Supplementary Material

A Combined Experimental and Theoretical Study on the Formation of the Elusive 2-Methyl-1-silacycloprop-2-enylidene Molecule under Single Collision Conditions via Reaction of the Silylidyne Radical (SiH; $X^2\Pi$) with Allene (H_2CCCH_2; X^1A_1) and D4-Allene (D_2CCCD_2; X^1A_1)

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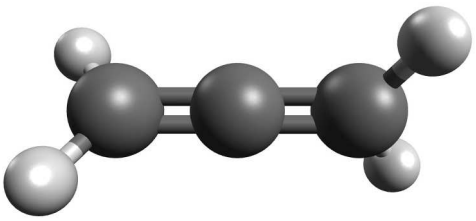
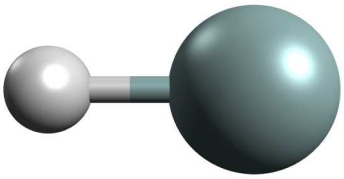
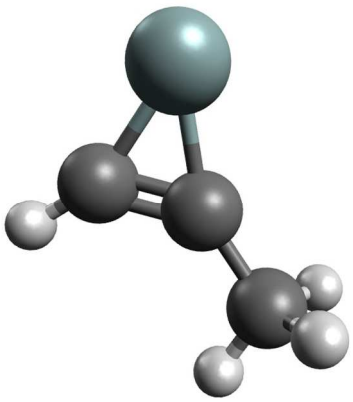
The zero-point vibration corrected relative energies (kJ mol^{-1}), point groups, symmetries of the electronic wave functions, and geometries (Ångstroms) of the reactants, products, intermediates, and transition states are given in the table below. The energies, geometries, and vibrational analyses were all calculated at the ωB97X-V/cc-pVTZ level.

Reactants							
H_2CCCH_2				SiH			
							
0				0			
D_{2d} – $^1A_1$				$C_{\infty v}$ – $^2\Pi$			
C	-7.512220	1.836330	0.000040	Si	-7.063060	1.620720	0.000000
C	-6.210180	1.823560	0.000150	H	-5.534020	1.620720	0.000000
C	-4.908230	1.810800	0.000270				
H	-8.068000	1.984400	-0.919490				
H	-8.070970	1.698440	0.9193500				
H	-4.360020	0.885480	-0.140010				
H	-4.342010	2.725330	0.139710				

Products

[p1]

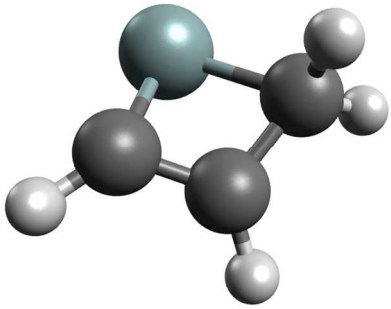


-19.931

$C_s - {}^1A'$

Si	-0.000450	0.531770	0.121220
C	-0.005400	-0.185320	1.787230
C	-1.250430	0.124280	1.390180
C	-2.625670	0.038020	1.952780
H	0.423160	-0.619410	2.684520
H	-3.259180	-0.565900	1.297380
H	-2.641320	-0.394260	2.957330
H	-3.075620	1.033970	1.988990

[p2]

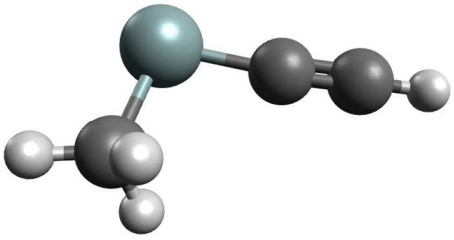


-1.193

$C_1 - {}^1A$

Si	-0.072960	0.286450	0.168280
C	1.806770	0.067770	1.262120
C	0.621320	0.399290	1.860830
C	1.844640	0.652470	-0.101170
H	2.539840	-0.653500	1.631710
H	0.336770	0.169040	2.880320
H	2.043320	1.720800	-0.106230
H	2.419310	0.133330	-0.867810

[p3]

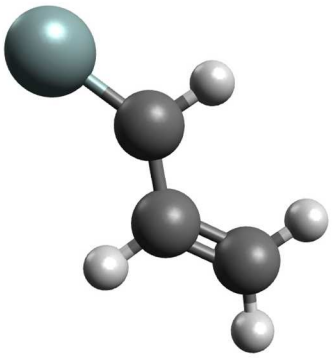


54.069

$C_s - {}^1A'$

Si	0.001877	-0.012444	-0.031075
C	0.007613	-0.002607	1.827437
C	0.126100	0.003639	3.031566
C	-1.884249	-0.021220	-0.252335
H	0.225171	0.009060	4.093980
H	-2.183940	-0.029650	-1.301841
H	-2.313535	-0.896269	0.250093
H	-2.319598	0.857960	0.237589

[p4]

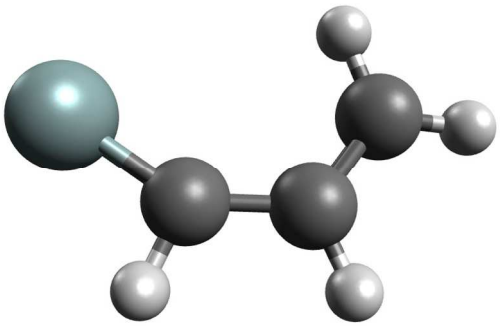


64.883

$C_s - {}^1A'$

Si	-0.001539	-0.000001	0.022764
C	0.004472	0.000000	1.736590
C	-1.007095	0.000000	2.786920
C	-0.751270	0.000000	4.096953
H	1.043898	0.000001	2.101102
H	-2.047249	0.000000	2.466746
H	-1.552697	0.000000	4.826776
H	0.267060	-0.000001	4.474013

[p5]

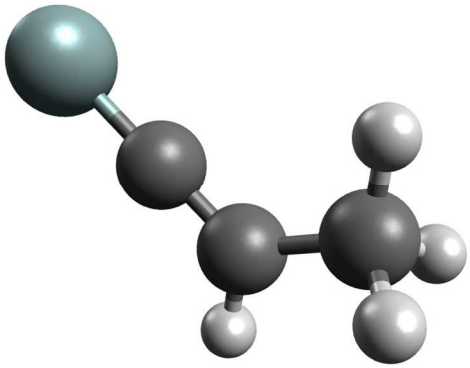


70.250

$C_s - {}^1A'$

Si	-0.347829	-0.000834	-0.542230
C	1.344427	-0.000080	-0.346974
C	2.648706	0.000099	-0.998258
C	2.854478	0.000115	-2.317062
H	1.383519	0.000281	0.763859
H	3.519358	0.000246	-0.346200
H	3.857790	0.000237	-2.726500
H	2.030920	0.000077	-3.024974

[p6]

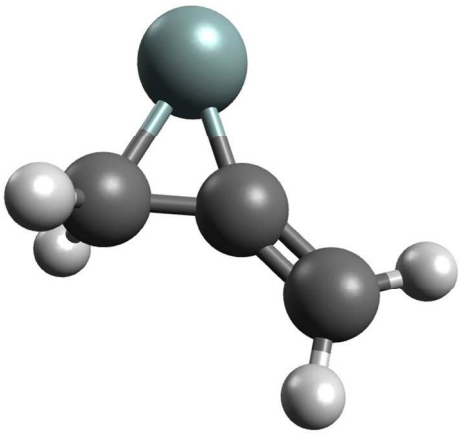


75.098

$C_s - {}^1A'$

Si	0.010056	-0.003660	0.021461
C	0.003404	-0.000954	1.706986
C	0.003083	0.000812	3.030169
C	1.182846	-0.317239	3.900107
H	-0.918998	0.250991	3.561925
H	2.060254	-0.556830	3.300167
H	0.947965	-1.162713	4.555074
H	1.408488	0.534209	4.550600

[p7]

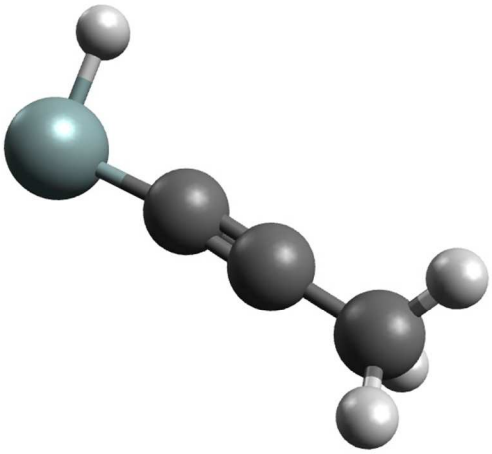


72.323

$C_s - {}^1A'$

Si	-0.021103	0.000441	0.013757
C	0.009541	-0.000058	1.859408
C	0.654905	0.000100	3.018055
C	-1.391521	0.000152	1.360029
H	1.741038	0.000090	3.055181
H	0.131770	0.000226	3.973724
H	-1.984894	-0.904226	1.499233
H	-1.985174	0.904192	1.500135

[p8]

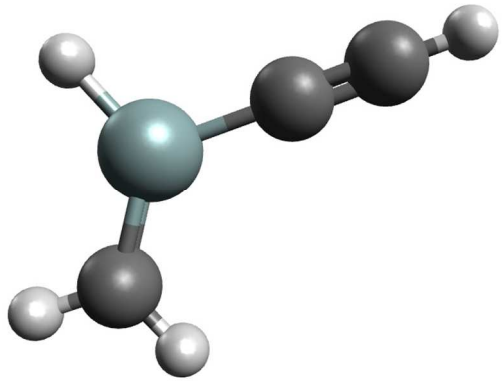


64.751

$C_s - {}^1A'$

Si	-0.001080	-0.006160	0.007180
C	1.823300	-0.004550	-0.182060
C	3.008700	-0.010510	-0.443430
C	4.437640	-0.011300	-0.738440
H	0.037850	0.008790	1.530590
H	5.020250	-0.330250	0.128390
H	4.658340	-0.674770	-1.577710
H	4.755710	0.997420	-1.014070

[p9]

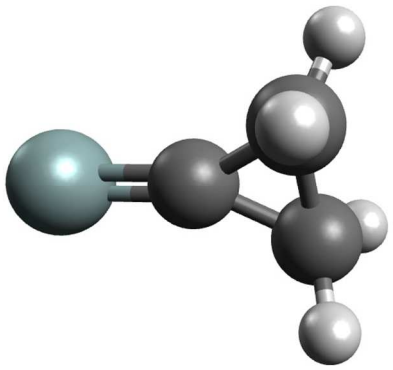


71.355

$C_s - {}^1A'$

Si	0.010056	-0.003660	0.021461
C	0.003404	-0.000954	1.706986
C	0.003083	0.000812	3.030169
C	1.182846	-0.317239	3.900107
H	-0.918998	0.250991	3.561925
H	2.060254	-0.556830	3.300167
H	0.947965	-1.162713	4.555074
H	1.408488	0.534209	4.550600

[p10]

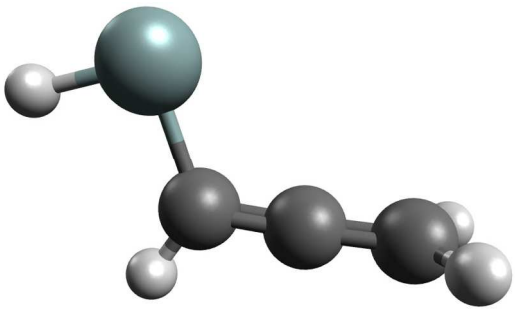


97.479

$C_s - {}^1A'$

Si	-0.000043	0.000332	0.019716
C	0.000020	-0.000366	1.702923
C	0.744072	0.000032	3.008418
C	-0.743133	-0.002639	3.008883
H	1.257929	0.915558	3.282279
H	1.261343	-0.913969	3.280930
H	-1.256941	-0.918492	3.281725
H	-1.260087	0.911046	3.283067

[p11]

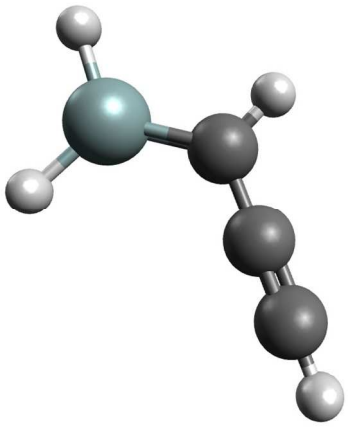


86.046

$C_s - {}^1A'$

Si	0.023630	-0.022090	-0.019590
C	1.896920	-0.016900	-0.142630
C	2.398350	-0.061270	-1.355990
C	2.833630	-0.107850	-2.580640
H	-0.011010	0.037970	1.507750
H	2.585330	0.018810	0.698790
H	3.017630	0.803970	-3.137320
H	3.026240	-1.059390	-3.062980

[p12]

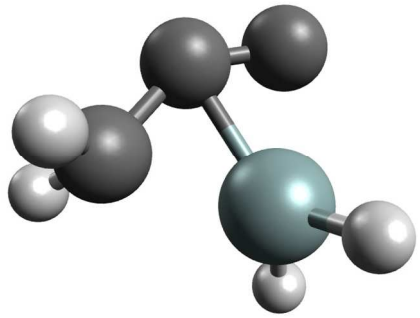


99.383

$C_s - {}^1A'$

Si	-0.022590	-0.000680	-0.011290
C	-1.438540	-0.001360	-0.972680
C	-2.760980	0.001300	-0.452830
C	-3.880270	0.004050	-0.010520
H	-0.055700	0.002850	1.464260
H	1.318440	-0.003920	-0.629700
H	-1.342270	-0.004370	-2.055020
H	-4.871770	0.006510	0.376690

[p13]

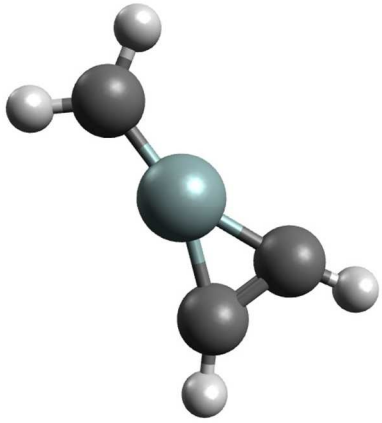


106.561

$C_s - {}^1A'$

Si	-0.004547	-0.023326	-0.002746
C	-1.598642	0.082415	-1.008166
C	-1.254667	1.275909	-0.791941
C	-1.228410	-1.311753	-0.773814
H	-0.007594	0.004112	1.471748
H	1.324780	0.002781	-0.640784
H	-0.904118	-1.876134	-1.644395
H	-1.874612	-1.875177	-0.105547

[p14]

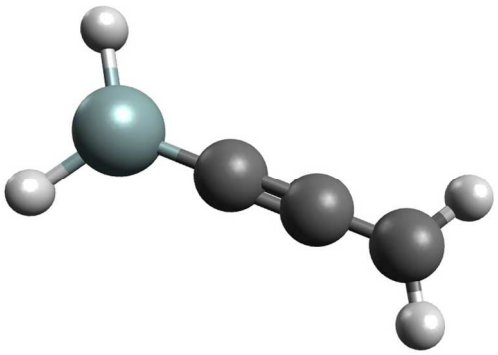


113.974

$C_{2v} - {}^1A_1$

Si	-0.000350	0.000000	-0.002231
C	-0.000120	0.000000	1.687454
C	-0.679107	0.000000	-1.648544
C	0.677576	0.000000	-1.648881
H	0.927223	0.000000	2.244083
H	-0.927415	0.000000	2.244172
H	1.416608	0.000000	-2.441050
H	-1.195329	0.000000	-2.542154

[p15]

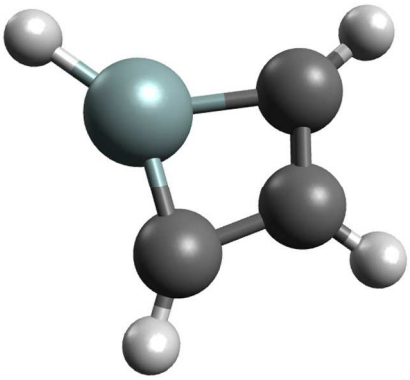


103.059

$C_{2v} - {}^1A_1$

Si	-0.012455	0.001709	-0.007677
C	-1.441566	0.008309	-0.894872
C	-2.521859	0.012454	-1.565080
C	-3.637593	0.017076	-2.257492
H	-0.008231	-0.001808	1.466932
H	1.311012	-0.000297	-0.658004
H	-4.599244	0.018445	-1.757855
H	-3.616685	0.019396	-3.341002

[p16]

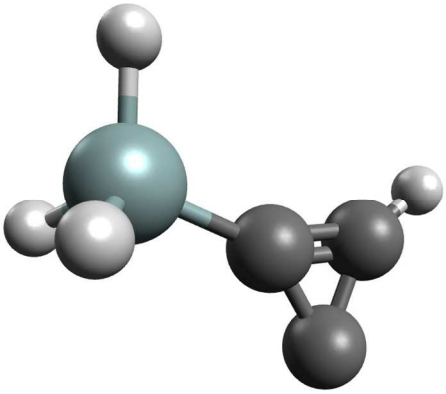


162.182

$C_s - {}^1A'$

Si	-0.001652	0.000077	-0.027121
C	1.088043	-0.000043	-1.328049
C	-0.176682	0.000115	-2.205859
C	-1.271400	-0.000046	-1.426119
H	-0.024804	0.000056	1.458869
H	2.108968	-0.000146	-1.665304
H	-0.154839	0.000134	-3.294679
H	-2.315713	-0.000147	-1.689707

[p17]

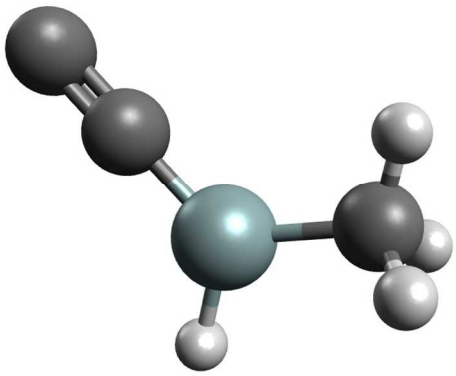


153.497

$C_s - {}^1A'$

Si	0.004334	-0.000181	0.002005
C	-0.803203	1.584153	-0.564362
C	-1.717663	2.299126	-1.214602
C	-0.740941	3.015555	-0.510774
H	-0.002573	0.005387	1.484086
H	1.392117	0.003139	-0.518443
H	-0.735323	-1.179251	-0.511981
H	-2.595580	2.305141	-1.843119

[p18]

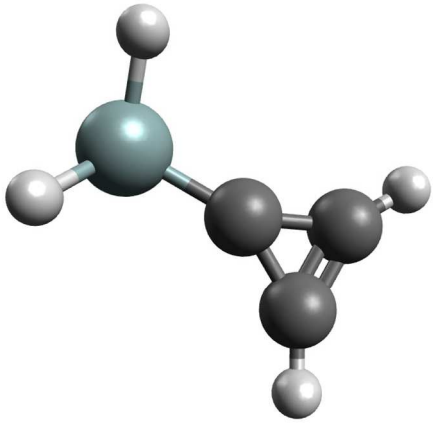


178.911

$C_s - {}^1A'$

Si	-0.001079	-0.006157	0.007180
C	1.823299	-0.004555	-0.182064
C	3.008697	-0.010508	-0.443431
C	4.437635	-0.011300	-0.738437
H	0.037849	0.008786	1.530586
H	5.020249	-0.330248	0.128389
H	4.658339	-0.674773	-1.577715
H	4.755707	0.997422	-1.014072

[p19]

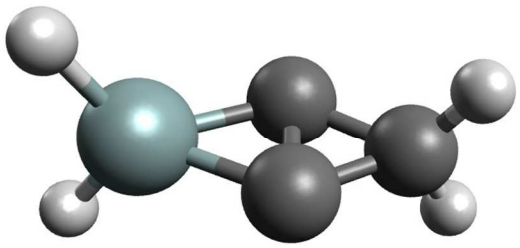


176.604

$C_s - {}^1A'$

Si	-0.005201	-0.003037	-0.001200
C	1.433875	0.002839	-0.888729
C	2.505471	0.005092	-1.557660
C	-1.709434	-0.003507	-0.719954
H	-0.008837	-0.010498	1.479531
H	-1.673055	0.026988	-1.808856
H	-2.273878	0.857153	-0.347870
H	-2.246839	-0.901868	-0.399468

[p20]

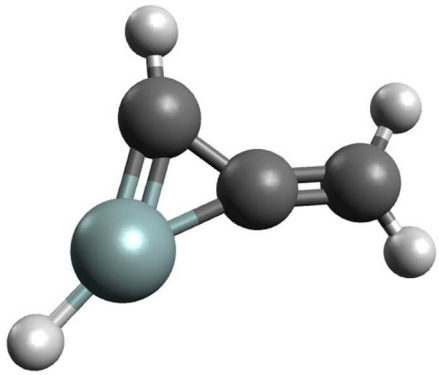


191.398

$C_{2v} - {}^1A_1$

Si	-0.012116	-0.000030	0.005720
C	-1.322180	-0.700443	-0.953352
C	-1.322647	0.700164	-0.952783
C	-2.371932	-0.000124	-1.719786
H	-0.053202	-0.000887	1.485663
H	1.385628	0.000866	-0.482292
H	-3.389674	-0.000670	-1.334431
H	-2.314044	0.000370	-2.806489

[p21]

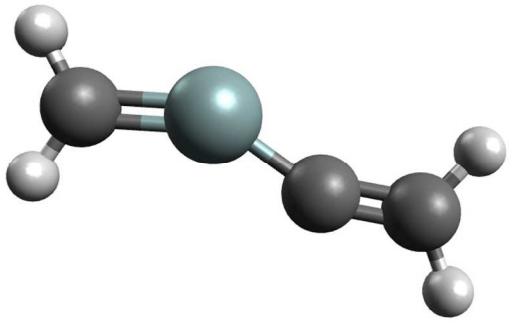


193.385

$C_s - {}^1A'$

Si	0.014366	0.000000	-0.023521
C	0.885142	0.000000	-1.461167
C	-0.585001	0.000000	-1.723398
C	-1.438916	0.000000	-2.741625
H	-0.049578	0.000000	1.450669
H	1.729896	0.000000	-2.134577
H	-2.509372	0.000000	-2.578677
H	-1.079818	0.000000	-3.766406

[p22]

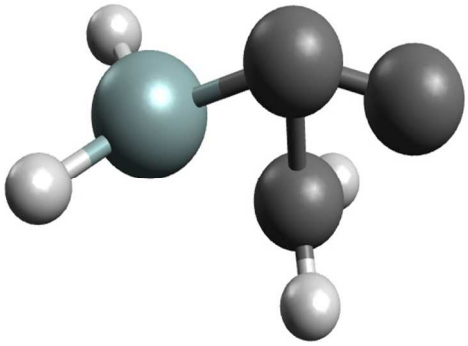


213.427

$C_s - {}^1A'$

Si	-0.269003	0.000008	0.093121
C	0.018618	-0.000231	1.763297
C	-1.416604	0.000095	-1.168790
C	-1.797755	0.000250	-2.424156
H	1.028159	0.000425	2.151104
H	-0.794110	-0.000070	2.478562
H	-1.103274	0.000127	-3.260910
H	-2.858443	-0.000131	-2.672367

[p23]

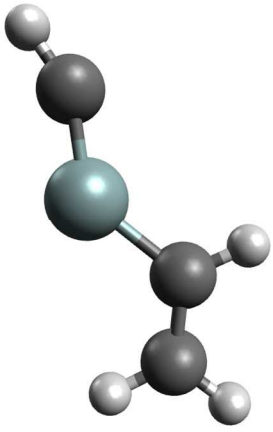


214.994

$C_s - {}^1A'$

Si	-0.009665	-0.001689	-0.003893
C	-1.330555	0.854343	-0.855206
C	-2.383937	0.619241	-1.533281
C	-1.422671	-0.856335	-0.910191
H	-0.007722	-0.005577	1.472056
H	1.333762	-0.010849	-0.615057
H	-1.172501	-1.361252	-1.836249
H	-2.162715	-1.357244	-0.296568

[p24]

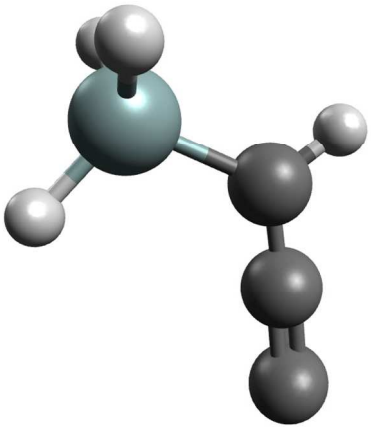


238.832

$C_s - {}^1A'$

Si	-0.096367	-0.005795	0.030176
C	0.040956	0.000800	1.648467
C	-1.484528	-0.007167	-1.198274
C	-1.277045	-0.012692	-2.513308
H	0.612500	0.003273	2.561016
H	-2.498193	-0.003375	-0.808082
H	-0.280369	-0.016906	-2.944298
H	-2.106936	-0.013574	-3.213940

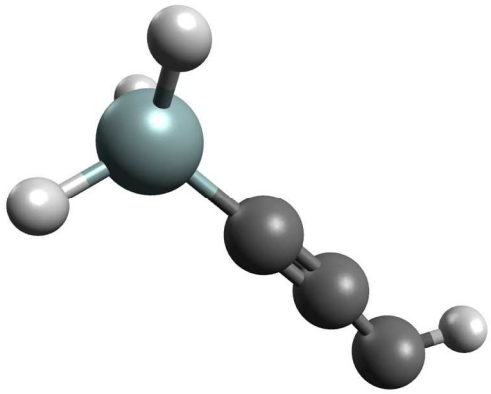
[p25]



252.184
$C_s - {}^1A'$

Si	-0.004567	-0.003107	0.001286
C	-0.886865	-1.545386	-0.658843
C	-1.424618	-2.450175	0.141487
C	-1.931123	-3.302048	0.959033
H	-0.042396	-0.022449	1.479329
H	1.389814	-0.029843	-0.508838
H	-0.704912	1.186118	-0.546792
H	-0.960444	-1.703162	-1.736828

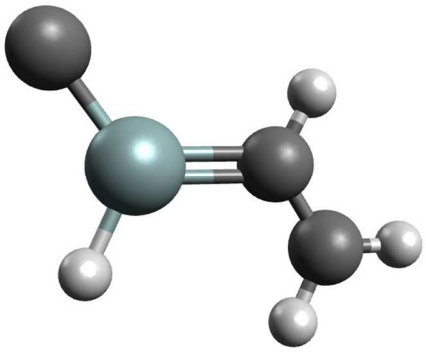
[p26]



248.933
$C_s - {}^1A'$

Si	0.001773	0.003776	0.005024
C	-0.912615	-1.451460	-0.635745
C	-1.564442	-2.410639	-1.074979
C	-2.351720	-3.437890	-1.426232
H	-0.031168	0.032211	1.486984
H	1.408806	-0.015095	-0.462759
H	-0.717869	1.172428	-0.557858
H	-2.083144	-3.890527	-2.388104

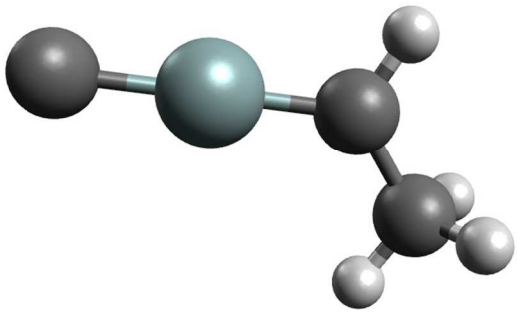
[p27]



408.155
$C_s - {}^1A'$

Si	-0.007945	0.000482	0.018110
C	1.570119	-0.000810	-0.790512
C	-1.651156	0.000187	-0.830798
C	-2.793446	0.000651	-0.144076
H	-0.045083	0.000488	1.500975
H	-1.684732	-0.000384	-1.917000
H	-2.813308	0.001189	0.942456
H	-3.758571	0.000474	-0.642617

[p28]

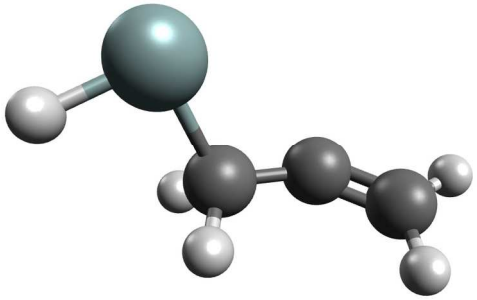


517.700
$C_s - {}^1A'$

Si	-0.003163	-0.001144	0.030693
C	0.003896	0.003579	1.747212
C	-1.184160	0.005053	2.665601
C	-0.013669	-0.006082	-1.727601
H	0.981708	0.007514	2.224514
H	-2.131829	-0.003554	2.125582
H	-1.155622	-0.869804	3.323335
H	-1.164063	0.890478	3.309461

Intermediates

[i1]

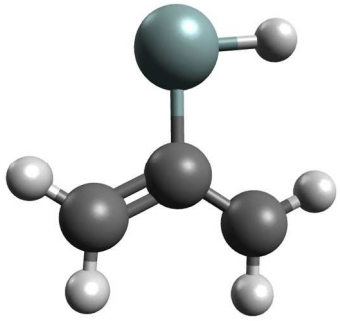


-36.600

$C_1 - {}^2A$

Si	0.024930	0.013540	-0.01140
C	1.944270	0.000140	-0.07076
C	2.527020	0.059890	-1.41193
C	3.224980	0.850000	-2.18511
H	0.001520	0.001110	1.51718
H	2.268140	-0.901210	0.46986
H	2.291860	0.847610	0.54946
H	3.450750	0.600100	-3.21784
H	3.619220	1.800390	-1.81374

[i2]

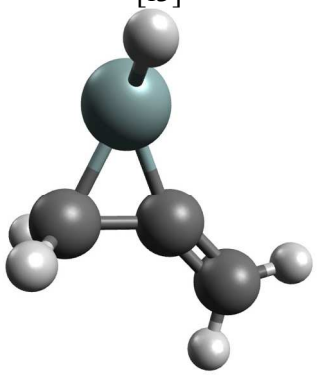


-124.163

$C_s - {}^2A'$

Si	0.009630	-0.016120	-0.000690
C	1.900430	-0.004340	-0.175780
C	2.386440	-0.036990	-1.478880
C	2.763010	0.036170	0.918660
H	0.004800	0.020210	1.525740
H	1.713300	-0.066410	-2.329320
H	3.453210	-0.034500	-1.691590
H	2.385340	0.059180	1.933460
H	3.843210	0.045950	0.785310

[i3]

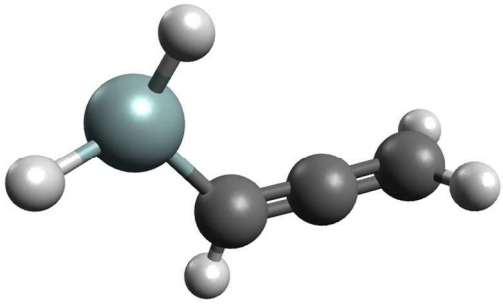


-140.913

$C_1 - {}^2A$

Si	-0.274790	0.102350	0.171240
C	-0.811520	-1.619270	0.695460
C	0.670180	-1.442810	0.354800
C	1.734480	-2.226040	0.358780
H	-0.120730	1.145920	1.230540
H	-1.061170	-1.836270	1.732850
H	-1.375040	-2.228980	-0.008540
H	1.675630	-3.266210	0.673930
H	2.707000	-1.859110	0.044890

[i4]

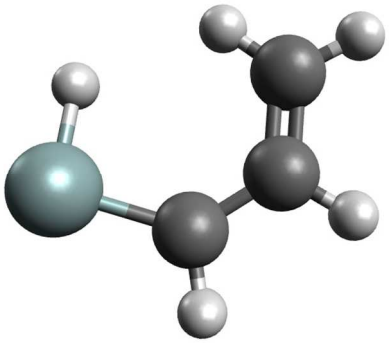


-182.497

$C_1 - {}^2A$

Si	-0.014570	0.009440	0.006690
C	-0.990260	1.428780	-0.686770
C	-1.880350	2.065470	0.030730
C	-2.753540	2.678240	0.777550
H	-0.035640	0.037100	1.494240
H	1.377980	0.005010	-0.523310
H	-0.864560	1.718200	-1.728320
H	-2.475570	3.553230	1.355290
H	-3.779530	2.330310	0.833300

[i5]

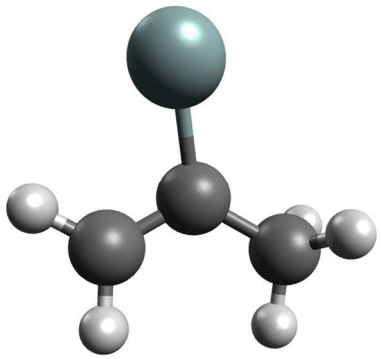


-141.544

$C_s - {}^2A'$

Si	0.003170	0.016510	0.022550
C	1.829680	-0.026590	-0.307380
C	2.900540	-0.515290	0.484710
C	2.835730	-0.847060	1.805730
H	0.052790	0.034670	1.546900
H	2.120410	0.213720	-1.331130
H	3.866750	-0.633210	-0.004860
H	1.920580	-0.731880	2.374210
H	3.710490	-1.220400	2.325410

[i6]

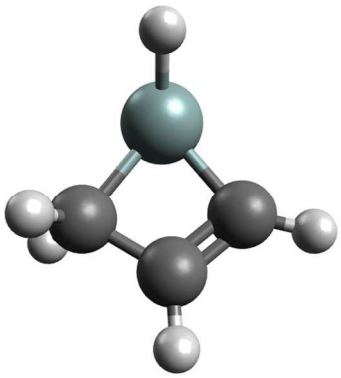


-176.593

$C_s - {}^2A'$

Si	0.025560	0.011720	0.019560
C	-0.003270	0.004370	1.883680
C	1.264040	-0.005330	2.339530
C	-1.172340	-0.299490	2.785490
H	2.102770	0.282270	1.707130
H	1.515150	-0.319970	3.352910
H	-1.749180	-1.150150	2.412610
H	-0.848760	-0.515040	3.808340
H	-1.854230	0.555510	2.821860

[i7]

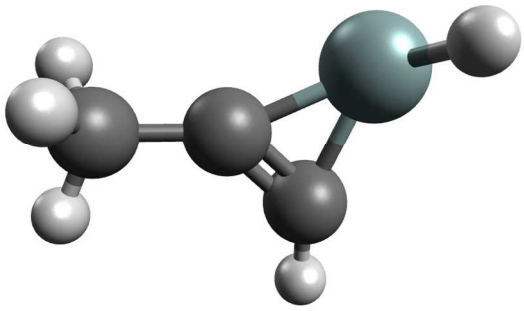


-232.358

$C_1 - {}^2A$

Si	0.003160	-0.012900	-0.005980
C	1.654090	-0.000290	-0.861930
C	1.422070	-1.232880	-1.347480
C	0.053560	-1.715120	-0.881850
H	-0.000880	-0.008850	1.493900
H	2.534210	0.608330	-1.025460
H	2.097650	-1.826310	-1.965650
H	-0.655350	-1.879630	-1.695710
H	0.084930	-2.608460	-0.253550

[i8]

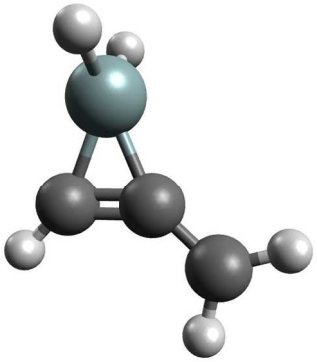


-172.644

$C_1 - {}^2A$

Si	0.010240	-0.006660	-0.004460
C	1.585020	-0.006680	-0.901020
C	1.019150	-1.221880	-0.914150
C	1.342930	-2.563880	-1.467010
H	-0.004880	-0.001700	1.504720
H	2.502850	0.407370	-1.303060
H	1.392460	-3.303440	-0.663460
H	2.293320	-2.562500	-2.008170
H	0.551010	-2.888040	-2.148160

[i9]

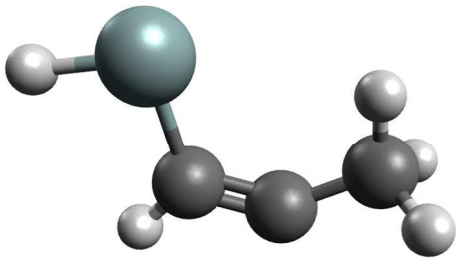


-165.421

$C_s - {}^2A'$

Si	-0.003570	-0.001300	-0.001830
C	-1.389860	0.678040	-0.948400
C	-1.398140	-0.694430	-0.957420
C	-2.184560	-1.705360	-1.498030
H	-0.004270	-0.000510	1.481670
H	1.378690	0.004530	-0.540400
H	-2.020970	1.445800	-1.377860
H	-1.948170	-2.750370	-1.338840
H	-3.059480	-1.466730	-2.096160

[i10]

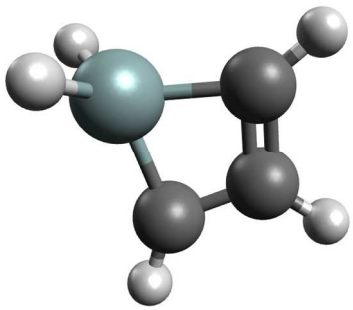


-72.987

$C_s - {}^2A'$

Si	0.030990	-0.004420	-0.039490
C	1.910010	-0.003930	-0.154280
C	2.461990	-0.015260	-1.352230
C	2.071260	-0.029700	-2.769760
H	-0.021830	0.009370	1.486460
H	2.547660	0.004910	0.730020
H	2.477450	0.846340	-3.282520
H	2.477170	-0.916240	-3.264380
H	0.978480	-0.030730	-2.884330

[i11]

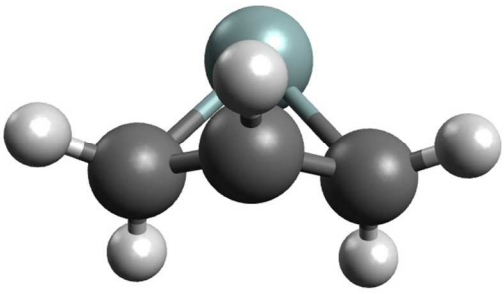


-243.273

$C_s - {}^2A'$

Si	-0.003088	-0.000621	-0.003109
C	-1.203463	1.127703	-0.888337
C	-1.869877	-0.003730	-1.381799
C	-1.200818	-1.132931	-0.886819
H	-0.008639	0.000394	1.486017
H	1.416706	0.000725	-0.452262
H	-1.452466	2.163478	-1.072296
H	-2.745767	-0.005100	-2.030994
H	-1.447290	-2.169535	-1.069512

[i12]

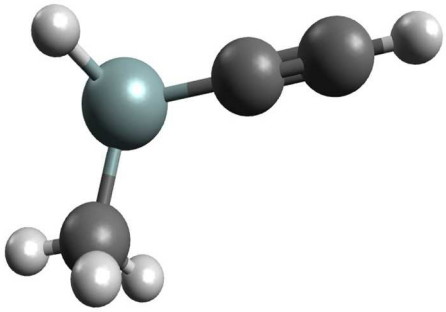


-233.736

$C_s - {}^2A'$

Si	-0.006753	-0.034939	0.035541
C	-0.005937	0.001307	2.082528
C	-0.508482	-1.251736	1.612737
C	-1.589254	-1.162073	0.681535
H	0.930575	0.017725	2.628701
H	-0.721418	0.765335	2.380239
H	0.102055	-2.146919	1.666105
H	-1.885661	-2.051459	0.136778
H	-2.398739	-0.467022	0.895805

[i13]

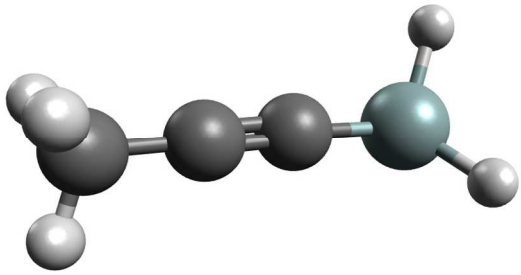


-213.566

$C_1 - {}^2A$

Si	-0.021544	0.013083	0.014969
C	1.695801	-0.000507	-0.614399
C	2.808221	0.073793	-1.077979
C	-1.025231	-1.397541	-0.715963
H	0.000005	-0.008210	1.503872
H	3.794020	0.132434	-1.480990
H	-1.027717	-1.342285	-1.806405
H	-2.058681	-1.362831	-0.364663
H	-0.591310	-2.358235	-0.422226

[i14]

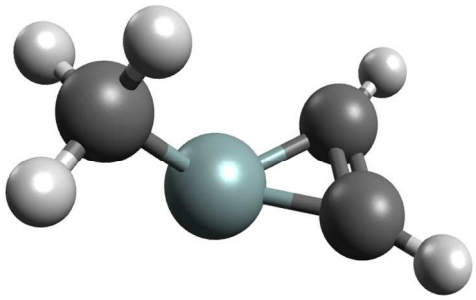


-206.251

$C_s - {}^2A'$

Si	-0.002426	-0.008265	0.001145
C	-1.016413	1.332439	-0.679293
C	-1.754347	2.154369	-1.173501
C	-2.632809	3.160642	-1.762943
H	0.002962	0.019332	1.487223
H	1.377357	0.024485	-0.550492
H	-2.571293	3.131355	-2.853070
H	-3.670127	2.982256	-1.470810
H	-2.348426	4.161156	-1.428680

[i15]

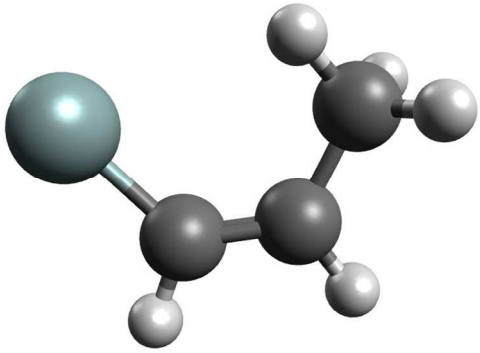


-188.510

$C_s - {}^2A'$

Si	0.002488	0.008657	0.003367
C	0.002672	0.010177	1.821072
C	-1.243880	0.002198	1.326472
C	0.391288	1.573237	-1.000446
H	0.417238	0.012615	2.822317
H	-2.232124	-0.004366	1.771094
H	-0.196321	1.596038	-1.920554
H	1.449850	1.606084	-1.266537
H	0.144996	2.449147	-0.393887

[i16]

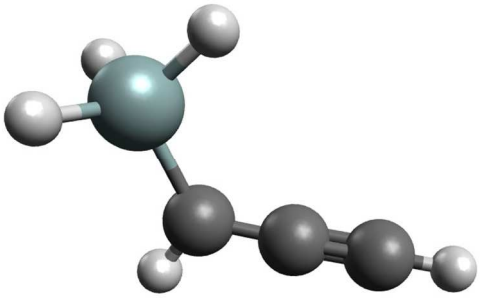


-181.918

$C_s - {}^2A'$

Si	-0.045538	-0.046298	0.030357
C	-0.018136	0.023234	1.869224
C	-1.068332	0.123885	2.710169
C	-2.498033	0.182266	2.258628
H	0.978173	0.011230	2.323629
H	-0.901175	0.189405	3.783996
H	-2.600210	-0.093824	1.202186
H	-3.127409	-0.496311	2.842086
H	-2.912272	1.189064	2.380879

[i17]

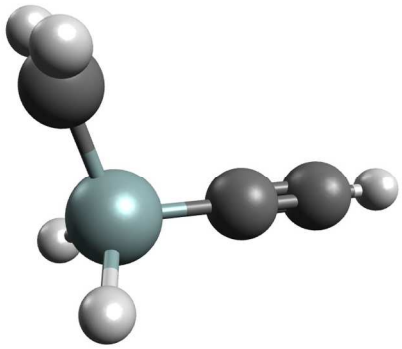


-178.928

$C_s - {}^2A'$

Si	-0.007371	0.003376	0.003076
C	-0.987858	1.432800	-0.684631
C	-1.776545	2.238462	0.101489
C	-2.463981	2.933246	0.829796
H	-0.224746	-0.081398	1.468356
H	1.440862	0.195093	-0.282480
H	-0.434630	-1.266823	-0.644835
H	-0.955481	1.663951	-1.746807
H	-3.066327	3.544450	1.460300

[i18]

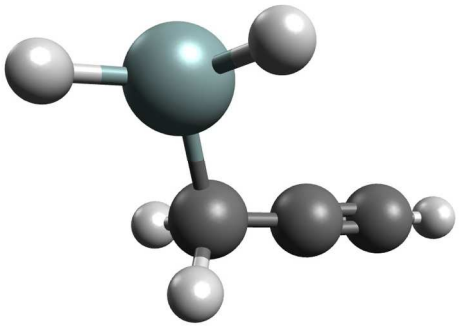


-171.528

$C_s - {}^2A'$

Si	0.009116	-0.007513	0.007601
C	-0.799995	1.548284	-0.567985
C	-1.334562	2.560090	-0.943690
C	-0.893982	-1.488596	-0.630309
H	0.002686	0.002696	1.492579
H	1.408283	0.001584	-0.490461
H	-1.805949	3.457659	-1.275128
H	-0.682899	-1.925745	-1.601131
H	-1.710328	-1.952097	-0.085492

[i19]

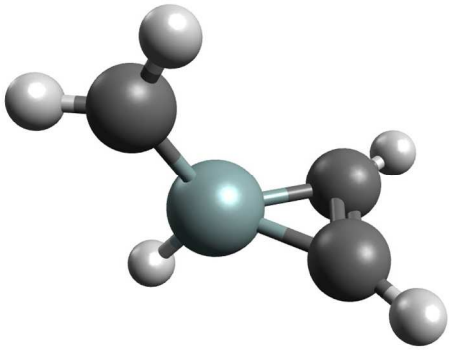


-155.408

$C_1 - {}^2A$

Si	0.025560	0.011720	0.019560
C	-0.003270	0.004370	1.883680
C	1.264040	-0.005330	2.339530
C	-1.172340	-0.299490	2.785490
H	2.102770	0.282270	1.707130
H	1.515150	-0.319970	3.352910
H	-1.749180	-1.150150	2.412610
H	-0.848760	-0.515040	3.808340
H	-1.854230	0.555510	2.821860

[i20]

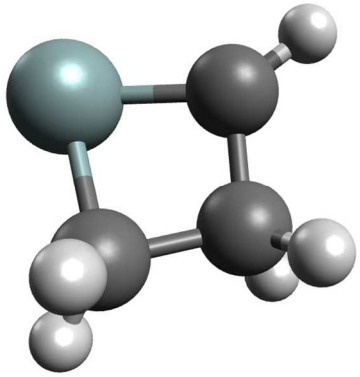


-151.648

$C_s - {}^2A'$

Si	-0.008017	0.000550	0.001486
C	1.690554	0.000376	-0.674550
C	-1.424667	0.669036	-0.921606
C	-1.425687	-0.662864	-0.923727
H	0.001755	-0.001892	1.484605
H	1.883662	0.002338	-1.742997
H	2.573810	-0.001722	-0.043031
H	-2.054601	1.442352	-1.344814
H	-2.056763	-1.433875	-1.349429

[i21]

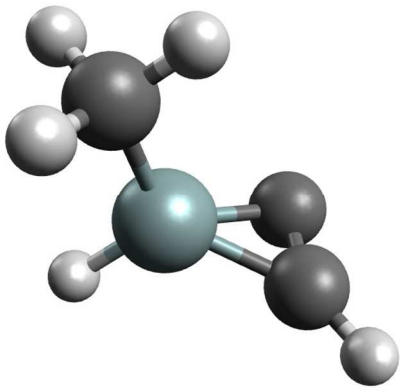


-149.857

$C_1 - {}^2A$

Si	-0.006732	-0.040232	-0.036596
C	-0.022291	-0.000475	1.790775
C	-1.490407	-0.335575	1.880195
C	-1.897361	0.010408	0.425150
H	0.641155	0.057906	2.648456
H	-1.705730	-1.367656	2.180282
H	-1.989318	0.306065	2.622776
H	-2.350692	1.001530	0.366360
H	-2.547446	-0.699342	-0.090961

[i22]

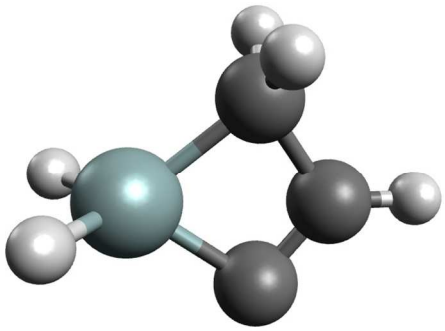


-148.256

$C_1 - {}^2A$

Si	0.002769	-0.004153	-0.006382
C	1.596453	0.001259	-0.922906
C	1.100070	1.203746	-0.922933
C	-1.573076	-0.697800	-0.724478
H	-0.003524	-0.013136	1.476658
H	1.233730	2.227988	-1.242425
H	-1.547249	-0.656412	-1.814882
H	-2.443839	-0.139031	-0.370558
H	-1.701772	-1.740433	-0.419104

[i23]

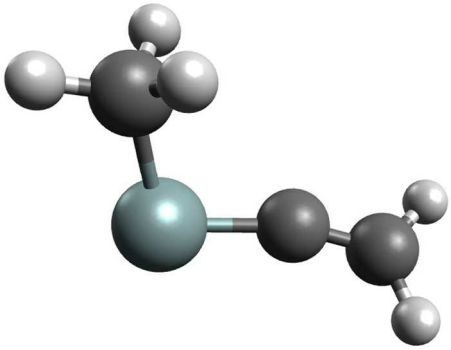


-143.527

$C_s - {}^2A'$

Si	-0.005611	-0.007672	-0.004156
C	-1.224635	1.103691	-0.880969
C	-1.930868	0.098658	-1.388444
C	-1.230921	-1.179525	-0.884373
H	-0.009497	-0.000726	1.482182
H	1.401826	-0.001691	-0.481994
H	-2.814258	0.116554	-2.023869
H	-1.865117	-1.791407	-0.238828
H	-0.821331	-1.792394	-1.690573

[i24]

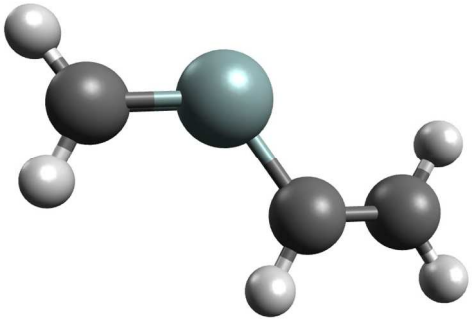


-140.460

$C_1 - {}^2A$

Si	0.038783	0.006912	-0.057025
C	0.010582	0.009525	1.742400
C	0.314828	-0.012816	3.011205
C	-1.400850	-1.187475	-0.443781
H	1.294610	-0.329141	3.368643
H	-0.409110	0.279171	3.772134
H	-1.416324	-1.454981	-1.502032
H	-1.309059	-2.098606	0.155970
H	-2.360607	-0.725588	-0.191892

[i25]

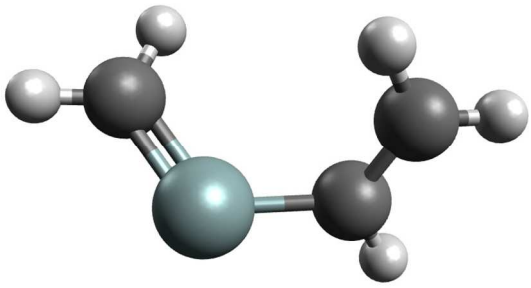


-136.974

$C_s - {}^2A'$

Si	-0.017236	-0.000001	-0.000864
C	0.005941	0.000000	1.704431
C	-1.606616	-0.000001	-0.979753
C	-1.668194	0.000000	-2.309471
H	0.914696	0.000000	2.292742
H	-0.926549	0.000002	2.264323
H	-2.530849	-0.000002	-0.401112
H	-0.773035	0.000001	-2.925144
H	-2.617105	0.000001	-2.838383

[i26]

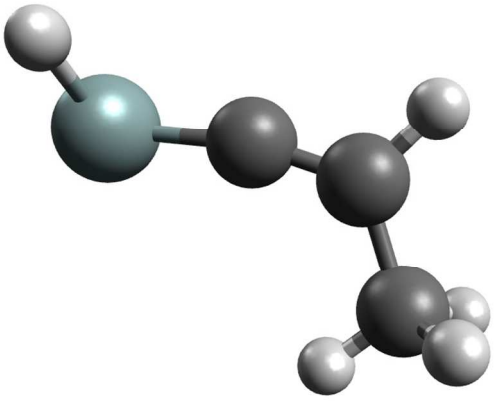


-132.788

$C_1 - {}^2A$

Si	-0.023264	0.170259	0.070953
C	0.047379	-0.085158	1.757110
C	-1.637977	0.438961	-0.833608
C	-2.571907	1.258761	-0.349731
H	0.975522	-0.156745	2.310226
H	-0.865139	-0.262151	2.321329
H	-1.815039	-0.066523	-1.779892
H	-2.428017	1.807364	0.576688
H	-3.520296	1.406300	-0.860815

[i27]

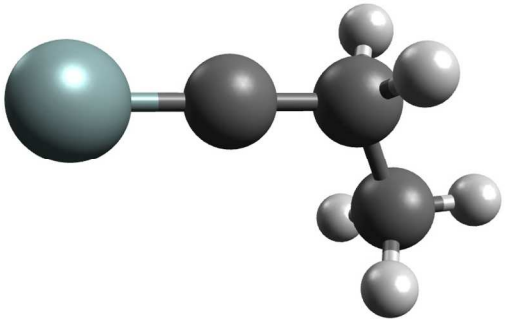


-120.466

$C_1 - {}^2A$

Si	-0.010300	0.009535	-0.013767
C	1.743823	-0.004401	-0.307462
C	2.958010	-0.201360	-0.753618
C	3.383129	-1.301256	-1.693083
H	0.052815	-0.021986	1.502137
H	3.743754	0.476540	-0.410958
H	2.530584	-1.907491	-1.999280
H	3.855286	-0.875368	-2.582762
H	4.120317	-1.947215	-1.207176

[i28]

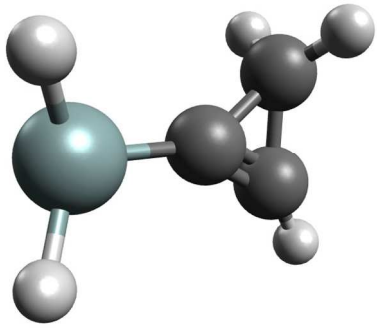


-115.430

$C_s - {}^2A'$

Si	-0.007915	0.012066	0.019900
C	-0.002032	0.004490	1.702004
C	0.006915	-0.001048	3.163153
C	-0.566477	1.257005	3.825268
H	-0.537142	-0.894665	3.502504
H	1.042152	-0.170186	3.494094
H	-1.606993	1.404801	3.528637
H	-0.002001	2.140651	3.520274
H	-0.524533	1.177666	4.914882

[i29]

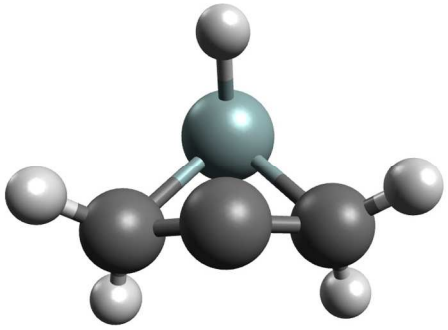


-111.993

$C_1 - {}^2A$

Si	-0.006289	-0.008892	0.000251
C	-1.080451	1.287981	-0.691480
C	-1.440370	2.077374	-1.666474
C	-2.384359	2.058005	-0.523124
H	0.010249	0.014149	1.485212
H	1.361885	0.017392	-0.580426
H	-1.230742	2.475067	-2.645213
H	-2.411053	2.893034	0.176475
H	-3.331936	1.527421	-0.618582

[i30]

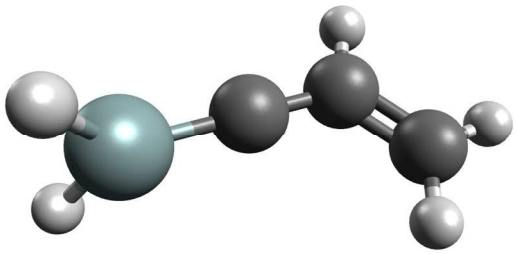


-110.724

$C_s - {}^2A'$

Si	0.015690	-0.012940	-0.001720
C	2.066105	-0.002214	-0.223176
C	1.652136	-1.255947	0.244220
C	0.553894	-1.992217	-0.217661
H	0.021989	-0.013873	1.515656
H	2.664330	0.627195	0.429273
H	2.294859	0.104438	-1.284724
H	0.109322	-2.734707	0.438688
H	0.509453	-2.244935	-1.278194

[i31]

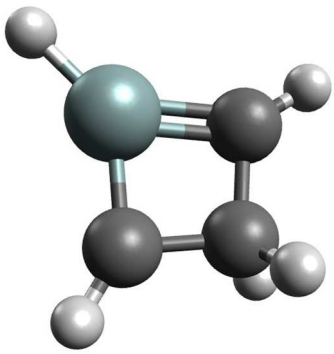


-107.620

$C_s - {}^2A'$

Si	-0.011216	0.005578	-0.006401
C	-1.429605	-0.011932	-0.896354
C	-2.589479	-0.019636	-1.624274
C	-3.258004	1.112155	-2.036706
H	-0.008456	0.004729	1.470750
H	1.319953	0.015727	-0.646603
H	-3.013620	-0.987483	-1.894891
H	-2.877115	2.096784	-1.792095
H	-4.174016	1.041191	-2.611130

[i32]

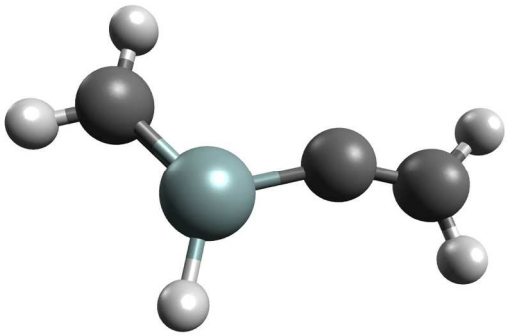


-106.868

$C_{2v} - {}^2A_1$

Si	0.000134	-0.001495	-0.010145
C	1.165908	0.000584	-1.326693
C	0.007591	-0.025419	-2.340574
C	-1.157176	-0.032443	-1.333577
H	-0.002275	0.000964	1.470545
H	2.217266	0.015013	-1.574628
H	-0.002998	0.853864	-2.997343
H	0.022142	-0.918818	-2.977956
H	-2.207059	-0.047449	-1.587628

[i33]

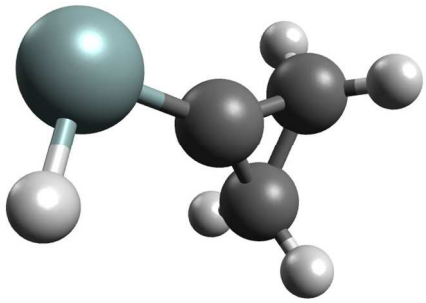


-91.155

$C_s - {}^2A'$

Si	-0.003197	0.000040	-0.051921
C	1.493397	-0.000027	-0.853687
C	-1.590905	0.000076	-0.925302
C	-2.893011	0.000029	-1.014381
H	-0.106435	0.000100	1.426564
H	1.571473	-0.000058	-1.934579
H	2.430437	-0.000042	-0.308773
H	-3.409704	0.000116	-1.975082
H	-3.535072	-0.000234	-0.129523

[i34]

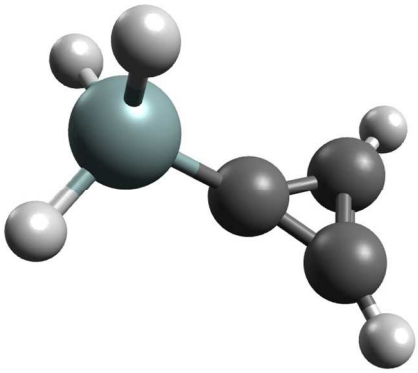


-90.409

$C_1 - {}^2A$

Si	-0.004298	-0.009457	-0.009392
C	1.755784	-0.007731	-0.321054
C	2.857594	0.175765	-1.288993
C	3.055895	-0.675387	-0.063510
H	0.036898	0.007742	1.510081
H	3.336644	1.149651	-1.325891
H	2.772631	-0.317653	-2.253436
H	3.115472	-1.752414	-0.182231
H	3.656699	-0.279612	0.751062

[i35]

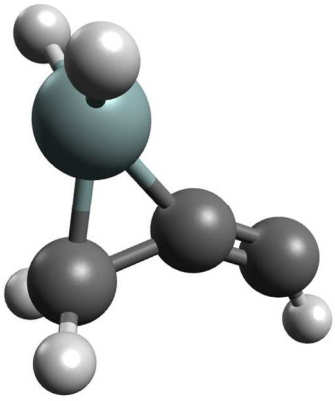


-82.275

$C_s - {}^2A'$

Si	0.004363	0.011666	0.003886
C	-0.818941	1.536237	-0.578167
C	-2.088512	2.239938	-0.675603
C	-1.334547	2.239800	-1.742343
H	0.007450	0.000580	1.491027
H	1.405451	-0.002296	-0.494540
H	-0.645169	-1.260952	-0.451353
H	-2.998375	2.544628	-0.186582
H	-1.177053	2.544363	-2.763264

[i36]

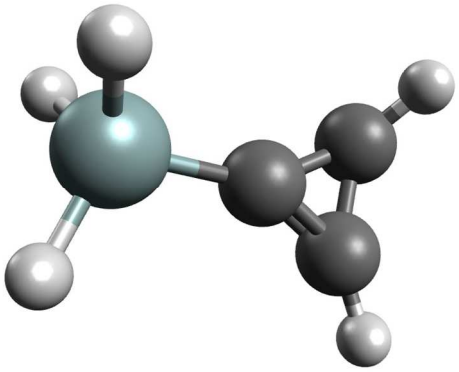


-76.167

$C_s - {}^2A'$

Si	-0.006281	0.008274	-0.004213
C	-1.418660	-0.724029	-0.923794
C	-2.116305	-1.700662	-1.379488
C	-1.405546	0.825590	-0.912879
H	-0.011215	-0.004516	1.474738
H	1.343623	-0.001471	-0.608459
H	-3.007286	-1.899332	-1.959550
H	-1.230504	1.286776	-1.881898
H	-2.220811	1.284406	-0.358651

[i37]

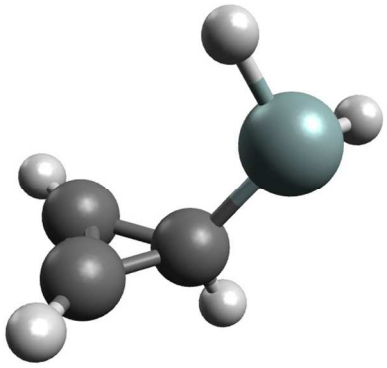


-75.598

$C_1 - {}^2A$

Si	0.001354	-0.002365	-0.001214
C	-0.876809	-1.494365	-0.639228
C	-1.530469	-2.625612	-0.431924
C	-1.374722	-2.283743	-1.798015
H	-0.017729	-0.004854	1.483855
H	1.405869	-0.020824	-0.485900
H	-0.667004	1.222858	-0.511099
H	-1.897810	-3.324591	0.303871
H	-0.835970	-2.782053	-2.602064

[i38]

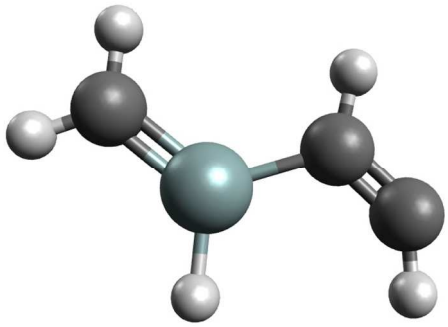


-74.535

$C_1 - {}^2A$

Si	-0.003876	0.009925	-0.013416
C	-0.979927	1.468587	-0.680599
C	-2.345356	1.827683	-0.125166
C	-1.392875	2.602906	0.247239
H	-0.067630	0.004845	1.479027
H	1.420618	0.035576	-0.464102
H	-0.791835	1.721757	-1.727296
H	-3.382063	1.538648	-0.107321
H	-1.026624	3.441872	0.813043

[i39]

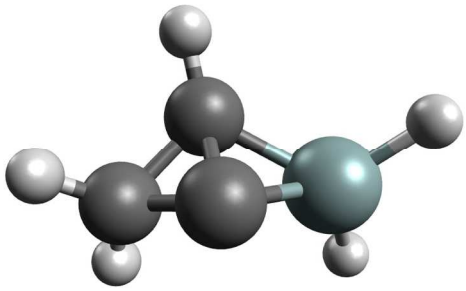


-70.348

$C_s - {}^2A'$

Si	-0.006846	0.000844	-0.014087
C	1.435901	0.001782	-0.909382
C	-1.710190	0.011243	-0.760287
C	-2.766773	0.009796	0.008364
H	-0.047119	-0.008560	1.465233
H	1.450106	0.008569	-1.993433
H	2.406298	-0.004696	-0.426341
H	-1.809211	0.018739	-1.846548
H	-2.975902	0.003596	1.071609

[i40]

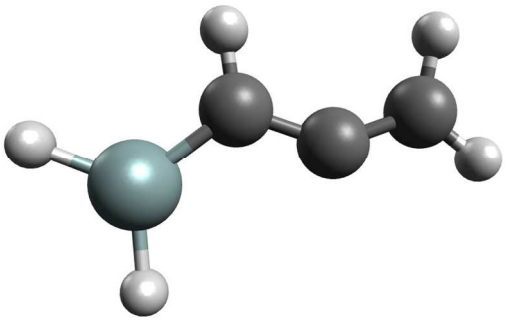


-65.763

$C_1 - {}^2A$

Si	-0.014138	0.004784	-0.003029
C	-1.487198	-0.714684	-0.785907
C	-1.730117	0.022245	-2.046059
C	-1.479483	0.808345	-0.778748
H	0.010518	0.009159	1.473549
H	1.337994	-0.011656	-0.614260
H	-2.761539	0.041008	-2.391387
H	-1.001274	0.007891	-2.854697
H	-2.208231	1.492858	-0.360456

[i41]

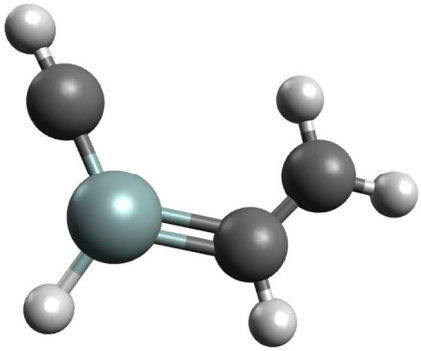


-65.425

$C_s - {}^2A'$

Si	-0.019329	-0.000021	-0.013450
C	-1.446391	0.000066	-0.963026
C	-2.765900	0.000087	-0.429462
C	-4.027025	-0.000013	-0.800968
H	-0.039599	-0.000090	1.462671
H	1.319319	-0.000031	-0.638254
H	-1.350181	0.000136	-2.052799
H	-4.842524	0.000129	-0.084130
H	-4.301031	-0.000263	-1.859131

[i42]

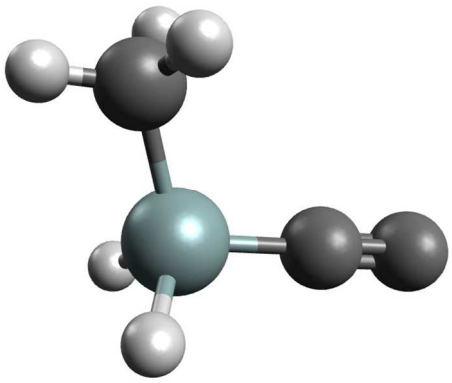


-63.884

$C_s - {}^2A'$

Si	-0.010047	0.001364	-0.003455
C	1.392806	-0.005238	-0.908852
C	-1.727590	-0.008073	-0.705147
C	-1.983812	-0.010712	-2.012237
H	0.018476	0.015849	1.477461
H	2.321827	-0.009141	-1.445443
H	-2.563360	-0.011327	-0.007417
H	-1.184482	-0.007173	-2.748151
H	-2.999867	-0.016338	-2.396748

[i43]

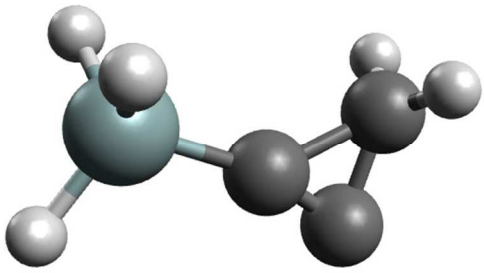


-37.457

$C_s - {}^2A'$

Si	0.009072	0.012642	0.006763
C	-0.787498	-1.554799	-0.565725
C	-1.315572	-2.577073	-0.944897
C	-0.933943	1.478813	-0.671765
H	0.000885	-0.000155	1.491814
H	1.414325	-0.000719	-0.473508
H	-1.970191	1.462882	-0.326519
H	-0.936451	1.462596	-1.764006
H	-0.475835	2.415166	-0.342507

[i44]

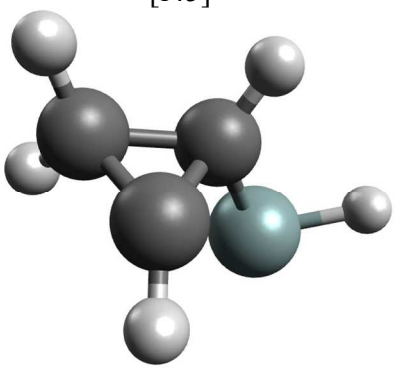


-35.140

$C_s - {}^2A'$

Si	0.000274	0.000100	-0.003529
C	-0.873944	1.502611	-0.621384
C	-1.516101	2.607736	-0.699847
C	-1.241172	2.142396	-2.068242
H	-0.008348	0.010619	1.479811
H	1.395940	0.010509	-0.509220
H	-0.695460	-1.208397	-0.512673
H	-2.018361	1.652716	-2.651603
H	-0.428221	2.577074	-2.646428

[i45]

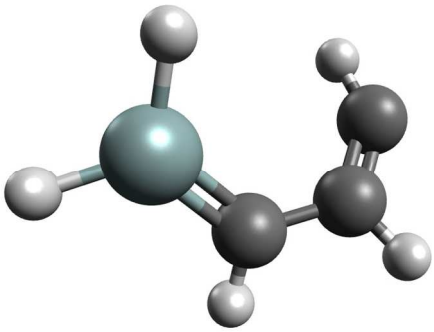


-30.865

$C_1 - {}^2A$

Si	0.035982	-0.032713	-0.040951
C	1.901618	-0.170503	-0.181241
C	2.344825	0.893292	-1.118808
C	2.525916	-0.480569	-1.552075
H	0.036510	0.326886	1.444112
H	2.536147	-0.339813	0.686026
H	1.887695	1.773063	-1.550130
H	3.531788	-0.890206	-1.529097
H	1.888706	-0.888370	-2.334812

[i46]

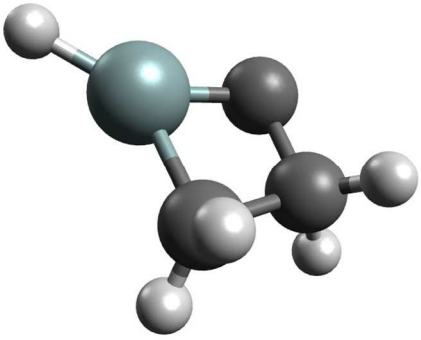


-30.278

$C_1 - {}^2A$

Si	-0.027795	-0.025083	-0.031443
C	-1.527660	0.063374	-0.849957
C	-1.711306	0.001498	-2.312443
C	-0.931156	0.575476	-3.201058
H	0.060152	0.080862	1.439765
H	1.257464	-0.213681	-0.735779
H	-2.438529	0.120231	-0.258268
H	-2.574572	-0.564051	-2.668099
H	-0.067791	1.228270	-3.202149

[i47]

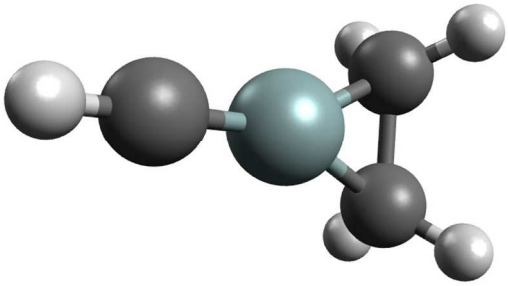


-9.783

$C_s - {}^2A'$

Si	0.002374	0.008040	-0.016213
C	1.086167	-0.003828	-1.336220
C	0.011477	0.054668	-2.404290
C	-1.239812	0.084587	-1.444888
H	-0.017006	-0.003625	1.462473
H	-0.007631	-0.820712	-3.060890
H	0.058777	0.953699	-3.026704
H	-1.819355	1.003345	-1.540189
H	-1.888948	-0.781915	-1.574927

[i48]

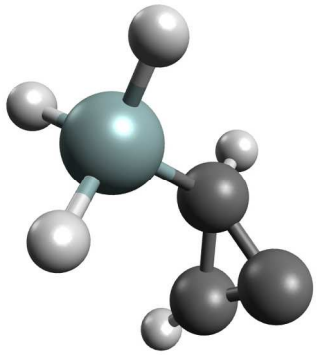


-1.870

$C_{2v} - {}^2A_1$

Si	-0.355377	-0.000106	0.128506
C	0.256144	0.000114	1.660023
C	-0.982297	-0.793334	-1.393671
C	-0.975634	0.801706	-1.391622
H	0.657461	0.000621	2.653525
H	-1.966332	-1.253458	-1.408978
H	-0.296676	-1.257243	-2.097084
H	-1.955767	1.270039	-1.406223
H	-0.285713	1.261839	-2.093349

[i49]

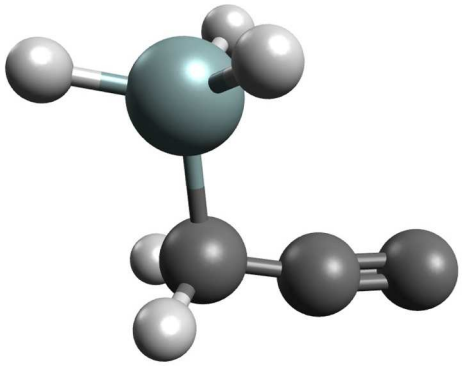


2.321

$C_1 - {}^2A$

Si	-0.008928	-0.003019	-0.002075
C	-0.935074	-1.503457	-0.656020
C	-1.121631	-2.759461	0.134851
C	-2.200257	-2.090118	0.180092
H	-0.050121	-0.017377	1.482903
H	1.403771	-0.022546	-0.471351
H	-0.646563	1.246265	-0.503428
H	-1.001232	-1.604080	-1.741867
H	-3.200702	-1.780353	0.412644

[i50]

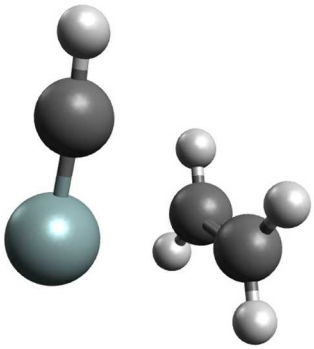


3.090

$C_s - {}^2A'$

Si	0.005588	-0.063651	0.003565
C	-0.998883	-1.553401	-0.694566
C	-0.348479	-2.739075	-0.239300
C	0.379695	-3.656370	0.269254
H	-0.008541	-0.123719	1.482882
H	1.388885	-0.126996	-0.520497
H	-0.678011	1.164322	-0.475312
H	-2.016840	-1.448611	-0.306674
H	-0.986814	-1.450902	-1.784071

[i51]

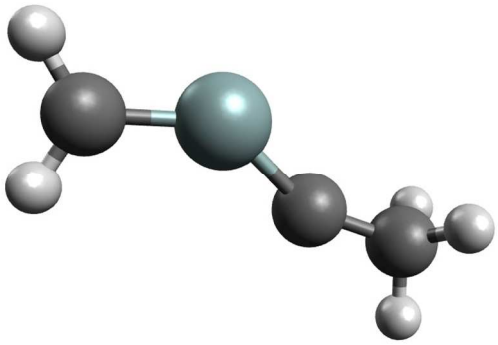


6.761

$C_1 - {}^2A$

Si	-0.063142	0.003881	-0.019719
C	-0.058741	0.027214	1.664755
C	-2.545893	1.449657	0.096780
C	-2.928978	0.173650	0.171563
H	0.013858	0.017135	2.741567
H	-2.364121	2.040158	0.987556
H	-2.420239	1.948415	-0.859062
H	-3.072380	-0.320197	1.125814
H	-3.129842	-0.411038	-0.720629

[i52]

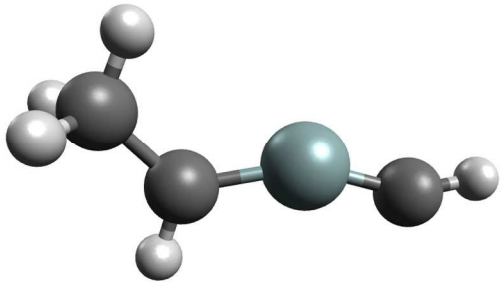


18.312

$C_s - {}^2A'$

Si	-0.111940	-0.010351	0.053585
C	-0.051817	-0.002604	1.741413
C	0.621112	0.000786	3.041612
C	-1.329402	-0.009570	-1.181562
H	1.265075	0.878507	3.164740
H	1.238015	-0.893532	3.182984
H	-0.126124	0.020357	3.842596
H	-1.065657	-0.016097	-2.230937
H	-2.384778	-0.002181	-0.936770

[i53]

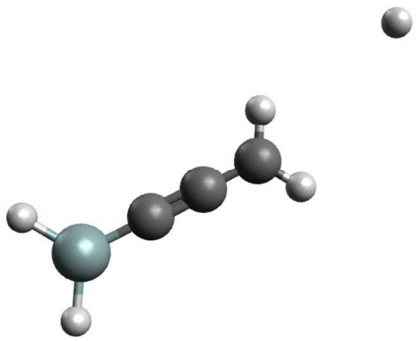


36.931

$C_s - {}^2A'$

Si	-0.274518	0.001524	0.075689
C	0.109553	0.011413	1.669090
C	-1.339537	-0.031706	-1.299835
C	-0.935202	0.007433	-2.745390
H	0.780909	0.034653	2.507814
H	-2.401980	-0.093641	-1.081187
H	0.146100	0.073994	-2.878386
H	-1.388798	0.867429	-3.249869
H	-1.283085	-0.889536	-3.269160

[i54]

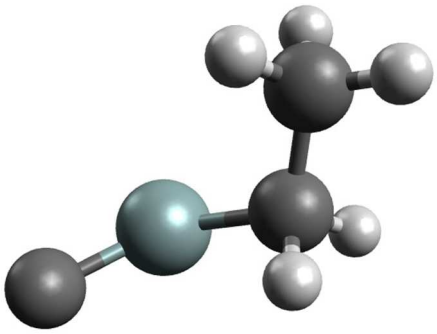


101.887

$C_1 - {}^2A$

Si	0.039466	-0.000072	0.015637
C	-1.371027	-0.000126	-0.900939
C	-2.443011	-0.000173	-1.584338
C	-3.549306	-0.000238	-2.291765
H	0.012315	0.000197	1.490002
H	1.376243	0.000017	-0.606814
H	-3.513979	-0.000463	-3.374925
H	-4.517661	0.000257	-1.805274
H	-7.575264	0.000601	-3.407957

[i55]

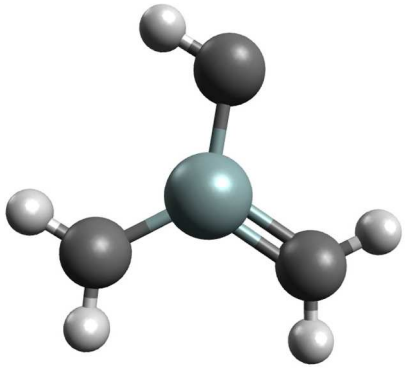


146.011

$C_1 - {}^2A$

Si	0.013112	0.060238	-0.005452
C	0.011525	-0.061297	1.702086
C	1.498637	0.006849	-1.185361
C	1.940672	1.389197	-1.682547
H	2.301938	-0.493795	-0.636798
H	1.233797	-0.644800	-2.023093
H	2.235955	2.032100	-0.850990
H	1.140557	1.895931	-2.227948
H	2.794873	1.294446	-2.357768

[i56]



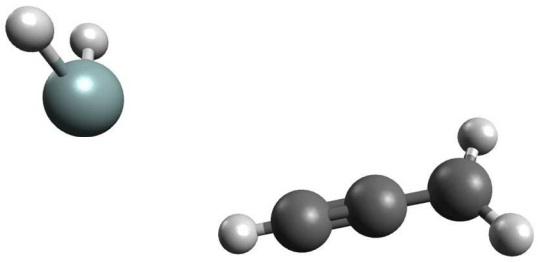
153.575

$C_s - {}^2A'$

Si	-0.000457	0.000885	0.019495
C	-0.000628	-0.000178	1.800371
C	-1.570291	-0.002730	-0.842929
C	1.645912	0.005645	-0.742293
H	0.943230	0.001931	2.335561
H	-0.892271	-0.003246	2.419389
H	-1.614839	-0.002060	-1.927494
H	-2.535382	-0.005110	-0.344026
H	1.587724	0.006829	-1.843413

Transition States

[r-i4]

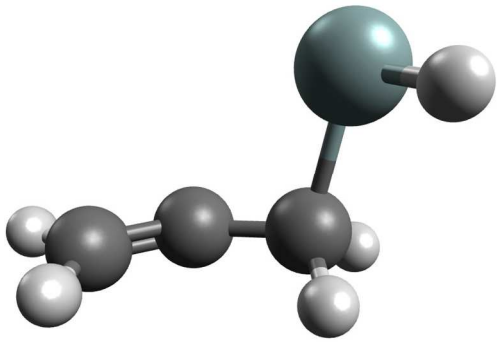


57.031

$C_1 - {}^2A$

Si	2.686700	-2.110350	-0.207080
C	-0.569070	0.214560	-0.959190
C	-1.343720	0.932280	-0.350960
C	-2.218650	1.743790	0.328150
H	2.588440	-3.211890	0.838310
H	3.947460	-1.537730	0.423820
H	0.108020	-0.413520	-1.492370
H	-2.553900	1.482850	1.323890
H	-2.586010	2.655730	-0.125570

[i1-i3]

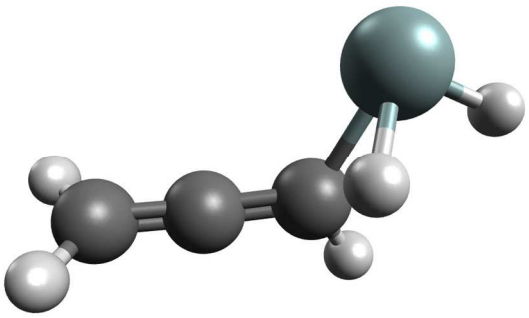


-31.772

$C_1 - {}^2A$

Si	0.168590	3.711230	1.045020
C	-3.275680	2.753440	0.183960
C	-2.209070	3.363140	-0.269510
C	-0.786510	3.107400	-0.524270
H	-4.225640	3.265760	0.306290
H	-3.255430	1.690060	0.438980
H	-0.617360	2.051480	-0.769940
H	-0.430530	3.703620	-1.376210
H	1.069190	2.479190	1.149210

[i1-i4]

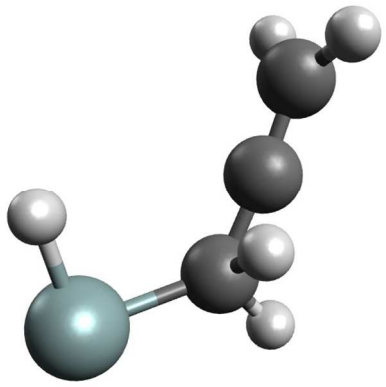


13.026

$C_1 - {}^2A$

Si	1.963460	-0.874180	0.342140
C	0.409310	-0.255360	-0.606020
C	-0.533010	0.478390	-0.000640
C	-1.420490	1.162590	0.655180
H	0.519160	-1.587830	0.280570
H	2.558320	-1.486690	-0.911170
H	0.278290	-0.458760	-1.667190
H	-1.311530	2.233220	0.803600
H	-2.302980	0.680250	1.067830

[i1-i5]

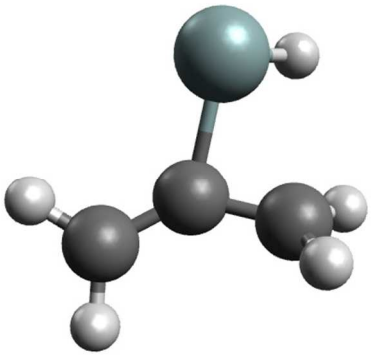


75.188

$C_1 - {}^2A$

Si	-2.074990	0.551860	-1.367080
C	-0.226440	0.620860	-0.917760
C	0.442870	0.071040	0.176170
C	0.985750	-0.415830	1.252910
H	-2.375970	-0.424480	-0.226840
H	0.435330	1.199150	-1.565170
H	0.145000	-0.562730	-1.013960
H	0.965100	0.157470	2.178770
H	1.470110	-1.387510	1.276940

[i2-i3]

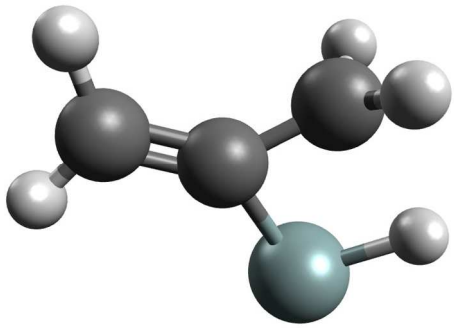


-89.605

$C_1 - {}^2A$

Si	-1.575240	0.999080	0.218950
C	-0.098920	-0.302790	-1.127400
C	0.062210	-0.014420	0.235950
C	1.065400	0.037380	1.118910
H	-2.507440	-0.086900	-0.289000
H	-0.814950	-1.040660	-1.464420
H	0.540610	0.158680	-1.874710
H	1.997670	-0.492750	0.940310
H	0.958910	0.564430	2.060530

[i2-i6]

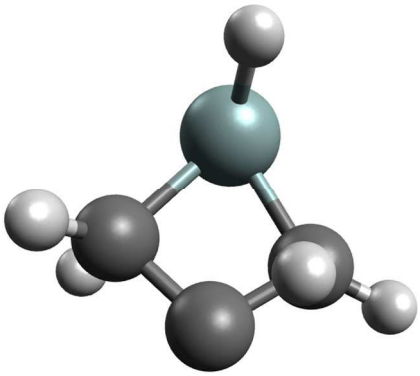


-64.010

$C_1 - {}^2A$

Si	-0.632170	-0.652390	-1.685350
C	0.303680	0.060000	-0.194990
C	1.574120	0.323670	0.097000
C	-0.928860	-0.135070	0.484830
H	2.340410	0.304670	-0.670070
H	1.885580	0.570870	1.108040
H	-1.953880	-0.212760	-1.000670
H	-1.089760	-1.019230	1.095610
H	-1.584330	0.704150	0.690500

[i3-i7]

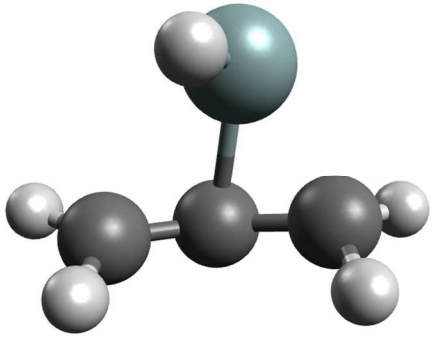


45.178

$C_1 - {}^2A$

Si	-0.749160	0.900190	0.749200
C	0.811700	0.848940	-0.394020
C	0.466390	-0.420760	-0.897860
C	-0.845760	-0.771670	-0.237190
H	-0.216540	0.565950	2.124980
H	1.611250	1.466460	-0.794830
H	1.393260	-0.082440	0.128310
H	-1.579680	-0.742650	-1.048880
H	-0.917810	-1.742790	0.252090

[i3-i8]

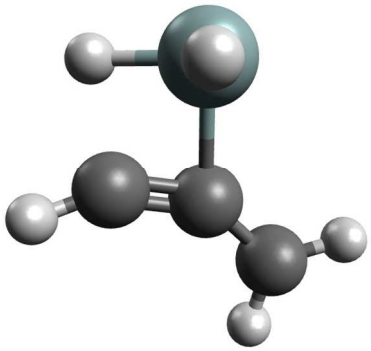


-72.311

$C_1 - {}^2A$

Si	-0.271550	1.053130	0.972230
C	-1.236250	-0.010930	-0.401350
C	-0.204820	-0.737600	0.303220
C	1.136170	-0.678110	0.131480
H	0.597540	1.903210	0.071800
H	-2.255880	-0.218000	-0.092090
H	-1.114450	0.165860	-1.472640
H	1.586690	-0.434980	-0.833610
H	1.806520	-1.024680	0.910800

[i3-i9]

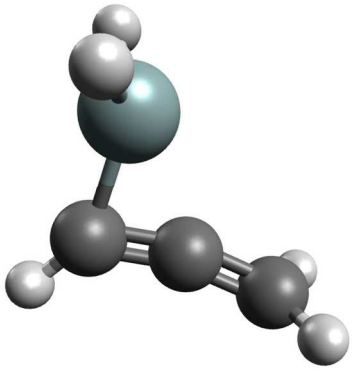


-0.981

$C_1 - {}^2A$

Si	1.512170	-0.011610	0.761530
C	-0.017460	1.086260	-0.206390
C	-0.149310	-0.204860	-0.271050
C	-0.953290	-1.256390	-0.654400
H	1.001370	0.350150	2.140660
H	1.644750	1.375790	0.110900
H	-0.389900	2.087740	-0.317080
H	-0.697980	-2.276340	-0.399080
H	-1.858300	-1.075660	-1.224180

[i4-i9]

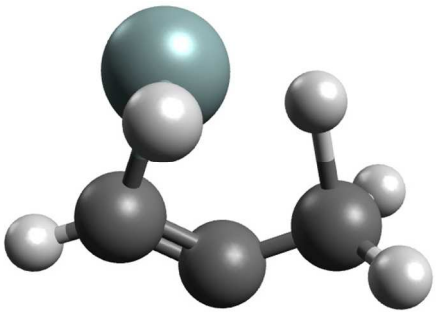


-113.396

$C_s - {}^2A'$

Si	1.108720	-1.020960	0.152910
C	0.553300	0.246780	-1.027950
C	-0.392080	0.419460	-0.134420
C	-1.484220	0.854340	0.544770
H	2.357530	-0.756260	0.910530
H	0.955940	-2.444020	-0.241010
H	0.712780	0.761590	-1.968090
H	-1.380500	1.599480	1.323860
H	-2.431230	0.339450	0.439270

[i4-i10]

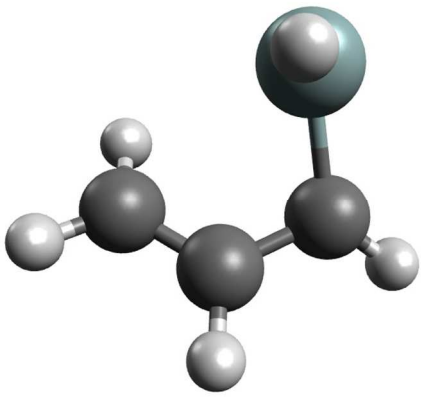


10.130

$C_1 - {}^2A$

Si	0.855430	-1.346530	-0.132220
C	0.141600	-0.060930	-1.385810
C	-0.546470	0.733450	-0.613290
C	-0.759950	0.592830	0.757130
H	2.167140	-0.726690	0.303810
H	0.301410	-0.008820	-2.455920
H	-0.184760	1.213660	1.442710
H	-1.763370	0.356480	1.110570
H	-0.203940	-0.767280	0.999490

[i5-i7]

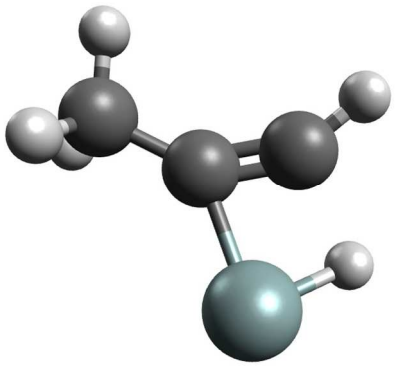


-112.239

$C_1 - {}^2A$

Si	-1.870650	0.098920	-0.143180
C	-0.361750	0.112140	-1.183680
C	0.710200	0.058910	-0.240150
C	0.606930	-0.631100	0.924560
H	-1.695570	1.446900	0.528570
H	-0.184330	0.166810	-2.251280
H	1.598200	0.671540	-0.407930
H	-0.129690	-1.419930	1.047090
H	1.326900	-0.503990	1.725510

[i6-i8]

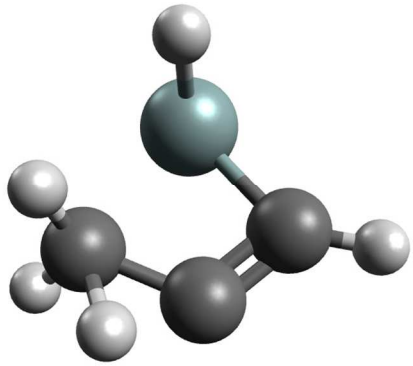


-61.228

$C_1 - {}^2A$

Si	0.695700	0.150140	-1.953760
C	0.045460	0.062510	-0.127200
C	1.304190	-0.016180	0.073400
C	-1.275960	-0.140370	0.521130
H	1.987710	0.723890	-1.304990
H	2.145970	-0.214050	0.714190
H	-1.822460	-0.932360	0.002240
H	-1.179750	-0.404970	1.575920
H	-1.872550	0.770700	0.431130

[i7-i8]

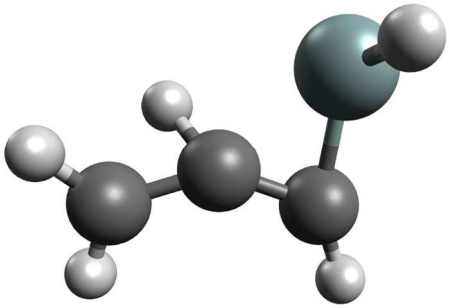


137.697

$C_1 - {}^2A$

Si	-1.156400	0.781190	0.539520
C	0.522170	1.357160	-0.153130
C	0.658830	0.184190	-0.740860
C	-0.315180	-0.956430	-0.350510
H	-0.719070	0.469110	1.974870
H	1.155460	2.230860	-0.210350
H	0.921850	-1.094740	-0.551550
H	-0.805570	-1.495940	-1.150550
H	-0.289460	-1.427970	0.638920

[i8-i9]

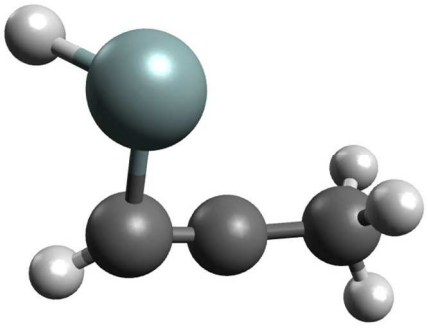


90.651

$C_1 - {}^2A$

Si	-1.311870	1.193150	0.787070
C	0.199320	1.302570	-0.153580
C	-0.048170	-0.066630	-0.055330
C	0.436700	-1.288290	-0.508620
H	-1.050420	1.194050	2.281520
H	1.067550	1.815590	-0.542520
H	0.039480	-2.210510	-0.099170
H	1.233750	-1.356330	-1.246510
H	-0.939610	-0.697410	-0.548360

[i8-i10]



-64.732

$C_1 - {}^2A$

Si	-1.179330	0.858760	1.311550
C	-0.011330	1.324410	-0.093310
C	0.383760	0.123650	-0.395040
C	0.226830	-1.310970	-0.646740
H	-0.515500	1.820140	2.300290
H	0.516190	2.252000	-0.309680
H	0.574750	-1.543320	-1.659010
H	0.825070	-1.897370	0.053650
H	-0.820420	-1.627290	-0.561660