

## ***SUPPORTING INFORMATION***

### **Thiol modifier effects of diphenyl diselenides: insight from experiment and DFT calculations**

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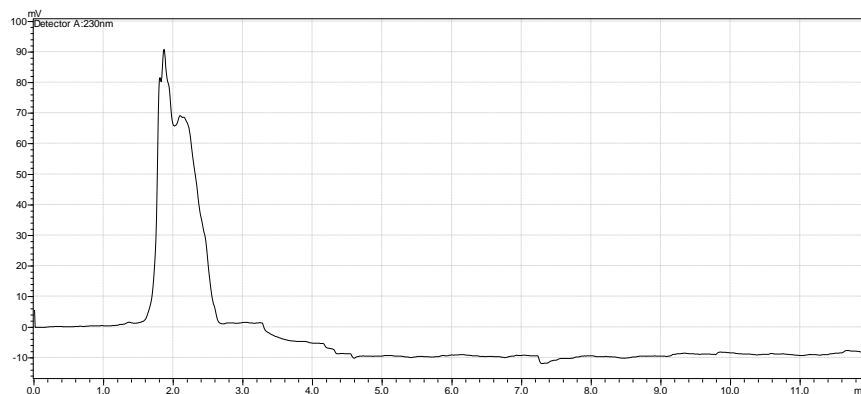
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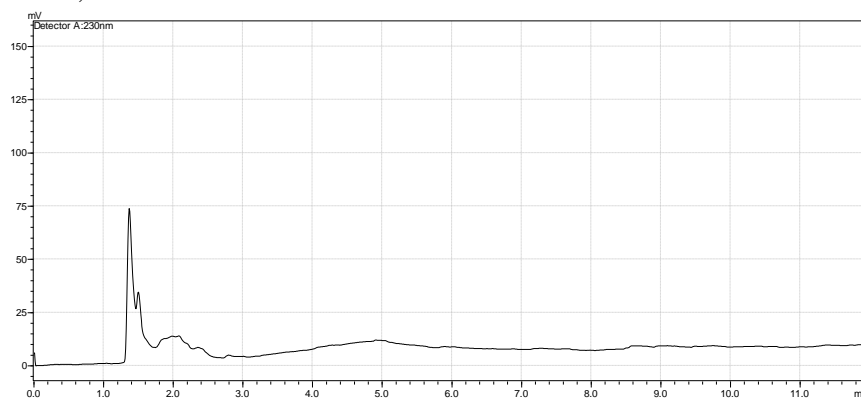
A) DTT reduced, 1 mM.



Retention time: 1.860.

Retention time: 2.094.

B) DTT oxidized, 1 mM.

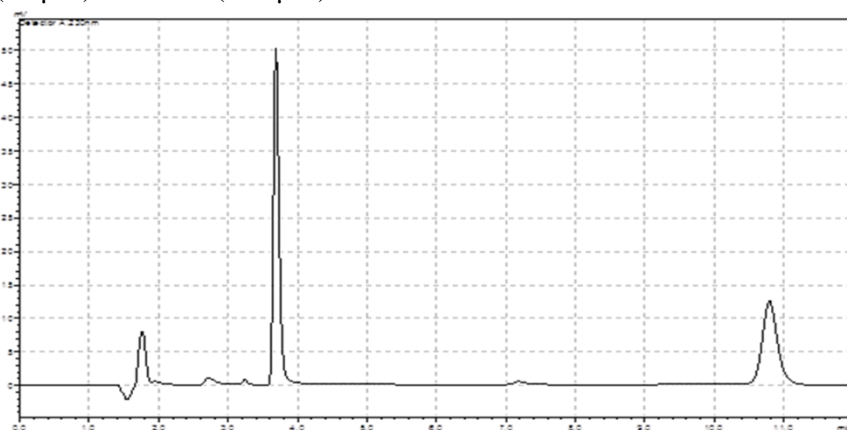


Retention time: 1.492.

Retention time: 1.981.

Retention time: 2.076.

C) (PhSe)<sub>2</sub> (50 μM) + NaBH<sub>4</sub> (250 μM)



Retention time: 10.913 min: (PhSe).

Retention time: 3.758 min: putative PhSeH.

**Figure S1.** Chromatographic detection of reduced (DTT-(SH)<sub>2</sub>) (A), oxidized DTT (DTT-(SS)) (B), and the reduction of (PhSe)<sub>2</sub> with NaBH<sub>4</sub> (C).

2. Cartesian coordinates (Å), energies (a.u.) and imaginary frequencies (cm<sup>-1</sup>) of the optimized structures. Level of theory: (COSMO)-ZORA-OLYP/TZ2P.

**Gas phase**

**MeS<sup>-</sup>**

E = -0.86001897  
 G = -0.84881110  
 N<sub>imag</sub> = not present.  
 S -9.625538 4.045012 -3.917616  
 C -7.817038 3.906355 -3.664923  
 H -7.252587 4.630108 -4.277113  
 H -7.526213 4.088024 -2.616288  
 H -7.433484 2.905971 -3.928231

**PhSeSePh**

E = -5.31483108  
 G = -5.17795782  
 N<sub>imag</sub> = not present.  
 Se -11.565199 1.683193 0.094184  
 C -13.418198 1.210710 -0.231276  
 C -14.385441 2.202179 -0.430966  
 C -15.721263 1.844792 -0.606420  
 C -16.100217 0.501539 -0.572760  
 C -15.137754 -0.486107 -0.366289  
 C -13.797069 -0.135804 -0.199545  
 H -14.094305 3.248181 -0.448635  
 H -16.468848 2.618984 -0.762573  
 H -17.143640 0.226646 -0.705489  
 H -15.426896 -1.534073 -0.339182  
 H -13.047224 -0.906446 -0.047174  
 Se -10.758095 2.259078 -2.045624  
 C -10.257228 0.551675 -2.818557  
 C -9.058526 -0.073089 -2.456241  
 C -8.686747 -1.270423 -3.065574  
 C -9.501064 -1.844125 -4.043670  
 C -10.692119 -1.218218 -4.409921  
 C -11.074616 -0.023841 -3.797564  
 H -8.419448 0.375783 -1.701732  
 H -7.754745 -1.752484 -2.779871  
 H -9.206082 -2.775805 -4.520009  
 H -11.330329 -1.660345 -5.171363  
 H -12.005947 0.458901 -4.078451

**PhSe<sup>-</sup>**

E = -2.69919684  
 G = -2.64342424  
 N<sub>imag</sub> = not present.  
 Se -11.554931 1.699855 0.043949  
 C -13.371053 1.220919 -0.202444  
 C -14.385129 2.189908 -0.416908  
 C -15.719606 1.837373 -0.601431  
 C -16.121851 0.495967 -0.582252  
 C -15.140609 -0.480705 -0.370684  
 C -13.805696 -0.129710 -0.186033  
 H -14.097725 3.238598 -0.436042  
 H -16.460227 2.622229 -0.763407  
 H -17.164928 0.221016 -0.727313  
 H -15.421919 -1.534842 -0.349854  
 H -13.062387 -0.906816 -0.023722

**MeSSePh**

E = -3.50684983  
 G = -3.41594105  
 N<sub>imag</sub> = not present.  
 Se -10.047850 2.519513 -2.087120  
 C -9.961380 0.867865 -3.115250  
 C -9.396790 -0.245755 -2.485373  
 C -9.381523 -1.479588 -3.138245  
 C -9.907012 -1.601115 -4.423699  
 C -10.458038 -0.482784 -5.052036  
 C -10.496543 0.748451 -4.399587  
 H -8.962478 -0.154860 -1.492934  
 H -8.942165 -2.341998 -2.642420  
 H -9.884920 -2.559909 -4.935138

H -10.871619 -0.569197 -6.054233  
 H -10.934621 1.611888 -4.890528  
 S -9.718821 4.099754 -3.568718  
 C -7.907366 4.203629 -3.742929  
 H -7.730489 5.038210 -4.430021  
 H -7.432789 4.418188 -2.783748  
 H -7.500695 3.288209 -4.176824

**MePhSeSePhMe**

E = -6.49076445  
 G = -6.30924858  
 N<sub>imag</sub> = not present.  
 Se -11.585888 1.758808 -0.005892  
 C -13.439165 1.266125 -0.275771  
 C -14.435646 2.246962 -0.339969  
 C -15.771337 1.879426 -0.472435  
 C -16.154045 0.531684 -0.540951  
 C -15.147054 -0.437672 -0.468839  
 C -13.804680 -0.081368 -0.339101  
 C -17.602729 0.148389 -0.702492  
 H -14.166333 3.297619 -0.283580  
 H -16.531107 2.657246 -0.518027  
 H -15.411492 -1.492048 -0.513687  
 H -13.043057 -0.853712 -0.285561  
 H -18.243461 0.709936 -0.014390  
 H -17.760555 -0.917608 -0.519734  
 H -17.954632 0.366372 -1.718727  
 Se -10.814308 2.257045 -2.182667  
 C -10.269231 0.536226 -2.884240  
 C -9.062309 -0.054512 -2.491881  
 C -8.661441 -1.263557 -3.051267  
 C -9.439098 -1.912849 -4.022252  
 C -10.639779 -1.307355 -4.408395  
 C -11.057363 -0.100082 -3.846794  
 C -8.980274 -3.211067 -4.635391  
 H -8.437351 0.430699 -1.747897  
 H -7.721133 -1.707750 -2.730405  
 H -11.267309 -1.786106 -5.157123  
 H -11.998668 0.343704 -4.157731  
 H -9.762219 -3.665495 -5.249051  
 H -8.689019 -3.934548 -3.866126  
 H -8.103626 -3.054342 -5.276144

**MePhSe<sup>-</sup>**

E = -3.28515938  
 G = -3.20603989  
 N<sub>imag</sub> = not present.  
 Se -11.565779 1.769494 -0.076885  
 C -13.387583 1.279355 -0.255742  
 C -14.432186 2.236647 -0.283646  
 C -15.769944 1.873778 -0.415703  
 C -16.168527 0.532704 -0.529100  
 C -15.144302 -0.426730 -0.497545  
 C -13.804654 -0.070717 -0.365798  
 C -17.614105 0.146484 -0.718511  
 H -14.170060 3.288344 -0.194198  
 H -16.528291 2.659127 -0.429436  
 H -15.401305 -1.484940 -0.576708  
 H -13.045067 -0.848714 -0.341408  
 H -18.290918 0.868582 -0.245241  
 H -17.830085 -0.838785 -0.286851  
 H -17.898376 0.095533 -1.782384

**MeSSePhMe**

E = -4.09461185  
 G = -3.98235972  
 N<sub>imag</sub> = not present.  
 Se -10.221607 2.593046 -2.222761  
 C -10.065534 0.909367 -3.181365  
 C -9.303389 -0.113795 -2.614697  
 C -9.238978 -1.363950 -3.233982

C	-9.909941	-1.616166	-4.434280
C	-10.663007	-0.571711	-4.993439
C	-10.752118	0.671412	-4.376154
C	-9.827690	-2.957575	-5.116906
H	-8.755615	0.058424	-1.692055
H	-8.642760	-2.149371	-2.774503
H	-11.201537	-0.736757	-5.924715
H	-11.352529	1.456649	-4.825667
H	-9.325475	-2.876475	-6.088513
H	-10.825885	-3.368440	-5.306240
H	-9.274167	-3.682654	-4.515038
S	-9.621994	4.098262	-3.708272
C	-7.801107	4.115915	-3.646290
H	-7.494998	4.909007	-4.337211
H	-7.443812	4.353771	-2.642572
H	-7.386289	3.164915	-3.986198

**MeOPhSeSePhOMe**

E = -6.92793242

G = -6.73652449

N<sub>imag</sub> = not present.

Se	-11.600005	1.667341	0.029350
C	-13.453826	1.203826	-0.243851
C	-14.443587	2.197331	-0.291929
C	-15.780896	1.856959	-0.424238
C	-16.164700	0.508302	-0.507378
C	-15.184482	-0.490623	-0.457270
C	-13.840460	-0.135421	-0.328131
H	-14.163072	3.244226	-0.223586
H	-16.550274	2.623105	-0.460122
H	-15.446563	-1.540598	-0.516387
H	-13.088634	-0.918364	-0.291515
O	-17.505287	0.287532	-0.631333
C	-17.975520	-1.053266	-0.713716
H	-19.060808	-0.978699	-0.802663
H	-17.725863	-1.625899	0.188451
H	-17.575860	-1.568941	-1.596112
Se	-10.806975	2.213183	-2.138108
C	-10.247672	0.520289	-2.878534
C	-9.002663	-0.037084	-2.549235
C	-8.581433	-1.220998	-3.134359
C	-9.394080	-1.876218	-4.074508
C	-10.636377	-1.325815	-4.412615
C	-11.053563	-0.137100	-3.810328
H	-8.359417	0.461359	-1.830140
H	-7.618001	-1.655368	-2.882617
H	-11.287134	-1.804859	-5.134863
H	-12.020934	0.278647	-4.076815
O	-8.878948	-3.028795	-4.591949
C	-9.636358	-3.743851	-5.561770
H	-9.816839	-3.139798	-6.459944
H	-10.595444	-4.087394	-5.153795
H	-9.028774	-4.610578	-5.828130

**MeOPhSe-**

E = -3.50072198

G = -3.41754322

N<sub>imag</sub> = not present.

Se	-11.546479	1.683885	0.022929
C	-13.371780	1.210190	-0.208298
C	-14.384228	2.180329	-0.420268
C	-15.721769	1.843027	-0.595002
C	-16.129758	0.503864	-0.567152
C	-15.163618	-0.484071	-0.358229
C	-13.821704	-0.128169	-0.184205
H	-14.096745	3.228595	-0.447204
H	-16.470635	2.617010	-0.756565
H	-15.430727	-1.536627	-0.327309
H	-13.090700	-0.917042	-0.023945
O	-17.495371	0.274768	-0.754376
C	-17.937487	-1.061081	-0.749153
H	-19.018843	-1.026577	-0.917181
H	-17.744757	-1.563206	0.212380
H	-17.473477	-1.659195	-1.549592

**MeSSePhOMe**

E = -4.31303603

G = -4.19625422

N<sub>imag</sub> = not present.

Se	-10.436426	2.762228	-2.493223
C	-10.174816	1.047557	-3.356679
C	-9.266357	0.123668	-2.821114
C	-9.109718	-1.129261	-3.397827
C	-9.855399	-1.484119	-4.532619
C	-10.765362	-0.565455	-5.073560
C	-10.921580	0.686664	-4.479358
H	-8.679452	0.384149	-1.944973
H	-8.408696	-1.849257	-2.985183
H	-11.360287	-0.809888	-5.945821
H	-11.634657	1.387248	-4.903946
O	-9.620691	-2.735179	-5.021991
C	-10.335120	-3.166933	-6.175504
H	-9.981095	-4.179366	-6.377579
H	-10.123687	-2.530430	-7.043895
H	-11.417155	-3.192461	-5.995188
S	-9.395851	4.183422	-3.822336
C	-7.650586	4.123823	-3.304270
H	-7.142861	4.886155	-3.905264
H	-7.544642	4.370566	-2.246026
H	-7.207712	3.148790	-3.517224

**ClPhSeSePhCl**

E = -5.19629341

G = -5.08208169

N<sub>imag</sub> = not present.

Se	-11.576203	1.727012	0.025744
C	-13.430760	1.243837	-0.252541
C	-14.420676	2.230681	-0.316035
C	-15.760858	1.880531	-0.460147
C	-16.111656	0.531643	-0.536172
C	-15.138039	-0.464927	-0.467976
C	-13.799291	-0.103718	-0.327154
Cl	-17.784964	0.088144	-0.714923
H	-14.148346	3.279893	-0.252246
H	-16.527757	2.646942	-0.508814
H	-15.422786	-1.510632	-0.525138
H	-13.041431	-0.879578	-0.275113
Se	-10.808849	2.249620	-2.145423
C	-10.268915	0.533673	-2.862877
C	-9.069698	-0.068096	-2.065657
C	-8.662711	-1.274151	-3.029682
C	-9.456945	-1.876184	-4.007552
C	-10.650671	-1.285660	-4.420985
C	-11.054540	-0.083294	-3.842150
Cl	-8.948114	-3.380225	-4.720384
H	-8.446192	0.403875	-1.712357
H	-7.732885	-1.740420	-2.719942
H	-11.260305	-1.761549	-5.182381
H	-11.988049	0.372403	-4.158643

**ClPhSe-**

E = -2.64796613

G = -2.60380380

N<sub>imag</sub> = not present.

Se	-11.556439	1.699342	0.040079
C	-13.368734	1.221453	-0.203068
C	-14.385150	2.187565	-0.416687
C	-15.722197	1.844619	-0.600737
C	-16.100804	0.501505	-0.577168
C	-15.139275	-0.488299	-0.368473
C	-13.806593	-0.127703	-0.186232
Cl	-17.794221	0.054995	-0.811839
H	-14.104651	3.237642	-0.437460
H	-16.468684	2.618658	-0.762362
H	-15.430669	-1.535786	-0.349021
H	-13.068574	-0.909440	-0.024942

**MeSSePhCl**

E = -3.44742340

G = -3.36823612

N<sub>imag</sub> = not present.

Se	-10.074126	2.576337	-2.094539
C	-9.980458	0.916688	-3.104200
C	-9.389102	-0.187315	-2.483365

C	-9.365956	-1.428225	-3.119921
C	-9.918816	-1.554444	-4.393009
C	-10.500482	-0.455398	-5.027642
C	-10.538780	0.774652	-4.376394
H	-8.934925	-0.089911	-1.500719
H	-8.907009	-2.284194	-2.635591
H	-10.930676	-0.563790	-6.018272
H	-11.000540	1.624145	-4.869964
Cl	-9.879830	-3.095945	-5.203113
S	-9.688260	4.133333	-3.588233
C	-7.872213	4.217839	-3.716683
H	-7.670856	5.040983	-4.410777
H	-7.420461	4.442579	-2.748904
H	-7.462619	3.293156	-4.127504

**CF<sub>3</sub>PhSeSePhCF<sub>3</sub>**

E = -6.57336209

G = -6.43374017

N<sub>imag</sub> = not present.

Se	-11,544678	1,856213	-0,047375
C	-13,386372	1,285806	-0,273391
C	-14,395069	2,212143	-0,558201
C	-15,717999	1,794696	-0,658231
C	-16,047332	0,449599	-0,460779
C	-15,042787	-0,475151	-0,172161
C	-13,715386	-0,058759	-0,081070
C	-17,485765	0,001026	-0,613381
H	-14,149700	3,260141	-0,698990
H	-16,494356	2,520965	-0,877380
H	-15,288220	-1,520818	-0,018940
H	-12,938887	-0,784934	0,138857
F	-18,361874	0,923123	-0,137188
F	-17,739260	-1,162070	0,035640
F	-17,804274	-0,201098	-1,924310
Se	-10,861925	2,322247	-2,247786
C	-10,328063	0,588849	-2,935933
C	-9,297236	-0,151584	-2,347637
C	-8,897363	-1,358299	-2,909756
C	-9,509042	-1,829542	-4,077224
C	-10,532783	-1,089079	-4,668343
C	-10,946175	0,113435	-4,095554
C	-9,083907	-3,162770	-4,654376
H	-8,804426	0,212707	-1,451810
H	-8,095945	-1,925240	-2,446174
H	-11,017986	-1,446942	-5,570263
H	-11,754286	0,675250	-4,554422
F	-9,451158	-3,311360	-5,950758
F	-9,639306	-4,201458	-3,965464
F	-7,737189	-3,335906	-4,598600

**CF<sub>3</sub>PhSe-**

E = -3.34581625

G = -3.29272820

N<sub>imag</sub> = not present.

Se	-11.552865	1.707326	-0.005637
C	-13.356278	1.224688	-0.214440
C	-14.367064	2.177780	-0.515924
C	-15.697941	1.825490	-0.672005
C	-16.114875	0.489208	-0.528658
C	-15.133600	-0.476575	-0.237512
C	-13.804212	-0.118213	-0.082725
C	-17.527175	0.098180	-0.760559
H	-14.075634	3.219091	-0.625259
H	-16.428490	2.597121	-0.902939
H	-15.419572	-1.519824	-0.125809
H	-13.069802	-0.885126	0.149132
F	-18.426675	1.088891	-0.459740
F	-17.916854	-1.001414	-0.038380
F	-17.806454	-0.236604	-2.080605

**MeSSePhCF<sub>3</sub>**

E = -4.13714356

G = -4.04829449

N<sub>imag</sub> = not present.

Se	-9.738766	2.434833	-1.960887
C	-9.802095	0.813054	-3.030679
C	-9.531473	-0.382761	-2.355966

C	-9.596497	-1.596572	-3.032662
C	-9.925756	-1.629558	-4.390549
C	-10.186846	-0.432017	-5.061266
C	-10.131666	0.783704	-4.385238
C	-9.937987	-2.942113	-5.138482
H	-9.265908	-0.378454	-1.301523
H	-9.386714	-2.517021	-2.497305
H	-10.445580	-0.442429	-6.115360
H	-10.349966	1.705698	-4.914536
F	-10.799806	-2.932225	-6.187971
F	-10.289677	-3.986685	-4.344367
F	-8.706379	-3.240483	-5.649582
S	-9.793358	4.069737	-3.408464
C	-8.050067	4.335365	-3.873578
H	-8.063403	5.199716	-4.546151
H	-7.442972	4.568806	-2.997518
H	-7.644875	3.471958	-4.403916

**TCI: [PhSeSePh+SMe]<sup>-</sup>**

E = -6.21909876

G = -6.05397160

N<sub>imag</sub> = not present.

Se	-11.548359	1.362392	0.192070
C	-13.383527	0.882452	-0.036846
C	-14.097759	1.136309	-1.224830
C	-15.438225	0.777175	-1.351749
C	-16.118653	0.153474	-0.302358
C	-15.423544	-0.104198	0.882926
C	-14.083015	0.251545	1.014138
H	-13.591424	1.624399	-2.051338
H	-15.958144	0.989048	-2.285736
H	-17.165144	-0.125630	-0.405437
H	-15.930310	-0.589927	1.716648
H	-13.560283	0.040083	1.943969
Se	-10.535346	2.648545	-2.172499
C	-10.218689	0.961634	-3.105483
C	-9.366065	-0.004305	-2.559888
C	-9.128972	-1.202517	-3.234498
C	-9.737779	-1.452915	-4.265091
C	-10.588556	-0.491746	-5.013400
C	-10.828198	0.705501	-4.338795
H	-8.898499	0.177317	-1.597543
H	-8.464857	-1.943782	-2.793048
H	-9.554175	-2.388449	-4.989628
H	-11.075367	-0.675419	-5.969832
H	-11.485710	1.450619	-4.775676
S	-9.591371	4.056601	-3.923270
C	-7.797089	3.895038	-3.654293
H	-7.291879	4.635546	-4.285521
H	-7.536292	4.090007	-2.609229
H	-7.438502	2.898502	-3.931721

**TCI: [MePhSeSePhMe+SMe]<sup>-</sup>**

E = -7.39213128

G = -7.17970172

N<sub>imag</sub> = not present.

Se	-11.528473	1.425835	0.184952
C	-13.357625	0.923873	-0.051100
C	-14.111084	1.278260	-1.186263
C	-15.447106	0.905289	-1.314881
C	-16.108643	0.163729	-0.326627
C	-15.361222	-0.186146	0.806333
C	-14.023883	0.178811	0.942836
H	-13.641189	1.860672	-1.972570
H	-15.989485	1.205187	-2.212083
H	-15.833218	-0.759954	1.604598
H	-13.480615	-0.114102	1.838237
C	-17.544780	-0.268927	-0.491234
H	-18.117052	0.451727	-1.086487
H	-18.047924	-0.374753	0.476706
H	-17.623824	-1.240422	-1.001936
Se	-10.528873	2.693937	-2.193960
C	-10.219223	0.984059	-3.088918
C	-9.302558	0.061319	-2.576294
C	-9.072858	-1.150471	-3.226635
C	-9.746838	-1.484035	-4.407697
C	-10.658781	-0.551205	-4.916427

C	-10.893923	0.661441	-4.270069
H	-8.772624	0.287022	-1.656234
H	-8.353047	-1.849376	-2.802090
H	-11.202038	-0.774899	-5.833854
H	-11.601555	1.367609	-4.693538
C	-9.526479	-2.814061	-5.085939
H	-9.682332	-2.745891	-6.167827
H	-10.222119	-3.575123	-4.705714
H	-8.512247	-3.190192	-4.914554
S	-9.591137	4.057468	-3.984413
C	-7.796055	3.917347	-3.708647
H	-7.294713	4.640267	-4.363027
H	-7.537382	4.147812	-2.670220
H	-7.430045	2.914842	-3.953173

C	-9.754128	-1.433992	-4.484685
C	-10.494264	-0.426565	-5.099387
C	-10.724262	0.765649	-4.413473
H	-9.099104	0.065929	-1.521146
H	-8.673533	-2.051111	-2.724776
H	-10.892519	-0.571488	-6.099101
H	-11.292263	1.552681	-4.898999
Cl	-9.456563	-2.937843	-5.341093
S	-9.618741	4.068871	-3.914803
C	-7.820557	3.918695	-3.666494
H	-7.331510	4.668806	-4.298587
H	-7.550666	4.109043	-2.623302
H	-7.457488	2.927660	-3.956391

**TCI: [MeOPhSeSePhOMe+SMe]<sup>-</sup>**

E = -7.82587018

G = -7.60489055

N<sub>imag</sub> = not present.

Se	-11.400189	1.628185	0.315266
C	-13.226962	1.152216	-0.006912
C	-14.176844	2.092240	-0.456484
C	-15.507735	1.749133	-0.661134
C	-15.950976	0.443169	-0.417355
C	-15.032025	-0.511043	0.025510
C	-13.692980	-0.152527	0.217040
H	-13.858247	3.112530	-0.649032
H	-16.223615	2.490379	-1.009756
H	-15.330851	-1.536147	0.219539
H	-12.990997	-0.912314	0.550446
O	-17.299311	0.210431	-0.645416
C	-17.791529	-1.093212	-0.418866
H	-18.858893	-1.058662	-0.655277
H	-17.668888	-1.407157	0.628553
H	-17.307232	-1.838216	-1.067523
Se	-10.476537	2.758871	-2.150726
C	-10.233780	1.004079	-2.952242
C	-9.128318	0.206609	-2.627176
C	-8.942977	-1.039470	-3.214249
C	-9.868619	-1.523721	-4.146899
C	-10.979297	-0.743294	-4.478436
C	-11.150136	0.508348	-3.879422
H	-8.408617	0.562279	-1.896029
H	-8.084496	-1.654906	-2.956637
H	-11.720929	-1.088355	-5.190514
H	-12.017798	1.104564	-4.145204
O	-9.592076	-2.771328	-4.671147
C	-10.500776	-3.315546	-5.609255
H	-10.096110	-4.292667	-5.886459
H	-10.583152	-2.693822	-6.512210
H	-11.503383	-3.452563	-5.180165
S	-9.670197	4.016493	-4.092713
C	-7.858272	3.949007	-3.916621
H	-7.419450	4.645519	-4.641085
H	-7.547673	4.250639	-2.911004
H	-7.471222	2.945581	-4.122749

**TCI: [ClPhSeSePhCl+SMe]<sup>-</sup>**

E = -6.11038423

G = -5.96772745

N<sub>imag</sub> = not present.

Se	-11.534942	1.365769	0.218085
C	-13.363768	0.875323	-0.008980
C	-14.063841	1.061802	-1.217291
C	-15.402611	0.700156	-1.353035
C	-16.080024	0.138177	-0.272411
C	-15.420876	-0.061521	0.939904
C	-14.082392	0.303831	1.061974
H	-13.551928	1.503484	-2.065962
H	-15.916260	0.856208	-2.297699
H	-15.947834	-0.499755	1.783037
H	-13.580050	0.142194	2.012336
Cl	-17.771061	-0.321581	-0.437018
Se	-10.528165	2.650728	-2.183333
C	-10.221929	0.966390	-3.123681
C	-9.483668	-0.060982	-2.527544
C	-9.247493	-1.260716	-3.198908

**TCI: [CF<sub>3</sub>PhSeSePhCF<sub>3</sub>+SMe]<sup>-</sup>**

E = -7.49761582

G = -7.33353016

N<sub>imag</sub> = not present.

Se	-11.582815	1.351162	0.245421
C	-13.410814	0.864290	0.110725
C	-14.105771	0.822400	-1.117516
C	-15.446093	0.464549	-1.184593
C	-16.157501	0.124037	-0.025902
C	-15.485090	0.165875	1.205356
C	-14.147044	0.524944	1.269554
H	-13.581717	1.079937	-2.032026
H	-15.941655	0.445915	-2.151045
H	-16.012263	-0.089254	2.120981
H	-13.648304	0.545221	2.234744
C	-17.612423	-0.210376	-0.077356
F	-18.026645	-0.635376	-1.305947
F	-18.423435	0.862404	0.233220
F	-17.967864	-1.192272	0.809637
Se	-10.551916	2.535900	-2.371899
C	-10.166227	0.883080	-3.354084
C	-10.125483	-0.340492	-2.668946
C	-9.858069	-1.525284	-3.347280
C	-9.625020	-1.522326	-4.726546
C	-9.664151	-0.303597	-5.412453
C	-9.935660	0.880563	-4.736081
H	-10.320289	-0.364366	-1.601484
H	-9.834981	-2.457479	-2.790648
H	-9.491624	-0.274173	-6.484611
H	-9.962149	1.816591	-5.284682
C	-9.275109	-2.789680	-5.451369
F	-9.723159	-2.804615	-6.740976
F	-9.779903	-3.904126	-4.852923
F	-7.916524	-2.989614	-5.529595
S	-9.753843	4.116172	-3.929683
C	-7.965531	4.166175	-3.581510
H	-7.550313	5.016228	-4.134101
H	-7.780889	4.313548	-2.514161
H	-7.466893	3.251219	-3.913801

**TCI: [PhSeSePh+SMe]<sup>-</sup> conformer a**

E = -6.21910960 Hartree

N<sub>imag</sub> = not present.

Se	-11.504567	1.369780	0.065720
C	-13.349222	0.895379	-0.084762
C	-14.102678	1.120548	-1.254139
C	-15.448937	0.767697	-1.324399
C	-16.096434	0.179402	-0.234484
C	-15.362223	-0.049602	0.932944
C	-14.015554	0.299443	1.007333
H	-13.622060	1.580941	-2.111356
H	-15.999600	0.956445	-2.245637
H	-17.147603	-0.094925	-0.293297
H	-15.842743	-0.507929	1.797159
H	-13.461856	0.109846	1.923852
Se	-10.542855	2.501383	-2.400538
C	-10.318174	0.761029	-3.259194
C	-9.481188	-0.208319	-2.695770
C	-9.309675	-1.445044	-3.318782
C	-9.969692	-1.731360	-4.514668
C	-10.805265	-0.767002	-5.080447
C	-10.979394	0.468848	-4.457365

H	-8.974525	0.001591	-1.759340
H	-8.656631	-2.188186	-2.864170
H	-9.837225	-2.696806	-4.998874
H	-11.331532	-0.978068	-6.009954
H	-11.625517	1.215790	-4.907884
S	-9.620061	3.787905	-4.252088
C	-7.823317	3.575846	-4.040585
H	-7.317804	4.267097	-4.725178
H	-7.516835	3.811056	-3.016428
H	-7.509245	2.555145	-4.281689

**TCI: [PhSeSePh+SMe]<sup>-</sup> conformer b**

E = -6.21910607 Hartree

N<sub>imag</sub> = not present.

Se	-11.878944	1.545819	0.354483
C	-13.628719	0.842152	0.048791
C	-14.333905	1.043134	-1.154664
C	-15.612851	0.520880	-1.337560
C	-16.238643	-0.219505	-0.330830
C	-15.551694	-0.427013	0.868944
C	-14.272241	0.091487	1.055891
H	-13.869871	1.619268	-1.948741
H	-16.127579	0.696426	-2.281903
H	-17.237212	-0.625697	-0.477571
H	-16.016456	-1.001545	1.670029
H	-13.754286	-0.083716	1.995871
Se	-10.941461	2.982629	-1.960751
C	-10.401434	1.361665	-2.907896
C	-9.472922	0.481969	-2.340838
C	-9.076441	-0.667562	-3.025181
C	-9.599108	-0.954364	-4.287014
C	-10.525200	-0.079086	-4.856668
C	-10.924492	1.069029	-4.172358
H	-9.071105	0.691096	-1.354721
H	-8.355162	-1.342124	-2.566801
H	-9.290970	-1.852012	-4.819321
H	-10.946266	-0.292506	-5.837815
H	-11.639841	1.748139	-4.625623
S	-10.108335	4.524187	-3.651761
C	-8.317285	4.561749	-3.322251
H	-7.879359	5.367922	-3.922539
H	-8.115421	4.763092	-2.265438
H	-7.838300	3.618389	-3.603764

**Water phase**

MeS<sup>-</sup>

E = -0.97168143

G = -0.95847800

N<sub>imag</sub> = not present.

S	0.000000	0.000000	-10.347919
C	0.000000	0.000000	-8.504374
H	0.511103	0.885256	-8.109940
H	-1.022206	0.000000	-8.109940
H	0.511103	-0.885256	-8.109940

**PhSeSePh**

E = -5.31880585

G = -5.18574462

N<sub>imag</sub> = not present.

Se	-11.567688	1.687709	0.074919
C	-13.424776	1.213354	-0.228544
C	-14.392483	2.206057	-0.425362
C	-15.731516	1.848653	-0.584742
C	-16.111650	0.505130	-0.537597
C	-15.147813	-0.483083	-0.332632
C	-13.804141	-0.133290	-0.181435
H	-14.104264	3.252832	-0.453269
H	-16.479307	2.622845	-0.738553
H	-17.156466	0.230568	-0.658075
H	-15.437704	-1.530276	-0.293685
H	-13.057064	-0.906364	-0.027222
Se	-10.781880	2.255072	-2.082094
C	-10.262300	0.547127	-2.843328
C	-9.080931	-0.087376	-2.440340
C	-8.695634	-1.285046	-3.042926
C	-9.477572	-1.847094	-4.055190

C	-10.650078	-1.209458	-4.462572
C	-11.047601	-0.015576	-3.856334
H	-8.463286	0.349892	-1.661313
H	-7.778357	-1.775112	-2.725644
H	-9.171890	-2.778063	-4.525721
H	-11.262392	-1.641299	-5.250452
H	-11.964206	0.473698	-4.172590

**PhSe<sup>-</sup>**

E = -2.78899960

G = -2.73243730

N<sub>imag</sub> = not present.

Se	-11.546266	1.702231	0.046230
C	-13.389035	1.216169	-0.204994
C	-14.383699	2.193391	-0.417236
C	-15.721128	1.839677	-0.601877
C	-16.113388	0.498222	-0.580832
C	-15.140853	-0.483500	-0.370660
C	-13.802799	-0.132106	-0.185818
H	-14.103406	3.243808	-0.437742
H	-16.461619	2.621071	-0.763596
H	-17.155274	0.223615	-0.725306
H	-15.423684	-1.534520	-0.350155
H	-13.064910	-0.914266	-0.024154

**MeS<sup>-</sup>SePh**

E = -3.50996639

G = -3.42150206

N<sub>imag</sub> = not present.

Se	-9.588007	2.377794	-1.914915
C	-9.751975	0.779642	-3.021219
C	-9.498377	-0.435273	-2.372297
C	-9.624309	-1.634959	-3.073960
C	-9.993817	-1.630592	-4.420768
C	-10.240246	-0.414922	-0.506803
C	-10.124000	0.791009	-4.365703
H	-9.202533	-0.454942	-1.325865
H	-9.426865	-2.574289	-2.562928
H	-10.086940	-2.565997	-4.966147
H	-10.528331	-0.398482	-6.109454
H	-10.323784	1.730475	-4.871783
S	-9.772168	4.058671	-3.304398
C	-8.081534	4.367880	-3.911323
H	-8.170753	5.254183	-4.547631
H	-7.404185	4.581020	-3.083198
H	-7.717275	3.529282	-4.506411

**MePhSeSePhMe**

E = -6.49490730

G = -6.31543138

N<sub>imag</sub> = not present.

Se	-11.593561	1.743090	-0.007468
C	-13.450151	1.259694	-0.271182
C	-14.441358	2.247326	-0.336140
C	-15.780202	1.886390	-0.465196
C	-16.170877	0.539312	-0.529113
C	-15.168258	-0.436443	-0.454495
C	-13.822804	-0.087124	-0.328505
C	-17.621185	0.163453	-0.686797
H	-14.170291	3.297914	-0.282711
H	-16.535136	2.668456	-0.511208
H	-15.438245	-1.489334	-0.494134
H	-13.068510	-0.866585	-0.271456
H	-18.256108	0.734640	-0.001618
H	-17.782923	-0.901074	-0.500811
H	-17.970242	0.381967	-1.703766
Se	-10.823339	2.245198	-2.193063
C	-10.267213	0.528033	-2.895042
C	-9.058547	-0.057268	-2.496515
C	-8.649406	-1.264767	-3.055752
C	-9.419935	-1.916625	-4.032578
C	-10.621902	-1.314637	-4.425329
C	-11.048160	-0.109303	-3.864005
C	-8.953504	-3.212104	-4.644066
H	-8.436155	0.427159	-1.749510
H	-7.709004	-1.704723	-2.730377
H	-11.243008	-1.793981	-5.178632

H	-11.988806	0.329361	-4.184501
H	-9.730869	-3.667096	-5.262556
H	-8.661466	-3.932202	-3.872237
H	-8.073144	-3.048558	-5.277761

**MePhSe<sup>-</sup>**

E = -3.37573615

G = -3.29410330

N<sub>imag</sub> = not present.

Se	-11.557694	1.771503	-0.070824
C	-13.407647	1.273878	-0.256214
C	-14.432966	2.239074	-0.284232
C	-15.773452	1.875173	-0.418519
C	-16.165894	0.533678	-0.532889
C	-15.146831	-0.429392	-0.500448
C	-13.804235	-0.073163	-0.366642
C	-17.612969	0.146652	-0.712905
H	-14.178133	3.292666	-0.196271
H	-16.529998	2.658557	-0.432395
H	-15.403377	-1.484952	-0.579703
H	-13.050131	-0.856547	-0.344329
H	-18.283978	0.872245	-0.242932
H	-17.821577	-0.838432	-0.284093
H	-17.882300	0.099223	-1.776762

**MeSSePhMe**

E = -4.09814845

G = -3.98665325

N<sub>imag</sub> = not present.

Se	-10.316653	2.642383	-2.336495
C	-10.133137	0.932603	-3.241690
C	-9.267312	-0.028646	-2.713161
C	-9.175972	-1.289524	-3.307134
C	-9.927598	-1.615911	-4.442631
C	-10.790791	-0.636505	-4.960366
C	-10.902664	0.618744	-4.367826
C	-9.805010	-2.964508	-5.103380
H	-8.663975	0.197717	-1.838436
H	-8.500250	-2.026061	-2.878171
H	-11.396342	-0.861804	-5.835743
H	-11.590452	1.349716	-4.783430
H	-9.195939	-2.896292	-6.013684
H	-10.784322	-3.352022	-5.401652
H	-9.331201	-3.694183	-4.442011
S	-9.521992	4.087106	-3.806338
C	-7.717942	4.089837	-3.556723
H	-7.337487	4.852247	-4.244333
H	-7.465214	4.366453	-2.531789
H	-7.284179	3.122525	-3.815866

**MeOPhSeSePhOMe**

E = -6.93730663

G = -6.74732550

N<sub>imag</sub> = not present.

Se	-11.651954	1.592680	-0.000719
C	-13.508044	1.141757	-0.273737
C	-14.491803	2.143009	-0.306757
C	-15.831764	1.810965	-0.443608
C	-16.223230	0.464266	-0.546780
C	-15.247871	-0.541810	-0.509739
C	-13.902321	-0.195717	-0.375749
H	-14.210313	3.188709	-0.223184
H	-16.592956	2.586105	-0.467439
H	-15.516115	-1.588941	-0.582944
H	-13.158748	-0.986912	-0.348236
O	-17.561706	0.248902	-0.675321
C	-18.039082	-1.100291	-0.782644
H	-19.122334	-1.018192	-0.874667
H	-17.790575	-1.679976	0.112475
H	-17.632709	-1.594078	-1.671508
Se	-10.851100	2.148101	-2.175401
C	-10.275697	0.462307	-2.917306
C	-9.012841	-0.067265	-2.607199
C	-8.581287	-1.249431	-3.190781
C	-9.401772	-1.930100	-4.107997
C	-10.661715	-1.405536	-4.427007
C	-11.088320	-0.218836	-3.828433

H	-8.361289	0.446855	-1.906589
H	-7.603503	-1.658603	-2.951257
H	-11.316970	-1.903534	-5.131574
H	-12.067864	0.174026	-4.085024
O	-8.880709	-3.077028	-4.625381
C	-9.657399	-3.824111	-5.573155
H	-9.865649	-3.230271	-6.469284
H	-10.596305	-4.170878	-5.129034
H	-9.041410	-4.683113	-5.840211

**MeOPhSe<sup>-</sup>**

E = -3.59500933

G = -3.51070760

N<sub>imag</sub> = not present.

Se	-11.538102	1.685785	0.030211
C	-13.390613	1.206830	-0.209597
C	-14.384389	2.185103	-0.419719
C	-15.722158	1.845936	-0.596429
C	-16.128038	0.503405	-0.570296
C	-15.162465	-0.487135	-0.361798
C	-13.820702	-0.129910	-0.185757
H	-14.105851	3.235729	-0.446166
H	-16.467259	2.621887	-0.572290
H	-15.430703	-1.537439	-0.333155
H	-13.094987	-0.923781	-0.026148
O	-17.471815	0.276184	-0.756809
C	-17.938908	-1.076075	-0.746572
H	-19.015345	-1.016996	-0.913983
H	-17.747991	-1.558865	0.218863
H	-17.478752	-1.664958	-1.548524

**MeSSePhOMe**

E = -4.31923053

G = -4.20305553

N<sub>imag</sub> = not present.

Se	-10.463851	2.780781	-2.564913
C	-10.187180	1.058165	-3.404247
C	-9.244471	0.160964	-2.880079
C	-9.079173	-1.096907	-3.444724
C	-9.852623	-1.484799	-4.551974
C	-10.798845	-0.593767	-5.078877
C	-10.960885	0.664935	-4.499590
H	-8.637556	0.441799	-2.042286
H	-8.350301	-1.792862	-3.038317
H	-11.415263	-0.864579	-5.927665
H	-11.702399	1.341170	-4.915377
O	-9.609962	-2.736102	-5.031731
C	-10.358185	-3.200209	-6.165242
H	-9.990239	-4.207283	-6.362968
H	-10.181796	-2.567501	-7.041380
H	-11.429686	-3.239337	-5.943061
S	-9.328073	4.180164	-3.854179
C	-7.617800	4.142372	-3.229362
H	-7.081522	4.890235	-3.822583
H	-7.580293	4.421070	-2.174900
H	-7.162048	3.163611	-3.388124

**ClPhSeSePhCl**

E = -5.20005103

G = -5.08634327

N<sub>imag</sub> = not present.

Se	-11.577764	1.725673	0.016205
C	-13.435342	1.243474	-0.250239
C	-14.422635	2.233260	-0.319575
C	-15.764972	1.884115	-0.454121
C	-16.115260	0.534479	-0.513539
C	-15.145875	-0.465519	-0.438703
C	-13.805183	-0.104995	-0.307761
Cl	-17.794176	0.091181	-0.680063
H	-14.152670	3.283673	-0.267651
H	-16.528097	2.653794	-0.507039
H	-15.429579	-1.512005	-0.482244
H	-13.052020	-0.884746	-0.248681
Se	-10.825354	2.245091	-2.167033
C	-10.273363	0.529214	-2.878207
C	-9.086866	-0.079320	-2.452662
C	-8.670623	-1.284398	-3.014046



C	-9.443606	-1.872985	-4.016563	H	-10.061109	1.749997	-4.952784
C	-10.623349	-1.276369	-4.459555	F	-8.410812	-2.468826	-6.545287
C	-11.037085	-0.075649	-3.882441	F	-10.142325	-3.563501	-5.788847
Cl	-8.921853	-3.378062	-4.728269	F	-8.255881	-3.611378	-4.691188
H	-8.477545	0.381506	-1.681125				
H	-7.751004	-1.754487	-2.681000				
H	-11.216970	-1.741229	-5.239972				
H	-11.959448	0.384124	-4.224267				

**ClPhSe<sup>-</sup>**

E = -2.73062582  
G = -2.68581906  
N<sub>imag</sub> = not present.

Se	-11.547776	1.701711	0.042708
C	-13.387456	1.216520	-0.205666
C	-14.384822	2.190239	-0.417234
C	-15.723722	1.845980	-0.601187
C	-16.097331	0.502434	-0.576530
C	-15.139949	-0.490277	-0.368664
C	-13.805044	-0.129931	-0.186300
Cl	-17.778561	0.059190	-0.808673
H	-14.112260	3.242203	-0.439476
H	-16.467469	2.620987	-0.762464
H	-15.428505	-1.537244	-0.348718
H	-13.073095	-0.917262	-0.025706

**MeSsePhCl**

E = -3.45060075  
G = -3.37340614

Se	-10.014653	2.552319	-2.063344
C	-9.954052	0.898960	-3.089694
C	-9.404949	-0.223586	-2.461657
C	-9.399699	-1.461090	-3.106532
C	-9.930345	-1.562261	-4.391371
C	-10.472631	-0.447625	-5.032548
C	-10.491382	0.780055	-4.373372
H	-8.971474	-0.147572	-1.468093
H	-8.972245	-2.329391	-2.615557
H	-10.886607	-0.535416	-6.031997
H	-10.923842	1.641016	-4.873352
Cl	-9.912711	-3.103564	-5.213454
S	-9.695290	4.128068	-3.559081
C	-7.887200	4.255119	-3.742182
H	-7.732848	5.087548	-4.436309
H	-7.413186	4.485064	-2.786773
H	-7.471996	3.342846	-4.173514

**CF<sub>3</sub>PhSeSePhCF<sub>3</sub>**

E = -6.58038964  
G = -6.44919427  
N<sub>imag</sub> = not present.

Se	-11.475792	1.603216	-0.060569
C	-13.347403	1.080344	-0.090776
C	-14.128670	0.979414	-1.242938
C	-15.459489	0.585720	-1.145812
C	-16.021130	0.286897	0.100315
C	-15.237669	0.389435	1.252080
C	-13.905727	0.784784	1.158097
C	-17.467156	-0.129965	0.169436
H	-13.710892	1.209512	-2.217201
H	-16.054850	0.511603	-2.050983
H	-15.654884	0.165222	2.227468
H	-13.313306	0.860028	2.066030
F	-18.307651	0.860569	-0.264381
F	-17.872581	-0.459093	1.420144
F	-17.728517	-1.212915	-0.624284
Se	-10.977363	2.239797	-2.237832
C	-10.398083	0.615787	-3.135227
C	-10.336639	-0.645249	-2.541455
C	-9.896610	-1.739506	-3.280233
C	-9.512004	-1.583744	-4.615837
C	-9.578782	-0.320531	-5.209815
C	-10.018695	0.775699	-4.473249
C	-9.075569	-2.789427	-5.406634
H	-10.624459	-0.783261	-1.504625
H	-9.853757	-2.714219	-2.804144
H	-9.288413	-0.179461	-6.245193

**CF<sub>3</sub>PhSe<sup>-</sup>**

E = -3.42376930  
G = -3.36823486  
N<sub>imag</sub> = not present.

Se	-11.544270	1.710349	-0.000007
C	-13.376681	1.219390	-0.215856
C	-14.367751	2.179194	-0.516532
C	-15.702594	1.825247	-0.675674
C	-16.105338	0.490549	-0.534441
C	-15.137568	-0.479669	-0.240959
C	-13.804150	-0.119969	-0.083130
C	-17.533351	0.096993	-0.758918
H	-14.084881	3.222563	-0.626368
H	-16.431021	2.596580	-0.907645
H	-15.421688	-1.522110	-0.130837
H	-13.076350	-0.892687	0.149107
F	-18.416290	1.089454	-0.453753
F	-17.907733	-0.993802	-0.031639
F	-17.787825	-0.232061	-2.074408

**MeSsePhCF<sub>3</sub>**

E = -4.14174705  
G = -4.05477487  
N<sub>imag</sub> = not present.

Se	-9.595980	2.390644	-1.923543
C	-9.728420	0.783829	-3.008732
C	-9.543083	-0.427462	-2.330130
C	-9.641417	-1.633604	-3.016057
C	-9.925627	-1.642340	-4.385912
C	-10.102925	-0.431143	-5.060871
C	-10.008625	0.777283	-4.375356
C	-9.980831	-2.945191	-5.139126
H	-9.322183	-0.441865	-1.265996
H	-9.496313	-2.563166	-2.475503
H	-10.321106	-0.419535	-6.123847
H	-10.159598	1.708798	-4.910882
F	-10.807179	-2.896234	-6.218279
F	-10.403687	-3.982827	-4.367994
F	-8.747815	-3.309806	-5.622107
S	-9.805594	4.048772	-3.336070
C	-8.112556	4.400109	-3.912160
H	-8.216437	5.276030	-4.560406
H	-7.459452	4.643715	-3.073191
H	-7.710962	3.566545	-4.489838

**TS: [PhSeSePh+SMe]<sup>-</sup>**

E = -6.28618592  
G = -6.12255558  
N<sub>imag</sub> = -38.513

Se	-11.266198	1.435970	-0.003273
C	-13.162296	1.175485	-0.312655
C	-14.014625	2.267830	-0.519434
C	-15.385036	2.062515	-0.681834
C	-15.915146	0.770929	-0.628495
C	-15.067814	-0.317503	-0.415675
C	-13.693832	-0.119375	-0.262261
H	-13.611464	3.275944	-0.551446
H	-16.040352	2.915355	-0.842269
H	-16.983980	0.614831	-0.750223
H	-15.472963	-1.325698	-0.372138
H	-13.039048	-0.971134	-0.102252
Se	-10.373842	2.001703	-2.164662
C	-10.104839	0.240619	-2.938593
C	-8.978110	-0.519001	-2.601728
C	-8.780192	-1.770791	-3.185917
C	-9.699574	-2.126797	-4.112531
C	-10.820501	-1.508675	-4.452736
C	-11.026080	-0.257790	-3.867160
H	-8.256293	-0.136530	-1.886002
H	-7.902833	-2.355451	-2.919500
H	-9.541665	-3.242150	-4.568350

H	-11.539685	-1.888865	-5.174348
H	-11.900923	0.327313	-4.135099
S	-8.690300	3.654646	-4.872339
C	-7.040319	3.183321	-4.216672
H	-6.921429	2.095093	-4.199263
H	-6.239336	3.601480	-4.836241
H	-6.903825	3.551806	-3.194605

**TS: [MePhSeSePhMe+SMe]<sup>-</sup>**

E = -7.46196571

G = -7.24991238

Nimag = -36.306

Se	-11.021030	1.769760	0.169399
C	-12.914767	1.511060	-0.134204
C	-13.779034	2.602893	-0.289523
C	-15.148038	2.398308	-0.446345
C	-15.699673	1.107285	-0.445614
C	-14.824799	0.025349	-0.281908
C	-13.450396	0.218253	-0.132516
H	-13.385282	3.615464	-0.283439
H	-15.800143	3.261625	-0.562210
H	-15.219072	-0.988524	-0.270826
H	-12.798538	-0.642062	-0.009485
C	-17.179998	0.897357	-0.633439
H	-17.457433	1.008594	-1.689447
H	-17.487172	-0.102080	-0.315001
H	-17.761736	1.633907	-0.070204
Se	-10.116979	2.321057	-2.005902
C	-9.846000	0.556913	-2.763574
C	-8.717832	-0.201329	-2.429379
C	-8.519732	-1.455964	-3.002393
C	-9.431536	-1.989436	-3.926223
C	-10.551674	-1.215081	-4.257693
C	-10.762228	0.039928	-3.685005
H	-7.989423	0.186015	-1.722662
H	-7.634303	-2.026662	-2.729793
H	-11.274971	-1.595261	-4.975976
H	-11.640489	0.615363	-3.963352
C	-9.221452	-3.357630	-4.521972
H	-8.162601	-3.548069	-4.721998
H	-9.564212	-4.138387	-3.830730
H	-9.777335	-3.478795	-5.455440
S	-8.542030	3.949204	-4.688331
C	-6.854636	3.348277	-4.282703
H	-6.813596	2.254500	-4.301202
H	-6.121570	3.727133	-5.003397
H	-6.548210	3.679109	-3.284703

**TS: [MeOPhSeSePhOMe+SMe]<sup>-</sup>**

E = -7.90371500

G = -7.67950156

Nimag = -34.424

Se	-11.028534	1.761475	0.171099
C	-12.920157	1.516896	-0.122094
C	-13.787926	2.617001	-0.217485
C	-15.154749	2.430903	-0.371531
C	-15.693785	1.133826	-0.427543
C	-14.837388	0.029201	-0.331069
C	-13.463182	0.229644	-0.183489
H	-13.393922	3.628135	-0.168551
H	-15.823229	3.284868	-0.442748
H	-15.218950	-0.984226	-0.369181
H	-12.813744	-0.638177	-0.111972
O	-17.048186	1.062663	-0.573107
C	-17.669102	-0.229354	-0.624421
H	-18.736243	-0.035145	-0.735745
H	-17.494130	-0.789890	0.300059
H	-17.311474	-0.807526	-1.483099
Se	-10.106739	2.308319	-2.020293
C	-9.828407	0.548865	-2.770530
C	-8.684547	-0.198201	-2.450919
C	-8.474769	-1.449343	-3.014255
C	-9.405259	-1.984574	-3.921490
C	-10.549094	-1.244815	-4.249701
C	-10.750721	0.010039	-3.671113
H	-7.949906	0.198471	-1.756195
H	-7.587303	-2.025255	-2.765380

H	-11.285861	-1.626751	-4.946386
H	-11.642911	0.569699	-3.936634
O	-9.101841	-3.217584	-4.420492
C	-10.002226	-3.822986	-5.358573
H	-9.554116	-4.783849	-5.613382
H	-10.100226	-3.214030	-6.263583
H	-10.988822	-3.987015	-4.912192
S	-8.612206	3.905101	-4.646242
C	-6.902848	3.333566	-4.297044
H	-6.833710	2.242963	-4.361559
H	-6.194838	3.761401	-5.015331
H	-6.586078	3.632047	-3.292140

**TS: [ClPhSeSePhCl+SMe]<sup>-</sup>**

E = -6.16861627

G = -6.02428845

Nimag = -36.700

Se	-11.025786	1.809101	0.200728
C	-12.911908	1.514998	-0.119581
C	-13.787175	2.588925	-0.322502
C	-15.151671	2.367898	-0.498688
C	-15.641062	1.061448	-0.461119
C	-14.787191	-0.020958	-0.205016
C	-13.422057	0.211789	-0.087696
H	-13.411115	3.607370	-0.343415
H	-15.825659	3.203832	-0.655807
H	-15.177066	-1.033315	-0.225994
H	-12.758038	-0.633099	0.068043
Cl	-17.351025	0.778497	-0.674773
Se	-10.136256	2.363481	-1.965003
C	-9.869507	0.598895	-2.724480
C	-8.751316	-0.167407	-2.377538
C	-8.552094	-1.426674	-2.940462
C	-9.478479	-1.914056	-3.862940
C	-10.595280	-1.162845	-4.227065
C	-10.786465	0.093367	-3.652245
H	-8.026041	0.211055	-1.663652
H	-7.683520	-2.017334	-2.667704
H	-11.309498	-1.550247	-4.946371
H	-11.657881	0.675404	-3.936101
Cl	-9.234554	-3.490577	-4.573845
S	-8.473458	4.039481	-4.702496
C	-6.851954	3.250513	-4.352678
H	-6.912140	2.163560	-4.467176
H	-6.081185	3.621106	-5.037435
H	-6.524628	3.462563	-3.329414

**TS: [CF<sub>3</sub>PhSeSePhCF<sub>3</sub>+SMe]<sup>-</sup>**

E = -7.54814325

G = -7.37879441

Nimag = -38.402

Se	-11.032635	1.682666	0.173014
C	-12.933963	1.414902	-0.100076
C	-13.653306	1.906209	-1.190357
C	-15.026316	1.685217	-1.281113
C	-15.693748	0.976474	-0.280048
C	-14.973888	0.489457	0.817836
C	-13.603037	0.701409	0.905362
H	-13.150868	2.462035	-1.975070
H	-15.568362	2.072808	-2.136886
H	-15.474784	-0.065899	1.605106
H	-13.060031	0.303821	1.758490
C	-17.178167	0.732390	-0.347053
F	-17.740252	1.151691	-1.507488
F	-17.489367	-0.593316	-0.218865
F	-17.849685	1.370734	0.662615
Se	-10.141699	2.381350	-1.910759
C	-9.888573	0.724600	-2.806569
C	-8.992210	-0.278946	-2.312187
C	-8.793531	-1.475997	-2.995668
C	-9.478375	-1.721134	-4.189004
C	-10.371730	-0.768749	-4.688242
C	-10.578747	0.422459	-3.996923
H	-8.442401	-0.093635	-1.395026
H	-8.094914	-2.205151	-2.600070
H	-10.912451	-0.948558	-5.611977
H	-11.276733	1.152801	-4.393084

C	-9.298355	-3.024980	-4.927715
F	-8.169640	-3.687668	-4.571596
F	-10.340730	-3.884969	-4.696830
F	-9.244026	-2.852693	-6.277882
S	-8.125589	4.171218	-4.514692
C	-6.661458	3.142567	-4.096666
H	-6.863860	2.081486	-4.273926
H	-5.795773	3.428123	-4.704376
H	-6.386305	3.259693	-3.043125