PG=C01 [X(C15H22N3O2)]\@

7Ac-4

NC-LX64I24\FOpt\RMF2-FC\6-31G(d)\C15H22N3O2(1+)\UJ271AC\20-May-2
006\0\#P MP2/6-31G(D) OPT\campacb013-mp2, mp2 optimization\1,\C,-2
.1490574331,0.3138737465,-2.1842626437\C,-2.1832328139,0.3571319264,-0
.819478274\C,-0.9795933417,0.436829527,-0.0534778829\C,0.2335466206,0.
4781956736,-0.8065193487\C,0.209999287,0.4156171765,-2.1732551507\N,-0
.9645289224,0.3360983506,-2.8710506406\N,-1.012302932,0.4721136537,1.2
791024544\C,0.1867893661,0.6204842535,2.1398418385\C,-0.4098355795,0.4
642990348,3.5558905443\C,-1.6170323976,-0.4434769643,3.3577607723\C,-2
.2106178316,0.0754497602,2.0542533556\C,0.8290577604,1.9988406394,1.97
46605886\C,1.0987949826,-0.5934118226,1.8603905421\O,0.6164694348,-1.6

481497057,1.4335525456\C,-1.0306373605,0.2721543412,-4.3464370143\O,-2
 .1253662775,0.2116636118,-4.8590289174\N,2.411099311,-0.4404674699,2.1
 527700577\C,3.3461466427,-1.5592022602,2.0033828048\C,3.7880586006,-1.
 7425418653,0.5579031017\C,0.2772164202,0.2862363731,-5.0809775697\H,-0
 .725050189,1.4495459597,3.9203328327\H,0.3308791591,0.0665166775,4.255
 50833538\H,-2.3315290298,-0.3883388245,4.182995053\H,-1.3020745202,-1.4
 815622361,3.2305777677\H,-2.8593747613,0.945810077,2.2134900766\H,-2.7
 64832323,-0.6930812286,1.5102000637\H,0.0517292669,2.7631304407,2.0565
 053272\H,1.3459879776,2.134925905,1.0227210175\H,1.5432136408,2.179516
 0419,2.7844926188\H,2.7586860696,0.4460939875,2.4935678115\H,2.8423386
 091,-2.4580511607,2.3660825835\H,4.1978661958,-1.3579978231,2.65766310
 67\H,4.2867762168,-0.8430283308,0.1866079151\H,4.4875793912,-2.5791710
 41,0.4779192237\H,2.919737563,-1.9606530819,-0.0678385141\H,1.20260364
 82,0.5043385059,-0.3268415768\H,1.1263695795,0.4134175117,-2.748881479
 \H,0.044538667,0.2309716078,-6.1440843289\H,0.8351087218,1.2056976369,
 -4.8844581035\H,0.8969815546,-0.5713733664,-4.8055096603\H,-3.03920103
 07,0.2653242587,-2.8007555976\H,-3.1546493954,0.3627682564,-0.34029060
 09\\Version=IA64-Linux-G03RevB.01\State=I-A\HF=-893.741517\MP2=-896.51
 53784\RMSD=8.369e-09\RMSE=6.095e-06\Dipole=0.4447136,1.3274399,-0.1989
 616\PG=C01 [X(C15H22N3O2)]\@

8-1

1\G\INC-LX64I153\FOpt\RMF2-FC\6-31G(d)\C20H23N3O2\UI271AC\24-May-2006
 \0\#P MP2/6-31G(D) OPT\camc004-mp2 , mp2 optimization\0,1\N,-2.866
 4619612,0.8009200034,-0.5616472388\C,-3.0081432423,0.6996672292,0.7727
 158193\C,-1.9726600057,0.8379895399,1.691654786\C,-0.6643231865,1.0914
 770098,1.2324869151\C,-0.4989577982,1.1754621763,-0.1659490958\C,-1.61
 06927274,1.0377191086,-0.9904230623\N,0.390294276,1.1866032957,2.12343
 61191\C,1.7698376671,1.5096807884,1.7245376127\C,2.5087404543,1.363349
 9373,3.0699853192\C,1.4971750726,1.8791219744,4.0930719157\C,0.1554027
 489,1.3717712151,3.560638333\C,1.9295311238,2.9227802154,1.1648978798\

C,2,-2.29794718,0.4603280343,0.7296577086\O,3.0708514153,0.7564995115,-0.1872280462\N,1.9064440836,-0.8176053285,1.0064649301\C,2,1017831861,-1.8700701291,0.0075916886\C,1.0501260569,-1.7988726894,-1.068015931\C,-0.2397286408,-2.2980231188,-0.8169004317\C,-1.2410318597,-2.0986282873,-1.7565587934\C,-0.9466271382,-1.4436765686,-2.9561019001\C,0.325601751,-0.963289366,-3.2479396334\C,1.3187251596,-1.1427090845,-2.2790122464\O,-2.0323030279,-1.3112176992,-3.7802169279\C,-3.1983968354,-1.6261403817,-2.9570364373\C,-2.6914209866,-2.5035411688,-1.800673075\H,-2.1893999396,0.7327047668,2.74970173\H,3.4520668855,1.9175517746,3.0674188219\H,2.7325055163,0.3072849656,3.2523486124\H,1.5038679611,2.9722874017,4.1221833305\H,1.7017586853,1.5212703945,5.1063405143\H,-0.6564349464,2.0888841462,3.7362734996\H,-0.134596043,0.4215763599,4.0320784843\H,1.2666274098,3.0976276383,0.3161870627\H,2.9582290943,3.0685271121,0.8292369064\H,1.6910906821,3.6566252384,1.9399032598\H,1.0803665626,-0.8889541094,1.5934469609\H,3.10222671,-1.7360299887,-0.4100059017\H,2.0733994613,-2.8329348537,0.52936139\H,-0.4543484177,-2.814792472,0.1200451925\H,-2.7978903936,-3.5732525153,-2.0196161863\H,-3.2283859407,-2.2841503112,-0.8728707013\H,-3.9243135075,-2.1143668614,-3.6097663164\H,-3.6022418289,-0.6853247989,-2.5719361756\H,0.527576996,-0.454587887,-4.1867397705\H,2.3164655177,-0.7448967761,-2.4511120132\H,0.4692989865,1.3393621633,-0.6246523478\H,-1.4867718396,1.1245225142,-2.0678439669\H,-4.0187473776,0.5030071978,1.1300365049\Version=IA64L-G03RevC.02\State=1-A\HF=-1083.8280581\MP2=-1087.2524209\RMSD=8.198e-09\RMSF=8.131e-06\Dipole=-0.0715679,-0.2983802,2.1947922\PG=C01 [X(C20H23N3O2)]\|

8-2

NC-LX64H157FOpt\RMp2-FC\6-31G(d)\C20H23N3O2\UJ271AC\24-May-2006
\0\#P MP2/6-31G(D) OPT\campc006-mp2 , mp2 optimization\0,1\N,-2.688
6155811,1.1565902827,-0.6816507749\C,-2.5835272952,1.0460328702,0.6561
561392\C,-1.4081470506,1.2275537619,1.377567411\C,-0.2134990411,1.537

0935735,0.6959723894\C,-0.3070625968,1.6377667092,-0.708108975\C,-1.54
05219686,1.4513611706,-1.3210347668\N,0.974266814,1.6919615144,1.37877
17899\C,2.2808754986,1.8880261026,0.7309603296\C,3.2420759569,1.713791
2886,1.9262250827\C,2.4491271776,2.2631906451,3.119046098\C,1.0290816
105,1.7716188735,2.8394439097\C,2.4425291162,3.2735594747,0.1069172295
\C,2.5304021487,0.778687393,-0.3126335635\O,3.0773682267,1.0053800382,
-1.3965587548\N,2.1413447587,-0.4574989538,0.1057675847\C,2.0442826555
,-1.6040303941,-0.8003135312\C,0.6274976687,-2.1094676548,-0.790263143
1\C,-0.3060527963,-1.6252222449,-1.7216014181\C,-1.6440979681,-1.96844
02049,-1.5822804291\C,-2.0473197781,-2.7883859796,-0.5233400057\C,-1.1
45663944,-3.3087012278,0.3991210082\C,0.1979108021,-2.9495885213,0.249
639452\O,-3.3951464156,-3.0314809707,-0.5128417743\C,-3.9742154792,-2.
058238347,-1.4346186107\C,-2.861866583,-1.6830620799,-2.4220493314\H,-
1.4274106472,1.1061270247,2.4558005503\H,4.1889450817,2.2336187285,1.7
521913764\H,3.4606863362,0.6514173147,2.0764563577\H,2.4743404642,3.35
67818143,3.1192005634\H,2.8314409191,1.9143164409,4.0757044145\H,0.266
065376,2.4607367379,3.2212694287\H,0.8485965359,0.7877092934,3.3005902
408\H,3.3958643411,3.3276826779,-0.4228619747\H,2.417308565,4.03341931
6,0.8931244155\H,1.6451095527,3.4952461205,-0.6036595257\H,1.514775291
3,-0.4746704451,0.9045075278\H,2.3501013786,-1.2513868355,-1.789569814
1\H,2.7468628045,-2.3854833502,-0.4857418692\H,0.0246372096,-0.9815429
966,-2.5355734414\H,-2.9461327841,-0.6383742586,-2.7302238558\H,-2.877
5941043,-2.3203022409,-3.3150581668\H,-4.2753305115,-1.1787187871,-0.8
562493057\H,-4.8484877327,-2.5293310736,-1.8869879289\H,-1.4814654567,
-3.9562924274,1.2042684012\H,0.9318536393,-3.3363616627,0.9567021563\H
0,0.5579491482,1.8467477784,-1.3268007473\H,-1.6126898339,1.5494123401,
-2.4042541547\H,-3.5030208039,0.7994147963,1.1861666657\Version=IA64L
-G03RevC.02\State=1-A\HF=-1083.8271193\MP2=-1087.2489942\RMSE=5.067e-0
9\RMSE=2.848e-06\Dipole=0.4662778,0.3246013,1.4026975\PG=C01 [X(C20H23
N3O2)]\@

8Ac-1

1\1\GINC-LX641151\FOpt\RMF2-FC\6-31G(d)\C22H26N3O3(1+)\UI271AC\29-Apr-2006\0\#P MP2\6-31G(D) OPT\campcac005-mp2\1,1\N,-2.0585282911,1.264123961,-0.266743875\C,-2.057788222,1.2249849941,1.0965141574\C,-0.8873315835,1.1801499185,1.8101123293\C,0.3761905674,1.1465072731,1.1476054179\C,0.3305845166,1.1451689289,-0.2774391164\C,-0.8675836638,1.21113338089,-0.934498812\N,1.5260161153,1.1317916152,1.8418021362\C,2.8923145607,1.0443703017,1.2374222492\C,3.7716413455,0.825034086,2.4841654475\C,3.0371940168,1.5718189182,3.5963442755\C,1.5706816047,1.2661305251,3.3137607243\C,3.2740535236,2.3399411097,0.5276793241\C,2.9321180396,-0.1550342737,0.2657285170,3.1877482145,-0.0085144411,-0.9327836459\C,-3.2912217581,1.3447039594,-1.0830671755\O,-3.1633913879,1.5640533041,-2.2671397308\N,2.6442584285,-1.3631209187,0.823375669\C,2.218232556,-2.4725794731,-0.0363756211\C,0.7793483984,-2.2766839541,-0.4470408013\C,0.4314527525,-1.9923737713,-1.7765944331\C,-0.9025131025,-1.7407458441,-2.0871000366\C,-1.8570521568,-1.7192356448,-1.0676996858\C,-1.5519059291,-2.0219210126,0.2558519258\C,-0.2141779985,-2.2929255872,0.5477412545\O,-3.1122195446,-1.376045513,-1.5060987707\C,-3.0747651426,-1.511520473,-2.9666060949\C,-1.5977981338,-1.3759626593,-3.3756807976\C,-4.5876824947,1.1726645556,-0.3541438887\H,-0.9605791258,1.1485895548,2.8906516114\H,4.7850537194,1.1962401963,2.308854538\H,3.8530402339,-0.238753424,2.7274904959\H,3.2174818753,2.6480337245,3.5304486368\H,3.3368737264,1.2440200188,4.5950510468\H,0.9013230348,2.0675283407,3.6405810411\H,1.2491131772,0.3286247173,3.7882908253\H,3.3411611562,3.1539057603,1.2540392359\H,2.5546688801,2.6220560383,-0.2416194318\H,4.244130761,2.2092208026,0.0431826269\H,2.2714324754,-1.3623303658,1.7661682419\H,2.8812286266,-2.4899161219,-0.9033906174\H,2.360823641,-3.4021786348,0.5234963859\H,1.1993508783,-1.9831177137,-2.5489339806\H,-1.3613739033,-0.3529158215,-3.6916956462\H,-1.3468433952,-2.0438257076,-4.204873035\H,-3.7259462713,-0.7383368812,-3.37454446638\H,-3.471469939,-2.5019044621,-3.2095336108\H,-2.3276881719,-2.0699254481,1.0158440008\H,0.0

538765355,-2.5698668543,1.5679910063\H,1.2272960499,1.0836729683,-0.87
98717337\H,-0.9405280711,1.2652196377,-2.0133850788\H,-5.3787796007,1.
1888622902,-1.1035619201\H,-4.607824278,0.2154647335,0.1705780551\H,-4
.7594052309,1.9877784482,0.3548332486\H,-3.0196889879,1.2453906841,1.5
929734337\Version=IA64L-G03RevC.02\State=1-A\HF=-1235.9985948\MP2=-12
39.8592691\RMSD=9.540e-09\RMSF=5.908e-06\Dipole=-0.8400095,0.931153,2.
3548282\PG=C01 [X(C22H26N3O3)]\@

8Ac-2

1\GINC-LX64I159\FOpt\RMP2-FC\6-31G(d)\C22H26N3O3(1+)\UI271AC\28-Apr-
2006\0\#P MP2/6-31G(D) OPT\campcac010-mp2\1,1\N,-0.8839232598,-0.95
69879165,-2.3400221338\C,-0.9053742317,-0.9816163745,-0.9729501997\C,0
.2502741298,-1.001307001,-0.2388447226\C,1.5249224125,-1.0115260258,-0
.8799989747\C,1.5017731757,-0.9548940501,-2.306934558\C,0.3184043024,-
0.9260911767,-2.9913064372\N,2.6794611888,-1.0777467953,-0.2105795343\
C,2.8079536026,-0.9926002412,1.269309893\C,4.3004191486,-0.6428444291,
1.4381148008\C,4.9778477379,-1.3064775144,0.2420601038\C,3.9927592764,
-1.0422798901,-0.8881609066\C,2.4687976685,-2.3428841941,1.9011238257\
C,1.9763840835,0.216378959,1.7363216346\O,1.9989248994,1.2600670574,1.
0781039508\C,-2.1125476427,-0.9558640644,-3.1677793349\O,-1.9837603948
,0.7723013917,-4.3578350676\N,1.2611052638,0.0778501825,2.878174883\C
,0.3412463961,1.1454065282,3.2898486307\C,-0.8575432676,1.1992580927,2
.375135042\C,-0.9038360243,2.1318364504,1.3251441118\C,-1.9989839907,2
.1300848809,0.470142483\C,-3.0150480342,1.1867843527,0.6412536452\C,-3
.0004901023,0.2452457274,1.6668311533\C,-1.8972711629,0.2660744464,2.5
289176843\O,-4.0041785671,1.285788946,-0.3102414563\C,-3.8167242836,2.
5996730884,-0.929076765\C,-2.3276814205,2.9338776551,-0.7629418286\C,-
3.401521878,-1.2025666378,-2.4476837382\H,0.1430717704,-0.9894491986,0
.8377659787\H,4.6820324788,-0.9834806225,2.4048384477\H,4.4190042932,0
.4435924013,1.3783538866\H,5.103017873,-2.3816647335,0.3994577945\H,5.
9624999314,-0.8827538574,0.0291649165\H,4.0338452943,-1.8003130323,-1.

6756473186\H,4.1429982402,-0.0501630136,-1.3325487934\H,2.6537240307,-
2.322222785,2.9799848262\H,3.1127870764,-3.117646282,1.4776202292\H,1
.4312584433,-2.6380852389,1.7211538597\H,1.2304928813,-0.8088213532,3.
3639429346\H,0.0471648332,0.9411510463,4.3234723412\H,0.8870724257,2.0
925027729,3.2704936912\H,-0.0901214001,2.8414114483,1.1965155241\H,-2.
1607718155,4.0085127149,-0.6482602522\H,-1.7369247953,2.5922308926,-1.
6228155792\H,-4.4468895218,3.3117893953,-0.3864413316\H,-4.1592600255,
2.5199994707,-1.9616487076\H,-3.828199162,-0.4448071622,1.8098510951\H
,-1.8712894993,-0.4320517872,3.3655357848\H,2.4166528519,-0.9193167735
,-2.8851955344\H,0.2575689848,-0.8778615632,-4.072525527\H,-4.17946183
65,-1.2766308709,-3.2077669322\H,-3.3610542478,-2.136271413,-1.8800682
584\H,-3.6442033537,-0.3820514855,-1.7631614591\H,-1.8719649731,-0.959
8261568,-0.486456793\Version=IA64L-G03RevC.02\State=1-A\HF=-1236.0074
156\MP2=-1239.8572638\RMSD=5.586e-09\RMSE=2.409e-06\Dipole=1.2605567,-
1.6314731,0.0270724\PG=C01 [X(C22H26N3O3)]\@

9

1\INGINC-LX64144\FOpt\RMPP2-FC\6-3IG(d)\C15H21N3O1S2\UI271AC\22-Apr-200
6\#\#P MP2/6-3IG(D) OPT MAXDISK=1GB\yama9mp2\0,1\C,0.5000345676,-0.
4364957984,-1.0330343327\N,0.4999852397,-0.436595899,0.3678368277\C,1.
8402032703,-0.4362948915,0.9842626564\C,2.6881326402,0.442028496,0.051
5031562\S,2.0325204961,0.1879182878,-1.6231932853\C,-0.6014131879,-0.1
210103625,1.1749174429\O,-0.5076631968,-0.1576581912,2.4032385554\C,2.
3836355474,-1.8582299003,1.2580489241\C,1.3348547215,-2.6427825735,2.0
525814802\S,-0.6706974241,-1.0019282568,-2.0187618183\C,-1.8607577052,
0.302480318,0.5074479693\C,-1.9162327582,1.4277105812,-0.335726629\C,-
3.1470055829,1.6942654761,-0.9418768662\C,-4.2465315547,0.8877894142,-
0.6402381167\N,-4.218228281,-0.1394338739,0.2252896647\C,-3.0292712554
,-0.403740094,0.792056717\N,-0.7339102284,2.1653714068,-0.5644474571\C
,-0.706957282,2.9520209769,-1.7898945444\C,-0.2894376311,2.9465208954,

0.5934345975\C,2.7132663784,-2.6365802656,-0.0178984914\C,3.6466377466
,-1.7227164143,2.1168875819\H,-3.2716218981,2.5313656027,-1.6215757804
\H,0.319245293,3.2934410584,-1.9495858751\H,-1.3640373334,3.8363430087,
-1.7573946351\H,-0.9928907603,2.3160502268,-2.6304831277\H,-0.91897787
64,3.8364735608,0.7542986365\H,0.7397994886,3.2770549187,0.4218654904\
H,-0.3185466189,2.3380255329,1.4988409266\H,1.7273398638,0.0580144998,
1.9556593484\H,4.4542841294,-1.203442498,1.5909222189\H,3.43441468,-1.
1807828784,3.0452290862\H,4.0179910121,-2.7166996453,2.3857966904\H,0.
4286346696,-2.7965944685,1.4596332763\H,1.7383870578,-3.6265118427,2.3
150469708\H,1.0556993158,-2.1213125412,2.971468148\H,3.0656901267,-3.6
366360633,0.2579562381\H,1.8324765184,-2.7582337029,-0.654707603\H,3.5
005832381,-2.1581341336,-0.607633218\H,3.744002392,0.1647222473,0.0730
535828\H,2.593694909,1.4957313441,0.3276253737\H,-2.9933711667,-1.2480
712036,1.4788512738\H,-5.2105352174,1.0894354272,-1.1048865279\Versio
n=IA64-Linux-G03RevB.01\State=I-A\HF=-1613.4518699\MP2=-1616.3341132R
MSD=6.451e-09\RMSEF=1.762e-06\Dipole=1.5543423,1.3375194,0.0697162\PG=C
01 [X(C15H21N3O1S2)]\@

9Ac-1

I\1\GINC-LX64I51\FOpt\RMF2-FC\6-31G(d)\C17H24N3O2S2(1+)\UI271AC\18-Apr
-2006\0\#P MP2/6-31G(D) MAXDISK=2GB SCF=TIGHT OPT=yamaac006-mp2, opt
imization calculation\1,1\S,0,0,0\C,-1.616844347,-0.644613086,-0.0
21542392\N,-1.617243392,-1.9018924579,-0.6525194816\C,-0.4887846891,-2
.1283133116,-1.5882672976\C,0.6912684644,-1.4313439003,-0.8923031035\C
,-2.452440152,-2.9499895171,-0.2996703367\O,-2.5367344754,-3.990459567
9,-0.9471379504\C,-0.7764082443,-1.6733772264,-3.037434242\C,-0.911028
2642,-0.1552148616,-3.1801875554\S,-2.9308509464,0.1253671188,0.578417
776\C,-3.1402190704,-2.859791246,1.035615645\C,-2.2901359274,-2.848209
5343,2.1128210215\N,-2.725166513,-3.0541799154,3.3901540329\C,-4.04365
35371,-3.3425333972,3.6049902335\C,-4.9341564774,-3.4056966947,2.56853
51266\C,-4.5374782036,-3.1293153152,1.2238118561\C,-1.71557665,-2.9833

844393,4.4705201379\O,-0.5690171607,-2.7610515959,4.153128518\N,-5.434
1335568,-3.1049254028,0.2336422262\C,-5.1568516787,-2.53308206,-1.0893
690803\C,-2.2136034541,-3.1914858812,5.8693266071\C,-6.8031855548,-3.5
909682005,0.4468301191\C,0.3776802894,-2.1734267259,-3.9162297575\C,-2
.0729673696,-2.3272865243,-3.5236288539\H,-1.2229040551,-2.6766775093,
2.0149562293\H,-1.3550830063,-3.0845359373,6.5318961412\H,-2.968291283
3,-2.4470942275,6.1372135904\H,-2.6390311294,-4.1908244208,5.995590707
9\H,-4.359999405,-3.5105639478,4.6274621773\H,-5.9675624006,-3.612550
8484,2.8169700409\H,-6.7933751812,-4.513603601,1.0284810391\H,-7.23521
808,-3.8109018675,-0.5286985296\H,-7.4165053151,-2.8348699117,0.947868
1351\H,-4.4134657848,-1.7413950279,-0.996081803\H,-6.0819280779,-2.082
857623,-1.4534465786\H,-4.8155756931,-3.3035565221,-1.7853891081\H,-0.
3229893107,-3.2120699581,-1.6072217563\H,1.3341059267,-1.709728854,-3.
6565374694\H,0.4890558544,-3.2607509267,-3.8434026561\H,0.1721892377,-
1.9275404133,-4.9622059553\H,-2.9333011183,-1.9584680465,-2.9575449498
\H,-2.2335339047,-2.0730932628,-4.5758310649\H,-2.036820948,-3.4156996
22,-3.4306871641\H,-1.1304922229,0.0826583544,-4.2260498771\H,-1.73132
23941,0.2412605065,-2.573918832\H,0.0061875547,0.3756187976,-2.9100247
035\H,1.436065357,-1.0763422494,-1.6063477374\H,1.1810281905,-2.101153
1357,-0.1800708365\Version=IA64-Linux-G03RevB.01\State=I-A\HF=-1765.6
175977\MP2=-1768.9275437\RMSE=5.595e-09\RMSE=1.162e-05\Dipole=-0.31897
05,2.282412,2.7705414\PG=C01 [X(C17H24N3O2S2)]\@

9Ac-2

1\GINC-LX64I25\FOPt\RMF2-FC\6-31G(d)\C17H24N3O2S2(1+)\UI271AC\20-Apr
-2006\0\#P MP2/6-31G(D) MAXDISK=2GB SCF=TIGHT OPT\yamaac005mp2\1,1\
S,-0.8037331371,-0.8606526747,-2.9071805718\C,-0.8043605707,-0.8615914
638,-1.1611244335\N,0.5207955942,-0.8621578353,-0.6924350729\C,1.51102
89038,-1.4330510854,-1.6371362569\C,1.0146196553,-0.9491496505,-3.0097
344181\C,0.9495277159,-0.200714062,0.4503252331\O,2.0819405257,-0.3265

408838,0.908910849\C,1.6984004339,-2.9607926403,-1.4947688562\C,0.4674
139646,-3.7635981565,-1.9233382056\S,-2.1528810326,-0.8838685333,-0.23
61002509\C,0.0318286953,0.840611485,1.0268308284\C,-0.2853027681,1.873
3831692,0.1769038358\N,-0.8545935272,3.0300367255,0.6175546392\C,-1.04
69415911,3.-2100225808,1.9606142632\C,-0.7191283688,2.2357879097,2.8599
090944\C,-0.2196373579,0.965668418,2.4340314787\C,-1.2805554377,4.1191
415912,-0.2916108747\O,-1.714367478,5.1306810507,0.2102072323\N,-0.029
0324457,-0.0290524415,3.3048630246\C,-0.0941965707,0.2142451616,4.7515
783286\C,-1.144311761,3.853419561,-1.7613494842\C,0.1553400741,-1.4272
458672,2.8999109531\C,2.9016323562,-3.3610658221,-2.3585370624\C,2.017
1296914,-3.2940576691,-0.0344878448\H,-0.0779049118,1.7995010616,-0.88
40468184\H,-1.5638160051,4.7150270344,-2.2804272817\H,-0.0936016954,3.
7470431457,-2.0466897919\H,-1.6867223587,2.9511042762,-2.0571912345\H,
-1.4817552314,4.1617753755,2.2437064855\H,-0.9254506087,2.4361456034,3
.9038709915\H,-0.3358796124,-1.5989673501,1.9417323131\H,-0.3366750776
,2.0532965904,3.646535955\H,1.2165754446,-1.6811967825,2.8387184428\H
,0.4193688339,1.1424674825,5.0046129519\H,0.4216341692,-0.605080724,5.
2510359191\H,-1.1319549173,0.2498656522,5.0988828566\H,2.4691339094,-0
.9569253949,-1.3975210173\H,2.7272129098,-3.1917218654,-3.4254470135\H
,3.802015057,-2.8114396019,-2.0632732012\H,3.1039978721,-4.4283179843,
-2.2293467646\H,1.1632130429,-3.0729987445,0.612742636\H,2.2330920394,
-4.3631551883,0.0537834561\H,2.8828961848,-2.7339293135,0.3281664757\H
,0.6736995397,-4.8290506439,-1.7795706351\H,-0.4125366318,-3.516059496
4,-1.3217714749\H,0.2172444044,-3.619569625,-2.97833287859\H,1.28915726
27,-1.6388323078,-3.8095133194\H,1.417188989,0.0389640742,-3.249090242
6\Version=IA64-Linux-G03RevB.01\State=1-A\HF=-1765.6165806\MP2=-1768.
9273388\RMSD=5.669e-09\RMSF=2.179e-06\Dipole=0.3836941,1.2526364,1.477
8105\PG=C01 [X(C17H24N3O2S2)]\@

10-1

1\1\GINC-LX64I47\FOpt\RMP2-FC\6-31G(d)\C25H24N2\UI271AB\09-May-2006\0\

\#P MP2(FC)/6-31G(D) SCF=(TIGHT,DIRECT) OPT\spiv01mp_003 mp2/6-31G(d)
) opt from rhf/3-21G structure\0,1\C,-1.2460145142,0.3655902715,-0.16
51564585\C,-1.2459888683,0.365640234,1.2506453794\C,0.0004679689,0.365
6260014,-0.9656239417\C,-2.4749764585,0.3128407262,-0.8354104902\N,-0.
032697546,0.4461101716,1.9506174113\C,-2.4982972861,0.2350408376,1.873
3013338\C,0.7701543696,1.6582145505,1.692715652\C,-0.0617095711,0.0915
333392,3.3708351515\C,2.2533638514,1.3535792195,1.5438265861\H,0.40150
59855,2.1338089463,0.782632319\H,0.6047022263,2.3772353525,2.5123890187
\H,2.8163309295,2.2834000535,1.4087784254\H,2.6496435681,0.8467476508,
2.4287161645\H,2.4163376241,0.7145459886,0.6739267889\C,-0.3348589238,
-1.3882918262,3.5966589017\H,0.9312780175,0.3280943218,3.7642361247\H,
-0.7706458735,0.7247502629,3.9330534694\H,-0.3308457806,-1.6099615857,
4.6691200943\H,-1.2992826635,-1.6954997087,3.1877546461\H,0.4364482872
, -1.9831048961,3.1059605616\C,-3.6561567619,0.1566087506,1.1015262538\
H,-2.5919448986,0.225921442,2.9540192524\N,-3.6762778047,0.2033396562,
-0.242045955\H,-4.6261028176,0.0629587323,1.5886636378\H,-2.4786272361
0,3257988406,-1.9263190733\C,0.3170291555,1.5004488678,-1.7763399144\
C,0.8318145273,-0.7596420135,-0.9778068237\C,1.5251289807,1.5009069596
, -2.5500914563\C,-0.4657416468,2.6880999365,-1.7536075623\C,1.84231660
72,2.6303293415,-3.3467671329\C,2.331826091,0.3375184733,-2.5613564859
\C,1.0491487494,3.7584076529,-3.3202182017\H,2.7491059349,2.6075848873
, -3.9497284262\C,-0.118231424,3.780033816,-2.5244126346\H,1.3069113466
, 4.622121794,-3.9287875916\H,-0.7358269584,4.6751029297,-2.4975098712\
H,-1.3693473521,2.7187120292,-1.150505291\C,2.005524874,-0.7471464727,
-1.7775617363\H,3.232254593,0.3215978404,-3.1743167266\H,2.6195387389,
-1.6450137101,-1.8119942762\C,0.5675719293,-1.966483562,-0.1640502225\
C,1.6195476823,-2.5373369826,0.5731140602\C,-0.6788038387,-2.613865599
4,-0.1737957028\C,1.4297813908,-3.7193045572,1.289686902\H,2.585370530
5,-2.0362320721,0.5979993614\C,0.1826826354,-4.3498069398,1.2830504183
\H,2.2553853935,-4.1479089178,1.8541431612\C,-0.8689223461,-3.79042654
14,0.5529183789\H,0.0323254088,-5.2713902396,1.8406317146\H,-1.8381689

382,-4.283808316,0.5293900239\H,-1.4934616872,-2.2102973202,-0.7687352
248\Version=IA64L-G03RevC.02\State=1-A\HF=-1069.570633\MP2=-1073.1186
586\RMSE=4.449e-09\RMSEF=1.743e-06\Dipole=1.0786344,0.2152923,0.6921045
\PG=C01 [X(C25H24N2)]\@

10-2

1\1\GINC-LX64I23\FOpt\RMP2-FC\6-31G(d)\C25H24N2\UI271AB\09-May-2006\0\
\#P MP2(FC)/6-31G(D) SCF=(TIGHT,DIRECT) OPT\spiv0Imp2_009 mp2/6-31G(d
) opt from thf/3-21G structure\0,1\C,-0.7137250026,1.4274856014,-3.63
39715154\C,-0.7134579173,1.4272006054,-2.2380884997\C,0.4983726263,1.4
264424078,-1.528321151\C,1.7044726562,1.4442169556,-2.2493686513\C,1.7
013742246,1.4558834979,-3.6444690102\C,0.4904253043,1.4474490954,-4.34
21925191\C,0.5384036369,1.5104696314,-0.05192224883\C,-0.2074424126,0.6
694282735,0.7796993951\C,-0.1311023679,0.8122368748,2.2020757133\C,0.7
506098223,1.7933577622,2.7661067478\C,1.4721326789,2.6464718933,1.8965
609523\C,1.3879264325,2.4874743151,0.531217808\C,0.8273923201,1.934295
4962,4.1750292234\C,0.1346282152,1.081334645,5.0084745868\C,-0.6941139
093,0.0781405588,4.4577937373\C,-0.8078843422,-0.0698038888,3.08959566
57\C,-1.1195501157,-0.3453739113,0.2046103653\C,-0.6754382923,-1.47050
35861,-0.5331773552\C,-1.6813451753,-2.2785427424,-1.0921872886\C,-3.0
247937931,-1.9701182919,-0.8919816327\N,-3.4607608474,-0.9247702786,-0
.1673140835\C,-2.4990413914,-0.1510828926,0.3633887273\N,0.6946546384,
-1.7166586409,-0.7161382512\C,1.0635279462,-2.6609293003,-1.7742435026
\C,0.7506068619,-2.1165278039,-3.1613977888\C,1.4762523696,-1.89108283
99,0.5202930232\C,1.1513343475,-3.1762999287,1.2772234474\H,2.53407856
17,-1.8666264733,0.2344590261\H,1.3042599468,-1.0291786416,1.165357545
8\H,1.7452011346,-3.2368858722,2.1951025157\H,0.0933191497,-3.19551627
55,1.5546804562\H,1.3659927006,-4.0650527973,0.6767151397\H,2.14602179
42,-2.8021259287,-1.6861568744\H,0.6130252853,-3.6570384582,-1.6304858
906\H,1.0690432817,-2.8347485952,-3.9244500873\H,-0.3157855607,-1.9261
733239,-3.2962983696\H,1.2776437024,-1.1742758257,-3.3144965208\H,-1.4

32904462,-3.1654438051,-1.6651401468\H,-3.7970090572,-2.6038894013,-1.
3265701508\H,-2.8411120392,0.711611644,0.936924645\H,1.4793116031,2.70
21406059,4.5894625649\H,0.2077023704,1.1928012501,6.087856793\H,-1.226
5957115,-0.603245063,5.1177014601\H,-1.4499641277,-0.8462694399,2.6829
408423\H,2.1208754601,3.4114655532,2.3215433406\H,1.930862509,3.162412
7821,-0.1275089488\H,2.6482169915,1.4290184564,-1.7072029197\H,2.64419
36288,1.4716499205,-4.1873806793\H,0.4854224827,1.4578112129,-5.429709
8825\H,-1.6604206066,1.4360238508,-4.1698185373\H,-1.6560184517,1.4518
024954,-1.6978469182\Version=IA64L-G03RevC.02\State=1-A\HF=-1069.5710
495\MP2=-1073.1173577\RMSE=5.240e-09\RMSE=2.874e-06\Dipole=1.2787237,-
0.3921616,-0.0540345\PG=C01 [X(C25H24N2)]\@

10-3

I\1\GINC-LX64I43\FOpt\RMP2-FC\6-31G(d)\C25H24N2\UI271AB\14-May-2006\0\
\#P MP2(FC)/6-31G(D) SCF=(TIGHT,DIRECT) OPT\spiv0Imp2_001 mp2/6-31G(d
) opt from thf/3-21G structure\0,1\C,-1.2361424906,0.1401798214,-0.24
19108912\C,-1.1873279289,0.1626377669,1.1729033824\C,-0.0162634597,0.2
005504978,-1.0777693476\C,-2.4755804924,-0.0563042078,-0.8644690909\N,
0.036442321,0.3747746122,1.8289822698\C,-2.3895654159,-0.1068737969,1.
8451468377\C,0.641110135,1.692702463,1.5761695892\C,0.100687411,-0.0955
417065,3.2140405328\C,-0.0397318433,2.837748582,2.3221542747\H,1.70276
08924,1.6374141249,1.8352206201\H,0.5961504651,1.875140443,0.501228683
7\H,0.4204365389,3.7930840914,2.0495726104\H,-1.1016446873,2.882977865
4,2.0623030606\H,0.0433634341,2.7242408641,3.4069636383\C,1.523215682,
-0.0989179508,3.7567824506\H,-0.5431448831,0.4882700959,3.8939472285\H
,-0.2791161444,-1.1226768433,3.2073956229\H,1.5395304975,-0.6152950898
4,4.7214616298\H,2.1855172901,-0.6277807439,3.0688994931\H,1.9091145927
0,9.104869742,3.9185411094\C,-3.5597559979,-0.3234569622,1.11871507\H,
-2.4346632904,-0.1220210295,2.9292811915\N,-3.634679839,-0.2871773349,
-0.2231289265\H,-4.4941128188,-0.5241451699,1.6417946344\H,-2.52078975
29,-0.0692789725,-1.9543442718\C,0.1743445876,1.2769268123,-1.998333338

59\C,0.9253270531,-0.8310973476,-0.996690365\C,1.3589929569,1.30868600
52,-2.8076108404\C,-0.7149384855,2.3850752235,-2.0622993467\C,1.546358
5646,2.3752411667,-3.7233808306\C,2.2814698431,0.2380863514,-2.7175144
307\C,0.6493800267,3.4213882981,-3.7822005114\H,2.4359706314,2.3756925
21,-4.3518513038\C,-0.4921235275,3.4197680707,-2.9490017567\H,0.808035
3255,4.2380059136,-4.4827879961\H,-1.1881153247,4.2549240412,-2.986724
4519\H,-1.5962605622,2.3970612182,-1.4263022567\C,2.0827659945,-0.7841
142426,-1.8148961232\H,3.1697025695,0.249502089,-3.3480890969\H,2.7898
548494,-1.6101271629,-1.7632971636\C,0.7696621459,-1.9627678847,-0.057
2811404\C,1.8302856652,-2.2948029453,0.800937668\C,-0.3994813882,-2.73
89195814,-0.0217580736\C,1.7145659935,-3.3573169892,1.6977179929\H,2.7
395039421,-1.6964959447,0.7761294473\C,0.5372702484,-4.1094177673,1.74
40200685\H,2.5422914711,-3.5979720385,2.3617535629\C,-0.5147265768,-3.
8000140893,0.8779540555\H,0.4447775066,-4.9378101806,2.4427032571\H,-1
425617571,-4.3944716924,0.8929534599\H,-1.2146218417,-2.5185798389,-0
.7062808398\Version=JA64L-G03RevC.02\State=1-A\HF=-1069.5713334\MP2=-
1073.1172394\RMSTD=9.114e-09\RMSEF=1.145e-05\Dipole=1.0357756,0.3519285,
0.7703796\PG=C01 [X(C25H24N2)]\@

10Ac-1

1\1\GINC-LX64I33\FOpt\RMP2-FC\6-31G(d)\C27H27N2O1(1+)\UI271AB\13-May-2
0060\#P MP2(FC)/6-31G(D) SCF=(TIGHT,DIRECT) OPT\spiv0\acmp2_008 mp2
/6-31G(d) opt from rhf/3-21G structure\1,1\C,-0.4370287608,0.21369803
27,0.2498557784\C,-0.4360895816,0.2016471057,1.6933886385\C,0.77511309
48,0.218095464,-0.5997025326\C,-1.6391846866,0.2658263054,-0.422300614
7\N,0.6443068112,-0.0377943725,2.458468672\C,-1.7017932141,0.505407210
1,2.2954403155\C,0.5898557369,0.1981648582,3.9158441588\C,1.8587221148
,0.7560578817,2.0071911821\C,0.6584244932,1.681415152,4.2574349705\H,
-0.3015830786,-0.2813674834,4.3332347151\H,1.4445567493,-0.3263956795,
4.3454158363\H,1.5807219086,2.116011298,3.8662874157\H,-0.1844838923,2
.2353353966,3.8369092811\H,0.643929044,1.8136065144,5.3431174183\C,3.1

515895692,0.0166914952,2.2310004313\H,1.8750441776,-1.6950182757,2.575
4279486\H,1.7434958832,-1.0133041906,0.9577500429\H,3.9859068395,-0.59
12979982,1.8685932947\H,3.1482178132,0.9603977874,1.6862298459\H,3.330
0741886,0.2180499674,3.2903145255\C,-2.8594214793,0.5230585204,1.56864
45284\H,-1.8042605613,0.6358940036,3.3642060095\N,-2.8408200379,0.3587
748636,0.2126569224\H,-3.8404348193,0.6579890083,2.0099622396\C,-4.133
0858278,0.2815005872,-0.4977632562\C,-4.0672370448,-0.0617164479,-1.95
62157965\O,-5.141861229,0.4759964126,0.1431082456\H,-3.5064629898,-0.9
858169352,-2.1256270305\H,-5.0938987435,-0.1829331309,-2.3016224242\H,
-3.596634761,0.7440921065,-2.5276044846\H,-1.6499469551,0.2562613841,-
1.5047716424\C,1.6750864474,1.3211994061,-0.4976562751\C,0.9744512367,
-0.7879349776,-1.5524253212\C,2.8867627827,1.2900630602,-1.2635958438\
C,1.4380566666,2.4281276105,0.3605183807\C,3.8194521594,2.3497750576,-
1.1286795309\C,3.0879744983,0.2380184257,-2.1923774921\C,3.5742315488,
3.3979980807,-0.2649303558\H,4.737740076,2.3198182759,-1.7124188817\C,
2.3610758076,3.4514660942,0.4586314794\H,4.2951409692,4.2060873658,-0.
1708229051\H,2.1566803713,4.3028758095,1.1038431211\H,0.4966346225,2.5
041963816,0.8993598125\C,2.1528638752,-0.7647766716,-2.3402448511\H,4.
0047997563,0.2201635221,-2.7794920698\H,2.316297931,-1.564181946,-3.05
99370521\C,-0.0083452863,-1.8783020857,-1.7511617775\C,-0.5691660845,-
2.0635153357,-3.0257010271\C,-0.4190741008,-2.7114317996,-0.6980130954
\C,-1.5325526833,-3.0528636683,-3.2382115998\H,-0.250231054,-1.4256584
871,-3.8487505071\C,-1.9449154891,-3.868558987,-2.1804287647\H,-1.9557
565838,-3.191198338,-4.2304094462\C,-1.3779626413,-3.7018659678,-0.912
9568797\H,-2.6881984741,-4.644059012,-2.3471654179\H,-1.6763460318,-4
3.531076923,-0.0947231421\H,0.0326611244,-2.60204576,0.2864392751\\Ver
sion=IA64L-G03RevC.02\State=1-A\HF=-1221.7459159\MP2=-1225.7209592\RMS
D=4.990e-09\RMSF=4.723e-06\Dipole=-0.3790593,0.0895636,1.0667145\PG=C0
1 [X(C27H27N2O1)]\@

10Ac-2

I:\GINC-LX64H14\SP\RM2-FC\6-311+G(d,p)\C27H27N2O1(1+)\UI271AB\18-May-2006\0\#P MP2(FC)/6-311+G(D,P) SCF=(TIGHT,DIRECT)\spiv0\acmp2_017 m p2(fc)/6-311+G(d,p)/mp2/6-31G(d) sp\1,C,1,1.44358802\C,1,1.48152 677,2,125.85352649\C,1,1.37853388,2,119.23212078,3,-179.28773307,0\N,2,1.34596356,1,125.25943259,4,170.76465383,0\C,2,1.43494336,1,114.49542 846,4,-10.92998366,0\C,5,1.48240439,2,125.21737844,1,-17.51340989,0\C, 5,1.47813174,2,120.24734181,1,177.63869856,0\C,7,1.52371743,5,114.0656 2273,2,120.49369521,0\H,7,1.09671598,5,105.80370125,2,-118.31437965,0\ H,7,1.0863919,5,108.77513149,2,-3.426529,0\H,9,1.09416972,7,108.324487 17,5,-179.06954548,0\H,9,1.08917931,7,111.31544989,5,-59.79563553,0\H, 9,1.09266535,7,112.24013958,5,62.57643613,0\C,8,1.52592802,5,112.71019 144,2,79.35589275,0\H,8,1.09063339,5,106.211417,2,-159.96524006,0\H,8, 1.09237427,5,109.12172255,2,-46.06353736,0\H,15,1.09206619,8,112.01683 975,5,-60.820282,0\H,15,1.0925072,8,110.78391995,5,60.11927486,0\H,15, 1.09359871,8,109.59442151,5,178.94368847,0\C,6,1.36638539,2,122.143371 45,1,11.92783815,0\H,6,1.08141343,2,121.45671113,1,-173.83147869,0\N,4 ,1.36208195,1,123.24488579,2,2.82788441,0\H,21,1.08409555,6,123.473320 28,2,175.08397682,0\C,23,1.47598815,4,123.06676444,1,-173.93073273,0\C ,25,1.49984759,23,116.21871523,4,6.16889801,0\O,25,1.21093156,23,117.7 7643296,4,-174.98670676,0\H,26,1.09414447,25,111.01278033,23,-67.17266 348,0\H,26,1.09419027,25,111.41680506,23,54.18940923,0\H,26,1.08993603 ,25,107.00998208,23,174.25919169,0\H,4,1.08262505,1,119.51384155,2,-17 8.17870331,0\C,3,1.42614464,1,118.71985546,4,111.98562569,0\C,3,1.3994 1143,1,119.94599826,4,-61.84962671,0\C,32,1.43379861,3,118.5270237,1,1 77.89107384,0\C,32,1.42041316,3,122.62348448,1,-0.27637843,0\C,34,1.41 80468,32,119.20444797,3,-177.85517173,0\C,34,1.41787132,32,119.0614662 7,3,5.95575251,0\C,36,1.38013259,34,120.65730499,32,0.61492779,0\H,36, 1.08851818,34,118.91045659,32,-179.96301964,0\C,35,1.38138939,32,120.5 1508134,3,178.42972337,0\H,38,1.0869831,36,120.04731507,34,-179.859636 06,0\H,40,1.08749126,35,119.7726202,32,178.9107858,0\H,35,1.08775395,3

2,119.86704471,3,-4.87823396,0\C,37,1.37923495,34,120.93537384,32,-1.4
9442147,0\H,37,1.08885756,34,118.98867011,32,179.57815413,0\H,44,1.088
01596,37,120.23210928,34,179.56589991,0\C,33,1.48119665,3,121.52220267
,1,-0.38589269,0\C,47,1.40425178,33,122.03704252,3,-55.94874279,0\C,47
,1.40473285,33,118.92712172,3,122.41327485,0\C,48,1.39519889,47,120.45
282319,33,178.01711201,0\H,48,1.08872516,47,119.83045614,33,-3.7473819
4,0\C,50,1.39821314,48,120.19619269,47,-0.47937193,0\H,50,1.08752235,4
8,119.86065914,47,178.92441166,0\C,49,1.39720174,47,120.45459693,33,-1
77.77392691,0\H,52,1.08700427,50,120.09005126,48,179.79452315,0\H,54,1
.08753529,49,119.81610445,47,-179.62939675,0\H,49,1.08907793,47,119.42
719135,33,2.01663848,0\Version=IA64L-G03RevC.02\State=1-A\HF=-1222.01
5185\MP2=-1226.3698479\RMSD=5.365e-09\PG=C01 [X(C27H27N2O1)]\@