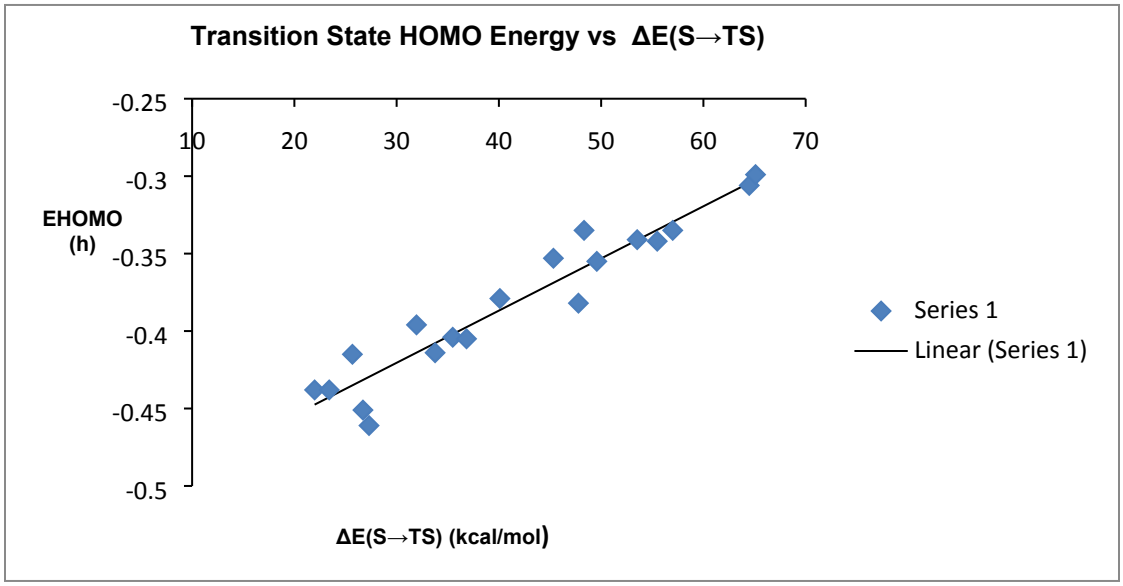
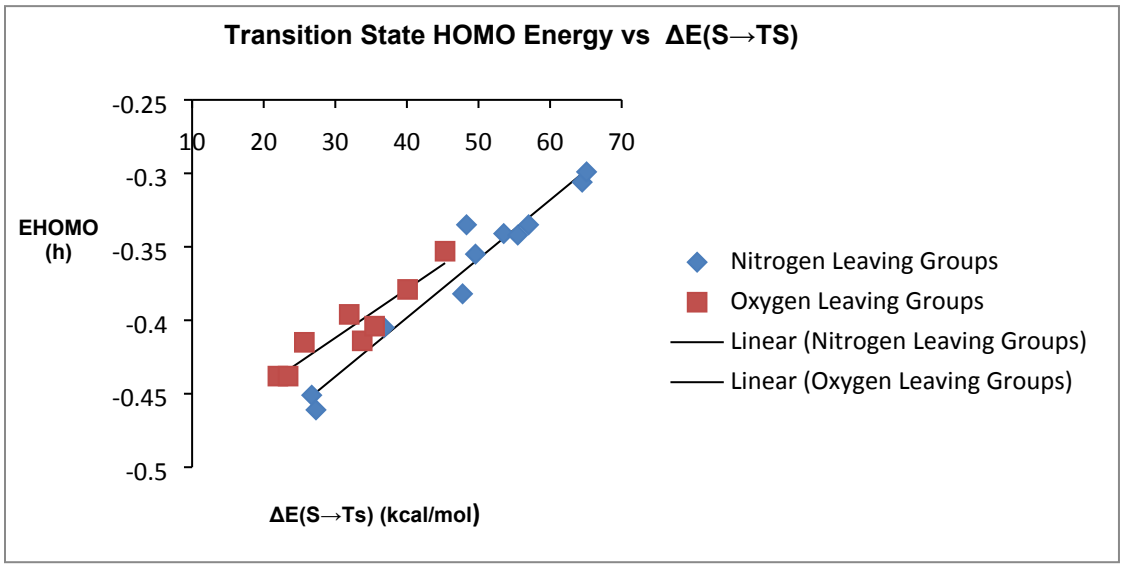
Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

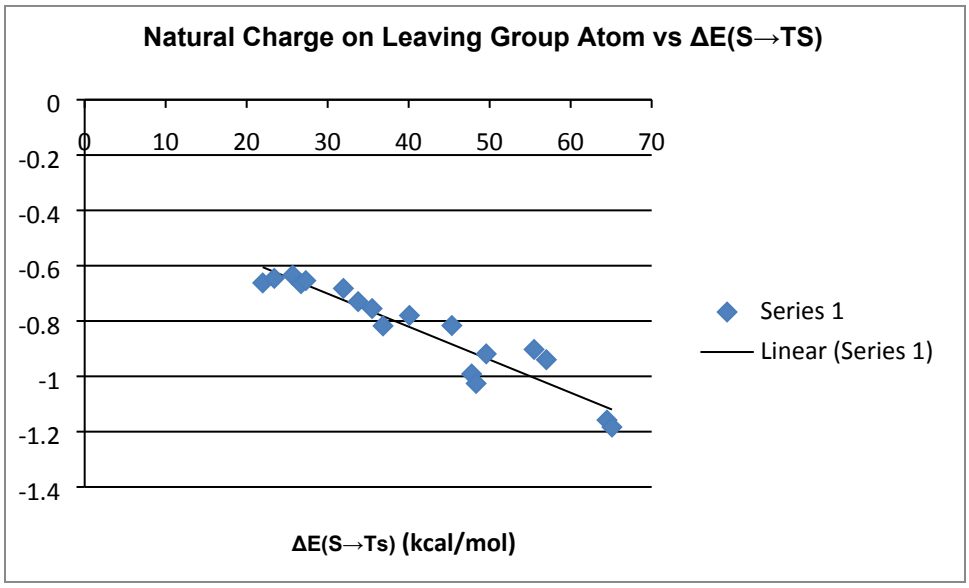
Supporting information

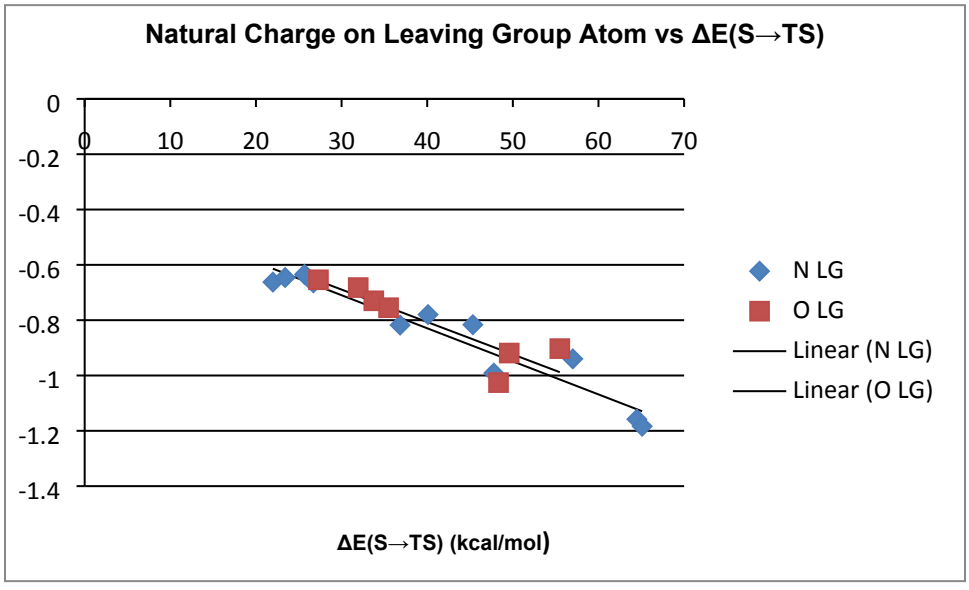
Contents

Correlations Between Barrier Height and Transition State Properties

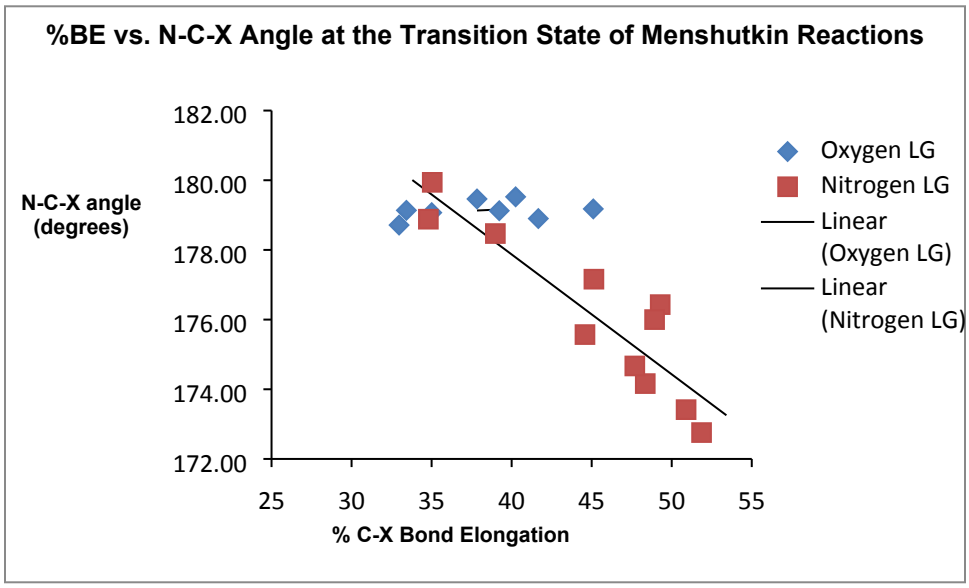





Natural Charge on Leaving Group Atom vs ΔE(S→TS)
0
-0.2
-0.4
-0.6
-0.8
-1
-1.2
-1.4
0
10
20
30
40
50
60
70
Series 1
Linear (Series 1)
ΔE(S→Ts) (kcal/mol)


Natural Charge on Leaving Group Atom vs ΔE(S→TS)
0
-0.2
-0.4
-0.6
-0.8
-1
-1.2
-1.4
0
10
20
30
40
50
60
70
N LG
O LG
Linear (N LG)
Linear (O LG)
ΔE(S→TS) (kcal/mol)

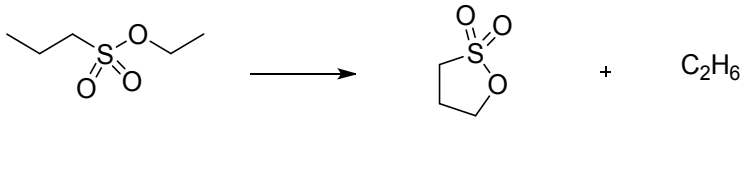
Transition State N-C-X Angle Contortion follows C-X bond elongation in Nitrogen Leaving Groups

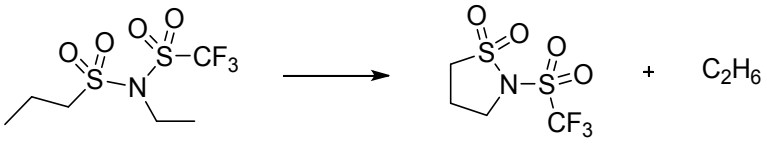


Calculation of Ring Strain in 1,3-Propanesultone, and N-Triflylpropanesutam

Computational method

Ring strain was calculated for 1,3-Propanesultone and N-Triflylpropanesultam using the following homeodesmotic reactions:



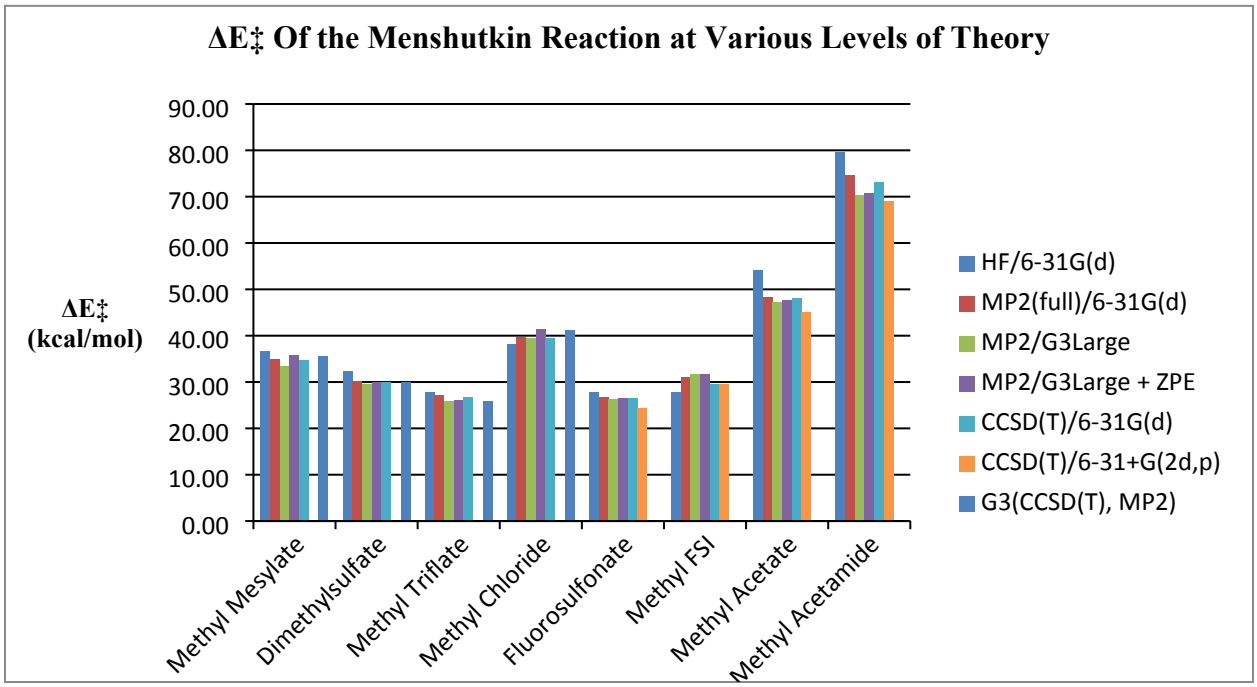


Structures were minimized at the B3LYP/6-31G(d) level of theory in GAMESS using the DFT=B3LYP keyword (as opposed to the slightly different DFT=B3LYP1 version). Ring strain was estimated to be 10.2 kcal/mol in 1,3-Propanesultone, and 9.0 kcal/mol in N-triflylpropanesultam.

Computational Benchmarks for $\Delta E^{\ddagger}$ Using High Level Calculations

A Table of $\Delta E^{\ddagger}$ Values for Various Nucleofuges (in kcal/mol)

	Geometric Optimizations		Single Points at MP2(full)/6-31G(d)				
	HF/6-31G(d)	MP2(full)/6-31G(d)	MP2/G3Large	MP2/G3Large + ZPE	CCSD(T)/6-31G(d)	CCSD(T)/6-31+G(2d,p)	G3(CCSD(T), MP2)
Methyl Mesylate	36.59	34.91	33.28	35.75	34.65		35.61
Dimethylsulfate	32.29	30.11	29.51	29.87	30.01		29.98
Methyl Triflate	27.70	27.08	25.78	26.03	26.68		25.85
Methyl Chloride	38.13	39.56	39.33	41.25	39.34		41.09
Methylfluorosulfonate	27.71	26.62	26.33	26.54	26.37	24.33	
Methyl FSI	27.74	30.89	31.71	31.72	29.42	29.38	
Methyl Acetate	54.02	48.20	47.17	47.61	48.01	45.00	
Methyl Acetamide	79.56	74.54	70.36	70.64	73.04	68.98	



MP2(full)/6-31G(d) Geometries and Energies of S_N2 transition states analyzed in cartesian coordinates

Methyl Mesylate, C_s, Energy: -758.53145

S	16.0	1.15939	-0.45877	0.00000
O	8.0	0.34332	0.83946	0.00000
C	6.0	-1.56443	0.25102	0.00000
C	6.0	2.83434	0.13571	0.00000
H	1.0	3.49926	-0.72871	0.00000
N	7.0	-3.39174	-0.29315	0.00000
H	1.0	-1.77836	1.30659	0.00000
H	1.0	-3.42903	-1.31310	0.00000
H	1.0	-3.88908	0.03958	-0.82614
H	1.0	-3.88908	0.03958	0.82614
H	1.0	-1.34932	-0.24862	-0.92968
H	1.0	-1.34932	-0.24862	0.92968
H	1.0	2.99358	0.73491	-0.89588
H	1.0	2.99358	0.73491	0.89588
O	8.0	0.95553	-1.21641	-1.25308
O	8.0	0.95553	-1.21641	1.25308

Dimethylsulfate, C_1, Energy: -833.56441

C	6.0	-3.23105	0.53029	0.56815
O	8.0	-2.38762	1.60405	0.11677
S	16.0	-1.09812	1.06888	-0.78967
O	8.0	-0.48480	2.41333	-1.11775
C	6.0	0.29671	3.22502	0.48992
O	8.0	-0.26375	0.29334	0.14471
O	8.0	-1.64534	0.37490	-1.94913
N	7.0	1.08021	4.04056	2.04906
H	1.0	-4.02379	1.00238	1.14786
H	1.0	-3.65542	-0.00086	-0.28628
H	1.0	-2.66470	-0.16271	1.19552
H	1.0	-0.70677	3.34643	0.86179
H	1.0	0.81085	2.29328	0.65588
H	1.0	0.70385	3.95738	-0.18691
H	1.0	0.74849	4.99383	2.19684
H	1.0	2.09771	4.06770	1.98137
H	1.0	0.83764	3.49160	2.87422

Methyl Triflate, C_1, Energy: -1055.61053

S	16.0	2.35501	0.45850	0.38755
O	8.0	2.11595	1.89145	0.14978
O	8.0	2.82997	0.01740	1.69291
O	8.0	3.09460	-0.19380	-0.77547
C	6.0	3.00518	0.78181	-2.45037
C	6.0	0.69775	-0.29530	0.20277
F	9.0	0.20757	-0.03145	-1.03440
F	9.0	-0.15989	0.20358	1.10085
F	9.0	0.74865	-1.62525	0.34790
N	7.0	2.95037	1.74648	-4.15797
H	1.0	2.06759	0.29666	-2.65665
H	1.0	3.01260	1.70453	-1.89490
H	1.0	3.92737	0.28607	-2.70168
H	1.0	3.77193	2.34060	-4.26976
H	1.0	2.12777	2.34956	-4.18146
H	1.0	2.90357	1.12215	-4.96329

Methylfluorosulfonate, C_1, Energy: -818.40115

S	16.0	-0.45745	-0.38751	1.66574
O	8.0	-0.73479	1.03262	1.46126
O	8.0	-0.66826	-0.99018	2.96502
O	8.0	0.82628	-0.82380	0.99410
C	6.0	1.03360	0.02595	-0.74241
F	9.0	-1.54639	-1.11887	0.67800
N	7.0	1.26902	0.86801	-2.48653
H	1.0	0.19039	-0.54494	-1.09193
H	1.0	0.87039	0.97787	-0.26719
H	1.0	2.01551	-0.41591	-0.75708
H	1.0	2.04944	1.52487	-2.48154
H	1.0	0.42573	1.39054	-2.72549
H	1.0	1.43614	0.18837	-3.22871

Methyl bis(trifluoromethanesulfonyl)imide (anti) C_1,

Energy: -1919.67259

C	6.0	-0.66116	-0.61732	0.85893
N	7.0	0.76965	0.64248	0.24164
S	16.0	2.28825	0.07028	0.04048
S	16.0	0.29060	2.15820	-0.14497
O	8.0	1.13996	2.84436	-1.10654
O	8.0	-1.16191	2.08861	-0.30589
O	8.0	2.38041	-1.12693	0.87802
O	8.0	3.32762	1.08767	0.03777
C	6.0	0.53203	3.01854	1.46019
F	9.0	0.13186	4.28929	1.35324
F	9.0	1.81216	2.98432	1.83089
F	9.0	-0.21007	2.41267	2.40979
C	6.0	2.19505	-0.58939	-1.67185
F	9.0	3.34478	-1.19444	-1.98500
F	9.0	1.95190	0.38496	-2.54919
F	9.0	1.19723	-1.49320	-1.74320
N	7.0	-2.06015	-1.84880	1.46472
H	1.0	0.12249	-1.32101	1.08911
H	1.0	-0.94777	0.12036	1.58802
H	1.0	-1.08444	-0.56937	-0.12863
H	1.0	-1.93545	-2.09763	2.44612
H	1.0	-2.05019	-2.71145	0.92037
H	1.0	-2.98197	-1.42349	1.36270

Methyl bis(trifluoromethanesulfonyl)imide (gauche) C_1,

Energy: -1919.67076

C	6.0	-3.87907	-1.83954	0.39261
N	7.0	-2.46911	-0.66098	-0.40728
S	16.0	-1.05071	-1.37594	-0.82492
S	16.0	-3.05201	0.69649	-1.12157
O	8.0	-2.15451	1.31547	-2.08550
O	8.0	-4.46939	0.47677	-1.41406
O	8.0	-1.05368	-2.66542	-0.12975
O	8.0	-0.71369	-1.28112	-2.23727
C	6.0	-3.07161	1.81762	0.33687
F	9.0	-3.58459	2.99752	-0.02300
F	9.0	-1.84005	2.00090	0.81939
F	9.0	-3.84154	1.29557	1.31448
C	6.0	0.21236	-0.37542	0.06172
F	9.0	0.29884	0.84929	-0.46056
F	9.0	1.39677	-0.98774	-0.05052
F	9.0	-0.10592	-0.27843	1.35979
N	7.0	-5.28215	-3.00105	1.17290
H	1.0	-3.12177	-2.59309	0.53190
H	1.0	-4.03898	-1.09180	1.14924
H	1.0	-4.42346	-1.76888	-0.53294
H	1.0	-5.07590	-3.24306	2.14198
H	1.0	-5.36234	-3.87042	0.64556
H	1.0	-6.19044	-2.53716	1.15092

Methyl bis(fluorosulfonyl)imide, C_1, Energy: -1445.25353

C	6.0	-1.16332	-0.57013	0.76693
N	7.0	0.23789	0.55663	-0.09700
S	16.0	1.79197	0.08379	-0.02432
S	16.0	-0.16317	2.09227	-0.43270
O	8.0	0.69968	2.72452	-1.40357
O	8.0	-1.61089	2.11438	-0.53546
O	8.0	2.69028	1.07449	0.52532
O	8.0	1.76682	-1.28644	0.45671
F	9.0	0.15377	2.82452	0.97651
F	9.0	2.16658	-0.02105	-1.58660
N	7.0	-2.55462	-1.69089	1.58284
H	1.0	-0.50627	-1.41217	0.62750
H	1.0	-1.07967	0.02351	1.66179
H	1.0	-1.83034	-0.24811	-0.01361
H	1.0	-2.20974	-2.15762	2.42195
H	1.0	-2.86906	-2.41160	0.93291
H	1.0	-3.36668	-1.13160	1.84525

Methyl bis(methylsulfonyl)imide (anti) C_1, Energy: -1325.52993

C	6.0	-0.90188	-0.77026	1.01037
N	7.0	0.57282	0.37880	0.16851
S	16.0	2.13085	0.04956	0.55812
S	16.0	0.15441	1.72961	-0.65742
O	8.0	1.05762	1.97950	-1.79024
O	8.0	-1.29032	1.58083	-0.90549
O	8.0	2.83856	1.23403	1.06923
O	8.0	2.04988	-1.15505	1.40218
C	6.0	0.36046	3.08876	0.47314
H	1.0	0.07588	4.00057	-0.05455
H	1.0	1.40447	3.11933	0.78265
H	1.0	-0.29198	2.92828	1.33173
C	6.0	2.92255	-0.41104	-0.96597
H	1.0	3.96082	-0.65469	-0.73449
H	1.0	2.85635	0.43160	-1.65300
H	1.0	2.40695	-1.28081	-1.37289
N	7.0	-2.27604	-1.85552	1.74458
H	1.0	-0.22703	-1.59409	0.85233
H	1.0	-0.78324	-0.19108	1.91016
H	1.0	-1.51230	-0.38219	0.21102
H	1.0	-1.93884	-2.36085	2.56473
H	1.0	-2.59571	-2.54128	1.06005
H	1.0	-3.08017	-1.29313	2.02451

Methyl bis(methylsulfonyl)imide (gauche) C_1, Energy: -1325.52302

C	6.0	-1.06997	-1.06292	0.37339
N	7.0	0.47826	0.13425	-0.29456
S	16.0	0.77880	-0.46294	-1.81098
S	16.0	0.18542	1.73729	-0.04374
O	8.0	0.20869	2.53612	-1.27794
O	8.0	-0.97466	1.83955	0.85874
O	8.0	1.17581	-1.86008	-1.57131
O	8.0	-0.33913	-0.21158	-2.73173
C	6.0	1.60757	2.22517	0.91248
H	1.0	1.47421	3.27192	1.19195
H	1.0	2.50235	2.10811	0.30094
H	1.0	1.66760	1.59679	1.80065
C	6.0	2.19991	0.40893	-2.42786
H	1.0	1.94467	1.46254	-2.53264
H	1.0	2.43613	-0.02782	-3.39992
H	1.0	3.02871	0.25597	-1.73627
N	7.0	-2.50727	-2.19857	0.98395
H	1.0	-0.35207	-1.86516	0.35027
H	1.0	-1.13760	-0.39700	1.21640
H	1.0	-1.60266	-0.80954	-0.52860
H	1.0	-2.29563	-2.63776	1.87953
H	1.0	-2.68341	-2.93659	0.30200
H	1.0	-3.36317	-1.65415	1.09124

Methyl MSA, C_1, Energy: -738.64549

C	6.0	-1.30251	-0.66876	0.30504
N	7.0	0.19773	0.67481	-0.52460
S	16.0	0.23801	0.45781	-2.10706
O	8.0	1.34285	-0.41401	-2.56768
O	8.0	-1.14025	0.10748	-2.54485
C	6.0	0.55593	2.05136	-2.85423
N	7.0	-2.61886	-1.74138	0.91736
H	1.0	-0.49270	-1.37337	0.40479
H	1.0	-1.38337	0.11501	1.04049
H	1.0	-1.70728	-0.49913	-0.68266
H	1.0	-2.45959	-2.07242	1.87005
H	1.0	-2.69837	-2.55369	0.30348
H	1.0	-3.51020	-1.24395	0.89449
H	1.0	1.15436	0.56209	-0.17789
H	1.0	0.52943	1.93270	-3.93872
H	1.0	1.54139	2.40051	-2.54249
H	1.0	-0.21478	2.74994	-2.52914

Methyl FSA, C_1, Energy: -798.52240

C	6.0	-1.19943	-0.77697	0.16278
N	7.0	0.43162	0.08935	-0.87921
S	16.0	-0.17642	1.20365	-1.80374
O	8.0	0.77442	2.08201	-2.47123
O	8.0	-1.32783	0.65982	-2.52223
F	9.0	-0.91823	2.23710	-0.71203
N	7.0	-2.69158	-1.51433	0.94819
H	1.0	-0.47177	-1.42425	0.62582
H	1.0	-1.35170	0.21199	0.56129
H	1.0	-1.50666	-0.97550	-0.85018
H	1.0	-2.68325	-1.42893	1.96554
H	1.0	-2.78539	-2.50283	0.71073
H	1.0	-3.51620	-1.02590	0.59484
H	1.0	1.27082	0.45106	-0.42114

MeiprFSA, C_1, Energy: -916.03637

C	6.0	-0.55910	-0.57798	0.51173
N	7.0	1.14889	0.04259	-0.61079
S	16.0	0.58564	0.93809	-1.76348
O	8.0	1.54941	1.65973	-2.59026
O	8.0	-0.56224	0.27135	-2.38087
F	9.0	-0.17324	2.19275	-0.93185
N	7.0	-2.05491	-1.12119	1.38979
H	1.0	0.16204	-1.09370	1.12841
H	1.0	-0.71244	0.47792	0.66585
H	1.0	-0.82453	-0.99309	-0.44652
H	1.0	-2.05987	-0.83085	2.36895
H	1.0	-2.15684	-2.13687	1.35578
H	1.0	-2.86788	-0.70673	0.93005
C	6.0	2.39504	0.42408	0.07307
H	1.0	2.42687	-0.24845	0.94370
C	6.0	2.41952	1.85866	0.59948
C	6.0	3.61997	0.11669	-0.78361
H	1.0	3.32047	2.02241	1.19983
H	1.0	1.54541	2.06661	1.22214
H	1.0	2.42414	2.57046	-0.22883
H	1.0	4.53926	0.26129	-0.20546
H	1.0	3.64292	0.77279	-1.65555
H	1.0	3.58153	-0.91958	-1.13011

Methyl acetate, C_s, Energy: -323.88097

C	6.0	2.71505	-0.28053	0.00000
C	6.0	1.21986	0.01855	0.00000
O	8.0	0.83498	1.21455	0.00000
O	8.0	0.46339	-1.02504	0.00000
C	6.0	-1.52119	-0.37468	0.00000
N	7.0	-3.22174	0.20938	0.00000
H	1.0	3.29119	0.64546	0.00000
H	1.0	-1.01488	0.58559	0.00000
H	1.0	-3.90645	-0.54807	0.00000
H	1.0	-3.38394	0.78874	-0.82474
H	1.0	-3.38394	0.78874	0.82474
H	1.0	-1.55695	-0.93747	-0.91937
H	1.0	-1.55695	-0.93747	0.91937
H	1.0	2.96968	-0.87697	-0.88004
H	1.0	2.96968	-0.87697	0.88004

Methyl trifluoroacetate, C_s, Energy: -620.97437

C	6.0	-2.74774	0.29836	0.00000
C	6.0	-1.25478	-0.07407	0.00000
O	8.0	-0.94712	-1.27898	0.00000
O	8.0	-0.50185	0.96265	0.00000
C	6.0	1.43691	0.36815	0.00000
N	7.0	3.21694	-0.16221	0.00000
H	1.0	1.02108	-0.62941	0.00000
H	1.0	3.86299	0.62802	0.00000
H	1.0	3.41129	-0.73166	-0.82442
H	1.0	3.41129	-0.73166	0.82442
H	1.0	1.48885	0.91979	-0.92412
H	1.0	1.48885	0.91979	0.92412
F	9.0	-3.55230	-0.77981	0.00000
F	9.0	-3.05977	1.03794	-1.09021
F	9.0	-3.05977	1.03794	1.09021

Methyl cyanoformate, C_s, Energy: -376.72778

C	6.0	-2.69698	0.22415	0.00000
C	6.0	-1.24349	-0.11266	0.00000
O	8.0	-0.93291	-1.31631	0.00000
O	8.0	-0.49173	0.92582	0.00000
C	6.0	1.44202	0.35379	0.00000
N	7.0	3.24599	-0.14958	0.00000
H	1.0	1.05365	-0.65397	0.00000
H	1.0	3.87723	0.65248	0.00000
H	1.0	3.45214	-0.71505	-0.82425
H	1.0	3.45214	-0.71505	0.82425
H	1.0	1.49444	0.90351	-0.92510
H	1.0	1.49444	0.90351	0.92510
N	7.0	-3.85118	0.47500	0.00000

Dimethylcarbonate, C_s, Energy: -398.92298

O	8.0	2.03073	0.31305	0.00000
C	6.0	0.64754	0.36460	0.00000
O	8.0	0.14739	1.50177	0.00000
O	8.0	0.04691	-0.77312	0.00000
C	6.0	-1.96009	-0.40610	0.00000
N	7.0	-3.75966	-0.03986	0.00000
C	6.0	2.59536	-0.99593	0.00000
H	1.0	3.67574	-0.84328	0.00000
H	1.0	-1.62111	0.62333	0.00000
H	1.0	-4.34362	-0.87706	0.00000
H	1.0	-3.99559	0.51406	-0.82420
H	1.0	-3.99559	0.51406	0.82420
H	1.0	-1.95109	-0.96455	-0.92205
H	1.0	-1.95109	-0.96455	0.92205
H	1.0	2.29741	-1.56072	-0.88658
H	1.0	2.29741	-1.56072	0.88658

Dimethylurethane, C_s, Energy: -379.04927

O	8.0	2.02579	0.47650	0.00000
C	6.0	0.66684	0.13493	0.00000
O	8.0	0.34646	-1.07929	0.00000
N	7.0	-0.15741	1.16869	0.00000
C	6.0	-2.18990	0.36842	0.00000
N	7.0	-3.75189	-0.46730	0.00000
C	6.0	2.90179	-0.64678	0.00000
H	1.0	3.91019	-0.22906	0.00000
H	1.0	-1.53527	-0.49858	0.00000
H	1.0	-4.55234	0.16691	0.00000
H	1.0	0.35677	2.04827	0.00000
H	1.0	-3.81515	-1.06606	-0.82479
H	1.0	-3.81515	-1.06606	0.82479
H	1.0	-2.29337	0.92365	-0.91858
H	1.0	-2.29337	0.92365	0.91858
H	1.0	2.75358	-1.26953	-0.88536
H	1.0	2.75358	-1.26953	0.88536

Methyl Acetamide, C_s, Energy: -304.00329

N	7.0	0.36989	0.72035	0.00000
O	8.0	0.56626	-1.56104	0.00000
C	6.0	1.08414	-0.40181	0.00000
C	6.0	2.61143	-0.34590	0.00000
H	1.0	0.95893	1.55229	0.00000
H	1.0	2.98632	-0.87554	0.87987
H	1.0	2.98632	-0.87554	-0.87987
C	6.0	-1.74849	0.13165	0.00000
H	1.0	-1.16436	-0.79005	0.00000
H	1.0	-1.79635	0.69735	-0.91752
H	1.0	-1.79635	0.69735	0.91752
N	7.0	-3.38196	-0.55392	0.00000
H	1.0	-4.12634	0.14517	0.00000
H	1.0	-3.49362	-1.14575	-0.82443
H	1.0	-3.49362	-1.14575	0.82443
H	1.0	3.00807	0.67358	0.00000

Methyl Trifluoroacetamide, C_s, Energy: -601.10242

C	6.0	2.11981	-0.52278	0.00000
C	6.0	0.58992	-0.40223	0.00000
O	8.0	-0.01703	-1.50505	0.00000
N	7.0	0.04913	0.80354	0.00000
C	6.0	-2.09064	0.55890	0.00000
N	7.0	-3.85725	0.17215	0.00000
F	9.0	2.76033	0.68086	0.00000
H	1.0	-1.71854	-0.46030	0.00000
H	1.0	-4.45550	0.99955	0.00000
H	1.0	0.74265	1.54876	0.00000
F	9.0	2.55559	-1.19283	-1.08864
F	9.0	2.55559	-1.19283	1.08864
H	1.0	-2.06198	1.11772	-0.92160
H	1.0	-2.06198	1.11772	0.92160
H	1.0	-4.08151	-0.38651	-0.82460
H	1.0	-4.08151	-0.38651	0.82460

Methylcyanoformamide, C_s, Energy: -356.85536

C	6.0	-2.13211	0.05823	0.00000
C	6.0	-0.65322	-0.13475	0.00000
O	8.0	-0.22872	-1.31677	0.00000
N	7.0	0.08105	0.96986	0.00000
N	7.0	-3.30421	0.21366	0.00000
H	1.0	-0.47753	1.82290	0.00000
C	6.0	2.15409	0.41429	0.00000
H	1.0	1.64901	-0.54449	0.00000
N	7.0	3.85744	-0.21663	0.00000
H	1.0	4.56232	0.52203	0.00000
H	1.0	2.20896	0.96893	-0.92261
H	1.0	2.20896	0.96893	0.92261
H	1.0	4.00477	-0.80038	-0.82462
H	1.0	4.00477	-0.80038	0.82462

Methyl Succinimide, C_s, Energy: -455.08510

N	7.0	0.05261	1.01151	0.00000
O	8.0	2.33705	0.61253	0.00000
O	8.0	-2.23756	0.72233	0.00000
C	6.0	1.17102	0.21489	0.00000
C	6.0	-1.08350	0.26114	0.00000
C	6.0	0.76545	-1.26900	0.00000
C	6.0	-0.75813	-1.23665	0.00000
H	1.0	1.19813	-1.75517	0.87941
H	1.0	1.19813	-1.75517	-0.87941
H	1.0	-1.21286	-1.70250	0.87953
H	1.0	-1.21286	-1.70250	-0.87953
C	6.0	-0.35264	3.13048	0.00000
H	1.0	-1.34340	2.69223	0.00000
H	1.0	0.21388	3.11421	-0.91761
H	1.0	0.21388	3.11421	0.91761
N	7.0	-0.80868	4.85024	0.00000
H	1.0	0.00960	5.46176	0.00000
H	1.0	-1.36974	5.06521	-0.82586
H	1.0	-1.36974	5.06521	0.82586

1, 3-Propanesultone, C_1, Energy: -796.52517

C	6.0	-3.45351	0.75616	0.30115
C	6.0	-2.19091	0.52215	-0.52144
C	6.0	-1.79074	-0.94950	-0.57062
O	8.0	-3.45727	-1.71120	0.31553
S	16.0	-4.49739	-0.65306	-0.06605
O	8.0	-5.67323	-0.63998	0.80762
O	8.0	-4.70828	-0.59716	-1.52723
N	7.0	-0.11650	-0.67549	-1.48034
H	1.0	-3.94260	1.69560	0.03500
H	1.0	-3.25237	0.73939	1.37412
H	1.0	-1.36522	1.11095	-0.10902
H	1.0	-2.37547	0.85603	-1.54511
H	1.0	-2.14297	-1.57827	-1.37184
H	1.0	-1.32008	-1.42299	0.27731
H	1.0	-0.27813	-0.23260	-2.38518
H	1.0	0.32686	-1.58056	-1.64854
H	1.0	0.54204	-0.09379	-0.96046

N-Triflylpropanesultam, C_1, Energy: -1660.59152

C	6.0	-6.80903	0.62350	0.94358
C	6.0	-6.26053	1.05260	2.30011
C	6.0	-5.04418	0.24503	2.73049
N	7.0	-4.41467	0.07993	0.77498
S	16.0	-5.48929	0.79614	-0.25481
O	8.0	-5.20853	2.23361	-0.36327
O	8.0	-5.78052	0.01902	-1.45839
S	16.0	-3.17308	-0.88152	0.43702
O	8.0	-3.27811	-1.65929	-0.79036
O	8.0	-2.80960	-1.51850	1.70950
C	6.0	-1.83920	0.33782	0.12987
F	9.0	-2.15599	1.10961	-0.91644
F	9.0	-0.68200	-0.28928	-0.11858
F	9.0	-1.67732	1.12280	1.21270
N	7.0	-5.31761	0.27377	4.63129
H	1.0	-7.12190	-0.42435	0.93553
H	1.0	-7.64294	1.25823	0.63005
H	1.0	-7.06380	0.95190	3.03707
H	1.0	-5.98698	2.11063	2.24992
H	1.0	-4.08081	0.71275	2.84873
H	1.0	-5.05721	-0.83451	2.70811
H	1.0	-5.41267	1.22307	4.99570
H	1.0	-4.49815	-0.15270	5.06855
H	1.0	-6.13924	-0.25975	4.92010

Methyl Chloride, C_{3v}, Energy: -555.66764

C	6.0	0.00000	0.00000	0.98077
H	1.0	-0.53245	0.92223	1.13760
H	1.0	-0.53245	-0.92223	1.13760
H	1.0	1.06490	0.00000	1.13760
H	1.0	0.47750	-0.82706	-1.18908
H	1.0	0.47750	0.82706	-1.18908
H	1.0	-0.95501	0.00000	-1.18908
Cl	17.0	0.00000	0.00000	3.41809
N	7.0	0.00000	0.00000	-0.82697

Methyl Fluoride, C_s, Energy: -195.59320

F	9.0	1.87241	-0.06110	0.00000
C	6.0	-0.24185	0.17504	0.00000
N	7.0	-1.86483	-0.08482	0.00000
H	1.0	0.33576	-0.74840	0.00000
H	1.0	-0.08458	0.74773	0.90368
H	1.0	-0.08458	0.74773	-0.90368
H	1.0	-2.13087	-0.62616	0.82517
H	1.0	-2.13087	-0.62616	-0.82517
H	1.0	-2.40897	0.78211	0.00000

Methyl Bromide, C_{3v}, Energy: -2668.48397

C	6.0	0.00000	0.00000	0.99427
H	1.0	-0.53392	0.92478	1.12971
H	1.0	-0.53392	-0.92478	1.12971
H	1.0	1.06784	0.00000	1.12971
H	1.0	0.47737	-0.82684	-1.21994
H	1.0	0.47737	0.82684	-1.21994
H	1.0	-0.95475	0.00000	-1.21994
Br	35.0	0.00000	0.00000	3.55196
N	7.0	0.00000	0.00000	-0.85810

MP2(full)/6-31G(d) Geometries and Energies of Van Der Waals complexes

Methyl Mesylate, C_1, Energy: -758.58709

S	16.0	2.07553	0.51573	0.18915
O	8.0	1.98721	1.90663	-0.25416
O	8.0	3.03576	0.15510	1.23078
O	8.0	2.26572	-0.44335	-1.10417
C	6.0	3.21452	0.05729	-2.09851
C	6.0	0.47676	-0.07754	0.65915
H	1.0	-0.23040	0.14685	-0.13785
H	1.0	0.20090	0.44264	1.57712
H	1.0	0.54040	-1.15053	0.83612
N	7.0	5.32093	1.83568	-0.17260
H	1.0	3.39137	-0.79804	-2.74665
H	1.0	2.75180	0.87475	-2.65164
H	1.0	4.13737	0.39319	-1.62272
H	1.0	4.61506	2.56859	-0.20399
H	1.0	6.21396	2.29069	0.00351
H	1.0	5.09539	1.28412	0.65259

Dimethylsulfate, C_1, Energy: -833.61240

C	6.0	-0.53204	-2.61811	0.15498
O	8.0	0.10826	-1.31517	0.15639
S	16.0	1.70441	-1.38677	-0.06897
O	8.0	1.84848	0.16909	-0.38204
C	6.0	3.02227	0.82869	0.19709
O	8.0	2.37762	-1.72019	1.17815
O	8.0	1.96618	-2.18795	-1.25647
N	7.0	5.05312	-1.66836	-0.70869
H	1.0	-1.57531	-2.40567	0.37460
H	1.0	-0.42705	-3.08419	-0.82454
H	1.0	-0.10311	-3.25026	0.93483
H	1.0	2.96440	1.83652	-0.20682
H	1.0	2.92959	0.83798	1.28227
H	1.0	3.92979	0.31584	-0.12212
H	1.0	5.98747	-1.86208	-1.06196
H	1.0	4.39412	-2.11560	-1.34245
H	1.0	4.96133	-2.16274	0.17586

Methyl Triflate, C_1, Energy: -1055.65367

S	16.0	2.20717	0.60708	0.29261
O	8.0	2.02832	1.94149	-0.25910
O	8.0	2.91878	0.36265	1.53519
O	8.0	2.70847	-0.42245	-0.82763
C	6.0	3.12432	0.14170	-2.11433
C	6.0	0.53321	-0.10498	0.51115
F	9.0	-0.13890	-0.02905	-0.64295
F	9.0	-0.11248	0.60054	1.44453
F	9.0	0.61466	-1.37976	0.89367
N	7.0	5.24527	1.74614	-0.13154
H	1.0	3.34404	-0.73845	-2.71390
H	1.0	2.30471	0.71340	-2.54797
H	1.0	4.00749	0.75565	-1.95000
H	1.0	4.84718	2.67830	-0.04216
H	1.0	6.24956	1.86479	-0.24715
H	1.0	5.10327	1.29429	0.76956

Methylfluorosulfonate, C_1, Energy: -818.44356

S	16.0	-0.61956	-0.01031	0.67213
O	8.0	-0.84288	1.30202	0.11379
O	8.0	0.00645	-0.23924	1.95035
O	8.0	0.00621	-1.00722	-0.38821
C	6.0	0.23617	-0.47692	-1.73065
F	9.0	-2.06612	-0.69736	0.77082
N	7.0	2.33568	1.16672	0.26904
H	1.0	0.60254	-1.33970	-2.28119
H	1.0	-0.69879	-0.11534	-2.15655
H	1.0	0.98718	0.30629	-1.66285
H	1.0	2.06008	2.14084	0.37115
H	1.0	3.33331	1.16487	0.06705
H	1.0	2.22440	0.74401	1.18854

Methyl bis(trifluoromethanesulfonyl)imide (anti) C_1,
Energy: -1919.72254

C	6.0	-0.26467	-1.53625	0.16484
N	7.0	0.41561	-0.23126	0.39525
S	16.0	1.61248	-0.12976	1.59217
S	16.0	0.09380	1.03733	-0.67679
O	8.0	1.22812	1.93340	-0.76902
O	8.0	-0.55561	0.44608	-1.83700
O	8.0	1.30838	-1.15564	2.57483
C	6.0	3.08627	-0.74737	0.67435
C	6.0	-1.22869	1.92895	0.24505
F	9.0	-1.63951	2.95437	-0.50540
F	9.0	-0.76557	2.37600	1.40824
F	9.0	-2.25420	1.09721	0.46151
O	8.0	1.85204	1.25943	1.92381
N	7.0	-3.27319	-1.16026	-1.31664
H	1.0	0.28315	-2.11954	-0.57529
H	1.0	-0.28348	-2.05745	1.11970
H	1.0	-1.28730	-1.36089	-0.17266
H	1.0	-4.03026	-0.57455	-0.97246
H	1.0	-3.70618	-1.89622	-1.87023
H	1.0	-2.73259	-0.58672	-1.96009
F	9.0	4.12992	-0.75323	1.50371
F	9.0	3.34498	0.02963	-0.37464
F	9.0	2.84185	-1.99517	0.25241

Methyl bis(trifluoromethanesulfonyl)imide (gauche) C_1,
Energy: -1919.71949

C	6.0	-3.63764	-2.16135	-0.08845
N	7.0	-2.65002	-1.06318	-0.28779
S	16.0	-1.01329	-1.43548	0.01436
S	16.0	-3.14598	0.36419	-1.03111
O	8.0	-1.99525	1.22201	-1.23136
O	8.0	-4.11198	0.05443	-2.07359
O	8.0	-1.01995	-2.83780	0.39523
O	8.0	-0.14290	-0.87986	-1.00114
C	6.0	-4.12482	1.12717	0.33468
F	9.0	-4.57789	2.30616	-0.09650
F	9.0	-3.35292	1.30963	1.40760
F	9.0	-5.15961	0.34697	0.66462
C	6.0	-0.70179	-0.50135	1.57348
F	9.0	-0.66844	0.80872	1.34499
F	9.0	0.47355	-0.90339	2.06028
F	9.0	-1.66904	-0.78079	2.45442
N	7.0	-6.71368	-1.52231	-1.28563
H	1.0	-3.31138	-3.04362	-0.63577
H	1.0	-3.70482	-2.38431	0.97618
H	1.0	-4.61261	-1.84472	-0.46398
H	1.0	-7.42086	-0.98022	-0.79443
H	1.0	-7.21403	-2.22207	-1.82937
H	1.0	-6.27433	-0.89124	-1.95199

Methyl bis(fluorosulfonyl)imide, C_1, Energy: -1445.30276

C	6.0	-0.83597	-0.92101	0.68570
N	7.0	0.26057	-0.15853	0.03331
S	16.0	1.77316	-0.83171	-0.20120
S	16.0	-0.00032	1.44807	-0.33436
O	8.0	-1.25556	1.82126	0.26870
O	8.0	1.22415	2.19124	-0.19725
O	8.0	2.37410	-0.25542	-1.37424
O	8.0	1.65240	-2.24543	0.05041
F	9.0	-0.28041	1.33325	-1.91105
F	9.0	2.55228	-0.22244	1.05854
N	7.0	-3.11589	-0.02290	-1.56959
H	1.0	-0.53618	-1.96603	0.68167
H	1.0	-0.97342	-0.57081	1.70872
H	1.0	-1.73650	-0.78848	0.08395
H	1.0	-3.37293	0.85147	-1.11727
H	1.0	-3.98272	-0.47669	-1.84960
H	1.0	-2.63218	0.23513	-2.42662

Methyl bis(methylsulfonyl)imide (anti) C_1, Energy: -1325.59716

C	6.0	-0.91580	-0.53634	1.16462
N	7.0	0.32220	0.17719	0.78978
S	16.0	1.12420	1.14196	1.95545
S	16.0	0.56593	0.49089	-0.86013
O	8.0	1.98593	0.79365	-1.01966
O	8.0	-0.04744	-0.64106	-1.55674
O	8.0	0.47362	0.83134	3.22596
C	6.0	2.75641	0.45260	1.96505
C	6.0	-0.38261	1.94798	-1.20549
H	1.0	-0.20706	2.19102	-2.25567
H	1.0	-0.02182	2.74552	-0.55717
H	1.0	-1.43657	1.71298	-1.04079
O	8.0	1.20009	2.51767	1.46588
N	7.0	-3.14985	0.06708	-1.46265
H	1.0	-0.88738	-1.52821	0.71574
H	1.0	-0.92754	-0.61816	2.24960
H	1.0	-1.80401	0.00133	0.82537
H	1.0	-3.60934	0.41138	-2.30310
H	1.0	-3.80087	-0.58630	-1.03252
H	1.0	-2.34570	-0.47849	-1.76958
H	1.0	3.33313	1.02151	2.69684
H	1.0	3.17675	0.55340	0.96585
H	1.0	2.68232	-0.59300	2.26269

Methyl bis(methylsulfonyl)imide (gauche) C_1, Energy: -1325.59135

C	6.0	-0.60345	-1.08454	0.59308
N	7.0	0.45232	-0.14910	0.13373
S	16.0	2.05582	-0.74612	0.44523
S	16.0	0.15176	0.54769	-1.39986
O	8.0	1.39961	1.18592	-1.81604
O	8.0	-0.53097	-0.41034	-2.27242
O	8.0	1.90420	-1.46530	1.70841
O	8.0	2.60600	-1.41060	-0.73122
C	6.0	-1.00596	1.81703	-0.95342
H	1.0	-1.17828	2.39382	-1.86507
H	1.0	-0.55225	2.44536	-0.18812
H	1.0	-1.93882	1.35809	-0.62107
C	6.0	2.94960	0.75260	0.75408
H	1.0	2.95473	1.35276	-0.15314
H	1.0	3.96169	0.44675	1.02623
H	1.0	2.47171	1.27101	1.58440
N	7.0	-3.50273	-0.38157	-1.16961
H	1.0	-0.53690	-2.05073	0.08625
H	1.0	-0.48537	-1.21652	1.66603
H	1.0	-1.57386	-0.63630	0.37982
H	1.0	-4.22919	0.10278	-1.69334
H	1.0	-3.92916	-1.23895	-0.82392
H	1.0	-2.79154	-0.66136	-1.84439

Methyl MSA, C_1, Energy: -738.74012

C	6.0	0.29660	-0.96040	1.56476
N	7.0	1.38978	-0.08339	1.14796
H	1.0	2.29714	-0.52363	1.01630
S	16.0	1.11500	1.08464	0.00513
O	8.0	-0.12475	1.76307	0.39542
O	8.0	2.37835	1.80203	-0.14314
C	6.0	0.78513	0.24371	-1.53005
N	7.0	-2.38816	-0.21797	-0.59323
H	1.0	0.65278	-1.55062	2.41035
H	1.0	-0.52779	-0.33386	1.90183
H	1.0	-0.06246	-1.63047	0.77631
H	1.0	-1.97799	0.62904	-0.20067
H	1.0	-3.01130	-0.59756	0.11641
H	1.0	-2.98534	0.07760	-1.36256
H	1.0	0.64067	1.01518	-2.28888
H	1.0	-0.12628	-0.34828	-1.42339
H	1.0	1.64863	-0.36906	-1.79255

Methyl FSA, C_1, Energy: -798.60455

C	6.0	0.26599	-1.01034	1.21145
N	7.0	1.39201	-0.27619	0.60706
H	1.0	2.17771	-0.83197	0.27763
S	16.0	1.07843	0.95996	-0.39351
O	8.0	-0.04715	1.70599	0.12390
O	8.0	2.32591	1.54862	-0.81861
F	9.0	0.50063	0.21460	-1.72081
N	7.0	-2.33177	-0.49680	-0.91025
H	1.0	0.69834	-1.84642	1.76055
H	1.0	-0.23563	-0.34657	1.91401
H	1.0	-0.45537	-1.36198	0.47071
H	1.0	-2.09204	0.43502	-0.57764
H	1.0	-3.34480	-0.57652	-0.85746
H	1.0	-2.08991	-0.50797	-1.89789

MeiprFSA, C_1, Energy: -916.11962

C	6.0	-0.14543	-1.18621	0.75151
N	7.0	0.86069	-0.15360	0.43946
C	6.0	2.25515	-0.48284	0.85894
S	16.0	0.62201	0.65794	-0.94614
O	8.0	-0.75302	1.10258	-1.03469
O	8.0	1.74177	1.53234	-1.21453
F	9.0	0.72827	-0.52536	-2.06457
N	7.0	-3.39035	-0.39663	-0.20120
H	1.0	0.10402	-2.13828	0.27073
H	1.0	-0.15009	-1.31550	1.83470
H	1.0	-1.14042	-0.86810	0.43931
H	1.0	-2.81037	0.30312	-0.65932
H	1.0	-4.06842	0.10977	0.36340
H	1.0	-3.91890	-0.86316	-0.93464
C	6.0	3.04897	-1.24595	-0.19605
H	1.0	2.08369	-1.15343	1.70724
C	6.0	2.98864	0.74177	1.38628
H	1.0	3.91018	0.42043	1.88086
H	1.0	2.36910	1.26838	2.11572
H	1.0	3.24651	1.42885	0.58146
H	1.0	3.99002	-1.59078	0.24163
H	1.0	3.28536	-0.60357	-1.04622
H	1.0	2.49994	-2.11917	-0.55669

Methyl acetate, C_1, Energy: -323.95778

C	6.0	-4.76330	-0.87502	0.56099
C	6.0	-3.48640	-0.13526	0.29454
O	8.0	-2.68648	-0.36043	-0.59484
O	8.0	-3.30869	0.86734	1.20657
C	6.0	-2.09098	1.61402	1.02202
N	7.0	-6.29875	2.16070	1.18625
H	1.0	-4.88517	-1.65388	-0.19018
H	1.0	-4.72516	-1.32253	1.55723
H	1.0	-5.60502	-0.17832	0.53898
H	1.0	-2.08778	2.35558	1.81839
H	1.0	-1.22546	0.95574	1.10386
H	1.0	-2.08180	2.09519	0.04315
H	1.0	-6.74213	2.36174	2.07912
H	1.0	-6.36621	3.01098	0.63224
H	1.0	-5.31062	2.00614	1.37478

Methyl trifluoroacetate, C_1, Energy: -621.03443

C	6.0	-1.75678	-0.01532	0.44186
C	6.0	-0.37804	0.65146	0.42408
O	8.0	0.54553	-0.29094	0.23608
O	8.0	-0.20424	1.84151	0.58277
F	9.0	-1.91152	-0.71456	1.58235
F	9.0	-2.72629	0.89983	0.36481
F	9.0	-1.89017	-0.87075	-0.59275
C	6.0	1.91810	0.17812	0.20045
H	1.0	2.47950	-0.68333	-0.14917
H	1.0	2.21883	0.49004	1.20088
H	1.0	1.99973	1.01833	-0.48857
N	7.0	1.48996	-2.76366	-1.32055
H	1.0	1.39698	-2.95790	-2.31484
H	1.0	1.46455	-3.66566	-0.85089
H	1.0	0.64837	-2.26680	-1.03817

Methyl cyanoformate, C_s, Energy: -376.78433

C	6.0	-1.47301	-0.77120	0.00000
C	6.0	-0.73161	0.49697	0.00000
O	8.0	0.57986	0.24591	0.00000
O	8.0	-1.27341	1.58460	0.00000
N	7.0	-2.11971	-1.75893	0.00000
C	6.0	1.42222	1.43332	0.00000
H	1.0	2.43222	1.03286	0.00000
N	7.0	3.46108	-1.18080	0.00000
H	1.0	2.47835	-1.44492	0.00000
H	1.0	1.21412	2.02517	-0.89140
H	1.0	1.21412	2.02517	0.89140
H	1.0	3.88029	-1.62369	-0.81425
H	1.0	3.88029	-1.62369	0.81425

Dimethylcarbonate, C_1, Energy: -398.99274

O	8.0	-1.71595	-1.64567	-0.34681
C	6.0	-0.66748	-0.81514	-0.46796
O	8.0	0.32101	-1.11461	-1.10910
O	8.0	-0.86388	0.34335	0.18726
C	6.0	-2.84908	-1.20995	0.42601
C	6.0	0.23999	1.27555	0.08546
H	1.0	-3.54950	-2.04128	0.37647
H	1.0	-0.08140	2.14169	0.65991
H	1.0	-3.29192	-0.31311	-0.00759
H	1.0	-2.56146	-1.01547	1.45935
H	1.0	0.39780	1.54388	-0.95969
H	1.0	1.14739	0.83630	0.49912
N	7.0	3.05507	-0.71645	0.47509
H	1.0	3.27864	-1.51546	1.06409
H	1.0	2.33736	-1.02664	-0.17824
H	1.0	3.88902	-0.52819	-0.07662

Dimethylurethane, C_1, Energy: -379.16693

O	8.0	0.04191	1.63211	0.12268
C	6.0	-0.00425	0.43002	-0.10942
N	7.0	-1.10517	-0.29066	-0.40633
O	8.0	1.10629	-0.38819	-0.08147
H	1.0	-0.99067	-1.27314	-0.67022
C	6.0	2.31080	0.31506	0.25469
C	6.0	-2.37522	0.38138	-0.57605
H	1.0	-3.16768	-0.36787	-0.54944
H	1.0	-2.43288	0.92663	-1.52439
H	1.0	-2.52691	1.09372	0.23628
H	1.0	3.09582	-0.43990	0.23699
H	1.0	2.23378	0.76334	1.24627
H	1.0	2.51772	1.09990	-0.47424
N	7.0	-0.20802	-3.07216	-1.02144
H	1.0	-0.07207	-3.45435	-1.95418
H	1.0	0.67082	-2.64108	-0.74028
H	1.0	-0.36983	-3.85984	-0.39864

Methyl Acetamide, C_1, Energy: -304.12207

C	6.0	-0.58441	-1.75116	-0.33760
C	6.0	0.69427	-0.98409	-0.60803
O	8.0	1.74947	-1.55792	-0.89954
N	7.0	0.59695	0.36353	-0.50903
C	6.0	1.76516	1.18265	-0.75155
N	7.0	-1.99959	1.82192	0.20970
H	1.0	-0.83598	-2.33883	-1.22328
H	1.0	-0.40745	-2.45155	0.48152
H	1.0	-1.42418	-1.10112	-0.08357
H	1.0	1.48857	2.22927	-0.61446
H	1.0	2.57168	0.92838	-0.05857
H	1.0	2.14185	1.03875	-1.76797
H	1.0	-2.20075	1.79949	1.20697
H	1.0	-2.83095	1.47116	-0.26089
H	1.0	-1.91824	2.80368	-0.04643
H	1.0	-0.29005	0.80918	-0.26822

Methyl Trifluoroacetamide, C_1, Energy: -601.21078

C	6.0	-0.82875	-0.56153	0.15288
O	8.0	-0.80045	-1.77822	-0.03209
N	7.0	-1.85164	0.26359	-0.11855
H	1.0	-1.77164	1.27590	0.05920
C	6.0	0.38976	0.16714	0.73801
F	9.0	1.35475	-0.68472	1.08379
F	9.0	0.05156	0.89101	1.83585
F	9.0	0.90633	1.04679	-0.16086
C	6.0	-3.06416	-0.27987	-0.69897
H	1.0	-3.77324	0.53671	-0.83466
H	1.0	-3.50126	-1.03572	-0.04201
H	1.0	-2.85776	-0.74710	-1.66533
N	7.0	-1.40375	3.13233	0.42482
H	1.0	-1.44356	3.29561	1.42829
H	1.0	-0.42197	3.19100	0.16428
H	1.0	-1.87974	3.91178	-0.02372

Methylcyanoformamide, C_s, Energy: -356.96347

N	7.0	-1.83570	-1.50407	0.00000
C	6.0	-0.74073	-1.06034	0.00000
C	6.0	0.63723	-0.51063	0.00000
O	8.0	1.62091	-1.25131	0.00000
N	7.0	0.63991	0.83336	0.00000
C	6.0	1.90428	1.54385	0.00000
H	1.0	-0.26184	1.33637	0.00000
H	1.0	1.69447	2.61327	0.00000
N	7.0	-2.10406	1.92527	0.00000
H	1.0	-2.60719	1.03890	0.00000
H	1.0	-2.42393	2.44214	-0.81642
H	1.0	-2.42393	2.44214	0.81642
H	1.0	2.49159	1.28779	-0.88526
H	1.0	2.49159	1.28779	0.88526

Methyl Succinimide, C_1, Energy: -455.18368

C	6.0	0.52917	-1.26291	-0.86215
C	6.0	1.76042	-0.83202	-0.08551
N	7.0	1.38135	0.14771	0.81472
C	6.0	0.02188	0.45676	0.76478
C	6.0	-0.61973	-0.44200	-0.27780
O	8.0	-0.52583	1.30054	1.45442
O	8.0	2.90039	-1.25874	-0.22177
C	6.0	2.31425	0.81389	1.71023
N	7.0	4.66504	-1.64816	2.40933
H	1.0	0.70344	-1.07043	-1.92439
H	1.0	0.40072	-2.34246	-0.74822
H	1.0	-1.38283	-1.05258	0.21272
H	1.0	-1.13219	0.18323	-1.01348
H	1.0	1.71974	1.38143	2.42535
H	1.0	2.93544	0.07381	2.21649
H	1.0	2.95198	1.49530	1.14227
H	1.0	4.30095	-1.62965	1.45794
H	1.0	4.64012	-2.61819	2.71474
H	1.0	5.64806	-1.39265	2.35189

1, 3-Propanesultone, C_1, Energy: -796.58767

C	6.0	-3.84229	0.75631	-0.06952
C	6.0	-2.58632	0.41009	-0.85058
C	6.0	-1.99255	-0.81172	-0.13710
O	8.0	-3.07688	-1.58382	0.44439
S	16.0	-4.53908	-0.86358	0.19264
O	8.0	-5.30841	-0.98887	1.42085
O	8.0	-5.08698	-1.34937	-1.07484
N	7.0	-6.48769	1.37912	-1.88668
H	1.0	-4.58130	1.35214	-0.61505
H	1.0	-3.62600	1.18153	0.91458
H	1.0	-1.87349	1.23697	-0.87655
H	1.0	-2.85960	0.15626	-1.87649
H	1.0	-1.44270	-1.46802	-0.81361
H	1.0	-1.34769	-0.51631	0.69471
H	1.0	-7.38886	1.55983	-1.45017
H	1.0	-6.39456	0.36670	-1.95086
H	1.0	-6.55907	1.72724	-2.84003

N-Triflylpropanesultam, C_1, Energy: -1660.66338

C	6.0	-6.53875	0.69446	1.10123
C	6.0	-5.68805	1.16524	2.26912
C	6.0	-4.38491	0.37091	2.17801
N	7.0	-4.08139	0.30374	0.73124
S	16.0	-5.42434	0.80259	-0.28481
O	8.0	-5.21655	2.20223	-0.64154
O	8.0	-5.69217	-0.19595	-1.31100
S	16.0	-2.78151	-0.57133	0.21035
O	8.0	-3.01004	-1.08554	-1.12846
O	8.0	-2.32875	-1.40146	1.32047
C	6.0	-1.54199	0.77269	0.03454
F	9.0	-1.96431	1.65378	-0.87233
F	9.0	-0.37569	0.25072	-0.35214
F	9.0	-1.38165	1.39053	1.21390
N	7.0	-5.52432	-2.52894	0.86250
H	1.0	-6.80796	-0.36070	1.19574
H	1.0	-7.40418	1.32330	0.88038
H	1.0	-6.18426	0.97369	3.22347
H	1.0	-5.49594	2.23828	2.18494
H	1.0	-3.56541	0.86521	2.70334
H	1.0	-4.52252	-0.64286	2.55743
H	1.0	-5.44561	-2.32132	-0.13276
H	1.0	-4.61498	-2.89066	1.14725
H	1.0	-6.17549	-3.30831	0.94198

Methyl Chloride, C_{3v}, Energy: -555.73069

C	6.0	0.00000	0.00000	1.91852
H	1.0	-0.51302	0.88858	1.56196
H	1.0	-0.51302	-0.88858	1.56196
H	1.0	1.02604	0.00000	1.56196
H	1.0	0.47000	-0.81406	-1.71285
H	1.0	0.47000	0.81406	-1.71285
H	1.0	-0.94000	0.00000	-1.71285
Cl	17.0	0.00000	0.00000	3.70220
N	7.0	0.00000	0.00000	-1.32406

Methyl Fluoride, C_{3v}, Energy: -195.70492

C	6.0	0.00000	0.00000	1.93797
H	1.0	-0.51418	0.89058	1.57738
H	1.0	-0.51418	-0.89058	1.57738
H	1.0	1.02835	0.00000	1.57738
H	1.0	0.47001	-0.81409	-1.63712
H	1.0	0.47001	0.81409	-1.63712
H	1.0	-0.94003	0.00000	-1.63712
F	9.0	0.00000	0.00000	3.33396
N	7.0	0.00000	0.00000	-1.24875

Methyl Bromide, C_{3v}, Energy: -2668.53500

C	6.0	0.00000	0.00000	1.90614
H	1.0	-0.51506	0.89211	1.56509
H	1.0	-0.51506	-0.89211	1.56509
H	1.0	1.03012	0.00000	1.56509
H	1.0	0.46981	-0.81373	-1.75015
H	1.0	0.46981	0.81373	-1.75015
H	1.0	-0.93961	0.00000	-1.75015
Br	35.0	0.00000	0.00000	3.85335
N	7.0	0.00000	0.00000	-1.36035

MP2(full)/6-31G(d) Geometries of Methyl Transfer Agents

Methyl Mesylate, C_s, Energy: -702.21914

S	16.0	-0.48793	0.59518	0.00000
O	8.0	0.74189	-0.48079	0.00000
C	6.0	2.05024	0.14658	0.00000
C	6.0	-1.78750	-0.60331	0.00000
H	1.0	-2.72724	-0.04971	0.00000
H	1.0	2.75493	-0.68149	0.00000
H	1.0	-1.70452	-1.21272	-0.89869
H	1.0	-1.70452	-1.21272	0.89869
H	1.0	2.17258	0.75409	-0.89797
H	1.0	2.17258	0.75409	0.89797
O	8.0	-0.48327	1.32550	-1.26391
O	8.0	-0.48327	1.32550	1.26391

Dimethylsulfate, C_1, Energy: -777.24377

C	6.0	-1.94327	-1.54122	0.02882
O	8.0	-1.26787	-0.26138	0.16975
S	16.0	0.29230	-0.32041	-0.21263
O	8.0	0.41024	1.27809	-0.33405
C	6.0	1.78363	1.75545	-0.32370
O	8.0	1.08668	-0.78435	0.91383
O	8.0	0.45285	-0.95375	-1.51198
H	1.0	-2.95766	-1.34542	0.36629
H	1.0	-1.93144	-1.85542	-1.01440
H	1.0	-1.46981	-2.28940	0.66698
H	1.0	1.69338	2.82986	-0.46080
H	1.0	2.25226	1.52071	0.63166
H	1.0	2.34201	1.31405	-1.15122

Methyl Triflate, C_1, Energy: -999.28488

S	16.0	0.25159	0.41701	0.83473
O	8.0	0.07720	1.75046	0.28263
O	8.0	0.96943	0.13787	2.05924
O	8.0	0.81877	-0.58589	-0.29120
C	6.0	0.71707	-0.15875	-1.68227
C	6.0	-1.42711	-0.29711	1.03422
F	9.0	-2.08031	-0.24174	-0.13658
F	9.0	-2.09407	0.41557	1.94346
F	9.0	-1.34499	-1.56608	1.43089
H	1.0	1.21648	-0.95207	-2.23302
H	1.0	-0.32836	-0.08190	-1.97734
H	1.0	1.22784	0.79245	-1.81832

Methylfluorosulfonate, C_1, Energy: -762.07625

S	16.0	-0.60047	0.32365	1.04387
O	8.0	-0.88595	1.67695	0.65859
O	8.0	0.30024	-0.05308	2.10684
O	8.0	-0.27758	-0.48448	-0.28811
C	6.0	0.14692	-1.86719	-0.10985
F	9.0	-2.00395	-0.37244	1.39800
H	1.0	0.32409	-2.22029	-1.12209
H	1.0	1.05819	-1.89960	0.48505
H	1.0	-0.65152	-2.43862	0.36382

Methyl bis(trifluoromethanesulfonyl)imide (anti) C_1,
Energy: -1863.35495

N	7.0	0.17552	0.23493	0.17590
S	16.0	0.43900	-1.37755	0.62715
S	16.0	-1.01820	0.70063	-0.93931
O	8.0	-0.59558	1.99214	-1.45403
O	8.0	-1.40403	-0.41878	-1.77282
O	8.0	1.17721	-1.34640	1.87842
O	8.0	-0.77508	-2.13839	0.42166
C	6.0	-2.41875	1.03803	0.20971
F	9.0	-3.45702	1.46415	-0.50953
F	9.0	-2.05184	1.99210	1.07545
F	9.0	-2.74842	-0.06349	0.87714
C	6.0	1.65825	-1.89764	-0.65200
F	9.0	1.12524	-1.81351	-1.86777
F	9.0	2.02968	-3.15258	-0.40263
F	9.0	2.72495	-1.08941	-0.57754
C	6.0	1.11958	1.28464	0.63431
H	1.0	0.54846	2.14726	0.97208
H	1.0	1.79542	1.57006	-0.17071
H	1.0	1.67563	0.87380	1.47449

Methyl bis(fluorosulfonyl)imide, C_1, Energy: -1388.93439

N	7.0	0.12598	0.85721	-0.43711
S	16.0	0.17991	-0.74351	0.10271
S	16.0	-1.35861	1.54537	-0.78570
O	8.0	-1.09995	2.82832	-1.38785
O	8.0	-2.21553	0.52898	-1.33205
O	8.0	-0.96600	-1.06044	0.91471
O	8.0	1.54614	-0.98483	0.49304
F	9.0	-1.88279	1.85606	0.69869
F	9.0	-0.04132	-1.46132	-1.30164
C	6.0	1.24220	1.74979	-0.04756
H	1.0	1.17936	2.63172	-0.68081
H	1.0	2.17296	1.22368	-0.24244
H	1.0	1.17679	2.03019	1.00543

Methyl bis(methylsulfonyl)imide (anti) C_1, Energy: -1269.22819

N	7.0	0.18569	0.23527	-0.72916
S	16.0	-0.02526	-1.44459	-0.89703
S	16.0	-1.19470	1.24290	-0.57807
O	8.0	-0.68432	2.59692	-0.77402
O	8.0	-2.27211	0.71724	-1.41653
O	8.0	-1.10049	-1.80835	0.02067
O	8.0	1.31052	-2.02036	-0.78488
C	6.0	-1.63882	1.02999	1.12318
H	1.0	-2.51134	1.66215	1.29904
H	1.0	-0.79905	1.35384	1.73718
H	1.0	-1.87133	-0.02041	1.28927
C	6.0	-0.59449	-1.68216	-2.56249
H	1.0	0.16590	-1.30695	-3.24863
H	1.0	-0.72473	-2.75684	-2.70243
H	1.0	-1.53800	-1.15121	-2.68209
C	6.0	1.39738	0.84298	-1.31282
H	1.0	1.59453	1.77865	-0.79397
H	1.0	1.28781	1.04332	-2.38254
H	1.0	2.21657	0.14727	-1.14029

Methyl MSA, C_1, Energy: -682.37105

C	6.0	-0.46679	-0.98040	1.39584
N	7.0	0.60191	-0.06732	1.00427
H	1.0	1.51463	-0.47669	0.82176
S	16.0	0.27618	1.19746	-0.01451
O	8.0	-0.92965	1.84720	0.49174
O	8.0	1.54382	1.90088	-0.18715
C	6.0	-0.15223	0.48393	-1.59370
H	1.0	-0.14236	-1.52469	2.28386
H	1.0	-1.33902	-0.38197	1.65753
H	1.0	-0.73913	-1.70185	0.61542
H	1.0	-0.39272	1.30803	-2.26707
H	1.0	-1.02420	-0.16124	-1.47872
H	1.0	0.70035	-0.07500	-1.98104

Methyl FSA, C_1, Energy: -742.23853

C	6.0	-0.47591	-1.08472	0.63071
N	7.0	0.77742	-0.37593	0.35091
H	1.0	1.15876	-0.49957	-0.58501
S	16.0	0.91353	1.17616	0.83132
O	8.0	0.46777	1.28713	2.19914
O	8.0	2.15882	1.69964	0.32390
F	9.0	-0.24927	1.89708	-0.04507
H	1.0	-0.31366	-2.13860	0.40637
H	1.0	-0.69531	-0.97950	1.69189
H	1.0	-1.31405	-0.70311	0.04073

MeiprFSA, C_1, Energy: -859.75289

C	6.0	-1.80722	-0.85772	0.47214
N	7.0	-0.79726	0.15979	0.14298
C	6.0	0.59710	-0.15701	0.57192
S	16.0	-1.04159	0.95216	-1.25824
O	8.0	-2.43176	1.33359	-1.36381
O	8.0	0.05565	1.85854	-1.51026
F	9.0	-0.86695	-0.24180	-2.35604
H	1.0	-1.59199	-1.81629	-0.01234
H	1.0	-1.80916	-0.98511	1.55533
H	1.0	-2.78819	-0.50207	0.16115
C	6.0	1.41497	-0.88805	-0.48732
H	1.0	0.43285	-0.84411	1.40886
C	6.0	1.30135	1.07545	1.12054
H	1.0	2.23665	0.77053	1.59903
H	1.0	0.67519	1.56923	1.86713
H	1.0	1.52976	1.78580	0.32701
H	1.0	2.35797	-1.22087	-0.04512
H	1.0	1.64644	-0.22725	-1.32439
H	1.0	0.88618	-1.76480	-0.86857

Methyl acetate, C_s, Energy: -267.59323

C	6.0	2.68274	-0.19511	0.00000
C	6.0	1.23130	0.19417	0.00000
O	8.0	0.79414	1.33134	0.00000
O	8.0	0.44331	-0.90962	0.00000
C	6.0	-0.96736	-0.62359	0.00000
H	1.0	3.29585	0.70458	0.00000
H	1.0	-1.45462	-1.59632	0.00000
H	1.0	-1.24089	-0.05332	-0.88859
H	1.0	-1.24089	-0.05332	0.88859
H	1.0	2.90425	-0.80029	-0.88168
H	1.0	2.90425	-0.80029	0.88168

Methyl trifluoroacetate, C_s, Energy: -564.66942

C	6.0	2.68783	-0.18717	0.00000
C	6.0	1.21056	0.21533	0.00000
O	8.0	0.82365	1.36512	0.00000
O	8.0	0.45829	-0.88853	0.00000
C	6.0	-0.96475	-0.63202	0.00000
H	1.0	-1.42554	-1.61614	0.00000
H	1.0	-1.24147	-0.06886	-0.89130
H	1.0	-1.24147	-0.06886	0.89130
F	9.0	2.97136	-0.92258	-1.09071
F	9.0	2.97136	-0.92258	1.09071
F	9.0	3.46795	0.89761	0.00000

Methyl cyanoformate, C_s, Energy: -320.41939

C	6.0	1.37723	-0.16951	0.00000
C	6.0	0.01780	0.38172	0.00000
O	8.0	-0.21986	1.57342	0.00000
O	8.0	-0.87322	-0.61542	0.00000
C	6.0	-2.25169	-0.17089	0.00000
H	1.0	-2.83598	-1.08702	0.00000
H	1.0	-2.45105	0.42337	-0.89167
H	1.0	-2.45105	0.42337	0.89167
N	7.0	2.49554	-0.54781	0.00000

Dimethylcarbonate, C_s, Energy: -342.62576

O	8.0	1.32894	-0.45491	0.00000
C	6.0	-0.01437	-0.45141	0.00000
O	8.0	-0.67479	-1.46683	0.00000
O	8.0	-0.51325	0.80765	0.00000
C	6.0	-1.95315	0.84933	0.00000
C	6.0	2.02034	0.80664	0.00000
H	1.0	3.07540	0.54013	0.00000
H	1.0	1.77468	1.38405	0.89158
H	1.0	1.77468	1.38405	-0.89158
H	1.0	-2.20380	1.90791	0.00000
H	1.0	-2.34489	0.35619	0.88966
H	1.0	-2.34489	0.35619	-0.88966

Dimethylurethane, C_1, Energy: -322.79444

O	8.0	-1.68705	2.70857	-0.07422
C	6.0	-1.68319	1.48714	-0.01669
N	7.0	-2.75114	0.69525	0.27394
O	8.0	-0.59305	0.70542	-0.26830
H	1.0	-2.55723	-0.28473	0.42707
C	6.0	0.57467	1.45616	-0.63476
C	6.0	-3.98495	1.26905	0.76937
H	1.0	-3.99845	1.35213	1.86158
H	1.0	-4.82779	0.65521	0.44694
H	1.0	-4.08382	2.26626	0.34329
H	1.0	1.35224	0.71044	-0.78915
H	1.0	0.85481	2.14578	0.16236
H	1.0	0.39661	2.02120	-1.55056

Methyl Acetamide, C_1, Energy: -247.75036

C	6.0	-2.63278	-0.41880	-0.00008
C	6.0	-1.32164	0.33824	-0.00008
N	7.0	-0.21658	-0.42195	0.25807
O	8.0	-1.26543	1.54426	-0.24354
C	6.0	1.12159	0.13121	0.23094
H	1.0	-2.58313	-1.36572	0.54296
H	1.0	-3.39653	0.21656	0.44900
H	1.0	-2.92879	-0.62105	-1.03287
H	1.0	-0.33358	-1.41158	0.42215
H	1.0	1.69942	-0.25824	-0.61273
H	1.0	1.01750	1.20998	0.12255
H	1.0	1.65173	-0.09100	1.16051

Methyl Trifluoroacetamide, C_s, Energy: -544.83515

C	6.0	0.49401	-0.00687	0.00000
C	6.0	-1.03527	0.07587	0.00000
O	8.0	-1.58336	1.17432	0.00000
N	7.0	-1.66595	-1.11551	0.00000
F	9.0	0.94330	-1.29065	0.00000
H	1.0	-1.12087	-1.96561	0.00000
F	9.0	0.99271	0.59792	1.08865
F	9.0	0.99271	0.59792	-1.08865
C	6.0	-3.11718	-1.16451	0.00000
H	1.0	-3.42912	-2.20812	0.00000
H	1.0	-3.51399	-0.66427	0.88576
H	1.0	-3.51399	-0.66427	-0.88576

Methylcyanoformamide, C_s, Energy: -300.58450

C	6.0	2.61562	-0.18309	0.00000
C	6.0	1.19688	0.22863	0.00000
O	8.0	0.86457	1.41048	0.00000
N	7.0	0.34474	-0.82117	0.00000
N	7.0	3.76025	-0.47562	0.00000
H	1.0	0.71669	-1.76205	0.00000
C	6.0	-1.09068	-0.59470	0.00000
H	1.0	-1.38667	-0.03003	-0.88642
H	1.0	-1.38667	-0.03003	0.88642
H	1.0	-1.59166	-1.56190	0.00000

Methyl Succinimide, C_s, Energy: -398.81698

N	7.0	-0.02919	0.96204	0.00000
O	8.0	2.26482	0.70480	0.00000
O	8.0	-2.32393	0.63450	0.00000
C	6.0	1.14492	0.21891	0.00000
C	6.0	-1.18736	0.18999	0.00000
C	6.0	0.76407	-1.25124	0.00000
C	6.0	-0.76528	-1.26945	0.00000
H	1.0	1.20551	-1.72785	0.87928
H	1.0	1.20551	-1.72785	-0.87928
H	1.0	-1.19543	-1.75653	0.87916
H	1.0	-1.19543	-1.75653	-0.87916
C	6.0	-0.03046	2.41152	0.00000
H	1.0	-1.07105	2.73425	0.00000
H	1.0	0.48307	2.78389	-0.88801
H	1.0	0.48307	2.78389	0.88801

Methyl Chloride, C_{3v}, Energy: -499.36908

C	6.0	0.00000	0.00000	1.91773
H	1.0	-0.51467	0.89144	1.56476
H	1.0	-0.51467	-0.89144	1.56476
H	1.0	1.02934	0.00000	1.56476
Cl	17.0	0.00000	0.00000	3.69460

Methyl Fluoride, C_{3v}, Energy: -139.34265

C	6.0	0.00000	0.00000	2.09315
H	1.0	-0.51566	0.89315	1.73532
H	1.0	-0.51566	-0.89315	1.73532
H	1.0	1.03132	0.00000	1.73532
F	9.0	0.00000	0.00000	3.48336

Methyl Bromide, C_{3v}, Energy: -2612.17333

C	6.0	0.00000	0.00000	1.97130
H	1.0	-0.51650	0.89461	1.63319
H	1.0	-0.51650	-0.89461	1.63319
H	1.0	1.03301	0.00000	1.63319
Br	35.0	0.00000	0.00000	3.91157

MP2(full)/6-31G(d) Geometries of Anions

Mesylate (-) C_{3v}, Energy: -662.53310

C	6.0	0.00000	0.00000	0.15191
S	16.0	0.00000	0.00000	1.95361
O	8.0	-0.72121	1.24918	2.31290
O	8.0	-0.72121	-1.24918	2.31290
O	8.0	1.44242	0.00000	2.31290
H	1.0	0.51566	-0.89315	-0.20542
H	1.0	0.51566	0.89315	-0.20542
H	1.0	-1.03132	0.00000	-0.20542

Methylsulfate (-) C_s, Energy: -737.57487

O	8.0	1.62257	0.37580	0.00000
S	16.0	0.50838	-0.58274	0.00000
O	8.0	-0.81510	0.48061	0.00000
C	6.0	-2.05606	-0.21083	0.00000
H	1.0	-2.83768	0.55435	0.00000
O	8.0	0.33447	-1.36721	-1.24145
O	8.0	0.33447	-1.36721	1.24145
H	1.0	-2.15525	-0.83840	-0.89199
H	1.0	-2.15525	-0.83840	0.89199

Triflate (-) C_{3v}, Energy: -959.63081

C	6.0	0.00000	0.00000	0.20921
S	16.0	0.00000	0.00000	2.04431
O	8.0	-0.72210	1.25071	2.35488
O	8.0	-0.72210	-1.25071	2.35488
O	8.0	1.44420	0.00000	2.35488
F	9.0	0.62744	-1.08676	-0.29674
F	9.0	0.62744	1.08676	-0.29674
F	9.0	-1.25489	0.00000	-0.29674

Fluorosulfonate (-) C_{3v}, Energy: -722.42035

F	9.0	0.00000	0.00000	0.29520
S	16.0	0.00000	0.00000	1.95804
O	8.0	-0.71849	1.24445	2.26366
O	8.0	-0.71849	-1.24445	2.26366
O	8.0	1.43697	0.00000	2.26366

Bis(trifluoromethanesulfonyl)imide (anti)(-) C_2,
Energy: -1823.69893

N	7.0	0.00000	0.00000	0.87210
S	16.0	1.41490	0.02268	0.11185
S	16.0	-1.41490	-0.02268	0.11185
O	8.0	1.41448	0.48851	-1.27785
O	8.0	-1.41448	-0.48851	-1.27785
O	8.0	2.42973	0.52762	1.03850
O	8.0	-2.42973	-0.52762	1.03850
C	6.0	1.80301	-1.76885	-0.01609
C	6.0	-1.80301	1.76885	-0.01609
F	9.0	2.98193	-1.93558	-0.64993
F	9.0	-2.98193	1.93558	-0.64993
F	9.0	0.86056	-2.42617	-0.70840
F	9.0	-0.86056	2.42617	-0.70840
F	9.0	1.90555	-2.33443	1.19802
F	9.0	-1.90555	2.33443	1.19802

Bis(fluorosulfonyl)imide (-)C_2, Energy -1349.28297

N	7.0	0.00000	0.00000	0.90199
S	16.0	1.34747	0.31716	0.10686
S	16.0	-1.34747	-0.31716	0.10686
F	9.0	1.79459	-1.15425	-0.44979
F	9.0	-1.79459	1.15425	-0.44979
O	8.0	1.19740	1.11481	-1.10277
O	8.0	-1.19740	-1.11481	-1.10277
O	8.0	2.37985	0.65209	1.07274
O	8.0	-2.37985	-0.65209	1.07274

Bis(methylsulfonyl)imide (anti)(-) C_2, Energy: -1229.53832

N	7.0	0.00000	0.00000	1.19069
S	16.0	1.39569	0.05051	0.37946
S	16.0	-1.39569	-0.05051	0.37946
O	8.0	1.36940	0.93808	-0.80902
O	8.0	-1.36940	-0.93808	-0.80902
O	8.0	2.46813	0.27777	1.36210
O	8.0	-2.46813	-0.27777	1.36210
C	6.0	1.63809	-1.59984	-0.26067
C	6.0	-1.63809	1.59984	-0.26067
H	1.0	2.58701	-1.61728	-0.80014
H	1.0	-2.58701	1.61728	-0.80014
H	1.0	0.80040	-1.83034	-0.91775
H	1.0	-0.80040	1.83034	-0.91775
H	1.0	1.66567	-2.29000	0.58283
H	1.0	-1.66567	2.29000	0.58283

MSA (-) C_1, Energy: -642.63252

N	7.0	0.57006	-0.10099	0.96594
H	1.0	1.48921	-0.50957	0.77668
S	16.0	0.38777	1.03873	-0.09430
O	8.0	-0.62712	2.02699	0.34904
O	8.0	1.66059	1.59170	-0.65248
C	6.0	-0.39514	0.32181	-1.56133
H	1.0	-0.57377	1.11028	-2.29622
H	1.0	-1.34108	-0.13545	-1.26657
H	1.0	0.26538	-0.43491	-1.991711

FSA (-) C_1, Energy: -702.52414

N	7.0	0.56722	-0.19330	0.15548
H	1.0	0.97222	-0.42577	-0.75429
S	16.0	0.52061	1.35184	0.22419
O	8.0	0.19381	1.84129	1.56672
O	8.0	1.54857	2.08606	-0.54186
F	9.0	-0.85883	1.81386	-0.63337

Isopropyl FSA (-) C_1, -820.03729

N	7.0	-1.16986	-0.12412	0.10324
C	6.0	0.17441	-0.43254	0.59246
S	16.0	-1.31598	0.71546	-1.18332
O	8.0	-2.70600	1.11600	-1.41984
O	8.0	-0.26330	1.70878	-1.49458
F	9.0	-1.06232	-0.37167	-2.45844
C	6.0	1.10384	-1.06709	-0.44532
H	1.0	0.00632	-1.18778	1.37443
C	6.0	0.84000	0.77038	1.26476
H	1.0	1.78322	0.48393	1.74879
H	1.0	0.16790	1.18169	2.02338
H	1.0	1.03613	1.54388	0.52087
H	1.0	2.03381	-1.40766	0.02768
H	1.0	1.35160	-0.34254	-1.22369
H	1.0	0.61212	-1.92015	-0.91840

Acetate (-) C_s, Energy: -227.85413

C	6.0	1.41889	0.17015	0.00000
C	6.0	-0.13047	-0.01033	0.00000
O	8.0	-0.81068	1.05306	0.00000
O	8.0	-0.51302	-1.21448	0.00000
H	1.0	1.70293	1.22674	0.00000
H	1.0	1.84816	-0.32279	-0.87991
H	1.0	1.84816	-0.32279	0.87991

Trifluoroacetate (-) C_s, Energy: -524.96954

C	6.0	-1.39578	-0.13102	0.00000
C	6.0	0.15647	0.01014	0.00000
O	8.0	0.78477	-1.07386	0.00000
O	8.0	0.51389	1.21294	0.00000
F	9.0	-1.96620	0.46561	-1.08925
F	9.0	-1.96620	0.46561	1.08925
F	9.0	-1.85640	-1.41109	0.00000

Cyanoformate (-) C_{2v}, Energy: -280.73023

C	6.0	0.00000	0.00000	-0.02555
C	6.0	0.00000	0.00000	1.51982
N	7.0	0.00000	0.00000	-1.20979
O	8.0	0.00000	-1.14998	2.00991
O	8.0	0.00000	1.14998	2.00991

Methylcarbonate (-) C_s, Energy: -302.90805

O	8.0	0.61675	0.77336	0.00000
C	6.0	-0.57910	-0.07927	0.00000
O	8.0	-1.62139	0.59762	0.00000
O	8.0	-0.34730	-1.30903	0.00000
C	6.0	1.82340	0.04709	0.00000
H	1.0	2.63345	0.78836	0.00000
H	1.0	1.92596	-0.59811	-0.88132
H	1.0	1.92596	-0.59811	0.88132

Methylurethane (-) C_s, Energy: -283.02333

O	8.0	2.05993	0.49488	0.00000
C	6.0	0.62469	0.13235	0.00000
O	8.0	0.37929	-1.09266	0.00000
N	7.0	-0.16535	1.17891	0.00000
C	6.0	2.90753	-0.62959	0.00000
H	1.0	3.93531	-0.24415	0.00000
H	1.0	0.44585	2.00010	0.00000
H	1.0	2.75986	-1.26547	-0.88135
H	1.0	2.75986	-1.26547	0.88135

Acetamide (-) C_s, Energy: -207.96859

N	7.0	-0.02089	-1.42154	0.00000
O	8.0	1.13446	0.59077	0.00000
C	6.0	0.06986	-0.09681	0.00000
C	6.0	-1.22754	0.76548	0.00000
H	1.0	-1.02004	-1.65591	0.00000
H	1.0	-1.21978	1.41923	0.87947
H	1.0	-1.21978	1.41923	-0.87947
H	1.0	-2.16072	0.18718	0.00000

Trifluoroacetamide (-) C_s, Energy: -505.08677

C	6.0	-0.45772	-0.03591	0.00000
C	6.0	1.09048	0.00643	0.00000
O	8.0	1.51171	1.19540	0.00000
N	7.0	1.75147	-1.13304	0.00000
F	9.0	-1.02417	-1.29038	0.00000
H	1.0	1.06639	-1.89247	0.00000
F	9.0	-0.98781	0.59077	-1.08749
F	9.0	-0.98781	0.59077	1.08749

Cyanoformamide (-) C_s, Energy: -260.84632

N	7.0	2.12924	-0.00457	0.00000
C	6.0	0.94410	0.01128	0.00000
C	6.0	-0.58354	-0.00423	0.00000
O	8.0	-1.08719	-1.15456	0.00000
N	7.0	-1.16580	1.18112	0.00000
H	1.0	-0.42817	1.89250	0.00000

Succinimide (-) C_{2v}, Energy: -359.07164

N	7.0	0.00000	0.00000	0.34286
O	8.0	-2.29645	0.00000	-0.07498
O	8.0	2.29645	0.00000	-0.07498
C	6.0	-1.11121	0.00000	-0.44605
C	6.0	1.11121	0.00000	-0.44605
C	6.0	-0.75752	0.00000	-1.95649
C	6.0	0.75752	0.00000	-1.95649
H	1.0	-1.20887	0.88031	-2.42744
H	1.0	1.20887	0.88031	-2.42744
H	1.0	-1.20887	-0.88031	-2.42744
H	1.0	1.20887	-0.88031	-2.42744