Supplementary Material

Computational study of phenyliodine diacetate intermediates during Lewis acid activation with TMSOTf

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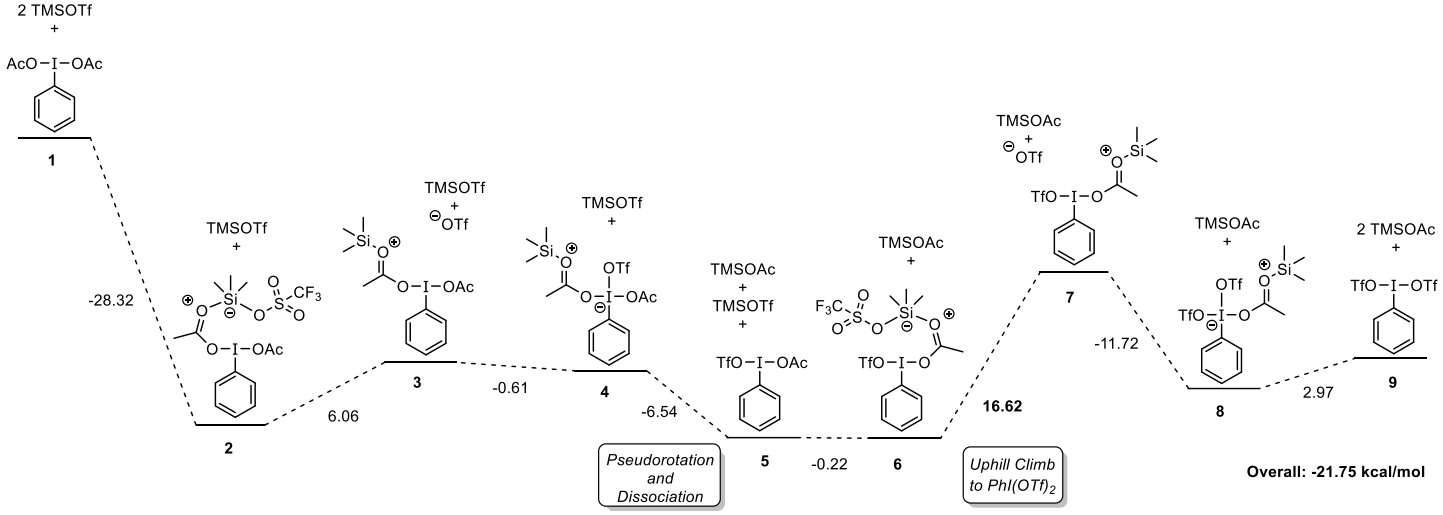
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+
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TMSOTf
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OTf
3
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TMSOTf
+
OTf
4
-6.54
TMSOAc
+
TMSOTf
+
TfO−I−OAc
5
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TMSOAc
+
TfO−I−O
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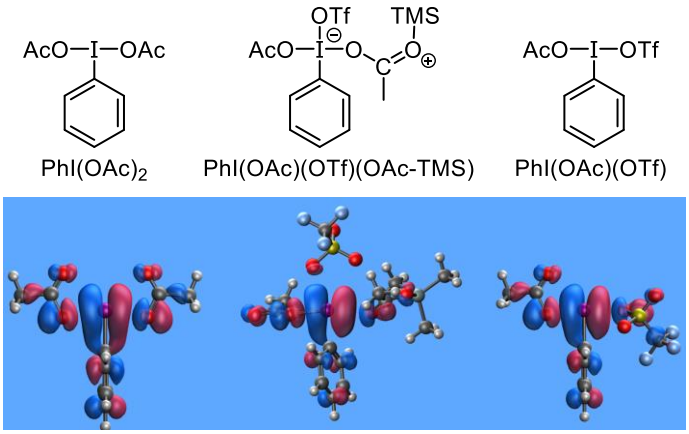
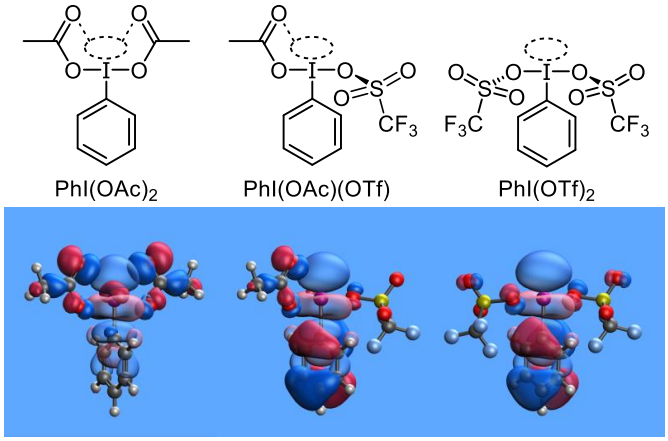
16.62
TMSOAc
+
OTf
TfO−I−O
7
-11.72
TMSOAc
+
OTf
TfO−I−O
8
2.97
2 TMSOAc
+
TfO−I−OTf
9
Pseudorotation and Dissociation
Uphill Climb to PhI(OTf)2
Overall: -21.75 kcal/mol


PhI(OAc)2
PhI(OAc)(OTf)(OAc-TMS)
PhI(OAc)(OTf)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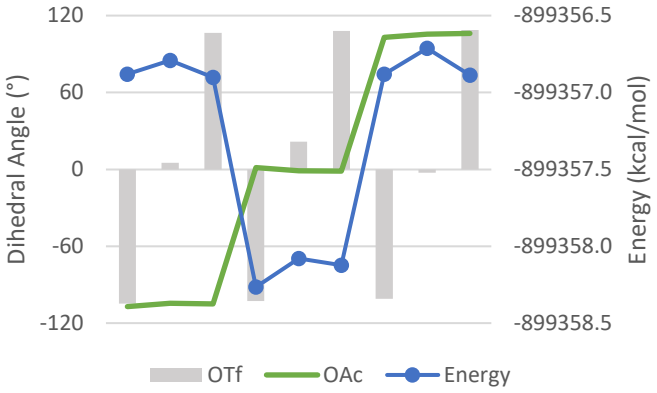
PhI(OAc)(OTf)
PhI(OTf)2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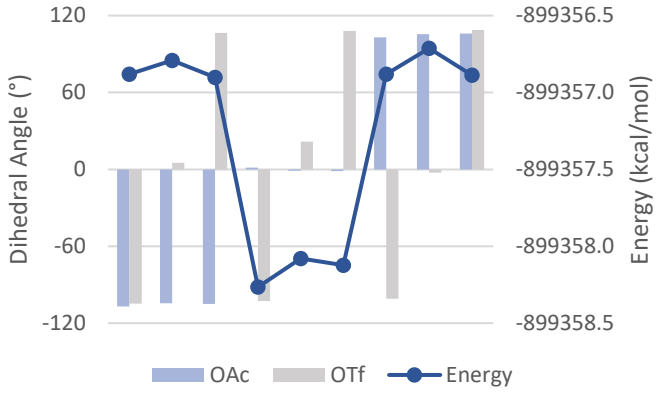
Dihedral Angle (°)
Energy (kcal/mol)
OTf
OAc
Energy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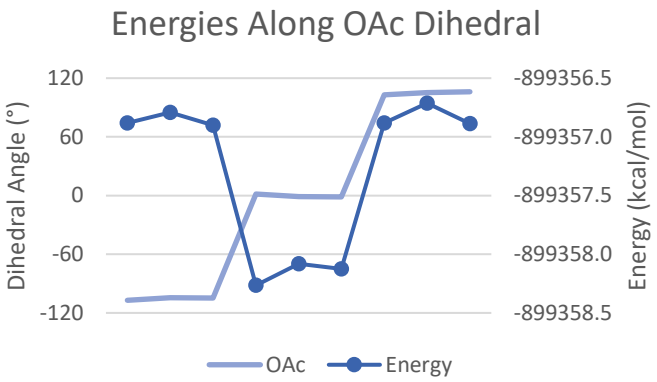
Dihedral Angle (°)
Energy (kcal/mol)
OAc
OTf
Energy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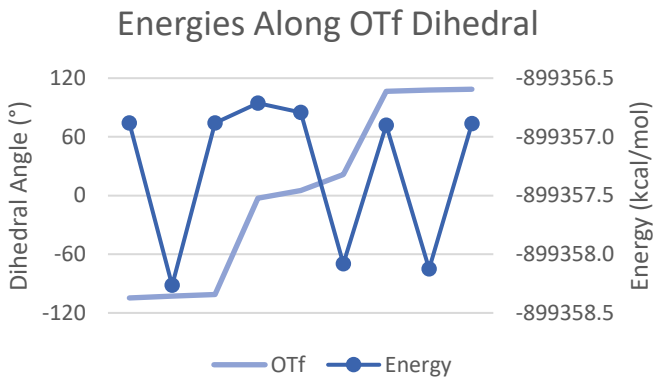
Dihedral Angle (°)
Energy (kcal/mol)
OAc
Energy


Energies Along OTf Dihedral
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60
0
-60
-120
-899356.5
-899357.0
-899357.5
-899358.0
-899358.5
Dihedral Angle (°)
Energy (kcal/mol)
OTf
Energy

Optimized Geometries and Electronic Energies

Compound 1

Optimized Geometry :

C	0.296318723	-1.277331630	-0.546967562
C	1.597869435	-1.806610429	-0.490026889
C	1.801657130	-3.188709927	-0.426308160
C	-0.794566181	-2.164423139	-0.538564401
C	-0.587114421	-3.546163211	-0.474763378
C	0.710070169	-4.058287846	-0.418660363
I	-0.013194480	0.808106295	-0.643144117
O	2.140883623	0.915915887	-0.578395053
C	2.711213152	2.206095382	-0.621626115
C	4.195312987	2.426734183	-0.822788737
O	-2.020736431	0.503309676	-0.685373644
C	-2.895423446	1.608850283	-0.755548788
C	-4.400453058	1.448536520	-0.788582053
O	1.917044360	3.204527418	-0.481688555
O	-2.363985705	2.776565948	-0.790372512
S	-8.149586558	8.077053583	3.270333577
O	-6.815441897	8.035843401	2.427790480
Si	-5.117352185	7.947464518	2.875214265
C	-4.840495036	6.310011313	3.729119481
C	-4.294134979	8.056112587	1.203585696
C	-4.759607255	9.413605259	3.976134867
O	-8.937362797	9.228895189	2.894464220
O	-7.885079317	7.759912332	4.663881097
C	-8.988360670	6.567574770	2.510350283
F	-10.162660818	6.385388148	3.110910776
F	-9.182052242	6.749658623	1.206710907
F	-8.229067623	5.483826367	2.693547042
S	6.006359370	9.195568405	-0.031987837
O	4.713551257	10.040126444	0.294957336
Si	3.026323551	9.605979328	0.532217184
C	2.926602219	8.529329139	2.054696475
C	2.247146142	11.286076707	0.764582120
C	2.458172805	8.731575938	-1.017689547
O	6.657951808	9.723034881	-1.209195451
O	5.740549705	7.774349889	0.116343019
C	7.046645241	9.720339142	1.451951714
F	8.215641098	9.085162076	1.398579958
F	7.256042425	11.034082589	1.432483624
F	6.420806979	9.392954030	2.585859131
H	2.810855773	-3.586484247	-0.382688039

H	-1.811651676	-1.800345231	-0.580972549
H	-1.436374511	-4.222363256	-0.468827473
H	0.869769556	-5.130882031	-0.369169259
H	4.701094242	1.454818983	-0.920595741
H	4.605856253	2.968010243	0.042355815
H	4.357381712	3.017696404	-1.736297319
H	-4.874199192	2.439799101	-0.843000351
H	-4.734086347	0.932576493	0.123816735
H	-4.686625056	0.856750350	-1.670564446
H	-5.430480980	6.240871527	4.646094857
H	-3.784802155	6.196805683	3.996157211
H	-5.113196216	5.471685716	3.082630091
H	-4.606034936	7.232524477	0.556239376
H	-3.205757545	8.006761979	1.309792666
H	-4.541975432	8.994884147	0.701930015
H	-5.334203152	9.359162758	4.904335794
H	-5.002906924	10.355571915	3.477306902
H	-3.697577833	9.439683762	4.240631076
H	3.492490972	7.604602423	1.919197774
H	1.885146315	8.262063155	2.260979612
H	3.319581395	9.045266043	2.934744538
H	2.677228242	11.804486277	1.625349782
H	1.170319719	11.187541262	0.934931398
H	2.393085794	11.914190811	-0.117773572
H	3.006651159	7.798044390	-1.167267723
H	2.599130277	9.357407606	-1.903010340
H	1.393423696	8.486905247	-0.947029491
H	2.466674553	-1.131963449	-0.495377873

Electronic Energy : -3442.12616133 Hartree

Compound 2

Optimized Geometry :

C	-5.94549	-6.20730	1.48639
C	-5.91653	-4.81807	1.37373
C	-6.24760	-4.24321	0.15104
C	-6.60418	-5.00866	-0.95432
C	-6.62762	-6.39647	-0.82443
C	-6.29948	-6.99329	0.39142
I	-6.20405	-2.13728	-0.03526
O	-8.30406	-2.32160	0.63147
C	-8.84551	-1.12856	0.72429
O	-8.23016	-0.09903	0.46638
C	-10.28848	-1.14688	1.17810
O	-4.12727	-2.51563	-0.64952
C	-3.54872	-1.36703	-0.93129
O	-4.14181	-0.29721	-0.85106
C	-2.09772	-1.49023	-1.33458
Si	-6.25487	3.18655	-0.13170
C	-5.59492	2.17722	1.28801
C	-6.57933	2.21046	-1.68304
C	-7.67357	4.30190	0.35963
O	-4.95697	4.26727	-0.67650
S	-4.05768	5.34627	0.01688
O	-4.03689	6.56097	-0.76930
O	-4.28522	5.38487	1.45245
C	-2.38468	4.51738	-0.24222
F	-1.43556	5.28850	0.30637
F	-2.12631	4.37418	-1.53989
F	-2.36212	3.32211	0.34705
S	13.48560	-1.50700	0.00118
O	12.98226	-0.22436	0.76424
Si	13.38198	1.48796	0.64431
C	12.86995	2.07492	-1.05151
C	12.35425	2.20368	2.02633
C	15.22281	1.62957	0.93654
O	13.99869	-2.47857	0.94153
O	14.23338	-1.14042	-1.19019
C	11.80793	-2.14431	-0.57670
F	11.99748	-3.25256	-1.29621
F	11.03162	-2.42730	0.46586
F	11.20793	-1.22788	-1.33878
H	-5.68944	-6.67076	2.43197
H	-5.64096	-4.20583	2.22257
H	-6.85823	-4.54258	-1.89748

H	-6.90266	-7.00711	-1.67647
H	-6.31888	-8.07284	0.48564
H	-10.88312	-1.75529	0.49359
H	-10.67824	-0.13131	1.21137
H	-10.35593	-1.60521	2.16717
H	-1.76800	-0.56552	-1.80459
H	-1.95454	-2.33678	-2.00676
H	-1.49690	-1.67042	-0.43910
H	-4.75051	1.56313	0.96639
H	-6.38637	1.50645	1.63592
H	-5.28067	2.81301	2.11879
H	-6.82883	2.86601	-2.52128
H	-7.41695	1.52915	-1.50725
H	-5.70517	1.61094	-1.94787
H	-8.53513	3.69382	0.65331
H	-7.98178	4.94512	-0.46909
H	-7.40614	4.93797	1.20757
H	13.38668	1.51293	-1.83308
H	13.12101	3.13368	-1.17343
H	11.79308	1.96913	-1.20274
H	11.28991	2.01651	1.86473
H	12.49864	3.28732	2.08408
H	12.63510	1.77362	2.99101
H	15.78727	1.11296	0.15590
H	15.50725	1.20513	1.90315
H	15.52789	2.68098	0.92967

Electronic Energy : -3442.17128900 Hartree

Compound 3

Optimized Geometry :

C	-5.774053	-7.119879	0.873171
C	-6.447680	-8.320893	0.662623
C	-5.653537	-6.789511	-1.549655
C	-6.327951	-7.994339	-1.734349
C	-6.721905	-8.754809	-0.633934
I	-4.378745	-4.558365	0.053632
O	-6.259211	-3.615773	0.111519
C	-6.058929	-2.308976	0.322210
C	-7.333880	-1.515266	0.389361
O	-2.391906	-5.952328	-0.037923
C	-1.278767	-5.404596	0.029246
C	-0.033459	-6.241561	-0.017329
O	-4.931555	-1.863024	0.440325
O	-1.209910	-4.106691	0.122167
C	-5.393068	-6.379429	-0.243840
Si	0.021608	-2.837811	0.310453
C	-0.982935	-1.304079	-0.002148
C	1.343729	-3.120485	-0.979105
C	0.640603	-2.987277	2.065767
S	-7.455528	9.165925	-0.107644
F	-9.181755	11.253576	-0.159299
F	-9.940691	9.524004	0.912997
F	-9.884711	9.516588	-1.257458
O	-7.722059	7.714976	-0.109565
O	-6.916632	9.711569	1.152490
O	-6.852289	9.703056	-1.342015
C	-9.202893	9.901611	-0.155226
S	12.359563	2.393872	-0.453462
O	11.345918	2.050471	0.706759
Si	9.597089	2.168992	0.844814
C	8.849223	0.994721	-0.399707
C	9.334342	1.634547	2.613755
C	9.138313	3.952544	0.531713
O	13.378292	3.297659	0.030241
O	11.649122	2.645497	-1.696229
C	13.164488	0.694883	-0.612097
F	14.067868	0.741134	-1.589138
F	13.762144	0.354703	0.526861
F	12.239782	-0.221217	-0.912555
H	-5.559515	-6.779863	1.877867
H	-6.756436	-8.914198	1.514810
H	-5.347354	-6.195965	-2.401146

H	-6.544160	-8.334396	-2.739931
H	-7.245693	-9.690746	-0.787639
H	-7.888681	-1.629230	-0.544014
H	-7.095605	-0.467866	0.559961
H	-7.962821	-1.895873	1.196561
H	0.658703	-5.947345	0.773578
H	0.466416	-6.084435	-0.977230
H	-0.290704	-7.293210	0.082294
H	-1.838217	-1.232066	0.674426
H	-1.359988	-1.274686	-1.027843
H	-0.364558	-0.413333	0.146719
H	0.919558	-3.212932	-1.982920
H	1.962647	-3.998143	-0.779945
H	2.012688	-2.253475	-0.993081
H	1.168279	-3.925949	2.254234
H	-0.176486	-2.901888	2.787034
H	1.345413	-2.175646	2.273659
H	9.122644	1.276924	-1.419171
H	7.757061	1.010392	-0.325205
H	9.180940	-0.032750	-0.228339
H	9.705399	0.619714	2.778258
H	8.268366	1.647293	2.862378
H	9.850828	2.301684	3.308409
H	9.395937	4.252884	-0.487160
H	9.650121	4.623792	1.226552
H	8.060638	4.095721	0.660795

Electronic Energy : -3442.16163346 Hartree

Compound 4

Optimized Geometry :

C	-5.103728	4.927168	0.359277
C	-4.894911	3.562720	0.554328
C	-5.681014	2.657465	-0.154633
C	-6.668256	3.077976	-1.043421
C	-6.870396	4.445655	-1.219298
C	-6.089025	5.366827	-0.523176
I	-5.386698	0.575303	0.140461
O	-3.091557	1.111766	-0.734066
C	-2.519281	0.546302	-1.677499
O	-1.220608	0.390759	-1.688741
C	-3.225786	-0.010569	-2.874937
O	-7.315225	0.467699	0.803911
C	-7.748036	0.172127	2.085309
O	-8.933867	0.221083	2.246155
C	-6.732738	-0.181040	3.135311
Si	-0.088503	0.641964	-0.370331
C	-0.748753	-0.178347	1.170825
C	0.142468	2.493321	-0.195660
C	1.440562	-0.198568	-1.038720
O	-5.544536	-1.999712	0.839789
O	-3.794185	-3.684717	1.419221
S	-4.354774	-2.805538	0.401341
C	-5.093977	-3.953295	-0.896566
F	-6.044086	-4.728970	-0.369393
F	-4.143156	-4.737285	-1.420587
F	-5.639503	-3.234614	-1.896584
O	-3.403154	-1.971325	-0.370582
H	-4.498867	5.643248	0.903377
H	-4.129495	3.220203	1.239009
H	-7.281624	2.362142	-1.575976
H	-7.639482	4.787173	-1.902165
H	-6.250315	6.428896	-0.666715
H	-4.155715	0.525045	-3.062105
H	-3.458907	-1.055210	-2.648422
H	-2.578672	0.021942	-3.750172
H	-6.192960	-1.082391	2.835898
H	-7.254163	-0.349609	4.075015
H	-6.005706	0.624978	3.267085
H	-1.205120	-1.143772	0.935995
H	-1.504870	0.437084	1.662210
H	0.066166	-0.348547	1.881900
H	0.493579	2.940730	-1.129692

H	0.886230	2.711997	0.577463
H	-0.791723	2.983484	0.088936
H	2.275143	-0.093255	-0.338491
H	1.747641	0.234328	-1.994551
H	1.264784	-1.266810	-1.190713
S	11.174818	-0.211640	0.971184
O	10.011565	-0.665479	0.005587
Si	8.296400	-0.285315	-0.066410
C	8.134817	1.537956	-0.436031
C	7.740515	-1.375712	-1.475608
C	7.555358	-0.763975	1.580195
O	11.831904	-1.369525	1.533448
O	10.743770	0.897089	1.806305
C	12.338062	0.499404	-0.333007
F	13.416695	0.985408	0.277884
F	12.705869	-0.445994	-1.193867
F	11.729072	1.484994	-0.998089
H	8.576282	2.140655	0.361192
H	7.078928	1.813581	-0.523997
H	8.627745	1.799787	-1.376014
H	8.269653	-1.126908	-2.399049
H	6.668615	-1.248238	-1.657420
H	7.922057	-2.430339	-1.253852
H	7.977842	-0.165705	2.391524
H	7.731546	-1.819302	1.805059
H	6.472974	-0.599932	1.571564

Electronic Energy : -3442.16260699 Hartree

Compound 5

Optimized Geometry :

C	2.43690	6.27152	0.73067
C	2.27715	4.88675	0.75231
C	1.00853	4.38134	1.01764
C	-0.09658	5.19581	1.24934
C	0.08798	6.57618	1.22418
C	1.35020	7.11058	0.96808
I	0.73942	2.28824	1.07346
O	0.90341	2.53045	3.18990
C	0.75381	1.34884	3.78248
O	0.56177	0.32770	3.14665
C	0.84496	1.42371	5.28640
S	1.58870	2.34493	-2.23412
C	0.99986	3.82305	-3.24946
F	0.93232	4.91865	-2.48223
F	1.86561	4.04765	-4.24028
F	-0.20450	3.58798	-3.76924
O	2.85937	2.75011	-1.63593
O	1.53349	1.20330	-3.12628
O	0.45638	2.30071	-1.16654
Si	8.67829	-4.63723	0.34948
O	7.08000	-4.03393	0.06925
C	9.75835	-4.22777	-1.12623
C	9.20125	-3.68345	1.87489
C	8.59100	-6.47954	0.68154
C	6.27667	-4.42556	-0.93693
O	6.60058	-5.25279	-1.75879
C	4.94562	-3.71757	-0.91327
S	-7.35504	-2.11294	0.73063
O	-6.12052	-2.16557	-0.25156
Si	-4.76174	-3.27001	-0.41098
C	-5.44286	-4.94149	-0.88980
C	-3.78611	-2.45245	-1.77611
C	-3.87026	-3.28889	1.23050
O	-7.41454	-0.82463	1.38278
O	-7.46304	-3.35117	1.48405
C	-8.72517	-2.13468	-0.56625
F	-9.90174	-2.12455	0.05698
F	-8.63460	-1.06860	-1.35708
F	-8.63180	-3.24090	-1.30932
H	3.41475	6.68817	0.52047
H	3.10924	4.23072	0.53688
H	-1.07472	4.77528	1.44278

H	-0.75802	7.22977	1.40118
H	1.48480	8.18574	0.94588
H	1.80871	1.84562	5.57796
H	0.72908	0.42632	5.70523
H	0.06502	2.08480	5.66993
H	10.79602	-4.52009	-0.93453
H	9.75025	-3.15444	-1.33753
H	9.41452	-4.75497	-2.01862
H	8.53157	-3.88343	2.71596
H	9.19476	-2.60570	1.68978
H	10.21435	-3.96451	2.17966
H	8.23256	-7.01685	-0.19898
H	7.91854	-6.70048	1.51564
H	9.58058	-6.86973	0.94111
H	5.10048	-2.63829	-0.98346
H	4.44164	-3.91103	0.03663
H	4.32799	-4.06091	-1.74063
H	-6.10174	-5.33432	-0.11182
H	-4.62549	-5.65548	-1.03386
H	-6.00900	-4.88914	-1.82352
H	-4.37856	-2.37335	-2.69120
H	-2.88847	-3.03527	-2.00597
H	-3.47068	-1.44659	-1.48783
H	-4.51009	-3.68727	2.02207
H	-3.54971	-2.28502	1.52172
H	-2.97825	-3.92080	1.17093

Electronic Energy : -3442.17303047 Hartree

Compound 6

Optimized Geometry :

C	5.96297	-1.3409	1.78733
C	4.57949	-1.30275	1.63015
C	4.07225	-0.99914	0.36972
C	4.88182	-0.72266	-0.7273
C	6.2632	-0.76319	-0.54353
C	6.79981	-1.07386	0.7043
I	1.97694	-0.94986	0.11778
O	2.12709	-3.08526	0.01274
C	0.92912	-3.6139	-0.19722
O	-0.07639	-2.92677	-0.2923
C	0.95394	-5.11761	-0.31197
Si	-3.33163	-1.02829	-0.5459
C	-2.64181	-0.73399	1.16387
C	-2.28413	-0.30721	-1.91045
C	-3.81264	-2.80747	-0.84409
O	-4.80274	-0.06584	-0.69344
S	-6.18964	-0.09795	0.05117
O	-7.26666	-0.22869	-0.90501
O	-6.12326	-0.94274	1.2329
C	-6.21086	1.68908	0.65475
F	-7.32578	1.88752	1.35766
F	-6.18469	2.52994	-0.37574
F	-5.15361	1.92027	1.43713
O	2.01843	1.28026	0.3806
S	2.29569	2.30832	-0.76017
O	2.95373	1.66185	-1.8938
O	1.16229	3.18607	-0.97671
C	3.61826	3.35529	0.08704
F	3.1369	3.91367	1.19592
F	4.67418	2.59698	0.40582
F	4.01546	4.3151	-0.74965
H	6.38197	-1.57528	2.75871
H	3.9245	-1.50404	2.4676
H	4.45739	-0.4518	-1.68429
H	6.91498	-0.54493	-1.38104
H	7.87514	-1.1007	0.83641
H	1.52103	-5.40223	-1.2013
H	-0.0639	-5.49452	-0.38722
H	1.45727	-5.55186	0.5534
H	-2.3778	0.316	1.31543
H	-1.74024	-1.33947	1.2972
H	-3.363	-1.02161	1.93249

H	-2.7982	-0.36555	-2.87323
H	-1.35017	-0.87166	-1.99163
H	-2.03786	0.74057	-1.72013
H	-2.91422	-3.43098	-0.80896
H	-4.2807	-2.93609	-1.82382
H	-4.50836	-3.16556	-0.08096
Si	-5.05002	-15.65307	-2.60585
O	-5.74943	-17.22021	-2.83375
C	-4.4432	-15.00393	-4.25579
C	-6.50262	-14.6592	-1.96377
C	-3.67695	-15.77097	-1.3359
C	-5.08608	-18.29826	-3.2908
O	-3.91431	-18.27546	-3.59269
C	-5.9693	-19.51716	-3.37842
H	-4.07784	-13.97689	-4.15261
H	-5.24645	-14.99669	-4.99841
H	-3.62719	-15.6195	-4.64011
H	-6.88779	-15.07868	-1.0302
H	-7.32222	-14.64278	-2.68753
H	-6.20777	-13.62324	-1.76859
H	-2.86128	-16.39791	-1.70214
H	-4.04155	-16.1965	-0.39637
H	-3.27244	-14.77771	-1.11515
H	-6.81388	-19.31396	-4.04109
H	-6.37975	-19.74705	-2.3923
H	-5.39701	-20.36399	-3.75158

Electronic Energy : -3442.17338890 Hartree

Compound 7

Optimized Geometry :

I	1.967708	-3.199638	-0.700805
C	2.702491	-5.068681	-0.071780
C	2.952856	-5.248332	1.287165
C	3.470236	-6.479073	1.684995
C	3.721199	-7.476627	0.742649
C	3.464044	-7.259778	-0.611584
C	2.948239	-6.039816	-1.041253
O	3.868361	-2.416217	-1.007696
S	4.777780	-1.791361	0.194889
O	6.153017	-2.101320	-0.096787
O	4.141395	-2.093604	1.465655
C	4.491794	0.049776	-0.159872
F	5.064382	0.758592	0.797495
F	4.999010	0.366636	-1.338067
F	3.172249	0.275682	-0.163014
O	-0.163738	-4.150152	-0.364602
C	-1.207705	-4.121565	-1.065748
C	-1.286046	-3.480170	-2.418556
O	-2.301197	-4.637268	-0.627612
Si	-2.692000	-5.417095	0.940326
C	-1.627179	-6.946606	1.040739
C	-2.341710	-4.149362	2.264426
C	-4.502199	-5.776902	0.712586
H	2.782236	-4.458517	2.006133
H	3.685145	-6.648881	2.733053
H	4.129079	-8.427391	1.064545
H	3.671934	-8.034339	-1.339783
H	2.759727	-5.859826	-2.091369
H	-1.598167	-2.438193	-2.288487
H	-2.041594	-3.976748	-3.024995
H	-0.323255	-3.492421	-2.928195
H	-1.796628	-7.607830	0.186576
H	-1.879586	-7.510946	1.944247
H	-0.563594	-6.702806	1.086592
H	-1.279202	-3.908090	2.336334
H	-2.660018	-4.539591	3.236607
H	-2.897524	-3.223833	2.090722
H	-4.902333	-6.275711	1.600810
H	-4.677862	-6.433680	-0.143246
H	-5.077196	-4.859668	0.561822
S	7.568601	8.334764	0.182133
F	4.929202	8.945476	0.144575

F	5.386917	7.133891	1.251767
F	5.413403	7.114847	-0.919178
O	8.237387	7.019990	0.201822
O	7.678757	9.122643	1.424384
O	7.709195	9.100767	-1.070684
C	5.732985	7.858357	0.163917
Si	-11.615371	3.900857	-0.013076
O	-13.332295	4.121388	-0.036454
C	-11.092758	2.973746	-1.555564
C	-10.987856	5.666142	-0.021490
C	-11.131909	3.002173	1.558740
C	-14.234919	3.123196	-0.038475
O	-13.927377	1.952765	-0.024280
C	-15.652768	3.635753	-0.060224
H	-10.001469	2.900692	-1.607497
H	-11.433871	3.485624	-2.460199
H	-11.503159	1.961788	-1.559429
H	-11.344802	6.217533	0.852824
H	-11.321943	6.201066	-0.914852
H	-9.893541	5.688831	-0.007556
H	-11.550250	1.993586	1.574421
H	-11.487748	3.535061	2.445383
H	-10.042573	2.921951	1.635032
H	-15.807699	4.254958	-0.946982
H	-15.829357	4.269678	0.811953
H	-16.349440	2.799980	-0.061847

Electronic Energy : -3442.14690004 Hartree

Compound 8

Optimized Geometry :

C	-1.04506	-4.18334	0.70562
C	-1.30825	-2.90475	0.21857
C	-1.96663	-2.00074	1.05025
C	-2.37251	-2.33895	2.34103
C	-2.10103	-3.62156	2.81030
C	-1.43697	-4.53845	1.99542
I	-2.36982	-0.05806	0.32517
O	-0.30665	0.37998	1.13494
C	0.04010	1.23740	2.00312
O	1.28648	1.42527	2.23019
C	-0.93175	1.97920	2.86141
Si	2.73916	0.87899	1.34162
C	2.44563	1.09640	-0.48089
C	2.98996	-0.89678	1.87344
C	4.01162	2.04038	2.05259
O	-2.19611	2.53292	-0.10795
O	-0.83574	3.27306	-2.07019
S	-1.09285	3.41077	-0.64000
C	-1.84057	5.12660	-0.42336
F	-2.95826	5.25586	-1.14453
F	-0.96941	6.06486	-0.81427
F	-2.14289	5.34658	0.86808
O	0.08102	3.41032	0.25757
O	-4.32403	-0.69468	-0.34728
S	-4.61686	-1.51931	-1.66842
O	-3.38313	-2.07388	-2.20882
O	-5.56619	-0.82403	-2.50749
C	-5.55778	-2.96125	-0.88768
F	-4.78083	-3.59651	-0.00445
F	-5.90534	-3.81480	-1.85062
F	-6.65221	-2.52580	-0.26978
H	-0.54034	-4.90168	0.07051
H	-1.02924	-2.63074	-0.79004
H	-2.89675	-1.62656	2.96591
H	-2.41297	-3.90347	3.80907
H	-1.23128	-5.53626	2.36533
H	-0.41440	2.74872	3.42769
H	-1.40423	1.27187	3.55131
H	-1.70266	2.42906	2.23532
H	2.07646	2.10033	-0.70134
H	1.72027	0.37779	-0.86690
H	3.39568	0.93659	-0.99883

H	3.08924	-0.98276	2.95906
H	3.91049	-1.27367	1.41785
H	2.16267	-1.53344	1.54973
H	4.99397	1.79112	1.64276
H	4.06244	1.96100	3.14185
H	3.78003	3.07725	1.79554
Si	8.11942	-2.01720	-0.83784
O	7.79354	-0.40877	-1.39681
C	6.69526	-3.13047	-1.33113
C	9.68979	-2.44633	-1.76127
C	8.39144	-1.97374	1.01570
C	6.75793	0.35894	-1.03418
O	5.90994	-0.00047	-0.24204
C	6.77175	1.70065	-1.72004
H	6.90502	-4.16780	-1.05075
H	6.53174	-3.10664	-2.41243
H	5.76951	-2.82512	-0.83901
H	10.49843	-1.75445	-1.51030
H	9.53539	-2.40389	-2.84291
H	10.02481	-3.45771	-1.51047
H	7.48314	-1.67188	1.54150
H	9.18912	-1.27369	1.28077
H	8.68498	-2.96291	1.38195
H	6.72192	1.55875	-2.80228
H	7.71146	2.21480	-1.50571
H	5.93071	2.30543	-1.38770

Electronic Energy : -3442.16555512 Hartree

Compound 9

Optimized Geometry :

I	0.22603	-1.23196	-0.24439
C	0.23451	-3.29811	0.11682
C	0.25620	-3.73387	1.43477
C	0.25901	-5.10351	1.65907
C	0.24530	-5.98863	0.58722
C	0.22619	-5.51983	-0.72134
C	0.21804	-4.15535	-0.97507
S	-2.86896	-1.76424	-1.27718
F	-2.89266	-4.01489	0.09882
F	-4.62370	-3.69477	-1.15333
F	-4.40874	-2.59745	0.69519
O	-2.09918	-2.42510	-2.30775
O	-3.85183	-0.77282	-1.60357
O	-1.92559	-1.25175	-0.14165
C	-3.76089	-3.10911	-0.33724
S	3.32401	-1.35712	0.90316
F	5.09300	-3.20206	1.44021
F	4.87145	-2.80043	-0.67092
F	3.36543	-3.94146	0.37459
O	4.29944	-0.30691	0.87135
O	2.37789	-1.26766	-0.33721
O	2.55816	-1.63369	2.09830
C	4.22652	-2.93508	0.47512
H	0.29490	-3.03588	2.26002
H	0.27828	-5.47397	2.67671
H	0.24955	-7.05632	0.77391
H	0.21129	-6.21373	-1.55289
H	0.17523	-3.77913	-1.98814
Si	14.29377	4.30443	-0.13477
O	12.66161	4.88135	-0.11984
C	14.57440	3.29129	-1.68613
C	15.27832	5.89817	-0.16230
C	14.61293	3.32090	1.42817
C	11.56935	4.09544	-0.09864
O	11.62398	2.88647	-0.08818
C	10.29097	4.89491	-0.08967
H	15.62442	2.99035	-1.76258
H	14.32815	3.86535	-2.58422
H	13.96028	2.38835	-1.67789
H	15.06536	6.51052	0.71835
H	15.04404	6.49326	-1.04933
H	16.35294	5.69006	-0.17323

H	13.99220	2.42289	1.45612
H	14.39744	3.91491	2.32117
H	15.66245	3.01310	1.47997
H	10.24967	5.53468	-0.97440
H	10.27160	5.55000	0.78452
H	9.43418	4.22445	-0.07319
Si	-13.05185	4.01784	0.21396
O	-14.68402	4.59475	0.22889
C	-12.77123	3.00470	-1.33740
C	-12.06731	5.61157	0.18643
C	-12.73270	3.03430	1.77690
C	-15.77627	3.80885	0.25009
O	-15.72165	2.59988	0.26055
C	-17.05466	4.60832	0.25906
H	-11.72121	2.70376	-1.41385
H	-13.01748	3.57876	-2.23549
H	-13.38535	2.10176	-1.32916
H	-12.28027	6.22393	1.06708
H	-12.30158	6.20666	-0.70060
H	-10.99269	5.40346	0.17550
H	-13.35342	2.13629	1.80485
H	-12.94819	3.62831	2.66990
H	-11.68318	2.72650	1.82871
H	-17.09595	5.24808	-0.62567
H	-17.07403	5.26341	1.13325
H	-17.91144	3.93785	0.27554

Electronic Energy : -3442.16082682 Hartree