

The distal effect of *N*-electron-withdrawing groups on the stability of peptide carbon radicals

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Accessory Publication

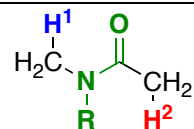
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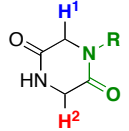
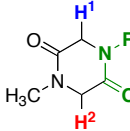
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Table S1. G3MP2-RAD enthalpies (Hartrees) calculated at 298 K for acetamides.



R		H298 (Hartree)	R		H298 (Hartree)
H	1	Acetamide	SO ₂ CF ₃	31	Acetamide
	2	CH ¹ -radical		32	CH ¹ -radical
	3	CH ² -radical		33	CH ² -radical
	4	Amide TS		34	Amide TS
	5	Amide TS CH ² radical		35	Amide TS CH ² radical
CH ₃	6	Acetamide	N...HF	36	Acetamide
	7	CH ¹ -radical		37	CH ¹ -radical
	8	CH ² -radical		38	CH ² -radical
	9	Amide TS			
	10	Amide TS CH ² radical			
CF ₃	11	Acetamide	O...HF	39	Acetamide
	12	CH ¹ -radical		40	CH ¹ -radical
	13	CH ² -radical		41	CH ² -radical
	14	Amide TS			
	15	Amide TS CH ² radical			
COCH ₃	16	Acetamide	NH ⁺	42	Acetamide
	17	CH ¹ -radical		43	CH ¹ -radical
	18	CH ² -radical		44	CH ² -radical
	19	Amide TS			
	20	Amide TS CH ² radical			
COCF ₃	21	Acetamide	OH ⁺	45	Acetamide
	22	CH ¹ -radical		46	CH ¹ -radical
	23	CH ² -radical		47	CH ² -radical
	24	Amide TS			
	25	Amide TS CH ² radical			
SO ₂ CH ₃	26	Acetamide			
	27	CH ¹ -radical			
	28	CH ² -radical			
	29	Amide TS			
	30	Amide TS CH ² radical			

Table S2. G3MP2-RAD enthalpies (Hartrees) calculated at 298 K for diketopiperazines.

							
R			H298 (Hartree)	R		H298 (Hartree)	
H	48	Diketopiperazine	-415.4211443	CH ₃	80	Diketopiperazine	-493.878139
	49	CH ¹ -radical	-414.7856961		81	CH ¹ -radical	-493.2429366
	50	CH ² -radical	-414.7856961		82	CH ² -radical	-493.2429366
CH ₃	51	Diketopiperazine	-454.6496015	CF ₃	83	Diketopiperazine	-791.3820312
	52	CH ¹ -radical	-454.0147475		84	CH ¹ -radical	-790.7414823
	53	CH ² -radical	-454.0137486		85	CH ² -radical	-790.7496106
CF ₃	54	Diketopiperazine	-752.153243	COCH ₃	86	Diketopiperazine	-607.0849173
	55	CH ¹ -radical	-751.5130301		87	CH ¹ -radical	-606.4428892
	56	CH ² -radical	-751.5198346		88	CH ² -radical	-606.4529585
COCH ₃	57	Diketopiperazine	-567.8563962	COCF ₃	89	Diketopiperazine	-904.5697276
	58	CH ¹ -radical	-567.2144816		90	CH ¹ -radical	-903.9259023
	59	CH ² -radical	-567.2234294		91	CH ² -radical	-903.9391433
COCF ₃	60	Diketopiperazine	-865.3409907	SO ₂ CH ₃	92	Diketopiperazine	-1041.911374
	61	CH ¹ -radical	-864.6972993		93	CH ¹ -radical	-1041.270362
	62	CH ² -radical	-864.7093418		94	CH ² -radical	-1041.278721
SO ₂ CH ₃	63	Diketopiperazine	-1002.682784	SO ₂ CF ₃	95	Diketopiperazine	-1339.387544
	64	CH ¹ -radical	-1002.042103		96	CH ¹ -radical	-1338.743598
	65	CH ² -radical	-1002.049125		97	CH ² -radical	-1338.756918
SO ₂ CF ₃	66	Diketopiperazine	-1300.158623				
	67	CH ¹ -radical	-1299.515068				
	68	CH ² -radical	-1299.526935				
N...HF	69	Diketopiperazine	-515.7809358				
	70	CH ² -radical	-515.1487011				
O...HF	71	Diketopiperazine	-515.7923563				
	72	CH ¹ -radical	-515.1580997				
	73	CH ² -radical	-515.1542814				
NH ⁺	74	Diketopiperazine	-415.7200351				
	75	CH ¹ -radical	-415.058456				
	76	CH ² -radical	-415.0953113				
OH ⁺	77	Diketopiperazine	-415.7427373				
	78	CH ¹ -radical	-415.1217937				
	79	CH ² -radical	-415.09502				

^a Convergence problem during geometry optimisation

Table S3. G3MP2-RAD enthalpies (Hartrees) calculated at 298 K for amino- and formamido-acetamides.

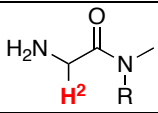
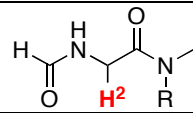
							
R			H298 (Hartree)	R		H298 (Hartree)	
H	98	Amino-acetamide	-303.398929	H	126	Formamino-acetamide	-416.6061482
	99	CH ² -radical	-302.7682142		127	CH ² -radical	-415.9703595
	100	Amide TS	-303.3756078		128	Amide TS	-416.5814439
	101	Amide TS CH ² radical	-302.7540247		129	Amide TS CH ² radical	-415.9510916
CH ₃	102	Amino-acetamide	-342.6217889	CH ₃	130	Formamino-acetamide	-455.8302925
	103	CH ² -radical	-341.991326		131	CH ² -radical	-455.1938264
	104	Amide TS	-342.6017324		132	Amide TS	-455.8077471
	105	Amide TS CH ² radical	-341.9800128		133	Amide TS CH ² radical	-455.1772631
CF ₃	106	Amino-acetamide	-640.1335209	CF ₃	134	Formamino-acetamide	-753.3383925
	107	CH ² -radical	-639.505971		135	CH ² -radical	-752.7046951
	108	Amide TS	-640.1197952		136	Amide TS	-753.3239682
	109	Amide TS CH ² radical	-639.4995298		137	Amide TS CH ² radical	-752.6949062
COCH ₃	110	Amino-acetamide	-455.8308578	COCH ₃	138	Formamino-acetamide	-569.0365837
	111	CH ² -radical	-455.2053485		139	CH ² -radical	-568.4025189
	112	Amide TS	-455.8183924		140	Amide TS	-569.0229848
	113	Amide TS CH ² radical	-455.1990821		141	Amide TS CH ² radical	-568.3945007
COCF ₃	114	Amino-acetamide	-753.3219682	COCF ₃	142	Formamino-acetamide	-866.5263871
	115	CH ² -radical	-752.6985698		143	CH ² -radical	-865.893847
	116	Amide TS	-753.3107061		144	Amide TS	-866.5139135
	117	Amide TS CH ² radical	-752.6921666		145	Amide TS CH ² radical	-865.8867685
SO ₂ CH ₃	118	Amino-acetamide	-890.6588507	SO ₂ CH ₃	146	Formamino-acetamide	-1003.864589
	119	CH ² -radical	-890.035849		147	CH ² -radical	-1003.2310055
	120	Amide TS	-890.6510153		148	Amide TS	-1003.849484
	121	Amide TS CH ² radical	-890.0302839		149	Amide TS CH ² radical	-1003.225316
SO ₂ CF ₃	122	Amino-acetamide	-1188.144086	SO ₂ CF ₃	150	Formamino-acetamide	-1301.347375
	123	CH ² -radical	-1187.519949		151	CH ² -radical	-1300.715345
	124	Amide TS	-1188.131835		152	Amide TS	-1301.333074
	125	Amide TS CH ² radical	-1187.511399		153	Amide TS CH ² radical	-1300.706224

Table S4. Calculated^a gas phase kinetic and thermodynamic parameters associated with hydrogen abstraction from diketopiperazines by bromine at 353 K.

	ΔG^\ddagger (kJ mol ⁻¹)	ΔG (kJ mol ⁻¹)	log(k ₃₅₃)	log(k ₃₅₃) (Q) ^b	Δq^c
Sarcosine anhydride (2a)	31.7	-23.6	9.56	9.89	0.093
<i>N</i> -acetylglycylsarcosine anhydride (1a)	31.0	-31.8	9.66	9.98	0.083

^a A spin-orbit correction of -5.3 mhartree¹ was applied for the bromine atom. ^b Rate constants corrected for the effects of tunneling. ^c Atomic charge of the α -carbon in the TS less that in the reactant. NPA charges calculated at the B3LYP/6-311+G(d,p) level.

The reaction rate constants were evaluated using variational transition state theory (VTST) based on equation (1)

$$\begin{aligned} k(T) &= \kappa(T) \frac{k_B T}{h} (c^\circ)^{1-m} e^{(-\Delta G^\ddagger / RT)} \\ &= \kappa(T) \frac{k_B T}{h} (c^\circ)^{1-m} \frac{Q^\ddagger}{\prod_{\text{reactants}} Q_i} e^{(-\Delta E^\ddagger / RT)} \end{aligned} \quad \text{Equation (1)}$$

where $\kappa(T)$ is the tunneling correction, T is the temperature (in Kelvin), k_B is Boltzmann's constant (1.380658×10^{-23} J mol⁻¹ K⁻¹), h is Planck's constant ($6.6260755 \times 10^{-34}$ J.s), c° is the standard unit of concentration (mol L⁻¹), m is the molecularity of the reaction, ΔG^\ddagger is the Gibbs free energy of activation, R is the universal gas constant (8.3142 J mol⁻¹ K⁻¹), Q and Q_i are the molecular partition functions of the transition state and the reactant i , respectively, and ΔE is the 0 K, zero-point energy corrected barrier for the reaction. The tunneling coefficient $\kappa(T)$ corrects for quantum effects in motion along the reaction path. In this work, Eckart tunneling coefficients² were evaluated using the imaginary frequency as an estimate of the curvature of the potential energy surface, as described previously.³ The ratio of the calculated rate constants of hydrogen abstraction from **1a** and **2a** correspond to a 1.2, which is close to unity, and is consistent with the observed rates of bromination of sarcosine anhydride and *N*-acetylglycylsarcosine anhydride.

¹ Curtiss, L. A.; Redfern, P. C.; Rassolov, V.; Kedziora, G.; Pople, J. A. *J. Chem. Phys.* **2001**, *114*, 9287.

² Eckart, C. *Phys. Rev.* **1930**, *35*, 1303.

³ Coote, M. L.; Collins, M. A.; Radom, L. *Mol. Phys.* **2003**, *101*, 1329.

Table S5. The gas phase geometries of all the species as numbered in Tables S1-3.

NOTE: All species had zero imaginary frequencies, as determined from frequency calculations at the B3LYP/6-31G(d) level.

Acetamides

NHMe 1

```
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LYP/6-31G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultrafine)\
SP Calc\0,1\C,0.0000373107,0.001630467,0.0056736645\C,0.002932341,0.0
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715892494,-0.3397503262\H,0.5268539332,0.8905754415,-0.3542447209\H,-1
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```

NHMe_c3 2

```
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278,0.0013025227\N,-0.7041246955,-0.6178332786,0.0001979805\H,-0.58236
05555,-1.6214078127,-0.0003885657\C,-1.9858756662,-0.1155137285,0.0006
077228\H,2.3313096611,-0.2858642205,0.8813446152\H,2.3312172831,-0.284
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```

NHMe_c6 3

```
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07,0.3502749298,-0.4684158327\H,-1.0176394554,0.148310082,-0.512353146
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```

NHMe-TS 4

```
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5053,-0.4157460199\H,-0.57240076,0.8589090813,-0.3923394679\H,-2.40605
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```

NHMe-TS_rad 5

```
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NMe2 6

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2\PG=C01 [X(C4H9N1O1)]\@

NMe2_c3 7

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UB3LYP/6-31G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultrafin
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NMe2_c6 8

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)\SP Calc\0,2\C,0.0989008302,0.1516807518,0.0971172576\C,0.031049345
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54810868\C,-1.2403288627,-0.2049423301,3.6076708492\H,1.0590361394,0.4
076152201,-0.3327577374\H,-0.6958414406,-0.1744269934,-0.5627500306\H,
-2.679124544,-1.2664733353,1.2607867806\H,-3.2669645116,0.2036318226,2
.0624145068\H,-2.4499356028,0.3335712785,0.5073002233\H,-1.5471651429,
-1.2279312555,3.8699426936\H,-0.2436100328,-0.0166818611,4.0041139524\
H,-1.9552994838,0.4945558265,4.0593863989\Version=IA64L-G03RevE.01\St
ate=2-A\HF=-287.1642215\S2=0.757075\S2-1=0.\S2A=0.750031\RMSD=4.795e-0
9\RMSF=8.844e-06\Thermal=0.\Dipole=-1.34478,-0.2409308,-0.4665341\PG=C
01 [X(C4H8N1O1)]\@

NMe2-TS 9

1\1\GINC-X8\FTS\RB3LYP\6-31G(d)\C4H9N1O1\JMH502\13-Sep-2010\0\#\# B3LYP
/6-31G(d) opt=(CalcFC,Noeigen,TS) freq=noraman maxdisk=458752000 INT(g
rid=ultrafine)\SP Calc\0,1\C,-0.0078263706,-0.0000659828,0.007359128
2\C,0.0697905085,0.0000328841,1.5141880806\O,1.1098795338,0.0000152376
,2.1348139263\N,-1.2363097816,0.0001530924,2.1611189312\C,-1.400654406
1,-1.2112300371,2.9754028635\C,-1.4005144691,1.211667198,2.9752361992\
H,-0.5728376212,-0.8769992894,-0.330365658\H,0.9906837925,-0.000157176
4,-0.4343157846\H,-0.5727300404,0.8768904411,-0.330485764\H,-2.4169998
685,-1.2233387201,3.3827917239\H,-1.2792027004,-2.0989625222,2.3450833
574\H,-0.6816462863,-1.2734393601,3.8080885218\H,-2.4168584339,1.22394
91611,3.3826236012\H,-0.6814990089,1.2739081766,3.8079131576\H,-1.2789
605043,2.0992989279,2.3447945329\Version=EM64L-G03RevE.01\State=1-A\H
F=-287.803788\RMSD=1.609e-09\RMSF=4.376e-06\Thermal=0.\Dipole=-0.67930
84,0.0000216,-0.265099\PG=C01 [X(C4H9N1O1)]\@

NMe2-TS_rad 10

1\1\GINC-X8\FTS\UB3LYP\6-31G(d)\C4H8N1O1(2)\JMH502\13-Sep-2010\0\#\# B3

LYP/6-31G(d) opt=(CalcFC,Noeigen,TS) freq=noraman maxdisk=458752000 INT(grid=ultrafine)\SP Calc\0,2\C,-0.0051766523,0.0007723662,0.0065404863\C,0.0646483726,-0.0008845988,1.4372757774\O,1.1445004629,-0.0027180494,2.0390547696\N,-1.214332249,-0.0002638801,2.1267364346\C,-1.3589432994,-1.2123838382,2.9426793106\C,-1.356320437,1.2103463141,2.9453760899\H,0.9159061663,0.000407735,-0.5668947256\H,-0.9613557101,0.0023734457,-0.5035683751\H,-2.3596143369,-1.2185984665,3.3873535221\H,-1.2653205094,-2.0978090127,2.3049525275\H,-0.611037634,-1.2818918546,3.7492631005\H,-2.3569763469,1.2177370786,3.3900662215\H,-0.6082672143,1.2764394496,3.7521099804\H,-1.2607796822,2.0969841907,2.3096217194\Version=EM64L-G03RevE.01\State=2-A\HF=-287.1441303\S2=0.766275\S2-1=0.\S2A=0.75008\RMSD=6.608e-09\RMSF=3.469e-06\Thermal=0.\Dipole=-0.6401873,0.0011109,-0.3814797\PG=C01 [X(C4H8N1O1)]\@

NCF3_11

1\1\GINC-AC1\FOpt\RB3LYP\6-31G(d)\C4H6F3N1O1\JMH502\13-Apr-2009\0\# B3LYP/6-31G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultrafine)\SP Calc\0,1\C,0.0043937165,-0.0039533607,0.0063426309\C,0.0030366359,-0.0163932624,1.5236833299\O,1.040599463,-0.023148323,2.1616408579\N,-1.2357087859,0.006015752,2.193027313\C,-1.2449576647,-0.0678501927,3.6615276858\C,-2.4748856112,-0.0824525888,1.5143955245\H,-0.272532081,0.9868672073,-0.366391845\H,-0.6927776541,-0.7285675091,-0.4200606908\H,1.0209576003,-0.2344083925,-0.313175984\H,-1.7732052853,0.7880138106,4.08779991\H,-1.7183967166,-0.9925804112,4.0045796626\H,-0.2032875904,-0.0527726072,3.974880592\F,-2.6074108492,0.8576652456,0.5538029639\F,-2.6605236249,-1.2799260203,0.9005063706\F,-3.4878479658,0.0758246767,2.3805061721\Version=IA64L-G03RevE.01\State=1-A\HF=-585.5541424\RMSD=6.214e-09\RMSF=2.423e-05\Thermal=0.\Dipole=-0.4261607,0.0295305,-0.0213689\PG=C01 [X(C4H6F3N1O1)]\@

NCF3_c3.a2_12

1\1\GINC-X137\FOpt\UB3LYP\6-31G(d)\C4H5F3N1O1(2)\JMH502\15-Apr-2009\0\# UB3LYP/6-31G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultrafine)\SP Calc\0,2\C,0.0883704025,0.0609250933,-0.0059456974\C,-0.0367440479,-0.0003479668,1.5023466927\O,0.9334812602,-0.0314714584,2.2358435676\N,-1.3361160297,-0.0024708506,2.08646736\C,-1.4414293052,-0.1062272791,3.4766657925\C,-2.5214600001,-0.0272894379,1.2864024305\H,-0.5855706948,-0.6293680745,-0.5174665812\H,1.1226052844,-0.1878285927,-0.2459807617\H,-0.1262772875,1.0712924321,-0.3685079214\H,-0.5099765954,-0.1022000386,4.0158385566\H,-2.4096451044,-0.0012360108,3.9327698852\F,-2.5312789935,0.9733314583,0.3843161896\F,-2.6435247499,-1.1814178605,0.5929764987\F,-3.6148685227,0.1002961448,2.0468368976\Version=EM64L-G03RevE.01\State=2-A\HF=-584.8893246\S2=0.754231\S2-1=0.\S2A=0.750013\RMSD=8.530e-09\RMSF=6.827e-06\Thermal=0.\Dipole=-0.4673351,0.0987633,-0.3382281\PG=C01 [X(C4H5F3N1O1)]\@

NCF3_c6_13

1\1\GINC-AC2\FOpt\UB3LYP\6-31G(d)\C4H5F3N1O1(2)\JMH502\08-Apr-2009\0\# UB3LYP/6-31G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultrafine)\SP Calc\0,2\N,-0.0405183147,-0.0400765292,-0.0032448919\C,0.1116068139,-0.4185889894,1.3500583975\C,1.363029659,-0.1507406619,2.0293461051\H,2.21984041,0.3286872307,1.5781529188\H,1.4102623285,-0.4666202605,3.0635947548\O,-0.816446309,-0.9717319857,1.9420268814\C,-1.3156629055,-0.3173260565,-0.6751288828\H,-1.9518186794,-0.8010476568,0.0631891114\H,-1.1707413102,-0.9841877954,-1.5296126297\H,-1.787061549,0.6083343251,-1.0169521286\C,0.9888549655,0.5976353822,-0.7307186891\F,1.362862738,1.7799414972,-0.1820751836\F,2.1178847791,-0.149606016,-0.8044961169\F,0.5862593737,0.8449875162,-1.9857456464\Version=IA64L-G03RevE.01\State=2-A\HF=-584.8892843\S2=0.758714\S2-1=0.\S2A=0.750041\RMSD=3.998e-09\RMSF=1.558e-05\Thermal=0.\Dipole=0.1991677,0.1737699,-0.2950347\PG=C01 [X(C4H5F3N1O1)]\@

NCF3-TS_14

1\1\GINC-X94\FTS\RB3LYP\6-31G(d)\C4H6F3N1O1\JMH502\13-Sep-2010\0\# B3LYP/6-31G(d) opt=(CalcFC,Noeigen,TS) freq=noraman maxdisk=458752000 INT(grid=ultrafine)\SP Calc\0,1\C,0.0317466202,0.0457733631,0.1372306518\C,0.0170834228,-0.1529089247,1.6275694379\O,0.9786843144,-0.4175990032,2.3033660188\N,-1.3234237237,0.0262589697,2.2148456924\C,-1.4264822513,1.2627102618,3.0095507783\C,-1.816325844,-1.1258819948,2.8629104732\H,-0.4376776259,1.0009243797,-0.1239564181\H,-0.5793507325,-0.7396174678,-0.3234582387\H,1.0523652375,0.0024778245,-0.2467006353\H,-2.4582401879,1.3752750059,3.348005771\H,-0.7514108714,1.2606100929,3.874193

6312\H,-1.1832155791,2.1119348662,2.3649384442\F,-1.6129781927,-2.2032
30909,2.0764819349\F,-1.2504400504,-1.3975351263,4.0657486772\F,-3.140
6754224,-1.0060069918,3.0903962569\\Version=EM64L-G03RevE.01\State=1-A
\HF=-585.5335697\RMSD=4.523e-09\RMSF=3.884e-06\Thermal=0.\Dipole=-0.22
57286,0.9509065,-0.7106282\PG=C01 [X(C4H6F3N1O1)]\@

NCF3-TS_rad 15

1\1\GINC-X94\FTS\UB3LYP\6-31G(d)\C4H5F3N1O1(2)\JMH502\13-Sep-2010\0\#\#
B3LYP/6-31G(d) opt=(CalcFC,Noeigen,TS) freq=noraman maxdisk=458752000
INT(grid=ultrafine)\SP Calc\0,2\N,0.0959156069,0.0110618309,-0.0851
698324\C,-0.0543748961,-0.1042773289,1.3691149666\C,1.1567561011,0.041
1202281,2.1115029346\H,2.1065390977,0.1898004347,1.611788041\H,1.11397
68285,-0.0080222598,3.1939732762\O,-1.1517965614,-0.2821777193,1.89583
24495\C,-0.468306486,1.2658462087,-0.6133558867\H,0.0426771969,2.10423
58212,-0.1324408663\H,-1.5469530955,1.3463460273,-0.4298446074\H,-0.27
34499136,1.3133269479,-1.6863249582\C,-0.2990456122,-1.144643216,-0.79
47451801\F,0.2060737595,-2.2397461105,-0.1957642293\F,-1.6406480337,-1
.3247574745,-0.8937204564\F,0.1657038958,-1.0965146638,-2.0610795376\\
Version=EM64L-G03RevE.01\State=2-A\HF=-584.8735653\S2=0.766615\S2-1=0.
\S2A=0.75008\RMSD=6.378e-09\RMSF=2.778e-05\Thermal=0.\Dipole=0.8827533
,0.9268929,0.2364803\PG=C01 [X(C4H5F3N1O1)]\@

NAC 16

1\1\GINC-AC30\FOpt\RB3LYP\6-31G(d)\C5H9N1O2\JMH502\13-Apr-2009\0\#\# B3
LYP/6-31G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultrafine)\
SP Calc\0,1\C,0.0026577464,-0.041130944,0.0069411795\C,0.0050125839,-
0.0144167153,1.5277188172\O,1.0554628972,-0.0008320175,2.1462589748\N,
-1.2553875298,-0.0066069664,2.1498188358\C,-2.4762186091,-0.0244361053
,1.3293498204\C,-1.4549539218,0.0175702844,3.5622734987\H,-0.500380460
3,-0.9320120029,-0.3844414417\H,1.043573086,-0.0449922182,-0.317586276
1\H,-0.5034060562,0.8337619391,-0.415386762\H,-2.5225779046,-0.9276186
009,0.7140425276\H,-3.3225091658,-0.0133350117,2.0122219828\H,-2.52600
67466,0.8547776755,0.6805593164\O,-2.5919380137,0.0220088191,4.0016399
58\C,-0.2634109494,0.0373097388,4.4912538552\H,0.3701141542,0.90938664
85,4.3136686231\H,-0.6619217313,0.0542473824,5.5072792531\H,0.37488641
33,-0.8370398033,4.3446572723\\Version=IA64L-G03RevE.01\State=1-A\HF=-
401.1737284\RMSD=9.009e-09\RMSF=9.363e-06\Thermal=0.\Dipole=-0.1306381
, -0.0195548, -1.110133\PG=C01 [X(C5H9N1O2)]\@

NAC_c3 17

1\1\GINC-AC29\FOpt\UB3LYP\6-31G(d)\C5H8N1O2(2)\JMH502\13-Apr-2009\0\#\#
UB3LYP/6-31G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultrafin
e)\SP Calc\0,2\C,-0.011853758,-0.1651262852,-0.0210042133\C,-0.00049
82599,0.1233091635,1.4681684999\O,1.0239691501,0.4520037094,2.03936413
05\N,-1.2391831874,-0.011709944,2.1483953637\C,-2.3748355947,-0.489134
8039,1.4954070163\C,-1.4262379355,0.352511421,3.5367866487\H,-0.205398
5377,-1.2256507478,-0.2210126814\H,0.975861468,0.0897489597,-0.4061449
436\H,-0.7760502741,0.4191018719,-0.5441960302\H,-2.2733810771,-0.9423
973558,0.5249633495\H,-3.2743198705,-0.5571475872,2.0826727658\O,-2.52
20611212,0.1731864878,4.0306982284\C,-0.2889090678,0.9540448983,4.3241
687686\H,0.1216135141,1.8417792971,3.8372326581\H,-0.6955155925,1.2094
461712,5.30454676\H,0.5408509984,0.2510858558,4.4286512595\\Version=IA
64L-G03RevE.01\State=2-A\HF=-400.5105149\S2=0.754555\S2-1=0.\S2A=0.750
015\RMSD=9.563e-09\RMSF=2.513e-05\Thermal=0.\Dipole=0.0892413,-0.18709
87,-0.9478544\PG=C01 [X(C5H8N1O2)]\@

NAC_c6.a2b2 18

1\1\GINC-AC20\FOpt\UB3LYP\6-31G(d)\C5H8N1O2(2)\JMH502\05-May-2009\0\#\#
UB3LYP/6-31G(d) INT(grid=ultrafine) OPT freq=noraman maxdisk=134217728
0\\NAC_c6 confsearch\0,2\C,-1.702755,-1.454844,0.001866\C,-1.365058,-
0.053088,-0.000097\O,-2.264279,0.793757,-0.002104\N,0.0011,0.385845,0.
000877\C,0.196528,1.843338,0.001035\C,1.116978,-0.462864,-0.000371\H,-
0.968744,-2.244147,0.00446\H,-2.766142,-1.663806,0.000594\H,-0.789039,
2.302399,0.006036\H,0.74661,2.166034,0.889858\H,0.737813,2.167772,-0.8
9266\O,1.042419,-1.681826,-0.001467\C,2.477602,0.218036,-0.000126\H,2.
618909,0.84733,0.885234\H,3.231506,-0.569578,-0.004006\H,2.616489,0.85
4163,-0.880918\\Version=IA64L-G03RevE.01\State=2-A\HF=-400.5102825\S2=
0.760721\S2-1=0.\S2A=0.750051\RMSD=8.926e-09\RMSF=1.563e-06\Thermal=0.
\Dipole=0.8208032,0.5487277,0.0031897\PG=C01 [X(C5H8N1O2)]\@

NAC-TS 19

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1\1\GINC-V1252\FTS\RB3LYP\6-31G(d)\C5H9N1O2\JMH502\14-Sep-2010\0\#\# B3
LYP/6-31G(d) opt=(CalcFC,Noeigen,TS) freq=noraman maxdisk=458752000 IN
T(grid=ultrafine)\SP Calc\0,1\C,0.0417542293,-0.008211492,0.02950978
69\C,0.0225514463,0.0075358855,1.539326515\O,1.0148523484,0.030408979,
2.227170376\N,-1.3008193495,-0.0899393992,2.1329430475\C,-1.6528260955
,-1.4127045239,2.6559892136\C,-1.995861745,1.0211880405,2.593442419\H,
-0.3746029905,-0.9596669287,-0.3249856933\H,1.0630115756,0.1043888625,
-0.3387966723\H,-0.5989101489,0.7810924075,-0.3774452253\H,-0.97008304
26,-1.7131618126,3.4593919946\H,-2.6678049371,-1.3448487452,3.04722131
31\H,-1.6156168332,-2.1591959469,1.8551755011\O,-3.0118502257,0.912217
2935,3.2630394195\C,-1.4167364564,2.3768621511,2.225842926\H,-1.16640
57069,2.4526700865,1.1589643066\H,-2.1545943056,3.1399496945,2.4727153
678\H,-0.5009440656,2.5643378711,2.7946551306\Version=EM64L-G03RevE.0
1\State=1-A\HF=-401.1564562\RMSD=5.583e-09\RMSF=8.508e-07\Thermal=0.\D
ipole=0.3598191,-0.2184964,-1.1955916\PG=C01 [X(C5H9N1O2)]\@
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NAC-TS_rad 20

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1\1\GINC-V1253\FTS\UB3LYP\6-31G(d)\C5H8N1O2(2)\JMH502\14-Sep-2010\0\#\#
B3LYP/6-31G(d) opt=(CalcFC,Noeigen,TS) freq=noraman maxdisk=458752000
INT(grid=ultrafine)\SP Calc\0,2\C,0.021611713,0.1861221645,-0.01890
35089\C,-0.081210586,-0.104954472,1.3790835292\O,0.8938371279,-0.42071
66402,2.0631558781\N,-1.3963968886,0.0341977819,1.9708140355\C,-1.6230
699381,1.2691855927,2.7245191783\C,-2.2158751793,-1.0623379051,2.20783
72394\H,-0.8422164417,0.4956393403,-0.5967404172\H,0.9894097263,0.1016
2281,-0.5013775676\H,-1.5111775211,2.138503733,2.0674265096\H,-2.63994
89296,1.2294600601,3.1146275519\H,-0.9152181359,1.3563570605,3.5574950
061\O,-3.2232724138,-0.9766041898,2.8936138243\C,-1.7930261822,-2.3663
701105,1.5510945824\H,-2.6086878173,-3.0816392269,1.6618269717\H,-1.56
25471676,-2.237021294,0.4876104503\H,-0.8966143706,-2.7654809385,2.039
019213\Version=EM64L-G03RevE.01\State=2-A\HF=-400.4974711\S2=0.76665\
S2-1=0.\S2A=0.750082\RMSD=4.432e-09\RMSF=1.258e-05\Thermal=0.\Dipole=0
.4594685,0.4498993,-1.277752\PG=C01 [X(C5H8N1O2)]\@
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NACCF3 21

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1\1\GINC-AC29\FOpt\RB3LYP\6-31G(d)\C5H6F3N1O2\JMH502\13-Apr-2009\0\#\#
B3LYP/6-31G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultrafine)
\SP Calc\0,1\C,-0.0020824581,-0.0000826028,0.0031669028\C,0.00569951
29,-0.0230246902,1.5121687659\O,1.0401304933,-0.0585820957,2.147835891
8\N,-1.2329933153,-0.0062697345,2.2418140746\C,-1.0802588286,-0.061182
5383,3.7118160892\C,-2.4660030213,0.1283941469,1.6267851368\H,-0.56067
62243,-0.8434738965,-0.4096211831\H,1.0414080967,-0.0408263366,-0.3134
619897\H,-0.4800996149,0.9039541957,-0.3825661229\H,-0.9552628663,0.94
1888144,4.1276949327\H,-1.9432629406,-0.5438777883,4.1606676088\H,-0.1
846807183,-0.6403092547,3.9247190157\O,-2.6660818223,0.1427065627,0.42
92991532\C,-3.7121033437,0.2829754857,2.5546115076\F,-3.5492108832,1.2
793469954,3.4503959016\F,-4.782575633,0.5610118385,1.8162568155\F,-3.9
599452315,-0.8588613537,3.2368297656\Version=IA64L-G03RevE.01\State=1
-A\HF=-698.8779501\RMSD=9.638e-09\RMSF=4.244e-06\Thermal=0.\Dipole=0.0
389677,-0.0558092,0.3044303\PG=C01 [X(C5H6F3N1O2)]\@
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NACCF3_c3.a2b2 22

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1\1\GINC-AC20\FOpt\UB3LYP\6-31G(d)\C5H5F3N1O2(2)\JMH502\05-May-2009\0\
\#UB3LYP/6-31G(d) INT(grid=ultrafine) OPT freq=noraman maxdisk=1342177
280\NACCF3_c3 confsearch\0,2\C,2.570968,1.375921,0.175121\C,2.185737
,-0.072121,0.016472\O,3.002646,-0.965142,-0.003702\N,0.774835,-0.44458
1,-0.080518\C,0.517864,-1.815882,-0.101452\C,-0.236453,0.518267,-0.143
972\H,2.356174,1.942887,-0.73403\H,3.642554,1.388726,0.381305\H,2.0208
35,1.864393,0.983114\H,-0.463022,-2.167726,-0.364117\H,1.371536,-2.460
288,0.016164\O,-0.060452,1.705886,-0.328066\C,-1.696983,0.018163,0.052
717\F,-1.823828,-0.705266,1.182102\F,-2.514951,1.06455,0.130391\F,-2.0
98585,-0.751279,-0.985602\Version=IA64L-G03RevE.01\State=2-A\HF=-698.
212683\S2=0.755768\S2-1=0.\S2A=0.750022\RMSD=9.450e-09\RMSF=1.322e-05\
Thermal=0.\Dipole=0.0488992,-0.097344,0.085008\PG=C01 [X(C5H5F3N1O2)]\
\@
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NACCF3_c6.a2b2 23

```
1\1\GINC-AC20\FOpt\UB3LYP\6-31G(d)\C5H5F3N1O2(2)\JMH502\05-May-2009\0\
\#UB3LYP/6-31G(d) INT(grid=ultrafine) OPT freq=noraman maxdisk=1342177
280\NACCF3_c6 confsearch\0,2\C,-2.6239110514,1.412967443,0.108162031
2\C,-2.2011087894,0.0444252308,-0.0182682169\O,-3.0229574605,-0.858503
3582,-0.1837281049\N,-0.8102933903,-0.3290512777,0.0849827116\C,-0.583
```

7872408,-1.7890474033,0.1197683012\C,0.2224165302,0.5839434975,0.00902
63755\H,-1.9537605328,2.2327130981,0.3112989292\H,-3.6895536681,1.5728
652681,-0.0062986201\H,-0.5622694062,-2.2061766236,-0.8905193952\H,0.3
467095502,-2.0102496972,0.6333087203\H,-1.4133973815,-2.2399528595,0.6
602467634\O,0.106534939,1.793531466,-0.0446981632\C,1.6761222596,0.016
1966914,-0.0192264796\F,1.842655245,-0.8817774128,-1.0133338527\F,2.53
76324475,1.0106145192,-0.211394996\F,1.9908619496,-0.5889255819,1.1495
889959\\Version=IA64L-G03RevE.01\State=2-A\HF=-698.2148304\S2=0.761988
\S2-1=0.\S2A=0.750057\RMSD=4.666e-09\RMSF=9.026e-06\Thermal=0.\Dipole=
-0.0913668,-0.2543852,0.202865\PG=C01 [X(C5H5F3N1O2)]\@

NACCF3-TS 24

1\1\GINC-V1249\FTS\RB3LYP\6-31G(d)\C5H6F3N1O2\JMH502\01-Nov-2010\0\#\
B3LYP/6-31G(d) opt=(CalcFC,Noeigen,TS) freq=noraman maxdisk=458752000
INT(grid=ultrafine)\SP Calc\0,1\C,0.0452833121,-0.0674231134,0.01675
63448\C,0.0516713124,0.002428497,1.5202402218\O,1.0355777742,0.0243025
678,2.2113016358\N,-1.2850452434,-0.0447764507,2.1378872032\C,-1.69235
5579,-1.387412422,2.5745773854\C,-1.9528502515,1.0221755625,2.67884387
01\H,-0.5506026082,-0.923418344,-0.3205812122\H,1.0669899485,-0.149958
0154,-0.3571822936\H,-0.4319418435,0.8315831024,-0.3847786883\H,-1.141
0324886,-1.690852664,3.4714525857\H,-2.7589597095,-1.3662977395,2.7968
5043\H,-1.4957501644,-2.1039435638,1.7717802372\O,-2.9209223166,0.9268
879522,3.4103334773\C,-1.4587271558,2.4316271396,2.2573463248\F,-1.473
6227409,2.5613734096,0.9053342513\F,-2.247084674,3.369950057,2.7714070
333\F,-0.1957167385,2.6578779184,2.6685962975\\Version=EM64L-G03RevE.0
1\State=1-A\HF=-698.8625577\RMSD=5.720e-09\RMSF=3.933e-06\Thermal=0.\D
ipole=0.1459994,-1.0378927,-1.1371053\PG=C01 [X(C5H6F3N1O2)]\@

NACCF3-TS_rad 25

1\1\GINC-V1406\FTS\UB3LYP\6-31G(d)\C5H5F3N1O2(2)\JMH502\01-Nov-2010\0\
B3LYP/6-31G(d) opt=(CalcFC,Noeigen,TS) freq=noraman maxdisk=4587520
00 INT(grid=ultrafine)\SP Calc\0,2\C,0.0000002874,0.0711724516,-0.00
95495829\C,0.0277778183,-0.0011047722,1.4161484274\O,1.0614468281,-0.0
127883457,2.0777019521\N,-1.2747328926,0.0173504032,2.085847708\C,-1.7
109443487,1.3433949487,2.541113877\C,-1.8776425641,-1.0816785609,2.639
7347552\H,-0.934006512,0.0717557322,-0.5589224917\H,0.9420596956,0.104
4055608,-0.5451744535\H,-1.6927780533,2.0413994879,1.6986558248\H,-2.7
259183765,1.252326168,2.9265947414\H,-1.0520646764,1.716627912,3.33328
36278\O,-2.8277176713,-1.0404210593,3.3989466493\C,-1.3039541177,-2.46
07602753,2.2199594417\F,-2.1467254405,-3.4326398221,2.5605639616\F,-1.
1052639345,-2.5263578854,0.8791157011\F,-0.1193952168,-2.6883539445,2.
8174826739\\Version=EM64L-G03RevE.01\State=2-A\HF=-698.2030391\S2=0.76
6539\S2-1=0.\S2A=0.750081\RMSD=3.552e-09\RMSF=1.137e-05\Thermal=0.\Dip
ole=0.0861975,1.0932722,-1.2988912\PG=C01 [X(C5H5F3N1O2)]\@

NSO2Me 26

1\1\GINC-AC1\FOpt\RB3LYP\6-31G(d)\C4H9N1O3S1\JMH502\13-Apr-2009\0\#\ B
3LYP/6-31G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultrafine)\
\SP Calc\0,1\C,0.0178310583,0.0019421466,0.005068417\C,0.023744775,-0
.003334974,1.519203406\O,1.0622823275,0.0258222146,2.1551091001\N,-1.1
907291251,-0.0367398038,2.2422999427\C,-1.0596205808,-0.0332088533,3.7
134050974\S,-2.7706713766,-0.1001630892,1.5679615884\H,-0.5748193777,-
0.8120532038,-0.4219014827\H,1.0567952691,-0.0970269722,-0.3121335161\
H,-0.4045152431,0.9337673814,-0.3780855583\H,-2.0523710089,0.017113799
9,4.1550074555\H,-0.5344223477,-0.9329070195,4.0456290903\H,-0.4778750
815,0.8388320571,4.0181262145\O,-3.6921391921,0.3109518306,2.624977641
3\O,-2.7541979449,0.5821977329,0.2767865102\C,-3.0313447819,-1.8620615
658,1.2726016602\H,-4.0383461166,-1.9677343404,0.8618919829\H,-2.29118
73028,-2.2258884732,0.5580053814\H,-2.9521059101,-2.3924111219,2.22330
18957\\Version=IA64L-G03RevE.01\State=1-A\HF=-836.3979523\RMSD=5.282e-
09\RMSF=2.099e-06\Thermal=0.\Dipole=-0.151286,-1.3618632,-0.1660644\PG
=C01 [X(C4H9N1O3S1)]\@

NSO2Me_c3 27

1\1\GINC-AC26\FOpt\UB3LYP\6-31G(d)\C4H8N1O3S1(2)\JMH502\15-Apr-2009\0\
B3LYP/6-31G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultrafi
ne)\SP Calc\0,2\C,-1.9347795359,0.9102720179,0.0390300433\C,-0.97302
53713,-0.2421909748,0.2359247276\O,-1.3425535326,-1.3961362631,0.39126
31365\N,0.3946750115,0.0869514452,0.2129323099\C,0.908064426,1.3389688
938,-0.1094713184\S,1.5543644903,-1.1485238346,0.7700143802\H,-1.70421
4364,1.7436193662,0.7106392049\H,-2.9409950624,0.5376620153,0.23439347
36\H,-1.8933403846,1.288303003,-0.9899906724\H,0.3005088322,1.99787812

9,-0.7121533646\H,1.9705535135,1.4813479482,0.0048220185\O,2.864728009
4,-0.5332934047,0.5629476169\O,1.1351287907,-1.5993337038,2.0896189622
\C,1.3430414886,-2.4709790166,-0.4317639811\H,2.0459994932,-3.25509768
38,-0.1389862051\H,0.3112489175,-2.8143707143,-0.3745505993\H,1.595394
2781,-2.0807442229,-1.4191547329\\Version=IA64L-G03RevE.01\State=2-A\H
F=-835.73652\S2=0.755457\S2-1=0.\S2A=0.75002\RMSD=6.683e-09\RMSF=1.783
e-05\Thermal=0.\Dipole=-0.4508112,0.5573814,-1.4694474\PG=C01 [X(C4H8N
103S1)]\@

NSO2Me_c6.a3b2 28

1\1\GINC-AC26\FOpt\UB3LYP\6-31G(d)\C4H8N103S1(2)\JMH502\06-May-2009\O\
\#UB3LYP/6-31G(d) INT(grid=ultrafine) OPT freq=noraman maxdisk=1342177
280\NSO2Me_c6 confsearch\0,2\C,-1.640002,-1.69448,-0.18167\C,-1.6767
39,-0.258081,-0.017704\O,-2.732982,0.325684,0.23204\N,-0.501026,0.5261
52,-0.174202\C,-0.68694,1.983357,-0.047674\S,1.102004,-0.08937,-0.1507
57\H,-0.784446,-2.234983,-0.560923\H,-2.570265,-2.208244,0.02728\H,0.2
4213,2.47751,-0.322136\H,-1.485698,2.28675,-0.72612\H,-0.979474,2.2563
81,0.971845\O,1.157528,-1.288958,-0.985522\O,1.983909,1.04506,-0.41379
1\C,1.337729,-0.596993,1.56587\H,2.350122,-1.000806,1.641065\H,1.22786
2,0.277833,2.209378\H,0.602959,-1.364691,1.816392\\Version=IA64L-G03Re
vE.01\State=2-A\HF=-835.734721\S2=0.759336\S2-1=0.\S2A=0.750043\RMSD=5
.538e-09\RMSF=1.425e-06\Thermal=0.\Dipole=0.0788559,-0.3679741,1.20150
88\PG=C01 [X(C4H8N103S1)]\@

NSO2Me-TS 29

1\1\GINC-V1293\FTS\RB3LYP\6-31G(d)\C4H9N103S1\JMH502\01-Nov-2010\O\
\#B3LYP/6-31G(d) opt=(CalcFC,Noeigen,TS) freq=noraman maxdisk=458752000
INT(grid=ultrafine)\SP Calc\0,1\C,0.0073949317,-0.0254743953,0.00528
15598\C,0.0083890571,0.0151759184,1.5056709503\O,0.9949755117,0.031099
3704,2.2026585247\N,-1.3423686006,0.0282120873,2.0839198197\C,-1.77624
95684,1.333374485,2.6055719867\S,-1.7464947455,-1.359084928,2.97890235
92\H,-0.4034179126,-0.9961358793,-0.2983045715\H,1.0196478293,0.095125
4286,-0.3844042145\H,-0.6594983137,0.741976628,-0.4023747326\H,-2.8041
883717,1.2355900645,2.9579492165\H,-1.1326052,1.7046046281,3.414842046
7\H,-1.760788728,2.0572619106,1.7844705097\O,-3.1564764192,-1.21830209
24,3.3419961906\O,-1.2607400251,-2.4780597387,2.1696693369\C,-0.778323
6127,-1.3098623448,4.5042542276\H,-1.0012707398,-2.2314074837,5.046863
564\H,0.2785175137,-1.2494412532,4.2440113081\H,-1.0878624341,-0.44362
00702,5.0924036887\\Version=EM64L-G03RevE.01\State=1-A\HF=-836.3840147
\RMSD=7.198e-09\RMSF=7.819e-06\Thermal=0.\Dipole=0.4996952,1.2797442,0
.1073387\PG=C01 [X(C4H9N103S1)]\@

NSO2Me-TS_rad 30

1\1\GINC-V1296\FTS\UB3LYP\6-31G(d)\C4H8N103S1(2)\JMH502\01-Nov-2010\O\
\#B3LYP/6-31G(d) opt=(CalcFC,Noeigen,TS) freq=noraman maxdisk=4587520
00 INT(grid=ultrafine)\SP Calc\0,2\C,-0.0883630484,-0.2865836252,-0.
1090601938\C,-0.0449062335,0.1480521349,1.2504223975\O,0.978903587,0.5
663063605,1.794607503\N,-1.309839027,0.0430036058,1.9742477048\C,-1.39
92107377,-1.0986969542,2.8979014437\S,-1.9742788259,1.5247616599,2.486
785036\H,-1.0170660188,-0.6109218452,-0.5625104843\H,0.8252511718,-0.2
650624091,-0.6928815109\H,-2.3938834252,-1.1010324582,3.3457834553\H,-
1.2762992362,-2.020041805,2.3198426112\H,-0.6309187023,-1.0706169974,3
.6831369206\O,-1.8255331089,2.4249400092,1.3438643896\O,-3.2826577372,
1.2061114135,3.0590464338\C,-0.9250140163,2.1376846134,3.8245203037\H,
-0.9786557594,1.4422252689,4.6645111334\H,0.0961792616,2.2251954052,3.
453268714\H,-1.3262714977,3.1109070663,4.1164262275\\Version=EM64L-G03
RevE.01\State=2-A\HF=-835.7234538\S2=0.765455\S2-1=0.\S2A=0.750074\RMS
D=4.203e-09\RMSF=1.813e-05\Thermal=0.\Dipole=0.8550107,-1.1407003,0.24
61734\PG=C01 [X(C4H8N103S1)]\@

NSO2CF3 31

1\1\GINC-AC13\FOpt\RB3LYP\6-31G(d)\C4H6F3N103S1\JMH502\13-Apr-2009\O\
\#B3LYP/6-31G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultrafin
e)\SP Calc\0,1\C,-0.0022607192,0.0029866339,0.006118446\C,0.00917921
32,-0.0055928149,1.516480632\O,1.0375899804,-0.0200348765,2.1606496656
\N,-1.2157054244,0.0245630732,2.257863181\C,-1.0696622545,0.0096293911
,3.7330123482\S,-2.7802003887,-0.0629543741,1.6197836913\H,-0.57863330
41,-0.8288143329,-0.4045802718\H,1.0379445907,-0.0736148365,-0.3126903
274\H,-0.4459376933,0.9241657873,-0.3786973307\H,-2.0470837477,0.16029
69005,4.1851395073\H,-0.6391089043,-0.9405337362,4.0575101786\H,-0.399
242465,0.8196942546,4.0211553617\O,-3.7116164542,0.43119402,2.62430756
67\O,-2.7874112716,0.4208559664,0.2470918526\C,-3.0639775536,-1.915467

9753,1.529941986\F,-4.2868267108,-2.1483035333,1.0656436488\F,-2.16117
75299,-2.4744690513,0.7162368985\F,-2.9354383156,-2.4401489776,2.75095
61966\\Version=IA64L-G03RevE.01\State=1-A\HF=-1134.0948361\RMSD=3.989e
-09\RMSF=2.676e-05\Thermal=0.\Dipole=0.2487892,-0.5017368,0.0637263\PG
=C01 [X(C4H6F3N1O3S1)]\@

NSO2CF3_c3.a1b2 32

1\1\GINC-AC25\FOpt\UB3LYP\6-31G(d)\C4H5F3N1O3S1(2)\JMH502\06-May-2009\
0\#\UB3LYP\6-31G(d) INT(grid=ultrafine) OPT freq=norman maxdisk=13421
77280\NSO2CF3_c3 confsearch\0,2\C,-2.0764859422,-1.650145192,0.40285
28216\C,-2.1387463871,-0.2590665885,-0.1780078053\O,-3.0852579458,0.14
31591424,-0.8189465585\N,-1.0464776889,0.6698525543,0.0326634472\C,-1.
1307231768,1.9381273038,-0.571040974\S,0.4386701601,0.3124348913,0.818
0602943\H,-1.18747184,-2.1953099397,0.0789303479\H,-2.9725874935,-2.16
72452842,0.0575773592\H,-2.0599405434,-1.6225177583,1.4950271422\H,-2.
0230862427,2.1210845413,-1.1457158657\H,-0.4552721951,2.7044175225,-0.
2285329366\O,1.0466344606,1.5737010224,1.2121336882\O,0.246939011,-0.7
879579003,1.7498406989\C,1.4804648765,-0.3570448395,-0.6006426624\F,2.
6442760632,-0.766956554,-0.1068430606\F,0.8477732791,-1.3864393062,-1.
1735780388\F,1.6792696048,0.5983573846,-1.5034568974\\Version=IA64L-G0
3RevE.01\State=2-A\HF=-1133.4278514\S2=0.753862\S2-1=0.\S2A=0.75001\RMS
D=4.829e-09\RMSF=3.985e-06\Thermal=0.\Dipole=0.0924003,-0.3732086,-0.
422752\PG=C01 [X(C4H5F3N1O3S1)]\@

NSO2CF3_c6.a1b2 33

1\1\GINC-AC26\FOpt\UB3LYP\6-31G(d)\C4H5F3N1O3S1(2)\JMH502\06-May-2009\
0\#\UB3LYP\6-31G(d) INT(grid=ultrafine) OPT freq=norman maxdisk=13421
77280\NSO2CF3_c6 confsearch\0,2\C,-2.024998,-1.655412,0.638465\C,-2.
057312,-0.40875,-0.081933\O,-2.956968,-0.146349,-0.876499\N,-1.065846,
0.614155,0.142164\C,-1.291335,1.877509,-0.597555\S,0.46634,0.370916,0.
811799\H,-1.318212,-1.884091,1.421538\H,-2.796045,-2.364586,0.36404\H,
-0.588651,2.623543,-0.233813\H,-1.168289,1.725907,-1.673278\H,-2.31340
9,2.201917,-0.401953\O,1.075703,1.673901,1.036351\O,0.40442,-0.643175,
1.856396\C,1.405876,-0.409971,-0.612432\F,2.649533,-0.675658,-0.227625
\F,0.795171,-1.54106,-0.978778\F,1.42257,0.435418,-1.645788\\Version=I
A64L-G03RevE.01\State=2-A\HF=-1133.4306956\S2=0.760133\S2-1=0.\S2A=0.7
50048\RMSD=5.101e-09\RMSF=2.565e-06\Thermal=0.\Dipole=-0.1664488,-0.25
4396,-0.4168098\PG=C01 [X(C4H5F3N1O3S1)]\@

NSO2CF3-TS 34

1\1\GINC-V1296\FTS\RB3LYP\6-31G(d)\C4H6F3N1O3S1\JMH502\01-Nov-2010\0\
B3LYP/6-31G(d) opt=(CalcFC,Noeigen,TS) freq=norman maxdisk=45875200
0 INT(grid=ultrafine)\SP Calc\0,1\C,0.0112766923,-0.0217416783,0.001
2636368\C,-0.0009376984,0.0124893179,1.5023335453\O,0.9659361657,0.030
4710773,2.2171656534\N,-1.3669567664,0.024634404,2.0684822354\C,-1.904
6008198,1.3480041768,2.4313510685\S,-1.8647936266,-1.3376948252,2.8914
48802\H,-0.3633609817,-1.003342745,-0.3139844267\H,1.0246505281,0.1299
7658,-0.3738597856\H,-0.6702041471,0.728188641,-0.4142138115\H,-2.9409
157286,1.2235248383,2.7473234635\H,-1.3216242835,1.8218330971,3.228097
5467\H,-1.8876180341,1.9812991845,1.5390645886\O,-3.2836230164,-1.1788
160954,3.1887974671\O,-1.3149224607,-2.4813873355,2.1724868885\C,-1.01
8833256,-1.3168746788,4.5742785528\F,-1.6391026355,-2.1893316752,5.367
4062506\F,0.262137837,-1.6457679428,4.4666342005\F,-1.1255461212,-0.08
78579421,5.0989770649\\Version=EM64L-G03RevE.01\State=1-A\HF=-1134.078
7771\RMSD=3.657e-09\RMSF=2.671e-06\Thermal=0.\Dipole=0.1716073,1.40817
98,-0.747194\PG=C01 [X(C4H6F3N1O3S1)]\@

NSO2CF3-TS_rad 35

1\1\GINC-V1297\FTS\UB3LYP\6-31G(d)\C4H5F3N1O3S1(2)\JMH502\01-Nov-2010\
0\#\B3LYP\6-31G(d) opt=(CalcFC,Noeigen,TS) freq=norman maxdisk=45875
2000 INT(grid=ultrafine)\SP Calc\0,2\C,0.021852026,-0.0059044272,0.0
752579273\C,-0.0270968621,0.008630447,1.5014176202\O,0.9652712108,0.00
89317933,2.2238210587\N,-1.3806823861,-0.0098602135,2.0716450168\C,-1.
9124007755,-1.3361924003,2.4337690924\S,-1.8808037235,1.3462281499,2.9
111716026\H,0.9913359452,-0.0333982119,-0.4093344254\H,-0.882222615,0.
0298198992,-0.5206891644\H,-2.9397167715,-1.2149845657,2.7783830848\H,
-1.9163723375,-1.9588232669,1.5339015616\H,-1.3086078435,-1.8186660502
,3.2098679436\O,-1.3529746479,2.5037021893,2.2005143254\O,-3.294423133
7,1.1664348737,3.2224103537\C,-1.0170805377,1.3148923454,4.5849353981\
F,-1.6502093931,2.1593612558,5.3983784006\F,-1.0905200262,0.0754742927
,5.0906099197\F,0.2544943625,1.6758325573,4.4717505915\\Version=EM64L-
G03RevE.01\State=2-A\HF=-1133.4183303\S2=0.766257\S2-1=0.\S2A=0.750078
\RMSD=4.356e-09\RMSF=2.922e-06\Thermal=0.\Dipole=0.2293223,-1.4542541,

-0.9080087\PG=C01 [X(C4H5F3N1O3S1)]\@

nhf-NHMe 36

1\1\GINC-X127\FOpt\RB3LYP\6-31G(d)\C3H8F1N1O1\JMH502\19-May-2009\0\#\B3LYP/6-31G(d) scf=tight opt freq=noraman maxdisk=671088640 INT(grid=ultrafine)\SP Calc\0,1\C,-0.0280102694,0.074410918,-0.1103682096\N,-0.0311793694,0.0010328532,1.3535158751\H,0.8892269048,-0.0536493816,1.7813046649\C,-0.945875069,0.8032170314,2.0579276579\O,-1.8819593767,1.3374495243,1.4945086412\C,-0.690481576,0.8695379005,3.5517880101\F,-0.1549521491,-2.2369597021,2.8919583592\H,-1.0496761321,-0.0612873274,-0.4660153162\H,0.6042641551,-0.7246511484,-0.50445763\H,0.3356474652,1.0427515609,-0.4750764716\H,-0.3154810568,-1.6340283257,2.1717003613\H,-1.5610782278,1.3072467501,4.0415107746\H,0.1851507672,1.4960938097,3.7638909066\H,-0.4963554893,-0.1341521643,3.942146006\Version=EM64L-G03RevE.01\State=1-A\HF=-348.9576262\RMSD=3.386e-09\RMSF=2.067e-06\Thermal=0.\Dipole=1.0710583,0.3567949,-0.3594984\PG=C01 [X(C3H8F1N1O1)]\@

nhf-NHMe_c3 37

1\1\GINC-V1251\Freq\UB3LYP\6-31G(d)\C3H7F1N1O1(2)\JMH502\27-Oct-2010\1\#\UB3LYP/6-31G(d) scf=tight freq=noraman maxdisk=458752000 INT(grid=ultrafine)\SP Calc\0,2\C\N,1,nc2\H,2,hn3,1,hnc3\C,2,cn4,3,cnh4,1,dih4,0\O,4,oc5,2,ocn5,1,dih5,0\C,4,cc6,2,ccn6,1,dih6,0\H,1,hc7,2,hcn7,4,dih7,0\H,1,hc8,2,hcn8,4,dih8,0\H,6,hc9,4,hcc9,2,dih9,0\H,6,hc10,4,hcc10,2,dih10,0\H,6,hc11,4,hcc11,2,dih11,0\H,2,hn12,4,hnc12,5,dih12,0\F,12,fh13,2,fhn13,1,dih13,0\nc2=1.393209\hn3=1.014967\hnc3=117.346\cn4=1.410304\cnh4=116.435\dih4=-157.659\oc5=1.216267\ocn5=120.681\dih5=9.653\cc6=1.514583\ccn6=114.215\dih6=-173.389\hc7=1.080198\hcn7=117.87\dih7=179.921\hc8=1.078839\hcn8=116.751\dih8=-15.604\hc9=1.095274\hcc9=109.129\dih9=-61.477\hc10=1.090296\hcc10=108.715\dih10=178.91\hc11=1.096886\hcc11=111.679\dih11=58.352\hn12=1.979419\hnc12=92.175\dih12=-104.426\fh13=0.944277\fhn13=151.733\dih13=179.75\Version=EM64L-G03RevE.01\State=2-A\HF=-348.2932647\S2=0.754329\S2-1=0.\S2A=0.750013\RMSD=8.919e-09\RMSF=3.207e-04\ZeroPoint=0.1000378\Thermal=0.1090034\Dipole=1.3034885,0.395038,-0.012642\@

nhf-NHMe_c6 38

1\1\GINC-X137\FOpt\UB3LYP\6-31G(d)\C3H7F1N1O1(2)\JMH502\19-May-2009\0\#\UB3LYP/6-31G(d) scf=tight opt=tight freq=noraman maxdisk=671088640 INT(grid=ultrafine)\SP Calc\0,2\C,-0.0951574614,-0.0510323105,-0.0334373841\N,0.0628407421,0.2035186403,1.4029405682\H,1.0003591528,0.0340207735,1.7551906335\C,-0.576397182,1.3278570684,1.9606397587\O,-1.4706803337,1.9230196319,1.3628237149\C,-0.1488865344,1.6951844578,3.2974374962\F,-0.3209520466,-2.4035379174,1.900542811\H,-1.1452335359,0.0910798038,-0.2895537774\H,0.1929226811,-1.0851742049,-0.2290884264\H,0.5064129266,0.6330497728,-0.6441868712\H,-0.4588296636,-1.4621241413,1.9286422454\H,-0.6299590677,2.5436287807,3.7673460645\H,0.6189543644,1.1523434752,3.8403456196\Version=EM64L-G03RevE.01\State=2-A\HF=-348.2914778\S2=0.75838\S2-1=0.\S2A=0.750039\RMSD=4.376e-09\RMSF=3.456e-07\Thermal=0.\Dipole=1.0861636,0.5400449,0.3019773\PG=C01 [X(C3H7F1N1O1)]\@

ohf-NHMe 39

1\1\GINC-X153\FOpt\RB3LYP\6-31G(d)\C3H8F1N1O1\JMH502\19-May-2009\0\#\B3LYP/6-31G(d) scf=tight opt freq=noraman maxdisk=671088640 INT(grid=ultrafine)\SP Calc\0,1\C,-0.0134985954,-0.0158553095,0.0057559351\N,-0.0058227656,-0.0850532637,1.4582793623\H,0.8786421023,-0.2083953751,1.9300442721\C,-1.1201787354,0.0417941562,2.2196616589\O,-2.2370417126,0.2144136978,1.7100852338\C,-0.9119021046,-0.0066455239,3.7213485639\H,-1.0527049458,0.0566473402,-0.3153286795\H,0.4373311278,-0.9154505269,-0.4270655643\H,0.5341787915,0.8640571827,-0.3514456699\H,-0.123439614,-0.7098551507,4.0084544988\H,-1.8575086183,-0.2792251799,4.1913334284\H,-0.6283747969,0.9905043,4.0798827963\H,-3.4540028818,0.0650331505,2.8071774774\F,-3.9759392876,-0.104668818,3.5977871774\Version=EM64L-G03RevE.01\State=1-A\HF=-348.9692937\RMSD=4.422e-09\RMSF=1.458e-05\Thermal=0.\Dipole=2.2989969,-0.0327232,-0.5715538\PG=C01 [X(C3H8F1N1O1)]\@

ohf-NHMe_c3 40

1\1\GINC-X147\FOpt\UB3LYP\6-31G(d)\C3H7F1N1O1(2)\JMH502\19-May-2009\0\#\UB3LYP/6-31G(d) scf=tight opt=tight freq=noraman maxdisk=671088640 INT(grid=ultrafine)\SP Calc\0,2\C,0.0007310666,0.0820452617,0.0862654658\N,0.0838904825,-0.0760824774,1.4514809767\H,0.9994754033,-0.0509550843,1.8815802006\C,-0.9923588641,-0.284243231,2.2789881466\O,-2.1380

863806,-0.3274983241,1.8096875279\C,-0.6795548494,-0.4874285319,3.7453
285164\H,0.9101450597,0.269881438,-0.463077517\H,-0.9788717897,0.05304
77248,-0.3626183827\H,-0.3897785119,-1.5309723934,3.9240566834\H,-1.58
58450679,-0.285866211,4.3178958128\H,0.137730668,0.1558439558,4.088815
8873\H,-3.2893910103,-0.3364397335,3.0023498602\F,-3.7418488127,-0.294
6523874,3.849029601\\Version=EM64L-G03RevE.01\State=2-A\HF=-348.309152
8\S2=0.755832\S2-1=0.\S2A=0.750022\RMSD=7.307e-09\RMSF=1.935e-07\Therm
al=0.\Dipole=2.2482226,0.0496511,-0.4818381\PG=C01 [X(C3H7F1N1O1)]\@

ohf-NHMe_c6 41

1\1\GINC-X154\FOpt\UB3LYP\6-31G(d)\C3H7F1N1O1(2)\JMH502\19-May-2009\0\
\# UB3LYP/6-31G(d) scf=tight opt=tight freq=noraman maxdisk=671088640
INT(grid=ultrafine)\SP Calc\1,2\C,0.0877925784,0.0982768925,-0.08386
86161\N,0.201772975,-0.4088534447,1.2713316306\H,1.0488298145,-0.22078
50185,1.7879691216\C,-0.7814047305,-1.1300524129,1.886039123\O,-1.8528
484665,-1.3960505598,1.3004170545\C,-0.5143256365,-1.5662147996,3.2453
258282\H,-0.8861908967,-0.2047250009,-0.4684456923\H,0.8736634444,-0.3
166078761,-0.7259657081\H,0.15752198,1.1922843245,-0.1010904569\H,-1.2
871424606,-2.1389367103,3.742590515\H,0.4161992117,-1.3353252209,3.754
226352\H,-2.8603843196,-2.2711533157,2.2588357987\F,-3.2482917363,-2.
7595610871,2.9936286346\\Version=EM64L-G03RevE.01\State=2-A\HF=-348.30
47089\S2=0.755119\S2-1=0.\S2A=0.750019\RMSD=7.272e-09\RMSF=1.834e-07\T
hermal=0.\Dipole=2.0751179,1.1168135,-0.3185806\PG=C01 [X(C3H7F1N1O1)]
\@

h+NHMe 42

1\1\GINC-X156\FOpt\RB3LYP\6-31G(d)\C3H8N1O1(1+)\JMH502\19-May-2009\0\
\# B3LYP/6-31G(d) scf=tight opt freq=noraman maxdisk=402653184 INT(grid
=ultrafine)\SP Calc\1,1\C,0.0072947341,0.0428671352,-0.0010931414\C,
0.0204737206,-0.0466926813,1.4881526147\O,0.9037211057,-0.0913089497,2
.2696683586\N,-1.4641653735,-0.0891084734,2.1160582917\H,-1.9677798809
,0.885551644,1.7050952747\C,-1.4752673108,-0.182698188,3.6191657638\
H,-0.5048607651,-0.8228289812,-0.4390349956\H,1.0393140579,0.070341567
, -0.355299642\H,-0.5159985564,0.948072522,-0.3330304272\H,-0.955161882
3,-1.0935228026,3.9126469226\H,-0.9563860205,0.6854148179,4.023352361\
H,-2.51356449,-0.2041759078,3.9522460331\H,-1.9713116066,0.7500058984,
1.806962907\\Version=EM64L-G03RevE.01\State=1-A\HF=-248.8539827\RMSD=9
.290e-09\RMSF=1.383e-05\Thermal=0.\Dipole=-1.7800912,0.0242512,-0.4856
46\PG=C01 [X(C3H8N1O1)]\@

h+NHMe_c3.a2 43

1\1\GINC-X152\FOpt\UB3LYP\6-31G(d)\C3H7N1O1(1+,2)\JMH502\26-Sep-2009\0\
\# UB3LYP/6-31G(d) scf=tight opt freq=noraman maxdisk=671088640 INT(g
rid=ultrafine)\SP Calc\1,2\C,-0.860606,1.371926,0.024925\C,-0.790598
, -0.106304,-0.00334\O,-1.531436,-1.004006,-0.08751\N,0.905898,-0.6696,
0.142923\H,0.89453,-1.477214,-0.491321\C,1.988178,0.216323,-0.116956\H
, -1.903894,1.669524,-0.103517\H,-0.241722,1.793814,-0.774479\H,-0.4791
75,1.744807,0.982926\H,2.309342,0.336646,-1.142221\H,2.375465,0.805496
,0.702171\H,0.933812,-1.045495,1.098283\\Version=EM64L-G03RevE.01\Stat
e=2-A\HF=-248.1748742\S2=0.755495\S2-1=0.\S2A=0.750021\RMSD=6.813e-09\
RMSF=6.084e-07\Thermal=0.\Dipole=1.1242093,0.2865427,0.2182175\PG=C01
[X(C3H7N1O1)]\@

h+NHMe_c6 44

1\1\GINC-X133\FOpt\UB3LYP\6-31G(d)\C3H7N1O1(1+,2)\JMH502\20-May-2009\0\
\# UB3LYP/6-31G(d) scf=tight opt=tight freq=noraman maxdisk=402653184
INT(grid=ultrafine)\SP Calc\1,2\C,0.0537556329,-0.3163261747,-0.011
6956917\C,-0.1523080648,0.328247793,1.2354828788\O,0.623994799,0.93473
11203,1.927782364\N,-1.6396757156,0.2227201625,1.7857103061\H,-1.8919
703998,-0.7702098523,1.8700435697\C,-1.8315442309,0.9155116244,3.11152
3977\H,1.0515046169,-0.2761541244,-0.4352018415\H,-0.7333238427,-0.837
5708145,-0.5472134653\H,-1.1617386312,0.4596242846,3.8391802607\H,-1.5
831172483,1.9687811126,2.9896033052\H,-2.8734658929,0.7918969069,3.408
7156995\H,-2.2802784031,0.6205532261,1.0871180472\\Version=EM64L-G03Re
vE.01\State=2-A\HF=-248.1925007\S2=0.764601\S2-1=0.\S2A=0.750069\RMSD=
8.296e-09\RMSF=3.115e-07\Thermal=0.\Dipole=-1.6511709,-0.8004129,-0.60
28869\PG=C01 [X(C3H7N1O1)]\@

oh+NHMe 45

1\1\GINC-X147\FOpt\RB3LYP\6-31G(d)\C3H8N1O1(1+)\JMH502\20-May-2009\0\
\# B3LYP/6-31G(d) scf=tight opt freq=noraman maxdisk=402653184 INT(grid
=ultrafine)\SP Calc\1,1\C,-0.0030552744,0.0018142518,0.0045066436\C,
0.0202586633,-0.0002907059,1.4974557245\O,1.1571285516,-0.0013399985,2

.1538753924\N,-1.0694000021,-0.0016334431,2.2131409418\H,-1.9468321458
, -0.0011483681,1.7021959685\C,-1.1557288974,-0.0040712993,3.6848399708
\H,0.5187597614,-0.8857747292,-0.3733952608\H,0.5188792417,0.890359662
6,-0.3709498367\H,-1.0206000771,0.0023971179,-0.3906494299\H,-0.153438
4907,-0.0012513088,4.1079887459\H,-1.6996506616,0.8874376355,4.0057505
074\H,-1.6935750194,-0.9001988588,4.0031304736\H,1.9305409383,-0.00059
34131,1.5605795177\Version=EM64L-G03RevE.01\State=1-A\HF=-248.8770824
\RMSD=2.566e-09\RMSF=2.221e-05\Thermal=0.\Dipole=-0.122614,0.0007774,-
0.68486\PG=C01 [X(C3H8N1O1)]\@

oh+NHMe_c3.a2 46

1\1\GINC-X136\FOpt\UB3LYP\6-31G(d)\C3H7N1O1(1+,2)\JMH502\20-May-2009\
\# UB3LYP/6-31G(d) scf=tight opt=tight freq=noraman maxdisk=402653184
INT(grid=ultrafine)\SP Calc\1,2\C,-0.0028506423,0.0000019205,0.00059
211022\C,0.0049969001,0.0000005132,1.4988575594\O,1.0981237703,0.00000
19185,2.230679928\N,-1.1334707271,-0.0000008236,2.2023445892\H,-1.9901
011896,-0.0000020799,1.6523014597\C,-1.2636955784,-0.0000006813,3.5582
13012\H,1.016590844,-0.00000084785,-0.387548924\H,-0.5158505414,0.88831
92212,-0.3825248398\H,-0.5158692258,-0.8883036446,-0.3825266761\H,-0.3
744684861,0.0000008761,4.17071911\H,-2.2643121451,-0.0000022369,3.9648
4892\H,1.9085953061,0.0000030799,1.6904558566\Version=EM64L-G03RevE.0
1\State=2-A\HF=-248.2134175\S2=0.763955\S2-1=0.\S2A=0.750071\RMSD=3.75
0e-09\RMSF=4.545e-06\Thermal=0.\Dipole=-0.2783525,0.0000007,-0.5330161
\PG=C01 [X(C3H7N1O1)]\@

oh+NHMe_c6.a2 47

1\1\GINC-X133\FOpt\UB3LYP\6-31G(d)\C3H7N1O1(1+,2)\JMH502\20-May-2009\
\# UB3LYP/6-31G(d) scf=tight opt=tight freq=noraman maxdisk=402653184
INT(grid=ultrafine)\SP Calc\1,2\C,0.0012957714,0.0000003063,0.01355
95089\C,-0.0045816126,-0.0000003477,1.4330880652\O,1.090898761,0.00000
04051,2.1723915175\N,-1.1376742515,-0.0000018172,2.120211945\H,-2.0031
683383,-0.0000014241,1.5903258944\C,-1.2156595484,-0.0000024432,3.5869
617356\H,0.934952291,0.0000015362,-0.5382004149\H,-0.9278461166,-0.000
0003376,-0.5450404762\H,-0.7197972264,-0.890624168,3.9835184501\H,-0.7
198165731,0.8906302152,3.9835184617\H,-2.2669524017,-0.000013722,3.870
5412946\H,1.9062750676,0.0000006628,1.6397739063\Version=EM64L-G03Rev
E.01\State=2-A\HF=-248.2131381\S2=0.760885\S2-1=0.\S2A=0.75005\RMSD=7.
891e-09\RMSF=2.545e-06\Thermal=0.\Dipole=-0.1579748,0.0000005,-0.83722
46\PG=C01 [X(C3H7N1O1)]\@

Amino-acetamides

h2n-ch2-conhme 98

1\1\GINC-V1298\FOpt\RB3LYP\6-31G(d)\C3H8N2O1\JMH502\01-Nov-2010\0\# B
3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine)\
SP Calc\0,1\N,0.0353846709,-0.1514149338,0.0495336113\C,0.020396656,-
0.020449881,1.4085217097\O,1.0330062663,0.1195462325,2.0856174783\C,-1
.3744793756,-0.0960881871,2.058310349\H,-0.8461513399,-0.2603466671,-0
.4321459647\C,1.2606558833,-0.1806249465,-0.7299858043\H,-1.6924103319
, -1.1485503562,2.041770181\N,-1.4239473906,0.3857040357,3.4303572607\H
, -2.1061619807,0.4549410886,1.453300922\H,-0.637989441,-0.0342528048,3
.9277876212\H,-1.2137838811,1.3837484467,3.4307698072\H,1.2763525406,0
.6239608478,-1.4746593478\H,2.0892124734,-0.0395399973,-0.0346292882\H
, 1.3845804321,-1.1410368902,-1.2450807969\Version=EM64L-G03RevE.01\St
ate=1-A\HF=-303.8656354\RMSD=4.645e-09\RMSF=8.281e-06\Thermal=0.\Dipol
e=-0.3606484,-0.0599684,-1.2966357\PG=C01 [X(C3H8N2O1)]\@

h2n-ch2-conhme_rad 99

1\1\GINC-V1258\FOpt\UB3LYP\6-31G(d)\C3H7N2O1(2)\JMH502\01-Nov-2010\0\
UB3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafin
e)\SP Calc\0,2\N,0.0363909801,-0.1909937132,0.0739920433\C,0.0150278
097,-0.0267108129,1.4465220693\O,1.052294623,0.1142764086,2.1168538601
\C,-1.2879088199,0.0182647072,2.0702771567\H,-0.8172246334,-0.49419868
61,-0.3737234698\C,1.2818086758,-0.3960728234,-0.6391985661\N,-1.31696
05853,0.0798186908,3.4389906232\H,-2.2263329451,-0.0720557514,1.535394
5074\H,-0.4073747268,0.2988714665,3.8376030509\H,-2.1110978723,0.51309
81344,3.8908921969\H,1.2358989311,0.076805408,-1.6260896915\H,2.077752
8853,0.0655805046,-0.0533963207\H,1.5245211245,-1.4610797027,-0.769660
5877\Version=EM64L-G03RevE.01\State=2-A\HF=-303.2294527\S2=0.753482\S
2-1=0.\S2A=0.75001\RMSD=4.162e-09\RMSF=2.996e-06\Thermal=0.\Dipole=-1.

2161765,0.04456,-0.4100096\PG=C01 [X(C3H7N2O1)]\@

h2n-ch2-conhme-TS 100

1\1\GINC-V1261\FTS\RB3LYP\6-31G(d)\C3H8N2O1\JMH502\01-Nov-2010\0\#\# B3LYP/6-31G(d) opt=(TS,CalcFC,Noeigen) freq=noraman maxdisk=458752000 INT(grid=ultrafine)\SP Calc\0,1\N,0.0274091972,-0.0191252774,0.0401577655\C,0.0039179907,0.0250933067,1.4923159474\O,1.001377165,0.0717629426,2.1798248292\C,-1.4022552127,-0.0027135817,2.0725170174\C,0.8210175078,-1.1611499047,-0.4582020246\H,0.4956758026,0.8370520193,-0.2641318316\H,-1.9046198669,-0.8946006327,1.672325455\N,-1.5052113118,0.0226829307,3.5217823088\H,-1.9553803146,0.8419581686,1.6387774427\H,-0.9726097566,-0.7588962432,3.902496899\H,-1.0264298188,0.8523713787,3.8708087136\H,0.8646032894,-1.1034293872,-1.5493878385\H,1.8429442991,-1.1981823765,-0.0559577285\H,0.3105666898,-2.093227454,-0.1938030342\Version=EM64L-G03RevE.01\State=1-A\HF=-303.8371894\RMSD=7.799e-09\RMSF=6.507e-06\Thermal=0.\Dipole=0.2039625,0.0078317,-0.5887176\PG=C01 [X(C3H8N2O1)]\@

h2n-ch2-conhme-TS_rad 101

1\1\GINC-V1262\FTS\UB3LYP\6-31G(d)\C3H7N2O1(2)\JMH502\01-Nov-2010\0\#\# B3LYP/6-31G(d) opt=(TS,CalcFC,Noeigen) freq=noraman maxdisk=458752000 INT(grid=ultrafine)\SP Calc\0,2\N,0.0131894069,0.0346162683,0.0391579143\C,-0.0021749735,-0.010346125,1.4882851651\O,1.0270264334,-0.0519033921,2.1874974764\C,-1.2993647226,0.0068497435,2.0755033628\H,0.4766011261,-0.8204660377,-0.2735789822\C,0.8011194617,1.1740706097,-0.464328112\N,-1.4033269868,-0.0830656297,3.4246598127\H,-2.2021497095,0.0526846217,1.4806737201\H,-0.5307982717,-0.022698486,3.9382136952\H,-2.2610074361,0.1405438216,3.9050902609\H,0.8546280001,1.1107101276,-1.5557346068\H,0.2847675336,2.1051013184,-0.2063083939\H,1.8204998176,1.2206206692,-0.055287636\Version=EM64L-G03RevE.01\State=2-A\HF=-303.2131857\S2=0.756239\S2-1=0.\S2A=0.750019\RMSD=3.845e-09\RMSF=2.707e-06\Thermal=0.\Dipole=-0.9925838,0.1532897,0.3911355\PG=C01 [X(C3H7N2O1)]\@

h2n-ch2-conme2 102

1\1\GINC-X14\FOpt\RB3LYP\6-31G(d)\C4H10N2O1\JMH502\13-Sep-2010\0\#\# B3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine)\SP Calc\0,1\N,-0.0303280771,0.1925885228,0.0351290533\C,-0.0873411271,0.0418206631,1.3985940088\O,0.9216722979,-0.1033727014,2.0843891054\C,-1.4754424953,0.0577093595,2.0792870805\C,-1.178987971,0.3667200838,-0.8366032124\C,1.2644227503,0.1809400591,-0.630195011\H,-2.1025985975,-0.738901604,1.6586773427\N,-1.421358672,-0.1085596989,3.5239504901\H,-1.986674015,1.0027023045,1.8547032738\H,-0.9154555608,-0.9720086216,3.7213637027\H,-0.8101448716,0.6161932607,3.9002609817\H,1.3151644656,-0.6382483953,-1.360049161\H,1.4322658232,1.1268510697,-1.1625202765\H,2.0370963167,0.045086413,0.1251777205\H,-1.2266271187,-0.4424379162,-1.5787628024\H,-2.1110018938,0.3663039511,-0.2738477789\H,-1.1086972576,1.3182020071,-1.3820261262\Version=EM64L-G03RevE.01\State=1-A\HF=-343.1725741\RMSD=4.546e-09\RMSF=1.061e-05\Thermal=0.\Dipole=-0.347026,0.1680357,-1.2812555\PG=C01 [X(C4H10N2O1)]\@

h2n-ch2-conme2_rad 103

1\1\GINC-X135\FOpt\UB3LYP\6-31G(d)\C4H9N2O1(2)\JMH502\13-Sep-2010\0\#\# B3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine)\SP Calc\0,2\N,0.006746566,-0.2250622452,0.0520948857\C,-0.0229495993,-0.0123084862,1.4229802873\O,1.0186124618,0.2011954508,2.0749809815\C,-1.2982937699,-0.01451923,2.1070191008\C,-1.1656545101,-0.6120801543,-0.7108045798\C,1.2995278388,-0.4148772777,-0.5847019798\N,-1.2494409818,0.1380289359,3.4664907225\H,-2.2594245884,-0.2201227204,1.6581322418\H,-0.3361100146,0.4355188841,3.7993521538\H,-2.0540360526,0.5110876749,3.9508167731\H,-0.9611654898,-0.451359833,-1.7735862668\H,-1.4401483337,-1.6701950484,-0.5741828487\H,-2.0274261762,0.0092511296,-0.450078823\H,1.3431478318,0.1460149125,-1.5264688681\H,2.0692377102,-0.0515927115,0.095033535\H,1.4930457789,-1.4761006623,-0.8054820914\Version=EM64L-G03RevE.01\State=2-A\HF=-342.5364979\S2=0.753443\S2-1=0.\S2A=0.750009\RMSD=5.229e-09\RMSF=1.883e-05\Thermal=0.\Dipole=-1.2202374,0.0311922,-0.3775379\PG=C01 [X(C4H9N2O1)]\@

h2n-ch2-conme2-TS 104

1\1\GINC-X88\FTS\RB3LYP\6-31G(d)\C4H10N2O1\JMH502\13-Sep-2010\0\#\# B3LYP/6-31G(d) opt=(TS,CalcFC,Noeigen) freq=noraman maxdisk=458752000 INT(grid=ultrafine)\SP Calc\0,1\N,0.1237912836,-0.0002114455,0.0656384853\C,0.0486325389,-0.0001300052,1.5155233825\O,1.0231012119,-0.0002710

309,2.2369027091\C,-1.3771710883,0.0001507096,2.048236818\C,0.797834817,-1.2132866655,-0.4163680054\C,0.7982689636,1.2125770832,-0.4164820736\H,-1.8915057546,-0.8688147551,1.6145942868\N,-1.5285907983,0.0002459803,3.4937594043\H,-1.8911942476,0.8692595832,1.6145123385\H,-1.0347794458,-0.8059500466,3.8754752946\H,-1.0344901787,0.8063007233,3.8753993367\H,0.7543191965,-1.2260024609,-1.5103746283\H,1.8515278947,-1.2765785968,-0.1005950498\H,0.2704841254,-2.0996321609,-0.0475417592\H,0.7547574789,1.2252058069,-1.5104898703\H,0.2712358626,2.099145983,-0.0477388112\H,1.8519847742,1.2755213442,-0.1007154511\Version=EM64L-G03RevE.01\State=1-A\HF=-343.1465994\RMSD=8.732e-09\RMSF=4.253e-06\Thermal=0.\Dipole=0.1095782,-0.0000487,-0.6221842\PG=C01 [X(C4H10N2O1)]\@

h2n-ch2-conme2-TS_rad 105

1\1\GINC-X75\FTS\UB3LYP\6-31G(d)\C4H9N2O1(2)\JMH502\13-Sep-2010\0\#\ B3LYP/6-31G(d) opt=(TS,CalcFC,Noeigen) freq=noraman maxdisk=458752000 INT(grid=ultrafine)\SP Calc\0,2\N,0.1212845446,0.002660499,0.0656346693\C,0.0517695693,0.002059001,1.5135912324\O,1.0566524618,0.0046476813,2.2481604191\C,-1.2658796578,0.0023022059,2.0545610111\C,0.8157621683,-1.1938874195,-0.4231619925\C,0.7682146748,1.2252194168,-0.4237585459\N,-1.4159831229,-0.046231929,3.4017694669\H,-2.1481797639,0.0050069537,1.4279035893\H,-0.5643874549,0.0515624008,3.943845127\H,-2.2955044309,0.170728401,3.844296795\H,0.7816186669,-1.2013373534,-1.5183529957\H,1.8686588199,-1.2441361093,-0.1011649548\H,0.2997704458,-2.0886818576,-0.0595376935\H,0.7348741073,1.230870175,-1.5189900845\H,0.2172759417,2.099635844,-0.0613954692\H,1.818377274,1.3173130536,-0.1013246971\Version=EM64L-G03RevE.01\State=2-A\HF=-342.5223955\S2=0.756315\S2-1=0.\S2A=0.750019\RMSD=4.115e-09\RMSF=3.795e-06\Thermal=0.\Dipole=-1.1263932,0.19566,0.3409328\PG=C01 [X(C4H9N2O1)]\@

h2n-ch2-concf3 106

1\1\GINC-X13\FOpt\RB3LYP\6-31G(d)\C4H7F3N2O1\JMH502\14-Sep-2010\0\#\ B3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine)\SP Calc\0,1\N,0.0045832196,0.1466506641,-0.0244072634\C,-0.0075332219,0.1055560454,1.3789157778\O,1.0377374397,0.1712031539,2.0039398142\C,-1.3567380323,0.0133528278,2.1207798041\C,-1.1620277573,-0.0576470428,-0.8017342963\C,1.2998371504,0.1881003589,-0.7215487789\H,-1.9862484589,-0.7592552558,1.6701325171\N,-1.2206302928,-0.2445551805,3.542949377\H,-1.8869538569,0.9615852793,1.9754388295\H,-0.7808968469,-1.1544005614,3.6761355763\H,-0.553227678,0.4216559978,3.9298407024\H,1.4668445602,-0.7296072822,-1.2934281963\H,1.3466406615,1.0470645947,-1.3944592335\H,2.0611719681,0.2798173454,0.0500797591\F,-1.6610341975,-1.3149272394,-0.6862314013\F,-2.1634440693,0.7795691764,-0.457380741\F,-0.8917866272,0.1416637341,-2.1005411627\Version=EM64L-G03RevE.01\State=1-A\HF=-640.8958588\RMSD=6.667e-09\RMSF=4.354e-05\Thermal=0.\Dipole=0.3563476,-0.0235153,-0.5935086\PG=C01 [X(C4H7F3N2O1)]\@

h2n-ch2-concf3_rad 107

1\1\GINC-X14\FOpt\UB3LYP\6-31G(d)\C4H6F3N2O1(2)\JMH502\14-Sep-2010\0\#\ B3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine)\SP Calc\0,2\N,0.005332601,-0.0260371777,-0.018042985\C,-0.0037624913,-0.0300252103,1.4028527354\O,1.0691278571,-0.0697775517,2.0252582546\C,-1.25314235,0.0357695822,2.1067293836\C,-1.1737602058,-0.1684465402,-0.7708706586\C,1.2971683434,-0.1478608887,-0.7018529228\N,-1.1878928558,-0.0611897117,3.4637414172\H,-2.2261172036,0.1010366453,1.6455682437\H,-0.2540225369,0.008971933,3.8543090648\H,-1.9571536069,0.2655340136,4.0295208448\F,-0.8953278392,-0.1700642949,-2.0842555737\F,-1.8511636581,-1.3153621114,-0.500490889\F,-2.0606918521,0.8367018886,-0.5460359945\H,1.407054591,0.6318284831,-1.4593081429\H,2.059940427,-0.0304258579,0.0652611228\H,1.4101901715,-1.1289036275,-1.175844681\Version=EM64L-G03RevE.01\State=2-A\HF=-640.2639368\S2=0.753849\S2-1=0.\S2A=0.750011\RMSD=6.181e-09\RMSF=9.007e-06\Thermal=0.\Dipole=-0.4854653,0.2864133,0.5196241\PG=C01 [X(C4H6F3N2O1)]\@

h2n-ch2-concf3-TS 108

1\1\GINC-V1251\FTS\RB3LYP\6-31G(d)\C4H7F3N2O1\JMH502\14-Sep-2010\0\#\ B3LYP/6-31G(d) opt=(TS,CalcFC,Noeigen) freq=noraman maxdisk=458752000 INT(grid=ultrafine)\SP Calc\0,1\N,0.0905650049,0.0268148336,0.0404698285\C,0.0377114878,0.0693473424,1.5081878399\O,1.0263814192,0.1592700038,2.1926168006\C,-1.3781522597,-0.0221305853,2.0505395363\C,0.6356454211,-1.2427734268,-0.4723758592\C,0.6496510634,1.1830391936,-0.5449749107\H,-1.8653505477,-0.8924919671,1.5898052566\N,-1.512234583,-0.0744854327,3.4932428487\H,-1.9191512332,0.8469390833,1.6505098623\H,-0.997

118329,-0.876635176,3.8532861097\H,-1.0556949136,0.7398641129,3.901614
9091\H,0.5566652479,-1.2419373612,-1.5611594385\H,1.680747863,-1.39771
87871,-0.177384154\H,0.0263189234,-2.0642956973,-0.0859669859\F,0.3693
362586,1.2247769035,-1.8632314264\F,0.1236332888,2.2790486401,0.040121
0455\F,1.998409875,1.2833257592,-0.4416190812\Version=EM64L-G03RevE.0
1\State=1-A\HF=-640.8760827\RMSD=4.073e-09\RMSF=9.751e-06\Thermal=0.\D
ipole=-0.2472213,-0.8352031,-0.1142816\PG=C01 [X(C4H7F3N2O1)]\@

h2n-ch2-concf3-TS_rad 109

1\1\GINC-V1327\FTS\UB3LYP\6-31G(d)\C4H6F3N2O1(2)\JMH502\14-Sep-2010\0\
\# B3LYP/6-31G(d) opt=(TS,CalcFC,Noeigen) freq=noraman maxdisk=4587520
00 INT(grid=ultrafine)\SP Calc\0,2\N,0.0922454775,-0.0407663724,0.05
06620978\C,0.0384826715,-0.0706403478,1.5091405464\O,1.0434861617,-0.2
208545972,2.2186343214\C,-1.2622048153,0.1145631188,2.0502080657\C,0.6
84880865,-1.1801680426,-0.5345769167\C,0.5946463951,1.2365162528,-0.48
4513844\N,-1.3975006568,0.2024552464,3.3941448577\H,-2.1423671774,0.21
03130768,1.4278929909\H,-0.568994289,-0.0022846177,3.9421356145\H,-2.2
985771296,0.1202056835,3.8392623046\F,0.3991204214,-1.2270690257,-1.85
67313649\F,2.0388970552,-1.2325368004,-0.4470544993\F,0.2047441293,-2.
2980961954,0.0392346301\H,0.535380944,1.2137398904,-1.5746067758\H,-0.
0501729998,2.0393040287,-0.1179599804\H,1.6287901716,1.4372374552,-0.1
767575463\Version=EM64L-G03RevE.01\State=2-A\HF=-640.2537731\S2=0.756
504\S2-1=0.\S2A=0.750019\RMSD=5.627e-09\RMSF=1.046e-05\Thermal=0.\Dipo
le=-1.5286965,0.8409548,0.8654838\PG=C01 [X(C4H6F3N2O1)]\@

h2n-ch2-concoch3 110

1\1\GINC-V1257\FOpt\RB3LYP\6-31G(d)\C5H10N2O2\JMH502\14-Sep-2010\0\#
B3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine)
\SP Calc\0,1\C,0.0123733767,-0.0001589637,-0.0036263332\C,-0.01349143
45,0.0002452968,1.5163442196\O,1.0231355919,0.00008962,2.1578662887\N,
-1.2829726502,0.0002380715,2.1182140862\C,-2.4933881581,-0.0000414897,
1.2808859208\C,-1.4944211319,0.0001274732,3.5257554964\H,-0.4856645152
, -0.882895914,-0.4191476058\H,1.0588593444,-0.0010767306,-0.3096776339
\H,-0.4841117837,0.8833329266,-0.4194254732\H,-2.5327564907,-0.8920776
677,0.6491429946\H,-3.3493066701,0.0009477546,1.9517997974\H,-2.531914
3144,0.890801311,0.6474458246\O,-2.6360616436,-0.0002348801,3.95644263
08\C,-0.3060281688,0.0004405483,4.5015982353\H,0.3301745039,0.86631509
1,4.2969352134\N,-0.7093554421,0.0004192313,5.8981531121\H,0.330544486
3,-0.8651846778,4.2970243176\H,-1.3114580348,0.8050864232,6.0688389565
\H,-1.3111218596,-0.804484455,6.0689083728\Version=EM64L-G03RevE.01\St
ate=1-A\HF=-456.5158498\RMSD=9.284e-09\RMSF=2.722e-05\Thermal=0.\Dipo
le=-0.6347677,0.0001602,-1.4450603\PG=C01 [X(C5H10N2O2)]\@

h2n-ch2-concoch3_rad 111

1\1\GINC-V1261\FOpt\UB3LYP\6-31G(d)\C5H9N2O2(2)\JMH502\14-Sep-2010\0\
\# B3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine)
\SP Calc\0,2\C,0.0268720687,0.0375030395,-0.0024284709\C,-0.0310744
041,0.0589098786,1.518550895\O,1.0034660658,0.1455862703,2.169793674\N
, -1.2974105318,-0.023600641,2.0897129741\C,-2.486639848,-0.1066571363,
1.2321308539\C,-1.5618530589,-0.0257377423,3.5053545537\H,-0.398667442
9,-0.8839342655,-0.4150534879\H,1.0774938871,0.1054734731,-0.286417802
2\H,-0.5201855033,0.8774477604,-0.4447117502\H,-2.458747347,-1.0023543
981,0.6037568388\H,-3.3516725541,-0.1574749656,1.8896215064\H,-2.57506
79837,0.7761310981,0.5911256433\O,-2.7431307133,-0.0734453352,3.898229
4289\C,-0.4949189159,0.021924001,4.4568659895\H,0.5472567978,0.0723818
893,4.1916399113\N,-0.8574537763,-0.0396120331,5.7632614501\H,-0.20164
29956,0.1990846629,6.4905891507\H,-1.8497957019,0.020111426,5.96047713
92\Version=EM64L-G03RevE.01\State=2-A\HF=-455.8871236\S2=0.754306\S2-
1=0.\S2A=0.750012\RMSD=5.062e-09\RMSF=7.705e-06\Thermal=0.\Dipole=-0.0
056447,0.1425217,-0.0231196\PG=C01 [X(C5H9N2O2)]\@

h2n-ch2-concoch3-TS 112

1\1\GINC-V1253\FTS\RB3LYP\6-31G(d)\C5H10N2O2\JMH502\14-Sep-2010\0\# B
3LYP/6-31G(d) opt=(CalcFC,Noeigen,TS) freq=noraman maxdisk=458752000 I
NT(grid=ultrafine)\SP Calc\0,1\C,0.0634033908,0.0067558837,0.0388620
082\C,0.0228131279,0.0270207951,1.5636351468\O,1.0150027106,0.06556172
24,2.2528858494\N,-1.3031334891,-0.0842748297,2.1396911428\C,-1.652942
5749,-1.4119577464,2.654565171\C,-2.010891384,1.0201790162,2.602071794
7\H,-0.4234279652,-0.9252857356,-0.2835882755\N,1.3762463389,0.1097499
201,-0.5690480485\H,-0.5893008383,0.8050336038,-0.3378469978\H,-0.9986
644592,-1.698056685,3.4864566817\H,-2.6837711031,-1.3613625293,3.00474
247\H,-1.5700244976,-2.1591246952,1.858391311\O,-3.0307703004,0.897636

1878,3.2621031852\C,-1.4393290332,2.3827289479,2.2455277138\H,-1.17282
84139,2.4651360945,1.1863714166\H,-2.1887753461,3.1375297531,2.4861463
181\H,-0.5357924321,2.5769969385,2.8346675376\H,1.814883121,0.98215118
72,-0.2774284405\H,1.9760902998,-0.624282573,-0.1950511083\Version=EM
64L-G03RevE.01\State=1-A\HF=-456.4987526\RMSD=9.264e-09\RMSF=2.171e-06
\Thermal=0.\Dipole=0.4956703,-0.1644342,-0.5973282\PG=C01 [X(C5H10N2O2
)]\@

h2n-ch2-concoch3-TS_rad 113

1\1\GINC-V1253\FTS\UB3LYP\6-31G(d)\C5H9N2O2(2)\JMH502\14-Sep-2010\0\#\
B3LYP/6-31G(d) opt=(CalcFC,Noeigen,TS) freq=noraman maxdisk=458752000
INT(grid=ultrafine)\SP Calc\0,2\C,-0.0015675503,0.012257171,0.07564
7238\C,-0.020138785,0.0058290562,1.4986263767\O,1.0242441984,0.0325557
296,2.1703283576\N,-1.3259911592,-0.0822878728,2.1146220777\C,-1.70579
68755,-1.406420599,2.6116871919\C,-1.9613431861,1.0334849735,2.6425157
15\H,-0.9041670098,-0.0248338434,-0.5213855022\N,1.1914480235,0.092072
4842,-0.5553188095\H,-1.0064052623,-1.7515555448,3.3827838211\H,-2.705
0916956,-1.3259774529,3.039131358\H,-1.7093822927,-2.1269513917,1.7868
846887\O,-2.9463951146,0.9373515302,3.3610204475\C,-1.3743393332,2.381
9825214,2.2559836346\H,-1.2794516539,2.488249578,1.1697740421\H,-2.032
738638,3.1606276326,2.6427841301\H,-0.3746685823,2.5018746546,2.687489
5002\H,2.0196391142,0.0556164639,0.0279024553\H,1.2846994572,-0.032931
5181,-1.5508342616\Version=EM64L-G03RevE.01\State=2-A\HF=-455.877556\
S2=0.756545\S2-1=0.\S2A=0.75002\RMSD=4.680e-09\RMSF=3.192e-06\Thermal=
0.\Dipole=0.9672165,-0.3467513,-2.2111142\PG=C01 [X(C5H9N2O2)]\@

h2n-ch2-concofc3 114

1\1\GINC-V1258\FOpt\RB3LYP\6-31G(d)\C5H7F3N2O2\JMH502\01-Nov-2010\0\#\
B3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine)
\SP Calc\0,1\C,0.0377373543,0.0244355625,-0.0199345452\C,-0.01698609
18,0.0727557456,1.5388395045\O,1.0421783337,0.1346287236,2.1290529798\
N,-1.2677318664,0.0370981476,2.1301793948\C,-2.5195590387,-0.001737003
5,1.3419937931\C,-1.4460251402,-0.0402518156,3.5518347534\F,-0.6526346
71,-1.0256656601,-0.5120692673\F,1.3018316919,-0.0876640893,-0.4159060
566\F,-0.4728319199,1.153998859,-0.5618209611\H,-2.7966879119,-1.03172
54122,1.1034470388\H,-3.3027485171,0.4381117795,1.955022306\H,-2.40440
73651,0.572457371,0.4271291167\O,-2.5783881748,-0.1458873272,3.9815620
216\C,-0.2437354295,0.0152433634,4.5075397429\H,0.3249271211,0.9309359
639,4.3190270298\N,-0.6200398637,-0.0551611271,5.9073568035\H,0.448025
4108,-0.797725547,4.266413223\H,-1.2693759753,0.7007772016,6.120299459
\H,-1.1538373949,-0.90771779,6.0703453738\Version=EM64L-G03RevE.01\St
ate=1-A\HF=-754.2196466\RMSD=4.522e-09\RMSF=4.884e-06\Thermal=0.\Dipol
e=-0.7935902,0.0022622,-0.4459164\PG=C01 [X(C5H7F3N2O2)]\@

h2n-ch2-concofc3_rad 115

1\1\GINC-V1261\FOpt\UB3LYP\6-31G(d)\C5H6F3N2O2(2)\JMH502\01-Nov-2010\
\# B3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafi
ne)\SP Calc\0,2\C,0.0368301888,-0.0364797308,-0.0187986196\C,-0.0172
341357,-0.0712932754,1.5390585926\O,1.0541686895,-0.131231492,2.121578
9424\N,-1.2562082385,-0.0321747702,2.1273467539\C,-2.5074821013,0.0201
141223,1.3445186158\C,-1.4555871113,0.05103547,3.5595032506\F,-0.47689
72199,-1.168073394,-0.5573831748\F,1.3021110512,0.066753914,-0.4192652
824\F,-0.6470786545,1.0118164971,-0.5270934112\H,-2.4036456269,-0.5598
672314,0.4317638257\H,-3.2941865135,-0.4037551661,1.9640384658\H,-2.77
41969983,1.0522982133,1.1013462754\O,-2.6172761639,0.1876737188,3.9807
307746\C,-0.3579663548,-0.032350825,4.4697442496\H,0.6691743523,-0.161
1229141,4.1737755563\N,-0.6640414784,0.0872605005,5.781544022\H,0.0239
649777,-0.069593169,6.5002385053\H,-1.6439242105,0.1512668855,6.029901
559\Version=EM64L-G03RevE.01\State=2-A\HF=-753.5932813\S2=0.754677\S2
-1=0.\S2A=0.750013\RMSD=5.236e-09\RMSF=1.325e-05\Thermal=0.\Dipole=-0.
137374,-0.1322818,1.0474866\PG=C01 [X(C5H6F3N2O2)]\@

h2n-ch2-concofc3-TS 116

1\1\GINC-V1262\FTS\RB3LYP\6-31G(d)\C5H7F3N2O2\JMH502\01-Nov-2010\0\#\
B3LYP/6-31G(d) opt=(CalcFC,Noeigen,TS) freq=noraman maxdisk=458752000
INT(grid=ultrafine)\SP Calc\0,1\C,0.0270179768,-0.0219252544,-0.0016
598331\C,0.037609502,0.0128198606,1.5212657849\O,1.0348007793,-0.01598
32124,2.1949650583\N,-1.2904179203,-0.0412779687,2.1477166272\C,-1.687
3361093,-1.3833233007,2.6003405672\C,-1.9649665441,1.0257477147,2.6834
039024\H,-0.534934884,-0.9197829323,-0.2994808629\N,1.3262152598,-0.01
81356393,-0.642020949\H,-0.5726167783,0.8218510135,-0.3573077788\H,-1.
1331994722,-1.6707573944,3.5005859849\H,-2.7540361325,-1.3668706698,2.

8220116947\H,-1.486057072,-2.107175162,1.8058504151\O,-2.9452605794,0.9286573289,3.3974318878\C,-1.4347773681,2.4371518106,2.3166460095\F,-1.3481529364,2.596450518,0.9708973472\F,-2.2482031845,3.3738373035,2.7919873406\F,-0.2019953333,2.6375290157,2.8237246799\H,1.810993441,0.8502530627,-0.421775282\H,1.9042730572,-0.7584231108,-0.2473860599\\Version=EM64L-G03RevE.01\State=1-A\HF=-754.204749\RMSD=6.327e-09\RMSF=2.268e-06\Thermal=0.\Dipole=0.2946501,-0.9208763,-0.5658955\PG=C01 [X(C5H7F3N2O2)]\@

h2n-ch2-concof3-TS_rad 117

1\1\GINC-V1265\FTS\UB3LYP\6-31G(d)\C5H6F3N2O2(2)\JMH502\01-Nov-2010\0\#\B3LYP/6-31G(d) opt=(CalcFC,Noeigen,TS) freq=noraman maxdisk=45875200 INT(grid=ultrafine)\SP Calc\0,2\C,0.003117127,-0.1120246416,-0.0159266778\C,0.0312624427,0.0300292325,1.3960946606\O,1.0806912936,0.1258391387,2.0451348547\N,-1.2695668294,-0.0057948173,2.0581875903\C,-1.7214686336,-1.3330319513,2.4951809154\C,-1.8360202614,1.0768207449,2.6765253801\H,-0.9191570319,-0.1606505921,-0.58045423\N,1.1770698598,-0.1966338255,-0.6803011219\H,-1.1514980124,-1.6733461992,3.3675822991\H,-2.7771966424,-1.2739357487,2.7600604637\H,-1.5787103706,-2.0415920506,1.6751337936\O,-2.7491006666,1.0124120464,3.4800683425\C,-1.2929491141,2.4736471031,2.2697991563\F,-1.1079230282,2.5718605782,0.9298376246\F,-2.1616286572,3.4197507009,2.6311423119\F,-0.1149508736,2.7289353328,2.8661279401\H,2.0184088957,-0.0371194188,-0.1371779264\H,1.2252899073,-0.0934797215,-1.6822994531\\Version=EM64L-G03RevE.01\State=2-A\HF=-753.5838698\S2=0.756664\S2-1=0.\S2A=0.75002\RMSD=9.552e-09\RMSF=1.345e-05\Thermal=0.\Dipole=0.6461665,-1.0934142,-2.2050134\PG=C01 [X(C5H6F3N2O2)]\@

h2n-ch2-conso2me.a3b2d2 118

1\1\GINC-V1301\FOpt\RB3LYP\6-31G(d)\C4H10N2O3S1\JMH502\02-Nov-2010\0\#\B3LYP/6-31G(d) opt freq=noraman INT(grid=ultrafine) maxdisk=458752000 \h2n-ch2-conso2me confsearch\0,1\C,2.551439,0.523278,-0.058931\C,1.185334,-0.190479,-0.057835\O,1.114727,-1.409407,-0.008916\N,0.054893,0.616892,-0.144202\C,0.12399,2.085235,-0.171871\S,-1.515376,-0.104822,0.166598\H,2.658266,1.085422,-0.996426\N,3.684633,-0.369719,0.091153\H,2.570705,1.27044,0.744074\H,-0.874729,2.467019,-0.37936\H,0.465886,2.492629,0.785945\H,0.798084,2.410829,-0.968276\O,-1.490496,-0.774998,1.462339\O,-2.471282,0.974831,-0.094356\C,-1.669392,-1.329966,-1.141618\H,-2.641955,-1.804884,-0.990713\H,-1.640234,-0.814467,-2.102835\H,-0.854967,-2.044548,-1.033635\H,3.593844,-0.869094,0.975177\H,3.62261,-1.098227,-0.619183\\Version=EM64L-G03RevE.01\State=1-A\HF=-891.7410816\RMSD=4.685e-09\RMSF=6.245e-06\Thermal=0.\Dipole=0.4608096,0.4059862,-1.1661404\PG=C01 [X(C4H10N2O3S1)]\@

h2n-ch2-conso2me_rad 119

1\1\GINC-V1256\FOpt\UB3LYP\6-31G(d)\C4H9N2O3S1(2)\JMH502\01-Nov-2010\0\#\UB3LYP/6-31G(d) INT(grid=ultrafine) OPT freq=noraman maxdisk=458752000\NSO2Me_c6 confsearch\0,2\C,-0.0165926922,0.0164690234,-0.0553744379\C,-0.0174194832,0.1345495866,1.3718858544\O,1.031111176,0.3548464421,1.9992318808\N,-1.2282904493,-0.0657563217,2.1137949395\C,-1.0714027369,-0.0773138371,3.579324526\S,-2.7728577284,0.3312252707,1.5070217227\H,-0.8771752863,-0.2643810046,-0.6424603241\N,1.1574537352,0.293992199,-0.6837996878\H,-1.9892872098,-0.4576998061,4.0224053904\H,-0.2370768533,-0.7372894895,3.8171398362\H,-0.8420698903,0.9187588531,3.9762983935\O,-2.9099927416,-0.2434591979,0.1672734756\O,-3.7329863087,0.0003797956,2.5585861871\C,-2.7350114075,2.129267197,1.3268086914\H,-3.7074601483,2.4313377486,0.9314109507\H,-2.5665039862,2.5787837299,2.3073324285\H,-1.9388815648,2.3967776264,0.6293580229\H,1.3138587048,-0.0342043568,-1.6251845384\H,1.9656748499,0.3915782152,-0.0780881007\\Version=EM64L-G03RevE.01\State=2-A\HF=-891.1110849\S2=0.754297\S2-1=0.\S2A=0.750012\RMSD=7.212e-09\RMSF=1.213e-06\Thermal=0.\Dipole=0.8682218,0.8803973,-0.7928224\PG=C01 [X(C4H9N2O3S1)]\@

h2n-ch2-conso2me-TS 120

1\1\GINC-V1260\FTS\RB3LYP\6-31G(d)\C4H10N2O3S1\JMH502\01-Nov-2010\0\#\B3LYP/6-31G(d) opt=(CalcFC,Noeigen,TS) freq=noraman maxdisk=458752000 INT(grid=ultrafine)\SP Calc\0,1\C,0.0306179595,0.0346916031,0.0173298041\C,0.0112710664,0.0221345969,1.5348427676\O,0.9987345934,0.0257270014,2.2324495979\N,-1.3415094743,-0.004291334,2.0952169039\C,-1.8149022053,1.2749807148,2.6470959557\S,-1.7369333336,-1.4289119775,2.9367536409\H,-0.4664887627,-0.8946409668,-0.2935746046\N,1.3335722527,0.1421180699,-0.6078550407\H,-0.6294816412,0.8411567704,-0.3304236561\H,-2.8

502794314,1.1463248118,2.9663203285\H,-1.2021208804,1.6302846514,3.486
9166301\H,-1.7906612176,2.0260152615,1.8513201455\O,-3.1569338228,-1.3
301050799,3.272148017\O,-1.2077804689,-2.5098563463,2.1035886235\C,-0.
8011796397,-1.4042154642,4.4827268079\H,-1.0123072295,-2.3469988737,4.
9926206718\H,0.2589227312,-1.3116118474,4.2457076188\H,-1.1428502414,-
0.5641046035,5.0906635849\H,1.8020283665,0.9869704496,-0.2840274992\H,
1.9204811457,-0.6295694224,-0.2949900376\\Version=EM64L-G03RevE.01\Sta
te=1-A\HF=-891.7263072\RMSD=9.891e-09\RMSF=5.218e-06\Thermal=0.\Dipole
=0.6050298,1.2894079,0.7481673\PG=C01 [X(C4H10N2O3S1)]\@

h2n-ch2-conso2me-TS_rad 121

1\1\GINC-V1261\FTS\UB3LYP\6-31G(d)\C4H9N2O3S1(2)\JMH502\01-Nov-2010\0\
\# B3LYP/6-31G(d) opt=(CalcFC,Noeigen,TS) freq=noraman maxdisk=4587520
00 INT(grid=ultrafine)\SP Calc\0,2\C,-0.0499201686,-0.0226749916,-0.
0161092847\C,-0.0180400289,0.1535670092,1.393395343\O,1.0356793926,0.3
736282234,2.0147119217\N,-1.3118106295,0.0519497574,2.043265186\C,-1.7
140605085,-1.2939403937,2.4794473265\S,-1.7542155211,1.3643139466,3.03
43237721\H,-0.9741743841,-0.1537774224,-0.5635390196\N,1.1211796914,-0
.0492929198,-0.6929894115\H,-2.7324759312,-1.2455889281,2.866529831\H,
-1.6993329342,-1.9558049624,1.6082744349\H,-1.0422376073,-1.7092309465
,3.24430747\O,-1.4408112867,2.5689164866,2.2674932061\O,-3.1159623266,
1.0795504052,3.494226488\C,-0.6669695199,1.316751219,4.4758965275\H,-0
.8520119621,0.3923900199,5.027223119\H,0.3630844453,1.3639111524,4.122
9323895\H,-0.9235401639,2.1805889125,5.0935367499\H,1.1458635241,0.055
323414,-1.6960672752\H,1.9483991172,0.2092819201,-0.1660042064\\Versio
n=EM64L-G03RevE.01\State=2-A\HF=-891.104612\S2=0.755879\S2-1=0.\S2A=0.
750017\RMSD=5.485e-09\RMSF=3.809e-06\Thermal=0.\Dipole=1.1854702,-1.34
4763,-1.0655691\PG=C01 [X(C4H9N2O3S1)]\@

h2n-ch2-conso2cf3 122

1\1\GINC-V1265\FOpt\RB3LYP\6-31G(d)\C4H7F3N2O3S1\JMH502\01-Nov-2010\0\
\# B3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafin
e)\SP Calc\0,1\C,0.0674632301,0.0518021984,-0.0131945583\C,0.0004056
985,-0.0236839773,1.5222950651\O,1.0082798857,-0.1192258893,2.19394680
16\N,-1.2413380771,0.0401902729,2.225069684\C,-1.1511237008,-0.0359358
01,3.703277784\S,-2.7835500339,0.0415441735,1.5277648147\H,-0.56948669
6,-0.7232599911,-0.4486676816\N,1.4145589236,-0.0791705541,-0.53454345
13\H,-0.3640532544,1.0030875299,-0.337948646\H,-2.1332616598,0.1632324
666,4.1259236448\H,-0.7950475667,-1.0227968388,4.0081719595\H,-0.44135
70761,0.7186077877,4.0431137386\O,-3.73005997,0.5423657195,2.514276194
6\O,-2.7126734222,0.5713659282,0.1742110225\C,-3.1387761369,-1.7939738
208,1.3629647527\F,-4.3472299743,-1.9594989587,0.8377247298\F,-2.22251
87639,-2.3633806104,0.5721565622\F,-3.0870053742,-2.3615207306,2.57041
99994\H,2.0071286772,0.6377381924,-0.1189060802\H,1.8153355405,-0.9626
446795,-0.223174016\\Version=EM64L-G03RevE.01\State=1-A\HF=-1189.43598
13\RMSD=5.151e-09\RMSF=3.010e-06\Thermal=0.\Dipole=0.2963829,-0.557581
9,0.6375251\PG=C01 [X(C4H7F3N2O3S1)]\@

h2n-ch2-conso2cf3_rad 123

1\1\GINC-V1265\FOpt\UB3LYP\6-31G(d)\C4H6F3N2O3S1(2)\JMH502\01-Nov-2010
\0\#UB3LYP/6-31G(d) INT(grid=ultrafine) OPT freq=noraman maxdisk=4587
52000\NSO2Me_c6 confsearch\0,2\C,0.0583752252,-0.1845886376,-0.05656
7756\C,-0.0008968207,0.1615922393,1.3241175365\O,0.9919755824,0.558459
0675,1.9492116404\N,-1.234397257,-0.0477239977,2.0672998417\C,-1.08109
48047,-0.01073388253,3.5395577758\S,-2.7530382379,0.3102412639,1.452793
3189\H,-0.7705748723,-0.5895746408,-0.6151463096\N,1.2453962924,-0.001
781141,-0.6800332687\H,-2.0065929447,-0.3634126213,3.9906757998\H,-0.2
621705504,-0.681984067,3.7990062738\H,-0.8381421619,0.9940538743,3.894
6182485\O,-2.8179039464,-0.0666868588,0.0446949663\O,-3.7547355489,-0.
1276602425,2.4164921966\C,-2.8110003881,2.1870595789,1.4650486586\F,-3
.9726890258,2.600145487,0.9642317386\F,-2.6820079008,2.6298010206,2.71
98592018\F,-1.807822435,2.6701860658,0.7251760148\H,1.3358837956,-0.08
94995847,-1.6796016115\H,1.9905601557,0.434918692,-0.1512048678\\Versi
on=EM64L-G03RevE.01\State=2-A\HF=-1188.8079687\S2=0.754629\S2-1=0.\S2A
=0.750013\RMSD=5.906e-09\RMSF=3.776e-06\Thermal=0.\Dipole=1.1863253,0.
1307932,-0.7674818\PG=C01 [X(C4H6F3N2O3S1)]\@

h2n-ch2-conso2cf3-TS 124

1\1\GINC-V1293\FTS\RB3LYP\6-31G(d)\C4H7F3N2O3S1\JMH502\01-Nov-2010\0\
\# B3LYP/6-31G(d) opt=(CalcFC,Noeigen,TS) freq=noraman maxdisk=45875200
0 INT(grid=ultrafine)\SP Calc\0,1\C,0.0245083687,0.0745213255,0.0149
263125\C,0.0717610835,0.0227172158,1.5329778811\O,1.0766869741,0.01402
19383,2.195126297\N,-1.2647033508,-0.0230256993,2.1530637432\C,-1.8267

55003,1.2659229926,2.5967937545\S,-1.7073793887,-1.4393761298,2.918195
935\H,-0.4550265657,-0.8625943484,-0.3011491769\N,1.2968261931,0.23612
22478,-0.656432469\H,-0.6709808478,0.8686553049,-0.2882864105\H,-2.852
8786664,1.0983768494,2.9259718087\H,-1.2393310785,1.7112397175,3.40657
01604\H,-1.8443653155,1.9457555504,1.7398681797\O,-3.1205824963,-1.333
6294615,3.2612287165\O,-1.1487193434,-2.5295025423,2.1266847657\C,-0.8
122627825,-1.4773947834,4.5746698747\F,-1.3779846895,-2.4109557388,5.3
377747592\F,0.4752692782,-1.7547730809,4.4116561141\F,-0.9430208632,-0
.2816228345,5.1664672366\H,1.7473828864,1.095269279,-0.3458569502\H,1.
9239294538,-0.51761455,-0.3805627239\\Version=EM64L-G03RevE.01\State=1
-A\HF=-1189.4210044\RMSD=9.067e-09\RMSF=8.008e-06\Thermal=0.\Dipole=0.
2847895,1.4562788,-0.1102628\PG=C01 [X(C4H7F3N2O3S1)]\@

h2n-ch2-conso2cf3-TS_rad 125

1\1\GINC-V1258\FTS\UB3LYP\6-31G(d)\C4H6F3N2O3S1(2)\JMH502\02-Nov-2010\0\#
B3LYP/6-31G(d) opt=(CalcFC,Noeigen,TS) freq=noraman maxdisk=45875
2000 INT(grid=ultrafine)\SP Calc\0,2\C,-0.0057359251,-0.0712476207,-
0.0095349302\C,0.0306324728,0.006161032,1.4086837089\O,1.0827717925,0.
05218171,2.0583813403\N,-1.2775957779,0.0252357894,2.0484077814\C,-1.9
711601506,-1.2653488771,2.2141523165\S,-1.5773321164,1.2594134819,3.14
28954623\H,-0.9282390898,-0.0418832956,-0.5748704893\N,1.1628985008,-0
.2104769903,-0.6760222832\H,-2.9625572398,-1.0798826838,2.6275598629\H
, -2.0810052224, -1.7230510784, 1.2270872014\H, -1.4129289941, -1.944070658
3, 2.8684044232\O, -1.0330929526, 2.4910800696, 2.5880358827\O, -2.96827454
9, 1.1214862155, 3.5664052442\C, -0.5739910324, 0.8839696645, 4.6979370326
\F, -0.5664259057, -0.440895936, 4.9049079797\F, 0.6687110427, 1.3297017136
, 4.59500544\F, -1.1747064042, 1.4825953885, 5.7284562623\H, 1.218113471, -0
.0555402041, -1.6712714698\H, 2.0100000439, -0.104339095, -0.1282807007\\V
ersion=EM64L-G03RevE.01\State=2-A\HF=-1188.799737\S2=0.756203\S2-1=0.\
S2A=0.750018\RMSD=8.803e-09\RMSF=7.141e-06\Thermal=0.\Dipole=0.5927008
, -1.4122326, -2.0511576\PG=C01 [X(C4H6F3N2O3S1)]\@

Formamido-acetamides

hconhch2conhme 126

1\1\GINC-V1266\FOpt\RB3LYP\6-31G(d)\C4H8N2O2\JMH502\02-Nov-2010\0\# B
3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine)\
SP Calc\0,1\N,0.007583688,0.0005633744,0.0158191973\C,0.0144227435,-0
.0001288214,1.3747977928\O,1.036940373,0.0001008288,2.0541229263\C,-1.
3754356325,-0.000313067,2.0199269363\H,-0.8836336479,0.0016518902,-0.4
609841872\C,1.2227755163,0.0023739008,-0.7818128312\H,-1.9459766169,-0
.8802639256,1.6912405845\N,-1.2121001669,-0.000924923,3.4525965527\H,
-1.9457797842,0.8800732697,1.6919969985\H,-0.2531697865,-0.0010055143,
3.7837350335\C,-2.2731613323,-0.0031555636,4.2946908504\O,-3.441027909
1,-0.0053518831,3.9351057559\H,-1.9679362082,-0.0050384562,5.359292397
\H,1.2787046329,-0.8894338298,-1.4163616142\H,1.275968851,0.8943692373
, -1.4163210073\H, 2.0670524126, 0.0036055993, -0.0916950722\\Version=EM64
L-G03RevE.01\State=1-A\HF=-417.2127058\RMSD=8.129e-09\RMSF=5.577e-05\T
hermal=0.\Dipole=0.7180042,0.0035003,-1.4454851\PG=C01 [X(C4H8N2O2)]\@
@

hconhch2conhme_rad 127

1\1\GINC-V1266\FOpt\UB3LYP\6-31G(d)\C4H7N2O2(2)\JMH502\02-Nov-2010\0\#
UB3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafin
e)\SP Calc\0,2\N,0.0441999354,-0.285243107,0.0767377537\C,0.02517872
54,-0.047053462,1.4262002159\O,1.0471744892,0.1761393567,2.0939475002\
C,-1.2835454285,-0.0679664197,2.0598560173\H,-0.8316334877,-0.45907729
94,-0.3951555181\C,1.2702881197,-0.2976191911,-0.6969530986\N,-1.29144
02236,0.1703376248,3.4041305429\H,-2.2337476544,-0.2499958891,1.576806
1347\H,-0.3673009398,0.3352563308,3.8010949103\C,-2.4176482286,0.19667
68258,4.1984378339\O,-3.5474757029,0.0078048038,3.7846273685\H,-2.1769
9958,0.4090208745,5.2544343944\H,1.255986948,0.4719410305,-1.478494810
3\H,2.0909343961,-0.0913360399,-0.0088055156\H,1.4345755466,-1.2747157
395,-1.1676614173\\Version=EM64L-G03RevE.01\State=2-A\HF=-416.5731785\
S2=0.755304\S2-1=0.\S2A=0.750021\RMSD=9.161e-09\RMSF=7.208e-06\Thermal
=0.\Dipole=0.3363952,-0.1124608,-0.8244394\PG=C01 [X(C4H7N2O2)]\@

hconhch2conhme-TS 128

1\1\GINC-V1269\FTS\RB3LYP\6-31G(d)\C4H8N2O2\JMH502\02-Nov-2010\0\# B3
LYP/6-31G(d) opt=(TS,CalcFC,Noeigen) freq=noraman maxdisk=458752000 IN

T(grid=ultrafine)\SP Calc\0,1\N,0.0276809091,0.0168473348,0.03813256
56\C,0.0071430473,-0.0230404522,1.4808453356\O,0.998834501,-0.06839803
1,2.1791505867\C,-1.3905726692,0.0087651902,2.051736621\H,0.4898658145
, -0.8410660149, -0.2696399807\C,0.8132805912,1.1619371059, -0.4703631014
\H, -1.9579905879, -0.8382095976,1.6404850733\N, -1.3518896094, -0.0198489
811,3.493557876\H, -1.9019630053,0.9051145961,1.6719014747\C, -2.4826585
035, -0.0162992033,4.245248007\H, -0.4342816621, -0.0512546541,3.92152848
41\O, -3.6143784881,0.0150892826,3.7899086507\H, -2.267148922, -0.0448949
378,5.3313839393\H,0.8438215291,1.0985554673, -1.5611647845\H,0.3013150
859,2.0918138865, -0.2031507083\H,1.8388416946,1.2014865889, -0.07911762
15\Version=EM64L-G03RevE.01\State=1-A\HF=-417.1830583\RMSD=7.833e-09\
RMSF=5.346e-06\Thermal=0.\Dipole=1.2287069, -0.0015816, -0.6607741\PG=C0
1 [X(C4H8N2O2)]\@

hconhch2conhme-TS_rad 129

1\1\GINC-V1269\FTS\UB3LYP\6-31G(d)\C4H7N2O2(2)\JMH502\02-Nov-2010\0\#\
B3LYP/6-31G(d) opt=(TS,CalcFC,Noeigen) freq=noraman maxdisk=458752000
INT(grid=ultrafine)\SP Calc\0,2\N,0.0209011181,0.0273967547,0.03871
75314\C,0.0037287646, -0.0114309523,1.4812024014\O,1.0232505683, -0.0531
847778,2.186811354\C, -1.300803617,0.0093817634,2.0711578923\H,0.468430
8507, -0.8357454241, -0.274225618\C,0.8150872527,1.1603914925, -0.4745002
212\H, -2.2220435732,0.0505121241,1.5085454798\N, -1.377017317, -0.027389
4712,3.4319209456\C, -2.5521820077, -0.0166603765,4.1654291537\H, -0.4771
103322, -0.0634727295,3.9077303097\O, -3.6606471279,0.0261644622,3.67271
09707\H, -2.3617786633, -0.0515567084,5.2520955645\H,0.8541743019,1.0908
140038, -1.5653321733\H,0.3085721852,2.095766629, -0.2150388986\H,1.8389
410899,1.1972389621, -0.0770697365\Version=EM64L-G03RevE.01\State=2-A\
HF=-416.5514579\S2=0.758568\S2-1=0.\S2A=0.750042\RMSD=6.587e-09\RMSF=5
.560e-06\Thermal=0.\Dipole=0.569623, -0.0471045,0.0867129\PG=C01 [X(C4H
7N2O2)]\@

hconhch2conme2 130

1\1\GINC-V1262\FOpt\RB3LYP\6-31G(d)\C5H10N2O2\JMH502\02-Nov-2010\0\#\
B3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine)\
\SP Calc\0,1\N,0.0024384987,0.0023305022,0.0316317203\C, -0.0059796045
,0.0014708891,1.3966080832\O,1.0255846385,0.0003151326,2.0685716921\C,
-1.3715485028,0.0027839447,2.0972713454\C, -1.180088546,0.0039790094, -0
.815000713\C,1.2788104006,0.0014554703, -0.6714647469\H, -1.9619487576, -
0.8756414107,1.80405132\N, -1.1422203666,0.0011611479,3.5217222654\H, -1
.9594498813,0.8833942576,1.8055443804\H, -0.1688767069, -0.0003003504,3.
8076505084\C, -2.1658402622,0.0002799028,4.4080512939\O, -3.3489105963,0
.0016150113,4.1003198067\H, -1.8148715656, -0.0010867208,5.4585374842\H,
1.3629867272, -0.8889532683, -1.3076539034\H,1.3639365158,0.8915609503, -
1.3079361295\H,2.0807580323,0.0011002445,0.0649132948\H, -1.1858811338,
0.8922415355, -1.4604847457\H, -1.1885877835, -0.8843301046, -1.4604056531
\H, -2.0957237412,0.0054203277, -0.2259272663\Version=EM64L-G03RevE.01\
State=1-A\HF=-456.5203843\RMSD=4.212e-09\RMSF=2.133e-05\Thermal=0.\Dip
ole=0.6668126,0.0004252, -1.5565243\PG=C01 [X(C5H10N2O2)]\@

hconhch2conme2_rad 131

1\1\GINC-V1263\FOpt\UB3LYP\6-31G(d)\C5H9N2O2(2)\JMH502\02-Nov-2010\0\#\
B3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine
)\SP Calc\0,2\N, -0.0088394561, -0.1792445661,0.0231802502\C, -0.043675
5257, -0.0097484131,1.389012964\O,0.9879950967,0.1576366394,2.066296074
8\C, -1.3334323502, -0.0203237055,2.0651278299\C, -1.1841462156, -0.447775
9978, -0.7898313226\C,1.2847310957, -0.3273431891, -0.6265975544\N, -1.276
3104682,0.1913739123,3.4131654201\H, -2.308890414, -0.2034510325,1.64320
59481\H, -0.3312976809,0.3337586039,3.7684874187\C, -2.3653263813,0.2066
016465,4.2576410817\O, -3.514811256,0.0360289504,3.8925857739\H, -2.0754
761216,0.3920670566,5.3063826147\H,1.3551193344,0.3491261893, -1.487187
1148\H,2.0615382733, -0.0828171253,0.0963573019\H,1.4334605127, -1.35704
21166, -0.982207527\H, -0.984899869, -0.1156064234, -1.8133503006\H, -1.439
9200955, -1.5172591314, -0.82250368\H, -2.0495140223,0.112069333, -0.42939
91028\Version=EM64L-G03RevE.01\State=2-A\HF=-455.8802953\S2=0.755298\
S2-1=0.\S2A=0.750021\RMSD=9.693e-09\RMSF=1.514e-05\Thermal=0.\Dipole=0
.3276169, -0.1277499, -0.8959928\PG=C01 [X(C5H9N2O2)]\@

hconhch2conme2-TS 132

1\1\GINC-V1264\FTS\RB3LYP\6-31G(d)\C5H10N2O2\JMH502\02-Nov-2010\0\#\ B
3LYP/6-31G(d) opt=(TS,CalcFC,Noeigen) freq=noraman maxdisk=458752000 I
NT(grid=ultrafine)\SP Calc\0,1\N,0.1179489144,0.0001324082,0.0670992
193\C,0.0587599959,0.0002085977,1.507975919\O,1.0332783991,0.000173288

4,2.2318024598\C,-1.3537951206,0.0003393992,2.0444634941\C,0.782245435
2,-1.2160304899,-0.4260040987\C,0.7824233474,1.2161489476,-0.426125408
8\H,-1.8841841226,-0.8721075053,1.636717074\N,-1.3499441844,0.00041025
41,3.4873135367\H,-1.8840544099,0.8728246409,1.6366301054\C,-2.4985026
063,0.0005175092,4.2112835046\H,-0.4423901377,0.0003694538,3.937423849
\O,-3.619171811,0.0005667086,3.7281129185\H,-2.3093646358,0.0005565362
,5.3026928351\H,0.7189908607,1.2253121535,-1.5186506736\H,0.2586064037
,2.1008541885,-0.0495741793\H,1.8406667693,1.2799356934,-0.1281553495\
H,0.7188116362,-1.2252934622,-1.5185284433\H,1.8404795084,-1.279942300
1,-0.1280276301\H,0.2582990996,-2.1006215131,-0.0493645646\\Version=EM
64L-G03RevE.01\State=1-A\HF=-456.4925272\RMSD=5.820e-09\RMSF=3.582e-06
\Thermal=0.\Dipole=1.1398076,-0.0001078,-0.6855115\PG=C01 [X(C5H10N2O2
)]\@

hconhch2conme2-TS_rad 133

1\1\GINC-V1278\FTS\UB3LYP\6-31G(d)\C5H9N2O2(2)\JMH502\02-Nov-2010\0\#\
B3LYP/6-31G(d) opt=(TS,CalcFC,Noeigen) freq=noraman maxdisk=458752000
INT(grid=ultrafine)\SP Calc\0,2\N,0.1176839939,0.0000164925,0.06738
16118\C,0.0603854863,-0.0001242246,1.508662672\O,1.0623354306,-0.00057
51586,2.2400900928\C,-1.2593520456,0.0002986673,2.0654516737\C,0.77848
66839,-1.2136150381,-0.430506861\C,0.7793804753,1.2132723955,-0.430235
0755\H,-2.1671697994,0.0006995483,1.47982181\N,-1.3696961806,0.0001859
588,3.4246963358\C,-2.5633150853,0.0005464054,4.1275377821\H,-0.481826
6545,-0.0001969758,3.923893627\O,-3.6592859472,0.0010092894,3.60561058
18\H,-2.4007376683,0.0003630139,5.2192616172\H,0.7245541395,1.21836286
57,-1.5238273408\H,0.2502370665,2.0969918847,-0.0590149251\H,1.8362379
433,1.2838709515,-0.1267444164\H,0.7236563439,-1.2184203583,-1.5241002
251\H,1.8352919456,-1.2850598257,-0.1270324568\H,0.2486926112,-2.09702
76355,-0.0594843559\\Version=EM64L-G03RevE.01\State=2-A\HF=-455.860770
4\S2=0.758632\S2-1=0.\S2A=0.750043\RMSD=8.583e-09\RMSF=3.293e-06\Therm
al=0.\Dipole=0.4601761,-0.0001778,0.0687218\PG=C01 [X(C5H9N2O2)]\@

hconhch2concf3 134

1\1\GINC-V1491\FOpt\RB3LYP\6-31G(d)\C5H7F3N2O2\JMH502\15-Sep-2010\0\#\
B3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine)
\SP Calc\0,1\N,-0.0227602209,0.0290197636,0.0053808826\C,-0.11439339
24,0.0897293805,1.3954484301\O,0.8914033245,0.0785890377,2.0890721845\
C,-1.4970254749,0.2123703493,2.0341732702\C,-1.1619010908,-0.127182568
, -0.8324635883\C,1.3073565197,-0.1262603655,-0.6078597211\H,-2.1929827
355,-0.5356588502,1.6426308425\N,-1.3523691177,0.0525076208,3.46225973
4\H,-1.9219315074,1.1922712787,1.7805981192\C,-2.4255715474,-0.1705616
138,4.2630466345\H,-0.4070926548,0.0605176332,3.8257050412\H,1.4032814
955,-1.105632272,-1.0854939489\H,1.4775055072,0.6577436726,-1.34807689
51\H,2.0337273942,-0.0417257858,0.1970917562\F,-1.7745105257,-1.322251
8791,-0.6622080297\F,-2.0938355602,0.819722767,-0.60622246\F,-0.794888
9466,-0.0445992846,-2.1184463304\O,-3.580862381,-0.2253998375,3.873132
8836\H,-2.1373292427,-0.2989340837,5.3244475872\\Version=EM64L-G03RevE
.01\State=1-A\HF=-754.2401996\RMSD=8.377e-09\RMSF=6.679e-07\Thermal=0.
\Dipole=1.3926952,0.1228094,-0.7275191\PG=C01 [X(C5H7F3N2O2)]\@

hconhch2concf3_rad 135

1\1\GINC-V1388\FOpt\UB3LYP\6-31G(d)\C5H6F3N2O2(2)\JMH502\15-Sep-2010\0
\# B3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafi
ne)\SP Calc\0,2\N,-0.0210289367,-0.068138114,-0.0013270994\C,-0.0987
702428,-0.0336773252,1.401555819\O,0.9317014997,0.0159344302,2.086969
9218\C,-1.3945317112,-0.0563934606,2.0436558939\C,-1.1748379175,-0.125
4036641,-0.8175450914\C,1.301908157,-0.0436677856,-0.6367406336\H,-2.3
611581855,-0.098716979,1.5685474888\N,-1.368087355,-0.0199124984,3.406
6036215\C,-2.4906404622,-0.033140527,4.2152667286\H,-0.4363385364,0.01
99160446,3.8155345307\H,1.465677636,-0.9466311458,-1.231287056\H,1.410
0310907,0.8350906346,-1.2784206208\H,2.0301025481,0.000401432,0.170446
0508\F,-1.9290141405,-1.2239114075,-0.574709103\F,-1.9946049607,0.9370
409936,-0.6337220984\F,-0.8238178067,-0.150009726,-2.1108982796\O,-3.6
296635548,-0.0792397959,3.7949900651\H,-2.2289832525,0.0033772212,5.28
65890134\\Version=EM64L-G03RevE.01\State=2-A\HF=-753.6035136\S2=0.7556
03\S2-1=0.\S2A=0.750024\RMSD=7.856e-09\RMSF=1.775e-05\Thermal=0.\Dipol
e=0.9491445,0.0295595,-0.0031322\PG=C01 [X(C5H6F3N2O2)]\@

hconhch2concf3-TS 136

1\1\GINC-V1262\FTS\RB3LYP\6-31G(d)\C5H7F3N2O2\JMH502\15-Sep-2010\0\#\
B3LYP/6-31G(d) opt=(TS,CalcFC,Noeigen) freq=noraman maxdisk=458752000
INT(grid=ultrafine)\SP Calc\0,1\N,0.00529233,0.0080005819,-0.0264691

954\C,-0.1086973583,0.0363342986,1.427043389\O,0.8425153509,-0.0238066
757,2.1683762443\C,-1.5364660686,0.1439818776,1.8951809143\C,0.4329332
434,-1.3081036757,-0.5398353874\C,0.7132943214,1.1086184643,-0.5646900
513\H,-2.1432191617,-0.6463862947,1.4348866005\N,-1.6145740904,0.07224
93396,3.333355332\H,-1.9357802278,1.0888018614,1.49446602\H,-0.7452597
614,0.1500583723,3.8467696618\C,-2.771234127,-0.2612776434,3.968387533
9\H,0.4052932364,-1.2777159035,-1.6303580825\H,1.4394172442,-1.5800609
826,-0.2006038224\H,-0.2815403308,-2.0620366666,-0.1994880934\F,0.4984
553514,1.19766504,-1.890009288\F,0.2818118829,2.2438307113,0.021327422
9\F,2.0569266843,1.0561045925,-0.3967470086\O,-3.8331586438,-0.4624114
91,3.4038820442\H,-2.6446501999,-0.3283408686,5.0658937828\Version=EM
64L-G03RevE.01\State=1-A\HF=-754.2200428\RMSD=6.477e-09\RMSF=3.928e-06
\Thermal=0.\Dipole=0.6422098,-0.4996894,-0.1076956\PG=C01 [X(C5H7F3N2O
2)]\@

hconhch2concf3-TS_rad 137

1\1\GINC-V1272\FTS\UB3LYP\6-31G(d)\C5H6F3N2O2(2)\JMH502\15-Sep-2010\O\
\# B3LYP/6-31G(d) opt=(TS,CalcFC,Noeigen) freq=noraman maxdisk=4587520
000 INT(grid=ultrafine)\SP Calc\0,2\N,-0.0057411035,0.0021321445,-0.0
228806699\C,-0.1036682016,-0.0011432061,1.4282451129\O,0.8826854124,-0
.007301777,2.1722855748\C,-1.4385165007,-0.031104896,1.9321034569\C,0.
4576103549,-1.2851233309,-0.5730384885\C,0.6579733726,1.1321315983,-0.
5543569612\H,-2.3245460709,-0.0154782488,1.3137610478\N,-1.6019000501,
-0.0735983356,3.2829445752\H,-0.7402026695,-0.0681570887,3.8254857944\
C,-2.8306504456,-0.1078621656,3.929485786\H,0.440004964,-1.2265607142,
-1.6628210568\H,1.4683199685,-1.542157357,-0.2329536803\H,-0.239598685
, -2.0653631868,-0.2572967885\F,0.4171902837,1.2325074676,-1.8782455669
\F,0.2101591753,2.249022574,0.0475440629\F,2.0078455836,1.1149061953,-
0.4176297944\O,-3.8965786835,-0.1164332878,3.3519784281\H,-2.720904794
, -0.1275857375,5.026944736\Version=EM64L-G03RevE.01\State=2-A\HF=-753
.5898558\S2=0.758695\S2-1=0.\S2A=0.750041\RMSD=7.353e-09\RMSF=3.347e-0
6\Thermal=0.\Dipole=-0.0603749,-0.795218,0.6220187\PG=C01 [X(C5H6F3N2O
2)]\@

hconhch2concoch3 138

1\1\GINC-V1250\FOpt\RB3LYP\6-31G(d)\C6H10N2O3\JMH502\01-Nov-2010\O\
\# B3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine)\
\SP Calc\0,1\C,-0.0355992126,-0.0001478974,-0.0074616179\C,0.01468707
11,-0.0002283727,1.5099359511\O,1.0763420387,0.0001812091,2.1052430778
\N,-1.2281726591,-0.0005244493,2.1768505188\C,-2.4794627487,-0.0010233
431,1.4001066748\C,-1.3692627585,-0.0006371377,3.5812926511\H,-0.55275
94165,-0.8834142985,-0.3975186049\H,0.9945234371,-0.0004056533,-0.3644
713188\H,-0.5521753277,0.8835545907,-0.3973324713\H,-2.5460591021,-0.8
933375798,0.7718426245\H,-3.3042501357,-0.0002833666,2.108407465\H,-2.
5457260799,0.8901905734,0.7702785105\O,-2.4861802966,-0.0015446463,4.0
794518486\C,-0.1351632156,-0.0003563722,4.4720624644\H,0.4959702646,0.
8677161342,4.2541779132\N,-0.5769820094,-0.001182827,5.8503674888\H,0.
4968856472,-0.867583271,4.2534462249\H,-1.5766688723,-0.0018642937,6.0
091847731\C,0.3039773254,-0.0011107413,6.881692326\O,1.5186614595,-0.0
002962213,6.7614561957\H,-0.2057371685,-0.0017606096,7.8658647933\Ver
sion=EM64L-G03RevE.01\State=1-A\HF=-569.8609498\RMSD=2.142e-09\RMSF=1.
820e-05\Thermal=0.\Dipole=-1.6406019,-0.0003734,-1.8872442\PG=C01 [X(C
6H10N2O3)]\@

hconhch2concoch3_rad 139

1\1\GINC-V1252\FOpt\UB3LYP\6-31G(d)\C6H9N2O3(2)\JMH502\01-Nov-2010\O\
\# B3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine
\)\SP Calc\0,2\C,-0.0327296687,-0.0805014499,-0.0212536401\C,0.000275
8078,-0.0527094935,1.4983430605\O,1.063093217,-0.1129604523,2.09599630
19\N,-1.2404927568,0.0442149702,2.1436323179\C,-2.4767720486,0.1122970
223,1.3503878389\C,-1.4160814505,0.0841166329,3.5575822173\H,-2.598623
231,-0.7854167794,0.7372474482\H,-3.3073546646,0.1828317431,2.04849199
41\H,-2.477680828,0.9929208811,0.7014164173\O,-2.562658399,0.171107303
5,4.0281939641\C,-0.2885145823,0.0255376104,4.4539803367\H,0.746078143
6,-0.0502071887,4.1687787055\N,-0.6080951711,0.0734901073,5.7794836727
\C,0.3084252591,0.0319825662,6.8162450486\H,-1.6037560027,0.1448880818
,5.9800526754\O,1.5101165649,-0.0523979756,6.6656906907\H,-0.185858396
4,0.0850328343,7.8022247409\H,-0.6034361582,-0.9346051202,-0.401745666
2\H,-0.4832150288,0.827580737,-0.4365110946\H,0.9993462144,-0.15765841
65,-0.3641530045\Version=EM64L-G03RevE.01\State=2-A\HF=-569.2252815\
S2=0.756188\S2-1=0.\S2A=0.750027\RMSD=4.073e-09\RMSF=2.445e-06\Thermal=
0.\Dipole=-1.3281009,0.0716501,-0.9317533\PG=C01 [X(C6H9N2O3)]\@

hconhch2concoch3-TS 140

```
1\1\GINC-V1257\FTS\RB3LYP\6-31G(d)\C6H10N2O3\JMH502\01-Nov-2010\0\#\# B
3LYP/6-31G(d) opt=(CalcFC,Noeigen,TS) freq=noraman maxdisk=458752000 I
NT(grid=ultrafine)\SP Calc\0,1\C,-0.1056820299,-0.0524320833,-0.0602
969438\C,-0.0301983015,-0.0219252354,1.4501113021\O,1.0185579814,-0.00
71038074,2.0548405557\N,-1.3049754695,-0.0890995757,2.1150854792\C,-1.
6520016883,-1.4044757665,2.6683458636\C,-1.9320360828,1.0438687384,2.6
387661452\H,-0.6487031969,-0.9632818506,-0.3567824076\N,1.2155201544,-
0.0020945196,-0.6359621702\H,-0.7263451901,0.7784130103,-0.4208515561\
H,-0.9502649278,-1.7001882275,3.456677515\H,-2.6543601239,-1.320928393
8,3.0875552017\H,-1.6447810935,-2.1587012932,1.8751438522\O,-2.8882922
562,0.9476148995,3.3884477739\C,-1.3590366504,2.3854646621,2.216725695
6\H,-1.25014536,2.4690664901,1.1299838809\H,-2.0338341934,3.166264889,
2.5688093478\H,-0.3713727165,2.5370115511,2.6666901252\C,1.4016954198,
0.1634892937,-1.9728209799\H,1.9977317219,-0.0298381878,0.0066420392\O
,0.4960741487,0.2497716873,-2.7851438706\H,2.4726575624,0.210793477,-2
.2484200603\Version=EM64L-G03RevE.01\State=1-A\HF=-569.8429122\RMSD=7
.242e-09\RMSF=6.492e-07\Thermal=0.\Dipole=0.7884711,-0.2854971,0.27413
7\PG=C01 [X(C6H10N2O3)]\@
```

hconhch2concoch3-TS_rad 141

```
1\1\GINC-V1258\FTS\UB3LYP\6-31G(d)\C6H9N2O3(2)\JMH502\01-Nov-2010\0\#\#
B3LYP/6-31G(d) opt=(CalcFC,Noeigen,TS) freq=noraman maxdisk=458752000
INT(grid=ultrafine)\SP Calc\0,2\C,-0.0497916664,-0.0537360571,-0.01
97640195\C,-0.0180299117,-0.032461496,1.4102291219\O,1.0511838676,-0.0
282330607,2.0337662562\N,-1.295258698,-0.0618605838,2.0733001816\C,-1.
7012397493,-1.3636486155,2.6117074448\C,-1.8799127286,1.0907543875,2.5
912136623\H,-0.9530689694,-0.0690167815,-0.6138217184\N,1.1420555237,-
0.0602593737,-0.678433551\H,-0.9917214985,-1.7143316657,3.3705151984\H
,-2.6837793333,-1.2364084848,3.0655982304\H,-1.7568435546,-2.100765434
1,1.8040352661\O,-2.8378624698,1.0388306687,3.3461824997\C,-1.26975694
9,2.4084794581,2.1433343469\H,-1.1945215689,2.4731262868,1.0520968651\
H,-1.902527703,3.2165736559,2.511667533\H,-0.2608077188,2.5232987301,2
.5547855778\H,1.9665442204,-0.0519529768,-0.0807054226\C,1.2811775145,
-0.0805186428,-2.0601391127\O,0.3454745649,-0.091468592,-2.831181307\H
,2.3395939159,-0.0854077395,-2.3706778615\Version=EM64L-G03RevE.01\St
ate=2-A\HF=-569.2137139\S2=0.758768\S2-1=0.\S2A=0.750042\RMSD=5.042e-0
9\RMSF=1.518e-06\Thermal=0.\Dipole=1.2313378,-0.2410258,-0.7220826\PG=
C01 [X(C6H9N2O3)]\@
```

hconhch2concoch3 142

```
1\1\GINC-V1471\FOpt\RB3LYP\6-31G(d)\C6H7F3N2O3\JMH502\03-Nov-2010\0\#\#
B3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine)
\SP Calc\0,1\C,-0.0025456672,0.0395458397,0.0163260524\C,0.002186277
6,-0.0543693339,1.57321318\O,1.0782179289,-0.1204003287,2.1276797159\N
,-1.2298789927,-0.0468690293,2.2140923525\C,-2.5136432099,-0.018333722
1,1.4767235448\C,-1.3567760666,0.007507166,3.6291792185\F,-0.519011825
2,-1.0808525506,-0.537254965\F,1.2434562785,0.1818015389,-0.4206577963
\F,-0.7267341321,1.0934628015,-0.413697638\O,-2.4728311097,0.087153198
6,4.1119680351\C,-0.1227003046,-0.0377298353,4.5145352054\H,0.55856258
79,0.7852193165,4.2701390024\N,-0.5548284797,0.0285679255,5.8928683539
\H,0.4555128,-0.9477724752,4.3180800107\H,-1.5507916566,0.085084952,6.
063431582\C,0.3407930875,0.03016931,6.9141103989\O,1.5510997494,-0.027
1778816,6.7735868536\H,-0.1528560429,0.0895788708,7.9039186909\H,-3.25
70533058,-0.5206849896,2.09139888\H,-2.836407772,1.0110952233,1.303159
2804\H,-2.4097835083,-0.54075575,0.5307623228\Version=EM64L-G03RevE.0
1\State=1-A\HF=-867.5633345\RMSD=5.194e-09\RMSF=4.288e-06\Thermal=0.\D
ipole=-1.7178195,0.0200917,-0.8426794\PG=C01 [X(C6H7F3N2O3)]\@
```

hconhch2concoch3_rad 143

```
1\1\GINC-V1261\FOpt\UB3LYP\6-31G(d)\C6H6F3N2O3(2)\JMH502\01-Nov-2010\0
\#\# B3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafi
ne)\SP Calc\0,2\C,0.0163859685,-0.0213089471,-0.0431951163\C,-0.0074
454606,-0.0375756743,1.5162552078\O,1.0678552823,-0.0495821163,2.08451
4957\N,-1.2445594203,-0.0314691431,2.1289932219\C,-2.5123921017,-0.033
1654542,1.3685464789\C,-1.4152180727,0.0817334178,3.5490459092\F,-0.47
58171044,-1.173654609,-0.5542097676\F,1.2692893427,0.1138914047,-0.466
031869\F,-0.7093510154,1.0011169622,-0.5440014591\H,-2.3912160405,-0.5
904288079,0.4446169446\H,-3.2667634595,-0.5122258322,1.9884226686\H,-2
.8372222122,0.9874856324,1.1499037993\O,-2.563863956,0.2227269637,3.99
27259246\C,-0.2961356798,0.0188438718,4.4502011913\H,0.7368941188,-0.1
115450718,4.1779877375\N,-0.6124743877,0.1415761244,5.7698984357\C,0.3
```

093122176,0.1021943075,6.806407454\H,-1.6026135534,0.2651241431,5.9718
937387\O,1.5026810645,-0.0460287277,6.6499905358\H,-0.1746065905,0.221
7680237,7.7910253693\\Version=EM64L-G03RevE.01\State=2-A\HF=-866.92942
73\S2=0.75657\S2-1=0.\S2A=0.750029\RMSD=9.386e-09\RMSF=7.696e-06\Therm
al=0.\Dipole=-1.3970981,0.0482919,0.1564005\PG=C01 [X(C6H6F3N2O3)]\@

hconhch2concofc3-TS 144

1\1\GINC-V1259\FTS\RB3LYP\6-31G(d)\C6H7F3N2O3\JMH502\01-Nov-2010\0\#\n
B3LYP/6-31G(d) opt=(CalcFC,Noeigen,TS) freq=noraman maxdisk=458752000
INT(grid=ultrafine)\SP Calc\0,1\C,-0.0813666103,0.315049775,-0.11025
30852\C,0.0392739219,0.1885765288,1.3925302426\O,1.0834355806,0.197138
8309,1.9919854657\N,-1.2378101349,0.019375136,2.0763750157\C,-1.620701
8328,-1.3828287835,2.3101429815\C,-1.8786357619,0.9789846474,2.8221719
455\H,-0.6898113892,-0.4982566827,-0.5216435568\N,1.2076724539,0.28547
96709,-0.7571290537\H,-0.6343500053,1.244047223,-0.3117696808\H,-1.078
1965134,-1.7991633005,3.1656230214\H,-2.6912729177,-1.4181204403,2.511
6706465\H,-1.3928558363,-1.9697174957,1.4164651883\O,-2.774360644,0.74
161095,3.6080138909\C,-1.4920883776,2.453095508,2.5278072934\F,-1.7807
991294,2.7581172785,1.2371004686\F,-2.1743364441,3.2753496593,3.315745
5132\F,-0.1744435258,2.6792090424,2.7069484895\C,1.4449649555,-0.53354
82256,-1.8248498901\H,1.9935452701,0.6712557043,-0.249285288\O,0.59395
46905,-1.1936855613,-2.3947184081\H,2.5073188548,-0.5218052488,-2.1314
598588\\Version=EM64L-G03RevE.01\State=1-A\HF=-867.5477028\RMSD=7.352e
-09\RMSF=2.756e-06\Thermal=0.\Dipole=0.6221428,-0.1371275,-0.1268151\PG
=C01 [X(C6H7F3N2O3)]\@

hconhch2concofc3-TS_rad 145

1\1\GINC-V1262\FTS\UB3LYP\6-31G(d)\C6H6F3N2O3(2)\JMH502\01-Nov-2010\0\#\n
#B3LYP/6-31G(d) opt=(CalcFC,Noeigen,TS) freq=noraman maxdisk=4587520
00 INT(grid=ultrafine)\SP Calc\0,2\C,-0.0313217419,-0.0695878812,-0.
0269993369\C,0.0173553209,0.0140764465,1.3954356748\O,1.0779990018,0.0
47529546,2.0246620919\N,-1.267389776,-0.0173117287,2.0747869533\C,-1.7
004307922,-1.3459966794,2.5300243743\C,-1.8511698419,1.0767889608,2.66
33162214\H,-0.9413490997,-0.089999992,-0.6099088774\N,1.1510858287,-0.
101245743,-0.6983109733\H,-1.0654023715,-1.7024037841,3.3488945056\H,-
2.7297725419,-1.2686536187,2.8788572292\H,-1.640632323,-2.0483785521,1
.6940235984\O,-2.77441507,1.0217461924,3.452933428\C,-1.2991332946,2.4
641026341,2.2391732527\F,-1.1455484844,2.5473050389,0.8945267759\F,-2.
1380321314,3.4252276459,2.6194823802\F,-0.098113527,2.6952340528,2.801
7646414\H,1.9864594951,-0.0530030596,-0.118343828\C,1.2672060357,-0.17
76905609,-2.0820317377\O,0.3182186641,-0.2400814476,-2.8329001537\H,2.
3198389673,-0.1766216107,-2.4106660115\\Version=EM64L-G03RevE.01\State
=2-A\HF=-866.9189735\S2=0.758769\S2-1=0.\S2A=0.750041\RMSD=8.207e-09\R
MSF=6.368e-06\Thermal=0.\Dipole=1.036827,-1.0375511,-0.7301279\PG=C01
[X(C6H6F3N2O3)]\@

hconhch2conso2me-ext 146

1\1\GINC-V1254\FOpt\RB3LYP\6-31G(d)\C5H10N2O4S1\JMH502\14-Nov-2010\0\#\n
#B3LYP/6-31G(d) opt freq=noraman INT(grid=ultrafine) maxdisk=458752000
\hconhch2conso2me confsearch\0,1\C,-1.841825,0.363921,-0.081143\C,-0
.457079,-0.276272,-0.011718\O,-0.321777,-1.492892,-0.037336\N,0.612411
,0.594274,0.095003\C,0.457846,2.05705,0.09609\S,2.237296,-0.050332,-0.
133339\H,-2.02988,0.990526,0.80041\N,-2.830735,-0.68176,-0.16536\H,-1.
894978,1.037319,-0.948669\H,1.432502,2.49784,0.299893\H,0.098683,2.422
883,-0.871575\H,-0.237346,2.358211,0.884041\O,2.292818,-0.76087,-1.404
876\O,3.114062,1.092867,0.12574\C,2.404395,-1.218894,1.223778\H,3.4084
78,-1.63986,1.129496\H,2.304925,-0.673451,2.163487\H,1.639784,-1.98576
3,1.109951\H,-2.47978,-1.628664,-0.250636\C,-4.151669,-0.416303,0.0035
73\O,-4.610708,0.699695,0.188172\H,-4.776027,-1.328745,-0.04755\\Versi
on=EM64L-G03RevE.01\State=1-A\HF=-1005.0858665\RMSD=7.283e-09\RMSF=1.2
60e-05\Thermal=0.\Dipole=0.3248081,-0.262025,1.023165\PG=C01 [X(C5H10N
2O4S1)]\@

hconhch2conso2me_rad 147

1\1\GINC-V1350\FOpt\UB3LYP\6-31G(d)\C5H9N2O4S1(2)\JMH502\01-Nov-2010\0\#\n
\\#UB3LYP/6-31G(d) INT(grid=ultrafine) OPT freq=noraman maxdisk=458752
000\\NSO2Me_c6 confsearch\0,2\C,0.0189408173,-0.0256387381,0.10693532
33\C,-0.013468854,-0.0532621618,1.5513908279\O,1.033450218,-0.20621507
88,2.1963747537\N,-1.2270737057,0.104623623,2.2581159869\C,-1.11742497
1,0.098356136,3.7282153094\S,-2.7910654581,-0.0196801762,1.5565244\H,-

0.8070883749,0.185760885,-0.55357466\N,1.2515993051,-0.225109707,-0.44
31153437\H,-2.0780651667,0.3892957054,4.1471276824\H,-0.8220290688,-0.
8892540148,4.0981028803\H,-0.3503194356,0.8180067663,4.0173310034\O,-3
.7410257371,0.3087149862,2.6158558504\O,-2.7881642103,0.7144185803,0.2
92653639\C,-2.9504435196,-1.7779736019,1.1796165939\H,-3.931268681,-1.
9145193229,0.7181557643\H,-2.160407939,-2.0668086195,0.4836966288\H,-2
.8843629543,-2.3444837876,2.1102927032\H,2.0066153484,-0.3529274579,0.
2283787179\C,1.5142118296,-0.2439411694,-1.8023789347\O,0.6661476659,-
0.1075823155,-2.6606649834\H,2.5860970062,-0.4006825263,-2.0131764677\
\Version=EM64L-G03RevE.01\State=2-A\HF=-1004.4488203\S2=0.75578\S2-1=0
\S2A=0.750025\RMSD=7.251e-09\RMSF=2.603e-05\Thermal=0.\Dipole=0.72721
74,-1.3713471,0.626385\PG=C01 [X(C5H9N2O4S1)]\@

hconhch2conso2me-TS.a2b2 148

1\1\GINC-V1296\FTS\RB3LYP\6-31G(d)\C5H10N2O4S1\JMH502\02-Nov-2010\0\#\
B3LYP/6-31G(d) OPT=(CalcFC,TS,Noeigen) freq=noraman maxdisk=458752000\
\hconhch2conso2me-TS confsearch\0,1\C,0.0260496721,-0.4523931697,0.11
26453348\C,-0.0162595012,-0.2312489753,1.607063116\O,0.9632689781,-0.1
911265032,2.3083726605\N,-1.3786572914,-0.08635266,2.1096289398\C,-1.7
276237643,1.3261002386,2.3798142386\S,-1.7582823127,-1.1872678239,3.38
98930314\H,-0.4646023068,-1.4208808128,-0.0742242687\N,1.3807374511,-0
.4140796066,-0.3807105857\H,-0.5745645847,0.2968831791,-0.4151284709\H
, -2.7954757902,1.4017693099,2.5980639489\H,-1.1554108833,1.7395320398,
3.216662562\H,-1.5278265484,1.9047170979,1.4730226654\O,-0.9618378538,
-2.3862505984,3.129092382\O,-1.7372756031,-0.5084642221,4.6869287047\C
, -3.4778624682,-1.5529172962,2.9850197556\H,-3.8302213748,-2.248199368
4,3.7506671226\H,-4.0685374618,-0.6357458485,3.0165359511\H,-3.5144073
698,-2.0132636287,1.997474899\H,2.1189734148,-0.6036363247,0.285930178
6\C,1.6804008694,0.0985292003,-1.6069050429\O,0.8541456811,0.476063627
4,-2.4206277481\H,2.7706933865,0.1298813013,-1.7923505821\Version=EM6
4L-G03RevE.01\State=1-A\HF=-1005.0657916\RMSD=4.941e-09\RMSF=4.221e-06
\Thermal=0.\Dipole=-1.1154108,0.3146719,-0.1670817\PG=C01 [X(C5H10N2O4
S1)]\@

hconhch2conso2me-TS_rad 149

1\1\GINC-V1351\FTS\UB3LYP\6-31G(d)\C5H9N2O4S1(2)\JMH502\01-Nov-2010\0\
#\B3LYP/6-31G(d) opt=(CalcFC,Noeigen,TS) freq=noraman maxdisk=4587520
00 INT(grid=ultrafine)\SP Calc\0,2\C,-0.1751799319,0.0510358238,-0.0
52271809\C,-0.0869671039,0.070211069,1.3707314714\O,0.998317542,0.1348
63656,1.9656123432\N,-1.3590847753,-0.0097799186,2.059354625\C,-1.7045
566847,-1.3359404021,2.5969794473\S,-1.7526295296,1.3523367178,3.00929
90275\H,-1.1044194415,0.0181455116,-0.6028652774\N,0.9863908831,0.0919
261275,-0.7583754223\H,-2.6978812256,-1.2769093708,3.0438047754\H,-1.7
385115306,-2.0456268592,1.7647722663\H,-0.9774105634,-1.695226609,3.33
81744795\O,-1.4053361189,2.5092433627,2.1856838034\O,-3.1135677587,1.1
25905239,3.4962450894\C,-0.6449835286,1.3256813384,4.4367736323\H,-0.8
525690863,0.4330028688,5.0302322956\H,0.3834212632,1.3257667574,4.0752
009022\H,-0.8629655141,2.2234521561,5.0198169358\C,1.0684271972,0.0698
889641,-2.146276038\H,1.8349490129,0.16095199,-0.2001094493\O,0.10539
45337,-0.0148117553,-2.8765707939\H,2.1110826185,0.1357455375,-2.50017
2675\Version=EM64L-G03RevE.01\State=2-A\HF=-1004.4395683\S2=0.758018\
S2-1=0.\S2A=0.750037\RMSD=6.595e-09\RMSF=4.628e-06\Thermal=0.\Dipole=1
.5900988,-1.2225977,0.4382275\PG=C01 [X(C5H9N2O4S1)]\@

hconhch2conso2cf3 150

1\1\GINC-V1300\FOpt\RB3LYP\6-31G(d)\C5H7F3N2O4S1\JMH502\01-Nov-2010\0\
#\B3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafin
e)\SP Calc\0,1\C,-0.0057092592,0.3059069234,-0.0284054256\C,-0.00467
51615,0.0965829689,1.4825609687\O,1.0369120161,0.0088192828,2.10647618
59\N,-1.2151684379,0.0493156376,2.2146252376\C,-1.0754481715,-0.134686
8227,3.679458941\S,-2.784688825,0.0556367148,1.5570595652\H,-0.6483115
088,-0.4056405827,-0.5510231765\N,1.34383838,0.1463124705,-0.523062923
2\H,-0.4105137127,1.3022282447,-0.2451773851\H,-2.0558991977,-0.033960
2381,4.138838461\H,-0.6499578558,-1.1176116558,3.8938530418\H,-0.40586
72287,0.6359401069,4.0625241744\O,-3.7105182792,0.4212817973,2.6183773
116\O,-2.765748951,0.7265805609,0.2665048375\C,-3.0701684496,-1.770263
3066,1.2216324905\F,-4.2894114295,-1.9309012078,0.7232914212\F,-2.1607
240176,-2.2162631217,0.352820884\F,-2.95323657,-2.4437279159,2.3681236
689\H,2.0947524589,0.3065504014,0.136644657\C,1.5971039853,-0.53534595
67,-1.6769368949\O,0.7455180159,-0.9499463004,-2.4442404407\H,2.682242
4025,-0.6611788414,-1.8539438746\Version=EM64L-G03RevE.01\State=1-A\H
F=-1302.7791374\RMSD=9.054e-09\RMSF=3.047e-06\Thermal=0.\Dipole=0.5796
454,-0.0984228,1.3472383\PG=C01 [X(C5H7F3N2O4S1)]\@

hconhch2conso2cf3_rad 151

1\1\GINC-V1351\FOpt\UB3LYP\6-31G(d)\C5H6F3N2O4S1(2)\JMH502\01-Nov-2010
\0\#UB3LYP/6-31G(d) INT(grid=ultrafine) OPT freq=noraman maxdisk=4587
52000\NSO2Me_c6 confsearch\0,2\C,0.0718668857,0.0447992218,0.0623616
665\C,-0.0111550311,-0.0972579262,1.4907999\O,0.9908011423,-0.36555029
07,2.1627256052\N,-1.2422830247,0.1210023859,2.1928651567\C,-1.1442633
721,0.0530994949,3.6691982302\S,-2.7848621968,0.0205555205,1.509936264
9\H,-0.7262075755,0.3275037948,-0.6044322382\N,1.3020336772,-0.1973087
761,-0.4722027607\H,-2.0786398229,0.4135927494,4.0933836268\H,-0.94021
30441,-0.9682340024,4.0015202209\H,-0.3211562351,0.6969697369,3.978422
0975\O,-3.7452177062,0.490898035,2.4973709279\O,-2.7576228175,0.531956
1862,0.1464832391\C,-3.043196701,-1.8335417633,1.3666007476\F,-4.23172
22967,-2.0719301165,0.8238190169\F,-2.0820851159,-2.3574582285,0.60041
28729\F,-2.9828626588,-2.3809501192,2.5834729925\H,2.0295486478,-0.441
4057302,0.1966737167\C,1.6003968225,-0.1126837809,-1.8244062191\O,0.79
15555708,0.1784450869,-2.6800536093\H,2.6603434206,-0.3424467058,-2.02
7301416\Version=EM64L-G03RevE.01\State=2-A\HF=-1302.1442662\S2=0.7560
53\S2-1=0.\S2A=0.750026\RMSD=9.607e-09\RMSF=7.955e-06\Thermal=0.\Dipol
e=1.1103571,-0.6557354,0.7880513\PG=C01 [X(C5H6F3N2O4S1)]\@e

hconhch2conso2cf3-TS.a3b2 152

1\1\GINC-V1304\FTS\RB3LYP\6-31G(d)\C5H7F3N2O4S1\JMH502\02-Nov-2010\0\
#B3LYP/6-31G(d) OPT=(CalcFC,TS,Noeigen) freq=noraman maxdisk=458752000
\hconhch2conso2cf3-TS confsearch\0,1\C,0.5969229443,-0.3595195207,0.
0511946032\C,0.2124101433,-0.0011599057,1.470008402\O,0.9570981674,0.4
853583081,2.2788494419\N,-1.1802950536,-0.3418845774,1.76833606\C,-2.1
330166089,0.7838084981,1.620332063\S,-1.424991204,-1.3915386466,3.0744
176686\H,0.5220029214,-1.455730106,-0.0243326413\N,1.906537388,0.13269
47819,-0.2945649934\H,-0.1212698252,0.0469516263,-0.6688746366\H,-3.15
22396429,0.3978056231,1.6330520925\H,-2.0073787086,1.5285576891,2.4118
094178\H,-1.9512109182,1.246835364,0.6465511633\O,-0.1569005911,-2.038
652886,3.3844390669\O,-2.2909565477,-0.7856248461,4.0788854698\C,-2.45
84329751,-2.6912638956,2.2046284038\F,-2.7921341806,-3.6304370698,3.08
52932861\F,-3.5673616929,-2.1346104853,1.7038472728\F,-1.7525374731,-3
.2365574829,1.2131180359\H,2.6101671102,0.1426689084,0.4328915687\C,2.
1108871422,0.8721391878,-1.4259597129\O,1.2697470363,1.0733568094,-2.2
842235451\H,3.1435231509,1.2622474885,-1.4880069677\Version=EM64L-G03
RevE.01\State=1-A\HF=-1302.7621624\RMSD=4.171e-09\RMSF=2.183e-06\Therm
al=0.\Dipole=-0.071236,0.1452489,-0.5528435\PG=C01 [X(C5H7F3N2O4S1)]\@
e

hconhch2conso2cf3-TS_rad 153

1\1\GINC-X69\FTS\UB3LYP\6-31G(d)\C5H6F3N2O4S1(2)\JMH502\02-Nov-2010\0\
\# B3LYP/6-31G(d) opt=(CalcFC,Noeigen,TS) freq=noraman maxdisk=4587520
00 INT(grid=ultrafine)\SP Calc\0,2\C,-0.0386120911,0.1264533306,-0.0
112120992\C,-0.0168196376,-0.0746357036,1.3996569343\O,1.0236488597,-0
.2667192333,2.0346829673\N,-1.326322623,-0.0617328155,2.0339096279\C,-
2.0087493883,-1.3619391577,2.1749794991\S,-1.6311242081,1.1611740703,3
.1383664386\H,-0.9315585229,0.3229973914,-0.5877446281\N,1.1479399209,
0.0801773474,-0.6732005974\H,-2.9996591468,-1.1886968347,2.5954010188\
H,-2.1222788109,-1.796466681,1.1775722763\H,-1.4434132982,-2.049595332
4,2.8128115324\O,-1.0057826347,2.3712286089,2.622030531\O,-3.041458230
9,1.0729131314,3.4996210527\C,-0.7067665878,0.7191497211,4.7199103132\
F,-0.8806400291,-0.584966077,4.9773566427\F,0.5880668689,0.9831009951,
4.6073589246\F,-1.222968833,1.4362094102,5.7176666251\C,1.287620551,0.
2487195706,-2.0476790866\H,1.9708591949,-0.0691745264,-0.0926552321\O,
0.354996224,0.4282044045,-2.799446589\H,2.341871601,0.1969923733,-2.36
66775212\Version=EM64L-G03RevE.01\State=2-A\HF=-1302.1343374\S2=0.758
461\S2-1=0.\S2A=0.750039\RMSD=8.928e-09\RMSF=1.371e-05\Thermal=0.\Dipo
le=0.9871476,-1.4494152,-0.6153284\PG=C01 [X(C5H6F3N2O4S1)]\@e

Glycine anhydrides

Dkp 48

1\1\GINC-AC30\FOpt\UB3LYP\6-31G(d)\C4H6N2O2\JMH502\09-Apr-2009\0\# UB
3LYP/6-31G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultrafine)\
\SP Calc\0,1\C,0.0097799347,0.0109261526,-0.00418692\N,0.0021635651,0
.0095660427,2.4983237784\C,0.81624147,-0.0206787573,1.2919753075\C,-1.

2417346639,0.5526550349,2.6118520921\N,-1.2855315947,0.4152018348,0.1134875832\H,1.5263226291,0.8198385693,1.2585222533\C,-1.8995842324,0.9855203581,1.3036945062\H,1.4076579479,-0.9400765874,1.2692337702\H,-1.8907792649,2.0860300432,1.2791300808\H,-2.94639868,0.6753218354,1.3631899632\O,0.5228227071,-0.3081437609,-1.0660178065\O,-1.8181469613,0.7006398495,3.6787884133\H,-1.7875443636,0.4747273542,-0.7647655755\H,0.4389837363,-0.2259828659,3.3818357023\\Version=IA64L-G03RevE.01\State=1-A\HF=-416.0068225\S2=0.\S2-1=0.\S2A=0.\RMSD=7.433e-09\RMSF=3.304e-05\Thermal=0.\Dipole=0.1125892,0.3039698,-0.0090795\PG=C01 [X(C4H6N2O2)]\@

dkp-rad 49 50

1\1\GINC-AC30\FOpt\UB3LYP\6-31G(d)\C4H5N2O2(2)\JMH502\09-Apr-2009\0\#\UB3LYP/6-31G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultrafine)\SP Calc\0,2\C,0.0061345906,0.047978677,-0.0319641608\N,0.0495045616,0.0008550621,2.4244111437\C,0.7133358325,-0.1065377806,1.2213180681\C,-1.2617525279,0.4171177981,2.5788986757\N,-1.3482666926,0.3153617589,0.094486668\C,-1.9528809426,0.867145558,1.2973310854\H,1.7607303605,-0.3697587938,1.2300981462\H,-1.9458442694,1.9712834222,1.3063526627\H,-2.9983618132,0.5545538795,1.372891766\O,0.5527268001,-0.1024595696,-1.1259652518\O,-1.7952156328,0.4715147578,3.6729347921\H,-1.8088703318,0.5017746173,-0.7879602481\H,0.5231732297,-0.2353751432,3.2901313704\Version=IA64L-G03RevE.01\State=2-A\HF=-415.3658728\S2=0.75673\S2-1=0.\S2A=0.750033\RMSD=5.721e-09\RMSF=1.023e-05\Thermal=0.\Dipole=-0.0619081,0.2648893,0.4690159\PG=C01 [X(C4H5N2O2)]\@

NMe 51

1\1\GINC-AC30\FOpt\UB3LYP\6-31G(d)\C5H8N2O2\JMH502\09-Apr-2009\0\#\UB3LYP/6-31G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultrafine)\SP Calc\0,1\C,0.0000631296,-0.0074471699,-0.000212362\N,0.0037182496,0.0074286106,2.5093180795\C,0.8050821641,-0.012558454,1.2974671057\C,-1.2498139951,0.5238107063,2.6121562\N,-1.3057152351,0.3819734748,0.0847715057\H,1.4973979287,0.8422594971,1.2536590318\C,-1.9155362133,0.915117099,1.296719978\H,1.4162600812,-0.9187692328,1.2738778862\H,-1.963965252,2.0152281422,1.2602017142\H,-2.9501377414,0.5618321512,1.3606565046\O,0.5527117703,-0.3322163021,-1.0442532845\O,-1.8355142146,0.6755449212,3.6739027397\C,-2.1027293166,0.4704518846,-1.1317025941\H,0.4508633491,-0.2053194361,3.3935394765\H,-1.5251510968,0.0398793545,-1.9488296198\H,-2.3402144379,1.5165424557,-1.3668986605\H,-3.0419661201,-0.0811141234,-1.0067239372\\Version=IA64L-G03RevE.01\State=1-A\HF=-455.3190886\S2=0.\S2-1=0.\S2A=0.\RMSD=3.236e-09\RMSF=1.533e-05\Thermal=0.\Dipole=0.0701198,0.2628691,-0.1276645\PG=C01 [X(C5H8N2O2)]\@

NMe_c3 52

1\1\GINC-AC30\FOpt\UB3LYP\6-31G(d)\C5H7N2O2(2)\JMH502\09-Apr-2009\0\#\UB3LYP/6-31G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultrafine)\SP Calc\0,2\C,0.0163680488,0.1622860573,-0.0036213109\C,0.0307626241,0.0238201648,2.4190315032\N,2.1006108921,-0.2710063035,1.0703697639\C,1.4081596855,-0.6184593765,2.2990628497\C,1.4275908711,-0.131526751,-0.1321866094\N,-0.6020235283,0.331402876,1.2184459507\H,1.2596471172,-1.7076085964,2.4102009441\H,-0.5711869002,0.335712323,-0.8940253871\H,1.9848560465,-0.2841409855,3.1652937699\O,-0.5003626033,0.1915128001,3.5053536769\O,1.9943263475,-0.1951729899,-1.2246802561\C,-1.9674206266,0.8625634377,1.2571678158\H,3.0602621084,-0.5791853328,0.9690613317\H,-1.9787486978,1.8976906866,0.9015201155\H,-2.3152058234,0.8236633962,2.2879801358\H,-2.6154242404,0.2540967943,0.6189801709\\Version=IA64L-G03RevE.01\State=2-A\HF=-454.678427\S2=0.756542\S2-1=0.\S2A=0.750031\RMSD=9.792e-09\RMSF=8.349e-06\Thermal=0.\Dipole=-0.5625448,-0.1432091,0.3947109\PG=C01 [X(C5H7N2O2)]\@

NMe_c6 53

1\1\GINC-AC15\FOpt\UB3LYP\6-31G(d)\C5H7N2O2(2)\JMH502\09-Apr-2009\0\#\UB3LYP/6-31G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultrafine)\SP Calc\0,2\C,-0.0034749301,0.0920535622,-0.0537275621\C,-0.017926582,0.0510653084,2.4480032637\N,2.1055028288,-0.0508488037,1.1981879315\C,1.4173134609,-0.1234571548,2.3881421902\C,1.5185578824,0.0893403225,-0.0433571872\N,-0.6512264436,0.2788310587,1.2350799624\H,1.9760814806,-0.2735627095,3.2999043549\O,-0.6175903373,0.0325116221,3.5277794892\O,2.1771710487,0.1661060948,-1.0663746432\C,-2.0968441718,0.4172236694,1.2070786705\H,3.1193394787,-0.092567324,1.1900207799\H,-2.3818484757,1.2893056542,0.6054229118\H,-2.4442637434,0.5450660548,2.2318251999\H,-2.5745464864,-0.4739783929,0.773898042\H,-0.3202281807,-0.8557668735,-0.5242164466\H,-0.3102800117,0.8895278561,-0.7421796161\\Version=

IA64L-G03RevE.01\State=2-A\HF=-454.6783541\S2=0.756154\S2-1=0.\S2A=0.750029\RMSD=6.048e-09\RMSF=8.632e-06\Thermal=0.\Dipole=0.2162931,-0.1067089,-0.3314401\PG=C01 [X(C5H7N2O2)]\@

NCF3 54

1\1\GINC-AC15\FOpt\UB3LYP\6-31G(d)\C5H5F3N2O2\JMH502\08-Apr-2009\0\#\UB3LYP/6-31G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultrafine)\SP Calc\0,1\C,0.0037669628,-0.0061754009,0.0001177894\N,0.0145789707,0.0171683979,2.4960937884\C,0.8203339637,-0.0101489334,1.2889039316\C,-1.1602047209,0.6947034466,2.6140269873\N,-1.2830301384,0.5060621777,0.1052160378\H,1.5199549378,0.839619445,1.2368018303\C,-1.7478624253,1.222428696,1.3067866161\H,1.4211466233,-0.9220366363,1.2659171227\H,-1.5233457731,2.2962905112,1.2360940063\H,-2.8272460803,1.1182427883,1.391988661\O,0.4815800018,-0.4156050321,-1.0386397256\O,-1.73056031,0.8908953451,3.6742767325\C,-2.0507089048,0.6082045727,-1.1053150777\F,-2.2100270322,-0.5816801803,-1.6907539607\F,-1.4868631041,1.4403801707,-1.9973847093\F,-3.2723381069,1.0978648754,-0.8174258569\H,0.4320362709,-0.279280072,3.3704415025\Version=IA64L-G03RevE.01\State=1-A\HF=-753.0335181\S2=0.\S2-1=0.\S2A=0.\RMSD=7.415e-09\RMSF=1.419e-05\Thermal=0.\Dipole=0.7507337,0.2211026,0.6077715\PG=C01 [X(C5H5F3N2O2)]\@

NCF3_c3 55

1\1\GINC-AC30\FOpt\UB3LYP\6-31G(d)\C5H4F3N2O2(2)\JMH502\08-Apr-2009\0\#\UB3LYP/6-31G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultrafine)\SP Calc\0,2\C,0.5088676713,1.1226913551,2.9545363747\N,-1.5743069981,-0.0852488038,2.3633888036\C,-0.7775373752,0.470657816,3.4424369694\C,-1.7326665333,0.5871191381,1.1639035247\N,0.4355945962,1.686984124,1.6633833719\C,-0.6811048951,1.5300881807,0.8443271669\O,1.5019334718,1.2101237285,3.6427660989\O,-2.6648453883,0.3677208334,0.390407054\H,-2.3658245067,-0.6648691607,2.6163210826\H,-0.7121273127,2.0693859109,-0.0874143446\C,1.5939600321,2.4295794972,1.1982223259\F,2.6669234316,1.6407617855,1.1054695509\F,1.8754839644,3.4422476421,2.0212312263\F,1.3416001668,2.9378769025,-0.0174545131\H,-0.4805047982,-0.3171171754,4.1383482873\H,-1.3202905265,1.236417226,4.0252320204\Version=IA64L-G03RevE.01\State=2-A\HF=-752.3879276\S2=0.757032\S2-1=0.\S2A=0.750033\RMSD=7.294e-09\RMSF=1.966e-05\Thermal=0.\Dipole=-0.297443,-0.010793,0.6697794\PG=C01 [X(C5H4F3N2O2)]\@

NCF3_c6 56

1\1\GINC-AC18\FOpt\UB3LYP\6-31G(d)\C5H4F3N2O2(2)\JMH502\09-Apr-2009\0\#\UB3LYP/6-31G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultrafine)\SP Calc\0,2\C,0.5807731313,0.9854238432,2.9169551547\N,-1.606501158,-0.0242957398,2.4187958785\C,-0.5452449773,0.161006556,3.2704495587\C,-1.8110201561,0.6987717136,1.2558760298\N,0.5044572852,1.5756241398,1.6298085525\C,-0.8056970524,1.8131791072,1.0040758782\H,-0.5352262157,-0.3689716326,4.2117232438\O,1.5518776297,1.1185860192,3.6553450623\O,-2.7630423697,0.4938997893,0.5273470574\H,-2.3168733551,-0.7181993753,2.6279934833\H,-1.2597459576,2.7520544008,1.3604225081\H,-0.6870650486,1.893710491,-0.0748480834\C,1.5795785567,2.4299540811,1.237026392\F,2.7549931967,1.8026930921,1.2972901595\F,1.6632974578,3.5476585388,1.9884486086\F,1.384225991,2.8305559757,-0.0380614843\Version=IA64L-G03RevE.01\State=2-A\HF=-752.3953215\S2=0.757982\S2-1=0.\S2A=0.750042\RMSD=9.607e-09\RMSF=1.945e-05\Thermal=0.\Dipole=-1.1387095,-0.5600881,0.2804231\PG=C01 [X(C5H4F3N2O2)]\@

NAC 57

1\1\GINC-AC15\FOpt\UB3LYP\6-31G(d)\C6H8N2O3\JMH502\08-Apr-2009\0\#\UB3LYP/6-31G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultrafine)\SP Calc\0,1\C,-0.0092792106,-0.0279149318,0.0070026617\N,0.0140188892,0.0195454514,2.491830063\C,0.8245757121,-0.0135785575,1.2893724925\C,-1.0959029933,0.8049217438,2.6038419163\N,-1.2295969747,0.6366291551,0.0882929044\H,1.5218028564,0.8389876153,1.2287385222\C,-1.5518460931,1.4326557685,1.2905173916\H,1.4258369371,-0.9240824164,1.271672978\H,-1.1141621016,2.4373763367,1.2077863779\H,-2.6311317849,1.5597338602,1.3289928182\O,0.4247446015,-0.5724218105,-0.99192881\O,-1.6798184926,1.0143150277,3.6537072239\H,0.3908723316,-0.3462141869,3.3578567283\C,-2.1817802454,0.7179757402,-0.9745549318\O,-3.1374604705,1.457962818,-0.8410179933\C,-1.9867152679,-0.1287913498,-2.2089502978\H,-2.8880702907,-0.0160121182,-2.8137203215\H,-1.8191410174,-1.1794129935,-1.959837476\H,-1.109617077,0.197899944,-2.7728865903\Version=IA64L-G03RevE.01\State=1-A\HF=-568.6597582\S2=0.\S2-1=0.\S2A=0.\RMSD=9.066e-09\RMSF=6.965e-05\Thermal=0.\Dipole=1.3306338,-0.3605216,-0.1177996\PG=C01 [X(C6H8N2O3)]\@

NAC_c3 58

```
1\1\GINC-AC18\FOpt\UB3LYP\6-31G(d)\C6H7N2O3(2)\JMH502\08-Apr-2009\0\#\
UB3LYP/6-31G(d) opt freq=norman maxdisk=1342177280 INT(grid=ultrafin
e)\SP Calc\0,2\C,0.0166612466,0.2100913099,0.0201654383\C,0.05556523
24,0.047951561,2.4483422663\N,2.1029327433,-0.273156752,1.0793335907\C
,1.3839451727,-0.6806014765,2.2699135332\C,1.4266625789,-0.0914832076,
-0.1150329964\N,-0.6096245425,0.402451201,1.2533203811\O,-0.4036737157
,0.2354632427,3.5566968258\O,1.9845607686,-0.1289250103,-1.2115486086\C
,-1.9591232382,0.9481186369,1.2041004219\H,3.0554350103,-0.6009155698
,0.9699148464\H,-0.5812607043,0.4118028388,-0.8538776733\H,1.973604644
9,-0.4645249822,3.1632911092\H,1.152456811,-1.7615290523,2.282916019\C
,-2.7092622422,1.1912485929,2.4873440456\H,-3.6873112752,1.5849915476,
2.2057930009\H,-2.1827845347,1.900734369,3.1303044482\H,-2.8214657891,
0.2730055495,3.0691623438\O,-2.4327689648,1.1828468909,0.1144745643\Version=IA64L-G03RevE.01\State=2-A\HF=-568.0123771\S2=0.756862\S2-1=0.\S2A=0.75003\RMSD=5.456e-09\RMSF=1.786e-05\Thermal=0.\Dipole=0.0944368,-0.5264597,1.3867788\PG=C01 [X(C6H7N2O3)]\@
```

NAC_c6 59

```
1\1\GINC-AC15\FOpt\UB3LYP\6-31G(d)\C6H7N2O3(2)\JMH502\08-Apr-2009\0\#\
UB3LYP/6-31G(d) opt freq=norman maxdisk=1342177280 INT(grid=ultrafin
e)\SP Calc\0,2\C,0.0852203414,0.3019682821,-0.0231033372\C,0.1429963
37,0.2517808592,2.4854898495\N,2.145350856,-0.3133879459,1.1641589584\C
,1.4715843338,-0.2856876334,2.3572297625\C,1.5715338126,-0.0001020327
,-0.0582107425\N,-0.4559704057,0.706685581,1.2865348456\O,-0.399730245
8,0.3235661006,3.5893351015\O,2.2147043936,-0.0261620033,-1.090295125\C
,-1.6789286855,1.4169897536,1.2154896983\H,3.1233271075,-0.5822222964
,1.130930508\H,1.9787855822,-0.6313593409,3.2464612949\C,-2.3122140664
,1.9451027564,2.4811640396\H,-3.1301623644,2.5994135112,2.1741797477\H
,-1.596594737,2.4881398513,3.1029105201\H,-2.6948864333,1.1261244564,3
.0949449753\O,-2.1758059671,1.606094362,0.1173520423\H,-0.4417816218,-
0.5877063599,-0.397625043\H,-0.115700211,1.0960611094,-0.7419588449\Version=IA64L-G03RevE.01\State=2-A\HF=-568.0230566\S2=0.757661\S2-1=0.\S2A=0.750038\RMSD=7.023e-09\RMSF=6.253e-06\Thermal=0.\Dipole=0.9987328,-0.5014144,0.7176936\PG=C01 [X(C6H7N2O3)]\@
```

NACCF3 60

```
1\1\GINC-AC11\FOpt\UB3LYP\6-31G(d)\C6H5F3N2O3\JMH502\08-Apr-2009\0\#\
UB3LYP/6-31G(d) opt freq=norman maxdisk=1342177280 INT(grid=ultrafine
)\SP Calc\0,1\C,0.0048985707,-0.0216450003,0.0026429976\N,0.00285804
03,0.0084150238,2.4942792326\C,0.818005461,-0.0029287903,1.294658406\C
,-1.1359645192,0.7514147558,2.6084340427\N,-1.3009637566,0.4854989899,
0.1157876235\H,1.5024620934,0.8596479367,1.2414230231\C,-1.6486849863,
1.319849839,1.2872676585\H,1.4372156293,-0.9024581395,1.2754913991\H,-
1.2632925908,2.3397681449,1.1553824082\H,-2.7325841377,1.3917451626,1.
3461618147\O,0.4941531639,-0.4114636325,-1.0333497174\O,-1.7130221938,
0.962035343,3.6605272185\H,0.4025303097,-0.3221649663,3.3644792995\C,-
2.2625279509,0.4540781143,-0.9053158539\O,-3.2200786103,1.194656218,-0
.8938087067\C,-2.1701453823,-0.6236693896,-2.0272917502\F,-3.400570951
4,-0.8004548521,-2.5241453024\F,-1.7471584883,-1.8075635372,-1.5528809
661\F,-1.3732225231,-0.2256383789,-3.0256253457\Version=IA64L-G03RevE
.01\State=1-A\HF=-866.356535\S2=0.\S2-1=0.\S2A=0.\RMSD=5.928e-09\RMSF=
1.355e-05\Thermal=0.\Dipole=1.4179422,0.038277,0.7264041\PG=C01 [X(C6H
5F3N2O3)]\@
```

NACCF3_c3 61

```
1\1\GINC-AC18\FOpt\UB3LYP\6-31G(d)\C6H4F3N2O3(2)\JMH502\08-Apr-2009\0\
\# UB3LYP/6-31G(d) opt freq=norman maxdisk=1342177280 INT(grid=ultrafin
e)\SP Calc\0,2\C,-0.0041846403,0.1959414701,0.0178783492\C,0.04572
14972,0.0861601327,2.4599879091\N,2.0748224,-0.2757921437,1.1068782465
\C,1.3492707046,-0.681964538,2.2958214723\C,1.4179347593,-0.070493975,
-0.0918820322\N,-0.6663062228,0.3127153057,1.241941794\O,-0.3732564519
,0.4469533507,3.5319380561\O,1.9917372649,-0.0674405979,-1.1795405864\C
,-2.017085239,0.7612812195,1.1837025457\H,3.0383287183,-0.5739665658,
1.0123322397\H,-0.5870710153,0.3896485912,-0.8686887733\H,1.9422496499
,-0.4804793569,3.1896644071\H,1.0941213918,-1.7572146716,2.2962233169\C
,-2.9654042302,0.5366816908,2.3979384827\F,-4.2199108398,0.5369557256
,1.9338087432\F,-2.8571269609,1.5138450242,3.3030757192\F,-2.745753004
4,-0.654150835,2.9834850574\O,-2.4721204421,1.2225225849,0.1648109563\
Version=IA64L-G03RevE.01\State=2-A\HF=-865.7073652\S2=0.757252\S2-1=0
.\S2A=0.750036\RMSD=9.081e-09\RMSF=1.746e-05\Thermal=0.\Dipole=0.77860
14,-0.8805532,0.7991212\PG=C01 [X(C6H4F3N2O3)]\@
```

NACCF3_c6 62

```
1\1\GINC-AC15\FOpt\UB3LYP\6-31G(d)\C6H4F3N2O3(2)\JMH502\08-Apr-2009\0\
\# UB3LYP/6-31G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultraf
ine)\SP Calc\0,2\C,0.0332048946,0.1668352038,-0.027735695\C,0.040075
4186,0.1214887247,2.4711383512\N,2.1232617854,-0.1792205314,1.20329647
99\C,1.4134735134,-0.2801222822,2.3709902739\C,1.5502389326,0.07361966
18,-0.0371879724\N,-0.5212839522,0.6301240764,1.2560463845\O,-0.594647
2123,0.0447182066,3.5171365699\O,2.218909566,0.1475514536,-1.048422470
9\C,-1.7093381858,1.3472497811,1.1611232393\H,3.1270377925,-0.32940852
33,1.1978827383\H,1.9182330981,-0.6413743937,3.2557953962\C,-2.2534253
643,2.1064039519,2.4072928882\F,-3.0149113775,3.1179380028,1.969663244
\F,-1.2633236482,2.6350992215,3.1486450607\F,-3.0151485277,1.316313735
4,3.172531312\O,-2.2974279244,1.4724756334,0.1061936993\H,-0.371556902
7,-0.8210831901,-0.2924015854\H,-0.2760537335,0.8571898476,-0.81119309
84\Version=IA64L-G03RevE.01\State=2-A\HF=-865.7213237\S2=0.759056\S2-
1=0.\S2A=0.750048\RMSD=6.983e-09\RMSF=1.264e-05\Thermal=0.\Dipole=1.66
05775,-0.8686997,0.1582793\PG=C01 [X(C6H4F3N2O3)]\@
```

NSO2Me 63

```
1\1\GINC-AC8\FOpt\UB3LYP\6-31G(d)\C5H8N2O4S1\JMH502\09-Apr-2009\0\# U
B3LYP/6-31G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultrafine)
\SP Calc\0,2\H,-0.0593196643,-0.034384373,0.0335479272\C,-0.01617029
98,0.0044224239,1.1308633186\C,2.4084562585,0.0037342343,1.7631770878\
N,1.0516079405,2.0834391553,1.8316628774\C,2.3481874276,1.5099502495,1
.5165436608\C,-0.1345111702,1.4643560003,1.5665023154\N,1.2032533805,-
0.6612764757,1.6292391097\H,2.6417621616,1.6870989439,0.4688535088\H,-
0.8854580029,-0.5290372025,1.5116240439\H,3.1153104362,1.9588615106,2.
1503655992\O,3.4576067863,-0.5422048495,2.0584207003\O,-1.2202154772,2
.0128171908,1.6472083457\S,1.1916696971,-2.4225279506,1.6176073718\H,0
.9893766648,3.0722436409,2.0425219906\O,-0.2313837392,-2.7600385728,1.
5818792034\O,2.0992918681,-2.89902622,0.5805043666\C,1.8531249939,-2.8
316430491,3.2387872606\H,1.8622421897,-3.9233456393,3.2879115837\H,1.1
870362513,-2.4188937724,3.9979328969\H,2.860150667,-2.4221443358,3.307
4728118\Version=IA64L-G03RevE.01\State=1-A\HF=-1003.8837899\S2=0.\S2-
1=0.\S2A=0.\RMSD=4.970e-09\RMSF=1.602e-05\Thermal=0.\Dipole=0.8255798,
0.9135921,0.7946624\PG=C01 [X(C5H8N2O4S1)]\@
```

NSO2Me_c3 64

```
1\1\GINC-AC30\FOpt\UB3LYP\6-31G(d)\C5H7N2O4S1(2)\JMH502\09-Apr-2009\0\
\# UB3LYP/6-31G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultraf
ine)\SP Calc\0,2\N,-0.1981995821,0.560798498,0.0013700432\C,-0.12023
94501,-0.1825785186,2.2732581455\C,1.9380521444,-0.2529914226,0.942603
0312\N,1.2026622065,-0.5706593121,2.0927645071\C,1.2460037419,0.720055
3981,-0.0043221045\C,-0.8987842469,0.3734646103,1.1831835154\H,-0.5768
097797,-0.3919872224,3.2284632368\H,1.6440468017,0.5244460906,-1.00242
86427\H,1.5683579363,1.7350846255,0.2896975177\O,3.0559333074,-0.68729
0821,0.7377938107\O,-2.1017105785,0.6080771562,1.2901418009\S,2.03215
0548,-1.3906483802,3.4546814927\H,-0.7242401568,1.0533764184,-0.710757
2504\C,2.509209198,-2.9586138625,2.7159434825\O,0.9689735199,-1.617218
0899,4.4288986825\O,3.2137263905,-0.6078268279,3.7829841233\H,3.173036
6478,-2.7464463841,1.8783762736\H,1.6035833845,-3.4821494528,2.4052049
975\H,3.0241397046,-3.5153158638,3.5031621089\Version=IA64L-G03RevE.0
1\State=2-A\HF=-1003.2380035\S2=0.757208\S2-1=0.\S2A=0.750036\RMSD=9.7
98e-09\RMSF=8.084e-06\Thermal=0.\Dipole=0.5875521,-0.6086211,-1.199493
9\PG=C01 [X(C5H7N2O4S1)]\@
```

NSO2Me_c6.a3 65

```
1\1\GINC-AC4\FOpt\UB3LYP\6-31G(d)\C5H7N2O4S1(2)\JMH502\12-Apr-2009\0\
\# UB3LYP/6-31G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultrafi
ne)\SP Calc\0,2\N,-0.0725091422,0.2427680604,-0.0179024158\C,-0.0308
770928,-0.1343885794,2.4120024983\C,2.0798943611,-0.2921788368,1.04357
33582\N,1.3451994536,-0.6218867125,2.2006713054\C,1.2970375736,0.17267
2979,-0.0714626039\C,-0.8269271859,0.0446061909,1.1283566822\H,1.79297
7777,0.4010103196,-1.0037609065\O,3.2969231,-0.4630386677,0.956850184\
O,-2.0418358445,0.082716922,1.1093351339\S,2.2089675374,-1.01208013,3.
668336455\H,-0.6075637565,0.4418018665,-0.8568830195\C,3.135238623,-2.
4792397894,3.1990727967\O,1.144595485,-1.3945177147,4.5992837105\O,3.1
33944476,0.0649447343,4.0071579521\H,3.8072447519,-2.2090586372,2.3855
839523\H,2.4273107396,-3.256612401,2.9081003324\H,3.6885593607,-2.7776
991592,4.09299387\H,-0.0328270124,0.8378158955,2.9276468077\H,-0.56788
42677,-0.8384529226,3.0470808246\Version=IA64L-G03RevE.01\State=2-A\H
```

F=-1003.2455312\S2=0.757055\S2-1=0.\S2A=0.750034\RMSD=4.848e-09\RMSF=1.050e-05\Thermal=0.\Dipole=-0.212769,-0.4847382,-1.6042971\PG=C01 [X(C5H7N2O4S1)]\@

NSO2CF3_a3 66

1\1\GINC-AC29\FOpt\UB3LYP\6-31G(d)\C5H5F3N2O4S1\JMH502\13-Apr-2009\0\#\ UB3LYP/6-31G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultrafine)\SP Calc\0,1\H,0.0363715191,0.0103516545,-0.0407051198\C,0.0252519796,-0.0465848395,1.0558359936\C,2.4345924708,0.1108646478,1.7528269073\N,0.8677908975,2.0274476287,2.0373921546\C,2.2303120832,1.6221125329,1.7449812099\C,-0.2405001012,1.3494154485,1.6226312098\N,1.2816736336,-0.6422604518,1.5540724315\H,2.5789612593,1.9951545591,0.7684407266\H,-0.8085706828,-0.6816520023,1.3475197021\H,2.9074015909,2.0238553077,2.5025982317\O,3.5340473621,-0.382677502,1.8966002813\O,-1.3726184956,1.7955689889,1.6771069723\S,1.3865918736,-2.3646889004,1.6846029317\H,0.6999413083,2.9735515564,2.3585853516\O,1.9862262465,-2.7368345978,2.9530454287\O,0.0787400324,-2.8484653078,1.2569720742\C,2.5919757792,-2.847238018,0.2977822616\F,2.1669047724,-4.0092821622,-0.1921229845\F,3.8215160691,-2.976374096,0.7583106714\F,2.5491790929,-1.9168822697,-0.6618415049\Version=IA64L-G03RevE.01\State=1-A\HF=-1301.5731244\S2=0.\S2-1=0.\S2A=0.\RMSD=6.485e-09\RMSF=2.120e-05\Thermal=0.\Dipole=0.6808235,1.433769,-0.7784942\PG=C01 [X(C5H5F3N2O4S1)]\@

NSO2CF3_c3.a2 67

1\1\GINC-AC30\FOpt\UB3LYP\6-31G(d)\C5H4F3N2O4S1(2)\JMH502\12-Apr-2009\0\#\ UB3LYP/6-31G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultrafine)\SP Calc\0,2\H,0.1236607381,-0.0622626502,-0.0122310391\C,0.0483253174,-0.0497799837,1.0640658307\C,1.2585215827,-0.1677510239,3.2066663581\N,-1.2001024906,0.0329478862,3.1053827652\C,-0.0033138209,0.3954631888,3.8449222412\C,-1.2418890537,0.0584161576,1.721297465\N,1.2149052543,-0.2427466634,1.8017464021\H,0.1381411997,1.4879353163,3.9263715304\H,-0.048576706,-0.0080996999,4.8587747341\O,2.2453980679,-0.4904113747,3.8320917491\O,-2.2914475756,0.1171174989,1.0839908471\S,2.7186740678,-0.5805181505,0.9377236708\H,-2.0946754345,0.2094431149,3.5467300977\O,2.3159591485,-0.7353136435,-0.4530116714\O,3.7350095675,0.3622350217,1.3668451541\C,3.1942024784,-2.3188133246,1.5582870785\F,3.7154054578,-2.9546264853,0.5134985987\F,2.1012206291,-2.953578772,1.9751050815\F,4.0839003916,-2.2330877385,2.5273446862\Version=IA64L-G03RevE.01\State=2-A\HF=-1300.9253927\S2=0.757233\S2-1=0.\S2A=0.750036\RMSD=6.026e-09\RMSF=1.307e-05\Thermal=0.\Dipole=-0.3204475,-0.0468835,1.1903853\PG=C01 [X(C5H4F3N2O4S1)]\@

NSO2CF3_c6 68

1\1\GINC-AC30\FOpt\UB3LYP\6-31G(d)\C5H4F3N2O4S1(2)\JMH502\09-Apr-2009\0\#\ UB3LYP/6-31G(d) opt freq=noraman maxdisk=1342177280 INT(grid=ultrafine)\SP Calc\0,2\H,-0.870648952,-0.35902104,1.4197867379\C,-0.1590261284,0.3985982482,1.7425701488\C,2.341696978,0.5591276825,1.9805982247\N,1.1150992454,2.1192623828,0.5382100801\C,2.2527947726,1.7756843467,1.22315712\C,-0.1140433805,1.4862390721,0.676537562\N,1.1560554157,-0.2268255949,1.9638798294\H,-0.5414170272,0.8505262188,2.6699371807\H,3.1188362004,2.4178999756,1.149563186\O,3.3561066213,0.1999702684,2.5693542654\O,-1.0880672054,1.8309889178,0.0388547474\S,1.2147171768,-1.8324614126,2.5445254165\H,1.1266753166,2.9005178771,-0.1096169198\O,-0.1665224652,-2.3021273878,2.4892231906\O,2.3139617077,-2.5506522094,1.9258389967\C,1.6081740004,-1.6433042216,4.3894739362\F,0.9661757354,-2.6191912598,5.0292265085\F,1.1468130626,-0.4587865907,4.8098558459\F,2.9047644495,-1.7358093296,4.6185445096\Version=IA64L-G03RevE.01\State=2-A\HF=-1300.9363768\S2=0.75806\S2-1=0.\S2A=0.750042\RMSD=7.028e-09\RMSF=2.257e-05\Thermal=0.\Dipole=-0.008667,1.9376555,-0.1234845\PG=C01 [X(C5H4F3N2O4S1)]\@

nhf-dkp 69

1\1\GINC-X127\FOpt\RB3LYP\6-31G(d)\C4H7F1N2O2\JMH502\19-May-2009\0\#\ B3LYP/6-31G(d) opt freq=noraman maxdisk=671088640 INT(grid=ultrafine)\SP Calc\0,1\C,0.0610463522,0.034703965,-0.0459067193\N,-0.0302251578,-0.0849208349,2.4456042416\C,0.8242648768,0.0233426255,1.2742355763\C,-1.2975438105,0.418195688,2.5471859101\N,-1.3158536476,0.1629574237,0.0664681904\H,1.4469680096,0.9314656521,1.2946521471\C,-1.9367308359,0.8305601233,1.2234031151\H,1.5090505541,-0.8289702875,1.2356789749\H,-1.8849005604,1.9245925048,1.1345253821\H,-2.9841989154,0.5342333951,1.275258816\O,0.627891699,-0.0962449663,-1.1130601466\O,-1.8916973228,0.5402003205,3.6034984379\H,-1.7543928998,0.3393783836,-0.8346492145\H,

0.4004848007,-0.3188497451,3.3325132233\H,-2.1074890496,-1.4877766521,
0.5357705312\F,-2.7696455659,-1.9519111683,1.0284257819\Version=EM64L
-G03RevE.01\State=1-A\HF=-516.4369408\RMSD=3.663e-09\RMSF=1.525e-05\Th
ermal=0.\Dipole=0.8642713,0.8515353,-0.3702354\PG=C01 [X(C4H7F1N2O2)]\
\@

nhf-dkp_c6 70

1\1\GINC-X69\FOpt\UB3LYP\6-31G(d)\C4H6F1N2O2(2)\JMH502\27-Oct-2010\0\
\# UB3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafin
e)\SP Calc\0,2\C,0.0021112835,0.1083776387,-0.0715387642\N,-0.036043
75,-0.0961700547,2.3663464541\C,0.6671222574,-0.0948861329,1.186216562
4\C,-1.3657421191,0.2895704232,2.5039146073\N,-1.4128226197,0.19967970
68,0.0216159058\C,-2.0082917455,0.8074260491,1.2234788513\H,1.73080226
62,-0.2825161335,1.2156074253\H,-1.9120615081,1.9044671775,1.225200425
5\H,-3.0679014892,0.5537816336,1.2714165032\O,0.576181944,0.1281370931
, -1.1575558195\O,-1.9209823083,0.2910965028,3.5827781657\H,-1.80240869
56,0.5375669795,-0.8551342055\H,0.4150782944,-0.3831173116,3.228717252
1\H,-2.032049573,-1.4371346855,0.4377961497\F,-2.4036304836,-2.0392751
422,1.0785110181\Version=EM64L-G03RevE.01\State=2-A\HF=-515.8005303\S
2=0.757669\S2-1=0.\S2A=0.750038\RMSD=7.654e-09\RMSF=1.702e-05\Thermal=
0.\Dipole=0.4884209,0.9372138,0.1073495\PG=C01 [X(C4H6F1N2O2)]\@

ohf-dkp 71

1\1\GINC-X137\FOpt\RB3LYP\6-31G(d)\C4H7F1N2O2\JMH502\19-May-2009\0\
\# B3LYP/6-31G(d) opt freq=noraman maxdisk=671088640 INT(grid=ultrafine)
\SP Calc\0,1\C,0.0111382011,0.0357452888,-0.029433338\N,0.0252233839,
-0.0078156996,2.449867942\C,0.8388572785,0.0448757608,1.2458410097\C,-
1.2296870587,0.5018103862,2.584902954\N,-1.2700510577,0.4394299544,0.0
821559578\H,1.4725684889,0.9458441596,1.2156337092\C,-1.8878407943,0.9
771869225,1.2891719578\H,1.5160966328,-0.8094661206,1.1937955754\H,-1.
8760846271,2.0767679464,1.2867061835\H,-2.9334986963,0.6635320742,1.33
27987799\O,0.4994101044,-0.3037752511,-1.1145484487\O,-1.820465703,0.5
884959716,3.6494589117\H,-1.7953329561,0.4535870246,-0.7848509354\H,0.
468465401,-0.2875513045,3.3168738792\H,1.9903674145,-0.9889931979,-0.9
128668906\F,2.7834545099,-1.3403188737,-0.4975164232\Version=EM64L-G0
3RevE.01\State=1-A\HF=-516.4521294\RMSD=8.545e-09\RMSF=1.996e-05\Therm
al=0.\Dipole=-0.8651551,0.8181173,-0.098541\PG=C01 [X(C4H7F1N2O2)]\@

ohf-dkp_c3 72

1\1\GINC-V1288\FOpt\UB3LYP\6-31G(d)\C4H6F1N2O2(2)\JMH502\27-Oct-2010\
\# UB3LYP/6-31G(d) opt freq=noraman INT(grid=ultrafine)\SP Calc\0,2
\C,-0.0724265945,0.1403778745,-0.15454463\N,0.1183779684,0.034932996,
2.2765325657\C,0.7086146286,-0.0589990659,1.0389578513\C,-1.1908302723,
0.4135867636,2.518716473\N,-1.3965299396,0.4372443293,0.0274831256\C,-
1.9968827011,0.8306063407,1.2932030591\H,1.7521275179,-0.3282443738,0.
9560748041\H,-2.1300780518,1.9223265798,1.3601117776\H,-2.9899791816,0
.3818905804,1.3985138494\O,0.4070235419,0.0157004778,-1.3014044651\O,-
1.6541624294,0.4549019159,3.6433269289\H,-1.9140379972,0.6096472126,-0.
8254858025\H,0.6553094547,-0.1913490444,3.1075865994\H,1.9907999897,-
0.3942201651,-1.2064115833\F,2.8665691496,-0.6106284518,-0.8620996408\
\Version=EM64L-G03RevE.01\State=2-A\HF=-515.8136192\S2=0.755054\S2-1=0
.\S2A=0.75002\RMSD=8.710e-09\RMSF=1.568e-05\Thermal=0.\Dipole=-1.20899
78,0.4684326,0.5450215\PG=C01 [X(C4H6F1N2O2)]\@

ohf-dkp_c6 73

1\1\GINC-X119\FOpt\UB3LYP\6-31G(d)\C4H6F1N2O2(2)\JMH502\19-May-2009\0\
\# UB3LYP/6-31G(d) opt freq=noraman maxdisk=671088640 INT(grid=ultrafi
ne)\SP Calc\0,2\C,-0.0181352566,0.0550230983,-0.0487127229\N,0.16494
47482,0.1740406857,2.4139384223\C,0.8728474379,-0.0912331447,1.1720012
064\C,-0.8538139606,1.1005919635,2.5374622328\N,-1.1165724622,0.860199
4852,0.1024950548\H,1.7270007467,0.5918297603,1.0160696234\C,-1.500649
928,1.4557205389,1.2873333808\H,1.2831731227,-1.1029485522,1.154275764
5\H,-2.3425210158,2.1317424192,1.274288516\O,0.2416128125,-0.456414273
9,-1.1401874362\O,-1.22987534,1.5465113755,3.6209273508\H,-1.668120045
8,0.9980997707,-0.7388271691\H,0.6493836591,-0.0276249228,3.2799855682
\H,1.5466048561,-1.519013376,-1.0043136766\F,2.2565036219,-2.025742809
4,-0.610884362\Version=EM64L-G03RevE.01\State=2-A\HF=-515.8081731\S2=
0.756866\S2-1=0.\S2A=0.750035\RMSD=5.976e-09\RMSF=5.783e-05\Thermal=0.
\Dipole=-0.5920784,0.7335956,-0.5110703\PG=C01 [X(C4H6F1N2O2)]\@

nh+dkp 74

1\1\GINC-X134\FOpt\RB3LYP\6-31G(d)\C4H7N2O2(1+)\JMH502\20-May-2009\0\
\# B3LYP/6-31G(d) opt freq=noraman maxdisk=402653184 INT(grid=ultrafine

)\SP Calc\1,1\C,0.0042531066,0.0016636728,-0.0000933177\N,-0.006171693,-0.0070357667,2.4908262532\C,0.881293213,0.0038713464,1.2610398663\C,-0.9512268689,1.2474067962,2.5439806914\N,-1.2366928376,0.5769316839,0.1868239888\H,1.5187103909,0.8915869582,1.3180030937\C,-1.510879789,1.5966030534,1.1864154848\H,1.5073127978,-0.8893556331,1.2655328422\H,-1.1095141584,2.5911767883,0.9295500833\H,-2.5930970043,1.7205119443,1.3064942135\O,0.3761450208,-0.5322584931,-1.0166509761\O,-1.0815790194,1.7887007511,3.5863174853\H,-1.8174271336,0.5917293478,-0.6472852381\H,0.5301482288,-0.0085007748,3.3693509782\H,-0.5889040584,-0.8567645778,2.488999152\Version=EM64L-G03RevE.01\State=1-A\HF=-416.3218698\RMSD=7.547e-09\RMSF=5.214e-05\Thermal=0.\Dipole=-0.0871317,-0.1017037,1.4344001\PG=C01 [X(C4H7N2O2)]\@

nh+dkp_c3 75

1\1\GINC-X127\FOpt\UB3LYP\6-31G(d)\C4H6N2O2(1+,2)\JMH502\20-May-2009\0\# UB3LYP/6-31G(d) opt freq=norman maxdisk=402653184 INT(grid=ultrafine)\SP Calc\1,2\C,0.0044650987,0.1010029787,0.0180743555\N,-0.0422613488,-0.3534834327,2.4418084513\C,0.7425464515,0.0291468347,1.273320197\C,-1.349003092,0.6098811561,2.6151860649\N,-1.3762948476,0.152099785,0.1885402978\C,-1.9663199745,0.9198143442,1.2742769747\H,1.8153313318,0.1312469524,1.3711291797\H,-1.8787533799,2.0123641918,1.1505194506\H,-3.036420454,0.6961787611,1.3560744533\O,0.577227583,0.0021638706,-1.0552990856\O,-1.6044734113,0.9612344761,3.7069465225\H,-1.8962049525,0.1597246879,-0.6848925064\H,0.4842029757,-0.3032407153,3.3241888028\H,-0.400283773,-1.3196513109,2.3482158951\Version=EM64L-G03RevE.01\State=2-A\HF=-415.6528839\S2=0.763255\S2-1=0.\S2A=0.750077\RMSD=4.131e-09\RMSF=2.607e-05\Thermal=0.\Dipole=-0.2350701,-0.4945731,1.4435457\PG=C01 [X(C4H6N2O2)]\@

nh+dkp_c6 76

1\1\GINC-X156\FOpt\UB3LYP\6-31G(d)\C4H6N2O2(1+,2)\JMH502\20-May-2009\0\# UB3LYP/6-31G(d) opt freq=norman maxdisk=402653184 INT(grid=ultrafine)\SP Calc\1,2\C,0.0027403301,0.0033814939,-0.0013815038\N,0.0261705569,0.0707767917,2.5019279408\C,0.8631391984,-0.0578885399,1.2577144676\C,-1.000103809,1.2894624984,2.4858392085\N,-1.1319030673,0.8261555226,0.0966769843\C,-1.5314162267,1.5195217494,1.199944188\H,1.4144754917,-0.999123205,1.274073553\H,-2.3126814646,2.2618604382,1.089930119\O,0.3003796456,-0.5580064462,-1.0237162245\O,-1.2016785352,1.8252427419,3.547041513\H,-1.6388403017,0.9532679645,-0.7778498257\H,0.6090329861,0.2182419244,3.3365352153\H,-0.5080281461,-0.7920767761,2.6748096801\H,1.5739647927,0.7753612497,1.2492124457\Version=EM64L-G03RevE.01\State=2-A\HF=-415.6971339\S2=0.759171\S2-1=0.\S2A=0.750048\RMSD=6.380e-09\RMSF=5.111e-05\Thermal=0.\Dipole=0.1951791,-0.4240259,0.6787476\PG=C01 [X(C4H6N2O2)]\@

oh+dkp 77

1\1\GINC-X156\FOpt\RB3LYP\6-31G(d)\C4H7N2O2(1+)\JMH502\20-May-2009\0\# B3LYP/6-31G(d) opt freq=norman maxdisk=402653184 INT(grid=ultrafine)\SP Calc\1,1\C,0.0036763996,0.0092348016,-0.0009494185\N,0.0068544017,0.0294247202,2.4427962551\C,0.8234827988,-0.0309292748,1.2539311582\C,-1.2742235446,0.5181296461,2.5302467149\N,-1.2442302963,0.3665748386,0.0086274614\H,1.5464112738,0.8017852487,1.1865899478\C,-1.9954940388,0.7864467674,1.20842622\H,1.4082316575,-0.9614434939,1.2446490404\H,-2.2130045711,1.8566407199,1.130061006\H,-2.9448893178,0.2454010003,1.2247965628\O,0.5266812258,-0.2770896641,-1.1678475208\O,-1.8530996362,0.7092710928,3.5739036586\H,-1.7289769978,0.379474117,-0.8900951235\H,0.4682501246,-0.1170335313,3.3350597145\H,1.4546899719,-0.5735699004,-1.1186818958\Version=EM64L-G03RevE.01\State=1-A\HF=-416.3429853\RMSD=3.784e-09\RMSF=3.260e-05\Thermal=0.\Dipole=1.5167766,-0.4154051,-2.1936288\PG=C01 [X(C4H7N2O2)]\@

oh+dkp_c3 78

1\1\GINC-X133\FOpt\UB3LYP\6-31G(d)\C4H6N2O2(1+,2)\JMH502\20-May-2009\0\# UB3LYP/6-31G(d) opt freq=norman maxdisk=402653184 INT(grid=ultrafine)\SP Calc\1,2\C,0.0035042688,0.0551985748,-0.0431326159\N,0.0611967039,0.0388774331,2.3461266285\C,0.696683825,-0.172388429,1.1645098546\C,-1.2722902364,0.4792952716,2.4812952396\N,-1.2580981041,0.471681815,-0.0316829588\C,-2.0346744016,0.7297887789,1.1849142647\H,1.7242136394,-0.5125788478,1.1840337333\H,-2.3721941684,1.7727242739,1.1918550199\H,-2.9273984941,0.0937112305,1.1937523515\O,0.5295525062,-0.1201640113,-1.245154712\O,-1.7661203542,0.6432569524,3.5653498797\H,-1.7066512551,0.6190140964,-0.9326604514\H,0.5502947732,-0.1214999987,3.22458328\H,1.454061725,-0.4237850216,-1.2182533345\Version=EM64L-G03RevE.01\

tate=2-A\HF=-415.7189351\S2=0.75365\S2-1=0.\S2A=0.750011\RMSD=6.455e-09\RMSF=1.870e-05\Thermal=0.\Dipole=1.1965647,-0.3949841,-1.3086658\PG=C01 [X(C4H6N2O2)]\@

oh+dkp_c6 79

1\1\GINC-X121\FOpt\UB3LYP\6-31G(d)\C4H6N2O2(1+,2)\JMH502\20-May-2009\0\# UB3LYP/6-31G(d) opt freq=noraman maxdisk=402653184 INT(grid=ultrafine)\SP Calc\1,2\C,-0.0197186387,0.0335491332,-0.0035678458\N,0.1102672486,0.2003786852,2.4229326468\C,0.8386881386,-0.1273018562,1.2147652283\C,-0.9971713099,1.026956057,2.4914693325\N,-1.1463371938,0.7299498558,0.0506540509\C,-1.6465689333,1.2936113448,1.2019223941\H,1.19332124,-1.1671334062,1.2564036687\H,-2.5497404102,1.883152238,1.1332569343\O,0.3084157021,-0.428882946,-1.1852632365\O,-1.4610642356,1.4620171104,3.5290555499\H,-1.6607587384,0.8449478562,-0.8258603799\H,0.56963913,0.0229887804,3.3100549968\H,1.1336292528,-0.9495439448,-1.1850507077\H,1.7331320777,0.5078212175,1.0657587409\Version=EM64L-G03RevE.01\State=2-A\HF=-415.6903384\S2=0.763133\S2-1=0.\S2A=0.750109\RMSD=8.633e-09\RMSF=2.796e-05\Thermal=0.\Dipole=1.2105905,-0.9506631,-2.2789872\PG=C01 [X(C4H6N2O2)]\@

Glycylsarcosine anhydrides

Sarcosine 80

1\1\GINC-V1255\FOpt\RB3LYP\6-31G(d)\C6H10N2O2\JMH502\24-Oct-2010\0\# B3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine)\SP Calc\0,1\C,-0.0336475811,-0.0793680714,0.0026202014\N,0.0118940576,0.0219644702,2.5392502763\C,0.753731226,-0.1833337433,1.3047374481\C,-1.1644361803,0.7073679747,2.5986760821\N,-1.2649699498,0.5006047019,0.0701378539\H,1.5987622198,0.5203090219,1.2351730275\C,-1.7815315912,1.1374200845,1.2718168992\H,1.1900823538,-1.1879800801,1.3120027698\H,-1.6865562317,2.2331365163,1.2050192111\H,-2.8529531346,0.9263184486,1.3566883792\O,0.4695349352,-0.5081888133,-1.0291912752\O,-1.7397268408,0.99815733,3.6409070367\C,-2.0405609367,0.6823022243,-1.1492214281\C,0.6813418911,-0.3633872798,3.7740541196\H,0.0103315175,-0.1494225507,4.6051871335\H,0.9220501369,-1.4328753031,3.7538205415\H,1.6136168156,0.2021764889,3.9047366123\H,-3.0509948174,0.2779722302,-1.0162276643\H,-2.1212673185,1.747325274,-1.4048558229\H,-1.5328171054,0.1554247457,-1.9563274733\Version=EM64L-G03RevE.01\State=1-A\HF=-494.631553\RMSD=9.974e-09\RMSF=1.115e-05\Thermal=0.\Dipole=0.0991449,0.1896056,-0.0144135\PG=C01 [X(C6H10N2O2)]\@

sarcosine_rad 81 82

1\1\GINC-V1256\FOpt\UB3LYP\6-31G(d)\C6H9N2O2(2)\JMH502\24-Oct-2010\0\# UB3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine)\SP Calc\0,2\C,0.0315470608,0.0694605605,0.0051360527\N,-0.0074973586,-0.1138478095,2.5214035062\C,0.7982774918,-0.0134639568,1.3181343956\C,-1.2930652531,0.3996277812,2.5793498641\N,-1.292115533,0.477087851,0.0909987823\H,1.4667623691,0.866611378,1.3532713226\C,-1.9040207045,0.7083296226,1.3042338213\H,1.4516085143,-0.8895329329,1.2372884731\H,-2.9182935199,1.0810631989,1.2936539936\O,0.5849417836,-0.1627582755,-1.0588385101\O,-1.9138617824,0.5495212839,3.6368752651\C,-2.0629548986,0.6481766068,-1.1433442838\C,0.7057701972,-0.3819921899,3.7578566304\H,-0.0228082872,-0.4179435021,4.5672962383\H,1.2331963715,-1.3408799089,3.687189642\H,1.4431550328,0.4051762015,3.976084537\H,-2.4948021936,1.6532249144,-1.169749237\H,-1.3858332623,0.5100618363,-1.9844745614\H,-2.8676669033,-0.0924082201,-1.1899864516\Version=EM64L-G03RevE.01\State=2-A\HF=-493.991011\S2=0.756008\S2-1=0.\S2A=0.750027\RMSD=9.407e-09\RMSF=4.309e-06\Thermal=0.\Dipole=0.1319235,0.1232718,-0.544364\PG=C01 [X(C6H9N2O2)]\@

NCF3 83

1\1\GINC-X86\FOpt\RB3LYP\6-31G(d)\C6H7F3N2O2\JMH502\14-Oct-2010\0\# B3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine)\SP Calc\0,1\C,-0.0124459231,0.004105429,0.0070339695\N,-0.0114873471,0.0170998161,2.5290589294\C,0.7798735202,0.0092007695,1.3093722793\C,-1.2106637167,0.6624612919,2.6078744989\N,-1.3096744299,0.4857462189,0.0937480929\H,1.476332907,0.8637740513,1.2741777218\C,-1.7892237729,1.1868404722,1.2951834749\H,1.394986598,-0.8947723766,1.2867129995\H,-1.5778488668,2.2640507379,1.2326437107\H,-2.8675998285,1.0692253256,1.3735608675\O,0.4929558245,-0.3921436783,-1.0241283328\O,-1.8258227985,0.8

525000838,3.6479647008\C,-2.0647245586,0.5840231508,-1.1239639492\F,-2.1898884595,-0.6028173776,-1.7238548519\F,-1.5092371476,1.4380006961,-2.0010221822\F,-3.3002117887,1.0432441738,-0.8453258014\C,0.6428297083,-0.4375734366,3.7497335444\H,-0.0796342183,-0.3772858029,4.5629313523\H,0.9835347225,-1.4717595849,3.6278883803\H,1.5088371489,0.1933260731,3.9903379116\\Version=EM64L-G03RevE.01\State=1-A\HF=-792.3461204\RMSD=4.839e-09\RMSF=1.516e-05\Thermal=0.\Dipole=0.7530975,0.1738917,0.7521934\PG=C01 [X(C6H7F3N2O2)]\@

NCF3_c3 84

1\1\GINC-X117\FOpt\UB3LYP\6-31G(d)\C6H6F3N2O2(2)\JMH502\14-Oct-2010\0\#\ UB3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine)\SP Calc\0,2\C,-0.007957116,0.0218342597,0.0028979912\N,0.0097457044,0.0696487017,2.5154063274\C,0.7935496535,0.0069288459,1.2954050862\C,-1.1695687092,0.7939070456,2.5659849033\N,-1.2599319368,0.6581066726,0.0811971268\C,-1.7795106945,1.1107139995,1.2910219019\O,0.4269908784,-0.4309623774,-1.0340699528\O,-1.7194484342,1.1220763337,3.6207162741\C,0.7148670738,-0.2160097919,3.7551791943\H,-2.7088341126,1.654637101,1.2764646272\C,-2.0182754094,0.7938323358,-1.1495082316\F,-2.334905538,-0.4007394466,-1.655363941\F,-1.3273575553,1.4775221867,-2.0643485334\F,-3.1570088862,1.458994587,-0.9029784703\H,1.3775813569,-0.9184725126,1.2792729259\H,1.5202121669,0.8383798752,1.2324896277\H,0.0038323788,-0.1329824168,4.5764361405\H,1.1297124823,-1.2296669179,3.7210557719\H,1.5373087036,0.4946324126,3.9247756842\\Version=EM64L-G03RevE.01\State=2-A\HF=-791.7005419\S2=0.756383\S2-1=0.\S2A=0.750029\RMSD=9.745e-09\RMSF=1.498e-05\Thermal=0.\Dipole=0.7058045,-0.0321947,0.2290378\PG=C01 [X(C6H6F3N2O2)]\@

NCF3_c6 85

1\1\GINC-X103\FOpt\UB3LYP\6-31G(d)\C6H6F3N2O2(2)\JMH502\14-Oct-2010\0\#\ UB3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine)\SP Calc\0,2\C,-0.0129214876,0.0190961588,0.0084548173\N,-0.0119234895,0.0114840814,2.491432535\C,0.6494160612,0.0474204543,1.2865672879\C,-1.388566963,0.1979820601,2.5699740342\N,-1.426972603,-0.0198282925,0.078734889\C,-2.0838791585,0.5491317783,1.2619920848\H,1.7301643757,0.0266345737,1.3008009144\O,0.6077696448,-0.0200489902,-1.049632046\O,-2.0003554503,0.1548944996,3.623032958\C,0.7464787317,-0.2281022282,3.7233010886\H,-2.1429693914,1.6484430839,1.2024483254\H,-3.0994290479,0.1662782122,1.3367838757\C,-2.1532845016,0.0025744515,-1.1490965986\F,-1.7837163479,-0.9915087145,-1.957133112\F,-2.0114360272,1.1641860946,-1.8233121931\F,-3.4713087075,-0.137255317,-0.8879285612\H,0.0712726231,-0.0904360586,4.5660059159\H,1.1418163588,-1.2484718341,3.7289679636\H,1.575485874,0.4829046794,3.7859747624\\Version=EM64L-G03RevE.01\State=2-A\HF=-791.7085262\S2=0.757683\S2-1=0.\S2A=0.750039\RMSD=6.737e-09\RMSF=1.972e-05\Thermal=0.\Dipole=0.5821137,0.1841682,1.4123727\PG=C01 [X(C6H6F3N2O2)]\@

NAC 86

1\1\GINC-X83\FOpt\RB3LYP\6-31G(d)\C7H10N2O3\JMH502\14-Oct-2010\0\#\ B3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine)\SP Calc\0,1\C,-0.0173126577,-0.0036241639,0.0085910098\N,-0.0057885556,0.0162346796,2.5156782857\C,0.7948501678,0.012823223,1.3028367866\C,-1.1370068062,0.7795928489,2.594891063\N,-1.2416636402,0.6502561329,0.0739708931\H,1.4866212899,0.8723896802,1.264703391\C,-1.5790425738,1.4220961332,1.2844241149\H,1.4109203119,-0.8889537336,1.2795591047\H,-1.1477850419,2.4313152301,1.2221724182\H,-2.6594054097,1.5414587271,1.3164147561\O,0.4359523036,-0.5440631932,-0.9844999049\O,-1.7639360982,0.9768718812,3.6260227167\C,0.5742080035,-0.5552794898,3.7231886138\C,-2.1778294745,0.7415871034,-1.0009339353\O,-3.1419617812,1.4710779653,-0.8697130972\C,-1.9540862422,-0.0814354893,-2.2461784646\H,-2.8428709357,0.0386251976,-2.8680389112\H,-1.7869576897,-1.1357221631,-2.0123996553\H,-1.0663575405,0.2584319316,-2.7854938838\H,-0.1677989244,-0.4809280321,4.5178595893\H,0.8358413395,-1.6057315716,3.5540288782\H,1.4785498079,-0.0104780987,4.0261252692\\Version=EM64L-G03RevE.01\State=1-A\HF=-607.9723924\RMSD=5.436e-09\RMSF=1.930e-05\Thermal=0.\Dipole=1.3400153,-0.3896223,0.0165712\PG=C01 [X(C7H10N2O3)]\@

NAC_c3 87

1\1\GINC-X73\FOpt\UB3LYP\6-31G(d)\C7H9N2O3(2)\JMH502\14-Oct-2010\0\#\ UB3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine)\SP Calc\0,2\C,-0.0180191666,0.0317163973,-0.0094433259\C,-0.0080974454,-0.004132552,2.4142105264\N,2.1227833033,-0.0687773709,1.077246874

4\C,1.4435170469,-0.4532435884,2.297233649\C,1.4249269312,-0.031919309
, -0.1185117101\N, -0.7036093236, 0.1524698512, 1.199028267\O, -0.516379433
5, 0.1402839672, 3.5083690874\O, 1.9758678875, -0.0064594138, -1.2220313601
\C, -2.1305064169, 0.4248057273, 1.1031678802\C, 3.5671807974, -0.232113504
6, 1.0502057773\H, -0.6166566403, 0.0926704868, -0.903776338\H, 1.960632023
9, -0.0241426803, 3.1606163301\H, 1.4482602245, -1.5504950864, 2.4419805409
\C, -2.9439097529, 0.5666157789, 2.362858873\H, -3.9738902254, 0.7457282871
, 2.0498549433\H, -2.5834803725, 1.3929166111, 2.9804081433\H, -2.884694293
2, -0.3303703347, 2.9843064566\O, -2.6134109481, 0.5209258747, -0.003381154
3\H, 3.9257117107, 0.0950991742, 0.0747458513\H, 4.025093871, 0.3747494904,
1.8393956348\H, 3.8594201537, -1.2821999052, 1.2005796614\\Version=EM64L-
G03RevE.01\State=2-A\HF=-607.3250921\S2=0.756175\S2-1=0.\S2A=0.750026\
RMSD=5.350e-09\RMSF=5.125e-06\Thermal=0.\Dipole=0.2912063,-0.3367482,1
.3913601\PG=C01 [X(C7H9N2O3)]\@

NAC_c6 88

1\1\GINC-X89\FOpt\UB3LYP\6-31G(d)\C7H9N2O3(2)\JMH502\14-Oct-2010\0\#\
UB3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine)
\SP Calc\0,2\C,-0.0179913668,-0.0354154479,-0.002440841\C,-0.0116320
654,-0.0443198723,2.4832883812\N,2.1300401266,-0.0071053338,1.21942844
28\C,1.4145587319,-0.2035821277,2.3740599041\C,1.4890443548,0.14699257
43,-0.008627937\N,-0.6874243541,0.2407400613,1.2757620412\O,-0.5714511
17,-0.1284995688,3.577931109\O,2.101791571,0.3472954617,-1.0427295517\
C,-2.0478873727,0.6134623251,1.1723020075\C,3.5934726129,0.0510510527,
1.2753986931\H,1.966387691,-0.416526169,3.2792206749\C,-2.8155864496,0
.9711992119,2.4233838015\H,-3.7663827545,1.3983050973,2.0994062415\H,-
2.2694160076,1.678408932,3.0521129721\H,-2.990415996,0.0842416407,3.03
71659761\O,-2.5574249452,0.6612408189,0.0646583203\H,-0.22709221,-1.06
41921701,-0.332694351\H,-0.4386555592,0.6215883145,-0.7622977198\H,3.9
655570763,0.096700553,0.2533350693\H,3.914697385,0.9407770253,1.825872
9289\H,3.976973643,-0.8432417874,1.7754714121\\Version=EM64L-G03RevE.0
1\State=2-A\HF=-607.3362574\S2=0.757353\S2-1=0.\S2A=0.750035\RMSD=6.03
7e-09\RMSF=1.421e-05\Thermal=0.\Dipole=1.3297225,-0.2268454,0.6939237\
PG=C01 [X(C7H9N2O3)]\@

NACCF3 89

1\1\GINC-X120\FOpt\RB3LYP\6-31G(d)\C7H7F3N2O3\JMH502\14-Oct-2010\0\#\
B3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine)\
\SP Calc\0,1\C,-0.0153616896,-0.0050440315,0.0087810175\N,-0.00391608
83,0.0208215798,2.523789571\C,0.7877992068,0.0149446497,1.3055946922\C
, -1.1518359734, 0.7576730204, 2.6088940669\N, -1.3158571642, 0.5116034992,
0.1111047204\H, 1.4802312542, 0.872862515, 1.2603051408\C, -1.6530128718, 1
.3374492272, 1.2885103866\H, 1.4074167886, -0.8855389974, 1.282797974\H, -1
.2579575203, 2.3547508778, 1.1640272726\H, -2.7358693071, 1.4195312514, 1.3
502046528\O, 0.4787853517, -0.4084877344, -1.0200411377\O, -1.7606026868, 0
.9727920427, 3.6461684769\C, 0.6124566291, -0.503624665, 3.7361551759\C, -2
.2747771048, 0.4948925556, -0.9118789423\O, -3.2297712085, 1.2388697945, -0
.8943274196\C, -2.1807883978, -0.5679704807, -2.0475161999\F, -3.406089615
6, -0.7226879393, -2.5637997266\F, -1.7788640811, -1.7632902826, -1.5835761
235\F, -1.3651703327, -0.1661488897, -3.0293537306\H, -0.1209013856, -0.441
1900424, 4.5396018925\H, 0.9101973157, -1.5465927388, 3.5826834665\H, 1.499
2832217, 0.0807247202, 4.0154492167\\Version=EM64L-G03RevE.01\State=1-A\
HF=-905.6692407\RMSD=4.010e-09\RMSF=1.707e-05\Thermal=0.\Dipole=1.4314
165,-0.0273859,0.8673658\PG=C01 [X(C7H7F3N2O3)]\@

NACCF3_c3 90

1\1\GINC-X90\FOpt\UB3LYP\6-31G(d)\C7H6F3N2O3(2)\JMH502\14-Oct-2010\0\#\
UB3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafin
e)\SP Calc\0,2\C,-0.0185109162,0.0198102756,-0.0052947313\C,-0.00656
32936,-0.0083711449,2.4277677376\N,2.1144530942,-0.0524487373,1.109219
2711\C,1.4308187106,-0.4898216873,2.3116155356\C,1.4302119418,0.021315
5507,-0.0909442646\N,-0.7247402193,0.0307059198,1.1977094589\O,-0.5090
229906,0.2859862717,3.4848459941\O,1.9883483749,0.11982429,-1.18546903
26\C,-2.135603638,0.1957799771,1.1005237544\C,3.5651390988,-0.16460272
19,1.0950602665\H,-0.602527593,0.0833380555,-0.9096952232\H,1.95124671
72,-0.1065856839,3.1931462575\H,1.4147856987,-1.5927152911,2.399184562
\C,-3.0462792545,-0.1709949423,2.3085017523\F,-4.2672635558,-0.4310764
232,1.8278738742\F,-3.1492747644,0.8372667882,3.1798681767\F,-2.610370
7765,-1.2760727314,2.9391102082\O,-2.6501930814,0.5201905523,0.0572298
281\H,3.9225549924,0.2099144757,0.1363768144\H,3.9913609302,0.43005915
99,1.9103922329\H,3.8904715041,-1.2086462346,1.2118200316\\Version=EM6
4L-G03RevE.01\State=2-A\HF=-905.0202167\S2=0.75658\S2-1=0.\S2A=0.75003
1\RMSD=9.968e-09\RMSF=1.539e-05\Thermal=0.\Dipole=1.0768855,-0.594883,

0.8195711\PG=C01 [X(C7H6F3N2O3)]\@

NAccF3_c6 91

1\1\GINC-X85\FOpt\UB3LYP\6-31G(d)\C7H6F3N2O3(2)\JMH502\14-Oct-2010\0\
UB3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine)
\SP Calc\0,2C,-0.0164395053,-0.0038030951,-0.0018452709\C,-0.0056
73923,-0.0116907976,2.4773790955\N,2.1298531976,-0.0133914741,1.215983
6435\C,1.408917535,-0.2210313678,2.3645124844\C,1.4957602915,0.1544795
029,-0.0165765754\N,-0.6421752406,0.3985042867,1.2653276583\O,-0.61205
31882,-0.1650575481,3.5320617671\O,2.1123386545,0.3459637683,-1.048218
3114\C,-1.9197724765,0.9348861288,1.1609270427\C,3.5952925619,0.013489
0282,1.2755826482\H,1.9496219404,-0.5092368931,3.2557634131\C,-2.57094
40648,1.6131743354,2.4019226213\F,-3.4796217248,2.4926487258,1.9592645
613\F,-1.6715024445,2.2933958883,3.1352680411\F,-3.2009860666,0.7226869
773,3.1769226642\O,-2.5176306579,0.9655413746,0.1041795876\H,-0.252953
398,-1.0524150687,-0.2360159806\H,-0.4297384369,0.604059992,-0.8049353
367\H,3.9712578257,0.0553686402,0.2548365228\H,3.9323536276,0.89404298
17,1.8305813422\H,3.9579792615,-0.891000391,1.772512143\Version=EM64L
-G03RevE.01\State=2-A\HF=-905.0347899\S2=0.758587\S2-1=0.\S2A=0.750044
\RMSD=8.229e-09\RMSF=1.030e-05\Thermal=0.\Dipole=2.0341182,-0.6242082,
0.1171107\PG=C01 [X(C7H6F3N2O3)]\@

NSO2Me 92

1\1\GINC-V1264\FOpt\RB3LYP\6-31G(d)\C6H10N2O4S1\JMH502\14-Oct-2010\0\
B3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine)
\SP Calc\0,1H,0.0089450511,-0.010034114,-0.0068358708\C,0.00023458
53,-0.014633367,1.0921624995\C,2.3817416792,-0.0015217402,1.8265936295
\N,0.9875761099,2.0822156722,1.9032349589\C,2.2955344193,1.5087144238,
1.62523471\C,-0.1656731563,1.4246683392,1.5779595906\N,1.2005102322,-0
.6861215241,1.6201012154\H,2.6311659193,1.7338592461,0.5985450561\H,-0
.8797750116,-0.5710594149,1.4098238204\H,3.0317222841,1.9472559088,2.3
034485781\O,3.4301825284,-0.5317295489,2.1527371039\O,-1.2806722753,1.
9228866653,1.6314503466\S,1.2196594408,-2.4441856459,1.5463825199\C,0.
93597646,3.4927332006,2.2665816203\O,-0.1943700041,-2.8032776435,1.437
4338756\O,2.1793847018,-2.8697083355,0.5341089817\C,1.8201215446,-2.89
82376992,3.179196782\H,1.8518756788,-3.9905673881,3.1905706436\H,1.113
5814253,-2.5268518247,3.9230047179\H,2.8139827086,-2.4703084366,3.3051
997168\H,-0.1060643487,3.7555259684,2.4461872317\H,1.5270161194,3.6689
586837,3.1722131662\H,1.3311632359,4.1230794069,1.4588837473\Version=
EM64L-G03RevE.01\State=1-A\HF=-1043.1962929\RMSD=3.147e-09\RMSF=1.050e
-05\Thermal=0.\Dipole=0.7227836,1.0265122,0.9055241\PG=C01 [X(C6H10N2O
4S1)]\@

NSO2Me_c3 93

1\1\GINC-V1270\FOpt\UB3LYP\6-31G(d)\C6H9N2O4S1(2)\JMH502\14-Oct-2010\
\# UB3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine)
\SP Calc\0,2N,-0.0491312203,0.0641389594,0.0076833783\C,-0.0032
386956,-0.0213498468,2.4115883601\C,2.1353416761,0.000538438,1.2335916
888\N,1.3817210474,-0.12608451,2.4036407751\C,1.3503311144,0.452509286
4,0.0102027481\C,-0.7789958189,0.0283201934,1.186947379\H,-0.501661078
7,-0.0623536887,3.3677999143\H,1.8550519424,0.0174737899,-0.8576815778
\H,1.4738346165,1.5491422005,-0.0656770743\O,3.336071315,-0.1979250126
1,1.976920265\O,-2.0111722353,-0.0074501832,1.2181920974\S,2.227006485
6,-0.2978304748,3.9748613836\C,-0.7598477645,0.2132591141,-1.252790102
4\C,3.1052167017,-1.8519890341,3.7619142766\O,1.1460121744,-0.47996844
27,4.938740093\O,3.1718320569,0.8029263913,4.0866447769\H,3.7855676719
,-1.7394609907,2.9182898735\H,2.3708146555,-2.6427358805,3.6000633145\
H,3.6492702306,-2.0179802765,4.6953068917\H,-1.7880626062,-0.114250492
3,-1.1027221987\H,-0.7674468463,1.2600217484,-1.591225523\H,-0.2810070
451,-0.4003025832,-2.0242098829\Version=EM64L-G03RevE.01\State=2-A\HF
=-1042.5504701\S2=0.756591\S2-1=0.\S2A=0.750031\RMSD=8.499e-09\RMSF=1.
110e-05\Thermal=0.\Dipole=0.736336,-0.8672323,-1.0430184\PG=C01 [X(C6H
9N2O4S1)]\@

NSO2Me_c6 94

1\1\GINC-V1271\FOpt\UB3LYP\6-31G(d)\C6H9N2O4S1(2)\JMH502\14-Oct-2010\
\# UB3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafine)
\SP Calc\0,2N,-0.0335138268,0.0024706741,-0.0022522527\C,0.0066
075603,0.0184584774,2.4733002151\C,2.1460964363,0.0145932036,1.1848742
003\N,1.4431489984,-0.2821351258,2.3680942415\C,1.3282381421,0.1856355
353,0.0127489909\C,-0.7624307298,-0.1665942998,1.173374903\H,1.8235234
229,0.3788800386,-0.9286332667\O,3.3766820766,0.0482081444,1.129263685

6\O,-1.9627942415,-0.3732433181,1.1742985087\S,2.3007626665,-0.3078148
744,3.8876921725\C,-0.7378047179,-0.043098284,-1.2877089346\C,3.482229
0299,-1.6392743932,3.6401153892\O,1.2830042755,-0.7391326786,4.8490005
537\O,3.0148823803,0.9501707544,4.085255942\H,4.1230712522,-1.36908849
84,2.8016598048\H,2.9298034944,-2.5617698731,3.4559362545\H,4.04970304
51,-1.7092794154,4.571422616\H,-0.1598784358,1.0567060758,2.7998203588
\H,-0.4428409508,-0.6343210711,3.2204572611\H,-1.8065757374,-0.0757702
649,-1.0840211099\H,-0.4927807011,0.8501269084,-1.8695269371\H,-0.4414
998725,-0.9350188632,-1.8484896019\Version=EM64L-G03RevE.01\State=2-A
\HF=-1042.5586572\S2=0.756772\S2-1=0.\S2A=0.750032\RMSD=4.904e-09\RMSF
=1.264e-05\Thermal=0.\Dipole=-0.2332877,-0.707837,-1.722211\PG=C01 [X(C
6H9N2O4S1)]\@

NSO2CF3_95

1\1\GINC-V1260\FOpt\RB3LYP\6-31G(d)\C6H7F3N2O4S1\JMH502\14-Oct-2010\O
\#\B3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultrafin
e)\SP Calc\0,1\H,0.0050570841,-0.0160120964,-0.0032546219\C,-0.00171
66961,-0.0158204157,1.0949324909\C,2.4066328689,-0.0036069768,1.763961
6573\N,0.9879769274,2.0671935652,1.9526680082\C,2.303764446,1.51409933
04,1.6767890361\C,-0.1608328949,1.4234566961,1.5885061161\N,1.20449918
59,-0.6841235889,1.6170089321\H,2.6749328626,1.8184560067,0.6837392012
\H,-0.8817233881,-0.5654404237,1.4216881938\H,3.0178669991,1.901652213
5,2.4092144593\O,3.4729287249,-0.5601969217,1.9278738077\O,-1.27369209
12,1.9263404292,1.6195328515\S,1.1839796593,-2.3995328406,1.8308737689
\C,0.9285473041,3.4670840383,2.3574474624\O,1.7718312707,-2.7534583742
,3.1100423682\O,-0.1609886018,-2.8061257273,1.439829175\C,2.3330435882
, -3.0354222933,0.4588532225\F,1.8237737434,-4.1900042637,0.0358124629\
F,3.5581359808,-3.2235954494,0.9114885409\F,2.3390902985,-2.1556391757
, -0.5483011603\H,-0.1148852774,3.7213909854,2.540069738\H,1.5146939928
,3.6160465657,3.2708349342\H,1.3251284767,4.1226600938,1.570903125\Ve
rsion=EM64L-G03RevE.01\State=1-A\HF=-1340.8857515\RMSD=3.502e-09\RMSF=
2.811e-05\Thermal=0.\Dipole=0.7191783,1.4791222,-0.7870038\PG=C01 [X(C
6H7F3N2O4S1)]\@

NSO2CF3_c3_96

1\1\GINC-V1261\FOpt\UB3LYP\6-31G(d)\C6H6F3N2O4S1(2)\JMH502\14-Oct-2010
\O\#\UB3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultr
afine)\SP Calc\0,2\H,0.0072405706,-0.0435233923,-0.0178875453\C,0.00
78176173,-0.0188766539,1.060696968\C,1.3576166919,0.0013826959,3.10851
63564\N,-1.1436643217,0.0006474175,3.1762564543\C,0.0852685788,0.41047
26851,3.8334215878\C,-1.2453930917,-0.0229343057,1.794244561\N,1.23676
45255,-0.077062012,1.7125221894\H,0.1308354196,1.5060240847,3.9773126\
H,0.140033117,-0.0423300456,4.8278411056\O,2.4106759854,-0.2059169938,
3.6735045533\O,-2.3198238543,-0.0870941882,1.1944323217\S,2.7068302638
, -0.2523954465,0.7500837397\C,-2.36122881,0.0847202735,3.9692312171\O,
2.2328912921,-0.4584168044,-0.6112473908\O,3.6402258783,0.7978888703,1
.1128154897\C,3.4110915676,-1.9241113713,1.3341012052\F,3.9321155605,-
2.5029527712,0.2565164709\F,2.4241926243,-2.6750659654,1.8180181919\F,
4.3456993832,-1.736412747,2.2447700527\H,-3.1916257431,-0.2554299961,3
.3514826077\H,-2.270984662,-0.5515688712,4.8566295588\H,-2.5599243712,
1.1164607658,4.2941468111\Version=EM64L-G03RevE.01\State=2-A\HF=-1340
.2379897\S2=0.756582\S2-1=0.\S2A=0.750031\RMSD=6.222e-09\RMSF=1.459e-0
5\Thermal=0.\Dipole=-0.3711627,-0.1655125,1.2663563\PG=C01 [X(C6H6F3N2
O4S1)]\@

NSO2CF3_c6_97

1\1\GINC-V1264\FOpt\UB3LYP\6-31G(d)\C6H6F3N2O4S1(2)\JMH502\14-Oct-2010
\O\#\UB3LYP/6-31G(d) opt freq=noraman maxdisk=458752000 INT(grid=ultr
afine)\SP Calc\0,2\H,-0.0091838591,-0.0334178679,0.0003375274\C,0.00
52534827,-0.016749262,1.0881536557\C,1.7218770909,-0.006607965,2.89899
31507\N,0.0443367137,1.8097976332,2.7559144045\C,0.9844958049,1.092917
6089,3.4546317755\C,-0.4646827139,1.3624772865,1.5351911384\N,1.358922
7104,-0.3328258329,1.5648673324\H,-0.7231649744,-0.7576465282,1.450856
8182\H,1.2268448733,1.4161972499,4.4577193569\O,2.6092245461,-0.601057
132,3.5026280644\O,-1.2876211093,1.9929386981,0.8984138013\S,2.3270334
71,-1.4127013215,0.6674295154\C,-0.4456843165,3.0787764774,3.306415415
8\O,1.6075888405,-1.6111623786,-0.587426737\O,3.717953354,-1.000750226
,0.7192278285\C,2.1736696366,-3.0559961565,1.5990560733\F,2.2187524886
, -4.0293776584,-0.6909164487\F,0.9894389019,-3.0876312009,2.2242018372\
F,3.1531015438,-3.2119152345,2.4702968553\H,-1.2747138538,3.4161764114
,2.6870008824\H,-0.7837120523,2.9237244112,4.3350177994\H,0.3532485159
,3.8261315884,3.2938624683\Version=EM64L-G03RevE.01\State=2-A\HF=-134

0.2497394\S2=0.757679\S2-1=0.\S2A=0.750038\RMSD=9.711e-09\RMSF=1.317e-05\Thermal=0.\Dipole=-1.3692249,0.9941745,1.3652777\PG=C01 [X(C6H6F3N2O4S1)]\@