

**Supporting Information:**

**The Effect of Solvation in Torquoselectivity:  
Ring Opening of Monosubstituted Cyclobutenes**

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# Energy components of solvation

	Cavitation				Dispersion				Repulsion			
	OMe-out	OMe-in	NH2-out	NH2-in	OMe-out	OMe-in	NH2-out	NH2-in	OMe-out	OMe-in	NH2-out	NH2-in
n-Hexane*	12.87	12.75	11.22	11.17	-10.23	-10.16	-9.05	-8.95	0.67	0.66	0.6	0.59
DCM	14.17	14.03	12.34	12.29	-9.94	-9.87	-8.81	-8.7	0.66	0.65	0.59	0.58
Acetone	13.6	13.47	11.84	11.8	-9.57	-9.5	-8.46	-8.38	0.64	0.63	0.57	0.56
Acetonitrile	16.31	16.15	14.21	14.15	-8.57	-8.5	-7.57	-7.5	0.57	0.56	0.51	0.5
DMSO	18.08	17.9	15.74	15.68	-12.18	-12.09	-10.77	-10.67	0.84	0.82	0.75	0.73
Water	18.78	18.59	16.35	16.28	-11.92	-11.82	-10.52	-10.44	0.85	0.83	0.76	0.74

  

	(Unpolarized solute)-solvent				(Polarized solute)-solvent				Solute polarization			
	OMe-out	OMe-in	NH2-out	NH2-in	OMe-out	OMe-in	NH2-out	NH2-in	OMe-out	OMe-in	NH2-out	NH2-in
n-Hexane	-0.8	-0.75	-1.13	-1.03	-0.88	-0.81	-1.24	-1.13	0.04	0.03	0.06	0.05
DCM	-1.8	-1.77	-2.54	-2.5	-2.25	-2.2	-3.13	-3.18	0.25	0.23	0.32	0.37
Acetone	-1.99	-1.98	-2.81	-2.81	-2.57	-2.54	-3.54	-3.71	0.32	0.30	0.40	0.49
Acetonitrile	-2.06	-2.05	-2.9	-2.92	-2.68	-2.66	-3.68	-3.9	0.34	0.33	0.43	0.54
DMSO	-2.08	-2.08	-2.93	-2.95	-2.72	-2.7	-3.73	-3.97	0.35	0.34	0.44	0.56
Water	-2.11	-2.11	-2.97	-3	-2.77	-2.76	-3.8	-4.05	0.36	0.36	0.45	0.58

  

	DeltaG				Total non-electrostatic				Total electrostatic			
	OMe-out	OMe-in	NH2-out	NH2-in	OMe-out	OMe-in	NH2-out	NH2-in	OMe-out	OMe-in	NH2-out	NH2-in
n-Hexane	2.48	2.47	1.58	1.73	3.31	3.25	2.77	2.81	-0.84	-0.78	-1.19	-1.08
DCM	2.88	2.84	1.32	1.35	4.89	4.81	4.12	4.16	-2.01	-1.97	-2.81	-2.81
Acetone	2.41	2.36	0.82	0.77	4.67	4.6	3.96	3.98	-2.25	-2.23	-3.14	-3.21
Acetonitrile	5.98	5.89	3.9	3.8	8.32	8.22	7.15	7.16	-2.34	-2.33	-3.25	-3.36
DMSO	4.37	4.27	2.43	2.34	6.73	6.64	5.72	5.75	-2.37	-2.36	-3.29	-3.41
Water	5.3	5.2	3.25	3.11	7.7	7.61	6.59	6.58	-2.41	-2.4	-3.34	-3.47

# Energy minima

3-CF3-Acetone

SCF Energy: -493.055574966

ZPE-corrected Energy: -492.962673

$\Delta U$ : -492.955782

$\Delta H$ : -492.954838

$\Delta G$ : -492.994279

Num. Imaginary Frequencies: 0

C	-0.449382	-0.006135	-0.670389
C	-1.456750	1.054149	-0.130165
C	-2.305021	-0.134455	0.261306
C	-1.439327	-1.041563	-0.184367
H	-0.280398	0.027463	-1.746486
H	-1.868928	1.703531	-0.900123
H	-1.081735	1.661023	0.693140
H	-3.279508	-0.201767	0.724017
H	-1.422607	-2.121258	-0.222020
C	0.894863	-0.008204	-0.003335
F	1.620478	-1.083463	-0.351894
F	0.813442	-0.017628	1.335068
F	1.617954	1.073119	-0.337266

3-CF3-Acetonitrile

SCF Energy: -493.055688843

ZPE-corrected Energy: -492.962800

$\Delta U$ : -492.955909

$\Delta H$ : -492.954965

$\Delta G$ : -492.994406

Num. Imaginary Frequencies: 0

C	-0.449450	-0.006116	-0.670507
C	-1.456804	1.054148	-0.130190
C	-2.304965	-0.134467	0.261477
C	-1.439306	-1.041597	-0.184327
H	-0.280552	0.027475	-1.746599
H	-1.869145	1.703265	-0.900259
H	-1.081862	1.661290	0.692956
H	-3.279522	-0.201724	0.724059
H	-1.422722	-2.121288	-0.222370
C	0.894710	-0.008181	-0.003510
F	1.620637	-1.083355	-0.351936
F	0.813428	-0.017792	1.335054
F	1.618013	1.073175	-0.337057

3-CF3-Dichloromethane

SCF Energy: -493.055246758

ZPE-corrected Energy: -492.962307

$\Delta U$ : -492.955418

$\Delta H$ : -492.954474

$\Delta G$ : -492.993913

Num. Imaginary Frequencies: 0

C	-0.449180	-0.006181	-0.670070
C	-1.456591	1.054151	-0.130111
C	-2.305151	-0.134426	0.260841
C	-1.439360	-1.041463	-0.184483
H	-0.279957	0.027431	-1.746177
H	-1.868340	1.704252	-0.899763
H	-1.081355	1.660299	0.693615
H	-3.279446	-0.201902	0.723910
H	-1.422267	-2.121167	-0.221075
C	0.895308	-0.008266	-0.002853
F	1.619969	-1.083831	-0.351672
F	0.813437	-0.017045	1.335107
F	1.617840	1.072898	-0.337931

3-CF3-DMSO

SCF Energy: -493.055726050

ZPE-corrected Energy: -492.962842

$\Delta U$ : -492.955950

$\Delta H$ : -492.955006

$\Delta G$ : -492.994448

Num. Imaginary Frequencies: 0

C	-0.449472	-0.006109	-0.670546
C	-1.456821	1.054148	-0.130198
C	-2.304946	-0.134471	0.261534
C	-1.439299	-1.041608	-0.184314
H	-0.280603	0.027479	-1.746637
H	-1.869218	1.703176	-0.900305
H	-1.081904	1.661380	0.692894
H	-3.279525	-0.201710	0.724073
H	-1.422759	-2.121298	-0.222487
C	0.894660	-0.008173	-0.003567
F	1.620687	-1.083323	-0.351945
F	0.813421	-0.017841	1.335050
F	1.618034	1.073191	-0.336992

3-CF3-Gas

SCF Energy: -493.052260465

ZPE-corrected Energy: -492.959028

$\Delta U$ : -492.952153

$\Delta H$ : -492.951209

$\Delta G$ : -492.990627

Num. Imaginary Frequencies: 0

C	-0.446971	-0.006322	-0.668512
C	-1.454687	1.054150	-0.130433
C	-2.304713	-0.134294	0.258015
C	-1.438451	-1.040501	-0.185851
H	-0.276094	0.027260	-1.744601
H	-1.864744	1.708547	-0.897896
H	-1.076690	1.655679	0.695323
H	-3.277420	-0.203369	0.724107
H	-1.418965	-2.120207	-0.215633
C	0.899427	-0.008614	0.000548
F	1.613797	-1.088888	-0.346175
F	0.810861	-0.008545	1.335425
F	1.618262	1.069164	-0.345238

3-CF3-n-Hexane

SCF Energy: -493.053555528

ZPE-corrected Energy: -492.960439

$\Delta U$ : -492.953558

$\Delta H$ : -492.952614

$\Delta G$ : -492.992040

Num. Imaginary Frequencies: 0

C	-0.448009	-0.006297	-0.668896
C	-1.455634	1.054161	-0.130131
C	-2.305234	-0.134334	0.258964
C	-1.439071	-1.040930	-0.185170
H	-0.277767	0.027317	-1.745013
H	-1.865990	1.707093	-0.898463
H	-1.079010	1.657366	0.695065
H	-3.278627	-0.202718	0.723729
H	-1.420428	-2.120644	-0.217413
C	0.897641	-0.008493	-0.000748
F	1.616677	-1.086477	-0.349096
F	0.812495	-0.012648	1.335305
F	1.617902	1.071008	-0.341989

3-CF3-Water

SCF Energy: -493.055774522

ZPE-corrected Energy: -492.962896

$\Delta U$ : -492.956004

$\Delta H$ : -492.955060

$\Delta G$ : -492.994502

Num. Imaginary Frequencies: 0

C	-0.449500	-0.006100	-0.670598
C	-1.456844	1.054148	-0.130210
C	-2.304920	-0.134476	0.261609
C	-1.439288	-1.041622	-0.184298
H	-0.280669	0.027485	-1.746687
H	-1.869314	1.703059	-0.900365
H	-1.081957	1.661498	0.692811
H	-3.279529	-0.201693	0.724092
H	-1.422807	-2.121311	-0.222641
C	0.894594	-0.008162	-0.003643
F	1.620750	-1.083282	-0.351954
F	0.813411	-0.017900	1.335044
F	1.618064	1.073209	-0.336909

3-CHO-Acetone

SCF Energy: -269.284767039

ZPE-corrected Energy: -269.187989

$\Delta U$ : -269.182331

$\Delta H$ : -269.181387

$\Delta G$ : -269.217370

Num. Imaginary Frequencies: 0

C	0.072202	0.002851	-0.520098
C	-1.012461	1.042949	-0.071011
C	-1.855957	-0.152045	0.294131
C	-0.955667	-1.042277	-0.116914
H	0.369904	0.035949	-1.566510
H	-1.381929	1.647553	-0.897553
H	-0.717613	1.699546	0.748743
H	-2.842507	-0.236567	0.728480
H	-0.919253	-2.122129	-0.150547
C	1.272863	0.011474	0.370282
O	2.415929	-0.032032	-0.006584
H	1.038076	0.054197	1.451715

3-CHO-Acetonitrile

SCF Energy: -269.284968628

ZPE-corrected Energy: -269.188193

$\Delta U$ : -269.182536

$\Delta H$ : -269.181591

$\Delta G$ : -269.217574

Num. Imaginary Frequencies: 0

C	0.072301	0.002313	-0.519956
C	-1.011941	1.043114	-0.070994
C	-1.856095	-0.151448	0.294001
C	-0.956180	-1.042220	-0.116850
H	0.369955	0.035390	-1.566385
H	-1.380828	1.647708	-0.897783
H	-0.716902	1.699621	0.748705
H	-2.842782	-0.235371	0.728137
H	-0.920266	-2.122090	-0.150469
C	1.272710	0.010810	0.370382
O	2.415981	-0.031676	-0.006688
H	1.038204	0.052736	1.451794



3-CHO-Dichloromethane  
SCF Energy: -269.284184456  
ZPE-corrected Energy: -269.187396  
 $\Delta U$ : -269.181739  
 $\Delta H$ : -269.180795  
 $\Delta G$ : -269.216777

Num. Imaginary Frequencies: 0

C	0.072006	0.002816	-0.520122
C	-1.012536	1.042948	-0.071190
C	-1.855899	-0.152077	0.294459
C	-0.955784	-1.042195	-0.117043
H	0.370117	0.035829	-1.566411
H	-1.382525	1.647514	-0.897564
H	-0.717466	1.699859	0.748313
H	-2.842318	-0.236779	0.729079
H	-0.919847	-2.122063	-0.150862
C	1.273419	0.011525	0.370249
O	2.415832	-0.032118	-0.006572
H	1.038152	0.054485	1.451895

### 3-CHO-DMSO

SCF Energy: -269.285034386  
ZPE-corrected Energy: -269.188260  
 $\Delta U$ : -269.182603  
 $\Delta H$ : -269.181658  
 $\Delta G$ : -269.217641

Num. Imaginary Frequencies: 0

C	0.072325	0.002305	-0.519946
C	-1.011922	1.043116	-0.070975
C	-1.856108	-0.151432	0.293958
C	-0.956180	-1.042228	-0.116832
H	0.369935	0.035387	-1.566389
H	-1.380736	1.647722	-0.897785
H	-0.716903	1.699580	0.748756
H	-2.842813	-0.235321	0.728058
H	-0.920222	-2.122096	-0.150423
C	1.272650	0.010794	0.370391
O	2.415992	-0.031662	-0.006696
H	1.038203	0.052686	1.451780

### 3-CHO-Gas

SCF Energy: -269.278904447  
ZPE-corrected Energy: -269.182058  
 $\Delta U$ : -269.176409  
 $\Delta H$ : -269.175465  
 $\Delta G$ : -269.211418

Num. Imaginary Frequencies: 0

C	0.070670	0.001761	-0.518252
C	-1.012905	1.042909	-0.072866
C	-1.856865	-0.151609	0.295143
C	-0.957620	-1.041397	-0.117457
H	0.373176	0.033419	-1.563314
H	-1.385222	1.648418	-0.897836
H	-0.716305	1.700420	0.746082
H	-2.842867	-0.236948	0.730625
H	-0.925862	-2.121476	-0.150540
C	1.279389	0.011900	0.371451
O	2.414943	-0.032917	-0.008532
H	1.041520	0.058125	1.455127

### 3-CHO-n-Hexane

SCF Energy: -269.281173974  
ZPE-corrected Energy: -269.184347  
 $\Delta U$ : -269.178694  
 $\Delta H$ : -269.177750  
 $\Delta G$ : -269.213719

Num. Imaginary Frequencies: 0

C	0.071147	0.002266	-0.519442
C	-1.012717	1.042950	-0.072142
C	-1.856207	-0.151854	0.295254
C	-0.956781	-1.041745	-0.117391
H	0.371571	0.034568	-1.565073
H	-1.384386	1.647917	-0.897658
H	-0.716583	1.700533	0.746752
H	-2.842256	-0.237012	0.730651
H	-0.923321	-2.121725	-0.151170
C	1.276661	0.011682	0.370642
O	2.415347	-0.032545	-0.007309
H	1.039585	0.056287	1.453435

3-CHO-Water

SCF Energy: -269.285119988

ZPE-corrected Energy: -269.188347

$\Delta U$ : -269.182690

$\Delta H$ : -269.181745

$\Delta G$ : -269.217728

Num. Imaginary Frequencies: 0

C	0.072356	0.002293	-0.519932
C	-1.011895	1.043120	-0.070951
C	-1.856125	-0.151408	0.293899
C	-0.956180	-1.042237	-0.116808
H	0.369910	0.035380	-1.566392
H	-1.380612	1.647741	-0.897787
H	-0.716901	1.699524	0.748823
H	-2.842855	-0.235251	0.727952
H	-0.920168	-2.122105	-0.150361
C	1.272573	0.010772	0.370403
O	2.416007	-0.031642	-0.006708
H	1.038204	0.052619	1.451762

3-COMe-Acetone

SCF Energy: -308.603992282

ZPE-corrected Energy: -308.479070

$\Delta U$ : -308.472010

$\Delta H$ : -308.471065

$\Delta G$ : -308.510375

Num. Imaginary Frequencies: 0

C	0.245279	-0.602132	-0.415362
C	1.194761	-0.702045	0.836434
C	2.051118	0.317137	0.126604
C	1.250970	0.405500	-0.933356
H	0.161839	-1.531177	-0.977234
H	1.632457	-1.690598	0.965258
H	0.749353	-0.383733	1.779624
H	2.984816	0.790260	0.398158
H	1.280030	0.976002	-1.851724
C	-1.141597	-0.115283	-0.076280
O	-2.098676	-0.851672	-0.173440
C	-1.282544	1.306534	0.395385
H	-0.477577	1.576936	1.078342
H	-1.198274	1.967025	-0.470342
H	-2.251163	1.450396	0.864886

3-COMe-Acetonitrile

SCF Energy: -308.604226359

ZPE-corrected Energy: -308.479313

$\Delta U$ : -308.472253

$\Delta H$ : -308.471308

$\Delta G$ : -308.510621

Num. Imaginary Frequencies: 0

C	0.245239	-0.601635	-0.415967
C	1.194617	-0.702782	0.835908
C	2.051167	0.316855	0.127006
C	1.251065	0.406399	-0.932910
H	0.161951	-1.530187	-0.978701
H	1.632059	-1.691547	0.963938
H	0.749220	-0.385020	1.779271
H	2.984863	0.789615	0.399182
H	1.279928	0.977904	-1.850647
C	-1.141442	-0.115094	-0.076381
O	-2.098559	-0.851833	-0.173534
C	-1.282677	1.306316	0.395787
H	-0.477708	1.576436	1.078854
H	-1.198404	1.967085	-0.469745
H	-2.251250	1.450019	0.865463

3-COMe-Dichloromethane

SCF Energy: -308.603319126

ZPE-corrected Energy: -308.478372

$\Delta U$ : -308.471313

$\Delta H$ : -308.470369

$\Delta G$ : -308.509672

Num. Imaginary Frequencies: 0

C	0.245455	-0.603497	-0.413552
C	1.195244	-0.699777	0.838021
C	2.051062	0.318033	0.125469
C	1.250867	0.402815	-0.934683
H	0.161588	-1.534039	-0.972817
H	1.633643	-1.687713	0.969264
H	0.749769	-0.379745	1.780644
H	2.984748	0.792236	0.395238
H	1.280527	0.970320	-1.854919
C	-1.142065	-0.115821	-0.075993
O	-2.098914	-0.851360	-0.173197
C	-1.282502	1.307133	0.394128
H	-0.477736	1.578441	1.076996
H	-1.198184	1.966894	-0.472137
H	-2.251408	1.451172	0.862966

3-COMe-DMSO

SCF Energy: -308.604302880

ZPE-corrected Energy: -308.479393

$\Delta U$ : -308.472332

$\Delta H$ : -308.471388

$\Delta G$ : -308.510702

Num. Imaginary Frequencies: 0

C	0.245221	-0.601511	-0.416140
C	1.194564	-0.702988	0.835767
C	2.051165	0.316774	0.127119
C	1.251085	0.406635	-0.932793
H	0.161968	-1.529927	-0.979109
H	1.631944	-1.691810	0.963561
H	0.749172	-0.385385	1.779179
H	2.984844	0.789456	0.399487
H	1.279884	0.978410	-1.850360
C	-1.141386	-0.115032	-0.076406
O	-2.098534	-0.851866	-0.173549
C	-1.282684	1.306261	0.395892
H	-0.477676	1.576316	1.078938
H	-1.198448	1.967090	-0.469602
H	-2.251213	1.449946	0.865668

3-COMe-Gas

SCF Energy: -308.597414192

ZPE-corrected Energy: -308.472322

$\Delta U$ : -308.465246

$\Delta H$ : -308.464302

$\Delta G$ : -308.503668

Num. Imaginary Frequencies: 0

C	0.247587	-0.611844	-0.400426
C	1.199553	-0.683044	0.849094
C	2.051883	0.324495	0.117414
C	1.251138	0.384456	-0.943514
H	0.159914	-1.552616	-0.941489
H	1.642948	-1.666387	0.998434
H	0.753827	-0.349356	1.787120
H	2.985125	0.806526	0.374761
H	1.284489	0.932117	-1.875765
C	-1.146013	-0.120110	-0.074350
O	-2.098772	-0.851352	-0.171746
C	-1.285894	1.311077	0.384946
H	-0.480431	1.593507	1.062749
H	-1.210193	1.966241	-0.485444
H	-2.255023	1.450603	0.854615

3-COMe-n-Hexane

SCF Energy: -308.599914622

ZPE-corrected Energy: -308.474877

$\Delta U$ : -308.467810

$\Delta H$ : -308.466866

$\Delta G$ : -308.506198

Num. Imaginary Frequencies: 0

C	0.246559	-0.608625	-0.405784
C	1.197637	-0.689966	0.844611
C	2.051407	0.321775	0.120659
C	1.250854	0.391845	-0.939998
H	0.160681	-1.545313	-0.954225
H	1.638700	-1.675281	0.986906
H	0.751842	-0.361656	1.784433
H	2.985098	0.800310	0.382816
H	1.282882	0.947500	-1.867491
C	-1.144328	-0.118358	-0.074955
O	-2.099147	-0.850968	-0.172379
C	-1.283865	1.309541	0.388788
H	-0.478606	1.586855	1.068809
H	-1.204029	1.966487	-0.479934
H	-2.252978	1.451567	0.857791

3-COMe-Water

SCF Energy: -308.604402599

ZPE-corrected Energy: -308.479497

$\Delta U$ : -308.472436

$\Delta H$ : -308.471491

$\Delta G$ : -308.510808

Num. Imaginary Frequencies: 0

C	0.245198	-0.601346	-0.416370
C	1.194498	-0.703265	0.835575
C	2.051164	0.316664	0.127264
C	1.251103	0.406957	-0.932634
H	0.161990	-1.529576	-0.979659
H	1.631795	-1.692163	0.963057
H	0.749117	-0.385871	1.779056
H	2.984824	0.789236	0.399879
H	1.279809	0.979103	-1.849968
C	-1.141312	-0.114954	-0.076440
O	-2.098502	-0.851909	-0.173570
C	-1.282688	1.306186	0.396038
H	-0.477642	1.576151	1.079069
H	-1.198491	1.967096	-0.469402
H	-2.251166	1.449845	0.865929

3-COOH-Acetone

SCF Energy: -344.552754453

ZPE-corrected Energy: -344.450038

$\Delta U$ : -344.443597

$\Delta H$ : -344.442652

$\Delta G$ : -344.481290

Num. Imaginary Frequencies: 0

C	0.230057	-0.535160	-0.440311
C	1.190092	-0.749606	0.786487
C	2.071525	0.283352	0.127973
C	1.251358	0.483820	-0.899509
H	0.118131	-1.414954	-1.069489
H	1.592268	-1.759113	0.852194
H	0.763424	-0.463845	1.747216
H	3.029920	0.697565	0.408365
H	1.273125	1.122402	-1.771358
C	-1.142409	-0.051987	-0.073329
O	-2.158928	-0.676548	-0.242141
O	-1.133426	1.158110	0.501892
H	-2.041778	1.382936	0.747199

3-COOH-Acetonitrile

SCF Energy: -344.553014571

ZPE-corrected Energy: -344.450312

$\Delta U$ : -344.443871

$\Delta H$ : -344.442927

$\Delta G$ : -344.481549

Num. Imaginary Frequencies: 0

C	0.230126	-0.533042	-0.442871
C	1.189568	-0.753286	0.783464
C	2.071435	0.282563	0.130083
C	1.251790	0.487806	-0.896937
H	0.118440	-1.410012	-1.076030
H	1.591615	-1.763112	0.844608
H	0.762535	-0.472058	1.745376
H	3.029843	0.695182	0.412798
H	1.274153	1.130149	-1.766008
C	-1.142261	-0.051516	-0.073718
O	-2.158471	-0.676968	-0.242394
O	-1.133853	1.157392	0.503440
H	-2.041940	1.381308	0.750767

3-COOH-Dichloromethane  
SCF Energy: -344.552002874  
ZPE-corrected Energy: -344.449247  
 $\Delta U$ : -344.442804  
 $\Delta H$ : -344.441860  
 $\Delta G$ : -344.480543

Num. Imaginary Frequencies: 0

C	0.229768	-0.542647	-0.431273
C	1.191673	-0.736269	0.797291
C	2.071846	0.285850	0.120526
C	1.249915	0.469279	-0.908579
H	0.116993	-1.432405	-1.046127
H	1.594086	-1.744469	0.879990
H	0.766092	-0.433859	1.753371
H	3.030195	0.705569	0.392699
H	1.269808	1.094502	-1.790072
C	-1.142899	-0.053559	-0.072063
O	-2.160647	-0.675069	-0.240848
O	-1.131642	1.160776	0.495855
H	-2.040682	1.389073	0.734682

3-COOH-DMSO  
SCF Energy: -344.553099561  
ZPE-corrected Energy: -344.450402  
 $\Delta U$ : -344.443961  
 $\Delta H$ : -344.443017  
 $\Delta G$ : -344.481632

Num. Imaginary Frequencies: 0

C	0.230175	-0.531928	-0.444140
C	1.189314	-0.755118	0.781940
C	2.071443	0.282121	0.131123
C	1.252035	0.489845	-0.895609
H	0.118624	-1.407466	-1.079301
H	1.591232	-1.765125	0.840833
H	0.762112	-0.476093	1.744424
H	3.029882	0.693887	0.414980
H	1.274682	1.134132	-1.763237
C	-1.142213	-0.051303	-0.073925
O	-2.158220	-0.677215	-0.242552
O	-1.134145	1.157042	0.504233
H	-2.042138	1.380350	0.752527



3-COOH-Gas

SCF Energy: -344.545273969

ZPE-corrected Energy: -344.442239

$\Delta U$ : -344.435793

$\Delta H$ : -344.434849

$\Delta G$ : -344.473678

Num. Imaginary Frequencies: 0

C	0.227768	-0.623765	-0.305545
C	1.209907	-0.555528	0.917466
C	2.071264	0.310709	0.031451
C	1.233085	0.273276	-0.998903
H	0.108257	-1.619079	-0.727070
H	1.623789	-1.522586	1.199684
H	0.795575	-0.063380	1.796247
H	3.027959	0.786476	0.195282
H	1.233717	0.707236	-1.988745
C	-1.146493	-0.070556	-0.053410
O	-2.171780	-0.676122	-0.196689
O	-1.119189	1.205677	0.377208
H	-2.034725	1.470086	0.534084

3-COOH-n-Hexane

SCF Energy: -344.548148502

ZPE-corrected Energy: -344.445227

$\Delta U$ : -344.438780

$\Delta H$ : -344.437836

$\Delta G$ : -344.476591

Num. Imaginary Frequencies: 0

C	0.228541	-0.585186	-0.373398
C	1.201606	-0.653482	0.858042
C	2.071485	0.300952	0.077159
C	1.240717	0.378606	-0.957468
H	0.111598	-1.529856	-0.899187
H	1.610050	-1.647089	1.036079
H	0.782266	-0.259308	1.782772
H	3.028772	0.751582	0.298682
H	1.250040	0.916326	-1.894980
C	-1.144894	-0.062447	-0.063174
O	-2.167622	-0.671906	-0.225492
O	-1.123741	1.180600	0.448344
H	-2.036548	1.428140	0.646849

3-COOH-Water

SCF Energy: -344.553210248

ZPE-corrected Energy: -344.450519

$\Delta U$ : -344.444078

$\Delta H$ : -344.443134

$\Delta G$ : -344.481738

Num. Imaginary Frequencies: 0

C	0.230249	-0.530198	-0.446124
C	1.188850	-0.757874	0.779647
C	2.071507	0.281317	0.132697
C	1.252463	0.492898	-0.893573
H	0.118867	-1.403585	-1.084265
H	1.590352	-1.768216	0.835362
H	0.761332	-0.481899	1.742878
H	3.029981	0.691779	0.418329
H	1.275546	1.140319	-1.758858
C	-1.142172	-0.050972	-0.074304
O	-2.157871	-0.677564	-0.242752
O	-1.134519	1.156527	0.505401
H	-2.042337	1.378877	0.755297

3-Me-Acetone

SCF Energy: -195.264889108

ZPE-corrected Energy: -195.149657

$\Delta U$ : -195.144530

$\Delta H$ : -195.143585

$\Delta G$ : -195.177298

Num. Imaginary Frequencies: 0

C	0.460058	-0.017936	-0.491265
C	-0.590876	1.052977	-0.049661
C	-1.483102	-0.122511	0.279879
C	-0.589628	-1.036587	-0.094703
H	0.656849	0.008868	-1.565064
H	-0.944852	1.713497	-0.841721
H	-0.272718	1.655803	0.802323
H	-2.489673	-0.181541	0.672990
H	-0.589831	-2.119351	-0.113319
C	1.763193	-0.035481	0.286189
H	2.347949	-0.926107	0.052420
H	2.370599	0.839374	0.050119
H	1.563802	-0.033318	1.359614

3-Me-Acetonitrile

SCF Energy: -195.264928435

ZPE-corrected Energy: -195.149707

$\Delta U$ : -195.144579

$\Delta H$ : -195.143635

$\Delta G$ : -195.177348

Num. Imaginary Frequencies: 0

C	0.460064	-0.017922	-0.491240
C	-0.590893	1.052982	-0.049666
C	-1.483145	-0.122522	0.279858
C	-0.589600	-1.036620	-0.094683
H	0.656883	0.008847	-1.565028
H	-0.944863	1.713515	-0.841717
H	-0.272778	1.655803	0.802336
H	-2.489752	-0.181537	0.672926
H	-0.589735	-2.119399	-0.113306
C	1.763216	-0.035467	0.286185
H	2.347862	-0.926181	0.052481
H	2.370641	0.839328	0.049951
H	1.563888	-0.033084	1.359634

3-Me-Dichloromethane

SCF Energy: -195.264777172

ZPE-corrected Energy: -195.149515

$\Delta U$ : -195.144389

$\Delta H$ : -195.143444

$\Delta G$ : -195.177156

Num. Imaginary Frequencies: 0

C	0.460041	-0.017972	-0.491340
C	-0.590827	1.052962	-0.049649
C	-1.482975	-0.122483	0.279946
C	-0.589705	-1.036493	-0.094761
H	0.656760	0.008928	-1.565165
H	-0.944827	1.713440	-0.841740
H	-0.272549	1.655819	0.802272
H	-2.489444	-0.181558	0.673181
H	-0.590103	-2.119214	-0.113368
C	1.763124	-0.035522	0.286205
H	2.348188	-0.925902	0.052261
H	2.370481	0.839500	0.050596
H	1.563554	-0.033968	1.359562

3-Me-DMSO

SCF Energy: -195.264941337

ZPE-corrected Energy: -195.149724

$\Delta U$ : -195.144596

$\Delta H$ : -195.143651

$\Delta G$ : -195.177365

Num. Imaginary Frequencies: 0

C	0.460066	-0.017918	-0.491231
C	-0.590899	1.052984	-0.049668
C	-1.483159	-0.122525	0.279851
C	-0.589591	-1.036631	-0.094677
H	0.656894	0.008840	-1.565017
H	-0.944867	1.713520	-0.841715
H	-0.272798	1.655803	0.802340
H	-2.489778	-0.181536	0.672905
H	-0.589703	-2.119415	-0.113302
C	1.763224	-0.035462	0.286184
H	2.347833	-0.926205	0.052501
H	2.370655	0.839313	0.049895
H	1.563915	-0.033007	1.359641

3-Me-Gas

SCF Energy: -195.263872477

ZPE-corrected Energy: -195.148381

$\Delta U$ : -195.143264

$\Delta H$ : -195.142320

$\Delta G$ : -195.176017

Num. Imaginary Frequencies: 0

C	0.459902	-0.018228	-0.491960
C	-0.590526	1.052817	-0.049647
C	-1.481893	-0.122317	0.280609
C	-0.590195	-1.035786	-0.095244
H	0.656365	0.009367	-1.565918
H	-0.944831	1.712828	-0.842013
H	-0.271319	1.656344	0.801469
H	-2.487534	-0.181835	0.674831
H	-0.592096	-2.118151	-0.114068
C	1.762471	-0.035810	0.286382
H	2.349683	-0.924493	0.051401
H	2.369637	0.840270	0.054188
H	1.561542	-0.038383	1.359267

3-Me-n-Hexane

SCF Energy: -195.264238452

ZPE-corrected Energy: -195.148838

$\Delta U$ : -195.143717

$\Delta H$ : -195.142772

$\Delta G$ : -195.176476

Num. Imaginary Frequencies: 0

C	0.459958	-0.018131	-0.491713
C	-0.590628	1.052881	-0.049638
C	-1.482332	-0.122371	0.280336
C	-0.590024	-1.036060	-0.095057
H	0.656471	0.009196	-1.565632
H	-0.944805	1.713081	-0.841901
H	-0.271778	1.656078	0.801843
H	-2.488305	-0.181695	0.674174
H	-0.591339	-2.118571	-0.113750
C	1.762745	-0.035703	0.286308
H	2.349150	-0.925024	0.051689
H	2.369958	0.839998	0.052795
H	1.562335	-0.036753	1.359368

3-Me-Water

SCF Energy: -195.264958182

ZPE-corrected Energy: -195.149745

$\Delta U$ : -195.144617

$\Delta H$ : -195.143673

$\Delta G$ : -195.177386

Num. Imaginary Frequencies: 0

C	0.460069	-0.017912	-0.491221
C	-0.590907	1.052986	-0.049670
C	-1.483178	-0.122530	0.279842
C	-0.589579	-1.036645	-0.094669
H	0.656910	0.008831	-1.565001
H	-0.944872	1.713527	-0.841714
H	-0.272823	1.655804	0.802344
H	-2.489811	-0.181534	0.672878
H	-0.589661	-2.119435	-0.113298
C	1.763234	-0.035456	0.286182
H	2.347795	-0.926237	0.052528
H	2.370673	0.839293	0.049823
H	1.563952	-0.032905	1.359649

3-NH2-Acetone

SCF Energy: -211.309741013

ZPE-corrected Energy: -211.205180

$\Delta U$ : -211.200119

$\Delta H$ : -211.199175

$\Delta G$ : -211.232810

Num. Imaginary Frequencies: 0

C	-0.484322	-0.016038	0.451392
C	0.570173	1.055163	0.033347
C	1.477498	-0.121515	-0.247248
C	0.567329	-1.037137	0.076940
H	-0.694459	0.011120	1.525950
H	0.889046	1.736080	0.822806
H	0.265122	1.627416	-0.842494
H	2.506593	-0.180245	-0.577009
H	0.560595	-2.119266	0.093765
N	-1.686335	-0.033109	-0.373292
H	-2.221640	-0.871726	-0.176714
H	-2.284979	0.745550	-0.119846

3-NH2-Acetonitrile

SCF Energy: -211.309954337

ZPE-corrected Energy: -211.205394

$\Delta U$ : -211.200334

$\Delta H$ : -211.199390

$\Delta G$ : -211.233024

Num. Imaginary Frequencies: 0

C	-0.484317	-0.016134	0.451381
C	0.570138	1.055170	0.033633
C	1.477451	-0.121450	-0.247528
C	0.567411	-1.037205	0.076941
H	-0.694982	0.010903	1.525768
H	0.889153	1.735622	0.823402
H	0.265127	1.628204	-0.841745
H	2.506564	-0.180045	-0.577313
H	0.560810	-2.119338	0.094206
N	-1.686312	-0.033235	-0.373604
H	-2.222286	-0.871059	-0.175230
H	-2.284300	0.746069	-0.120428

3-NH2-Dichloromethane  
SCF Energy: -211.309147714  
ZPE-corrected Energy: -211.204581  
 $\Delta U$ : -211.199518  
 $\Delta H$ : -211.198574  
 $\Delta G$ : -211.232212

Num. Imaginary Frequencies: 0

C	-0.484336	-0.015774	0.451483
C	0.570257	1.055151	0.032595
C	1.477584	-0.121686	-0.246570
C	0.567123	-1.036950	0.076984
H	-0.693062	0.011730	1.526493
H	0.888811	1.737329	0.821179
H	0.264990	1.625277	-0.844475
H	2.506608	-0.180778	-0.576333
H	0.560076	-2.119064	0.092729
N	-1.686364	-0.032762	-0.372466
H	-2.219730	-0.873637	-0.181025
H	-2.286910	0.744029	-0.118261

3-NH2-DMSO  
SCF Energy: -211.310024918  
ZPE-corrected Energy: -211.205465  
 $\Delta U$ : -211.200405  
 $\Delta H$ : -211.199461  
 $\Delta G$ : -211.233094

Num. Imaginary Frequencies: 0

C	-0.484315	-0.016166	0.451380
C	0.570127	1.055173	0.033730
C	1.477434	-0.121428	-0.247624
C	0.567439	-1.037227	0.076943
H	-0.695158	0.010832	1.525710
H	0.889191	1.735471	0.823600
H	0.265123	1.628467	-0.841493
H	2.506552	-0.179978	-0.577421
H	0.560884	-2.119362	0.094360
N	-1.686303	-0.033277	-0.373709
H	-2.222495	-0.870841	-0.174747
H	-2.284078	0.746237	-0.120621

3-NH2-Gas

SCF Energy: -211.304852182  
ZPE-corrected Energy: -211.200220  
 $\Delta U$ : -211.195129  
 $\Delta H$ : -211.194185  
 $\Delta G$ : -211.227893

Num. Imaginary Frequencies: 0

C	-0.484362	-0.013321	0.454742
C	0.570717	1.055340	0.028394
C	1.476107	-0.123194	-0.245543
C	0.565328	-1.035535	0.079688
H	-0.685912	0.017361	1.532015
H	0.890885	1.744049	0.810846
H	0.260046	1.613257	-0.854257
H	2.503478	-0.185502	-0.578731
H	0.556896	-2.117433	0.092920
N	-1.684260	-0.030091	-0.368074
H	-2.199564	-0.889816	-0.222364
H	-2.302752	0.728986	-0.107601

3-NH2-n-Hexane

SCF Energy: -211.306506441  
ZPE-corrected Energy: -211.201894  
 $\Delta U$ : -211.196821  
 $\Delta H$ : -211.195877  
 $\Delta G$ : -211.229537

Num. Imaginary Frequencies: 0

C	-0.484374	-0.014559	0.452961
C	0.570400	1.055205	0.029895
C	1.477104	-0.122345	-0.245219
C	0.566299	-1.036099	0.078047
H	-0.687953	0.014604	1.529604
H	0.888986	1.742000	0.814700
H	0.262513	1.617260	-0.851231
H	2.505398	-0.183093	-0.576287
H	0.558554	-2.118103	0.091132
N	-1.685576	-0.031295	-0.369468
H	-2.209184	-0.882866	-0.203577
H	-2.295859	0.736057	-0.112168



3-NH2-Water

SCF Energy: -211.310117537  
ZPE-corrected Energy: -211.205557  
 $\Delta U$ : -211.200498  
 $\Delta H$ : -211.199554  
 $\Delta G$ : -211.233186

Num. Imaginary Frequencies: 0

C	-0.484313	-0.016207	0.451381
C	0.570111	1.055177	0.033858
C	1.477410	-0.121398	-0.247754
C	0.567477	-1.037257	0.076948
H	-0.695390	0.010739	1.525634
H	0.889243	1.735271	0.823860
H	0.265115	1.628812	-0.841160
H	2.506534	-0.179889	-0.577566
H	0.560985	-2.119393	0.094568
N	-1.686291	-0.033332	-0.373848
H	-2.222765	-0.870558	-0.174119
H	-2.283789	0.746454	-0.120875

3-NO2-Acetone

SCF Energy: -360.478747578  
ZPE-corrected Energy: -360.387955  
 $\Delta U$ : -360.381821  
 $\Delta H$ : -360.380877  
 $\Delta G$ : -360.419286

Num. Imaginary Frequencies: 0

C	-0.204973	-0.289563	0.576636
C	-1.103799	-1.004304	-0.479935
C	-2.054512	0.144279	-0.231534
C	-1.247302	0.785594	0.610460
H	0.003079	-0.850903	1.481323
H	-1.434780	-1.998246	-0.187025
H	-0.664714	-1.038650	-1.476020
H	-3.049432	0.341578	-0.603870
H	-1.304535	1.704969	1.172878
N	1.134764	0.088187	0.014896
O	1.213956	1.089398	-0.658620
O	2.057363	-0.663410	0.240454

3-NO<sub>2</sub>-Acetonitrile

SCF Energy: -360.479034602  
ZPE-corrected Energy: -360.388246  
 $\Delta U$ : -360.382113  
 $\Delta H$ : -360.381169  
 $\Delta G$ : -360.419550

Num. Imaginary Frequencies: 0

C	-0.204866	-0.291149	0.576069
C	-1.104233	-1.002996	-0.482078
C	-2.054583	0.145161	-0.230484
C	-1.246984	0.784135	0.612968
H	0.003495	-0.854645	1.479301
H	-1.435391	-1.997442	-0.191179
H	-0.665635	-1.035233	-1.478434
H	-3.049736	0.343331	-0.601728
H	-1.304013	1.701690	1.178390
N	1.134645	0.087989	0.014743
O	1.212718	1.087981	-0.660886
O	2.058877	-0.661047	0.242336

3-NO<sub>2</sub>-Dichloromethane

SCF Energy: -360.477921697  
ZPE-corrected Energy: -360.387121  
 $\Delta U$ : -360.380981  
 $\Delta H$ : -360.380037  
 $\Delta G$ : -360.418557

Num. Imaginary Frequencies: 0

C	-0.205277	-0.285034	0.578208
C	-1.102593	-1.007965	-0.473822
C	-2.054316	0.141798	-0.234490
C	-1.248178	0.789757	0.603295
H	0.001837	-0.840229	1.487008
H	-1.433091	-2.000439	-0.175188
H	-0.662115	-1.048331	-1.469105
H	-3.048600	0.336585	-0.609861
H	-1.305955	1.714246	1.157158
N	1.135121	0.088718	0.015329
O	1.217553	1.093371	-0.652171
O	2.052980	-0.670146	0.235113

3-NO2-DMSO

SCF Energy: -360.479128435  
ZPE-corrected Energy: -360.388341  
 $\Delta U$ : -360.382209  
 $\Delta H$ : -360.381265  
 $\Delta G$ : -360.419638

Num. Imaginary Frequencies: 0

C	-0.204829	-0.291688	0.575871
C	-1.104383	-1.002549	-0.482804
C	-2.054609	0.145461	-0.230122
C	-1.246874	0.783639	0.613819
H	0.003636	-0.855917	1.478609
H	-1.435599	-1.997169	-0.192594
H	-0.665952	-1.034065	-1.479252
H	-3.049840	0.343930	-0.600995
H	-1.303828	1.700577	1.180254
N	1.134608	0.087921	0.014689
O	1.212299	1.087500	-0.661653
O	2.059388	-0.660247	0.242974

3-NO2-Gas

SCF Energy: -360.470528809  
ZPE-corrected Energy: -360.379592  
 $\Delta U$ : -360.373437  
 $\Delta H$ : -360.372493  
 $\Delta G$ : -360.411405

Num. Imaginary Frequencies: 0

C	-0.203592	-0.272012	0.581702
C	-1.097382	-1.019211	-0.454016
C	-2.053317	0.132877	-0.241418
C	-1.249627	0.800669	0.581800
H	0.000363	-0.809161	1.502599
H	-1.425587	-2.009105	-0.142713
H	-0.650862	-1.073746	-1.446194
H	-3.044229	0.323103	-0.628253
H	-1.306181	1.744372	1.102089
N	1.138569	0.091462	0.015102
O	1.223306	1.108836	-0.629306
O	2.036697	-0.692541	0.216599

3-NO2-n-Hexane

SCF Energy: -360.473704913

ZPE-corrected Energy: -360.382818

$\Delta U$ : -360.376673

$\Delta H$ : -360.375728

$\Delta G$ : -360.414386

Num. Imaginary Frequencies: 0

C	-0.205394	-0.270816	0.582575
C	-1.098456	-1.019237	-0.453825
C	-2.053562	0.133682	-0.243046
C	-1.250386	0.802452	0.580448
H	-0.001650	-0.806563	1.504156
H	-1.427217	-2.007504	-0.138694
H	-0.652848	-1.077503	-1.446122
H	-3.045405	0.321452	-0.628522
H	-1.308563	1.743980	1.104544
N	1.137036	0.090523	0.016155
O	1.227782	1.106697	-0.630550
O	2.037620	-0.692197	0.217380

3-NO2-Water

SCF Energy: -360.479250717

ZPE-corrected Energy: -360.388465

$\Delta U$ : -360.382333

$\Delta H$ : -360.381389

$\Delta G$ : -360.419755

Num. Imaginary Frequencies: 0

C	-0.204772	-0.292472	0.575591
C	-1.104684	-1.002017	-0.483676
C	-2.054593	0.145965	-0.229684
C	-1.246628	0.783025	0.614904
H	0.003874	-0.857633	1.477692
H	-1.436070	-1.996812	-0.194298
H	-0.666450	-1.032772	-1.480232
H	-3.049900	0.344940	-0.600072
H	-1.303424	1.699090	1.182771
N	1.134544	0.087761	0.014586
O	1.211736	1.086958	-0.662554
O	2.060042	-0.659226	0.243706

3-OMe-Acetone  
SCF Energy: -270.479673167  
ZPE-corrected Energy: -270.359247  
 $\Delta U$ : -270.353111  
 $\Delta H$ : -270.352167  
 $\Delta G$ : -270.388785

Num. Imaginary Frequencies: 0

C	0.021309	-0.226896	0.421579
C	0.767028	1.091900	0.027934
C	1.951777	0.182113	-0.212808
C	1.292359	-0.944272	0.052405
H	-0.230454	-0.269466	1.487962
H	0.872965	1.845400	0.808530
H	0.352208	1.549553	-0.870193
H	2.980041	0.393809	-0.474013
H	1.558007	-1.992436	0.058167
O	-1.097842	-0.574781	-0.349697
C	-2.226372	0.205746	-0.020825
H	-3.044534	-0.108045	-0.664165
H	-2.512106	0.058030	1.025308
H	-2.029999	1.269861	-0.183730

3-OMe-Acetonitrile  
SCF Energy: -270.479821755  
ZPE-corrected Energy: -270.359403  
 $\Delta U$ : -270.353265  
 $\Delta H$ : -270.352321  
 $\Delta G$ : -270.388943

Num. Imaginary Frequencies: 0

C	0.021394	-0.226902	0.421735
C	0.766974	1.091899	0.028089
C	1.951713	0.182183	-0.213127
C	1.292456	-0.944273	0.052467
H	-0.230640	-0.269574	1.487990
H	0.873200	1.845070	0.808921
H	0.351947	1.550060	-0.869688
H	2.979942	0.393988	-0.474406
H	1.558437	-1.992377	0.058763
O	-1.097771	-0.574826	-0.349866
C	-2.226518	0.205730	-0.020842
H	-3.044607	-0.107807	-0.664397
H	-2.512257	0.057604	1.025174
H	-2.029975	1.269824	-0.183362

3-OMe-Dichloromethane  
SCF Energy: -270.479254279  
ZPE-corrected Energy: -270.358810  
 $\Delta U$ : -270.352676  
 $\Delta H$ : -270.351732  
 $\Delta G$ : -270.388344

Num. Imaginary Frequencies: 0

C	0.021068	-0.226832	0.421194
C	0.767243	1.091917	0.027550
C	1.951941	0.181851	-0.212014
C	1.292045	-0.944289	0.052277
H	-0.230006	-0.269113	1.487914
H	0.872519	1.846261	0.807531
H	0.352962	1.548277	-0.871470
H	2.980286	0.393182	-0.473120
H	1.556729	-1.992626	0.056617
O	-1.098008	-0.574584	-0.349241
C	-2.225994	0.205753	-0.020812
H	-3.044260	-0.108682	-0.663713
H	-2.511846	0.059000	1.025586
H	-2.030134	1.269969	-0.184578

3-OMe-DMSO  
SCF Energy: -270.479870672  
ZPE-corrected Energy: -270.359454  
 $\Delta U$ : -270.353316  
 $\Delta H$ : -270.352372  
 $\Delta G$ : -270.388995

Num. Imaginary Frequencies: 0

C	0.021423	-0.226902	0.421791
C	0.766958	1.091900	0.028146
C	1.951688	0.182204	-0.213240
C	1.292487	-0.944274	0.052489
H	-0.230705	-0.269610	1.488003
H	0.873289	1.844956	0.809059
H	0.351856	1.550236	-0.869509
H	2.979903	0.394044	-0.474556
H	1.558577	-1.992358	0.058965
O	-1.097745	-0.574841	-0.349921
C	-2.226565	0.205724	-0.020852
H	-3.044626	-0.107726	-0.664487
H	-2.512315	0.057458	1.025122
H	-2.029966	1.269811	-0.183237

3-OMe-Gas

SCF Energy: -270.476006557

ZPE-corrected Energy: -270.355452

$\Delta U$ : -270.349322

$\Delta H$ : -270.348377

$\Delta G$ : -270.384993

Num. Imaginary Frequencies: 0

C	0.019251	-0.225136	0.420100
C	0.770306	1.092320	0.026023
C	1.952406	0.178312	-0.208870
C	1.288392	-0.944833	0.052286
H	-0.227979	-0.265128	1.488887
H	0.874671	1.850912	0.802597
H	0.358341	1.542707	-0.877065
H	2.980996	0.385354	-0.471706
H	1.545636	-1.994490	0.048259
O	-1.097940	-0.571195	-0.346423
C	-2.223830	0.204703	-0.021673
H	-3.039907	-0.112778	-0.666083
H	-2.514482	0.059914	1.024846
H	-2.032907	1.270873	-0.185555

3-OMe-n-Hexane

SCF Energy: -270.477299671

ZPE-corrected Energy: -270.356785

$\Delta U$ : -270.350655

$\Delta H$ : -270.349711

$\Delta G$ : -270.386318

Num. Imaginary Frequencies: 0

C	0.020001	-0.226069	0.420493
C	0.768677	1.092212	0.026639
C	1.952183	0.180023	-0.209845
C	1.290032	-0.944513	0.052182
H	-0.228626	-0.267095	1.488478
H	0.872914	1.849552	0.804155
H	0.355846	1.543882	-0.875393
H	2.980473	0.389111	-0.472495
H	1.549886	-1.993735	0.050693
O	-1.098066	-0.573024	-0.347230
C	-2.224299	0.205367	-0.021446
H	-3.041666	-0.111168	-0.664562
H	-2.512756	0.060987	1.025299
H	-2.031114	1.270541	-0.186475

3-OMe-Water

SCF Energy: -270.479934675

ZPE-corrected Energy: -270.359521

$\Delta U$ : -270.353383

$\Delta H$ : -270.352439

$\Delta G$ : -270.389063

Num. Imaginary Frequencies: 0

C	0.021461	-0.226904	0.421872
C	0.766935	1.091903	0.028228
C	1.951652	0.182232	-0.213400
C	1.292527	-0.944275	0.052521
H	-0.230796	-0.269659	1.488023
H	0.873416	1.844801	0.809251
H	0.351729	1.550476	-0.869260
H	2.979844	0.394116	-0.474777
H	1.558760	-1.992333	0.059235
O	-1.097708	-0.574860	-0.349990
C	-2.226625	0.205715	-0.020871
H	-3.044642	-0.107618	-0.664619
H	-2.512400	0.057265	1.025046
H	-2.029949	1.269795	-0.183076

E-CF3-Acetone

SCF Energy: -493.064459807

ZPE-corrected Energy: -492.973031

$\Delta U$ : -492.965211

$\Delta H$ : -492.964267

$\Delta G$ : -493.006246

Num. Imaginary Frequencies: 0

C	0.226193	-0.271448	0.218742
C	3.211745	-0.664742	-0.080730
C	2.574440	0.485795	0.106055
C	1.127340	0.663332	-0.055797
H	0.490443	-1.241456	0.620389
H	2.686656	-1.558652	-0.394460
H	4.281335	-0.740048	0.057034
H	3.136696	1.375166	0.366302
H	0.789330	1.631157	-0.408411
C	-1.233575	-0.066244	0.011744
F	-1.538523	1.147975	-0.457539
F	-1.740140	-0.959251	-0.857158
F	-1.923706	-0.227205	1.154593



E-CF3-Acetonitrile

SCF Energy: -493.064586911

ZPE-corrected Energy: -492.973167

$\Delta U$ : -492.965347

$\Delta H$ : -492.964403

$\Delta G$ : -493.006381

Num. Imaginary Frequencies: 0

C	0.226326	-0.271863	0.218062
C	3.211751	-0.664848	-0.080481
C	2.574538	0.485889	0.105669
C	1.127344	0.663382	-0.055530
H	0.490568	-1.242505	0.618190
H	2.686559	-1.559155	-0.392935
H	4.281438	-0.739920	0.056718
H	3.136873	1.375515	0.364815
H	0.789280	1.631666	-0.406805
C	-1.233381	-0.066271	0.011726
F	-1.538659	1.148695	-0.455540
F	-1.740490	-0.957814	-0.858523
F	-1.923539	-0.229030	1.154434

E-CF3-Dichloromethane

SCF Energy: -493.064093525

ZPE-corrected Energy: -492.972636

$\Delta U$ : -492.964817

$\Delta H$ : -492.963873

$\Delta G$ : -493.005850

Num. Imaginary Frequencies: 0

C	0.225809	-0.270290	0.220663
C	3.211736	-0.664429	-0.081429
C	2.574156	0.485531	0.107142
C	1.127317	0.663174	-0.056549
H	0.490079	-1.238501	0.626593
H	2.686940	-1.557213	-0.398758
H	4.281050	-0.740393	0.057930
H	3.136176	1.374181	0.370499
H	0.789442	1.629687	-0.412938
C	-1.234141	-0.066175	0.011795
F	-1.538105	1.145907	-0.463239
F	-1.739162	-0.963329	-0.853249
F	-1.924172	-0.221981	1.155037

E-CF3-DMSO

SCF Energy: -493.064628436

ZPE-corrected Energy: -492.973211

$\Delta U$ : -492.965391

$\Delta H$ : -492.964447

$\Delta G$ : -493.006426

Num. Imaginary Frequencies: 0

C	0.226369	-0.272000	0.217839
C	3.211754	-0.664882	-0.080400
C	2.574570	0.485920	0.105542
C	1.127345	0.663398	-0.055442
H	0.490608	-1.242849	0.617469
H	2.686528	-1.559319	-0.392435
H	4.281472	-0.739878	0.056615
H	3.136930	1.375630	0.364327
H	0.789262	1.631832	-0.406278
C	-1.233318	-0.066280	0.011720
F	-1.538702	1.148929	-0.454887
F	-1.740605	-0.957344	-0.858967
F	-1.923484	-0.229624	1.154382

E-CF3-Gas

SCF Energy: -493.060800582

ZPE-corrected Energy: -492.969058

$\Delta U$ : -492.961264

$\Delta H$ : -492.960320

$\Delta G$ : -493.002215

Num. Imaginary Frequencies: 0

C	0.222629	-0.263301	0.231545
C	3.212326	-0.661790	-0.085975
C	2.571720	0.483629	0.113638
C	1.126237	0.662224	-0.060953
H	0.488378	-1.220013	0.662629
H	2.690548	-1.547660	-0.426088
H	4.279609	-0.741443	0.065200
H	3.132421	1.367113	0.397695
H	0.788411	1.620561	-0.438629
C	-1.239806	-0.066218	0.012056
F	-1.535133	1.134276	-0.495409
F	-1.732014	-0.986232	-0.830854
F	-1.925965	-0.193137	1.157076

E-CF3-n-Hexane

SCF Energy: -493.062216920

ZPE-corrected Energy: -492.970595

$\Delta U$ : -492.962793

$\Delta H$ : -492.961848

$\Delta G$ : -493.003774

Num. Imaginary Frequencies: 0

C	0.224028	-0.265261	0.229089
C	3.211771	-0.662892	-0.084307
C	2.572716	0.484366	0.111771
C	1.126889	0.662398	-0.060017
H	0.488560	-1.225284	0.653790
H	2.688495	-1.550659	-0.417403
H	4.279822	-0.741643	0.062308
H	3.133683	1.369708	0.388926
H	0.789211	1.622714	-0.433087
C	-1.237270	-0.066254	0.012108
F	-1.535770	1.136725	-0.487750
F	-1.734601	-0.980715	-0.836340
F	-1.926138	-0.199229	1.156713

E-CF3-Water

SCF Energy: -493.064682530

ZPE-corrected Energy: -492.973269

$\Delta U$ : -492.965449

$\Delta H$ : -492.964505

$\Delta G$ : -493.006483

Num. Imaginary Frequencies: 0

C	0.226425	-0.272179	0.217549
C	3.211757	-0.664927	-0.080294
C	2.574611	0.485961	0.105376
C	1.127345	0.663418	-0.055327
H	0.490660	-1.243299	0.616529
H	2.686488	-1.559532	-0.391781
H	4.281517	-0.739822	0.056480
H	3.137003	1.375780	0.363690
H	0.789238	1.632046	-0.405590
C	-1.233236	-0.066292	0.011712
F	-1.538757	1.149234	-0.454039
F	-1.740756	-0.956733	-0.859545
F	-1.923412	-0.230397	1.154314

E-Me-Acetone

SCF Energy: -195.280667552

ZPE-corrected Energy: -195.166808

$\Delta U$ : -195.160696

$\Delta H$ : -195.159752

$\Delta G$ : -195.195746

Num. Imaginary Frequencies: 0

C	0.885256	-0.295821	-0.156140
C	-2.147697	-0.605713	0.101548
C	-1.460268	0.516074	-0.093803
C	-0.009121	0.661854	0.080208
H	0.535407	-1.253461	-0.532291
H	-1.664226	-1.511622	0.446992
H	-3.214678	-0.647064	-0.069650
H	-1.996379	1.411846	-0.391652
H	0.343025	1.637291	0.404141
C	2.358693	-0.152760	0.044331
H	2.722665	-0.885419	0.767624
H	2.898877	-0.336252	-0.886339
H	2.614134	0.842881	0.404313

E-Me-Acetonitrile

SCF Energy: -195.280753734

ZPE-corrected Energy: -195.166900

$\Delta U$ : -195.160788

$\Delta H$ : -195.159844

$\Delta G$ : -195.195839

Num. Imaginary Frequencies: 0

C	0.885255	-0.296026	-0.155593
C	-2.147734	-0.605819	0.101219
C	-1.460342	0.516182	-0.093453
C	-0.009067	0.662000	0.079879
H	0.535402	-1.254240	-0.530306
H	-1.664190	-1.512207	0.445349
H	-3.214824	-0.646874	-0.069437
H	-1.996618	1.412225	-0.390191
H	0.343188	1.637820	0.402526
C	2.358756	-0.152688	0.044192
H	2.722918	-0.884545	0.768199
H	2.898568	-0.337472	-0.886434
H	2.614352	0.843400	0.402828

E-Me-Dichloromethane  
SCF Energy: -195.280424284  
ZPE-corrected Energy: -195.166546  
 $\Delta U$ : -195.160435  
 $\Delta H$ : -195.159491  
 $\Delta G$ : -195.195482

Num. Imaginary Frequencies: 0

C	0.885250	-0.295262	-0.157635
C	-2.147577	-0.605428	0.102445
C	-1.460066	0.515782	-0.094754
C	-0.009271	0.661454	0.081098
H	0.535407	-1.251318	-0.537716
H	-1.664289	-1.510006	0.451469
H	-3.214259	-0.647607	-0.070216
H	-1.995732	1.410803	-0.395630
H	0.342582	1.635830	0.408560
C	2.358511	-0.152956	0.044710
H	2.721984	-0.887824	0.766018
H	2.899715	-0.332865	-0.886073
H	2.613516	0.841445	0.408406

E-Me-DMSO  
SCF Energy: -195.280782088  
ZPE-corrected Energy: -195.166930  
 $\Delta U$ : -195.160818  
 $\Delta H$ : -195.159874  
 $\Delta G$ : -195.195869

Num. Imaginary Frequencies: 0

C	0.885254	-0.296095	-0.155411
C	-2.147745	-0.605854	0.101109
C	-1.460367	0.516218	-0.093337
C	-0.009049	0.662049	0.079770
H	0.535400	-1.254498	-0.529647
H	-1.664176	-1.512401	0.444803
H	-3.214871	-0.646812	-0.069366
H	-1.996698	1.412351	-0.389705
H	0.343242	1.637995	0.401990
C	2.358776	-0.152664	0.044147
H	2.723003	-0.884256	0.768388
H	2.898465	-0.337875	-0.886466
H	2.614423	0.843571	0.402337

E-Me-Gas

SCF Energy: -195.278556226

ZPE-corrected Energy: -195.164518

$\Delta U$ : -195.158417

$\Delta H$ : -195.157473

$\Delta G$ : -195.193432

Num. Imaginary Frequencies: 0

C	0.885000	-0.291653	-0.167206
C	-2.146308	-0.603636	0.108116
C	-1.458809	0.513943	-0.100652
C	-0.010337	0.658827	0.086488
H	0.535132	-1.237114	-0.572272
H	-1.663842	-1.499383	0.479263
H	-3.211006	-0.651493	-0.073276
H	-1.991753	1.403893	-0.420417
H	0.339769	1.625928	0.436727
C	2.357055	-0.154172	0.047188
H	2.717886	-0.903147	0.755246
H	2.905179	-0.310423	-0.883873
H	2.609026	0.831883	0.435004

E-Me-n-Hexane

SCF Energy: -195.279292080

ZPE-corrected Energy: -195.165314

$\Delta U$ : -195.159211

$\Delta H$ : -195.158267

$\Delta G$ : -195.194234

Num. Imaginary Frequencies: 0

C	0.884882	-0.292932	-0.163631
C	-2.146408	-0.604474	0.106056
C	-1.459241	0.514736	-0.098319
C	-0.010022	0.660038	0.084553
H	0.534725	-1.242316	-0.559413
H	-1.663184	-1.503326	0.469031
H	-3.211746	-0.650783	-0.072655
H	-1.993395	1.406322	-0.411590
H	0.340865	1.629965	0.426011
C	2.357454	-0.153825	0.046195
H	2.719218	-0.897735	0.759085
H	2.902895	-0.318664	-0.884916
H	2.610636	0.835277	0.425318

E-Me-Water

SCF Energy: -195.280819172

ZPE-corrected Energy: -195.166970

$\Delta U$ : -195.160858

$\Delta H$ : -195.159914

$\Delta G$ : -195.195908

Num. Imaginary Frequencies: 0

C	0.885253	-0.296184	-0.155172
C	-2.147760	-0.605900	0.100966
C	-1.460399	0.516265	-0.093184
C	-0.009026	0.662112	0.079626
H	0.535397	-1.254836	-0.528782
H	-1.664157	-1.512655	0.444085
H	-3.214933	-0.646731	-0.069272
H	-1.996804	1.412516	-0.389066
H	0.343313	1.638224	0.401286
C	2.358803	-0.152633	0.044086
H	2.723114	-0.883877	0.768634
H	2.898330	-0.338401	-0.886508
H	2.614516	0.843795	0.401694

E-NH2-Acetone

SCF Energy: -211.335115740

ZPE-corrected Energy: -211.232114

$\Delta U$ : -211.226113

$\Delta H$ : -211.225169

$\Delta G$ : -211.260818

Num. Imaginary Frequencies: 0

C	0.915485	-0.287579	-0.110417
C	-2.109081	-0.618764	0.092679
C	-1.424010	0.513694	-0.075970
C	0.018760	0.696238	0.058036
H	0.581852	-1.279705	-0.394189
H	-1.627312	-1.538884	0.401265
H	-3.176970	-0.653071	-0.072562
H	-1.982278	1.408636	-0.335421
H	0.376242	1.697527	0.273805
N	2.281713	-0.156922	-0.034738
H	2.639434	0.641076	0.465925
H	2.810112	-0.998660	0.118375

E-NH2-Acetonitrile

SCF Energy: -211.335363298

ZPE-corrected Energy: -211.232371

$\Delta U$ : -211.226368

$\Delta H$ : -211.225424

$\Delta G$ : -211.261082

Num. Imaginary Frequencies: 0

C	0.915646	-0.287967	-0.109168
C	-2.109337	-0.618883	0.091680
C	-1.424010	0.513857	-0.075030
C	0.018891	0.696443	0.057260
H	0.582013	-1.281067	-0.389568
H	-1.627644	-1.540250	0.396692
H	-3.177538	-0.652069	-0.071841
H	-1.982577	1.409546	-0.331279
H	0.376608	1.698190	0.270439
N	2.281613	-0.157046	-0.034940
H	2.640194	0.642598	0.462520
H	2.810509	-0.998323	0.119159

E-NH2-Dichloromethane

SCF Energy: -211.334413990

ZPE-corrected Energy: -211.231392

$\Delta U$ : -211.225394

$\Delta H$ : -211.224450

$\Delta G$ : -211.260085

Num. Imaginary Frequencies: 0

C	0.915032	-0.286475	-0.113870
C	-2.108351	-0.618438	0.095429
C	-1.424008	0.513232	-0.078580
C	0.018390	0.695678	0.060175
H	0.581395	-1.275843	-0.406946
H	-1.626372	-1.535032	0.413886
H	-3.175366	-0.655889	-0.074486
H	-1.981437	1.406058	-0.346847
H	0.375188	1.695662	0.283179
N	2.281986	-0.156593	-0.034168
H	2.637323	0.636809	0.475272
H	2.808997	-0.999604	0.116194



E-NH2-DMSO

SCF Energy: -211.335444626  
ZPE-corrected Energy: -211.232456  
 $\Delta U$ : -211.226452  
 $\Delta H$ : -211.225508  
 $\Delta G$ : -211.261169

Num. Imaginary Frequencies: 0

C	0.915699	-0.288094	-0.108754
C	-2.109421	-0.618923	0.091348
C	-1.424010	0.513910	-0.074718
C	0.018934	0.696511	0.057003
H	0.582066	-1.281515	-0.388034
H	-1.627753	-1.540700	0.395174
H	-3.177724	-0.651739	-0.071600
H	-1.982676	1.409845	-0.329905
H	0.376727	1.698408	0.269325
N	2.281580	-0.157087	-0.035007
H	2.640446	0.643101	0.461387
H	2.810639	-0.998212	0.119419

E-NH2-Gas

SCF Energy: -211.328864118  
ZPE-corrected Energy: -211.225678  
 $\Delta U$ : -211.219694  
 $\Delta H$ : -211.218750  
 $\Delta G$ : -211.254318

Num. Imaginary Frequencies: 0

C	0.912112	-0.279276	-0.136011
C	-2.103921	-0.615721	0.112484
C	-1.423949	0.509894	-0.095460
C	0.016007	0.691114	0.073488
H	0.579338	-1.249183	-0.488031
H	-1.621524	-1.507929	0.492597
H	-3.165178	-0.673162	-0.083919
H	-1.974725	1.388305	-0.418328
H	0.367920	1.680807	0.346261
N	2.284182	-0.154282	-0.030573
H	2.621615	0.609616	0.531981
H	2.801782	-1.004546	0.106442

E-NH2-n-Hexane

SCF Energy: -211.331088164

ZPE-corrected Energy: -211.227985

$\Delta U$ : -211.221990

$\Delta H$ : -211.221046

$\Delta G$ : -211.256650

Num. Imaginary Frequencies: 0

C	0.913117	-0.281600	-0.128314
C	-2.105230	-0.616939	0.106713
C	-1.423944	0.511091	-0.089514
C	0.016805	0.693193	0.068847
H	0.579641	-1.258598	-0.459851
H	-1.622774	-1.517869	0.465952
H	-3.168463	-0.667733	-0.081408
H	-1.977502	1.394454	-0.394034
H	0.370359	1.686978	0.323367
N	2.283092	-0.155284	-0.031481
H	2.628037	0.618532	0.513133
H	2.804565	-1.003254	0.106817

E-NH2-Water

SCF Energy: -211.335550902

ZPE-corrected Energy: -211.232567

$\Delta U$ : -211.226562

$\Delta H$ : -211.225618

$\Delta G$ : -211.261283

Num. Imaginary Frequencies: 0

C	0.915769	-0.288260	-0.108209
C	-2.109531	-0.618975	0.090911
C	-1.424010	0.513979	-0.074308
C	0.018990	0.696600	0.056666
H	0.582134	-1.282102	-0.386016
H	-1.627895	-1.541289	0.393177
H	-3.177969	-0.651306	-0.071281
H	-1.982805	1.410237	-0.328097
H	0.376883	1.698695	0.267863
N	2.281536	-0.157143	-0.035094
H	2.640777	0.643761	0.459893
H	2.810811	-0.998066	0.119762

E-NO2-Acetone

SCF Energy: -360.490248538

ZPE-corrected Energy: -360.400768

$\Delta U$ : -360.393922

$\Delta H$ : -360.392978

$\Delta G$ : -360.432257

Num. Imaginary Frequencies: 0

C	0.105446	-0.338474	-0.145828
C	-2.861073	-0.628686	0.217322
C	-2.218628	0.468348	-0.172244
C	-0.773638	0.652474	-0.062982
H	-0.098120	-1.379033	-0.335658
H	-3.934235	-0.709639	0.117111
H	-2.339998	-1.463770	0.668437
H	-2.775159	1.310582	-0.564570
H	-0.394730	1.657716	0.075843
N	1.524275	-0.073958	0.005581
O	1.908318	1.059097	0.208048
O	2.261640	-1.036613	-0.085277

E-NO2-Acetonitrile

SCF Energy: -360.490530970

ZPE-corrected Energy: -360.401057

$\Delta U$ : -360.394211

$\Delta H$ : -360.393267

$\Delta G$ : -360.432546

Num. Imaginary Frequencies: 0

C	0.105402	-0.338670	-0.145253
C	-2.860982	-0.628981	0.216466
C	-2.218651	0.468729	-0.171553
C	-0.773641	0.652499	-0.062872
H	-0.098174	-1.379397	-0.334099
H	-3.934244	-0.709445	0.116894
H	-2.339808	-1.465086	0.665562
H	-2.775225	1.311827	-0.561889
H	-0.394780	1.657849	0.075132
N	1.523944	-0.074007	0.005554
O	1.908473	1.059126	0.207425
O	2.261759	-1.036521	-0.085076

E-NO<sub>2</sub>-Dichloromethane  
SCF Energy: -360.489432989  
ZPE-corrected Energy: -360.399936  
 $\Delta U$ : -360.393088  
 $\Delta H$ : -360.392144  
 $\Delta G$ : -360.431429

Num. Imaginary Frequencies: 0

C	0.105589	-0.337874	-0.147965
C	-2.861270	-0.627885	0.219777
C	-2.218544	0.467279	-0.174044
C	-0.773600	0.652393	-0.063241
H	-0.097851	-1.377892	-0.340991
H	-3.934131	-0.710278	0.117689
H	-2.340462	-1.460061	0.676569
H	-2.774959	1.307128	-0.571788
H	-0.394549	1.657234	0.078473
N	1.525208	-0.073806	0.005599
O	1.907802	1.059064	0.209669
O	2.261253	-1.036935	-0.085458

E-NO<sub>2</sub>-DMSO

SCF Energy: -360.490623161  
ZPE-corrected Energy: -360.401151  
 $\Delta U$ : -360.394306  
 $\Delta H$ : -360.393362  
 $\Delta G$ : -360.432641

Num. Imaginary Frequencies: 0

C	0.105386	-0.338723	-0.145146
C	-2.860931	-0.629054	0.216313
C	-2.218658	0.468816	-0.171407
C	-0.773645	0.652514	-0.062882
H	-0.098180	-1.379488	-0.333782
H	-3.934210	-0.709450	0.116866
H	-2.339700	-1.465374	0.664940
H	-2.775237	1.312102	-0.561305
H	-0.394826	1.657898	0.074918
N	1.523833	-0.074022	0.005550
O	1.908504	1.059126	0.207323
O	2.261797	-1.036481	-0.085041

E-NO2-Gas

SCF Energy: -360.482107207  
ZPE-corrected Energy: -360.392477  
 $\Delta U$ : -360.385633  
 $\Delta H$ : -360.384689  
 $\Delta G$ : -360.423978

Num. Imaginary Frequencies: 0

C	0.108017	-0.335531	-0.162810
C	-2.866189	-0.619931	0.236664
C	-2.217466	0.459108	-0.186803
C	-0.772532	0.649053	-0.064682
H	-0.092516	-1.372214	-0.377612
H	-3.936912	-0.710028	0.120498
H	-2.350155	-1.431593	0.733904
H	-2.770983	1.281564	-0.624465
H	-0.389728	1.649899	0.097645
N	1.533660	-0.072352	0.005835
O	1.902105	1.060347	0.220082
O	2.259608	-1.038768	-0.085711

E-NO2-n-Hexane

SCF Energy: -360.485244174  
ZPE-corrected Energy: -360.395658  
 $\Delta U$ : -360.388812  
 $\Delta H$ : -360.387868  
 $\Delta G$ : -360.427161

Num. Imaginary Frequencies: 0

C	0.106744	-0.335938	-0.157767
C	-2.863708	-0.623398	0.230417
C	-2.218088	0.462298	-0.182014
C	-0.773191	0.650847	-0.063942
H	-0.095063	-1.373631	-0.365465
H	-3.935302	-0.710932	0.120162
H	-2.345273	-1.442692	0.712489
H	-2.773060	1.291465	-0.604343
H	-0.392415	1.653313	0.091519
N	1.530121	-0.072949	0.005645
O	1.904949	1.059489	0.216173
O	2.260016	-1.038207	-0.085428

E-NO2-Water

SCF Energy: -360.490743104

ZPE-corrected Energy: -360.401276

$\Delta U$ : -360.394429

$\Delta H$ : -360.393485

$\Delta G$ : -360.432770

Num. Imaginary Frequencies: 0

C	0.105225	-0.338675	-0.144671
C	-2.860664	-0.629352	0.215806
C	-2.218776	0.469035	-0.171076
C	-0.773574	0.652822	-0.062737
H	-0.098532	-1.379466	-0.332856
H	-3.933998	-0.709770	0.117174
H	-2.338855	-1.466087	0.662940
H	-2.775497	1.312638	-0.560007
H	-0.394763	1.658198	0.074798
N	1.523681	-0.074068	0.005489
O	1.908677	1.059074	0.206930
O	2.261649	-1.036576	-0.084980

E-OMe-Acetone

SCF Energy: -270.496424532

ZPE-corrected Energy: -270.377465

$\Delta U$ : -270.370235

$\Delta H$ : -270.369291

$\Delta G$ : -270.408838

Num. Imaginary Frequencies: 0

C	-0.374636	-0.007178	0.023023
C	2.536925	0.827388	-0.120985
C	2.049490	-0.374213	0.182571
C	0.676370	-0.823414	-0.048186
H	-0.273218	1.037820	0.305477
H	1.936682	1.571515	-0.630391
H	3.554842	1.095754	0.126078
H	2.712614	-1.101652	0.640399
H	0.504474	-1.872636	-0.257989
O	-1.629041	-0.421323	-0.253931
C	-2.657520	0.471788	0.149002
H	-3.595820	0.048670	-0.195889
H	-2.678607	0.570890	1.235189
H	-2.512412	1.454001	-0.303974

E-OMe-Acetonitrile  
SCF Energy: -270.496597117  
ZPE-corrected Energy: -270.377638  
 $\Delta U$ : -270.370409  
 $\Delta H$ : -270.369465  
 $\Delta G$ : -270.408998

Num. Imaginary Frequencies: 0

C	-0.374651	-0.007559	0.023413
C	2.536563	0.828117	-0.120505
C	2.049861	-0.374260	0.181418
C	0.676553	-0.823650	-0.048142
H	-0.273479	1.037678	0.304960
H	1.935370	1.573325	-0.627236
H	3.554799	1.096152	0.125641
H	2.713847	-1.102384	0.636900
H	0.504863	-1.873078	-0.257207
O	-1.629118	-0.422426	-0.251996
C	-2.657627	0.472526	0.147770
H	-3.595994	0.048066	-0.195235
H	-2.678277	0.575771	1.233528
H	-2.512380	1.452830	-0.309113

E-OMe-Dichloromethane  
SCF Energy: -270.495936308  
ZPE-corrected Energy: -270.376971  
 $\Delta U$ : -270.369740  
 $\Delta H$ : -270.368796  
 $\Delta G$ : -270.408363

Num. Imaginary Frequencies: 0

C	-0.374559	-0.005905	0.021658
C	2.538003	0.825186	-0.122328
C	2.048398	-0.374134	0.185967
C	0.675787	-0.822714	-0.048200
H	-0.272363	1.038481	0.306426
H	1.940519	1.566185	-0.639389
H	3.555008	1.094491	0.127345
H	2.708978	-1.099583	0.650581
H	0.503207	-1.871393	-0.259849
O	-1.628775	-0.417887	-0.259896
C	-2.657240	0.469449	0.152842
H	-3.595265	0.050721	-0.198249
H	-2.679906	0.555311	1.240267
H	-2.512309	1.457587	-0.287596

E-OMe-DMSO

SCF Energy: -270.496653861

ZPE-corrected Energy: -270.377695

$\Delta U$ : -270.370467

$\Delta H$ : -270.369522

$\Delta G$ : -270.409051

Num. Imaginary Frequencies: 0

C	-0.374655	-0.007675	0.023529
C	2.536448	0.828350	-0.120347
C	2.049981	-0.374277	0.181048
C	0.676610	-0.823725	-0.048122
H	-0.273561	1.037644	0.304767
H	1.934949	1.573908	-0.626209
H	3.554788	1.096275	0.125501
H	2.714243	-1.102625	0.635769
H	0.504984	-1.873222	-0.256932
O	-1.629141	-0.422772	-0.251386
C	-2.657663	0.472756	0.147384
H	-3.596048	0.047886	-0.195051
H	-2.678192	0.577280	1.233005
H	-2.512358	1.452464	-0.310704

E-OMe-Gas

SCF Energy: -270.492079346

ZPE-corrected Energy: -270.372899

$\Delta U$ : -270.365734

$\Delta H$ : -270.364790

$\Delta G$ : -270.404076

Num. Imaginary Frequencies: 0

C	-0.373336	0.003127	0.013100
C	2.543163	0.811237	-0.129385
C	2.041373	-0.374388	0.205486
C	0.671559	-0.818438	-0.048311
H	-0.264908	1.044094	0.310052
H	1.961465	1.532514	-0.689845
H	3.554389	1.087052	0.135042
H	2.686335	-1.087528	0.709220
H	0.492843	-1.863560	-0.270480
O	-1.626906	-0.394639	-0.295975
C	-2.653845	0.453184	0.176101
H	-3.590652	0.063407	-0.211287
H	-2.686288	0.457753	1.267852
H	-2.511420	1.475051	-0.184697



E-OMe-n-Hexane  
SCF Energy: -270.493629668  
ZPE-corrected Energy: -270.374528  
 $\Delta U$ : -270.367345  
 $\Delta H$ : -270.366401  
 $\Delta G$ : -270.405758

Num. Imaginary Frequencies: 0

C	-0.373878	0.000217	0.015322
C	2.541961	0.815757	-0.127157
C	2.043714	-0.374224	0.199487
C	0.672991	-0.819802	-0.048045
H	-0.267764	1.042458	0.307897
H	1.955404	1.543721	-0.673973
H	3.555213	1.089053	0.132593
H	2.693711	-1.091546	0.690788
H	0.496676	-1.866329	-0.266073
O	-1.627508	-0.402347	-0.284949
C	-2.655484	0.458627	0.169138
H	-3.592416	0.060066	-0.208247
H	-2.685302	0.487225	1.260098
H	-2.511282	1.470681	-0.215959

E-OMe-Water  
SCF Energy: -270.496728047  
ZPE-corrected Energy: -270.377768  
 $\Delta U$ : -270.370541  
 $\Delta H$ : -270.369597  
 $\Delta G$ : -270.409119

Num. Imaginary Frequencies: 0

C	-0.374658	-0.007818	0.023671
C	2.536300	0.828648	-0.120142
C	2.050135	-0.374302	0.180569
C	0.676682	-0.823823	-0.048093
H	-0.273666	1.037609	0.304499
H	1.934403	1.574660	-0.624873
H	3.554775	1.096431	0.125320
H	2.714753	-1.102938	0.634305
H	0.505137	-1.873411	-0.256562
O	-1.629168	-0.423213	-0.250607
C	-2.657712	0.473047	0.146892
H	-3.596116	0.047664	-0.194833
H	-2.678096	0.579185	1.232337
H	-2.512320	1.451999	-0.312714

E-trans-CHO-Acetone  
SCF Energy: -269.304395699  
ZPE-corrected Energy: -269.208484  
 $\Delta U$ : -269.202043  
 $\Delta H$ : -269.201099  
 $\Delta G$ : -269.238717

Num. Imaginary Frequencies: 0

C	-0.455268	-0.160584	0.116476
C	2.514278	-0.744384	-0.104240
C	1.962195	0.448490	0.100220
C	0.533317	0.727934	-0.034700
H	-0.276046	-1.193785	0.389160
H	3.579089	-0.893106	0.008413
H	1.923887	-1.599645	-0.408633
H	2.593105	1.292396	0.353154
H	0.262342	1.754840	-0.264241
C	-1.842234	0.256542	-0.073457
O	-2.796735	-0.481495	0.027396
H	-1.982217	1.323275	-0.322812

E-trans-CHO-Acetonitrile  
SCF Energy: -269.304653134  
ZPE-corrected Energy: -269.208744  
 $\Delta U$ : -269.202302  
 $\Delta H$ : -269.201357  
 $\Delta G$ : -269.238983

Num. Imaginary Frequencies: 0

C	-0.455277	-0.160853	0.115819
C	2.514146	-0.744516	-0.103727
C	1.962203	0.448643	0.099781
C	0.533271	0.728014	-0.034492
H	-0.275947	-1.194439	0.387017
H	3.579061	-0.893018	0.008292
H	1.923631	-1.600273	-0.406500
H	2.593217	1.292879	0.351269
H	0.262198	1.755146	-0.262783
C	-1.841972	0.256692	-0.073161
O	-2.796788	-0.481466	0.027339
H	-1.982077	1.323549	-0.321326

E-trans-CHO-Dichloromethane  
SCF Energy: -269.30365514  
ZPE-corrected Energy: -269.207741  
 $\Delta U$ : -269.201303  
 $\Delta H$ : -269.200358  
 $\Delta G$ : -269.237963

Num. Imaginary Frequencies: 0

C	-0.455272	-0.159875	0.117970
C	2.514756	-0.744036	-0.105438
C	1.962239	0.448112	0.101145
C	0.533445	0.727724	-0.035136
H	-0.276511	-1.192219	0.394044
H	3.579292	-0.893288	0.008921
H	1.924707	-1.598241	-0.413361
H	2.592920	1.291247	0.357442
H	0.262684	1.754115	-0.267554
C	-1.843066	0.256183	-0.074104
O	-2.796613	-0.481621	0.027497
H	-1.982802	1.322711	-0.326097

E-trans-CHO-DMSO  
SCF Energy: -269.304737295  
ZPE-corrected Energy: -269.208829  
 $\Delta U$ : -269.202386  
 $\Delta H$ : -269.201442  
 $\Delta G$ : -269.239069

Num. Imaginary Frequencies: 0

C	-0.455280	-0.160922	0.115667
C	2.514095	-0.744551	-0.103617
C	1.962196	0.448677	0.099708
C	0.533259	0.728038	-0.034452
H	-0.275901	-1.194591	0.386540
H	3.579036	-0.893005	0.008242
H	1.923550	-1.600403	-0.406070
H	2.593225	1.292987	0.350884
H	0.262176	1.755219	-0.262470
C	-1.841879	0.256730	-0.073113
O	-2.796801	-0.481454	0.027346
H	-1.982016	1.323591	-0.321051

E-trans-CHO-Gas

SCF Energy: -269.297217198

ZPE-corrected Energy: -269.201355

$\Delta U$ : -269.194914

$\Delta H$ : -269.193970

$\Delta G$ : -269.231559

Num. Imaginary Frequencies: 0

C	-0.455533	-0.151950	0.128009
C	2.518278	-0.741700	-0.115742
C	1.962579	0.444009	0.110907
C	0.535189	0.727254	-0.039311
H	-0.280677	-1.177097	0.431806
H	3.579941	-0.896983	0.014690
H	1.931273	-1.584880	-0.457454
H	2.591129	1.278834	0.399498
H	0.268275	1.749419	-0.295832
C	-1.850936	0.253607	-0.081462
O	-2.794567	-0.484173	0.031525
H	-1.990864	1.316771	-0.359319

E-trans-CHO-n-Hexane

SCF Energy: -269.299926403

ZPE-corrected Energy: -269.204042

$\Delta U$ : -269.197602

$\Delta H$ : -269.196657

$\Delta G$ : -269.234254

Num. Imaginary Frequencies: 0

C	-0.455361	-0.155571	0.124347
C	2.516868	-0.742565	-0.111484
C	1.962449	0.445857	0.106641
C	0.534359	0.727213	-0.037536
H	-0.278845	-1.183639	0.417030
H	3.579831	-0.895096	0.011960
H	1.928536	-1.590574	-0.438855
H	2.591911	1.284446	0.381292
H	0.265520	1.751068	-0.284332
C	-1.847495	0.254565	-0.078141
O	-2.795610	-0.482822	0.029349
H	-1.986986	1.319384	-0.344855

E-trans-CHO-Water  
SCF Energy: -269.304846966  
ZPE-corrected Energy: -269.208940  
 $\Delta U$ : -269.202497  
 $\Delta H$ : -269.201552  
 $\Delta G$ : -269.239183

Num. Imaginary Frequencies: 0

C	-0.455282	-0.161020	0.115431
C	2.514027	-0.744602	-0.103444
C	1.962189	0.448729	0.099585
C	0.533242	0.728073	-0.034390
H	-0.275836	-1.194817	0.385801
H	3.579005	-0.892985	0.008180
H	1.923434	-1.600602	-0.405398
H	2.593247	1.293146	0.350292
H	0.262139	1.755330	-0.261987
C	-1.841760	0.256785	-0.073031
O	-2.796818	-0.481440	0.027351
H	-1.981944	1.323667	-0.320604

E-trans-COMe-Acetone  
SCF Energy: -308.621605816  
ZPE-corrected Energy: -308.497526  
 $\Delta U$ : -308.489669  
 $\Delta H$ : -308.488725  
 $\Delta G$ : -308.529883

Num. Imaginary Frequencies: 0

C	0.040127	-0.399053	-0.140757
C	-2.965325	-0.552012	0.228357
C	-2.270160	0.510684	-0.166473
C	-0.812800	0.626845	-0.076993
H	-0.312547	-1.411985	-0.298702
H	-4.041994	-0.581067	0.135037
H	-2.482100	-1.413386	0.672630
H	-2.794786	1.375584	-0.556118
H	-0.422621	1.633060	0.032620
C	1.505691	-0.265025	-0.018868
O	2.204662	-1.259344	-0.068415
C	2.110806	1.102726	0.163899
H	1.846159	1.750032	-0.672416
H	1.729954	1.568254	1.073074
H	3.190609	1.009276	0.226205

E-trans-COMe-Acetonitrile  
SCF Energy: -308.621879320  
ZPE-corrected Energy: -308.497801  
 $\Delta U$ : -308.489945  
 $\Delta H$ : -308.489001  
 $\Delta G$ : -308.530157

Num. Imaginary Frequencies: 0

C	0.040178	-0.399223	-0.140246
C	-2.965293	-0.552091	0.228121
C	-2.270092	0.510742	-0.166433
C	-0.812729	0.626822	-0.077110
H	-0.312582	-1.412272	-0.297388
H	-4.042003	-0.580869	0.135100
H	-2.482171	-1.413790	0.671896
H	-2.794614	1.375927	-0.555538
H	-0.422589	1.633112	0.031736
C	1.505543	-0.264867	-0.018799
O	2.204802	-1.259313	-0.068671
C	2.110640	1.102716	0.163906
H	1.845438	1.750209	-0.672068
H	1.730112	1.568024	1.073316
H	3.190508	1.009559	0.225679

E-trans-COMe-Dichloromethane  
SCF Energy: -308.620823338  
ZPE-corrected Energy: -308.496737  
 $\Delta U$ : -308.488877  
 $\Delta H$ : -308.487933  
 $\Delta G$ : -308.529100

Num. Imaginary Frequencies: 0

C	0.039986	-0.398565	-0.142168
C	-2.965418	-0.551711	0.229307
C	-2.270379	0.510419	-0.166813
C	-0.813033	0.626909	-0.076905
H	-0.312413	-1.411213	-0.302179
H	-4.041969	-0.581627	0.135139
H	-2.481890	-1.411924	0.675437
H	-2.795316	1.374312	-0.558408
H	-0.422811	1.632966	0.034608
C	1.506115	-0.265451	-0.019087
O	2.204268	-1.259405	-0.067915
C	2.111312	1.102725	0.164149
H	1.847821	1.749930	-0.672665
H	1.729967	1.568402	1.073083
H	3.190968	1.008438	0.227413

E-trans-COMe-DMSO  
SCF Energy: -308.621968894  
ZPE-corrected Energy: -308.497891  
 $\Delta U$ : -308.490036  
 $\Delta H$ : -308.489092  
 $\Delta G$ : -308.530247

Num. Imaginary Frequencies: 0

C	0.040195	-0.399277	-0.140080
C	-2.965282	-0.552114	0.228058
C	-2.270071	0.510757	-0.166430
C	-0.812707	0.626815	-0.077159
H	-0.312592	-1.412367	-0.296951
H	-4.042005	-0.580805	0.135135
H	-2.482191	-1.413909	0.671689
H	-2.794560	1.376025	-0.555377
H	-0.422583	1.633132	0.031425
C	1.505495	-0.264814	-0.018777
O	2.204848	-1.259301	-0.068764
C	2.110587	1.102712	0.163920
H	1.845185	1.750284	-0.671921
H	1.730182	1.567926	1.073426
H	3.190478	1.009651	0.225496

E-trans-COMe-Gas  
SCF Energy: -308.614199080  
ZPE-corrected Energy: -308.490049  
 $\Delta U$ : -308.482181  
 $\Delta H$ : -308.481237  
 $\Delta G$ : -308.522403

Num. Imaginary Frequencies: 0

C	0.039257	-0.395951	-0.150586
C	-2.967827	-0.546046	0.244422
C	-2.272709	0.505135	-0.176494
C	-0.815660	0.625967	-0.082949
H	-0.309389	-1.408361	-0.319467
H	-4.043278	-0.583892	0.142794
H	-2.483048	-1.390018	0.718800
H	-2.799146	1.355148	-0.596447
H	-0.426720	1.632304	0.034445
C	1.509925	-0.268305	-0.020659
O	2.202879	-1.258029	-0.071117
C	2.115568	1.102385	0.173651
H	1.857759	1.756506	-0.659914
H	1.735029	1.562765	1.085971
H	3.194438	1.000668	0.238444

E-trans-COMe-n-Hexane  
SCF Energy: -308.616953719  
ZPE-corrected Energy: -308.492848  
 $\Delta U$ : -308.484973  
 $\Delta H$ : -308.484029  
 $\Delta G$ : -308.525238

Num. Imaginary Frequencies: 0

C	0.039467	-0.396568	-0.148310
C	-2.966320	-0.549078	0.237176
C	-2.271712	0.507900	-0.171198
C	-0.814499	0.626759	-0.079505
H	-0.310959	-1.408639	-0.315368
H	-4.042270	-0.583688	0.138989
H	-2.481550	-1.400905	0.697533
H	-2.797956	1.364647	-0.577093
H	-0.424796	1.632685	0.037466
C	1.508270	-0.267239	-0.020218
O	2.202902	-1.259040	-0.068264
C	2.113898	1.102506	0.168578
H	1.853295	1.753246	-0.666615
H	1.733279	1.565208	1.079559
H	3.193107	1.004091	0.232502

E-trans-COMe-Water  
SCF Energy: -308.622085741  
ZPE-corrected Energy: -308.498009  
 $\Delta U$ : -308.490154  
 $\Delta H$ : -308.489210  
 $\Delta G$ : -308.530364

Num. Imaginary Frequencies: 0

C	0.040217	-0.399348	-0.139864
C	-2.965266	-0.552142	0.227985
C	-2.270044	0.510773	-0.166434
C	-0.812679	0.626806	-0.077232
H	-0.312604	-1.412491	-0.296378
H	-4.042006	-0.580723	0.135192
H	-2.482216	-1.414051	0.671446
H	-2.794492	1.376143	-0.555189
H	-0.422579	1.633160	0.031004
C	1.505432	-0.264744	-0.018750
O	2.204907	-1.259285	-0.068892
C	2.110519	1.102705	0.163948
H	1.844841	1.750396	-0.671704
H	1.730290	1.567780	1.073595
H	3.190440	1.009769	0.225246



E-trans-COOH-Acetone  
SCF Energy: -344.570069424  
ZPE-corrected Energy: -344.468400  
 $\Delta U$ : -344.461204  
 $\Delta H$ : -344.460260  
 $\Delta G$ : -344.500157

Num. Imaginary Frequencies: 0

C	0.060932	-0.374222	-0.144622
C	-2.934886	-0.598265	0.219158
C	-2.264277	0.484166	-0.163828
C	-0.810992	0.632522	-0.067225
H	-0.252531	-1.394441	-0.320610
H	-4.010392	-0.651710	0.123577
H	-2.432557	-1.451879	0.657206
H	-2.806700	1.341154	-0.546080
H	-0.430113	1.639292	0.060350
C	1.515715	-0.196544	-0.014940
O	2.308296	-1.106454	-0.072251
O	1.900310	1.074611	0.173693
H	2.864487	1.086393	0.242761

E-trans-COOH-Acetonitrile  
SCF Energy: -344.570329426  
ZPE-corrected Energy: -344.468672  
 $\Delta U$ : -344.461477  
 $\Delta H$ : -344.460532  
 $\Delta G$ : -344.500430

Num. Imaginary Frequencies: 0

C	0.060916	-0.373882	-0.143933
C	-2.934998	-0.598584	0.218400
C	-2.264474	0.484408	-0.163274
C	-0.811147	0.632878	-0.067024
H	-0.252962	-1.394145	-0.319114
H	-4.010531	-0.651736	0.122930
H	-2.432773	-1.452977	0.655056
H	-2.807036	1.341919	-0.544125
H	-0.430550	1.639856	0.059766
C	1.515808	-0.196441	-0.014961
O	2.308009	-1.106937	-0.072241
O	1.900982	1.074412	0.173305
H	2.865296	1.087010	0.241728

E-trans-COOH-Dichloromethane  
SCF Energy: -344.569316377  
ZPE-corrected Energy: -344.467620  
 $\Delta U$ : -344.460427  
 $\Delta H$ : -344.459483  
 $\Delta G$ : -344.499374

Num. Imaginary Frequencies: 0

C	0.060814	-0.374016	-0.146559
C	-2.934606	-0.597666	0.221414
C	-2.264226	0.483429	-0.165306
C	-0.811063	0.632443	-0.067682
H	-0.252405	-1.393842	-0.325073
H	-4.009932	-0.652596	0.124858
H	-2.431767	-1.448727	0.663780
H	-2.806798	1.338483	-0.551776
H	-0.429990	1.638878	0.062077
C	1.515745	-0.196972	-0.015216
O	2.308240	-1.106154	-0.072316
O	1.900109	1.074896	0.174959
H	2.864115	1.084564	0.245082

E-trans-COOH-DMSO  
SCF Energy: -344.570414271  
ZPE-corrected Energy: -344.468761  
 $\Delta U$ : -344.461565  
 $\Delta H$ : -344.460620  
 $\Delta G$ : -344.500518

Num. Imaginary Frequencies: 0

C	0.060929	-0.373883	-0.143841
C	-2.934993	-0.598632	0.218286
C	-2.264481	0.484450	-0.163202
C	-0.811150	0.632892	-0.066999
H	-0.252970	-1.394166	-0.318887
H	-4.010539	-0.651711	0.122894
H	-2.432776	-1.453160	0.654691
H	-2.807029	1.342070	-0.543814
H	-0.430592	1.639896	0.059688
C	1.515796	-0.196387	-0.014943
O	2.308005	-1.106970	-0.072237
O	1.900993	1.074376	0.173239
H	2.865324	1.087181	0.241616

E-trans-COOH-Gas

SCF Energy: -344.562442857

ZPE-corrected Energy: -344.460529

$\Delta U$ : -344.453345

$\Delta H$ : -344.452401

$\Delta G$ : -344.492267

Num. Imaginary Frequencies: 0

C	0.060701	-0.374367	-0.156645
C	-2.936178	-0.591944	0.235094
C	-2.263499	0.477998	-0.174683
C	-0.810883	0.630043	-0.071290
H	-0.249624	-1.392519	-0.348672
H	-4.010299	-0.653049	0.130677
H	-2.434215	-1.427880	0.705947
H	-2.805710	1.320773	-0.588649
H	-0.427480	1.634359	0.068974
C	1.517440	-0.200724	-0.016866
O	2.309694	-1.102697	-0.073429
O	1.897997	1.077824	0.183445
H	2.860313	1.071254	0.257933

E-trans-COOH-n-Hexane

SCF Energy: -344.565405569

ZPE-corrected Energy: -344.463583

$\Delta U$ : -344.456394

$\Delta H$ : -344.455449

$\Delta G$ : -344.495336

Num. Imaginary Frequencies: 0

C	0.060591	-0.373762	-0.152850
C	-2.934963	-0.594576	0.229757
C	-2.263824	0.480215	-0.170975
C	-0.811045	0.631495	-0.069736
H	-0.251417	-1.392358	-0.339925
H	-4.009546	-0.653811	0.128501
H	-2.432098	-1.436255	0.689471
H	-2.806549	1.327740	-0.574057
H	-0.428823	1.636719	0.066724
C	1.516569	-0.199217	-0.016246
O	2.308717	-1.104394	-0.073012
O	1.899075	1.076441	0.180055
H	2.862137	1.076662	0.253243

E-trans-COOH-Water  
SCF Energy: -344.570524686  
ZPE-corrected Energy: -344.468875  
 $\Delta U$ : -344.461679  
 $\Delta H$ : -344.460735  
 $\Delta G$ : -344.500634

Num. Imaginary Frequencies: 0

C	0.060947	-0.373884	-0.143723
C	-2.934987	-0.598694	0.218137
C	-2.264491	0.484505	-0.163108
C	-0.811153	0.632910	-0.066967
H	-0.252979	-1.394192	-0.318592
H	-4.010549	-0.651679	0.122846
H	-2.432782	-1.453398	0.654218
H	-2.807020	1.342267	-0.543409
H	-0.430647	1.639948	0.059587
C	1.515780	-0.196316	-0.014920
O	2.307999	-1.107014	-0.072232
O	1.901006	1.074329	0.173153
H	2.865360	1.087404	0.241469

Z-CF3-Acetone  
SCF Energy: -493.059288398  
ZPE-corrected Energy: -492.967705  
 $\Delta U$ : -492.959995  
 $\Delta H$ : -492.959051  
 $\Delta G$ : -493.000557

Num. Imaginary Frequencies: 0

C	-0.131517	1.172892	0.281956
C	2.159171	-1.014125	0.206238
C	2.146067	0.229163	-0.258713
C	1.187182	1.265639	0.140924
H	-0.706493	2.021816	0.624870
H	1.426286	-1.361645	0.922793
H	2.919482	-1.716333	-0.106945
H	2.930658	0.555791	-0.932621
H	1.620018	2.240355	0.341535
C	-0.971909	-0.028159	-0.016478
F	-1.025759	-0.897243	1.011101
F	-0.570469	-0.724239	-1.085428
F	-2.239762	0.344543	-0.256028

Z-CF3-Acetonitrile

SCF Energy: -493.059420559

ZPE-corrected Energy: -492.967848

$\Delta U$ : -492.960138

$\Delta H$ : -492.959194

$\Delta G$ : -493.000700

Num. Imaginary Frequencies: 0

C	-0.131547	1.172936	0.282211
C	2.159551	-1.014058	0.206317
C	2.145981	0.229153	-0.258937
C	1.187160	1.265607	0.140985
H	-0.706441	2.021833	0.625317
H	1.427126	-1.361551	0.923377
H	2.919997	-1.716121	-0.106893
H	2.930290	0.555879	-0.933124
H	1.620066	2.240272	0.341598
C	-0.971884	-0.027995	-0.016368
F	-1.025539	-0.897743	1.010733
F	-0.570807	-0.723830	-1.085800
F	-2.239943	0.344442	-0.255546

Z-CF3-Dichloromethane

SCF Energy: -493.058909352

ZPE-corrected Energy: -492.967295

$\Delta U$ : -492.959586

$\Delta H$ : -492.958642

$\Delta G$ : -493.000149

Num. Imaginary Frequencies: 0

C	-0.131449	1.172778	0.281219
C	2.158091	-1.014326	0.205987
C	2.146320	0.229201	-0.258050
C	1.187228	1.265734	0.140746
H	-0.706658	2.021792	0.623552
H	1.423872	-1.361961	0.921057
H	2.918060	-1.716911	-0.107098
H	2.931753	0.555587	-0.931098
H	1.619867	2.240597	0.341332
C	-0.972002	-0.028623	-0.016786
F	-1.026126	-0.895968	1.012035
F	-0.569670	-0.725227	-1.084539
F	-2.239318	0.344786	-0.257101

Z-CF3-DMSO

SCF Energy: -493.059463806

ZPE-corrected Energy: -492.967895

$\Delta U$ : -492.960185

$\Delta H$ : -492.959241

$\Delta G$ : -493.000747

Num. Imaginary Frequencies: 0

C	-0.131557	1.172951	0.282294
C	2.159675	-1.014036	0.206342
C	2.145953	0.229151	-0.259009
C	1.187153	1.265596	0.141005
H	-0.706424	2.021839	0.625462
H	1.427401	-1.361522	0.923565
H	2.920168	-1.716050	-0.106877
H	2.930172	0.555910	-0.933285
H	1.620081	2.240245	0.341617
C	-0.971877	-0.027941	-0.016331
F	-1.025457	-0.897913	1.010608
F	-0.570925	-0.723688	-1.085930
F	-2.240005	0.344407	-0.255377

Z-CF3-Gas

SCF Energy: -493.055628337

ZPE-corrected Energy: -492.963746

$\Delta U$ : -492.956052

$\Delta H$ : -492.955108

$\Delta G$ : -492.996570

Num. Imaginary Frequencies: 0

C	-0.131630	1.173264	0.272586
C	2.146455	-1.017568	0.201905
C	2.148921	0.229701	-0.249922
C	1.187095	1.267148	0.138498
H	-0.708887	2.024378	0.606197
H	1.397194	-1.368570	0.898945
H	2.906507	-1.721391	-0.107648
H	2.946153	0.555945	-0.909099
H	1.618141	2.243530	0.336738
C	-0.973440	-0.032049	-0.019132
F	-1.016819	-0.889895	1.016116
F	-0.569434	-0.727075	-1.083754
F	-2.238581	0.343984	-0.253332

Z-CF3-n-Hexane

SCF Energy: -493.057010532

ZPE-corrected Energy: -492.965257

$\Delta U$ : -492.957547

$\Delta H$ : -492.956603

$\Delta G$ : -492.998134

Num. Imaginary Frequencies: 0

C	-0.131459	1.172743	0.276795
C	2.151983	-1.015796	0.204114
C	2.147618	0.229474	-0.253975
C	1.187183	1.266432	0.139639
H	-0.707853	2.022654	0.614963
H	1.410075	-1.364824	0.910198
H	2.911354	-1.719476	-0.107608
H	2.938673	0.555362	-0.920695
H	1.618903	2.242097	0.339376
C	-0.972718	-0.030746	-0.018194
F	-1.022942	-0.891726	1.014988
F	-0.568345	-0.727348	-1.082977
F	-2.238357	0.344801	-0.257178

Z-CF3-Water

SCF Energy: -493.059520194

ZPE-corrected Energy: -492.967956

$\Delta U$ : -492.960246

$\Delta H$ : -492.959302

$\Delta G$ : -493.000809

Num. Imaginary Frequencies: 0

C	-0.131571	1.172971	0.282403
C	2.159838	-1.014008	0.206373
C	2.145917	0.229148	-0.259103
C	1.187143	1.265583	0.141031
H	-0.706404	2.021848	0.625649
H	1.427759	-1.361486	0.923809
H	2.920393	-1.715956	-0.106855
H	2.930019	0.555952	-0.933492
H	1.620101	2.240210	0.341642
C	-0.971868	-0.027871	-0.016283
F	-1.025342	-0.898140	1.010441
F	-0.571084	-0.723498	-1.086104
F	-2.240089	0.344360	-0.255146

Z-Me-Acetone

SCF Energy: -195.279003535

ZPE-corrected Energy: -195.164652

$\Delta U$ : -195.158745

$\Delta H$ : -195.157801

$\Delta G$ : -195.193421

Num. Imaginary Frequencies: 0

C	-1.179572	0.565787	0.119932
C	1.621368	-0.846782	0.179709
C	1.303996	0.385293	-0.210415
C	0.048474	1.087920	0.078087
H	-1.993783	1.243799	0.353712
H	0.950282	-1.444367	0.782771
H	2.577989	-1.282997	-0.074870
H	2.041764	0.956199	-0.766482
H	0.144157	2.156388	0.241841
C	-1.572494	-0.852334	-0.150526
H	-1.701476	-1.409099	0.781003
H	-2.527184	-0.886089	-0.674903
H	-0.822376	-1.373141	-0.743792

Z-Me-Acetonitrile

SCF Energy: -195.279082608

ZPE-corrected Energy: -195.164735

$\Delta U$ : -195.158829

$\Delta H$ : -195.157885

$\Delta G$ : -195.193500

Num. Imaginary Frequencies: 0

C	-1.179583	0.565914	0.119640
C	1.621151	-0.847151	0.179301
C	1.304246	0.385410	-0.209882
C	0.048544	1.088029	0.077988
H	-1.993823	1.244074	0.352906
H	0.949477	-1.445471	0.780980
H	2.578039	-1.283074	-0.074814
H	2.042639	0.956812	-0.764616
H	0.144163	2.156569	0.241340
C	-1.572567	-0.852294	-0.150285
H	-1.700638	-1.408929	0.781444
H	-2.527706	-0.886204	-0.673797
H	-0.822890	-1.373228	-0.744013



Z-Me-Dichloromethane  
SCF Energy: -195.278780581  
ZPE-corrected Energy: -195.164413  
 $\Delta U$ : -195.158506  
 $\Delta H$ : -195.157562  
 $\Delta G$ : -195.193183

Num. Imaginary Frequencies: 0

C	-1.179552	0.565406	0.120811
C	1.621917	-0.845698	0.180916
C	1.303226	0.384976	-0.211965
C	0.048239	1.087661	0.078351
H	-1.993733	1.242925	0.356075
H	0.952549	-1.441135	0.788016
H	2.577738	-1.282820	-0.075019
H	2.039200	0.954376	-0.771919
H	0.144093	2.155915	0.243284
C	-1.572157	-0.852489	-0.151244
H	-1.703377	-1.409808	0.779648
H	-2.525697	-0.885910	-0.677838
H	-0.820812	-1.372683	-0.743455

Z-Me-DMSO  
SCF Energy: -195.279108635  
ZPE-corrected Energy: -195.164761  
 $\Delta U$ : -195.158857  
 $\Delta H$ : -195.157913  
 $\Delta G$ : -195.193525

Num. Imaginary Frequencies: 0

C	-1.179587	0.565954	0.119546
C	1.621078	-0.847271	0.179170
C	1.304326	0.385448	-0.209711
C	0.048566	1.088066	0.077955
H	-1.993837	1.244160	0.352648
H	0.949213	-1.445825	0.780404
H	2.578051	-1.283102	-0.074795
H	2.042922	0.957008	-0.764014
H	0.144165	2.156629	0.241178
C	-1.572588	-0.852281	-0.150207
H	-1.700356	-1.408879	0.781585
H	-2.527875	-0.886243	-0.673434
H	-0.823055	-1.373252	-0.744090

Z-Me-Gas

SCF Energy: -195.277072506

ZPE-corrected Energy: -195.162551

$\Delta U$ : -195.156648

$\Delta H$ : -195.155704

$\Delta G$ : -195.191315

Num. Imaginary Frequencies: 0

C	-1.179355	0.563178	0.125947
C	1.625425	-0.838753	0.188232
C	1.298324	0.382819	-0.221602
C	0.046785	1.085660	0.080033
H	-1.992933	1.237914	0.370515
H	0.966583	-1.420416	0.819490
H	2.576360	-1.281240	-0.075325
H	2.022729	0.943042	-0.805213
H	0.143595	2.152613	0.251917
C	-1.570110	-0.853334	-0.155426
H	-1.714325	-1.414036	0.771577
H	-2.516666	-0.884918	-0.695044
H	-0.811762	-1.370375	-0.741022

Z-Me-n-Hexane

SCF Energy: -195.277745398

ZPE-corrected Energy: -195.163274

$\Delta U$ : -195.157377

$\Delta H$ : -195.156433

$\Delta G$ : -195.192020

Num. Imaginary Frequencies: 0

C	-1.179355	0.563946	0.124266
C	1.624271	-0.841327	0.185612
C	1.300207	0.383581	-0.218136
C	0.047404	1.086410	0.079441
H	-1.993199	1.239776	0.365208
H	0.961759	-1.428080	0.808389
H	2.576966	-1.281934	-0.075337
H	2.028826	0.946966	-0.793467
H	0.143878	2.153843	0.248721
C	-1.571115	-0.852953	-0.153974
H	-1.711853	-1.412254	0.774381
H	-2.519786	-0.884770	-0.689769
H	-0.815061	-1.371489	-0.741382

Z-Me-Water

SCF Energy: -195.279142684

ZPE-corrected Energy: -195.164796

$\Delta U$ : -195.158893

$\Delta H$ : -195.157948

$\Delta G$ : -195.193556

Num. Imaginary Frequencies: 0

C	-1.179591	0.566007	0.119424
C	1.620982	-0.847425	0.179002
C	1.304430	0.385498	-0.209489
C	0.048595	1.088115	0.077913
H	-1.993855	1.244271	0.352316
H	0.948869	-1.446282	0.779659
H	2.578063	-1.283142	-0.074769
H	2.043289	0.957260	-0.763236
H	0.144168	2.156708	0.240969
C	-1.572613	-0.852265	-0.150108
H	-1.699985	-1.408818	0.781764
H	-2.528094	-0.886295	-0.672960
H	-0.823266	-1.373281	-0.744194

Z-NH2-Acetone

SCF Energy: -211.337139862

ZPE-corrected Energy: -211.233131

$\Delta U$ : -211.227520

$\Delta H$ : -211.226576

$\Delta G$ : -211.261401

Num. Imaginary Frequencies: 0

C	-1.219902	0.471656	-0.075000
C	1.624316	-0.821963	-0.123370
C	1.276873	0.443998	0.134142
C	-0.018901	1.079140	-0.055513
H	-2.108514	1.076583	-0.206588
H	0.953191	-1.534385	-0.583721
H	2.631028	-1.163950	0.073907
H	2.050990	1.098723	0.524421
H	-0.026446	2.157167	-0.138462
N	-1.474374	-0.873606	0.035369
H	-0.752409	-1.438267	0.458380
H	-2.401545	-1.117616	0.342932

Z-NH2-Acetonitrile

SCF Energy: -211.337352655

ZPE-corrected Energy: -211.233352

$\Delta U$ : -211.227740

$\Delta H$ : -211.226796

$\Delta G$ : -211.261625

Num. Imaginary Frequencies: 0

C	-1.220006	0.471795	-0.074444
C	1.624573	-0.822449	-0.122401
C	1.277294	0.444101	0.132972
C	-0.018716	1.079108	-0.055080
H	-2.108499	1.077135	-0.204992
H	0.952821	-1.536571	-0.579156
H	2.631868	-1.163542	0.073507
H	2.052237	1.099758	0.520075
H	-0.026348	2.157241	-0.136886
N	-1.474926	-0.873232	0.034754
H	-0.753818	-1.439299	0.457295
H	-2.402648	-1.117420	0.340596

Z-NH2-Dichloromethane

SCF Energy: -211.336539692

ZPE-corrected Energy: -211.232506

$\Delta U$ : -211.226900

$\Delta H$ : -211.225955

$\Delta G$ : -211.260771

Num. Imaginary Frequencies: 0

C	-1.219671	0.471263	-0.076503
C	1.623678	-0.820559	-0.126022
C	1.275600	0.443729	0.137321
C	-0.019472	1.079245	-0.056591
H	-2.108638	1.074940	-0.211253
H	0.954523	-1.528553	-0.596048
H	2.628887	-1.164784	0.074823
H	2.047452	1.095922	0.536115
H	-0.026740	2.156965	-0.142763
N	-1.472752	-0.874699	0.037014
H	-0.748580	-1.435341	0.461732
H	-2.398450	-1.118327	0.349065

Z-NH2-DMSO

SCF Energy: -211.337421876  
ZPE-corrected Energy: -211.233418  
 $\Delta U$ : -211.227806  
 $\Delta H$ : -211.226862  
 $\Delta G$ : -211.261691

Num. Imaginary Frequencies: 0

C	-1.219920	0.471675	-0.074408
C	1.624830	-0.822575	-0.122132
C	1.277486	0.444214	0.132349
C	-0.018464	1.078664	-0.054809
H	-2.108293	1.077392	-0.204726
H	0.952227	-1.536819	-0.577589
H	2.631940	-1.164030	0.074038
H	2.051929	1.100574	0.519515
H	-0.026262	2.156921	-0.136396
N	-1.475359	-0.872712	0.034668
H	-0.754538	-1.440196	0.455839
H	-2.403075	-1.116728	0.340642

Z-NH2-Gas

SCF Energy: -211.331920691  
ZPE-corrected Energy: -211.227662  
 $\Delta U$ : -211.222092  
 $\Delta H$ : -211.221148  
 $\Delta G$ : -211.255878

Num. Imaginary Frequencies: 0

C	-1.217405	0.468640	-0.086131
C	1.617055	-0.811003	-0.143864
C	1.266622	0.441880	0.158293
C	-0.023080	1.080608	-0.064149
H	-2.109477	1.063087	-0.239687
H	0.959414	-1.485029	-0.676805
H	2.610210	-1.174224	0.080486
H	2.021634	1.075345	0.614727
H	-0.028845	2.156476	-0.168896
N	-1.459650	-0.882324	0.047919
H	-0.719605	-1.416078	0.481037
H	-2.374933	-1.124058	0.388815

Z-NH2-n-Hexane

SCF Energy: -211.333747399

ZPE-corrected Energy: -211.229585

$\Delta U$ : -211.224000

$\Delta H$ : -211.223055

$\Delta G$ : -211.257821

Num. Imaginary Frequencies: 0

C	-1.218169	0.469705	-0.082868
C	1.619422	-0.814755	-0.137468
C	1.270151	0.442487	0.150713
C	-0.021608	1.080123	-0.061391
H	-2.108976	1.067819	-0.229587
H	0.957205	-1.501306	-0.647952
H	2.617093	-1.170993	0.078524
H	2.031743	1.082901	0.586236
H	-0.027779	2.156693	-0.159363
N	-1.464712	-0.879458	0.044073
H	-0.730921	-1.422689	0.475590
H	-2.384152	-1.121579	0.374132

Z-NH2-Water

SCF Energy: -211.337514312

ZPE-corrected Energy: -211.233521

$\Delta U$ : -211.227907

$\Delta H$ : -211.226963

$\Delta G$ : -211.261796

Num. Imaginary Frequencies: 0

C	-1.220098	0.471898	-0.073983
C	1.624760	-0.822815	-0.121646
C	1.277599	0.444193	0.132040
C	-0.018595	1.079100	-0.054721
H	-2.108511	1.077515	-0.203804
H	0.952554	-1.538314	-0.575534
H	2.632516	-1.163188	0.073189
H	2.053189	1.100555	0.516671
H	-0.026290	2.157306	-0.135700
N	-1.475308	-0.872958	0.034265
H	-0.754855	-1.440091	0.456446
H	-2.403448	-1.117335	0.338739

Z-NO2-Acetone

SCF Energy: -360.481851068  
ZPE-corrected Energy: -360.392150  
 $\Delta U$ : -360.385377  
 $\Delta H$ : -360.384433  
 $\Delta G$ : -360.423948

Num. Imaginary Frequencies: 0

C	-0.502657	1.034547	-0.209511
C	2.178343	-0.902558	-0.190590
C	1.924071	0.310787	0.288019
C	0.810934	1.194042	-0.056412
H	-1.169978	1.852904	-0.420365
H	1.512947	-1.403031	-0.876463
H	3.092524	-1.410236	0.085929
H	2.662486	0.784150	0.925941
H	1.107897	2.232914	-0.168784
N	-1.245870	-0.190254	0.001772
O	-0.669185	-1.255540	0.047153
O	-2.449432	-0.062689	0.134384

Z-NO2-Acetonitrile

SCF Energy: -360.482143800  
ZPE-corrected Energy: -360.392456  
 $\Delta U$ : -360.385681  
 $\Delta H$ : -360.384737  
 $\Delta G$ : -360.424282

Num. Imaginary Frequencies: 0

C	-0.502503	1.034693	-0.208000
C	2.178350	-0.902137	-0.194060
C	1.924362	0.309988	0.287903
C	0.811196	1.193820	-0.054821
H	-1.169562	1.853261	-0.418732
H	1.512439	-1.400540	-0.881066
H	3.092743	-1.410630	0.080246
H	2.663005	0.782079	0.926479
H	1.108271	2.232737	-0.166373
N	-1.245817	-0.189948	0.002312
O	-0.669074	-1.255017	0.052929
O	-2.450253	-0.063164	0.129212

Z-NO2-Dichloromethane  
SCF Energy: -360.481014535  
ZPE-corrected Energy: -360.391278  
 $\Delta U$ : -360.384512  
 $\Delta H$ : -360.383567  
 $\Delta G$ : -360.423022

Num. Imaginary Frequencies: 0

C	-0.503179	1.034239	-0.213608
C	2.178085	-0.903685	-0.181624
C	1.923162	0.312831	0.288445
C	0.810138	1.194657	-0.060511
H	-1.171269	1.851947	-0.424857
H	1.513854	-1.409155	-0.864748
H	3.091628	-1.409406	0.100542
H	2.660871	0.789362	0.924903
H	1.106868	2.233407	-0.175062
N	-1.245986	-0.191114	0.000343
O	-0.669017	-1.256463	0.032070
O	-2.447144	-0.061863	0.148007

Z-NO2-DMSO

SCF Energy: -360.482239715  
ZPE-corrected Energy: -360.392557  
 $\Delta U$ : -360.385781  
 $\Delta H$ : -360.384836  
 $\Delta G$ : -360.424396

Num. Imaginary Frequencies: 0

C	-0.502394	1.034747	-0.207369
C	2.178343	-0.901986	-0.195378
C	1.924523	0.309671	0.287813
C	0.811334	1.193726	-0.054217
H	-1.169344	1.853410	-0.418047
H	1.512197	-1.399643	-0.882717
H	3.092805	-1.410803	0.078091
H	2.663282	0.781285	0.926595
H	1.108463	2.232655	-0.165475
N	-1.245808	-0.189841	0.002530
O	-0.669152	-1.254893	0.055150
O	-2.450545	-0.063227	0.127193



Z-NO2-Gas

SCF Energy: -360.473948973  
ZPE-corrected Energy: -360.384042  
 $\Delta U$ : -360.377261  
 $\Delta H$ : -360.376317  
 $\Delta G$ : -360.415847

Num. Imaginary Frequencies: 0

C	-0.504143	1.032848	-0.227426
C	2.171264	-0.914260	-0.133000
C	1.924097	0.323383	0.281511
C	0.808000	1.197835	-0.080125
H	-1.176456	1.848431	-0.435978
H	1.499376	-1.451859	-0.781961
H	3.084682	-1.407776	0.170561
H	2.669943	0.820091	0.893113
H	1.103006	2.236180	-0.204921
N	-1.248309	-0.196062	-0.005485
O	-0.671601	-1.260031	-0.042624
O	-2.433112	-0.053902	0.211601

Z-NO2-n-Hexane

SCF Energy: -360.476884892  
ZPE-corrected Energy: -360.387014  
 $\Delta U$ : -360.380251  
 $\Delta H$ : -360.379306  
 $\Delta G$ : -360.418780

Num. Imaginary Frequencies: 0

C	-0.504103	1.032996	-0.226528
C	2.174940	-0.909206	-0.148555
C	1.921456	0.319854	0.287602
C	0.808165	1.196794	-0.075111
H	-1.174976	1.848653	-0.438402
H	1.510774	-1.433774	-0.816343
H	3.086368	-1.407949	0.152318
H	2.659754	0.808442	0.914528
H	1.104234	2.234997	-0.197773
N	-1.246888	-0.194480	-0.004323
O	-0.670559	-1.259534	-0.021981
O	-2.437026	-0.056921	0.195917

Z-NO2-Water  
SCF Energy: -360.482364881  
ZPE-corrected Energy: -360.392689  
 $\Delta U$ : -360.385911  
 $\Delta H$ : -360.384966  
 $\Delta G$ : -360.424550

Num. Imaginary Frequencies: 0

C	-0.502231	1.034821	-0.206530
C	2.178228	-0.901821	-0.197148
C	1.924726	0.309246	0.287669
C	0.811535	1.193625	-0.053386
H	-1.169050	1.853596	-0.417135
H	1.511734	-1.398484	-0.884890
H	3.092766	-1.411115	0.075174
H	2.663717	0.780181	0.926667
H	1.108726	2.232576	-0.164215
N	-1.245770	-0.189682	0.002825
O	-0.669226	-1.254706	0.058143
O	-2.450905	-0.063320	0.124481

Z-OMe-Acetone  
SCF Energy: -270.498165622  
ZPE-corrected Energy: -270.378613  
 $\Delta U$ : -270.371494  
 $\Delta H$ : -270.370550  
 $\Delta G$ : -270.409940

Num. Imaginary Frequencies: 0

C	-0.484675	0.877061	0.000005
C	1.833403	-1.184087	-0.000023
C	1.917975	0.149051	0.000086
C	0.830130	1.120559	-0.000016
H	-1.204380	1.689811	-0.000065
H	0.887156	-1.703455	-0.000152
H	2.735042	-1.781941	-0.000080
H	2.910155	0.588691	-0.000030
H	1.105383	2.166075	-0.000173
O	-1.008610	-0.362503	0.000036
C	-2.429825	-0.416775	-0.000005
H	-2.704418	-1.466796	-0.000243
H	-2.831072	0.066203	0.891641
H	-2.831038	0.066582	-0.891466

Z-OMe-Acetonitrile  
SCF Energy: -270.498359180  
ZPE-corrected Energy: -270.378808  
 $\Delta U$ : -270.371691  
 $\Delta H$ : -270.370747  
 $\Delta G$ : -270.410120

Num. Imaginary Frequencies: 0

C	-0.484788	0.877193	-0.000028
C	1.833477	-1.184193	-0.000033
C	1.917869	0.149056	0.000120
C	0.830119	1.120702	-0.000013
H	-1.204573	1.689854	-0.000110
H	0.887347	-1.703817	-0.000234
H	2.735226	-1.781900	-0.000054
H	2.910066	0.588680	0.000070
H	1.105504	2.166181	-0.000163
O	-1.008445	-0.362401	-0.000028
C	-2.429947	-0.416959	0.000045
H	-2.704248	-1.467038	-0.000291
H	-2.831011	0.065937	0.891745
H	-2.831131	0.066524	-0.891289

Z-OMe-Dichloromethane  
SCF Energy: -270.497619347  
ZPE-corrected Energy: -270.378059  
 $\Delta U$ : -270.370934  
 $\Delta H$ : -270.369990  
 $\Delta G$ : -270.409421

Num. Imaginary Frequencies: 0

C	-0.484354	0.876740	0.000097
C	1.833129	-1.183808	-0.000002
C	1.918244	0.149015	-0.000010
C	0.830164	1.120175	-0.000023
H	-1.203862	1.689720	0.000056
H	0.886552	-1.702453	0.000072
H	2.734448	-1.782093	-0.000157
H	2.910389	0.588666	-0.000307
H	1.105081	2.165787	-0.000211
O	-1.009040	-0.362777	0.000236
C	-2.429433	-0.416280	-0.000155
H	-2.704830	-1.466147	-0.000085
H	-2.831234	0.066978	0.891295
H	-2.830728	0.066703	-0.891986

Z-OMe-DMSO

SCF Energy: -270.498422869

ZPE-corrected Energy: -270.378872

$\Delta U$ : -270.371756

$\Delta H$ : -270.370812

$\Delta G$ : -270.410179

Num. Imaginary Frequencies: 0

C	-0.484826	0.877238	-0.000038
C	1.833499	-1.184229	-0.000036
C	1.917832	0.149057	0.000131
C	0.830115	1.120750	-0.000013
H	-1.204638	1.689869	-0.000125
H	0.887407	-1.703936	-0.000261
H	2.735283	-1.781888	-0.000046
H	2.910036	0.588674	0.000102
H	1.105546	2.166217	-0.000161
O	-1.008389	-0.362367	-0.000047
C	-2.429985	-0.417021	0.000061
H	-2.704190	-1.467119	-0.000304
H	-2.830992	0.065853	0.891775
H	-2.831158	0.066502	-0.891233

Z-OMe-Gas

SCF Energy: -270.493389715

ZPE-corrected Energy: -270.373708

$\Delta U$ : -270.366580

$\Delta H$ : -270.365636

$\Delta G$ : -270.405187

Num. Imaginary Frequencies: 0

C	-0.482107	0.876166	-0.000058
C	1.829469	-1.182266	-0.000064
C	1.919253	0.148224	0.000100
C	0.830284	1.118060	-0.000039
H	-1.201160	1.689934	-0.000115
H	0.880953	-1.696437	-0.000359
H	2.728267	-1.783818	0.000085
H	2.911503	0.586812	0.000349
H	1.103684	2.164118	-0.000102
O	-1.011440	-0.364675	-0.000009
C	-2.424618	-0.413541	0.000059
H	-2.705678	-1.462485	-0.000057
H	-2.829821	0.069595	0.891771
H	-2.829912	0.069827	-0.891484

Z-OMe-n-Hexane

SCF Energy: -270.495068959

ZPE-corrected Energy: -270.375437

$\Delta U$ : -270.368309

$\Delta H$ : -270.367365

$\Delta G$ : -270.406874

Num. Imaginary Frequencies: 0

C	-0.482923	0.876113	-0.000135
C	1.830941	-1.182840	-0.000086
C	1.918943	0.148555	0.000185
C	0.830297	1.118834	-0.000051
H	-1.202003	1.689729	-0.000198
H	0.883038	-1.698497	-0.000614
H	2.730685	-1.783208	0.000181
H	2.911176	0.587578	0.000671
H	1.104182	2.164739	-0.000092
O	-1.010532	-0.363885	-0.000180
C	-2.426705	-0.414465	0.000195
H	-2.705559	-1.463735	-0.000425
H	-2.830028	0.068050	0.892383
H	-2.830547	0.069239	-0.891117

Z-OMe-Water

SCF Energy: -270.498506175

ZPE-corrected Energy: -270.378956

$\Delta U$ : -270.371841

$\Delta H$ : -270.370897

$\Delta G$ : -270.410255

Num. Imaginary Frequencies: 0

C	-0.484874	0.877299	-0.000052
C	1.833525	-1.184276	-0.000041
C	1.917784	0.149057	0.000145
C	0.830111	1.120813	-0.000012
H	-1.204724	1.689889	-0.000145
H	0.887482	-1.704093	-0.000296
H	2.735354	-1.781874	-0.000035
H	2.909997	0.588663	0.000144
H	1.105601	2.166264	-0.000158
O	-1.008314	-0.362323	-0.000070
C	-2.430033	-0.417103	0.000080
H	-2.704110	-1.467226	-0.000319
H	-2.830967	0.065745	0.891810
H	-2.831191	0.066469	-0.891164

Z-trans-CHO-Acetone  
SCF Energy: -269.300336649  
ZPE-corrected Energy: -269.204125  
 $\Delta U$ : -269.197907  
 $\Delta H$ : -269.196963  
 $\Delta G$ : -269.234030

Num. Imaginary Frequencies: 0

C	-0.598676	0.919753	-0.147645
C	1.776844	-1.107300	-0.254180
C	1.741581	0.119339	0.258352
C	0.722748	1.120979	-0.057797
H	-1.252316	1.727634	-0.453160
H	1.036035	-1.442177	-0.969688
H	2.568351	-1.798079	0.001935
H	2.545773	0.448563	0.907762
H	1.094563	2.125067	-0.236211
C	-1.272325	-0.329630	0.218641
O	-2.442752	-0.541015	-0.014994
H	-0.671419	-1.071734	0.765091

Z-trans-CHO-Acetonitrile  
SCF Energy: -269.300575263  
ZPE-corrected Energy: -269.204366  
 $\Delta U$ : -269.198149  
 $\Delta H$ : -269.197205  
 $\Delta G$ : -269.234270

Num. Imaginary Frequencies: 0

C	-0.598746	0.919709	-0.147869
C	1.776756	-1.107311	-0.254170
C	1.741531	0.119339	0.258433
C	0.722748	1.120941	-0.057715
H	-1.252194	1.727753	-0.453402
H	1.035942	-1.442219	-0.969666
H	2.568339	-1.798034	0.001868
H	2.545761	0.448693	0.907704
H	1.094523	2.125084	-0.235812
C	-1.272062	-0.329532	0.218415
O	-2.442832	-0.541051	-0.014714
H	-0.671079	-1.071751	0.764466

Z-trans-CHO-Dichloromethane  
SCF Energy: -269.299647767  
ZPE-corrected Energy: -269.203430  
 $\Delta U$ : -269.197211  
 $\Delta H$ : -269.196267  
 $\Delta G$ : -269.233340

Num. Imaginary Frequencies: 0

C	-0.598454	0.919892	-0.146985
C	1.777024	-1.107305	-0.254198
C	1.741736	0.119327	0.258087
C	0.722776	1.121095	-0.058033
H	-1.252625	1.727334	-0.452428
H	1.036154	-1.442087	-0.969663
H	2.568294	-1.798269	0.002118
H	2.545866	0.448165	0.907839
H	1.094718	2.125021	-0.237343
C	-1.273073	-0.329894	0.219310
O	-2.442507	-0.540898	-0.015818
H	-0.672407	-1.071661	0.766939

Z-trans-CHO-DMSO  
SCF Energy: -269.300653159  
ZPE-corrected Energy: -269.204445  
 $\Delta U$ : -269.198228  
 $\Delta H$ : -269.197284  
 $\Delta G$ : -269.234348

Num. Imaginary Frequencies: 0

C	-0.598768	0.919696	-0.147942
C	1.776724	-1.107316	-0.254167
C	1.741515	0.119338	0.258458
C	0.722749	1.120929	-0.057688
H	-1.252153	1.727794	-0.453480
H	1.035905	-1.442234	-0.969656
H	2.568331	-1.798022	0.001846
H	2.545760	0.448734	0.907681
H	1.094511	2.125090	-0.235682
C	-1.271975	-0.329499	0.218342
O	-2.442857	-0.541062	-0.014624
H	-0.670968	-1.071755	0.764264

Z-trans-CHO-Gas

SCF Energy: -269.293493082

ZPE-corrected Energy: -269.197291

$\Delta U$ : -269.191049

$\Delta H$ : -269.190105

$\Delta G$ : -269.227258

Num. Imaginary Frequencies: 0

C	-0.595661	0.920603	-0.140483
C	1.776595	-1.108381	-0.253665
C	1.744025	0.119139	0.254348
C	0.723997	1.122245	-0.059964
H	-1.253994	1.725353	-0.444180
H	1.031736	-1.442846	-0.964866
H	2.565683	-1.801392	0.003494
H	2.549796	0.445057	0.904017
H	1.096807	2.124860	-0.246250
C	-1.279453	-0.332438	0.225221
O	-2.440626	-0.538213	-0.023469
H	-0.682037	-1.072335	0.782798

Z-trans-CHO-n-Hexane

SCF Energy: -269.296116865

ZPE-corrected Energy: -269.199896

$\Delta U$ : -269.193667

$\Delta H$ : -269.192723

$\Delta G$ : -269.229833

Num. Imaginary Frequencies: 0

C	-0.596818	0.920882	-0.143174
C	1.775979	-1.108170	-0.254049
C	1.742773	0.118930	0.255926
C	0.723578	1.121889	-0.059177
H	-1.253429	1.726613	-0.447784
H	1.032830	-1.442443	-0.967249
H	2.565537	-1.800796	0.002922
H	2.547816	0.445585	0.905949
H	1.096398	2.124861	-0.242913
C	-1.276366	-0.330856	0.222995
O	-2.440838	-0.539862	-0.020356
H	-0.677327	-1.070978	0.776797



Z-trans-CHO-Water

SCF Energy: -269.300754585

ZPE-corrected Energy: -269.204548

$\Delta U$ : -269.198331

$\Delta H$ : -269.197387

$\Delta G$ : -269.234451

Num. Imaginary Frequencies: 0

C	-0.598796	0.919679	-0.148036
C	1.776679	-1.107323	-0.254162
C	1.741494	0.119336	0.258489
C	0.722752	1.120913	-0.057653
H	-1.252097	1.727848	-0.453580
H	1.035852	-1.442255	-0.969640
H	2.568317	-1.798009	0.001816
H	2.545760	0.448786	0.907648
H	1.094497	2.125098	-0.235511
C	-1.271861	-0.329455	0.218247
O	-2.442889	-0.541076	-0.014507
H	-0.670824	-1.071758	0.764003

Z-trans-COMe-Acetone

SCF Energy: -308.614198362

ZPE-corrected Energy: -308.490186

$\Delta U$ : -308.482427

$\Delta H$ : -308.481483

$\Delta G$ : -308.522612

Num. Imaginary Frequencies: 0

C	-0.289854	1.203842	0.119494
C	1.803055	-0.947991	-0.725350
C	1.920895	0.016818	0.180665
C	1.039196	1.184001	0.249462
H	-0.796214	2.160815	0.066398
H	1.027198	-0.917513	-1.481262
H	2.490162	-1.782664	-0.751854
H	2.750102	-0.003169	0.880085
H	1.539232	2.138022	0.385494
C	-1.215643	0.046948	-0.008356
O	-2.210117	0.168309	-0.695963
C	-0.995480	-1.222026	0.780551
H	-0.813389	-2.048977	0.095285
H	-0.168299	-1.149839	1.478968
H	-1.920872	-1.432705	1.315798

Z-trans-COMe-Acetonitrile  
SCF Energy: -308.614446883  
ZPE-corrected Energy: -308.490433  
 $\Delta U$ : -308.482679  
 $\Delta H$ : -308.481735  
 $\Delta G$ : -308.522846

Num. Imaginary Frequencies: 0

C	-0.290507	1.203474	0.118854
C	1.804650	-0.947232	-0.724934
C	1.921184	0.017772	0.181072
C	1.038585	1.184267	0.249196
H	-0.797063	2.160341	0.065499
H	1.029081	-0.917668	-1.481183
H	2.492520	-1.781288	-0.750992
H	2.750033	-0.001281	0.880918
H	1.537930	2.138650	0.385205
C	-1.215967	0.046527	-0.008222
O	-2.211931	0.168337	-0.694064
C	-0.994433	-1.223134	0.778904
H	-0.811210	-2.048935	0.092529
H	-0.167356	-1.150914	1.477410
H	-1.919547	-1.435643	1.313906

Z-trans-COMe-Dichloromethane  
SCF Energy: -308.613485384  
ZPE-corrected Energy: -308.489480  
 $\Delta U$ : -308.481705  
 $\Delta H$ : -308.480761  
 $\Delta G$ : -308.521971

Num. Imaginary Frequencies: 0

C	-0.287943	1.204881	0.121281
C	1.798472	-0.950209	-0.726497
C	1.920103	0.014080	0.179490
C	1.040985	1.183220	0.250228
H	-0.793722	2.162167	0.068930
H	1.021732	-0.917171	-1.481379
H	2.483376	-1.786652	-0.754267
H	2.750361	-0.008568	0.877651
H	1.542994	2.136194	0.386375
C	-1.214701	0.048175	-0.008756
O	-2.204907	0.168274	-0.701386
C	-0.998559	-1.218828	0.785256
H	-0.819773	-2.049061	0.103168
H	-0.171094	-1.146822	1.483430
H	-1.924758	-1.424193	1.321171

Z-trans-COMe-DMSO

SCF Energy: -308.614528197

ZPE-corrected Energy: -308.490515

$\Delta U$ : -308.482762

$\Delta H$ : -308.481818

$\Delta G$ : -308.522923

Num. Imaginary Frequencies: 0

C	-0.290717	1.203354	0.118645
C	1.805163	-0.946990	-0.724797
C	1.921280	0.018080	0.181203
C	1.038390	1.184352	0.249109
H	-0.797335	2.160187	0.065207
H	1.029682	-0.917727	-1.481150
H	2.493279	-1.780847	-0.750710
H	2.750017	-0.000668	0.881181
H	1.537511	2.138853	0.385112
C	-1.216071	0.046392	-0.008178
O	-2.212517	0.168349	-0.693449
C	-0.994099	-1.223491	0.778369
H	-0.810526	-2.048921	0.091635
H	-0.167049	-1.151270	1.476899
H	-1.919120	-1.436582	1.313301

Z-trans-COMe-Gas

SCF Energy: -308.607312588

ZPE-corrected Energy: -308.483295

$\Delta U$ : -308.475451

$\Delta H$ : -308.474507

$\Delta G$ : -308.516089

Num. Imaginary Frequencies: 0

C	-0.265038	1.214419	0.137784
C	1.747026	-0.980946	-0.731548
C	1.915485	-0.014749	0.164443
C	1.063016	1.173231	0.255929
H	-0.762711	2.176321	0.096897
H	0.953123	-0.931023	-1.467289
H	2.409535	-1.834690	-0.771182
H	2.762542	-0.057832	0.841527
H	1.584584	2.114969	0.396367
C	-1.202767	0.062407	-0.014404
O	-2.145726	0.169736	-0.761990
C	-1.039309	-1.179436	0.836319
H	-0.948950	-2.051712	0.190997
H	-0.185379	-1.131388	1.504346
H	-1.957408	-1.292085	1.413115

Z-trans-COMe-n-Hexane  
SCF Energy: -308.609912919  
ZPE-corrected Energy: -308.485957  
 $\Delta U$ : -308.478091  
 $\Delta H$ : -308.477146  
 $\Delta G$ : -308.519039

Num. Imaginary Frequencies: 0

C	-0.271671	1.211774	0.133391
C	1.761132	-0.972524	-0.730935
C	1.916785	-0.006948	0.168278
C	1.056778	1.175706	0.254675
H	-0.771290	2.172606	0.089549
H	0.971978	-0.927385	-1.472142
H	2.430213	-1.821297	-0.767788
H	2.759537	-0.044055	0.850918
H	1.572777	2.120589	0.394488
C	-1.205409	0.058428	-0.012871
O	-2.161886	0.168425	-0.746811
C	-1.028117	-1.189274	0.823880
H	-0.921535	-2.053276	0.169747
H	-0.177198	-1.136023	1.495075
H	-1.946379	-1.321532	1.396137

Z-trans-COMe-Water  
SCF Energy: -308.614634213  
ZPE-corrected Energy: -308.490621  
 $\Delta U$ : -308.482870  
 $\Delta H$ : -308.481926  
 $\Delta G$ : -308.523026

Num. Imaginary Frequencies: 0

C	-0.290983	1.203200	0.118375
C	1.805818	-0.946681	-0.724620
C	1.921405	0.018474	0.181369
C	1.038142	1.184460	0.249000
H	-0.797678	2.159992	0.064829
H	1.030446	-0.917807	-1.481102
H	2.494248	-1.780284	-0.750348
H	2.750000	0.000118	0.881515
H	1.536975	2.139109	0.385001
C	-1.216200	0.046219	-0.008123
O	-2.213268	0.168365	-0.692661
C	-0.993674	-1.223945	0.777687
H	-0.809667	-2.048906	0.090494
H	-0.166655	-1.151729	1.476240
H	-1.918573	-1.437770	1.312536

Z-trans-COOH-Acetone  
SCF Energy: -344.562287142  
ZPE-corrected Energy: -344.460769  
 $\Delta U$ : -344.453602  
 $\Delta H$ : -344.452658  
 $\Delta G$ : -344.492951

Num. Imaginary Frequencies: 0

C	0.321411	1.175904	-0.032770
C	-1.851635	-1.012587	0.616961
C	-1.928949	0.043066	-0.183639
C	-1.007914	1.182570	-0.138655
H	0.847925	2.111766	0.099129
H	-1.064694	-1.103800	1.355815
H	-2.580855	-1.809448	0.566770
H	-2.761410	0.134298	-0.873117
H	-1.483747	2.158204	-0.165247
C	1.229262	0.004725	-0.023020
O	2.246704	-0.024059	0.625928
O	0.870415	-0.995516	-0.833872
H	1.532777	-1.696481	-0.753052

Z-trans-COOH-Acetonitrile  
SCF Energy: -344.562571943  
ZPE-corrected Energy: -344.461068  
 $\Delta U$ : -344.453898  
 $\Delta H$ : -344.452954  
 $\Delta G$ : -344.493261

Num. Imaginary Frequencies: 0

C	0.320454	1.176256	-0.033201
C	-1.849363	-1.014456	0.616743
C	-1.929128	0.042032	-0.182610
C	-1.008950	1.182260	-0.138486
H	0.846535	2.112477	0.098092
H	-1.060994	-1.105933	1.354061
H	-2.578042	-1.811850	0.567017
H	-2.763045	0.133281	-0.870330
H	-1.485277	2.157603	-0.165468
C	1.228658	0.005334	-0.022991
O	2.244147	-0.024472	0.629175
O	0.872908	-0.992950	-0.837239
H	1.534364	-1.694758	-0.755590

Z-trans-COOH-Dichloromethane  
SCF Energy: -344.561467475  
ZPE-corrected Energy: -344.459915  
 $\Delta U$ : -344.452751  
 $\Delta H$ : -344.451807  
 $\Delta G$ : -344.492091

Num. Imaginary Frequencies: 0

C	0.322938	1.175077	-0.031993
C	-1.855871	-1.009153	0.617175
C	-1.928799	0.045075	-0.185451
C	-1.006206	1.183237	-0.138922
H	0.850455	2.110182	0.100948
H	-1.071481	-1.099897	1.358744
H	-2.585847	-1.805213	0.565766
H	-2.758501	0.136072	-0.878292
H	-1.480831	2.159530	-0.165227
C	1.230536	0.003602	-0.022878
O	2.251715	-0.022824	0.619343
O	0.865831	-1.000690	-0.827121
H	1.530251	-1.699589	-0.747293

Z-trans-COOH-DMSO  
SCF Energy: -344.562665099  
ZPE-corrected Energy: -344.461165  
 $\Delta U$ : -344.453995  
 $\Delta H$ : -344.453050  
 $\Delta G$ : -344.493356

Num. Imaginary Frequencies: 0

C	0.320504	1.176271	-0.033223
C	-1.849364	-1.014539	0.616629
C	-1.929157	0.042113	-0.182532
C	-1.008923	1.182310	-0.138391
H	0.846599	2.112519	0.097867
H	-1.060919	-1.106259	1.353834
H	-2.578154	-1.811833	0.566856
H	-2.763185	0.133570	-0.870092
H	-1.485201	2.157669	-0.165385
C	1.228656	0.005319	-0.023046
O	2.244182	-0.024488	0.629164
O	0.872868	-0.992957	-0.837179
H	1.534164	-1.694950	-0.755590

Z-trans-COOH-Gas

SCF Energy: -344.554227697

ZPE-corrected Energy: -344.452485

$\Delta U$ : -344.445275

$\Delta H$ : -344.444330

$\Delta G$ : -344.485112

Num. Imaginary Frequencies: 0

C	0.348974	1.158850	-0.012939
C	-1.931053	-0.968159	0.590794
C	-1.938015	0.089493	-0.208502
C	-0.978608	1.195077	-0.131548
H	0.891771	2.083250	0.130712
H	-1.170496	-1.093154	1.350953
H	-2.690218	-1.734124	0.514540
H	-2.743271	0.212651	-0.925060
H	-1.427264	2.184477	-0.149477
C	1.253763	-0.015027	-0.020340
O	2.336267	0.000221	0.502243
O	0.803015	-1.082670	-0.699899
H	1.494856	-1.754908	-0.645215

Z-trans-COOH-n-Hexane

SCF Energy: -344.557300889

ZPE-corrected Energy: -344.455621

$\Delta U$ : -344.448447

$\Delta H$ : -344.447503

$\Delta G$ : -344.487933

Num. Imaginary Frequencies: 0

C	0.330193	1.170842	-0.028261
C	-1.876748	-0.994570	0.614539
C	-1.929850	0.056301	-0.192879
C	-0.998186	1.186707	-0.138980
H	0.862755	2.102353	0.108580
H	-1.101897	-1.088331	1.365379
H	-2.612300	-1.784902	0.556889
H	-2.749242	0.150246	-0.897571
H	-1.466286	2.166508	-0.163336
C	1.237384	-0.001618	-0.022092
O	2.276121	-0.015834	0.586509
O	0.845108	-1.026383	-0.792420
H	1.520382	-1.714114	-0.716618

Z-trans-COOH-Water  
SCF Energy: -344.562786461  
ZPE-corrected Energy: -344.461291  
 $\Delta U$ : -344.454121  
 $\Delta H$ : -344.453176  
 $\Delta G$ : -344.493478

Num. Imaginary Frequencies: 0

C	0.320374	1.176357	-0.033324
C	-1.848958	-1.014930	0.616535
C	-1.929206	0.041958	-0.182308
C	-1.009082	1.182261	-0.138316
H	0.846375	2.112694	0.097564
H	-1.060193	-1.106852	1.353376
H	-2.577734	-1.812248	0.566858
H	-2.763575	0.133561	-0.869433
H	-1.485457	2.157563	-0.165330
C	1.228536	0.005428	-0.023087
O	2.243684	-0.024606	0.629835
O	0.873343	-0.992450	-0.837821
H	1.534379	-1.694712	-0.756144



## Transition states

TS-con-in-3-CF3-Acetone  
SCF Energy: -492.991413139  
ZPE-corrected Energy: -492.901112  
 $\Delta U$ : -492.894390  
 $\Delta H$ : -492.893446  
 $\Delta G$ : -492.932415

Num. Imaginary Frequencies: 1

Imaginary Frequency: -664.4875

C	0.285177	0.608665	-0.763966
C	1.582732	-1.063654	-0.323738
C	2.056724	0.042365	0.411925
C	1.435538	1.137457	-0.140999
H	-0.121151	1.043705	-1.677240
H	1.693416	-1.060829	-1.396691
H	1.442785	-2.047106	0.119859
H	2.702000	-0.011432	1.279649
H	1.763453	2.167072	-0.190677
C	-0.851840	0.007903	0.007306
F	-0.576760	-0.403216	1.246063
F	-1.424077	-1.026430	-0.637331
F	-1.835886	0.930999	0.138149

TS-con-in-3-CF3-Acetonitrile  
SCF Energy: -492.991538580  
ZPE-corrected Energy: -492.901251  
 $\Delta U$ : -492.894528  
 $\Delta H$ : -492.893584  
 $\Delta G$ : -492.932555

Num. Imaginary Frequencies: 1

Imaginary Frequency: -664.4987

C	0.285228	0.608627	-0.764046
C	1.582883	-1.063692	-0.323675
C	2.056807	0.042409	0.411967
C	1.435533	1.137472	-0.140931
H	-0.120936	1.043523	-1.677439
H	1.693433	-1.060786	-1.396652
H	1.443297	-2.047206	0.119906
H	2.702385	-0.011356	1.279471
H	1.763413	2.167088	-0.190729
C	-0.851653	0.007943	0.007141
F	-0.576922	-0.403078	1.246113
F	-1.424183	-1.026508	-0.637216
F	-1.836048	0.930939	0.138071

TS-con-in-3-CF3-Dichloromethane  
SCF Energy: -492.991050048  
ZPE-corrected Energy: -492.900711  
 $\Delta U$ : -492.893991  
 $\Delta H$ : -492.893047  
 $\Delta G$ : -492.932012

Num. Imaginary Frequencies: 1

Imaginary Frequency: -664.4678

C	0.285034	0.608792	-0.763717
C	1.582283	-1.063545	-0.323923
C	2.056489	0.042221	0.411807
C	1.435564	1.137412	-0.141181
H	-0.121741	1.044228	-1.676669
H	1.693322	-1.060926	-1.396809
H	1.441300	-2.046824	0.119703
H	2.700919	-0.011688	1.280141
H	1.763614	2.167011	-0.190552
C	-0.852386	0.007791	0.007773
F	-0.576322	-0.403517	1.245959
F	-1.423697	-1.026270	-0.637616
F	-1.835461	0.931140	0.138282

TS-con-in-3-CF3-DMSO  
SCF Energy: -492.991579499  
ZPE-corrected Energy: -492.901296  
 $\Delta U$ : -492.894573  
 $\Delta H$ : -492.893629  
 $\Delta G$ : -492.932601

Num. Imaginary Frequencies: 1

Imaginary Frequency: -664.5029

C	0.285244	0.608615	-0.764072
C	1.582932	-1.063704	-0.323655
C	2.056834	0.042423	0.411980
C	1.435531	1.137477	-0.140908
H	-0.120864	1.043463	-1.677504
H	1.693437	-1.060771	-1.396640
H	1.443463	-2.047239	0.119920
H	2.702512	-0.011332	1.279412
H	1.763402	2.167093	-0.190748
C	-0.851592	0.007956	0.007087
F	-0.576976	-0.403029	1.246132
F	-1.424214	-1.026536	-0.637176
F	-1.836104	0.930918	0.138041

TS-con-in-3-CF3-Gas

SCF Energy: -492.987697697

ZPE-corrected Energy: -492.897061

$\Delta U$ : -492.890356

$\Delta H$ : -492.889411

$\Delta G$ : -492.928360

Num. Imaginary Frequencies: 1

Imaginary Frequency: -664.9740

C	0.283771	0.611022	-0.760624
C	1.577213	-1.062503	-0.325926
C	2.054449	0.040064	0.410837
C	1.436249	1.136994	-0.142009
H	-0.125823	1.049301	-1.671385
H	1.690094	-1.060402	-1.398368
H	1.426785	-2.044535	0.117111
H	2.692748	-0.016022	1.283494
H	1.767612	2.165681	-0.190651
C	-0.857583	0.006861	0.011639
F	-0.573275	-0.403798	1.246164
F	-1.417769	-1.026412	-0.639150
F	-1.832957	0.931471	0.137018

TS-con-in-3-CF3-n-Hexane  
SCF Energy: -492.989155995  
ZPE-corrected Energy: -492.898638  
 $\Delta U$ : -492.891928  
 $\Delta H$ : -492.890983  
 $\Delta G$ : -492.929937

Num. Imaginary Frequencies: 1

Imaginary Frequency: -664.6241

C	0.284313	0.609833	-0.762121
C	1.579635	-1.062962	-0.324989
C	2.055324	0.041169	0.411243
C	1.435860	1.137179	-0.141812
H	-0.124281	1.046990	-1.673716
H	1.691970	-1.060878	-1.397591
H	1.433347	-2.045488	0.118453
H	2.695963	-0.013749	1.282278
H	1.765384	2.166411	-0.190394
C	-0.855311	0.007241	0.010033
F	-0.574475	-0.403966	1.245931
F	-1.420715	-1.026169	-0.638586
F	-1.833843	0.931463	0.137860

TS-con-in-3-CF3-Water  
SCF Energy: -492.991632756  
ZPE-corrected Energy: -492.901355  
 $\Delta U$ : -492.894632  
 $\Delta H$ : -492.893687  
 $\Delta G$ : -492.932661

Num. Imaginary Frequencies: 1

Imaginary Frequency: -664.5087

C	0.285266	0.608601	-0.764105
C	1.582994	-1.063720	-0.323629
C	2.056869	0.042441	0.411998
C	1.435530	1.137484	-0.140878
H	-0.120770	1.043385	-1.677589
H	1.693441	-1.060750	-1.396624
H	1.443680	-2.047283	0.119938
H	2.702679	-0.011303	1.279335
H	1.763389	2.167099	-0.190772
C	-0.851513	0.007973	0.007016
F	-0.577048	-0.402961	1.246157
F	-1.424252	-1.026575	-0.637123
F	-1.836177	0.930890	0.137999

TS-con-in-3-CHO-Acetone  
SCF Energy: -269.240925332  
ZPE-corrected Energy: -269.145782  
 $\Delta U$ : -269.140536  
 $\Delta H$ : -269.139592  
 $\Delta G$ : -269.174460

Num. Imaginary Frequencies: 1

Imaginary Frequency: -586.6634

C	-0.158291	-0.726966	0.439542
C	0.867524	1.145434	0.401218
C	1.661825	0.237545	-0.354584
C	1.147783	-0.992522	-0.066556
H	-0.601637	-1.289709	1.259501
H	0.828431	1.030414	1.474397
H	0.608311	2.139826	0.045316
H	2.439199	0.512694	-1.054962
H	1.596852	-1.971380	-0.163691
C	-1.138403	-0.007716	-0.376569
O	-2.299192	0.164315	-0.057787
H	-0.760245	0.328988	-1.356583

TS-con-in-3-CHO-Acetonitrile  
SCF Energy: -269.241220701  
ZPE-corrected Energy: -269.146078  
 $\Delta U$ : -269.140833  
 $\Delta H$ : -269.139889  
 $\Delta G$ : -269.174755

Num. Imaginary Frequencies: 1

Imaginary Frequency: -585.9618

C	-0.158088	-0.727829	0.439100
C	0.865693	1.145659	0.401147
C	1.661698	0.238420	-0.353930
C	1.148560	-0.992049	-0.066624
H	-0.600896	-1.290825	1.259158
H	0.826174	1.030892	1.474354
H	0.605768	2.139679	0.044761
H	2.439597	0.514414	-1.053366
H	1.598207	-1.970568	-0.164326
C	-1.137610	-0.008344	-0.376581
O	-2.298832	0.164119	-0.057833
H	-0.759709	0.328310	-1.356586

TS-con-in-3-CHO-Dichloromethane

SCF Energy: -269.240075509

ZPE-corrected Energy: -269.144933

$\Delta U$ : -269.139686

$\Delta H$ : -269.138742

$\Delta G$ : -269.173613

Num. Imaginary Frequencies: 1

Imaginary Frequency: -588.6293

C	-0.158498	-0.725078	0.440362
C	0.871316	1.144839	0.401406
C	1.662291	0.235948	-0.355909
C	1.146516	-0.993460	-0.066234
H	-0.603198	-1.287806	1.259672
H	0.833025	1.029587	1.474535
H	0.612846	2.139719	0.046193
H	2.438220	0.509776	-1.058485
H	1.594429	-1.972960	-0.162672
C	-1.140566	-0.006519	-0.376738
O	-2.299969	0.164681	-0.057440
H	-0.761930	0.329867	-1.357051

TS-con-in-3-CHO-DMSO

SCF Energy: -269.241317247

ZPE-corrected Energy: -269.146174

$\Delta U$ : -269.140930

$\Delta H$ : -269.139986

$\Delta G$ : -269.174851

Num. Imaginary Frequencies: 1

Imaginary Frequency: -585.7300

C	-0.158021	-0.728116	0.438954
C	0.865091	1.145735	0.401122
C	1.661653	0.238707	-0.353715
C	1.148812	-0.991893	-0.066647
H	-0.600654	-1.291193	1.259046
H	0.825432	1.031050	1.474339
H	0.604936	2.139633	0.044577
H	2.439734	0.514976	-1.052831
H	1.598649	-1.970300	-0.164538
C	-1.137348	-0.008549	-0.376585
O	-2.298712	0.164056	-0.057848
H	-0.759528	0.328088	-1.356585

TS-con-in-3-CHO-Gas  
SCF Energy: -269.232626053  
ZPE-corrected Energy: -269.137512  
 $\Delta U$ : -269.132245  
 $\Delta H$ : -269.131300  
 $\Delta G$ : -269.166230

Num. Imaginary Frequencies: 1

Imaginary Frequency: -603.9854

C	-0.162984	-0.705150	0.449314
C	0.912878	1.138857	0.402903
C	1.665201	0.215714	-0.370112
C	1.128426	-1.004078	-0.064956
H	-0.620422	-1.261174	1.266820
H	0.885812	1.017995	1.475349
H	0.672064	2.141933	0.057606
H	2.429252	0.470743	-1.092930
H	1.564462	-1.990601	-0.146588
C	-1.158626	0.009283	-0.377252
O	-2.308286	0.168014	-0.055327
H	-0.774254	0.349238	-1.357023

TS-con-in-3-CHO-n-Hexane  
SCF Energy: -269.235775529  
ZPE-corrected Energy: -269.140638  
 $\Delta U$ : -269.135381  
 $\Delta H$ : -269.134437  
 $\Delta G$ : -269.169337

Num. Imaginary Frequencies: 1

Imaginary Frequency: -597.5732

C	-0.161009	-0.714315	0.445481
C	0.895006	1.141558	0.402656
C	1.663526	0.224784	-0.364441
C	1.136374	-0.999473	-0.065417
H	-0.612990	-1.273598	1.263498
H	0.862832	1.022070	1.475304
H	0.646004	2.141464	0.054298
H	2.432169	0.488195	-1.079182
H	1.577384	-1.983070	-0.153845
C	-1.150835	0.002326	-0.376895
O	-2.304410	0.166897	-0.056432
H	-0.768484	0.340479	-1.356921

TS-con-in-3-CHO-Water  
SCF Energy: -269.241443050  
ZPE-corrected Energy: -269.146300  
 $\Delta U$ : -269.141056  
 $\Delta H$ : -269.140112  
 $\Delta G$ : -269.174977

Num. Imaginary Frequencies: 1

Imaginary Frequency: -585.4265

C	-0.157935	-0.728492	0.438764
C	0.864305	1.145835	0.401090
C	1.661594	0.239082	-0.353434
C	1.149142	-0.991691	-0.066676
H	-0.600339	-1.291677	1.258897
H	0.824461	1.031257	1.474319
H	0.603850	2.139572	0.044337
H	2.439914	0.515712	-1.052129
H	1.599228	-1.969951	-0.164820
C	-1.137004	-0.008817	-0.376589
O	-2.298555	0.163973	-0.057868
H	-0.759291	0.327803	-1.356584

TS-con-in-3-COMe-Acetone  
SCF Energy: -308.553426109  
ZPE-corrected Energy: -308.430554  
 $\Delta U$ : -308.423716  
 $\Delta H$ : -308.422771  
 $\Delta G$ : -308.461410

Num. Imaginary Frequencies: 1

Imaginary Frequency: -612.3167

C	0.159940	-0.971477	-0.330272
C	1.068132	0.183730	1.226329
C	1.811470	0.449305	0.044940
C	1.397778	-0.499022	-0.846045
H	-0.099609	-2.029388	-0.361103
H	1.163355	-0.785717	1.692592
H	0.712079	0.970213	1.888670
H	2.477991	1.289183	-0.104257
H	1.894000	-0.880215	-1.728515
C	-1.040332	-0.147685	-0.071452
O	-2.033200	-0.680470	0.403542
C	-1.120862	1.303696	-0.493498
H	-1.464583	1.899150	0.350569
H	-0.190661	1.707348	-0.876340
H	-1.883723	1.361899	-1.269966



TS-con-in-3-COMe-Acetonitrile  
SCF Energy: -308.553732383  
ZPE-corrected Energy: -308.430857  
 $\Delta U$ : -308.424026  
 $\Delta H$ : -308.423082  
 $\Delta G$ : -308.461689

Num. Imaginary Frequencies: 1

Imaginary Frequency: -611.9232

C	0.159856	-0.969212	-0.336191
C	1.068279	0.176758	1.227840
C	1.811603	0.449182	0.047956
C	1.397641	-0.493256	-0.849029
H	-0.099371	-2.026998	-0.373603
H	1.163044	-0.795609	1.688102
H	0.712774	0.959441	1.894936
H	2.478662	1.289546	-0.095862
H	1.893322	-0.868216	-1.734451
C	-1.039707	-0.147152	-0.071422
O	-2.031981	-0.682416	0.403173
C	-1.122321	1.305126	-0.489330
H	-1.482842	1.895413	0.351219
H	-0.188940	1.715676	-0.856703
H	-1.872908	1.361394	-1.277975

TS-con-in-3-COMe-Dichloromethane

SCF Energy: -308.552546576

ZPE-corrected Energy: -308.429647

$\Delta U$ : -308.422812

$\Delta H$ : -308.421868

$\Delta G$ : -308.460492

Num. Imaginary Frequencies: 1

Imaginary Frequency: -614.0424

C	0.160299	-0.967954	-0.335842
C	1.073591	0.174506	1.227352
C	1.812534	0.450078	0.046011
C	1.396626	-0.491981	-0.851102
H	-0.100090	-2.025442	-0.374543
H	1.169092	-0.799210	1.684458
H	0.719821	0.954945	1.898058
H	2.478054	1.291580	-0.098881
H	1.891716	-0.867898	-1.736524
C	-1.042279	-0.147076	-0.070574
O	-2.032244	-0.684219	0.402294
C	-1.125126	1.306331	-0.485914
H	-1.484094	1.894798	0.356515
H	-0.192429	1.717220	-0.854890
H	-1.877987	1.364340	-1.272134

TS-con-in-3-COMe-DMSO  
SCF Energy: -308.553833206  
ZPE-corrected Energy: -308.430960  
 $\Delta U$ : -308.424129  
 $\Delta H$ : -308.423185  
 $\Delta G$ : -308.461792

Num. Imaginary Frequencies: 1

Imaginary Frequency: -611.7312

C	0.159789	-0.969461	-0.335870
C	1.067825	0.177412	1.227802
C	1.811535	0.449072	0.047937
C	1.397719	-0.493737	-0.848669
H	-0.099359	-2.027283	-0.372760
H	1.162490	-0.794656	1.688729
H	0.712181	0.960576	1.894253
H	2.478738	1.289273	-0.096111
H	1.893407	-0.868960	-1.733969
C	-1.039496	-0.147175	-0.071473
O	-2.032036	-0.682120	0.403315
C	-1.121986	1.304922	-0.489908
H	-1.482416	1.895579	0.350427
H	-0.188558	1.715264	-0.857372
H	-1.872512	1.360974	-1.278636

TS-con-in-3-COMe-Gas  
SCF Energy: -308.545116018  
ZPE-corrected Energy: -308.422176  
 $\Delta U$ : -308.415273  
 $\Delta H$ : -308.414329  
 $\Delta G$ : -308.453243

Num. Imaginary Frequencies: 1

Imaginary Frequency: -625.0615

C	0.161985	-0.969955	-0.314428
C	1.097738	0.188633	1.219900
C	1.816416	0.453588	0.026569
C	1.392009	-0.506529	-0.850241
H	-0.106317	-2.026318	-0.336170
H	1.198763	-0.780740	1.684216
H	0.750939	0.973563	1.889370
H	2.474674	1.296930	-0.141419
H	1.886810	-0.907416	-1.725162
C	-1.056656	-0.148186	-0.066487
O	-2.037305	-0.686099	0.400196
C	-1.132981	1.307510	-0.484863
H	-1.435871	1.903875	0.374101
H	-0.212966	1.700240	-0.903628
H	-1.928657	1.378291	-1.225578

TS-con-in-3-COMe-n-Hexane  
SCF Energy: -308.548213430  
ZPE-corrected Energy: -308.425278  
 $\Delta U$ : -308.418408  
 $\Delta H$ : -308.417464  
 $\Delta G$ : -308.456229

Num. Imaginary Frequencies: 1

Imaginary Frequency: -620.9313

C	0.162019	-0.965454	-0.332407
C	1.087815	0.171810	1.225050
C	1.815023	0.452996	0.039524
C	1.394402	-0.491117	-0.855144
H	-0.102096	-2.022204	-0.371209
H	1.185957	-0.804005	1.676639
H	0.737616	0.947959	1.902816
H	2.476374	1.297164	-0.110515
H	1.889871	-0.873373	-1.737866
C	-1.050541	-0.147304	-0.068447
O	-2.032960	-0.688939	0.400097
C	-1.132686	1.309116	-0.478641
H	-1.480739	1.894236	0.370632
H	-0.203027	1.718632	-0.857498
H	-1.896470	1.372816	-1.253388

TS-con-in-3-COMe-Water  
SCF Energy: -308.553965833  
ZPE-corrected Energy: -308.431109  
 $\Delta U$ : -308.424270  
 $\Delta H$ : -308.423326  
 $\Delta G$ : -308.461967

Num. Imaginary Frequencies: 1

Imaginary Frequency: -611.4218

C	0.159432	-0.972762	-0.328212
C	1.066743	0.187426	1.226028
C	1.811277	0.448684	0.044216
C	1.397871	-0.501800	-0.844323
H	-0.100027	-2.030771	-0.356087
H	1.161450	-0.780440	1.695717
H	0.710713	0.976531	1.885214
H	2.478911	1.287343	-0.106593
H	1.893733	-0.884496	-1.726311
C	-1.039429	-0.147794	-0.071584
O	-2.033608	-0.679003	0.404448
C	-1.119559	1.302684	-0.496381
H	-1.459463	1.900609	0.347492
H	-0.189910	1.704261	-0.882676
H	-1.884551	1.360360	-1.270808

TS-con-in-3-COOH-Acetone  
SCF Energy: -344.498403445  
ZPE-corrected Energy: -344.398146  
 $\Delta U$ : -344.391939  
 $\Delta H$ : -344.390995  
 $\Delta G$ : -344.428360

Num. Imaginary Frequencies: 1

Imaginary Frequency: -636.7155

C	-0.117991	0.998140	-0.061566
C	-1.128485	-0.475111	1.152011
C	-1.801766	-0.431595	-0.093137
C	-1.346696	0.703631	-0.706151
H	0.189923	2.018417	0.155543
H	-1.226298	0.361319	1.826776
H	-0.819075	-1.406829	1.620898
H	-2.456852	-1.202412	-0.478069
H	-1.811687	1.308393	-1.473294
C	1.057733	0.106293	-0.059469
O	2.093607	0.391457	0.503164
O	0.951422	-1.015855	-0.795513
H	1.786989	-1.491851	-0.703189

TS-con-in-3-COOH-Acetonitrile  
SCF Energy: -344.498699855  
ZPE-corrected Energy: -344.398455  
 $\Delta U$ : -344.392248  
 $\Delta H$ : -344.391304  
 $\Delta G$ : -344.428668

Num. Imaginary Frequencies: 1

Imaginary Frequency: -636.5008

C	-0.118060	0.998197	-0.061791
C	-1.127882	-0.475543	1.152116
C	-1.801781	-0.431781	-0.092757
C	-1.346976	0.703421	-0.705972
H	0.189403	2.018574	0.155454
H	-1.225409	0.360828	1.827017
H	-0.818319	-1.407355	1.620695
H	-2.457440	-1.202374	-0.477174
H	-1.812251	1.308126	-1.472982
C	1.057439	0.106409	-0.059620
O	2.093179	0.391124	0.504077
O	0.951925	-1.014867	-0.796751
H	1.786752	-1.492058	-0.703479

TS-con-in-3-COOH-Dichloromethane  
SCF Energy: -344.497548891  
ZPE-corrected Energy: -344.397254  
 $\Delta U$ : -344.391048  
 $\Delta H$ : -344.390104  
 $\Delta G$ : -344.427473

Num. Imaginary Frequencies: 1

Imaginary Frequency: -637.3163

C	-0.117787	0.997982	-0.060714
C	-1.130223	-0.474253	1.151566
C	-1.801784	-0.431028	-0.094333
C	-1.345925	0.704418	-0.706465
H	0.191367	2.017931	0.156290
H	-1.228802	0.362138	1.826204
H	-0.821240	-1.405869	1.620989
H	-2.455420	-1.202268	-0.480842
H	-1.810130	1.309593	-1.473775
C	1.058592	0.105975	-0.059013
O	2.094805	0.392284	0.500712
O	0.950103	-1.018412	-0.792274
H	1.787718	-1.491061	-0.702622

TS-con-in-3-COOH-DMSO  
SCF Energy: -344.498796674  
ZPE-corrected Energy: -344.398556  
 $\Delta U$ : -344.392349  
 $\Delta H$ : -344.391405  
 $\Delta G$ : -344.428769

Num. Imaginary Frequencies: 1

Imaginary Frequency: -636.4295

C	-0.118082	0.998217	-0.061853
C	-1.127683	-0.475696	1.152144
C	-1.801785	-0.431840	-0.092637
C	-1.347067	0.703361	-0.705906
H	0.189234	2.018625	0.155447
H	-1.225118	0.360648	1.827099
H	-0.818067	-1.407544	1.620610
H	-2.457629	-1.202356	-0.476895
H	-1.812437	1.308058	-1.472864
C	1.057342	0.106447	-0.059669
O	2.093042	0.391011	0.504371
O	0.952082	-1.014542	-0.797157
H	1.786668	-1.492124	-0.703586

TS-con-in-3-COOH-Gas  
SCF Energy: -344.489910347  
ZPE-corrected Energy: -344.389323  
 $\Delta U$ : -344.383120  
 $\Delta H$ : -344.382176  
 $\Delta G$ : -344.419597

Num. Imaginary Frequencies: 1

Imaginary Frequency: -641.6836

C	-0.114187	0.997806	-0.039511
C	-1.147349	-0.483031	1.139722
C	-1.802811	-0.421881	-0.112285
C	-1.337647	0.723428	-0.699624
H	0.205923	2.011659	0.191495
H	-1.252564	0.343218	1.825264
H	-0.844043	-1.421680	1.598911
H	-2.446582	-1.188884	-0.522747
H	-1.794610	1.344918	-1.458356
C	1.066862	0.103379	-0.053660
O	2.108751	0.394882	0.477297
O	0.935637	-1.035376	-0.769587
H	1.787559	-1.483490	-0.704098



TS-con-in-3-COOH-n-Hexane  
SCF Energy: -344.493174620  
ZPE-corrected Energy: -344.392704  
 $\Delta U$ : -344.386501  
 $\Delta H$ : -344.385557  
 $\Delta G$ : -344.422954

Num. Imaginary Frequencies: 1

Imaginary Frequency: -639.9514

C	-0.116181	0.997919	-0.051098
C	-1.138943	-0.476663	1.146317
C	-1.801982	-0.426823	-0.102931
C	-1.341734	0.713092	-0.703971
H	0.199041	2.015083	0.171158
H	-1.241354	0.355467	1.825343
H	-0.832221	-1.410893	1.612180
H	-2.449475	-1.197183	-0.501185
H	-1.802266	1.325240	-1.468048
C	1.063064	0.104636	-0.056310
O	2.101919	0.394256	0.488012
O	0.942154	-1.028508	-0.779104
H	1.788352	-1.486674	-0.702750

TS-con-in-3-COOH-Water  
SCF Energy: -344.498922783  
ZPE-corrected Energy: -344.398688  
 $\Delta U$ : -344.392481  
 $\Delta H$ : -344.391537  
 $\Delta G$ : -344.428900

Num. Imaginary Frequencies: 1

Imaginary Frequency: -636.3352

C	-0.118110	0.998247	-0.061920
C	-1.127420	-0.475907	1.152175
C	-1.801787	-0.431912	-0.092486
C	-1.347183	0.703295	-0.705812
H	0.189016	2.018692	0.155463
H	-1.224738	0.360393	1.827210
H	-0.817737	-1.407808	1.620482
H	-2.457868	-1.202329	-0.476548
H	-1.812678	1.307991	-1.472692
C	1.057216	0.106498	-0.059733
O	2.092870	0.390861	0.504744
O	0.952276	-1.014118	-0.797684
H	1.786547	-1.492211	-0.703737

TS-con-in-3-Me-Acetone  
SCF Energy: -195.199515336  
ZPE-corrected Energy: -195.086746  
 $\Delta U$ : -195.081761  
 $\Delta H$ : -195.080817  
 $\Delta G$ : -195.114268

Num. Imaginary Frequencies: 1

Imaginary Frequency: -705.6738

C	-0.667273	-0.435650	0.489777
C	0.903352	1.037401	0.335443
C	1.321023	-0.079129	-0.420629
C	0.482682	-1.094123	-0.019271
H	-1.153870	-0.858472	1.373726
H	0.884925	0.956451	1.411597
H	0.943818	2.058521	-0.040959
H	2.087521	-0.078335	-1.187280
H	0.683245	-2.157047	0.055747
C	-1.653955	0.329717	-0.364188
H	-2.482447	-0.335748	-0.627042
H	-2.084736	1.176875	0.169380
H	-1.193428	0.688460	-1.281960

TS-con-in-3-Me-Acetonitrile  
SCF Energy: -195.199565832  
ZPE-corrected Energy: -195.086808  
 $\Delta U$ : -195.081821  
 $\Delta H$ : -195.080877  
 $\Delta G$ : -195.114330

Num. Imaginary Frequencies: 1

Imaginary Frequency: -705.6778

C	-0.667218	-0.435773	0.489692
C	0.903136	1.037487	0.335484
C	1.321129	-0.078969	-0.420563
C	0.482853	-1.094137	-0.019324
H	-1.153739	-0.858522	1.373689
H	0.884311	0.956507	1.411649
H	0.943272	2.058605	-0.040931
H	2.087677	-0.077968	-1.187185
H	0.683549	-2.157039	0.055836
C	-1.653955	0.329591	-0.364215
H	-2.482397	-0.335956	-0.627016
H	-2.084814	1.176621	0.169477
H	-1.193524	0.688556	-1.281964

TS-con-in-3-Me-Dichloromethane  
SCF Energy: -195.199373127  
ZPE-corrected Energy: -195.086571  
 $\Delta U$ : -195.081589  
 $\Delta H$ : -195.080644  
 $\Delta G$ : -195.114091

Num. Imaginary Frequencies: 1

Imaginary Frequency: -705.7750

C	-0.667240	-0.435569	0.489981
C	0.903279	1.037273	0.335424
C	1.320749	-0.079288	-0.420689
C	0.482471	-1.094096	-0.019208
H	-1.154308	-0.858665	1.373619
H	0.885883	0.956448	1.411537
H	0.944437	2.058439	-0.040893
H	2.087041	-0.078447	-1.187480
H	0.683063	-2.156988	0.055380
C	-1.653707	0.329877	-0.364159
H	-2.482006	-0.335505	-0.627844
H	-2.084773	1.177012	0.169251
H	-1.192649	0.688525	-1.281664

TS-con-in-3-Me-DMSO  
SCF Energy: -195.199582468  
ZPE-corrected Energy: -195.086828  
 $\Delta U$ : -195.081841  
 $\Delta H$ : -195.080897  
 $\Delta G$ : -195.114351

Num. Imaginary Frequencies: 1

Imaginary Frequency: -705.6789

C	-0.667200	-0.435813	0.489664
C	0.903064	1.037516	0.335498
C	1.321163	-0.078915	-0.420542
C	0.482910	-1.094142	-0.019341
H	-1.153695	-0.858538	1.373678
H	0.884108	0.956525	1.411666
H	0.943091	2.058633	-0.040921
H	2.087729	-0.077846	-1.187154
H	0.683650	-2.157037	0.055866
C	-1.653956	0.329549	-0.364224
H	-2.482380	-0.336025	-0.627007
H	-2.084839	1.176537	0.169509
H	-1.193555	0.688587	-1.281965

TS-con-in-3-Me-Gas  
SCF Energy: -195.198297924  
ZPE-corrected Energy: -195.085250  
 $\Delta U$ : -195.080287  
 $\Delta H$ : -195.079343  
 $\Delta G$ : -195.112756

Num. Imaginary Frequencies: 1

Imaginary Frequency: -705.4206

C	-0.668131	-0.433573	0.491543
C	0.906947	1.035564	0.334902
C	1.318287	-0.081836	-0.422213
C	0.479534	-1.093810	-0.018112
H	-1.156247	-0.858061	1.374420
H	0.896849	0.954914	1.410753
H	0.953774	2.056925	-0.040619
H	2.083645	-0.084445	-1.189474
H	0.678252	-2.156994	0.052958
C	-1.653358	0.332093	-0.363678
H	-2.483508	-0.331055	-0.627324
H	-2.081959	1.182515	0.166655
H	-1.190478	0.685573	-1.282022

TS-con-in-3-Me-n-Hexane  
SCF Energy: -195.198719601  
ZPE-corrected Energy: -195.085772  
 $\Delta U$ : -195.080801  
 $\Delta H$ : -195.079857  
 $\Delta G$ : -195.113285

Num. Imaginary Frequencies: 1

Imaginary Frequency: -705.4798

C	-0.667990	-0.433888	0.491069
C	0.906462	1.036071	0.334978
C	1.319218	-0.081326	-0.421804
C	0.480239	-1.093959	-0.018496
H	-1.155730	-0.857516	1.374398
H	0.893795	0.955361	1.410932
H	0.951553	2.057286	-0.041001
H	2.084923	-0.083347	-1.188908
H	0.679130	-2.157103	0.054607
C	-1.653811	0.331509	-0.363816
H	-2.483125	-0.332685	-0.627406
H	-2.083466	1.180631	0.167718
H	-1.191786	0.686938	-1.281921

TS-con-in-3-Me-Water  
SCF Energy: -195.199604243  
ZPE-corrected Energy: -195.086855  
 $\Delta U$ : -195.081868  
 $\Delta H$ : -195.080923  
 $\Delta G$ : -195.114377

Num. Imaginary Frequencies: 1

Imaginary Frequency: -705.6802

C	-0.667175	-0.435867	0.489627
C	0.902970	1.037553	0.335517
C	1.321208	-0.078845	-0.420514
C	0.482985	-1.094149	-0.019364
H	-1.153638	-0.858560	1.373662
H	0.883841	0.956548	1.411690
H	0.942852	2.058669	-0.040906
H	2.087795	-0.077684	-1.187114
H	0.683783	-2.157034	0.055906
C	-1.653955	0.329494	-0.364236
H	-2.482359	-0.336115	-0.626995
H	-2.084872	1.176427	0.169551
H	-1.193596	0.688629	-1.281967

TS-con-in-3-NH2-Acetone  
SCF Energy: -211.239677565  
ZPE-corrected Energy: -211.137884  
 $\Delta U$ : -211.132877  
 $\Delta H$ : -211.131933  
 $\Delta G$ : -211.165482

Num. Imaginary Frequencies: 1

Imaginary Frequency: -730.5841

C	-0.696066	-0.399578	0.461910
C	0.894747	1.036085	0.307620
C	1.310091	-0.106451	-0.408048
C	0.452511	-1.097498	0.008375
H	-1.234320	-0.792510	1.330194
H	0.867257	0.987989	1.385409
H	0.948489	2.043335	-0.101782
H	2.082630	-0.132934	-1.168230
H	0.625956	-2.161576	0.118728
N	-1.544352	0.348922	-0.451358
H	-2.390811	-0.194566	-0.599351
H	-1.856442	1.212454	-0.024604

TS-con-in-3-NH2-Acetonitrile  
SCF Energy: -211.239898954  
ZPE-corrected Energy: -211.138108  
 $\Delta U$ : -211.133101  
 $\Delta H$ : -211.132157  
 $\Delta G$ : -211.165705

Num. Imaginary Frequencies: 1

Imaginary Frequency: -730.7574

C	-0.695946	-0.399855	0.461447
C	0.894307	1.036306	0.307619
C	1.310610	-0.106108	-0.407792
C	0.453016	-1.097439	0.008152
H	-1.234042	-0.792731	1.329757
H	0.865700	0.988201	1.385393
H	0.947888	2.043657	-0.101575
H	2.084011	-0.132445	-1.167138
H	0.626860	-2.161399	0.119144
N	-1.544938	0.348378	-0.451524
H	-2.392583	-0.194206	-0.596189
H	-1.855194	1.212852	-0.025278

TS-con-in-3-NH2-Dichloromethane  
SCF Energy: -211.239061679  
ZPE-corrected Energy: -211.137261  
 $\Delta U$ : -211.132253  
 $\Delta H$ : -211.131309  
 $\Delta G$ : -211.164862

Num. Imaginary Frequencies: 1

Imaginary Frequency: -730.1003

C	-0.696379	-0.398939	0.463127
C	0.895820	1.035486	0.307757
C	1.308624	-0.107235	-0.408883
C	0.451343	-1.097630	0.008958
H	-1.235064	-0.792181	1.331266
H	0.871712	0.987231	1.385578
H	0.949764	2.042550	-0.102035
H	2.078799	-0.133986	-1.171350
H	0.623907	-2.161998	0.117570
N	-1.542856	0.350246	-0.450910
H	-2.386494	-0.195177	-0.607123
H	-1.859079	1.211751	-0.023289

TS-con-in-3-NH2-DMSO  
SCF Energy: -211.239972179  
ZPE-corrected Energy: -211.138182  
 $\Delta U$ : -211.133176  
 $\Delta H$ : -211.132231  
 $\Delta G$ : -211.165779

Num. Imaginary Frequencies: 1

Imaginary Frequency: -730.8157

C	-0.695904	-0.399953	0.461290
C	0.894152	1.036382	0.307620
C	1.310784	-0.105988	-0.407705
C	0.453191	-1.097418	0.008076
H	-1.233945	-0.792814	1.329608
H	0.865166	0.988271	1.385389
H	0.947672	2.043767	-0.101502
H	2.084475	-0.132270	-1.166770
H	0.627174	-2.161338	0.119278
N	-1.545133	0.348192	-0.451578
H	-2.393174	-0.194085	-0.595134
H	-1.854770	1.212985	-0.025508

TS-con-in-3-NH2-Gas  
SCF Energy: -211.234671907  
ZPE-corrected Energy: -211.132820  
 $\Delta U$ : -211.127797  
 $\Delta H$ : -211.126853  
 $\Delta G$ : -211.160445

Num. Imaginary Frequencies: 1

Imaginary Frequency: -726.8113

C	-0.698818	-0.393357	0.471912
C	0.904213	1.031249	0.307416
C	1.299542	-0.113338	-0.413966
C	0.441868	-1.098295	0.012731
H	-1.238297	-0.785036	1.341827
H	0.896478	0.982695	1.385133
H	0.961553	2.036936	-0.105150
H	2.056506	-0.143726	-1.188766
H	0.608096	-2.164172	0.113549
N	-1.532937	0.359410	-0.447057
H	-2.348615	-0.202659	-0.672292
H	-1.885989	1.202540	-0.013462

TS-con-in-3-NH2-n-Hexane  
SCF Energy: -211.236341758  
ZPE-corrected Energy: -211.134527  
 $\Delta U$ : -211.129504  
 $\Delta H$ : -211.128560  
 $\Delta G$ : -211.162153

Num. Imaginary Frequencies: 1

Imaginary Frequency: -728.0531

C	-0.697840	-0.395385	0.468699
C	0.901086	1.032849	0.307593
C	1.302819	-0.111169	-0.412058
C	0.445309	-1.098141	0.011431
H	-1.237392	-0.788045	1.337621
H	0.887946	0.984557	1.385393
H	0.957190	2.038906	-0.104272
H	2.063932	-0.140127	-1.183078
H	0.613772	-2.163527	0.114762
N	-1.536370	0.356237	-0.448602
H	-2.363012	-0.200231	-0.647890
H	-1.876087	1.205889	-0.016309

TS-con-in-3-NH2-Water

SCF Energy: -211.240068250

ZPE-corrected Energy: -211.138279

$\Delta U$ : -211.133273

$\Delta H$ : -211.132329

$\Delta G$ : -211.165875

Num. Imaginary Frequencies: 1

Imaginary Frequency: -730.8882

C	-0.695841	-0.400121	0.461073
C	0.893886	1.036497	0.307641
C	1.311010	-0.105792	-0.407592
C	0.453466	-1.097391	0.007979
H	-1.233795	-0.792961	1.329412
H	0.864378	0.988366	1.385399
H	0.947286	2.043938	-0.101371
H	2.085037	-0.131935	-1.166334
H	0.627689	-2.161248	0.119435
N	-1.545371	0.347926	-0.451654
H	-2.393932	-0.193940	-0.593760
H	-1.854194	1.213133	-0.025807



TS-con-in-3-NO2-Acetone  
SCF Energy: -360.417155129  
ZPE-corrected Energy: -360.328975  
 $\Delta U$ : -360.323109  
 $\Delta H$ : -360.322165  
 $\Delta G$ : -360.359010

Num. Imaginary Frequencies: 1

Imaginary Frequency: -642.7447

C	-0.043416	0.914534	0.277647
C	-1.178696	-0.808845	0.930019
C	-1.778502	-0.310754	-0.246572
C	-1.260082	0.946712	-0.427226
H	0.420940	1.751806	0.782476
H	-1.250736	-0.231625	1.838340
H	-0.941268	-1.861267	1.064818
H	-2.433318	-0.876488	-0.896498
H	-1.661363	1.802158	-0.952246
N	1.048249	0.003081	-0.117429
O	0.935818	-0.758181	-1.054299
O	2.075704	0.126177	0.527037

TS-con-in-3-NO2-Acetonitrile  
SCF Energy: -360.417489205  
ZPE-corrected Energy: -360.329320  
 $\Delta U$ : -360.323454  
 $\Delta H$ : -360.322510  
 $\Delta G$ : -360.359352

Num. Imaginary Frequencies: 1

Imaginary Frequency: -642.4159

C	-0.043318	0.913687	0.280141
C	-1.178340	-0.812102	0.927607
C	-1.778838	-0.310194	-0.247149
C	-1.260254	0.947569	-0.424563
H	0.420307	1.749506	0.787977
H	-1.249645	-0.237586	1.837711
H	-0.941118	-1.864989	1.059081
H	-2.434832	-0.873635	-0.897883
H	-1.661614	1.804574	-0.946952
N	1.047943	0.003938	-0.117345
O	0.936748	-0.753502	-1.057774
O	2.075227	0.123603	0.528433

TS-con-in-3-NO2-Dichloromethane

SCF Energy: -360.416195448

ZPE-corrected Energy: -360.327987

$\Delta U$ : -360.322122

$\Delta H$ : -360.321178

$\Delta G$ : -360.358027

Num. Imaginary Frequencies: 1

Imaginary Frequency: -643.5913

C	-0.043481	0.917122	0.269777
C	-1.180075	-0.798434	0.937605
C	-1.777490	-0.312276	-0.244890
C	-1.259362	0.944093	-0.435810
H	0.422929	1.758907	0.765316
H	-1.254307	-0.212564	1.840136
H	-0.942158	-1.849361	1.082909
H	-2.428757	-0.885127	-0.892130
H	-1.660305	1.794913	-0.968602
N	1.049134	0.000302	-0.117552
O	0.932628	-0.773509	-1.042663
O	2.077510	0.134520	0.522056

TS-con-in-3-NO2-DMSO

SCF Energy: -360.417598479

ZPE-corrected Energy: -360.329432

$\Delta U$ : -360.323567

$\Delta H$ : -360.322623

$\Delta G$ : -360.359464

Num. Imaginary Frequencies: 1

Imaginary Frequency: -642.3062

C	-0.043294	0.913386	0.281056
C	-1.178188	-0.813310	0.926699
C	-1.778961	-0.309992	-0.247346
C	-1.260326	0.947883	-0.423555
H	0.420088	1.748667	0.789975
H	-1.249204	-0.239811	1.837472
H	-0.941034	-1.866367	1.056924
H	-2.435398	-0.872577	-0.898376
H	-1.661710	1.805442	-0.945009
N	1.047842	0.004251	-0.117324
O	0.937081	-0.751765	-1.059057
O	2.075042	0.122651	0.528951

TS-con-in-3-NO2-Gas  
SCF Energy: -360.407847257  
ZPE-corrected Energy: -360.319426  
 $\Delta U$ : -360.313564  
 $\Delta H$ : -360.312620  
 $\Delta G$ : -360.349519

Num. Imaginary Frequencies: 1

Imaginary Frequency: -647.7627

C	-0.040349	0.931262	0.222674
C	-1.199651	-0.724672	0.979257
C	-1.770618	-0.313079	-0.241250
C	-1.247491	0.933303	-0.491523
H	0.444817	1.796065	0.658480
H	-1.293544	-0.085232	1.842283
H	-0.965129	-1.764931	1.191765
H	-2.394996	-0.928536	-0.875711
H	-1.640281	1.755679	-1.073244
N	1.057414	-0.024678	-0.114395
O	0.900861	-0.893949	-0.936747
O	2.098625	0.198801	0.467027

TS-con-in-3-NO2-n-Hexane  
SCF Energy: -360.411367425  
ZPE-corrected Energy: -360.323021  
 $\Delta U$ : -360.317159  
 $\Delta H$ : -360.316215  
 $\Delta G$ : -360.353096

Num. Imaginary Frequencies: 1

Imaginary Frequency: -646.8095

C	-0.042296	0.926911	0.237557
C	-1.190407	-0.751206	0.967189
C	-1.773280	-0.315280	-0.240319
C	-1.253270	0.934850	-0.472843
H	0.435022	1.785634	0.692940
H	-1.276765	-0.129137	1.843811
H	-0.953796	-1.795206	1.157862
H	-2.408543	-0.916768	-0.877376
H	-1.650485	1.766230	-1.038380
N	1.053995	-0.014123	-0.116557
O	0.915222	-0.846502	-0.981847
O	2.088793	0.173560	0.492789

TS-con-in-3-NO2-Water  
SCF Energy: -360.417740915  
ZPE-corrected Energy: -360.329579  
 $\Delta U$ : -360.323713  
 $\Delta H$ : -360.322769  
 $\Delta G$ : -360.359610

Num. Imaginary Frequencies: 1

Imaginary Frequency: -642.1709

C	-0.043266	0.912976	0.282263
C	-1.178025	-0.814859	0.925525
C	-1.779115	-0.309726	-0.247621
C	-1.260403	0.948288	-0.422265
H	0.419792	1.747545	0.792614
H	-1.248705	-0.242670	1.837155
H	-0.940971	-1.868133	1.054155
H	-2.436092	-0.871212	-0.899059
H	-1.661812	1.806566	-0.942508
N	1.047714	0.004652	-0.117287
O	0.937523	-0.749499	-1.060724
O	2.074806	0.121407	0.529629

TS-con-in-3-OMe-Acetone  
SCF Energy: -270.406619956  
ZPE-corrected Energy: -270.289306  
 $\Delta U$ : -270.283106  
 $\Delta H$ : -270.282161  
 $\Delta G$ : -270.319148

Num. Imaginary Frequencies: 1

Imaginary Frequency: -734.5740

C	-0.147190	-0.235675	0.660744
C	1.556214	0.955075	0.166305
C	1.675741	-0.252472	-0.553063
C	0.795012	-1.112331	0.065364
H	-0.631392	-0.498987	1.606712
H	1.730084	0.937921	1.230902
H	1.658661	1.933085	-0.298856
H	2.280176	-0.405644	-1.440080
H	0.852570	-2.183662	0.214864
O	-0.987106	0.590022	-0.087931
C	-2.253297	-0.020758	-0.276281
H	-2.878788	0.695966	-0.802793
H	-2.158344	-0.933943	-0.869880
H	-2.714999	-0.267940	0.684165

TS-con-in-3-OMe-Acetonitrile  
SCF Energy: -270.406767284  
ZPE-corrected Energy: -270.289463  
 $\Delta U$ : -270.283260  
 $\Delta H$ : -270.282316  
 $\Delta G$ : -270.319309

Num. Imaginary Frequencies: 1

Imaginary Frequency: -734.6362

C	-0.147307	-0.235533	0.660319
C	1.556656	0.955049	0.166551
C	1.676242	-0.252617	-0.552778
C	0.795036	-1.112282	0.065264
H	-0.631740	-0.498633	1.606159
H	1.729852	0.937851	1.231272
H	1.660156	1.933020	-0.298536
H	2.281475	-0.406037	-1.439222
H	0.852427	-2.183559	0.215178
O	-0.987207	0.589870	-0.088871
C	-2.254000	-0.020657	-0.275726
H	-2.879434	0.695628	-0.802891
H	-2.159709	-0.934686	-0.868086
H	-2.715138	-0.266301	0.685313

TS-con-in-3-OMe-Dichloromethane  
SCF Energy: -270.406207463

ZPE-corrected Energy: -270.288866  
 $\Delta U$ : -270.282672  
 $\Delta H$ : -270.281727  
 $\Delta G$ : -270.318696

Num. Imaginary Frequencies: 1

Imaginary Frequency: -734.3080

C	-0.146770	-0.235509	0.662500
C	1.555368	0.954880	0.165082
C	1.673655	-0.252698	-0.554258
C	0.794233	-1.112428	0.065999
H	-0.629930	-0.498740	1.609216
H	1.731363	0.937958	1.229288
H	1.655408	1.932851	-0.300505
H	2.275429	-0.405610	-1.443086
H	0.851884	-2.183793	0.215338
O	-0.986801	0.590967	-0.084636
C	-2.250777	-0.021224	-0.278355
H	-2.876360	0.696492	-0.803446
H	-2.152912	-0.931863	-0.875501
H	-2.714723	-0.273155	0.679987

TS-con-in-3-OMe-DMSO  
SCF Energy: -270.406815900  
ZPE-corrected Energy: -270.289514  
 $\Delta U$ : -270.283312  
 $\Delta H$ : -270.282367  
 $\Delta G$ : -270.319362

Num. Imaginary Frequencies: 1

Imaginary Frequency: -734.6577

C	-0.147350	-0.235498	0.660154
C	1.556792	0.955046	0.166652
C	1.676438	-0.252644	-0.552665
C	0.795068	-1.112268	0.065216
H	-0.631875	-0.498547	1.605939
H	1.729748	0.937830	1.231417
H	1.660626	1.933010	-0.298401
H	2.281945	-0.406130	-1.438914
H	0.852413	-2.183528	0.215253
O	-0.987244	0.589803	-0.089216
C	-2.254254	-0.020620	-0.275519
H	-2.879687	0.695529	-0.802865
H	-2.160221	-0.934929	-0.867475
H	-2.715162	-0.265754	0.685736

TS-con-in-3-OMe-Gas  
SCF Energy: -270.403122572  
ZPE-corrected Energy: -270.285588  
 $\Delta U$ : -270.279431  
 $\Delta H$ : -270.278487  
 $\Delta G$ : -270.315332

Num. Imaginary Frequencies: 1

Imaginary Frequency: -732.2113

C	-0.144486	-0.237138	0.672059
C	1.547727	0.954581	0.159710
C	1.661505	-0.251149	-0.561212
C	0.791539	-1.113285	0.068336
H	-0.622899	-0.503435	1.621568
H	1.738008	0.937639	1.221114
H	1.629739	1.933288	-0.306818
H	2.247220	-0.399806	-1.461144
H	0.852400	-2.185045	0.213387
O	-0.984453	0.594544	-0.065343
C	-2.235233	-0.022888	-0.290060
H	-2.861558	0.702660	-0.803784
H	-2.122273	-0.917291	-0.909825
H	-2.711318	-0.305095	0.655248

TS-con-in-3-OMe-n-Hexane  
SCF Energy: -270.404329313  
ZPE-corrected Energy: -270.286868  
 $\Delta U$ : -270.280699  
 $\Delta H$ : -270.279755  
 $\Delta G$ : -270.316640

Num. Imaginary Frequencies: 1

Imaginary Frequency: -733.1152

C	-0.145330	-0.235951	0.668972
C	1.550570	0.954649	0.161130
C	1.665865	-0.252167	-0.558673
C	0.792234	-1.113068	0.067876
H	-0.625361	-0.500801	1.617619
H	1.736201	0.938302	1.223495
H	1.638734	1.932862	-0.305665
H	2.257309	-0.402851	-1.454614
H	0.851920	-2.184692	0.214589
O	-0.985414	0.593797	-0.071960
C	-2.240635	-0.022730	-0.286191
H	-2.867378	0.700040	-0.803124
H	-2.132336	-0.922163	-0.898994
H	-2.712002	-0.295480	0.663698

TS-con-in-3-OMe-Water  
SCF Energy: -270.406879597  
ZPE-corrected Energy: -270.289582  
 $\Delta U$ : -270.283379  
 $\Delta H$ : -270.282434  
 $\Delta G$ : -270.319432

Num. Imaginary Frequencies: 1

Imaginary Frequency: -734.6839

C	-0.147406	-0.235444	0.659942
C	1.556976	0.955039	0.166779
C	1.676696	-0.252683	-0.552513
C	0.795108	-1.112251	0.065156
H	-0.632047	-0.498424	1.605657
H	1.729616	0.937809	1.231601
H	1.661232	1.932990	-0.298241
H	2.282551	-0.406258	-1.438516
H	0.852386	-2.183489	0.215355
O	-0.987298	0.589722	-0.089663
C	-2.254585	-0.020576	-0.275250
H	-2.880040	0.695409	-0.802787
H	-2.160884	-0.935221	-0.866723
H	-2.715168	-0.265100	0.686283

TS-con-out-3-CF3-Acetone  
SCF Energy: -492.993272597  
ZPE-corrected Energy: -492.903181  
 $\Delta U$ : -492.896167  
 $\Delta H$ : -492.895223  
 $\Delta G$ : -492.936052

Num. Imaginary Frequencies: 1

Imaginary Frequency: -652.0912

C	0.389825	0.018580	-0.466458
C	2.167284	-0.994176	0.085544
C	2.494746	0.378709	-0.007461
C	1.282385	1.023322	-0.023740
H	0.532785	-0.445004	-1.431230
H	2.750080	-1.773735	-0.400880
H	1.577584	-1.332165	0.923736
H	3.488208	0.784248	-0.146419
H	1.022360	2.031079	0.272985
C	-1.039234	-0.037486	-0.019553
F	-1.475133	-1.302372	0.083041
F	-1.225696	0.544050	1.172229
F	-1.870399	0.580754	-0.880624

TS-con-out-3-CF3-Acetonitrile  
SCF Energy: -492.993385981  
ZPE-corrected Energy: -492.903312  
 $\Delta U$ : -492.896295  
 $\Delta H$ : -492.895351  
 $\Delta G$ : -492.936207

Num. Imaginary Frequencies: 1

Imaginary Frequency: -652.1189

C	0.389890	0.018371	-0.466462
C	2.167659	-0.994111	0.085645
C	2.494759	0.378861	-0.007399
C	1.282283	1.023293	-0.023742
H	0.532959	-0.445475	-1.431099
H	2.750547	-1.773488	-0.400907
H	1.577887	-1.332216	0.923752
H	3.488134	0.784532	-0.146583
H	1.022210	2.031177	0.272575
C	-1.039074	-0.037582	-0.019619
F	-1.477148	-1.302205	0.077191
F	-1.224758	0.538703	1.174957
F	-1.869743	0.586000	-0.877512



TS-con-out-3-CF3-Dichloromethane  
SCF Energy: -492.992945019  
ZPE-corrected Energy: -492.902808  
 $\Delta U$ : -492.895798  
 $\Delta H$ : -492.894854  
 $\Delta G$ : -492.935668

Num. Imaginary Frequencies: 1

Imaginary Frequency: -652.0009

C	0.389583	0.019199	-0.466655
C	2.166267	-0.994307	0.085365
C	2.494628	0.378334	-0.007614
C	1.282566	1.023429	-0.023885
H	0.532468	-0.443852	-1.431677
H	2.748971	-1.774393	-0.400471
H	1.576526	-1.331918	0.923653
H	3.488326	0.783543	-0.145875
H	1.022632	2.030816	0.273996
C	-1.039674	-0.037254	-0.019371
F	-1.470982	-1.302652	0.094048
F	-1.227270	0.554080	1.167090
F	-1.871653	0.570728	-0.886322

TS-con-out-3-CF3-DMSO  
SCF Energy: -492.993422964  
ZPE-corrected Energy: -492.903356  
 $\Delta U$ : -492.896337  
 $\Delta H$ : -492.895393  
 $\Delta G$ : -492.936270

Num. Imaginary Frequencies: 1

Imaginary Frequency: -652.1943

C	0.389937	0.018064	-0.466337
C	2.167858	-0.994136	0.085564
C	2.494747	0.378926	-0.007275
C	1.282180	1.023159	-0.023613
H	0.532956	-0.445705	-1.431024
H	2.750821	-1.773293	-0.401235
H	1.578287	-1.332473	0.923705
H	3.488052	0.784766	-0.146468
H	1.021965	2.031066	0.272548
C	-1.039008	-0.037720	-0.019634
F	-1.478354	-1.302055	0.075198
F	-1.224425	0.536863	1.175869
F	-1.869040	0.588068	-0.876596

TS-con-out-3-CF3-Gas  
SCF Energy: -492.989995429  
ZPE-corrected Energy: -492.899514  
 $\Delta U$ : -492.892533  
 $\Delta H$ : -492.891589  
 $\Delta G$ : -492.932547

Num. Imaginary Frequencies: 1

Imaginary Frequency: -660.1795

C	0.384545	0.028560	-0.498889
C	2.145785	-0.999777	0.077638
C	2.484086	0.370977	0.006309
C	1.276385	1.022610	-0.030997
H	0.543564	-0.429902	-1.462271
H	2.739685	-1.778906	-0.397095
H	1.529616	-1.342013	0.894659
H	3.482356	0.773149	-0.106091
H	1.010866	2.028405	0.264936
C	-1.040730	-0.037575	-0.028602
F	-1.841819	-0.624822	-0.923635
F	-1.157294	-0.733058	1.114642
F	-1.534944	1.184602	0.214893

TS-con-out-3-CF3-n-Hexane  
SCF Energy: -492.991192235  
ZPE-corrected Energy: -492.900904  
 $\Delta U$ : -492.893883  
 $\Delta H$ : -492.892939  
 $\Delta G$ : -492.934383

Num. Imaginary Frequencies: 1

Imaginary Frequency: -658.7451

C	0.384727	0.022164	-0.496746
C	2.157085	-0.997093	0.080167
C	2.483830	0.376047	0.005580
C	1.272033	1.020599	-0.030395
H	0.544569	-0.439078	-1.458635
H	2.755794	-1.772446	-0.394127
H	1.542925	-1.341770	0.897784
H	3.479130	0.784637	-0.110019
H	1.003319	2.026302	0.264348
C	-1.039640	-0.040695	-0.028891
F	-1.796573	-0.814217	-0.814898
F	-1.139373	-0.534053	1.216850
F	-1.605603	1.176738	0.000532

TS-con-out-3-CF3-Water  
SCF Energy: -492.993471194  
ZPE-corrected Energy: -492.903410  
 $\Delta U$ : -492.896392  
 $\Delta H$ : -492.895448  
 $\Delta G$ : -492.936316

Num. Imaginary Frequencies: 1

Imaginary Frequency: -652.1271

C	0.389940	0.018177	-0.466409
C	2.168013	-0.994051	0.085699
C	2.494779	0.379003	-0.007362
C	1.282191	1.023252	-0.023708
H	0.533048	-0.445808	-1.430976
H	2.750992	-1.773251	-0.400987
H	1.578248	-1.332283	0.923766
H	3.488070	0.784818	-0.146721
H	1.022055	2.031220	0.272328
C	-1.038971	-0.037677	-0.019673
F	-1.478855	-1.302049	0.072327
F	-1.224004	0.534230	1.177197
F	-1.869156	0.590385	-0.874933

TS-con-out-3-CHO-Acetone  
SCF Energy: -269.230844881  
ZPE-corrected Energy: -269.136539  
 $\Delta U$ : -269.130947  
 $\Delta H$ : -269.130003  
 $\Delta G$ : -269.165743

Num. Imaginary Frequencies: 1

Imaginary Frequency: -659.7457

C	0.192173	0.159580	0.383859
C	-1.399005	-1.109196	-0.172189
C	-1.964790	0.185856	-0.033730
C	-0.884293	1.022270	0.014496
H	0.142504	-0.393486	1.313056
H	-1.817252	-1.991013	0.308482
H	-0.781755	-1.318599	-1.032458
H	-3.014841	0.403931	0.111537
H	-0.811483	2.080585	-0.202442
C	1.541008	0.324988	-0.171407
O	2.462331	-0.436068	0.025263
H	1.673625	1.206134	-0.826455

TS-con-out-3-CHO-Acetonitrile  
SCF Energy: -269.231077504  
ZPE-corrected Energy: -269.136776  
 $\Delta U$ : -269.131184  
 $\Delta H$ : -269.130240  
 $\Delta G$ : -269.165980

Num. Imaginary Frequencies: 1

Imaginary Frequency: -659.7557

C	0.192268	0.159465	0.383859
C	-1.399129	-1.109236	-0.172160
C	-1.964730	0.185967	-0.033760
C	-0.884211	1.022288	0.014517
H	0.142598	-0.393597	1.313084
H	-1.817470	-1.990862	0.308748
H	-0.781992	-1.318728	-1.032500
H	-3.014817	0.403989	0.111289
H	-0.811299	2.080685	-0.201955
C	1.540779	0.324991	-0.171470
O	2.462477	-0.436031	0.025255
H	1.673304	1.205919	-0.826621

TS-con-out-3-CHO-Dichloromethane  
SCF Energy: -269.230175504  
ZPE-corrected Energy: -269.135857  
 $\Delta U$ : -269.130266  
 $\Delta H$ : -269.129322  
 $\Delta G$ : -269.165064

Num. Imaginary Frequencies: 1

Imaginary Frequency: -659.8378

C	0.191869	0.160075	0.384085
C	-1.398457	-1.109129	-0.172169
C	-1.964991	0.185452	-0.033711
C	-0.884560	1.022167	0.014462
H	0.142496	-0.392614	1.313444
H	-1.816535	-1.991483	0.307748
H	-0.780608	-1.318134	-1.032071
H	-3.015112	0.403415	0.111171
H	-0.812018	2.080196	-0.204060
C	1.541539	0.324959	-0.171126
O	2.461911	-0.436136	0.025089
H	1.674091	1.206561	-0.826190

TS-con-out-3-CHO-DMSO  
SCF Energy: -269.231153534  
ZPE-corrected Energy: -269.136854  
 $\Delta U$ : -269.131262  
 $\Delta H$ : -269.130318  
 $\Delta G$ : -269.166057

Num. Imaginary Frequencies: 1

Imaginary Frequency: -659.7624

C	0.192295	0.159457	0.383878
C	-1.399124	-1.109260	-0.172147
C	-1.964711	0.185977	-0.033782
C	-0.884203	1.022293	0.014526
H	0.142630	-0.393593	1.313120
H	-1.817468	-1.990831	0.308846
H	-0.782016	-1.318768	-1.032508
H	-3.014815	0.403959	0.111184
H	-0.811278	2.080714	-0.201820
C	1.540692	0.325001	-0.171490
O	2.462509	-0.436017	0.025246
H	1.673181	1.205839	-0.826702

TS-con-out-3-CHO-Gas  
SCF Energy: -269.224281867  
ZPE-corrected Energy: -269.129933  
 $\Delta U$ : -269.124333  
 $\Delta H$ : -269.123388  
 $\Delta G$ : -269.159181

Num. Imaginary Frequencies: 1

Imaginary Frequency: -660.9785

C	0.190531	0.161562	0.383760
C	-1.398493	-1.107591	-0.173181
C	-1.966613	0.184679	-0.031596
C	-0.885211	1.021539	0.015528
H	0.143692	-0.388931	1.314068
H	-1.818434	-1.993362	0.299552
H	-0.778986	-1.314083	-1.032242
H	-3.016404	0.403712	0.114500
H	-0.812059	2.077237	-0.214534
C	1.547026	0.322780	-0.172569
O	2.460111	-0.435948	0.027337
H	1.677864	1.205193	-0.831688

TS-con-out-3-CHO-n-Hexane  
SCF Energy: -269.226780851  
ZPE-corrected Energy: -269.132434  
 $\Delta U$ : -269.126839  
 $\Delta H$ : -269.125894  
 $\Delta G$ : -269.161663

Num. Imaginary Frequencies: 1

Imaginary Frequency: -660.4193

C	0.190876	0.161414	0.384640
C	-1.397748	-1.108466	-0.172420
C	-1.965736	0.184609	-0.033314
C	-0.885079	1.021873	0.014686
H	0.142518	-0.389876	1.314556
H	-1.816656	-1.992640	0.303861
H	-0.777968	-1.316458	-1.031020
H	-3.015808	0.402883	0.111826
H	-0.812486	2.078463	-0.211170
C	1.544628	0.324306	-0.170799
O	2.460227	-0.436611	0.025131
H	1.676930	1.208095	-0.825851

TS-con-out-3-CHO-Water  
SCF Energy: -269.231252599  
ZPE-corrected Energy: -269.136955  
 $\Delta U$ : -269.131363  
 $\Delta H$ : -269.130419  
 $\Delta G$ : -269.166158

Num. Imaginary Frequencies: 1

Imaginary Frequency: -659.7734

C	0.192325	0.159484	0.383927
C	-1.399066	-1.109302	-0.172126
C	-1.964684	0.185961	-0.033825
C	-0.884215	1.022302	0.014534
H	0.142668	-0.393542	1.313196
H	-1.817379	-1.990813	0.308990
H	-0.781989	-1.318823	-1.032513
H	-3.014818	0.403866	0.111019
H	-0.811297	2.080747	-0.201678
C	1.540570	0.325032	-0.171510
O	2.462527	-0.436004	0.025225
H	1.673019	1.205740	-0.826814

TS-con-out-3-COMe-Acetone  
SCF Energy: -308.550213279  
ZPE-corrected Energy: -308.427811  
 $\Delta U$ : -308.420730  
 $\Delta H$ : -308.419785  
 $\Delta G$ : -308.459368

Num. Imaginary Frequencies: 1

Imaginary Frequency: -652.5222

C	0.164878	-0.211301	-0.490968
C	1.891148	-0.860421	0.554800
C	2.226486	0.392093	-0.019369
C	1.024812	0.922991	-0.403616
H	0.428766	-1.019494	-1.160120
H	2.514153	-1.745902	0.447869
H	1.222324	-0.882741	1.401736
H	3.229795	0.757928	-0.195871
H	0.748789	1.956097	-0.573071
C	-1.264955	-0.213488	-0.099602
O	-1.927860	-1.229576	-0.184684
C	-1.842883	1.069534	0.434280
H	-1.338559	1.340961	1.362905
H	-1.672137	1.883246	-0.272273
H	-2.907162	0.950060	0.613158

TS-con-out-3-COMe-Acetonitrile  
SCF Energy: -308.550473739  
ZPE-corrected Energy: -308.428078  
 $\Delta U$ : -308.420997  
 $\Delta H$ : -308.420053  
 $\Delta G$ : -308.459634  
Num. Imaginary Frequencies: 1  
Imaginary Frequency: -652.5274

C	0.164692	-0.211851	-0.490901
C	1.890865	-0.860067	0.555966
C	2.226437	0.391644	-0.019912
C	1.024955	0.922376	-0.404879
H	0.428456	-1.020848	-1.159159
H	2.513731	-1.745770	0.450141
H	1.222026	-0.880998	1.402950
H	3.229863	0.756991	-0.196744
H	0.749278	1.955274	-0.576092
C	-1.264949	-0.213115	-0.099672
O	-1.928721	-1.228920	-0.185482
C	-1.841936	1.069674	0.435221
H	-1.338122	1.339015	1.364733
H	-1.669287	1.884219	-0.269881
H	-2.906560	0.951502	0.612966



TS-con-out-3-COMe-Dichloromethane

SCF Energy: -308.549468803

ZPE-corrected Energy: -308.427044

$\Delta U$ : -308.419964

$\Delta H$ : -308.419019

$\Delta G$ : -308.458601

Num. Imaginary Frequencies: 1

Imaginary Frequency: -652.5036

C	0.165386	-0.209839	-0.491155
C	1.891874	-0.861304	0.551787
C	2.226640	0.393257	-0.017954
C	1.024473	0.924586	-0.400350
H	0.429571	-1.015940	-1.162631
H	2.515261	-1.746202	0.442046
H	1.223087	-0.887223	1.398590
H	3.229647	0.760361	-0.193593
H	0.747534	1.958225	-0.565158
C	-1.264989	-0.214492	-0.099422
O	-1.925552	-1.231287	-0.182620
C	-1.845437	1.069148	0.431835
H	-1.339638	1.346244	1.357968
H	-1.679997	1.880608	-0.278636
H	-2.908731	0.946085	0.613940

TS-con-out-3-COMe-DMSO  
SCF Energy: -308.550559081  
ZPE-corrected Energy: -308.428166  
 $\Delta U$ : -308.421085  
 $\Delta H$ : -308.420141  
 $\Delta G$ : -308.459723

Num. Imaginary Frequencies: 1

Imaginary Frequency: -652.5286

C	0.164630	-0.212036	-0.490878
C	1.890769	-0.859945	0.556360
C	2.226422	0.391493	-0.020096
C	1.025005	0.922168	-0.405305
H	0.428351	-1.021303	-1.158835
H	2.513589	-1.745723	0.450911
H	1.221927	-0.880408	1.403361
H	3.229887	0.756674	-0.197040
H	0.749443	1.954995	-0.577110
C	-1.264948	-0.212990	-0.099695
O	-1.929010	-1.228699	-0.185751
C	-1.841620	1.069721	0.435539
H	-1.337973	1.338368	1.365343
H	-1.668344	1.884543	-0.269079
H	-2.906358	0.951979	0.612912

TS-con-out-3-COMe-Gas  
SCF Energy: -308.543123289  
ZPE-corrected Energy: -308.420535  
 $\Delta U$ : -308.413455  
 $\Delta H$ : -308.412511  
 $\Delta G$ : -308.452090

Num. Imaginary Frequencies: 1

Imaginary Frequency: -652.9253

C	0.168562	-0.203101	-0.493269
C	1.893205	-0.863182	0.541880
C	2.228520	0.397137	-0.012308
C	1.025047	0.930290	-0.389708
H	0.432281	-1.001809	-1.173184
H	2.518634	-1.746259	0.426611
H	1.222798	-0.900896	1.386659
H	3.230716	0.768714	-0.183412
H	0.744099	1.966231	-0.532500
C	-1.266010	-0.219838	-0.099117
O	-1.913964	-1.237659	-0.175410
C	-1.858261	1.067174	0.423342
H	-1.340989	1.375118	1.333247
H	-1.727665	1.867541	-0.307224
H	-2.914537	0.921755	0.628159

TS-con-out-3-COMe-n-Hexane  
SCF Energy: -308.545778834  
ZPE-corrected Energy: -308.423246  
 $\Delta U$ : -308.416168  
 $\Delta H$ : -308.415224  
 $\Delta G$ : -308.454793

Num. Imaginary Frequencies: 1

Imaginary Frequency: -652.6004

C	0.167435	-0.204893	-0.492318
C	1.893485	-0.863348	0.543262
C	2.227628	0.396566	-0.013533
C	1.024193	0.929265	-0.391130
H	0.431912	-1.004814	-1.170705
H	2.518279	-1.746606	0.427050
H	1.224104	-0.899478	1.389024
H	3.229850	0.767371	-0.186074
H	0.744244	1.964591	-0.540049
C	-1.265451	-0.218173	-0.099034
O	-1.917355	-1.236440	-0.176569
C	-1.854485	1.067755	0.424710
H	-1.341610	1.366064	1.340276
H	-1.711411	1.871166	-0.299960
H	-2.913362	0.930192	0.621249

TS-con-out-3-COMe-Water  
SCF Energy: -308.550670442  
ZPE-corrected Energy: -308.428280  
 $\Delta U$ : -308.421199  
 $\Delta H$ : -308.420255  
 $\Delta G$ : -308.459838

Num. Imaginary Frequencies: 1

Imaginary Frequency: -652.5297

C	0.164549	-0.212281	-0.490848
C	1.890643	-0.859783	0.556885
C	2.226403	0.391292	-0.020340
C	1.025072	0.921891	-0.405873
H	0.428211	-1.021907	-1.158404
H	2.513402	-1.745659	0.451935
H	1.221796	-0.879623	1.403908
H	3.229920	0.756254	-0.197433
H	0.749662	1.954625	-0.578460
C	-1.264946	-0.212825	-0.099726
O	-1.929391	-1.228405	-0.186110
C	-1.841203	1.069782	0.435960
H	-1.337775	1.337513	1.366148
H	-1.667103	1.884970	-0.268018
H	-2.906090	0.952607	0.612848

TS-con-out-3-COOH-Acetone  
SCF Energy: -344.498959600  
ZPE-corrected Energy: -344.398630  
 $\Delta U$ : -344.392309  
 $\Delta H$ : -344.391365  
 $\Delta G$ : -344.429347

Num. Imaginary Frequencies: 1

Imaginary Frequency: -653.3546

C	0.145456	-0.186434	-0.472744
C	1.870454	-0.910221	0.523569
C	2.228810	0.343715	-0.033163
C	1.034967	0.919792	-0.374753
H	0.356534	-0.981724	-1.171445
H	2.464959	-1.810556	0.383054
H	1.222256	-0.930791	1.386173
H	3.238186	0.683471	-0.225141
H	0.776027	1.961116	-0.511687
C	-1.278694	-0.136954	-0.080395
O	-2.060424	-1.048140	-0.213239
O	-1.626496	1.035583	0.472650
H	-2.568567	0.999562	0.688687

TS-con-out-3-COOH-Acetonitrile  
SCF Energy: -344.499218704  
ZPE-corrected Energy: -344.398902  
 $\Delta U$ : -344.392581  
 $\Delta H$ : -344.391637  
 $\Delta G$ : -344.429618

Num. Imaginary Frequencies: 1

Imaginary Frequency: -653.2859

C	0.145353	-0.186583	-0.472656
C	1.870512	-0.910110	0.523916
C	2.228796	0.343651	-0.033310
C	1.034989	0.919655	-0.375114
H	0.356472	-0.982137	-1.171069
H	2.464962	-1.810470	0.383486
H	1.222303	-0.930397	1.386532
H	3.238189	0.683173	-0.225591
H	0.776352	1.960937	-0.513051
C	-1.278681	-0.136754	-0.080348
O	-2.060701	-1.047922	-0.213633
O	-1.626262	1.035377	0.473074
H	-2.568386	1.000094	0.689228

TS-con-out-3-COOH-Dichloromethane

SCF Energy: -344.498209651

ZPE-corrected Energy: -344.397844

$\Delta U$ : -344.391524

$\Delta H$ : -344.390580

$\Delta G$ : -344.428565

Num. Imaginary Frequencies: 1

Imaginary Frequency: -653.5522

C	0.145756	-0.185974	-0.473038
C	1.870272	-0.910564	0.522531
C	2.228840	0.343906	-0.032701
C	1.034900	0.920212	-0.373666
H	0.356737	-0.980451	-1.172627
H	2.464965	-1.810805	0.381739
H	1.222071	-0.932001	1.385077
H	3.238168	0.684337	-0.223777
H	0.775089	1.961662	-0.507653
C	-1.278726	-0.137537	-0.080549
O	-2.059576	-1.048818	-0.212050
O	-1.627195	1.036185	0.471385
H	-2.569114	0.998056	0.687089

TS-con-out-3-COOH-DMSO  
SCF Energy: -344.499303218  
ZPE-corrected Energy: -344.398991  
 $\Delta U$ : -344.392670  
 $\Delta H$ : -344.391726  
 $\Delta G$ : -344.429707

Num. Imaginary Frequencies: 1

Imaginary Frequency: -653.2633

C	0.145318	-0.186631	-0.472628
C	1.870531	-0.910074	0.524031
C	2.228791	0.343630	-0.033358
C	1.034996	0.919610	-0.375232
H	0.356452	-0.982271	-1.170947
H	2.464963	-1.810441	0.383629
H	1.222317	-0.930267	1.386650
H	3.238191	0.683074	-0.225738
H	0.776459	1.960879	-0.513499
C	-1.278677	-0.136688	-0.080333
O	-2.060792	-1.047851	-0.213762
O	-1.626185	1.035310	0.473214
H	-2.568325	1.000267	0.689406

TS-con-out-3-COOH-Gas  
SCF Energy: -344.491362180  
ZPE-corrected Energy: -344.390722  
 $\Delta U$ : -344.384405  
 $\Delta H$ : -344.383460  
 $\Delta G$ : -344.421482

Num. Imaginary Frequencies: 1

Imaginary Frequency: -654.9955

C	0.147787	-0.182095	-0.476299
C	1.868415	-0.913220	0.514767
C	2.228908	0.345062	-0.028958
C	1.034403	0.923252	-0.365677
H	0.358195	-0.969923	-1.183176
H	2.465555	-1.812287	0.373139
H	1.219284	-0.941094	1.376220
H	3.238050	0.690383	-0.212299
H	0.767555	1.965402	-0.476114
C	-1.279240	-0.142272	-0.081923
O	-2.052807	-1.053726	-0.202685
O	-1.631965	1.041155	0.462106
H	-2.572100	0.983733	0.675399

TS-con-out-3-COOH-n-Hexane  
SCF Energy: -344.494315724  
ZPE-corrected Energy: -344.393787  
 $\Delta U$ : -344.387468  
 $\Delta H$ : -344.386524  
 $\Delta G$ : -344.424534

Num. Imaginary Frequencies: 1

Imaginary Frequency: -654.4367

C	0.147040	-0.183651	-0.474797
C	1.869215	-0.912161	0.517858
C	2.228928	0.344624	-0.030501
C	1.034635	0.922106	-0.368780
H	0.357619	-0.974223	-1.178669
H	2.465120	-1.811829	0.376315
H	1.220637	-0.937458	1.379882
H	3.238121	0.687995	-0.217143
H	0.770724	1.964049	-0.488800
C	-1.278978	-0.140326	-0.081369
O	-2.055526	-1.051839	-0.206505
O	-1.630232	1.039089	0.465743
H	-2.571191	0.989917	0.680037

TS-con-out-3-COOH-Water  
SCF Energy: -344.499413210  
ZPE-corrected Energy: -344.399107  
 $\Delta U$ : -344.392785  
 $\Delta H$ : -344.391841  
 $\Delta G$ : -344.429822

Num. Imaginary Frequencies: 1

Imaginary Frequency: -653.2337

C	0.145274	-0.186694	-0.472592
C	1.870555	-0.910026	0.524181
C	2.228785	0.343602	-0.033420
C	1.035006	0.919552	-0.375387
H	0.356425	-0.982446	-1.170789
H	2.464964	-1.810404	0.383817
H	1.222334	-0.930098	1.386803
H	3.238192	0.682944	-0.225930
H	0.776600	1.960802	-0.514083
C	-1.278672	-0.136602	-0.080314
O	-2.060910	-1.047757	-0.213931
O	-1.626084	1.035222	0.473397
H	-2.568246	1.000491	0.689640



TS-con-out-3-Me-Acetone  
SCF Energy: -195.209798830  
ZPE-corrected Energy: -195.097539  
 $\Delta U$ : -195.092150  
 $\Delta H$ : -195.091205  
 $\Delta G$ : -195.125990

Num. Imaginary Frequencies: 1

Imaginary Frequency: -649.8397

C	0.601212	-0.018144	0.402822
C	-1.211687	-0.982970	-0.119355
C	-1.515452	0.398635	-0.052445
C	-0.284330	1.006418	-0.027748
H	0.402076	-0.454142	1.370806
H	-1.823382	-1.746243	0.359093
H	-0.624756	-1.345156	-0.950499
H	-2.500625	0.834748	0.063242
H	0.013793	1.996124	-0.355616
C	1.991470	-0.179691	-0.136502
H	2.661945	-0.670898	0.565715
H	1.984659	-0.761600	-1.060921
H	2.399020	0.801682	-0.392455

TS-con-out-3-Me-Acetonitrile  
SCF Energy: -195.209862523  
ZPE-corrected Energy: -195.097615  
 $\Delta U$ : -195.092224  
 $\Delta H$ : -195.091280  
 $\Delta G$ : -195.126068

Num. Imaginary Frequencies: 1

Imaginary Frequency: -649.8933

C	0.601187	-0.017998	0.402840
C	-1.211384	-0.983091	-0.119368
C	-1.515539	0.398471	-0.052512
C	-0.284492	1.006571	-0.027679
H	0.402055	-0.454124	1.370787
H	-1.822778	-1.746525	0.359202
H	-0.624142	-1.345185	-0.950351
H	-2.500845	0.834345	0.063113
H	0.013578	1.996276	-0.355624
C	1.991385	-0.179619	-0.136520
H	2.661816	-0.670637	0.565861
H	1.984506	-0.761839	-1.060743
H	2.398870	0.801685	-0.392812

TS-con-out-3-Me-Dichloromethane  
SCF Energy: -195.209617950  
ZPE-corrected Energy: -195.097327  
 $\Delta U$ : -195.091939  
 $\Delta H$ : -195.090995  
 $\Delta G$ : -195.125779

Num. Imaginary Frequencies: 1

Imaginary Frequency: -649.7993

C	0.601253	-0.018341	0.402724
C	-1.212190	-0.982781	-0.119320
C	-1.515317	0.398844	-0.052256
C	-0.284127	1.006192	-0.027933
H	0.402161	-0.453921	1.370853
H	-1.824296	-1.745824	0.359004
H	-0.626135	-1.345082	-0.950971
H	-2.500237	0.835382	0.063505
H	0.013923	1.995923	-0.355680
C	1.991677	-0.179785	-0.136428
H	2.662560	-0.669724	0.566328
H	1.985364	-0.762917	-1.060086
H	2.398876	0.801386	-0.393672

TS-con-out-3-Me-DMSO  
SCF Energy: -195.209883339  
ZPE-corrected Energy: -195.097642  
 $\Delta U$ : -195.092250  
 $\Delta H$ : -195.091306  
 $\Delta G$ : -195.126103

Num. Imaginary Frequencies: 1

Imaginary Frequency: -649.8470

C	0.601220	-0.017848	0.402568
C	-1.211377	-0.983219	-0.119418
C	-1.515693	0.398393	-0.052325
C	-0.284626	1.006644	-0.027844
H	0.402225	-0.453855	1.370617
H	-1.822379	-1.746828	0.359369
H	-0.624218	-1.345131	-0.950557
H	-2.500979	0.834228	0.063662
H	0.013075	1.996389	-0.355973
C	1.991528	-0.179567	-0.136442
H	2.661143	-0.671302	0.566248
H	1.984958	-0.761531	-1.060785
H	2.399863	0.801611	-0.391817

TS-con-out-3-Me-Gas  
SCF Energy: -195.208180659  
ZPE-corrected Energy: -195.095670  
 $\Delta U$ : -195.090284  
 $\Delta H$ : -195.089340  
 $\Delta G$ : -195.124166

Num. Imaginary Frequencies: 1

Imaginary Frequency: -650.0843

C	0.601352	-0.020388	0.401739
C	-1.216412	-0.981063	-0.119224
C	-1.514213	0.400812	-0.050686
C	-0.282249	1.004171	-0.029484
H	0.402637	-0.453535	1.370614
H	-1.831566	-1.742254	0.358248
H	-0.637200	-1.344457	-0.954721
H	-2.496977	0.840772	0.066493
H	0.015620	1.994205	-0.355622
C	1.993356	-0.180455	-0.135727
H	2.667291	-0.661364	0.570646
H	1.991614	-0.771600	-1.054345
H	2.397580	0.799769	-0.401023

TS-con-out-3-Me-n-Hexane  
SCF Energy: -195.208756491  
ZPE-corrected Energy: -195.096328  
 $\Delta U$ : -195.090943  
 $\Delta H$ : -195.089999  
 $\Delta G$ : -195.124801

Num. Imaginary Frequencies: 1

Imaginary Frequency: -649.7723

C	0.601378	-0.019577	0.402203
C	-1.214878	-0.981718	-0.119238
C	-1.514608	0.400086	-0.051327
C	-0.282931	1.004931	-0.028875
H	0.402456	-0.453595	1.370810
H	-1.829038	-1.743583	0.358416
H	-0.632880	-1.344692	-0.953167
H	-2.498189	0.838795	0.065272
H	0.015016	1.994829	-0.355702
C	1.992704	-0.180273	-0.136040
H	2.665044	-0.666363	0.568169
H	1.988805	-0.766599	-1.057708
H	2.398797	0.800516	-0.396423

TS-con-out-3-Me-Water  
SCF Energy: -195.209910749  
ZPE-corrected Energy: -195.097671  
 $\Delta U$ : -195.092280  
 $\Delta H$ : -195.091336  
 $\Delta G$ : -195.126126

Num. Imaginary Frequencies: 1

Imaginary Frequency: -649.9525

C	0.601152	-0.017872	0.402911
C	-1.211078	-0.983191	-0.119362
C	-1.515601	0.398334	-0.052590
C	-0.284625	1.006661	-0.027627
H	0.402046	-0.454060	1.370849
H	-1.822240	-1.746756	0.359287
H	-0.623634	-1.345201	-0.950255
H	-2.501011	0.834025	0.062953
H	0.013381	1.996396	-0.355565
C	1.991288	-0.179530	-0.136547
H	2.662183	-0.668964	0.566493
H	1.984409	-0.763416	-1.059726
H	2.398049	0.801565	-0.394747

TS-con-out-3-NH2-Acetone  
SCF Energy: -211.273807716  
ZPE-corrected Energy: -211.171897  
 $\Delta U$ : -211.166951  
 $\Delta H$ : -211.166006  
 $\Delta G$ : -211.199314

Num. Imaginary Frequencies: 1

Imaginary Frequency: -595.3618

C	0.634946	-0.010692	0.391554
C	-1.136336	-1.007069	-0.119602
C	-1.477324	0.375143	-0.054064
C	-0.277602	1.024579	-0.005720
H	0.533910	-0.416374	1.387021
H	-1.742056	-1.777326	0.354319
H	-0.590309	-1.352544	-0.985969
H	-2.471826	0.797135	0.044006
H	0.000370	2.037163	-0.273652
N	1.897966	-0.115311	-0.131551
H	2.010618	0.047786	-1.118433
H	2.511430	-0.820435	0.240562

TS-con-out-3-NH2-Acetonitrile  
SCF Energy: -211.273991501  
ZPE-corrected Energy: -211.172090  
 $\Delta U$ : -211.167145  
 $\Delta H$ : -211.166200  
 $\Delta G$ : -211.199507

Num. Imaginary Frequencies: 1

Imaginary Frequency: -595.7935

C	0.634849	-0.010333	0.391647
C	-1.135493	-1.007315	-0.119547
C	-1.477513	0.374741	-0.054137
C	-0.277999	1.024715	-0.005723
H	0.533932	-0.415639	1.387314
H	-1.740551	-1.778000	0.354544
H	-0.589134	-1.352477	-0.985870
H	-2.472275	0.796182	0.043861
H	-0.000267	2.037163	-0.274491
N	1.897897	-0.114747	-0.131446
H	2.009619	0.046302	-1.118845
H	2.510333	-0.821146	0.240172

TS-con-out-3-NH2-Dichloromethane  
SCF Energy: -211.273281376  
ZPE-corrected Energy: -211.171331  
 $\Delta U$ : -211.166387  
 $\Delta H$ : -211.165443  
 $\Delta G$ : -211.198747

Num. Imaginary Frequencies: 1

Imaginary Frequency: -594.2079

C	0.635015	-0.011302	0.391244
C	-1.138539	-1.006316	-0.119878
C	-1.476959	0.376092	-0.053699
C	-0.276440	1.024176	-0.006042
H	0.533032	-0.417953	1.386150
H	-1.745589	-1.775718	0.353653
H	-0.593021	-1.352473	-0.986206
H	-2.470740	0.799258	0.045860
H	0.002376	2.036515	-0.273772
N	1.898829	-0.115974	-0.131206
H	2.011833	0.047634	-1.117865
H	2.511842	-0.821345	0.240872

TS-con-out-3-NH2-DMSO  
SCF Energy: -211.274051648  
ZPE-corrected Energy: -211.172159  
 $\Delta U$ : -211.167212  
 $\Delta H$ : -211.166268  
 $\Delta G$ : -211.199575

Num. Imaginary Frequencies: 1

Imaginary Frequency: -596.0780

C	0.634822	-0.010321	0.391787
C	-1.135144	-1.007359	-0.119443
C	-1.477624	0.374579	-0.054325
C	-0.277978	1.024938	-0.005592
H	0.534487	-0.415173	1.387719
H	-1.740157	-1.778126	0.354597
H	-0.588857	-1.352586	-0.985813
H	-2.472554	0.795606	0.043809
H	-0.000265	2.037315	-0.274654
N	1.897590	-0.114829	-0.131637
H	2.009184	0.046349	-1.119025
H	2.510576	-0.820605	0.240266

TS-con-out-3-NH2-Gas  
SCF Energy: -211.268824811  
ZPE-corrected Energy: -211.166599  
 $\Delta U$ : -211.161664  
 $\Delta H$ : -211.160720  
 $\Delta G$ : -211.194014

Num. Imaginary Frequencies: 1

Imaginary Frequency: -589.6049

C	0.634307	-0.016064	0.389067
C	-1.153927	-1.000624	-0.122577
C	-1.474678	0.382805	-0.050531
C	-0.268198	1.020841	-0.009176
H	0.525113	-0.430867	1.379359
H	-1.768548	-1.764734	0.349081
H	-0.611989	-1.350708	-0.988924
H	-2.462989	0.813910	0.062194
H	0.016825	2.031544	-0.274818
N	1.905600	-0.120188	-0.128457
H	2.020030	0.044583	-1.113826
H	2.517337	-0.824160	0.245436

TS-con-out-3-NH2-n-Hexane  
SCF Energy: -211.270673089  
ZPE-corrected Energy: -211.168551  
 $\Delta U$ : -211.163614  
 $\Delta H$ : -211.162670  
 $\Delta G$ : -211.195964

Num. Imaginary Frequencies: 1

Imaginary Frequency: -590.5015

C	0.634797	-0.014130	0.389591
C	-1.148106	-1.002878	-0.121363
C	-1.475542	0.380165	-0.051622
C	-0.271286	1.022239	-0.008343
H	0.528336	-0.425143	1.381943
H	-1.760363	-1.768956	0.350431
H	-0.604935	-1.351471	-0.987800
H	-2.465912	0.808404	0.056129
H	0.011011	2.033982	-0.273462
N	1.902895	-0.118864	-0.129354
H	2.017559	0.046631	-1.114956
H	2.514856	-0.823782	0.243610

TS-con-out-3-NH2-Water  
SCF Energy: -211.274130085  
ZPE-corrected Energy: -211.172243  
 $\Delta U$ : -211.167296  
 $\Delta H$ : -211.166352  
 $\Delta G$ : -211.199660

Num. Imaginary Frequencies: 1

Imaginary Frequency: -596.2596

C	0.634818	-0.010238	0.391834
C	-1.134847	-1.007460	-0.119409
C	-1.477672	0.374448	-0.054375
C	-0.278142	1.024995	-0.005532
H	0.534603	-0.414979	1.387834
H	-1.739678	-1.778349	0.354675
H	-0.588456	-1.352587	-0.985765
H	-2.472703	0.795312	0.043544
H	-0.000536	2.037378	-0.274717
N	1.897492	-0.114706	-0.131671
H	2.008957	0.046295	-1.119122
H	2.510430	-0.820601	0.240142

TS-con-out-3-NO2-Acetone  
SCF Energy: -360.424575233  
ZPE-corrected Energy: -360.336373  
 $\Delta U$ : -360.330407  
 $\Delta H$ : -360.329463  
 $\Delta G$ : -360.366751

Num. Imaginary Frequencies: 1

Imaginary Frequency: -633.7762

C	-0.104198	-0.173015	0.425510
C	-1.843081	-0.925719	-0.496014
C	-2.178291	0.324334	0.074219
C	-0.979155	0.931884	0.344878
H	-0.186954	-0.956826	1.159521
H	-2.424476	-1.826441	-0.315009
H	-1.233702	-0.948939	-1.386014
H	-3.175990	0.641121	0.346856
H	-0.724658	1.971282	0.492852
N	1.292908	-0.027183	0.012596
O	1.616012	0.994045	-0.560427
O	2.049460	-0.948398	0.250685

TS-con-out-3-NO2-Acetonitrile  
SCF Energy: -360.424878082  
ZPE-corrected Energy: -360.336687  
 $\Delta U$ : -360.330721  
 $\Delta H$ : -360.329777  
 $\Delta G$ : -360.367060

Num. Imaginary Frequencies: 1

Imaginary Frequency: -633.5243

C	-0.104142	-0.173349	0.425410
C	-1.843321	-0.925548	-0.496403
C	-2.178258	0.324379	0.074344
C	-0.979133	0.931694	0.345336
H	-0.186820	-0.957475	1.159096
H	-2.424642	-1.826255	-0.315281
H	-1.233840	-0.948640	-1.386341
H	-3.175922	0.640984	0.347277
H	-0.724971	1.970952	0.494980
N	1.292654	-0.027185	0.012629
O	1.615785	0.993720	-0.561232
O	2.050057	-0.947760	0.251199



TS-con-out-3-NO2-Dichloromethane

SCF Energy: -360.423702846

ZPE-corrected Energy: -360.335471

$\Delta U$ : -360.329504

$\Delta H$ : -360.328560

$\Delta G$ : -360.365859

Num. Imaginary Frequencies: 1

Imaginary Frequency: -634.4637

C	-0.104367	-0.172124	0.425794
C	-1.842335	-0.926122	-0.495004
C	-2.178356	0.324158	0.073853
C	-0.979180	0.932377	0.343691
H	-0.187355	-0.955035	1.160743
H	-2.423952	-1.826896	-0.314427
H	-1.233293	-0.949615	-1.385235
H	-3.176078	0.641371	0.346046
H	-0.723731	1.972141	0.487084
N	1.293608	-0.027179	0.012497
O	1.616521	0.994930	-0.558283
O	2.047801	-0.950111	0.249321

TS-con-out-3-NO2-DMSO

SCF Energy: -360.424976841

ZPE-corrected Energy: -360.336789

$\Delta U$ : -360.330824

$\Delta H$ : -360.329879

$\Delta G$ : -360.367161

Num. Imaginary Frequencies: 1

Imaginary Frequency: -633.4728

C	-0.104264	-0.173332	0.425539
C	-1.843595	-0.925433	-0.496492
C	-2.178346	0.324446	0.074602
C	-0.978932	0.931792	0.345091
H	-0.186795	-0.957485	1.159197
H	-2.425682	-1.825763	-0.316039
H	-1.233916	-0.948276	-1.386242
H	-3.176007	0.640633	0.347934
H	-0.724230	1.970970	0.494496
N	1.292684	-0.027289	0.012613
O	1.615972	0.993598	-0.561202
O	2.050111	-0.947835	0.251191

TS-con-out-3-NO2-Gas  
SCF Energy: -360.415927028  
ZPE-corrected Energy: -360.327468  
 $\Delta U$ : -360.321506  
 $\Delta H$ : -360.320562  
 $\Delta G$ : -360.357894

Num. Imaginary Frequencies: 1

Imaginary Frequency: -637.9293

C	-0.103975	-0.166320	0.428918
C	-1.837565	-0.928370	-0.488638
C	-2.178645	0.323034	0.072838
C	-0.978456	0.934680	0.336741
H	-0.188986	-0.944697	1.168493
H	-2.421833	-1.829494	-0.314154
H	-1.228009	-0.952556	-1.378424
H	-3.177539	0.643826	0.337290
H	-0.713769	1.976198	0.444271
N	1.299472	-0.027336	0.011076
O	1.617350	1.002018	-0.543653
O	2.035860	-0.962027	0.239383

TS-con-out-3-NO2-n-Hexane  
SCF Energy: -360.419250345  
ZPE-corrected Energy: -360.330878  
 $\Delta U$ : -360.324913  
 $\Delta H$ : -360.323969  
 $\Delta G$ : -360.361296

Num. Imaginary Frequencies: 1

Imaginary Frequency: -636.9663

C	-0.104496	-0.168465	0.427594
C	-1.839215	-0.927615	-0.491035
C	-2.178565	0.323340	0.072872
C	-0.978972	0.934039	0.339285
H	-0.188545	-0.948165	1.165864
H	-2.422308	-1.828616	-0.313777
H	-1.230369	-0.951699	-1.381371
H	-3.176821	0.642599	0.341294
H	-0.718514	1.975107	0.461365
N	1.297045	-0.027202	0.011790
O	1.617518	0.999044	-0.549391
O	2.040573	-0.957369	0.243366

TS-con-out-3-NO2-Water  
SCF Energy: -360.425105762  
ZPE-corrected Energy: -360.336923  
 $\Delta U$ : -360.330957  
 $\Delta H$ : -360.330013  
 $\Delta G$ : -360.367292

Num. Imaginary Frequencies: 1

Imaginary Frequency: -633.3743

C	-0.104226	-0.173487	0.425487
C	-1.843741	-0.925359	-0.496658
C	-2.178317	0.324490	0.074642
C	-0.978899	0.931711	0.345309
H	-0.186723	-0.957774	1.159010
H	-2.425882	-1.825611	-0.316075
H	-1.234016	-0.948239	-1.386359
H	-3.175968	0.640603	0.348087
H	-0.724334	1.970814	0.495505
N	1.292580	-0.027292	0.012628
O	1.615867	0.993448	-0.561573
O	2.050378	-0.947558	0.251416

TS-con-out-3-OMe-Acetone  
SCF Energy: -270.436044502  
ZPE-corrected Energy: -270.318151  
 $\Delta U$ : -270.311924  
 $\Delta H$ : -270.310980  
 $\Delta G$ : -270.348056

Num. Imaginary Frequencies: 1

Imaginary Frequency: -593.0446

C	-0.126409	-0.193669	0.257151
C	1.459410	1.125472	-0.160415
C	2.039861	-0.146871	0.070627
C	0.993486	-1.032202	0.013169
H	-0.222352	0.304066	1.213892
H	1.836260	2.032528	0.307462
H	0.939645	1.289796	-1.092825
H	3.068052	-0.342117	0.353028
H	0.956552	-2.087588	-0.223073
O	-1.283713	-0.376913	-0.406742
C	-2.404274	0.309895	0.136497
H	-2.604213	-0.027695	1.154129
H	-2.221262	1.385840	0.137372
H	-3.255424	0.084727	-0.498225

TS-con-out-3-OMe-Acetonitrile  
SCF Energy: -270.436179736  
ZPE-corrected Energy: -270.318299  
 $\Delta U$ : -270.312071  
 $\Delta H$ : -270.311127  
 $\Delta G$ : -270.348206

Num. Imaginary Frequencies: 1

Imaginary Frequency: -593.4298

C	-0.126330	-0.193704	0.257312
C	1.459223	1.125547	-0.160392
C	2.039957	-0.146768	0.070464
C	0.993620	-1.032225	0.013230
H	-0.222487	0.303964	1.214055
H	1.835847	2.032606	0.307629
H	0.939008	1.289971	-1.092547
H	3.068231	-0.341834	0.352724
H	0.956831	-2.087687	-0.222828
O	-1.283570	-0.376922	-0.406863
C	-2.404437	0.309816	0.136498
H	-2.604903	-0.028833	1.153620
H	-2.220929	1.385629	0.138568
H	-3.255241	0.085568	-0.498991

TS-con-out-3-OMe-Dichloromethane  
SCF Energy: -270.435659536

ZPE-corrected Energy: -270.317730  
 $\Delta U$ : -270.311508  
 $\Delta H$ : -270.310564  
 $\Delta G$ : -270.347630

Num. Imaginary Frequencies: 1

Imaginary Frequency: -592.1193

C	-0.126583	-0.193618	0.256937
C	1.459941	1.125312	-0.160471
C	2.039661	-0.147174	0.071015
C	0.993134	-1.032093	0.013095
H	-0.222194	0.304092	1.213741
H	1.837578	2.032414	0.306764
H	0.941036	1.289240	-1.093385
H	3.067767	-0.342888	0.353257
H	0.955844	-2.087166	-0.224139
O	-1.284204	-0.377003	-0.406404
C	-2.403825	0.310178	0.136393
H	-2.603937	-0.026233	1.154543
H	-2.221029	1.386290	0.136341
H	-3.255393	0.084638	-0.497709

TS-con-out-3-OMe-DMSO  
SCF Energy: -270.436224124  
ZPE-corrected Energy: -270.318348  
 $\Delta U$ : -270.312119  
 $\Delta H$ : -270.311175  
 $\Delta G$ : -270.348256

Num. Imaginary Frequencies: 1

Imaginary Frequency: -593.5450

C	-0.126303	-0.193670	0.257307
C	1.459168	1.125543	-0.160388
C	2.039976	-0.146752	0.070428
C	0.993646	-1.032243	0.013232
H	-0.222453	0.304034	1.214030
H	1.835645	2.032586	0.307772
H	0.938918	1.290039	-1.092519
H	3.068229	-0.341767	0.352819
H	0.956869	-2.087742	-0.222707
O	-1.283469	-0.376828	-0.406918
C	-2.404515	0.309726	0.136529
H	-2.604619	-0.028753	1.153762
H	-2.221316	1.385575	0.138280
H	-3.255353	0.085026	-0.498745

TS-con-out-3-OMe-Gas  
SCF Energy: -270.432495619  
ZPE-corrected Energy: -270.314320  
 $\Delta U$ : -270.308124  
 $\Delta H$ : -270.307179  
 $\Delta G$ : -270.344201

Num. Imaginary Frequencies: 1

Imaginary Frequency: -587.3029

C	-0.127696	-0.192524	0.255173
C	1.466257	1.123740	-0.161134
C	2.038187	-0.150526	0.073786
C	0.989400	-1.031456	0.011907
H	-0.219951	0.306845	1.211547
H	1.850185	2.030127	0.302615
H	0.952963	1.286853	-1.096962
H	3.064923	-0.350847	0.356548
H	0.948485	-2.085006	-0.228845
O	-1.289049	-0.377226	-0.403994
C	-2.400648	0.312429	0.135768
H	-2.608657	-0.022529	1.154191
H	-2.215104	1.389162	0.139588
H	-3.253456	0.093223	-0.499720

TS-con-out-3-OMe-n-Hexane  
SCF Energy: -270.433792904  
ZPE-corrected Energy: -270.315713  
 $\Delta U$ : -270.309507  
 $\Delta H$ : -270.308563  
 $\Delta G$ : -270.345596

Num. Imaginary Frequencies: 1

Imaginary Frequency: -588.8385

C	-0.127377	-0.193055	0.255730
C	1.463619	1.124415	-0.160799
C	2.038761	-0.149137	0.072797
C	0.990974	-1.031660	0.012520
H	-0.221075	0.305433	1.212396
H	1.845391	2.031191	0.303938
H	0.948453	1.287569	-1.095712
H	3.066162	-0.347677	0.354929
H	0.951550	-2.085716	-0.227282
O	-1.287152	-0.377309	-0.405017
C	-2.401863	0.311667	0.136093
H	-3.254557	0.089226	-0.498042
H	-2.605889	-0.023105	1.154795
H	-2.217512	1.388173	0.137071

TS-con-out-3-OMe-Water  
SCF Energy: -270.436282066  
ZPE-corrected Energy: -270.318412  
 $\Delta U$ : -270.312181  
 $\Delta H$ : -270.311237  
 $\Delta G$ : -270.348323

Num. Imaginary Frequencies: 1

Imaginary Frequency: -593.6905

C	-0.126255	-0.193498	0.257240
C	1.459250	1.125475	-0.160388
C	2.040015	-0.146837	0.070421
C	0.993624	-1.032270	0.013223
H	-0.222321	0.304331	1.213903
H	1.835514	2.032440	0.308086
H	0.939082	1.290153	-1.092543
H	3.068186	-0.341880	0.353114
H	0.956750	-2.087821	-0.222514
O	-1.283313	-0.376492	-0.407057
C	-2.404738	0.309493	0.136623
H	-2.604177	-0.028839	1.154014
H	-2.222298	1.385441	0.137969
H	-3.255606	0.083935	-0.498296