Supporting Information

Gas Phase Formation of c-SiC_3 Molecules in the Circumstellar Envelope of Carbon Stars

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Experimental

It is important to note that both species – silylidyne (SiH) and atomic silicon (Si) – are present in the beam as the result of the disilane (Si_2H_6) photolysis. However, since the reaction dynamics of the SiH($X^2\Pi$) radicals with allene and methylacetylene have been already disseminated (*1, 2*) and atomic silicon is lighter by 1 amu compared to the silylidyne radical, it is possible to untangle the reaction dynamics of the silicon atoms from those of the silylidyne radical. Also, it is important to note that atomic silicon can be formed in its ground (^3P) and/or first electronically excited state (^1D). Therefore, we exploited laser induced fluorescence (LIF) to probe the electronic state(s) of the silicon atoms (*3, 4*). Briefly, fluorescence of ground and electronically excited silicon atoms was probed by utilizing excitations from dye lasers and detected by photomultiplier tube (PMT; Hamamatsu R955). Details of the LIF of the SiH($X^2\Pi$) radical beam have been compiled in a previous publication(*2*); therefore, only those results relevant to atomic silicon are reported here. Silicon atoms in the ground (triplet) and excited (singlet) spin states were detected via their $3p^2\ ^3P \rightarrow 3p4s\ ^3P$ and $3p^2\ ^1D \rightarrow 3p4s\ ^1P$ transitions around 251 nm and 288 nm, respectively. Photons near 251 nm were produced by a Lambda Physik Scanmate dye laser with circulating Coumarin 503 dye, frequency doubled in a BBO II nonlinear crystal in Lambda Physik Scanmate frequency conversion unit. The dye laser was pumped by the third harmonic of a Nd:YAG laser operating at 10 Hz repetition rate and 10 ns pulse duration. The pulse energy was attenuated to 9 nJ by turning off the amplification stages of the dye laser and reducing the iris diameter in the beam path. The 288 nm radiation was obtained by using Rhodamine 590 dye pumped by third harmonic of the Nd:YAG with a frequency doubled output with energy value of 36 nJ per pulse. The excitation LIF of the silicon atoms recorded via the $3p^2\ ^3P \rightarrow 3p4s\ ^3P$ and $3p^2\ ^1D \rightarrow 3p4s\ ^1P$ transitions are presented in Fig. S1 (a) & (b). As evident, the supersonic beam contains silicon atoms both in their ground (^3P) and first electronically excited (^1D) states. Based on the NIST Atomic Spectra Database and using the values of Einstein coefficients of the detected transitions ($3p^2\ ^3P \rightarrow 3p4s\ ^3P$ and $3p^2\ ^1D \rightarrow 3p4s\ ^1P$), we estimated relative number densities of ground to excited state silicon atoms of about one to one.

To discriminate the reactive scattering signal of ground state silicon atoms (^3P) from silicon in its first electronically excited state (^1D), a supersonic beam of solely ground state silicon atoms was generated via a laser ablation source described in detail elsewhere (*5, 6*). Briefly, in the current experiments, ablated silicon atoms entrained in the supersonic expansion

of helium depicted peak velocities (v_p) and speed ratio (S) values of 1474 ± 22 ms^{-1} and 2.2 ± 0.8, respectively. This section of the beam was also characterized via LIF under identical conditions (pulse energy, detection system) as described above. Our data reveal that only silicon atoms in their electronic ground state are present in this section of the supersonic beam as shown in Fig. S1 (c) & (d) generated via laser ablation. Therefore, each crossed molecular beam experiment of the silicon atoms with allene or methylacetylene was conducted twice: first, with the ablation source, which contained only ground state atomic silicon (^{3}P) and second, with the photolysis source which produced ground (^{3}P) and the first electronically excited state (^{1}D).

Laboratory Data

We also probed the reactive scattering signal originating from reactions of solely ground state silicon atoms (Si(^{3}P)) prepared in the ablation source with allene and methylacetylene at collision energies between 15 and 32 $kJmol^{-1}$. However, our crossed beam studies of allene and methylacetylene with ground state silicon atoms (^{3}P) did not reveal any reactive scattering signal; neither atomic nor molecular hydrogen, nor methyl or methane loss channels could be monitored. Therefore, we have to conclude that ground state silicon atoms do not react with allene and methylacetylene at collision energies of between 15 and 32 $kJmol^{-1}$. Hence although ground state silicon atoms (^{3}P) are present in the photolytically generated silicon beam, they do not interfere with the reactive scattering signal.

Branching Ratio Calculations

We performed RRKM calculations (*7*) via direct counting of vibrational states (*8*) to determine the unimolecular reaction rate constants for the silicon–methylacetylene, silicon–allene, and silicon–D3-methylacetylene systems. We also applied a tunneling correction to the reaction rates by approximating the barriers as Eckart potentials (*9*). These rate constants were used to form the coupled systems of equations for each network, which was then solved and evaluated in the long-time limit to extract branching ratios.

For the silicon–methylacetylene system, the trimmed reaction network of reactions considered in the RRKM calculations is given in Fig. S3. For this system our network began with a unit population in isomer [i1] and no population in any other isomers, corresponding to the entrance channel for this reaction. Using the tunneling-corrected rates, we predicted a branching ratio of 38.2% **p1**, 0.6% **p2**, 11.1% **p3**, and 45.8% **p4**. For the silicon–allene system, the same

reaction network and rates were used as in the silicon–methylacetylene case. For this system, however, our network began with unit population in isomer [i7]. While we observed that the silicon–allene system has entrance channels leading to both isomers [i7] and [i10], we note that all flux out of isomer [i7] into the reaction network must proceed through [i10] according to our network. Using the tunneling-corrected rates, we predicted a branching ratio of 38.7% **p1**, 0.5% **p2**, 11.3% **p3**, and 46.5% **p4**.

Comparison of the silicon–methylacetylene and silicon–allene branching ratios shows similar branching ratios for each product. While the reaction rates show the fastest isomerization from [i1] to be [i1]→[i4], exit from this channel is stifled by the high barrier to form product **p2** going through intermediate [i13]. This allows for the other channels out of [i1] to be expressed, particularly [i1]→[i5] and [i1]→[i6]. Both of these channels can eventually lead to isomers [i6], [i9], and [i12], from which we see much lower overall barriers to for products **p4**, **p1**, and **p3**, respectively. Starting from isomer [i7], we predict fast isomerization to [i10], which then preferentially isomerizes to [i6] over [i2]. From [i6] we have facile isomerization to isomers [i9] and [i12] via ring opening. These computational results corroborate the experimental results for these systems, where the product translational energy distributions of the silicon–methylacetylene and silicon–allene systems are nearly identical.

We also examined the branching ratios for hydrogen atom and methyl loss in the silicon–methylacetylene and silicon–allene systems. These channels were found to contribute negligibly (4.2% for methylacetylene, 2.9% for allene) to the overall product stream, corroborating the experimental findings. Specifically, when considering the silicon–methylacetylene and silicon–allene networks, we included exits to atomic hydrogen loss products **n1**, **n2**, **n3**, **n4**, and **n6** and methyl loss product **m2**. For the silicon–methylacetylene system, we predicted branching ratio of 3.9% **n1**, 0.06% **n2**, 0.02% **n3**, 0.01% **n4**, 0.01% **n6**, and 0.2% **m2**. For the silicon–allene system, we predicted branching ratio of 2.7% **n1**, 0.03% **n2**, 0.02% **n3**, 0.01% **n4**, 0.004% **n6**, and 0.1% **m2**. These lower branching ratios are due to the higher barriers for hydrogen atom or methyl loss when compared to the more favorable molecular hydrogen loss channels.

For the silicon–D3-methylacetylene system, we begin from the same reaction network as in the non-deuterated case. From here, we expanded the reaction network to include all possible constitutional isomers for each corresponding non-deuterated isomer to account for the potential of hydrogen-deuterium scrambling. Hydrogen-deuterium scrambling reaction can occur for the

[i2]↔[i3], [i2]↔[i10], [i6]↔[i10], and [i6]→[i9]→[i8]→[i12]→[i6] reactions. We further included the [i2]→[i2] and [i2]→[i3] reactions in our reaction network. Using the tunneling-corrected rates, we predicted a branching ratio of 21.7% **p1a** + HD, 11.0% **p1b** + D_2, 0.3% **p2a** + HD, 0.01% **p2b** + D_2, 0.01% **p2c** + D_2, 2.6% **p3a** + D_2, 1.8% **p3b** + D_2, 5.2% **p3c** + HD, 27.7% **p4a** + D_2, and 29.5% **p4b** + HD. Therefore, we predicted a total branching ratio of 56.8% HD loss products and 43.2% D_2 loss products. These values are in good agreement with the experimental findings of 60 ± 15% HD loss and 40 ± 15% D_2 loss. Furthermore, this corroborates the non-deuterated results, which utilize the same general reaction network framework. Reaction rate constants, imaginary transition state frequencies, and reaction path degeneracies are reported in Table S9.

Astrochemical Modeling

Previous circumstellar models postulated that the formation of c-SiC_3 involves complex networks of ion-molecule reactions terminated by dissociative recombination reactions (1) – (4) along with oxidative destruction of SiC_4 (reaction (5)). Further, photolysis (hν) or cosmic ray (CR) degradation of SiC_3H has been proposed to contribute to c-SiC_3 (reactions (6) – (7)). It must be noted that none of these reactions has yet been studied in the laboratory and hence previous networks must be considered as unproven hypotheses.

(1) $SiC_3H^+ + e \rightarrow c\text{-}SiC_3 + H$

(2) $SiC_3H_2^+ + e \rightarrow c\text{-}SiC_3 + H_2$

(3) $SiC_4^+ + e \rightarrow c\text{-}SiC_3 + C$

(4) $SiC_4H^+ + e \rightarrow c\text{-}SiC_3 + CH$

(5) $O + SiC_4 \rightarrow c\text{-}SiC_3 + CO$

(6) $SiC_3H + h\nu \rightarrow c\text{-}SiC_3 + H$

(7) $SiC_3H + CR \rightarrow c\text{-}SiC_3 + H$

References

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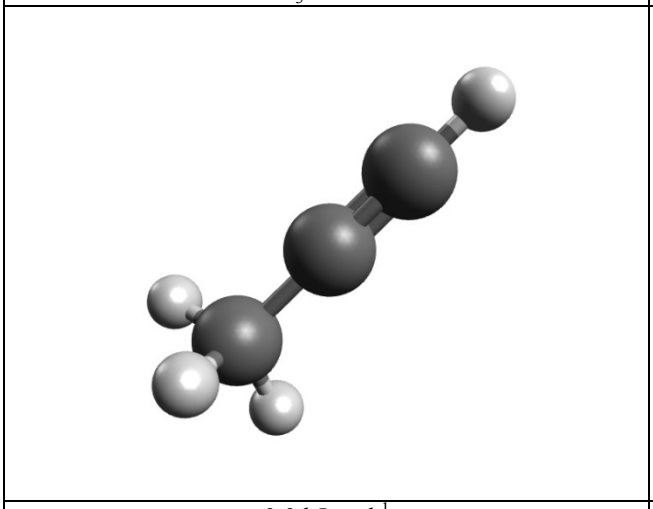
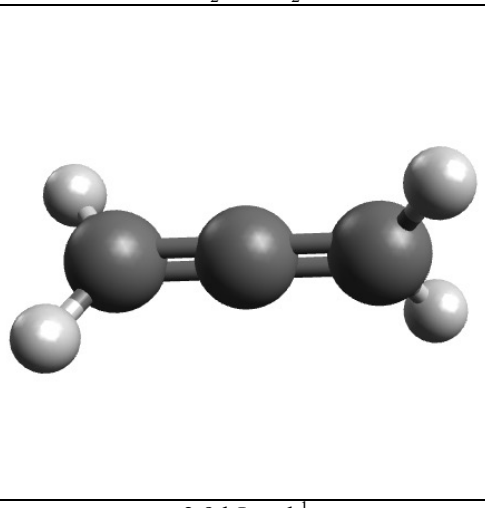
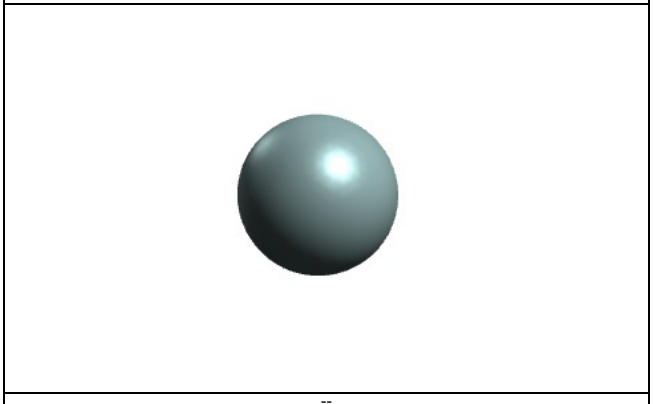
Table S1: Reactants, products, intermediates, and transition state structures relevant to the reaction of electronically excited atomic silicon with methylacetylene and allene. Geometries were calculated at the ωB97X-V//cc-pVTZ level of theory; relative energies were calculated at the CCSD(T)//CBS level of theory.

Reactants							
H_3CCCH				H_2CCCH_2			
							
0.0 kJ mol^{-1}				3.9 kJ mol^{-1}			
C_{3v}-$^1A_1$				D_{2d} – $^1A_1$			
C	-1.919449	1.519750	0.000000	C	-7.512217	1.836332	0.000036
C	-0.721221	1.524736	0.000000	C	-6.210183	1.823559	0.000153
C	-3.382029	1.513693	0.000000	C	-4.908232	1.810798	0.000267
H	0.343441	1.529181	0.000000	H	-8.068002	1.984399	-0.919492
H	-3.768514	1.986640	-0.905294	H	-8.070971	1.698436	0.919347
H	-3.768812	2.058826	0.863618	H	-4.360016	0.885485	-0.140011
H	-3.762327	0.490833	0.041676	H	-4.342009	2.725331	0.139709
Si							
							
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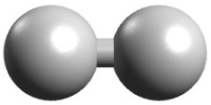
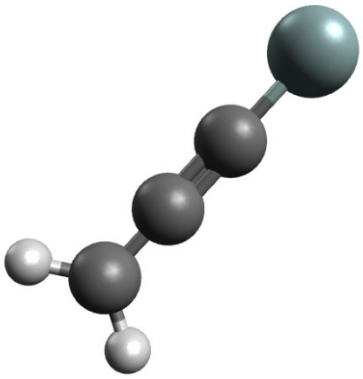
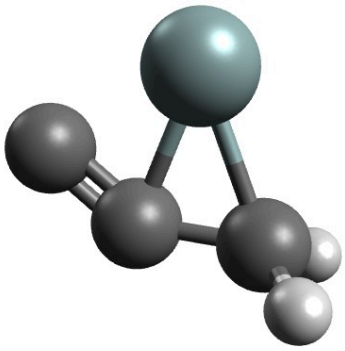
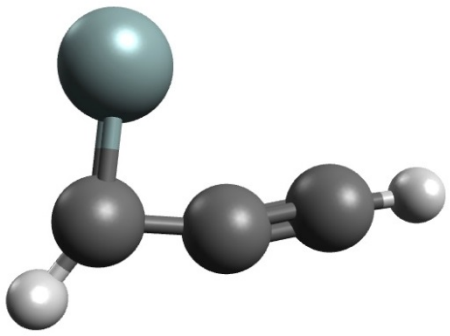
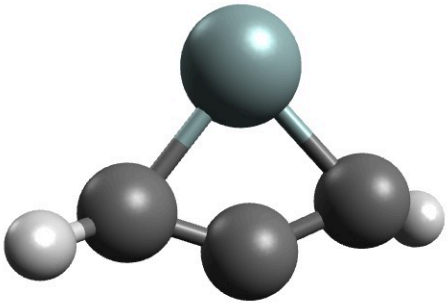
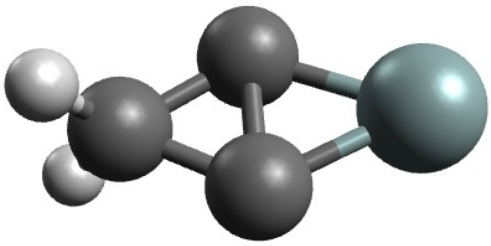
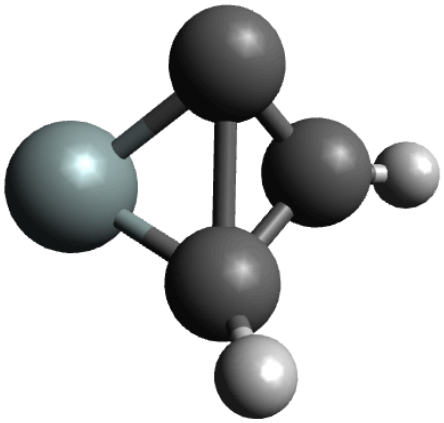
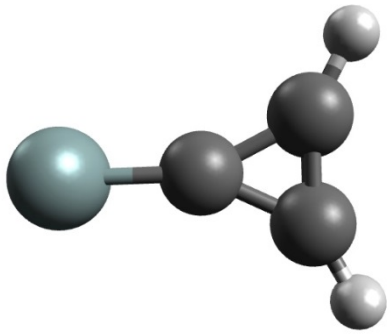
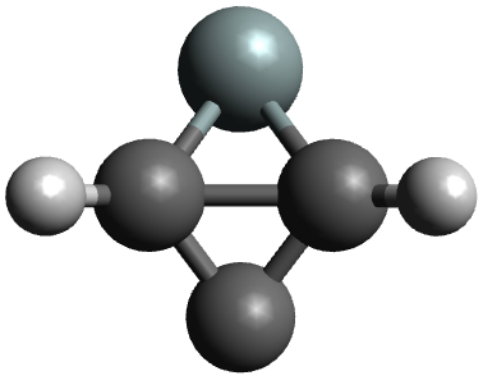
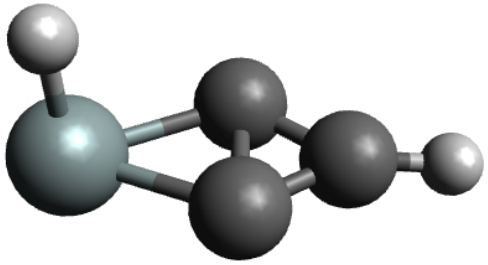
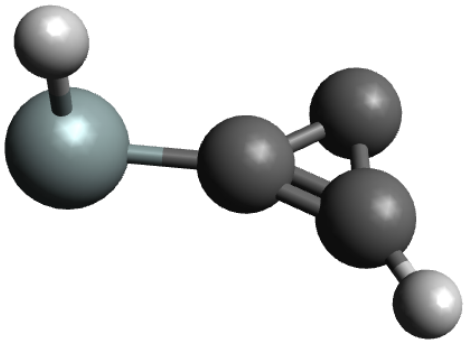
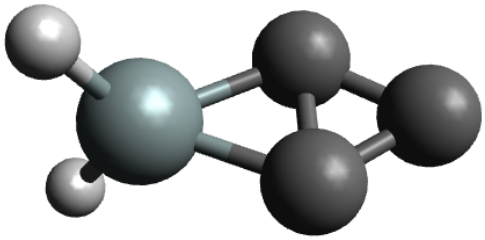
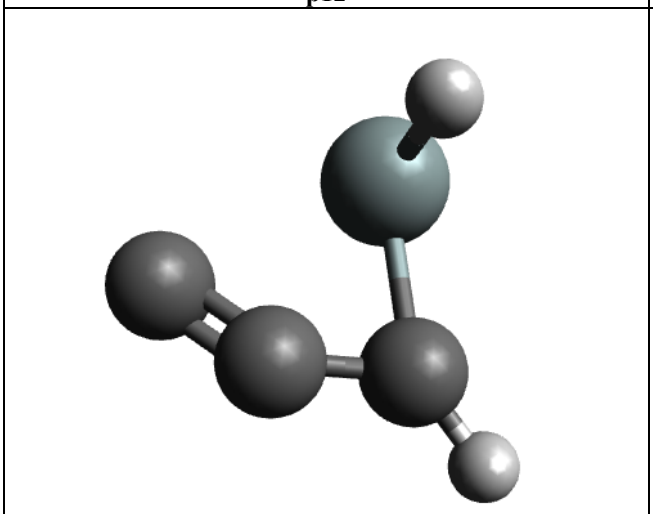
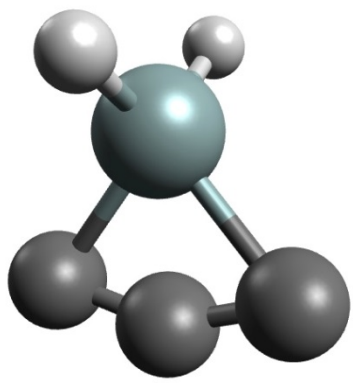
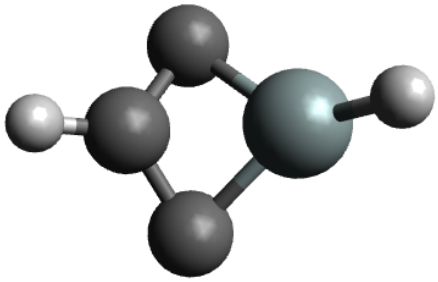
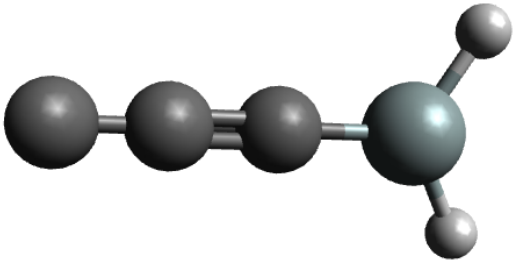
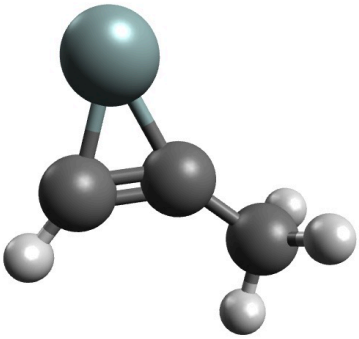
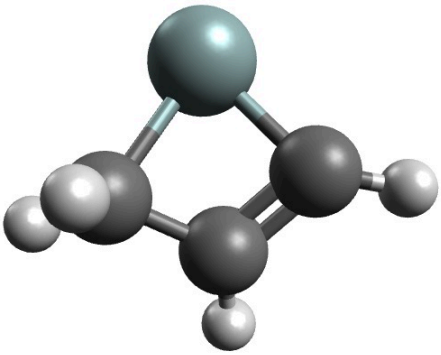
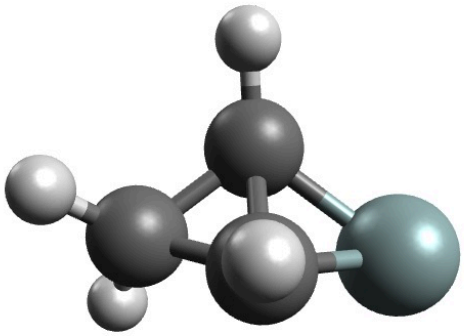
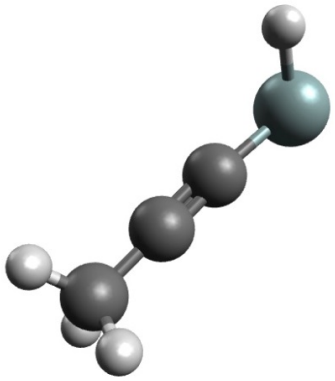
^1D							
Si	0.000000	0.000000	0.000000				

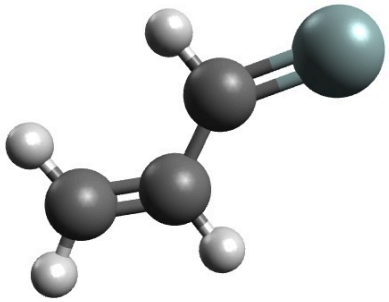
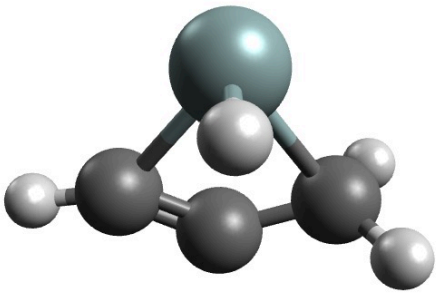
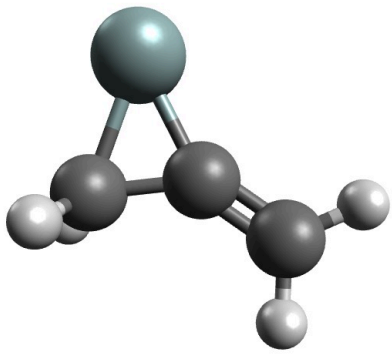
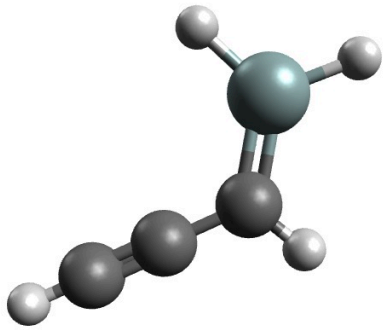
Products							
H_2				**p1**			
							
--				-189.6 kJ mol^{-1}			
$D_{\infty h} - {}^1\Sigma$				$C_{2v} - {}^1A_1$			
H	0.003216	0.000000	0.000000	Si	-2.667415	2.191276	0.000000
H	0.746784	0.000000	0.000000	C	-0.985018	2.220382	0.000000
				C	0.298405	2.242563	0.000000
				C	1.607796	2.265203	0.000000
				H	2.142021	3.207971	0.000000
				H	2.174299	1.341470	0.000000
p2				**p3**			
							
-173.9 kJ mol^{-1}				-163.4 kJ mol^{-1}			
$C_s - {}^1A'$				$C_s - {}^1A'$			
Si	-3.530077	0.607099	0.333008	Si	-1.440031	2.135965	1.571949
C	-2.115964	1.751749	-0.167586	C	-1.258585	1.493357	-0.509032
C	-1.762971	0.449585	-0.634584	C	-1.918764	2.648067	0.002796
C	-2.980050	2.474570	0.443216	C	-0.632564	0.456668	-0.644013
H	-0.954113	-0.065250	-0.122807	H	-2.429665	3.372178	-0.610959
H	-1.792019	0.273905	-1.706863	H	-0.091486	-0.444116	-0.815669

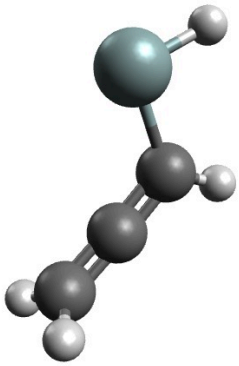
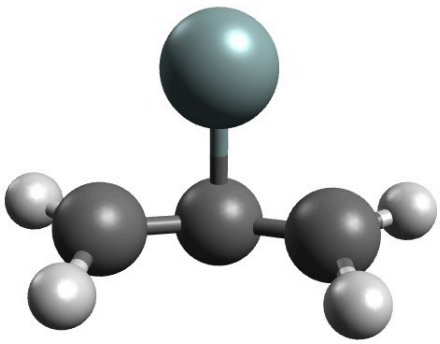
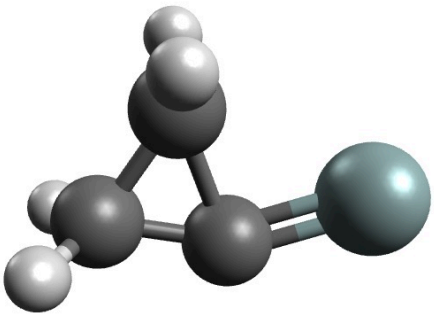
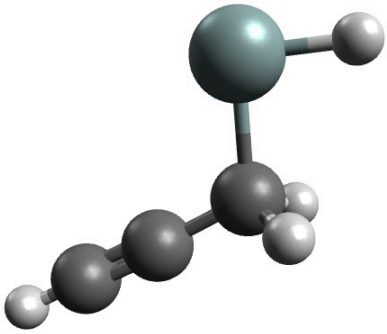
p4				**p5**			
							
-159.3 kJ mol^{-1}				-138.6 kJ mol^{-1}			
$C_2 - {}^1A_1$				$C_{2v} - {}^1A_1$			
Si	0.015583	1.421694	0.441321	Si	-0.153925	2.791130	0.597108
C	-1.710909	1.657474	1.228824	C	-0.701267	1.901637	-0.854814
C	-1.833196	1.452865	-0.080188	C	-1.470675	0.643621	-0.899626
C	-1.051473	1.232997	-1.134185	C	-1.079103	1.277031	0.374194
H	-2.213088	1.188068	2.060067	H	-0.958764	-0.265564	-1.204780
H	-1.030405	1.710504	-2.101157	H	-2.515112	0.686694	-1.198739
p6				**p7**			
							
-99.8 kJ mol^{-1}				-83.5 kJ mol^{-1}			
$C_1 - {}^1A$				$C_{2v} - {}^1A_1$			
Si	0.000000	0.000000	0.000000	Si	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.806628	C	0.000000	0.000000	1.719212
C	-1.286808	0.627089	1.815653	C	0.639430	0.000000	3.039625
C	-0.765193	1.502612	0.924959	C	-0.652963	-0.004736	3.033189
H	0.697327	0.000000	2.637474	H	1.582650	0.005577	3.557070
H	-2.217623	0.494213	2.353974	H	-1.601967	-0.006606	3.539526

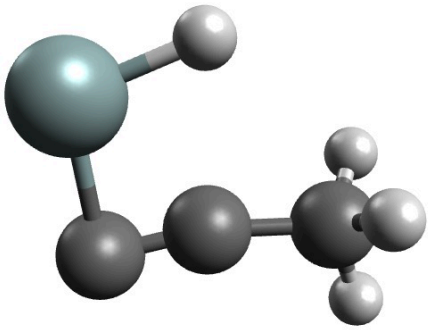
p8				p9			
							
-70.6 kJ mol^{-1}				-62.1 kJ mol^{-1}			
$C_s - {}^1A'$				$C_s - {}^1A'$			
Si	0.000000	0.000000	0.000000	Si	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.843287	C	1.937037	0.000000	-0.025559
C	-1.401563	-0.160952	2.078228	C	2.673224	1.126057	-0.140369
C	-0.973371	-1.112994	1.101537	C	1.353436	1.386523	-0.023475
H	-1.159475	-2.178800	1.178760	H	0.000000	0.000000	1.517171
H	0.745816	0.000000	2.630932	H	3.661304	1.544024	-0.241081
p10				**p11**			
							
-6.0 kJ mol^{-1}				26.5 kJ mol^{-1}			
$C_1 - {}^1A$				$C_{2v} - {}^1A_1$			
Si	0.000000	0.000000	0.000000	Si	0.000000	0.000000	0.000000
C	1.834756	0.000000	-0.012712	C	-1.406915	-0.732528	-0.876099
C	3.087703	0.481614	-0.103968	C	-2.436321	0.000674	-1.517362
C	2.999800	-0.889315	-0.084047	C	-1.406701	0.733908	-0.875881
H	0.000000	0.000000	1.519674	H	0.000000	0.000000	1.472112
H	3.675556	1.385395	-0.152491	H	1.321012	0.000000	-0.649666

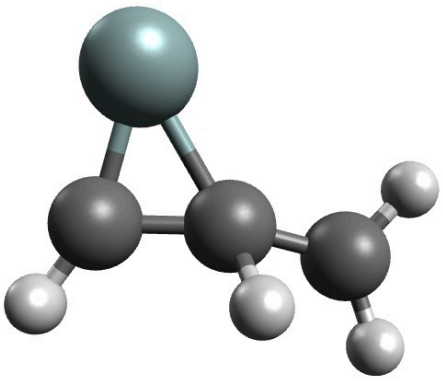
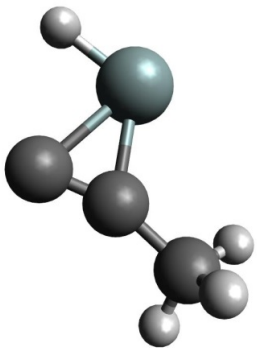
p12				**p13**			
							
58.7 kJ mol^{-1}				82.7 kJ mol^{-1}			
$C_1 - {}^1A$				$C_{2v} - {}^1A_1$			
Si	0.000000	0.000000	0.000000	Si	0.000000	0.000000	0.000000
C	1.906751	0.000000	-0.088904	C	-1.604147	-0.000599	-0.965813
C	1.719817	-1.323251	-0.158049	C	-1.321163	1.286223	-0.796186
C	0.828888	-2.195636	-0.498761	C	-1.319392	-1.286995	-0.795253
H	0.000000	0.000000	1.522410	H	0.000000	0.000000	1.471313
H	2.826815	0.569597	-0.151117	H	1.299958	0.000000	-0.689114
p14				**p15**			
							
127.8 kJ mol^{-1}				147.4 kJ mol^{-1}			
$C_s - {}^1A'$				$C_{2v} - {}^1A_1$			
Si	0.000000	0.000000	0.000000	Si	0.000000	0.000000	0.000000
C	1.264017	0.000000	-1.312498	C	-1.482108	0.004467	-0.835693
C	0.536426	-1.228541	-1.454983	C	-2.602584	0.005168	-1.467455
C	-0.859350	-0.926376	-1.313170	C	-3.727678	0.003497	-2.101864
H	0.000000	0.000000	1.476786	H	0.000000	0.000000	1.469804
H	0.950336	-2.176678	-1.791926	H	1.257655	0.000000	-0.760691

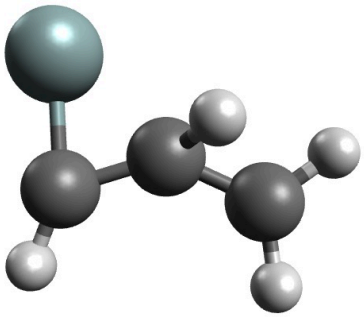
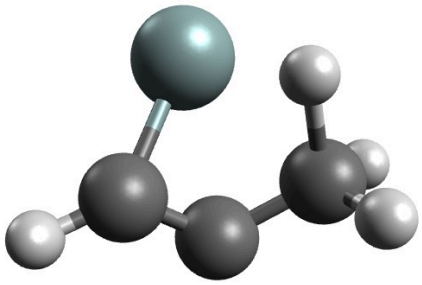
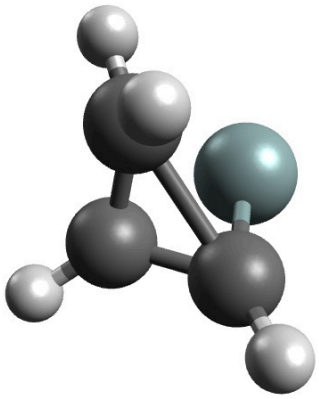
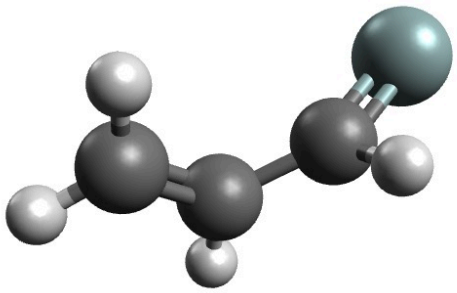
Intermediates							
[i1]				[i2]			
							
-381.9 kJ mol^{-1}				-366.5 kJ mol^{-1}			
$C_s - {}^1A'$				$C_1 - {}^1A$			
Si	-1.656605	1.891479	-0.619303	Si	1.217161	2.092109	-0.478041
C	-3.043502	0.820878	-0.149821	C	-0.718085	2.105551	-0.106733
C	-1.887126	0.137774	-0.160470	C	0.896350	0.503330	0.378512
C	-1.441882	-1.256744	0.108866	C	-0.384938	0.659690	-0.076621
H	-2.267948	-1.914363	0.393239	H	-1.435881	2.452625	-0.849645
H	-0.951711	-1.667938	-0.777728	H	-0.927003	2.520049	0.875808
H	-0.695679	-1.260617	0.907968	H	-1.014639	-0.115450	-0.520096
H	-4.076299	0.569772	0.067786	H	1.393630	-0.440136	0.568491
[i3]				[i4]			
							
-307.0 kJ mol^{-1}				-306.5 kJ mol^{-1}			
$C_s - {}^1A'$				$C_1 - {}^1A$			
Si	-2.584650	2.826243	0.102164	Si	2.269227	0.314672	0.012013
C	-1.277255	1.533566	0.133824	C	0.446698	0.519161	0.002884
C	-2.614644	1.183903	0.928846	C	-0.767059	0.515702	-0.005318
C	-1.976747	0.221766	-0.020795	C	-2.225868	0.529673	-0.008062
H	-1.488341	-0.647336	0.417639	H	2.557659	1.810564	-0.006117
H	-2.696767	0.944785	1.983522	H	-2.625510	-0.364956	-0.490733
H	-2.476241	-0.001272	-0.958483	H	-2.607844	1.412410	-0.525637
H	-0.273455	1.579469	0.542808	H	-2.593502	0.553573	1.020967

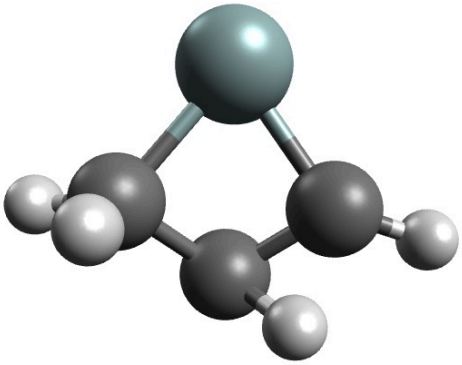
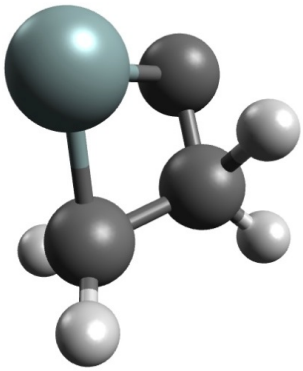
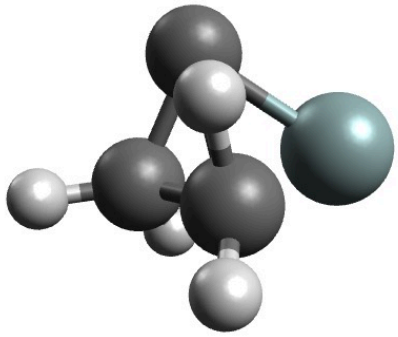
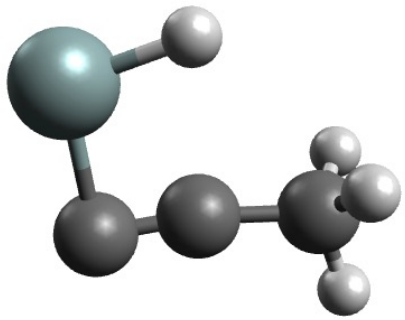
[i5]				[i6]			
							
-305.2 kJ mol^{-1}				-301.9 kJ mol^{-1}			
$C_s - {}^1A'$				$C_1 - {}^1A$			
Si	-2.791074	1.331229	0.575045	Si	1.271276	2.401422	0.597200
C	0.041883	1.957213	0.098223	C	-0.676445	2.076496	-0.045615
C	1.276133	1.530665	-0.176961	C	1.201685	0.439514	-0.022520
C	-1.134334	1.101465	0.199981	C	0.071228	0.921046	-0.285832
H	-0.109806	3.022058	0.263830	H	1.712703	2.984364	-0.742591
H	2.111404	2.219175	-0.232581	H	-0.965219	2.689118	-0.894417
H	1.481749	0.478866	-0.350967	H	-1.396336	2.031078	0.765002
H	-0.944290	0.035021	0.000428	H	1.843949	-0.418828	-0.047808
[i7]				[i8]			
							
-292.0 kJ mol^{-1}				-280.5 kJ mol^{-1}			
$C_s - {}^1A'$				$C_s - {}^1A'$			
Si	-0.002314	3.177910	-0.169760	Si	-2.123430	2.732956	0.435983
C	-0.649663	1.369072	-0.142375	C	-0.578881	1.995631	0.420032
C	0.826543	1.531957	-0.066304	C	-0.360326	0.594266	0.333811
C	1.909821	0.771693	0.020207	C	-0.179590	-0.593207	0.258429
H	-1.073424	0.953192	-1.057167	H	-2.265622	4.199834	0.528920
H	-1.173338	1.016264	0.746817	H	-3.379454	1.961598	0.360797
H	1.853963	-0.315790	0.055069	H	0.306230	2.623143	0.479257
H	2.902621	1.211905	0.059823	H	-0.015456	-1.642789	0.191810

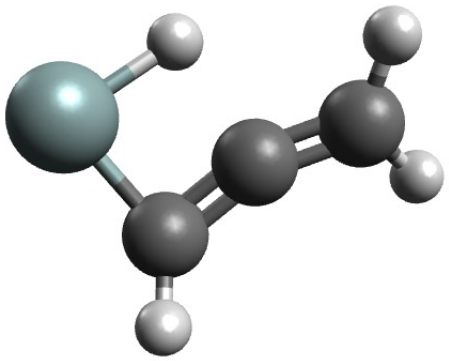
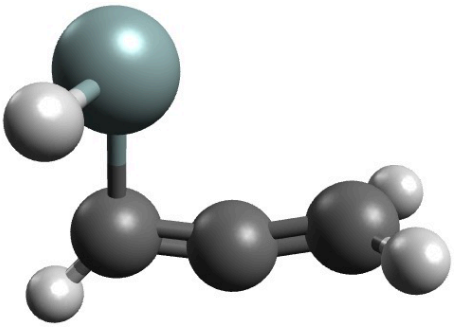
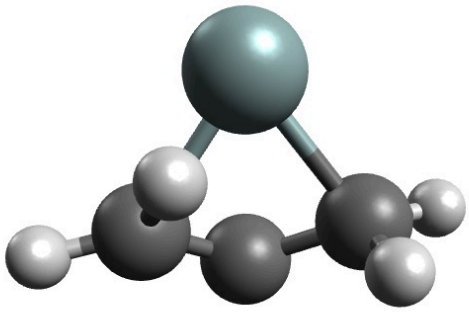
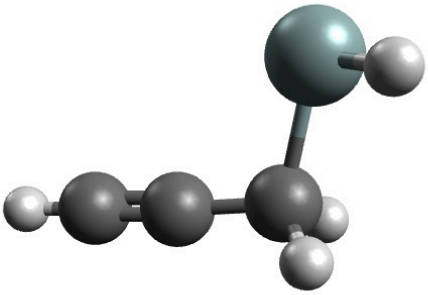
[i9]				[i10]			
							
-279.4 kJ mol^{-1}				-277.3 kJ mol^{-1}			
$C_s - {}^1A'$				$C_s - {}^1A'$			
Si	-0.948677	2.863727	0.654535	Si	-0.333163	1.486867	-0.671031
C	-1.217505	1.006333	0.704275	C	-0.144820	0.334917	0.683483
C	-0.284681	0.271592	0.142353	C	-1.419478	-0.081122	0.274337
C	0.670871	-0.400535	-0.428995	C	1.062694	0.035706	0.040856
H	-2.235815	3.206243	1.405402	H	-1.610019	-1.027212	-0.240233
H	-2.068992	0.501898	1.155645	H	-2.282879	0.366410	0.756404
H	1.531568	-0.731501	0.140907	H	1.241688	-0.893852	-0.506956
H	0.619686	-0.645957	-1.483673	H	1.954699	0.571689	0.349342
[i11]				[i12]			
							
-273.3 kJ mol^{-1}				-247.9 kJ mol^{-1}			
$C_s - {}^1A'$				$C_s - {}^1A'$			
Si	1.409563	2.464346	0.895067	Si	-0.980308	2.921623	1.046459
C	-0.674602	1.916613	-0.147441	C	-1.407690	1.314359	0.084885
C	0.532533	1.098713	0.523749	C	-0.359350	0.302722	0.082071
C	-0.611275	0.405511	-0.024987	C	0.531367	-0.500595	0.106582
H	-0.564797	2.315714	-1.149586	H	-2.336725	3.551344	0.727266
H	-1.405816	2.412592	0.481019	H	-1.671387	1.607227	-0.940700
H	-0.477705	-0.147527	-0.951107	H	-2.336671	0.913777	0.513390
H	-1.312873	-0.051284	0.668184	H	1.315662	-1.220461	0.122189

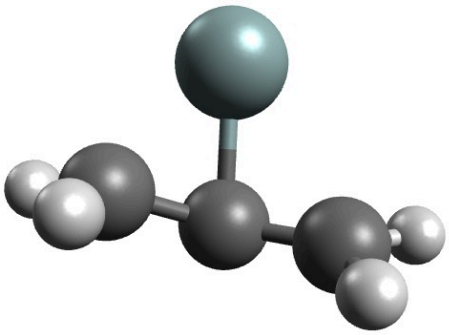
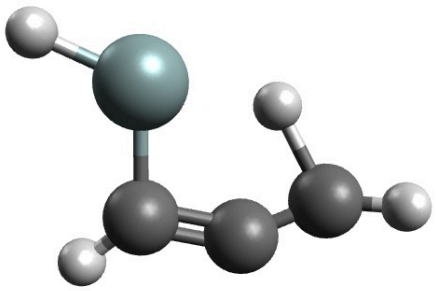
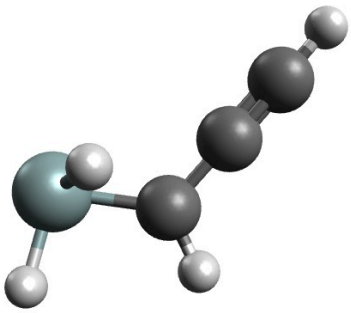
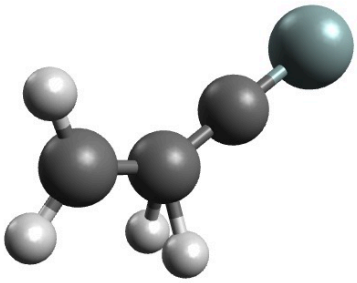
[i13]			
			
-224.0 kJ mol^{-1}			
$C_s - {}^1A'$			
Si	-1.688737	2.624682	0.616789
C	-0.244907	1.218317	-0.220340
C	1.218639	1.272651	-0.343790
C	-1.465384	0.927557	-0.237325
H	-0.260660	3.204713	0.754427
H	1.524821	2.129620	-0.945098
H	1.687125	1.351436	0.638071
H	1.564998	0.357273	-0.829223

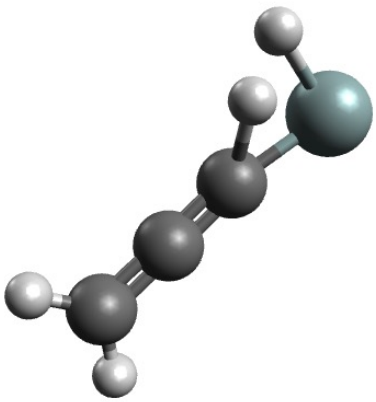
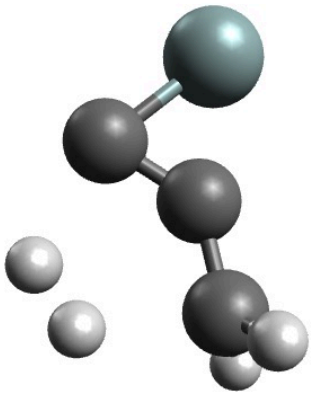
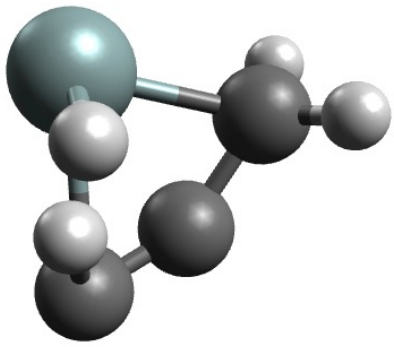
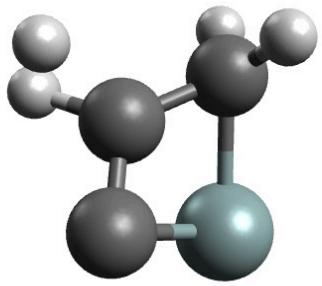
Transition State Structures							
[i1]→[i2]				[i1]→[i4]			
							
-77.0 kJ mol^{-1}				-194.1 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	0.387656	1.918057	-0.868165	Si	-2.122577	1.493357	-0.465731
C	0.507204	-1.109474	-0.273582	C	-3.577778	0.142016	0.174868
C	-0.001009	0.171130	-0.093798	C	-2.426216	-0.379803	0.065365
C	-0.892669	1.297958	0.108223	C	-1.341337	-1.393100	0.060616
H	1.347937	-1.296852	-0.939211	H	-1.737882	-2.337896	-0.315266
H	0.177136	-0.265142	0.972772	H	-0.507637	-1.078652	-0.566987
H	0.170559	-1.954642	0.325094	H	-0.973850	-1.547956	1.076886
H	-1.765240	1.299326	0.746709	H	-3.309526	2.412152	-0.373543

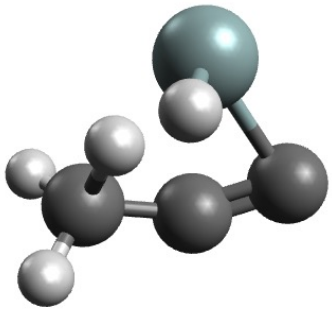
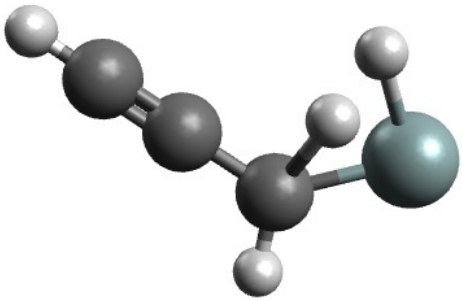
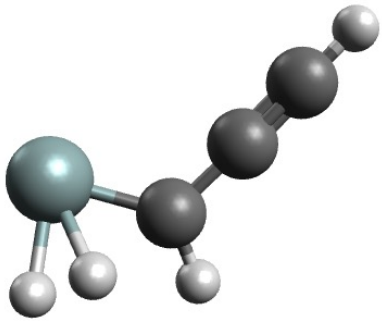
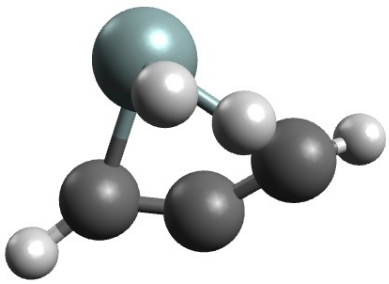
[i1]→[i5]				[i1]→[i6]			
							
-142.6 kJ mol^{-1}				-125.8 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	0.485782	2.153579	-0.469008	Si	0.778035	1.356341	0.013393
C	0.332198	-1.132452	-0.095064	C	-1.041349	0.972089	0.089159
C	0.161878	0.240941	-0.155304	C	-0.726348	-0.144886	-0.571048
C	-0.869881	1.190140	0.041691	C	0.465469	-0.839573	-0.180070
H	1.058802	-0.010869	0.587659	H	0.248932	-1.572742	0.597463
H	-0.474833	-1.810179	0.181935	H	1.180352	-1.204148	-0.916275
H	1.295799	-1.572078	-0.331053	H	1.081984	-0.069503	0.844891
H	-1.919433	1.016042	0.235748	H	-1.980789	1.508295	0.137363
[i2]→[i3]				[i2]→[i5]			
							
-188.1 kJ mol^{-1}				-294.1 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-2.150053	2.178667	0.625370	Si	0.342188	2.735051	-0.130811
C	-0.578457	1.585315	-0.456669	C	0.391241	-1.205372	-0.299825
C	-1.232877	0.355972	-0.039025	C	0.039692	-0.188254	0.478770
C	-0.432102	1.821019	0.963102	C	-0.308252	1.168082	-0.001663
H	0.445188	1.756078	1.604662	H	0.000480	-0.344895	1.555941
H	0.020532	1.864829	-1.311772	H	0.632717	-2.174234	0.123862
H	-0.716789	-0.405155	0.544939	H	0.451087	-1.098752	-1.378354
H	-2.145988	-0.008539	-0.518207	H	-1.322618	1.262237	-0.434147

[i2]→[i10]				[i2]→[i11]			
							
-27.6 kJ mol^{-1}				8.3 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	0.728857	1.050351	-1.035226	Si	0.711581	1.120945	-1.147132
C	0.745086	-0.738470	-0.340304	C	0.472146	-0.659767	-0.443763
C	0.053676	-0.073521	0.854344	C	-0.426581	0.126484	0.507436
C	-0.693567	0.957443	0.165361	C	0.185285	1.423246	0.742216
H	1.677882	-1.260348	-0.131790	H	-1.131751	-0.376092	1.184455
H	0.063165	-1.398234	-0.873462	H	1.329286	-1.008742	0.132221
H	-1.158678	-0.176597	0.686967	H	0.056519	-1.475193	-1.037839
H	-1.402374	1.604957	0.677393	H	-1.169658	0.875873	-0.033549
[i3]→[i11]				[i4]→[i13]			
							
-25.7 kJ mol^{-1}				-224.8 kJ mol^{-1}			
$C_1 - {}^1A$				$C_s - {}^1A'$			
Si	-2.117498	2.386481	0.331886	Si	-1.742300	2.701762	0.558436
C	-1.109699	0.390124	0.271138	C	-1.453027	0.995062	-0.232032
C	-0.453814	1.674840	-0.208502	C	-0.226982	1.212635	-0.272076
C	-1.026002	1.305652	1.486479	C	1.233250	1.262100	-0.377354
H	-2.106608	0.234772	-0.198696	H	-0.321943	3.146011	0.987967
H	0.243508	1.734296	-1.034771	H	1.549669	2.031502	-1.083304
H	-0.560203	-0.548099	0.270135	H	1.675869	1.477113	0.596678
H	0.211278	1.873915	0.737564	H	1.597521	0.293445	-0.727392

[i5]→[i9]				[i6]→[i9]			
							
-206.4 kJ mol^{-1}				-259.9 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-1.992862	2.228890	0.527181	Si	1.820646	2.497868	0.585175
C	-1.168691	0.701841	0.088179	C	1.254585	0.742483	0.074294
C	0.014708	1.354943	0.010861	C	0.032876	1.141174	-0.073976
C	1.299058	1.583736	-0.198471	C	-1.054450	1.887589	-0.083800
H	-0.660165	2.892930	0.016175	H	2.460246	2.819309	-0.774176
H	-1.325198	-0.327819	0.375544	H	1.690241	-0.197006	-0.235942
H	1.802093	2.476996	0.142678	H	-1.294651	2.500444	-0.946357
H	1.862043	0.843052	-0.756205	H	-1.774537	1.839849	0.726578
[i6]→[i10]				[i6]→[i12]			
							
-159.1 kJ mol^{-1}				-241.9 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	1.108893	2.428844	0.896755	Si	0.852609	1.635684	0.581065
C	1.254157	0.804122	-0.190514	C	-0.565860	0.423002	0.059391
C	-0.047399	0.766331	0.066469	C	0.001882	-0.919555	0.000234
C	-0.677368	2.066019	0.073662	C	0.544992	-1.989473	-0.037835
H	2.054356	0.150676	-0.497980	H	0.555684	2.682867	-0.493235
H	1.608219	2.139909	-0.662094	H	-1.048992	0.683920	-0.883382
H	-0.645862	2.587746	-0.883451	H	-1.329382	0.463880	0.848535
H	-1.601289	2.227878	0.621898	H	1.001958	-2.950630	-0.071481

[i7]→[i10]				[i8]→[i9]			
							
-276.7 kJ mol^{-1}				-56.0 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-1.965407	2.054224	0.949023	Si	1.041061	0.917892	0.436916
C	-2.941031	0.741834	-0.252682	C	0.760892	-0.738193	-0.161392
C	-1.529983	0.959789	-0.397630	C	-0.609128	-0.750344	-0.306514
C	-0.519325	0.330323	0.274811	C	-1.670823	-0.094074	-0.212414
H	-3.585322	1.284613	-0.938932	H	2.501462	1.265763	0.648959
H	-3.363470	-0.192898	0.123519	H	-0.818889	0.943557	0.334551
H	-0.582867	-0.703830	0.623728	H	1.411713	-1.596634	-0.075037
H	0.457528	0.798760	0.345200	H	-2.618347	0.185964	-0.624789
[i8]→[i12]				[i5]→**p1**			
							
-115.2 kJ mol^{-1}				36.0 kJ mol^{-1}			
$C_1 - {}^1A$				$C_s - {}^1A'$			
Si	-2.521663	2.463165	1.136938	Si	-2.989127	-0.912311	-0.067647
C	-0.857503	2.002660	0.565118	C	-1.436574	-0.366039	-0.033811
C	-0.462648	0.671903	0.277186	C	-0.145854	0.096600	-0.001158
C	-0.127979	-0.463490	0.061318	C	1.148919	-0.335722	0.029154
H	-0.053439	2.725894	0.410733	H	1.968519	0.370590	0.051314
H	0.166755	-1.470185	-0.125512	H	1.364749	-1.396295	0.033802
H	-2.334378	3.957638	1.028947	H	-0.052376	1.252833	0.469567
H	-2.405675	1.983846	-0.345689	H	-0.028713	1.251089	-0.470006

[i9]→**p1**				[i1]→**p2**			
							
-88.7 kJ mol^{-1}				7.0 kJ mol^{-1}			
$C_1 - {}^1A$				$C_s - {}^1A'$			
Si	-0.744770	2.157892	1.133843	Si	0.528665	2.400596	-0.746415
C	-0.117447	0.739329	0.301978	C	0.638969	-0.741790	0.047537
C	0.508868	-0.265289	-0.184605	C	0.334217	0.578629	-0.236986
C	1.137912	-1.291212	-0.706981	C	-0.782728	1.293996	-0.211915
H	2.192710	-1.451493	-0.511820	H	1.142678	-0.981263	0.980498
H	0.620937	-2.000203	-1.344227	H	0.810919	-1.435189	-0.771673
H	-1.537155	0.742156	0.712436	H	-1.559747	-0.175915	0.315690
H	-2.215299	1.527879	0.692674	H	-1.065292	-0.900941	0.410427
[i6]→**p2**				[i11]→**p2**			
							
-46.2 kJ mol^{-1}				98.6 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	1.178923	2.205371	0.803390	Si	0.042413	-0.714013	0.848100
C	-0.641206	2.137118	-0.050763	C	-0.717668	0.642379	-0.366158
C	-0.130702	0.814244	0.053579	C	0.748846	0.531954	-0.607018
C	0.888991	0.086553	0.200705	C	1.444960	-0.634113	-0.453494
H	-0.835280	2.504167	-1.054512	H	-1.128405	1.560574	0.057494
H	-1.380706	2.457777	0.683302	H	-1.303184	0.282882	-1.207928
H	1.725043	1.088245	-0.475804	H	1.486648	1.537155	-0.404833
H	1.923344	2.086626	-0.687100	H	1.243355	1.496133	-1.295948

[i13]→**p2**				[i12]→**p3**			
							
-45.6 kJ mol^{-1}				-70.6 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-0.830773	0.883817	0.953003	Si	-1.151997	1.718947	0.728726
C	-1.811287	-0.696687	0.301549	C	-0.793552	-0.036891	0.485201
C	-0.590983	-0.923847	0.102221	C	0.356363	-0.744575	0.018188
C	0.749568	-0.461799	-0.040845	C	1.337204	-1.326892	-0.364743
H	1.185475	-0.546441	-1.038520	H	-1.597641	-0.704860	0.800559
H	1.455315	-0.696271	0.749183	H	2.205962	-1.845464	-0.696218
H	0.271987	0.942873	-0.437740	H	-0.463884	1.036474	-0.582223
H	-0.545547	1.525644	-0.576927	H	0.061553	1.931814	-0.358027
[i12]→**p3′**				[i6]→**p4**			
							
-76.3 kJ mol^{-1}				-114.2 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-1.555112	0.642765	0.911988	Si	0.831125	0.640403	0.777373
C	0.049390	0.418870	0.114001	C	-1.185225	0.266693	0.157410
C	0.581034	-0.893905	-0.073288	C	-0.415827	-0.797532	0.102736
C	1.006592	-2.011224	-0.207659	C	0.854625	-1.135711	0.195070
H	0.726733	1.208649	-0.209397	H	-2.051331	0.445181	0.777573
H	1.387736	-2.997804	-0.330653	H	1.482402	-1.878498	-0.264555
H	-1.435106	2.141508	0.235326	H	-0.203090	1.162708	-0.807825
H	-1.002771	1.445970	-0.426216	H	0.676107	1.295027	-0.933420

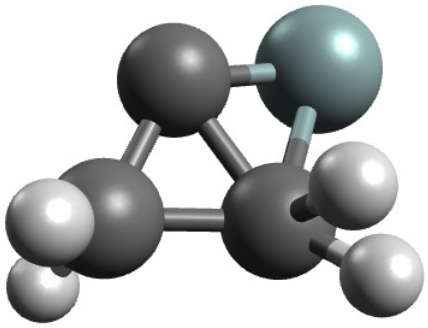
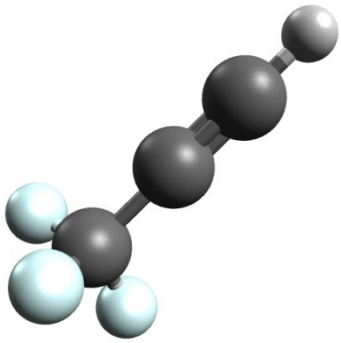
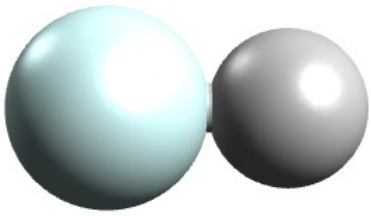
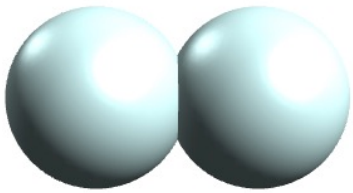
[i11]→**p5**			
			
66.7 kJ mol^{-1}			
C_1 – ^{1}A			
Si	-0.987538	1.955490	-0.108967
C	0.391227	0.544056	-0.099353
C	-0.222777	-0.796271	-0.455253
C	-1.149070	0.247028	-0.031728
H	-0.029086	-1.630912	0.222284
H	-0.176856	-1.062271	-1.507519
H	1.344670	0.560033	0.664829
H	0.776750	0.207977	1.273359

Table S2: Reactants, products, intermediates, and transition state structures relevant to the reaction of electronically excited atomic silicon with D3-methylacetylene. Geometries were calculated at the ωB97X-V//cc-pVTZ level of theory; relative energies were calculated at the CCSD(T)//CBS level of theory.

Reactants							
D_3CCCH				Si			
							
C_{3v}-$^1A_1$				^1D			
C	-1.919449	1.519750	0.000000	Si	0.000000	0.000000	0.000000
C	-0.721221	1.524736	0.000000				
C	-3.382029	1.513693	0.000000				
H	0.343441	1.529181	0.000000				
D	-3.768514	1.986640	-0.905294				
D	-3.768812	2.058826	0.863618				
D	-3.762327	0.490833	0.041676				
Products							
HD				D_2			
							
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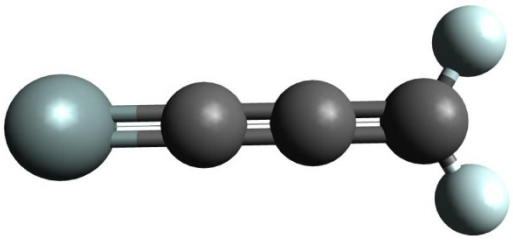
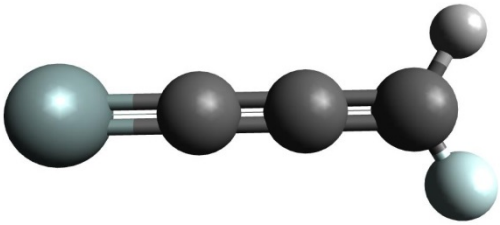
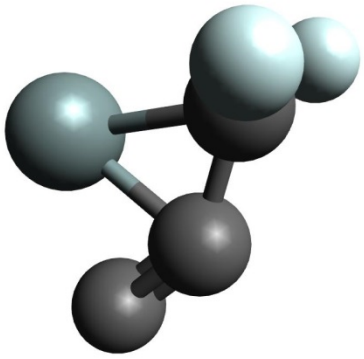
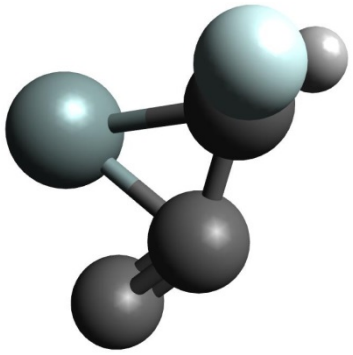
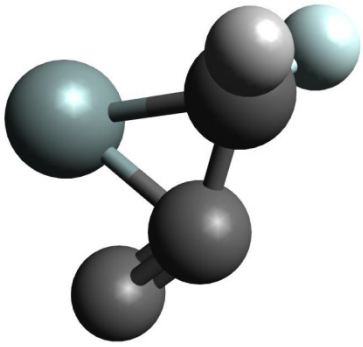
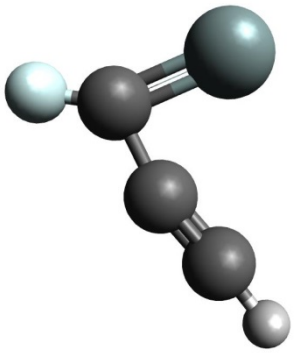
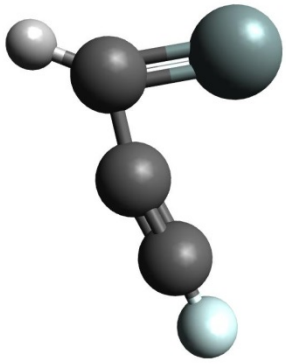
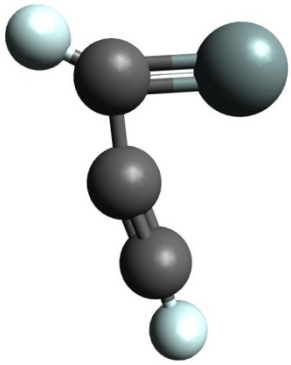
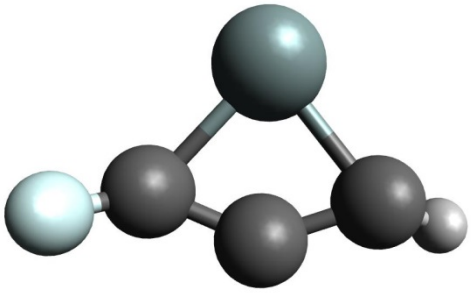
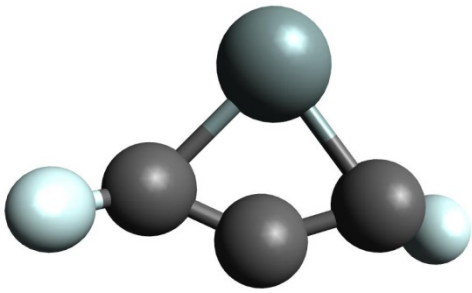
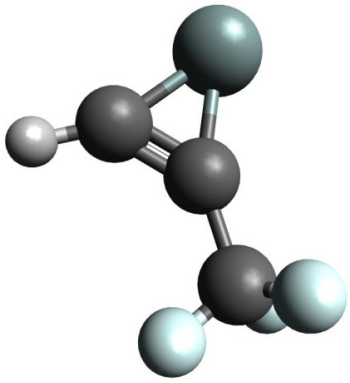
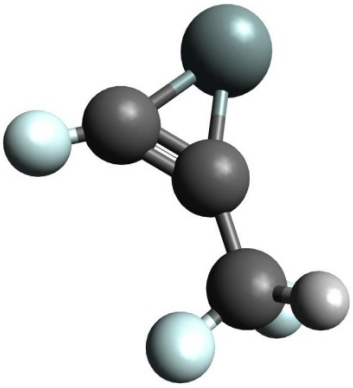
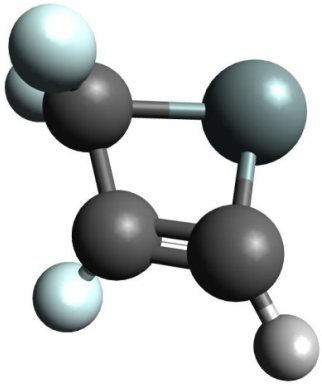
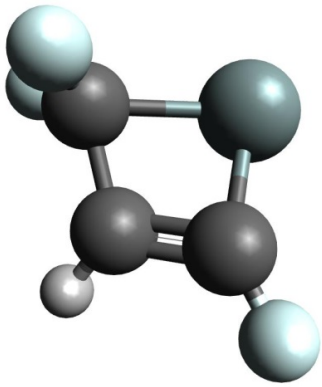
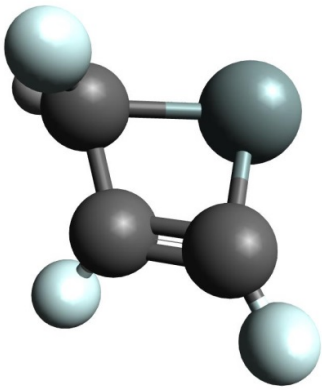
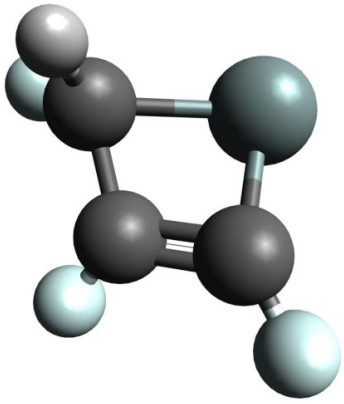
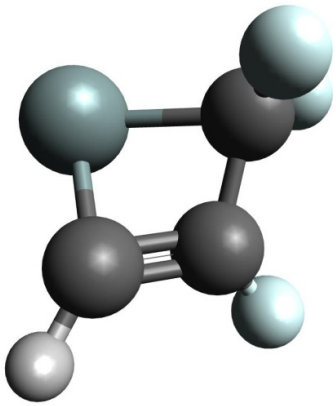
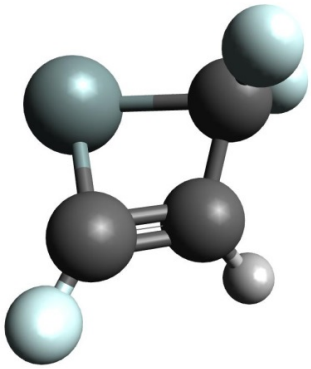
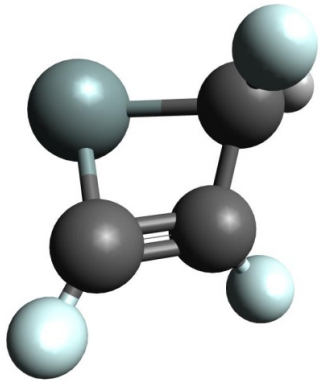
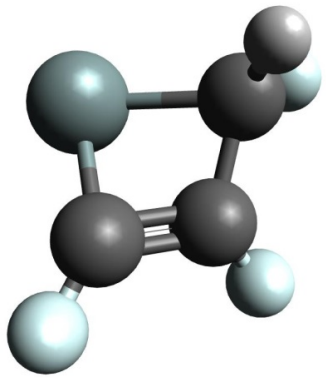
$C_{\infty v} - {}^1\Sigma$				$D_{\infty h} - {}^1\Sigma$			
D	0.003216	0.000000	0.000000	D	0.003216	0.000000	0.000000
H	0.746784	0.000000	0.000000	D	0.746784	0.000000	0.000000

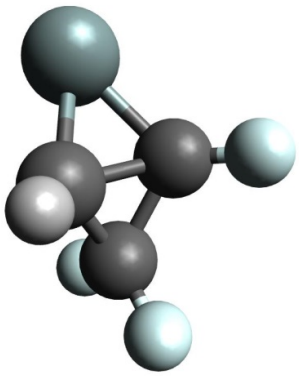
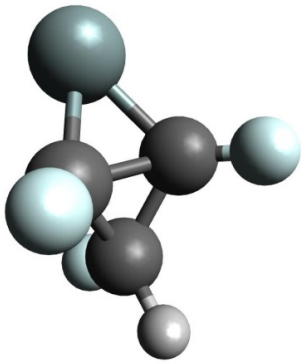
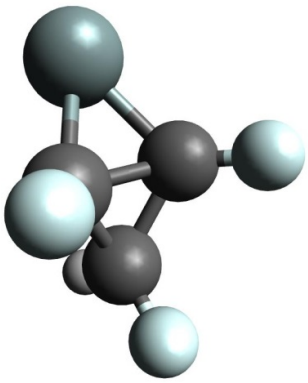
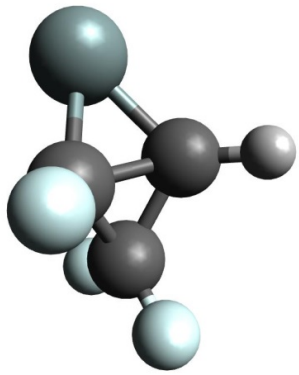
p1a				**p1b**			
							
-183.1 kJ mol^{-1}				-179.8 kJ mol^{-1}			
$C_{2v} - {}^1A_1$				$C_s - {}^1A'$			
Si	-2.667415	2.191276	0.000000	Si	-2.667415	2.191276	0.000000
C	-0.985018	2.220382	0.000000	C	-0.985018	2.220382	0.000000
C	0.298405	2.242563	0.000000	C	0.298405	2.242563	0.000000
C	1.607796	2.265203	0.000000	C	1.607796	2.265203	0.000000
D	2.142021	3.207971	0.000000	H	2.142021	3.207971	0.000000
D	2.174299	1.341470	0.000000	D	2.174299	1.341470	0.000000
p2a				**p2b**			
							
-169.2 kJ mol^{-1}				-165.1 kJ mol^{-1}			
$C_s - {}^1A'$				$C_1 - {}^1A$			
Si	-3.530077	0.607099	0.333008	Si	-3.530077	0.607099	0.333008
C	-2.115964	1.751749	-0.167586	C	-2.115964	1.751749	-0.167586
C	-1.762971	0.449585	-0.634584	C	-1.762971	0.449585	-0.634584
C	-2.980050	2.474570	0.443216	C	-2.980050	2.474570	0.443216
D	-0.954113	-0.065250	-0.122807	H	-0.954113	-0.065250	-0.122807
D	-1.792019	0.273905	-1.706863	D	-1.792019	0.273905	-1.706863

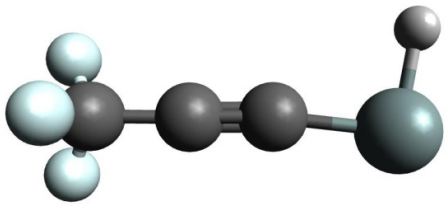
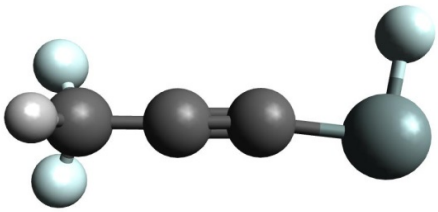
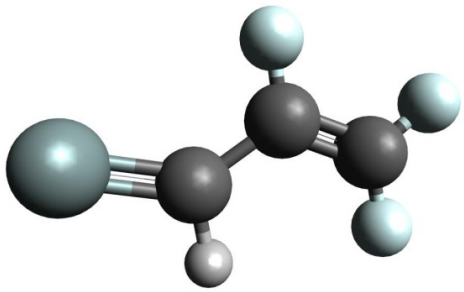
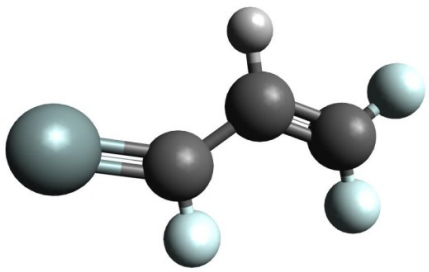
p2c				**p3a**			
							
-165.1 kJ mol^{-1}				-154.0 kJ mol^{-1}			
$C_1 - {}^1A$				$C_s - {}^1A'$			
Si	-3.530077	0.607099	0.333008	Si	-1.440031	2.135965	1.571949
C	-2.115964	1.751749	-0.167586	C	-1.258585	1.493357	-0.509032
C	-1.762971	0.449585	-0.634584	C	-1.918764	2.648067	0.002796
C	-2.980050	2.474570	0.443216	C	-0.632564	0.456668	-0.644013
D	-0.954113	-0.065250	-0.122807	D	-2.429665	3.372178	-0.610959
H	-1.792019	0.273905	-1.706863	H	-0.091486	-0.444116	-0.815669
p3b				**p3c**			
							
-153.5 kJ mol^{-1}				-157.0 kJ mol^{-1}			
$C_s - {}^1A'$				$C_s - {}^1A'$			
Si	-1.440031	2.135965	1.571949	Si	-1.440031	2.135965	1.571949
C	-1.258585	1.493357	-0.509032	C	-1.258585	1.493357	-0.509032
C	-1.918764	2.648067	0.002796	C	-1.918764	2.648067	0.002796
C	-0.632564	0.456668	-0.644013	C	-0.632564	0.456668	-0.644013
H	-2.429665	3.372178	-0.610959	D	-2.429665	3.372178	-0.610959
D	-0.091486	-0.444116	-0.815669	D	-0.091486	-0.444116	-0.815669

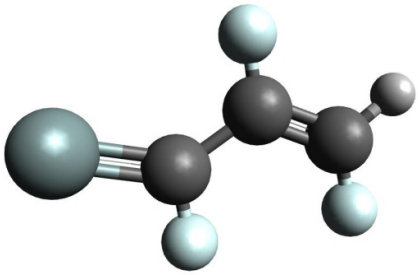
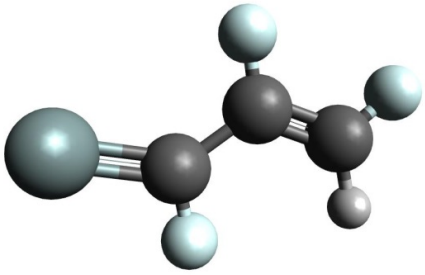
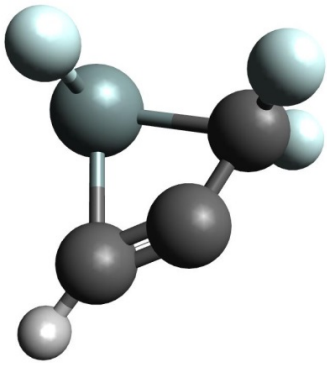
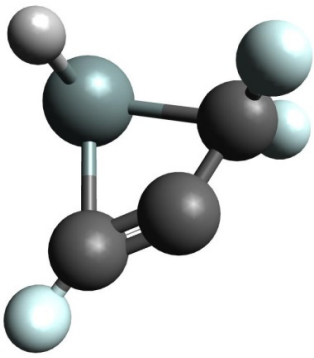
p4a				**p4b**			
							
-149.7 kJ mol^{-1}				-153.1 kJ mol^{-1}			
$C_1 - {}^1A$				$C_2 - {}^1A_1$			
Si	0.015583	1.421694	0.441321	Si	0.015583	1.421694	0.441321
C	-1.710909	1.657474	1.228824	C	-1.710909	1.657474	1.228824
C	-1.833196	1.452865	-0.080188	C	-1.833196	1.452865	-0.080188
C	-1.051473	1.232997	-1.134185	C	-1.051473	1.232997	-1.134185
H	-2.213088	1.188068	2.060067	D	-2.213088	1.188068	2.060067
D	-1.030405	1.710504	-2.101157	D	-1.030405	1.710504	-2.101157
Intermediates							
[i1a]				[i1b]			
							
-381.9 kJ mol^{-1}				-381.2 kJ mol^{-1}			
$C_s - {}^1A'$				$C_1 - {}^1A$			
Si	-1.656605	1.891479	-0.619303	Si	-1.656605	1.891479	-0.619303
C	-3.043502	0.820878	-0.149821	C	-3.043502	0.820878	-0.149821
C	-1.887126	0.137774	-0.160470	C	-1.887126	0.137774	-0.160470
C	-1.441882	-1.256744	0.108866	C	-1.441882	-1.256744	0.108866
D	-2.267948	-1.914363	0.393239	D	-2.267948	-1.914363	0.393239
D	-0.951711	-1.667938	-0.777728	D	-0.951711	-1.667938	-0.777728
D	-0.695679	-1.260617	0.907968	H	-0.695679	-1.260617	0.907968
H	-4.076299	0.569772	0.067786	D	-4.076299	0.569772	0.067786

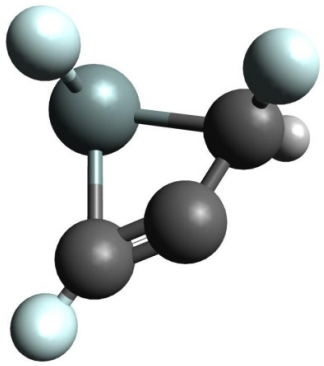
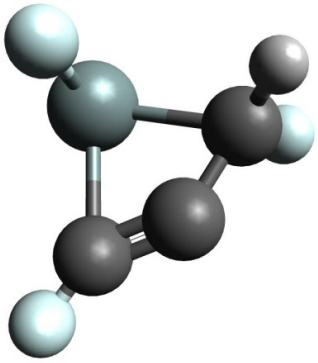
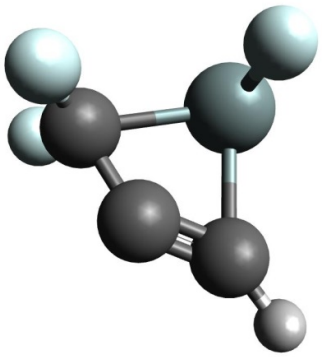
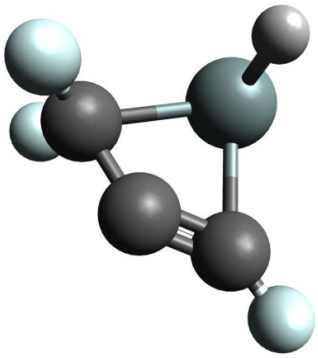
[i2a]				[i2b]			
							
-366.5 kJ mol^{-1}				-366.5 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	1.217161	2.092109	-0.478041	Si	1.217161	2.092109	-0.478041
C	-0.718085	2.105551	-0.106733	C	-0.718085	2.105551	-0.106733
C	0.896350	0.503330	0.378512	C	0.896350	0.503330	0.378512
C	-0.384938	0.659690	-0.076621	C	-0.384938	0.659690	-0.076621
D	-1.435881	2.452625	-0.849645	D	-1.435881	2.452625	-0.849645
D	-0.927003	2.520049	0.875808	D	-0.927003	2.520049	0.875808
D	-1.014639	-0.115450	-0.520096	H	-1.014639	-0.115450	-0.520096
H	1.393630	-0.440136	0.568491	D	1.393630	-0.440136	0.568491
[i2c]				[i2d]			
							
-366.2 kJ mol^{-1}				-366.2 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	1.217161	2.092109	-0.478041	Si	1.217161	2.092109	-0.478041
C	-0.718085	2.105551	-0.106733	C	-0.718085	2.105551	-0.106733
C	0.896350	0.503330	0.378512	C	0.896350	0.503330	0.378512
C	-0.384938	0.659690	-0.076621	C	-0.384938	0.659690	-0.076621
H	-1.435881	2.452625	-0.849645	D	-1.435881	2.452625	-0.849645
D	-0.927003	2.520049	0.875808	H	-0.927003	2.520049	0.875808
D	-1.014639	-0.115450	-0.520096	D	-1.014639	-0.115450	-0.520096
D	1.393630	-0.440136	0.568491	D	1.393630	-0.440136	0.568491

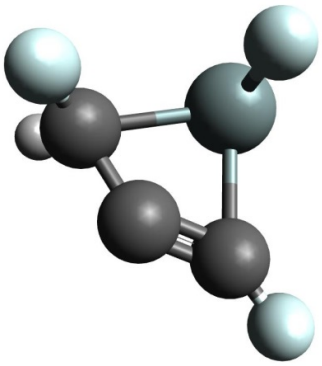
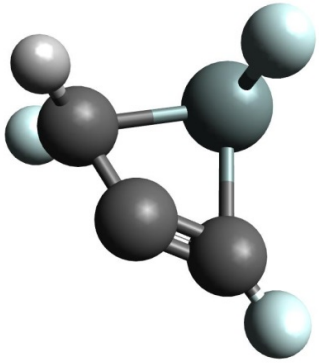
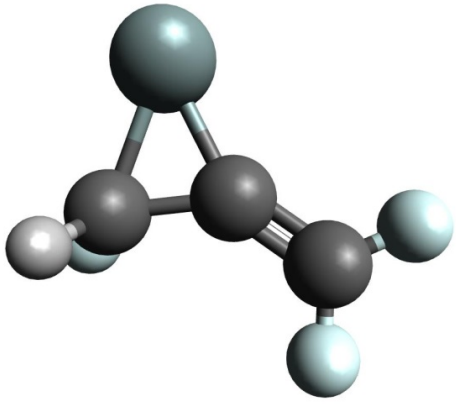
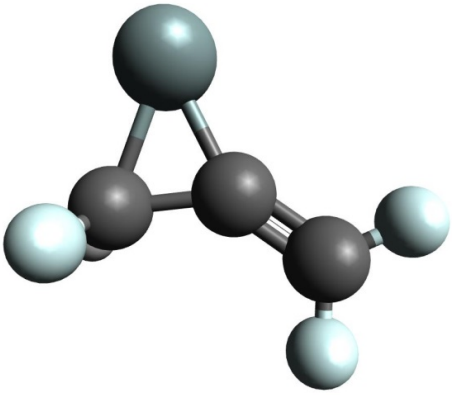
[i2e]				[i2f]			
							
-366.5 kJ mol^{-1}				-366.5 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-1.217161	2.092109	-0.478041	Si	-1.217161	2.092109	-0.478041
C	0.718085	2.105551	-0.106733	C	0.718085	2.105551	-0.106733
C	-0.896350	0.503330	0.378512	C	-0.896350	0.503330	0.378512
C	0.384938	0.659690	-0.076621	C	0.384938	0.659690	-0.076621
D	1.435881	2.452625	-0.849645	D	1.435881	2.452625	-0.849645
D	0.927003	2.520049	0.875808	D	0.927003	2.520049	0.875808
D	1.014639	-0.115450	-0.520096	H	1.014639	-0.115450	-0.520096
H	-1.393630	-0.440136	0.568491	D	-1.393630	-0.440136	0.568491
[i2g]				[i2h]			
							
-366.2 kJ mol^{-1}				-366.2 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-1.217161	2.092109	-0.478041	Si	-1.217161	2.092109	-0.478041
C	0.718085	2.105551	-0.106733	C	0.718085	2.105551	-0.106733
C	-0.896350	0.503330	0.378512	C	-0.896350	0.503330	0.378512
C	0.384938	0.659690	-0.076621	C	0.384938	0.659690	-0.076621
H	1.435881	2.452625	-0.849645	D	1.435881	2.452625	-0.849645
D	0.927003	2.520049	0.875808	H	0.927003	2.520049	0.875808
D	1.014639	-0.115450	-0.520096	D	1.014639	-0.115450	-0.520096
D	-1.393630	-0.440136	0.568491	D	-1.393630	-0.440136	0.568491

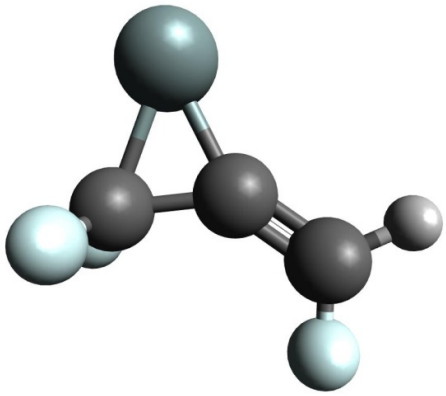
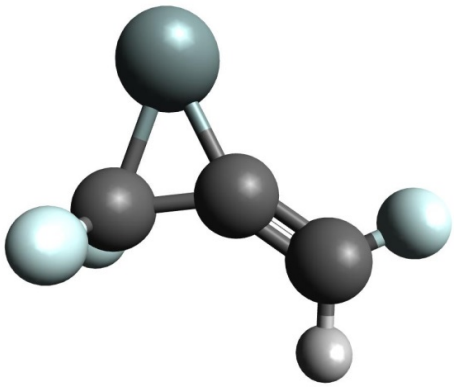
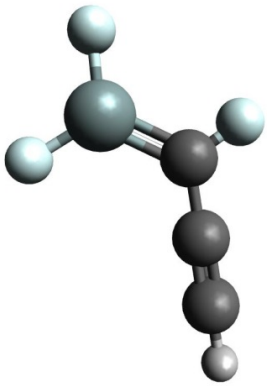
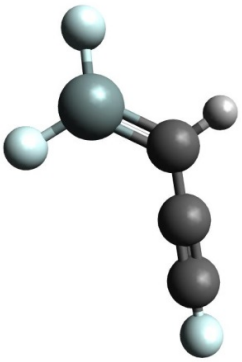
[i3a]				[i3b]			
							
-307.7 kJ mol^{-1}				-307.3 kJ mol^{-1}			
$C_1 - {}^1A$				$C_s - {}^1A'$			
Si	-2.584650	2.826243	0.102164	Si	-2.584650	2.826243	0.102164
C	-1.277255	1.533566	0.133824	C	-1.277255	1.533566	0.133824
C	-2.614644	1.183903	0.928846	C	-2.614644	1.183903	0.928846
C	-1.976747	0.221766	-0.020795	C	-1.976747	0.221766	-0.020795
D	-1.488341	-0.647336	0.417639	H	-1.488341	-0.647336	0.417639
H	-2.696767	0.944785	1.983522	D	-2.696767	0.944785	1.983522
D	-2.476241	-0.001272	-0.958483	D	-2.476241	-0.001272	-0.958483
D	-0.273455	1.579469	0.542808	D	-0.273455	1.579469	0.542808
[i3c]				[i3d]			
							
-307.2 kJ mol^{-1}				-307.7 kJ mol^{-1}			
$C_s - {}^1A'$				$C_1 - {}^1A$			
Si	-2.584650	2.826243	0.102164	Si	-2.584650	2.826243	0.102164
C	-1.277255	1.533566	0.133824	C	-1.277255	1.533566	0.133824
C	-2.614644	1.183903	0.928846	C	-2.614644	1.183903	0.928846
C	-1.976747	0.221766	-0.020795	C	-1.976747	0.221766	-0.020795
D	-1.488341	-0.647336	0.417639	D	-1.488341	-0.647336	0.417639
D	-2.696767	0.944785	1.983522	D	-2.696767	0.944785	1.983522
H	-2.476241	-0.001272	-0.958483	D	-2.476241	-0.001272	-0.958483
D	-0.273455	1.579469	0.542808	H	-0.273455	1.579469	0.542808

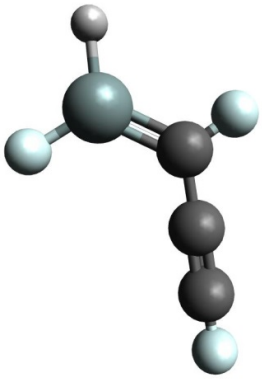
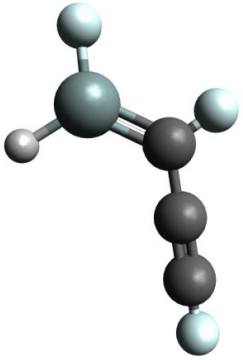
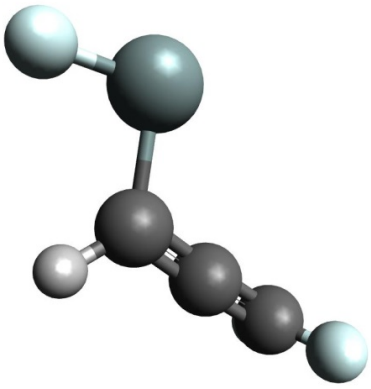
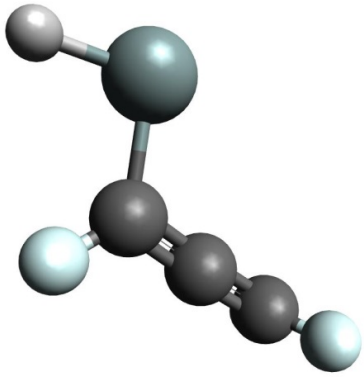
[i4a]				[i4b]			
							
-306.4 kJ mol^{-1}				-302.8 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	2.269227	0.314672	0.012013	Si	2.269227	0.314672	0.012013
C	0.446698	0.519161	0.002884	C	0.446698	0.519161	0.002884
C	-0.767059	0.515702	-0.005318	C	-0.767059	0.515702	-0.005318
C	-2.225868	0.529673	-0.008062	C	-2.225868	0.529673	-0.008062
H	2.557659	1.810564	-0.006117	D	2.557659	1.810564	-0.006117
D	-2.625510	-0.364956	-0.490733	D	-2.625510	-0.364956	-0.490733
D	-2.607844	1.412410	-0.525637	D	-2.607844	1.412410	-0.525637
D	-2.593502	0.553573	1.020967	H	-2.593502	0.553573	1.020967
[i5a]				[i5b]			
							
-305.2 kJ mol^{-1}				-304.1 kJ mol^{-1}			
$C_s - {}^1A'$				$C_s - {}^1A'$			
Si	-2.791074	1.331229	0.575045	Si	-2.791074	1.331229	0.575045
C	0.041883	1.957213	0.098223	C	0.041883	1.957213	0.098223
C	1.276133	1.530665	-0.176961	C	1.276133	1.530665	-0.176961
C	-1.134334	1.101465	0.199981	C	-1.134334	1.101465	0.199981
D	-0.109806	3.022058	0.263830	H	-0.109806	3.022058	0.263830
D	2.111404	2.219175	-0.232581	D	2.111404	2.219175	-0.232581
D	1.481749	0.478866	-0.350967	D	1.481749	0.478866	-0.350967
H	-0.944290	0.035021	0.000428	D	-0.944290	0.035021	0.000428

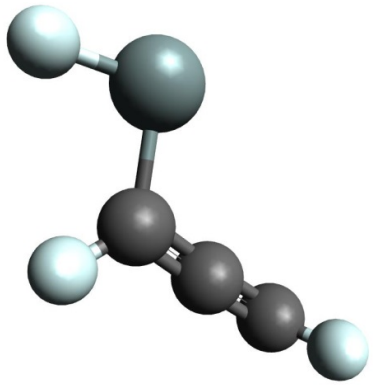
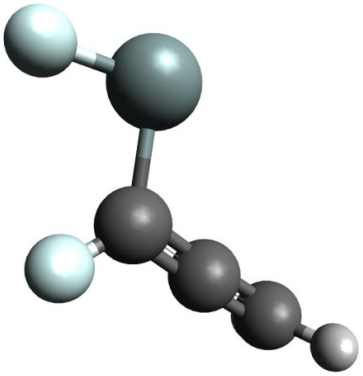
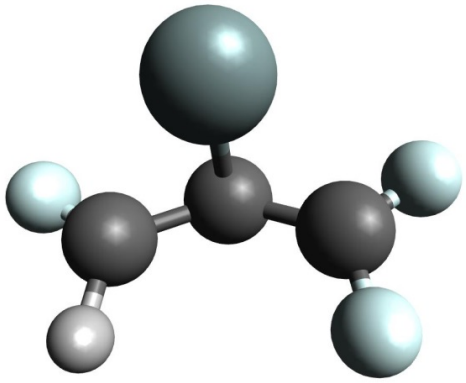
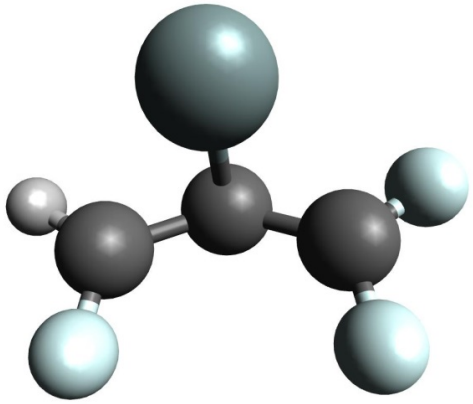
[i5c]				[i5d]			
							
-304.3 kJ mol^{-1}				-304.4 kJ mol^{-1}			
$C_s - {}^1A'$				$C_s - {}^1A'$			
Si	-2.791074	1.331229	0.575045	Si	-2.791074	1.331229	0.575045
C	0.041883	1.957213	0.098223	C	0.041883	1.957213	0.098223
C	1.276133	1.530665	-0.176961	C	1.276133	1.530665	-0.176961
C	-1.134334	1.101465	0.199981	C	-1.134334	1.101465	0.199981
D	-0.109806	3.022058	0.263830	D	-0.109806	3.022058	0.263830
H	2.111404	2.219175	-0.232581	D	2.111404	2.219175	-0.232581
D	1.481749	0.478866	-0.350967	H	1.481749	0.478866	-0.350967
D	-0.944290	0.035021	0.000428	D	-0.944290	0.035021	0.000428
[i6a]				[i6b]			
							
-299.6 kJ mol^{-1}				-301.5 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	1.271276	2.401422	0.597200	Si	1.271276	2.401422	0.597200
C	-0.676445	2.076496	-0.045615	C	-0.676445	2.076496	-0.045615
C	1.201685	0.439514	-0.022520	C	1.201685	0.439514	-0.022520
C	0.071228	0.921046	-0.285832	C	0.071228	0.921046	-0.285832
D	1.712703	2.984364	-0.742591	H	1.712703	2.984364	-0.742591
D	-0.965219	2.689118	-0.894417	D	-0.965219	2.689118	-0.894417
D	-1.396336	2.031078	0.765002	D	-1.396336	2.031078	0.765002
H	1.843949	-0.418828	-0.047808	D	1.843949	-0.418828	-0.047808

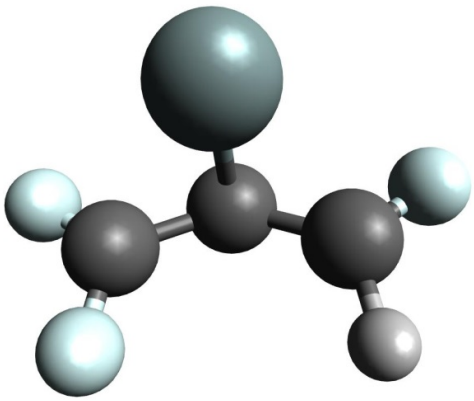
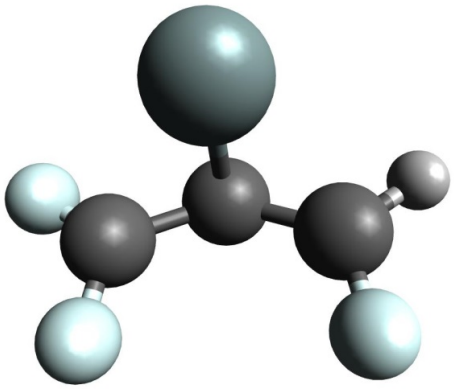
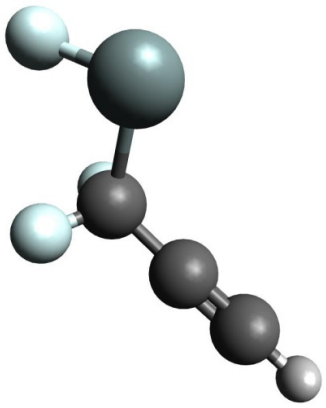
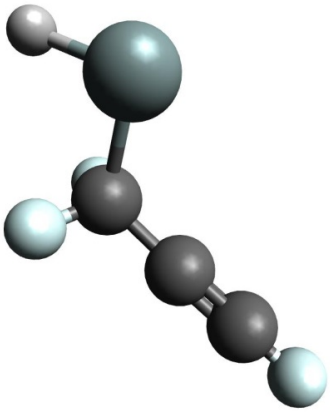
[i6c]				[i6d]			
							
-298.9 kJ mol^{-1}				-299.0 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	1.271276	2.401422	0.597200	Si	1.271276	2.401422	0.597200
C	-0.676445	2.076496	-0.045615	C	-0.676445	2.076496	-0.045615
C	1.201685	0.439514	-0.022520	C	1.201685	0.439514	-0.022520
C	0.071228	0.921046	-0.285832	C	0.071228	0.921046	-0.285832
D	1.712703	2.984364	-0.742591	D	1.712703	2.984364	-0.742591
D	-0.965219	2.689118	-0.894417	H	-0.965219	2.689118	-0.894417
H	-1.396336	2.031078	0.765002	D	-1.396336	2.031078	0.765002
D	1.843949	-0.418828	-0.047808	D	1.843949	-0.418828	-0.047808
[i6e]				[i6f]			
							
-299.6 kJ mol^{-1}				-301.5 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-1.271276	2.401422	0.597200	Si	-1.271276	2.401422	0.597200
C	0.676445	2.076496	-0.045615	C	0.676445	2.076496	-0.045615
C	-1.201685	0.439514	-0.022520	C	-1.201685	0.439514	-0.022520
C	-0.071228	0.921046	-0.285832	C	-0.071228	0.921046	-0.285832
D	-1.712703	2.984364	-0.742591	H	-1.712703	2.984364	-0.742591
D	0.965219	2.689118	-0.894417	D	0.965219	2.689118	-0.894417
D	1.396336	2.031078	0.765002	D	1.396336	2.031078	0.765002
H	-1.843949	-0.418828	-0.047808	D	-1.843949	-0.418828	-0.047808

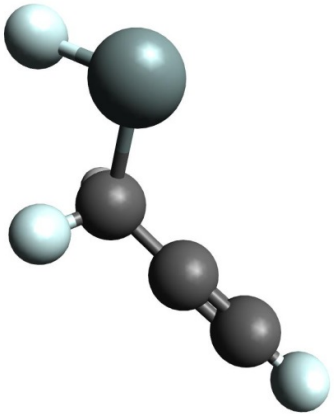
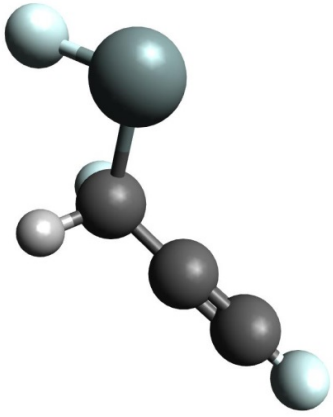
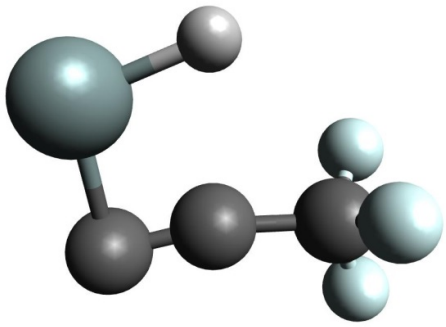
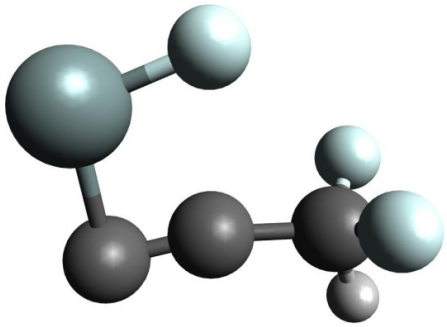
[i6g]				[i6h]			
							
-298.9 kJ mol^{-1}				-299.0 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-1.271276	2.401422	0.597200	Si	-1.271276	2.401422	0.597200
C	0.676445	2.076496	-0.045615	C	0.676445	2.076496	-0.045615
C	-1.201685	0.439514	-0.022520	C	-1.201685	0.439514	-0.022520
C	-0.071228	0.921046	-0.285832	C	-0.071228	0.921046	-0.285832
D	-1.712703	2.984364	-0.742591	D	-1.712703	2.984364	-0.742591
D	0.965219	2.689118	-0.894417	H	0.965219	2.689118	-0.894417
H	1.396336	2.031078	0.765002	D	1.396336	2.031078	0.765002
D	-1.843949	-0.418828	-0.047808	D	-1.843949	-0.418828	-0.047808
[i7a]				[i7b]			
							
-291.2 kJ mol^{-1}				-291.2 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-0.002314	3.177910	-0.169760	Si	-0.002314	3.177910	-0.169760
C	-0.649663	1.369072	-0.142375	C	-0.649663	1.369072	-0.142375
C	0.826543	1.531957	-0.066304	C	0.826543	1.531957	-0.066304
C	1.909821	0.771693	0.020207	C	1.909821	0.771693	0.020207
D	-1.073424	0.953192	-1.057167	H	-1.073424	0.953192	-1.057167
H	-1.173338	1.016264	0.746817	D	-1.173338	1.016264	0.746817
D	1.853963	-0.315790	0.055069	D	1.853963	-0.315790	0.055069
D	2.902621	1.211905	0.059823	D	2.902621	1.211905	0.059823

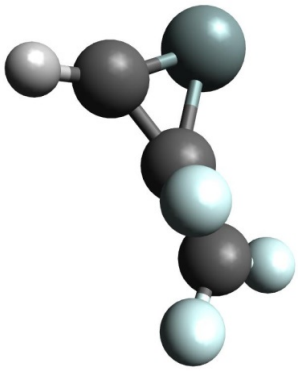
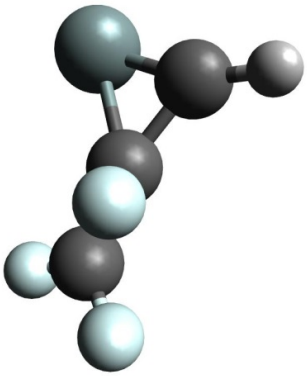
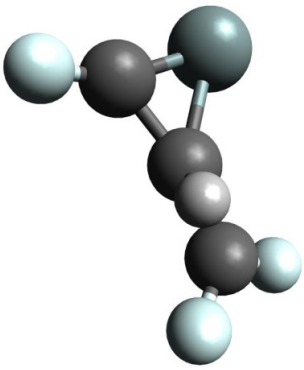
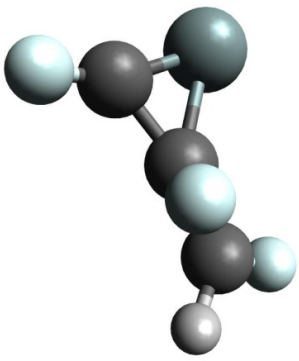
[i7c]				[i7d]			
							
-290.9 kJ mol^{-1}				-291.1 kJ mol^{-1}			
$C_s - {}^1A'$				$C_s - {}^1A'$			
Si	-0.002314	3.177910	-0.169760	Si	-0.002314	3.177910	-0.169760
C	-0.649663	1.369072	-0.142375	C	-0.649663	1.369072	-0.142375
C	0.826543	1.531957	-0.066304	C	0.826543	1.531957	-0.066304
C	1.909821	0.771693	0.020207	C	1.909821	0.771693	0.020207
D	-1.073424	0.953192	-1.057167	D	-1.073424	0.953192	-1.057167
D	-1.173338	1.016264	0.746817	D	-1.173338	1.016264	0.746817
D	1.853963	-0.315790	0.055069	H	1.853963	-0.315790	0.055069
H	2.902621	1.211905	0.059823	D	2.902621	1.211905	0.059823
[i8a]				[i8b]			
							
-275.2 kJ mol^{-1}				-274.7 kJ mol^{-1}			
$C_s - {}^1A'$				$C_s - {}^1A'$			
Si	-2.123430	2.732956	0.435983	Si	-2.123430	2.732956	0.435983
C	-0.578881	1.995631	0.420032	C	-0.578881	1.995631	0.420032
C	-0.360326	0.594266	0.333811	C	-0.360326	0.594266	0.333811
C	-0.179590	-0.593207	0.258429	C	-0.179590	-0.593207	0.258429
D	-2.265622	4.199834	0.528920	D	-2.265622	4.199834	0.528920
D	-3.379454	1.961598	0.360797	D	-3.379454	1.961598	0.360797
D	0.306230	2.623143	0.479257	H	0.306230	2.623143	0.479257
H	-0.015456	-1.642789	0.191810	D	-0.015456	-1.642789	0.191810

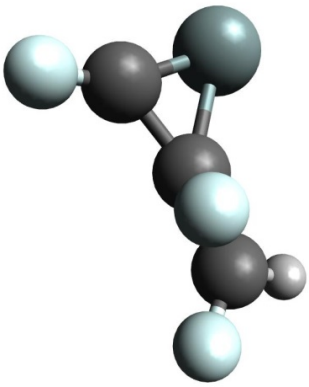
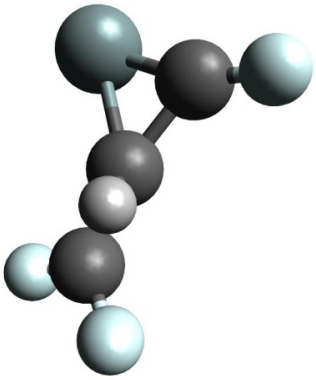
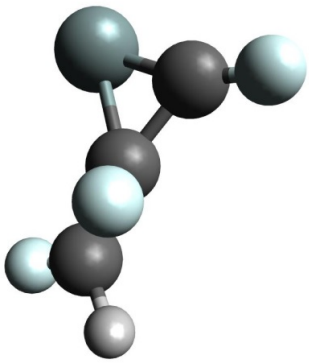
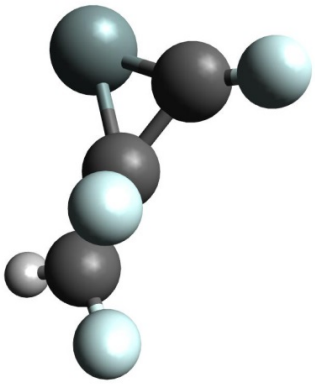
[i8c]				[i8d]			
							
-276.8 kJ mol^{-1}				-276.9 kJ mol^{-1}			
$C_s - {}^1A'$				$C_s - {}^1A'$			
Si	-2.123430	2.732956	0.435983	Si	-2.123430	2.732956	0.435983
C	-0.578881	1.995631	0.420032	C	-0.578881	1.995631	0.420032
C	-0.360326	0.594266	0.333811	C	-0.360326	0.594266	0.333811
C	-0.179590	-0.593207	0.258429	C	-0.179590	-0.593207	0.258429
H	-2.265622	4.199834	0.528920	D	-2.265622	4.199834	0.528920
D	-3.379454	1.961598	0.360797	H	-3.379454	1.961598	0.360797
D	0.306230	2.623143	0.479257	D	0.306230	2.623143	0.479257
D	-0.015456	-1.642789	0.191810	D	-0.015456	-1.642789	0.191810
[i9a]				[i9b]			
							
-275.3 kJ mol^{-1}				-278.3 kJ mol^{-1}			
$C_s - {}^1A'$				$C_s - {}^1A'$			
Si	-0.948677	2.863727	0.654535	Si	-0.948677	2.863727	0.654535
C	-1.217505	1.006333	0.704275	C	-1.217505	1.006333	0.704275
C	-0.284681	0.271592	0.142353	C	-0.284681	0.271592	0.142353
C	0.670871	-0.400535	-0.428995	C	0.670871	-0.400535	-0.428995
D	-2.235815	3.206243	1.405402	H	-2.235815	3.206243	1.405402
H	-2.068992	0.501898	1.155645	D	-2.068992	0.501898	1.155645
D	1.531568	-0.731501	0.140907	D	1.531568	-0.731501	0.140907
D	0.619686	-0.645957	-1.483673	D	0.619686	-0.645957	-1.483673

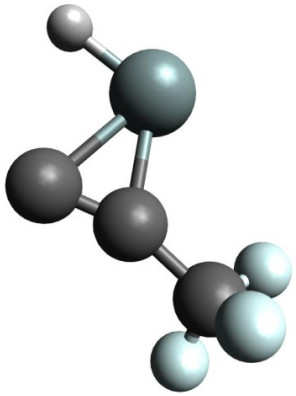
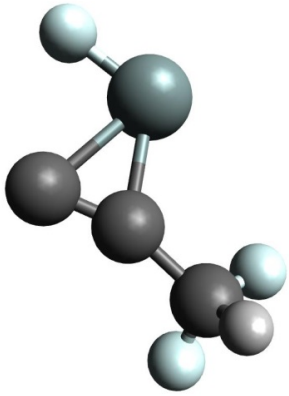
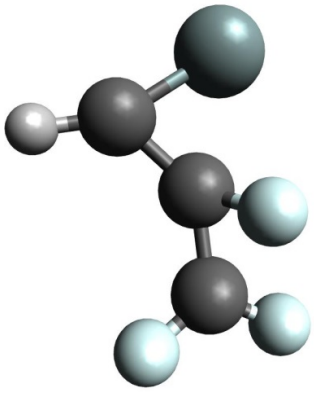
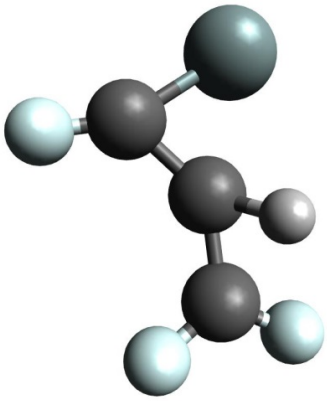
[i9c]				[i9d]			
							
-275.4 kJ mol^{-1}				-275.4 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-0.948677	2.863727	0.654535	Si	-0.948677	2.863727	0.654535
C	-1.217505	1.006333	0.704275	C	-1.217505	1.006333	0.704275
C	-0.284681	0.271592	0.142353	C	-0.284681	0.271592	0.142353
C	0.670871	-0.400535	-0.428995	C	0.670871	-0.400535	-0.428995
D	-2.235815	3.206243	1.405402	D	-2.235815	3.206243	1.405402
D	-2.068992	0.501898	1.155645	D	-2.068992	0.501898	1.155645
D	1.531568	-0.731501	0.140907	H	1.531568	-0.731501	0.140907
H	0.619686	-0.645957	-1.483673	D	0.619686	-0.645957	-1.483673
[i10a]				[i10b]			
							
-277.4 kJ mol^{-1}				-277.1 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-0.333163	1.486867	-0.671031	Si	-0.333163	1.486867	-0.671031
C	-0.144820	0.334917	0.683483	C	-0.144820	0.334917	0.683483
C	-1.419478	-0.081122	0.274337	C	-1.419478	-0.081122	0.274337
C	1.062694	0.035706	0.040856	C	1.062694	0.035706	0.040856
H	-1.610019	-1.027212	-0.240233	D	-1.610019	-1.027212	-0.240233
D	-2.282879	0.366410	0.756404	H	-2.282879	0.366410	0.756404
D	1.241688	-0.893852	-0.506956	D	1.241688	-0.893852	-0.506956
D	1.954699	0.571689	0.349342	D	1.954699	0.571689	0.349342

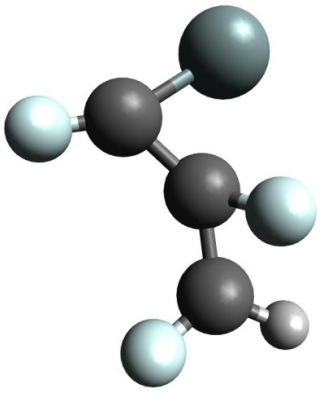
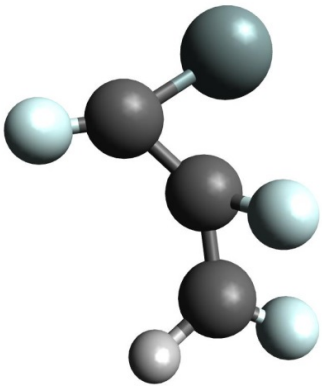
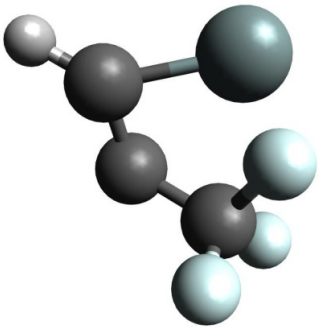
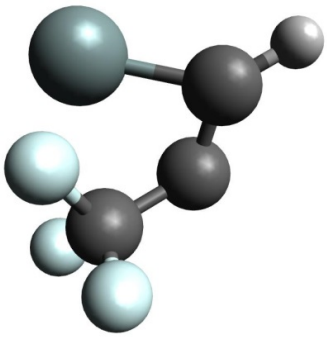
[i10c]				[i10d]			
							
-277.4 kJ mol^{-1}				-277.1 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-0.333163	1.486867	-0.671031	Si	-0.333163	1.486867	-0.671031
C	-0.144820	0.334917	0.683483	C	-0.144820	0.334917	0.683483
C	-1.419478	-0.081122	0.274337	C	-1.419478	-0.081122	0.274337
C	1.062694	0.035706	0.040856	C	1.062694	0.035706	0.040856
D	-1.610019	-1.027212	-0.240233	D	-1.610019	-1.027212	-0.240233
D	-2.282879	0.366410	0.756404	D	-2.282879	0.366410	0.756404
H	1.241688	-0.893852	-0.506956	D	1.241688	-0.893852	-0.506956
D	1.954699	0.571689	0.349342	H	1.954699	0.571689	0.349342
[i12a]				[i12b]			
							
-244.3 kJ mol^{-1}				-246.7 kJ mol^{-1}			
$C_s - {}^1A'$				$C_s - {}^1A'$			
Si	-0.980308	2.921623	1.046459	Si	-0.980308	2.921623	1.046459
C	-1.407690	1.314359	0.084885	C	-1.407690	1.314359	0.084885
C	-0.359350	0.302722	0.082071	C	-0.359350	0.302722	0.082071
C	0.531367	-0.500595	0.106582	C	0.531367	-0.500595	0.106582
D	-2.336725	3.551344	0.727266	H	-2.336725	3.551344	0.727266
D	-1.671387	1.607227	-0.940700	D	-1.671387	1.607227	-0.940700
D	-2.336671	0.913777	0.513390	D	-2.336671	0.913777	0.513390
H	1.315662	-1.220461	0.122189	D	1.315662	-1.220461	0.122189

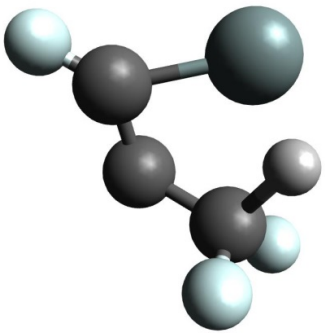
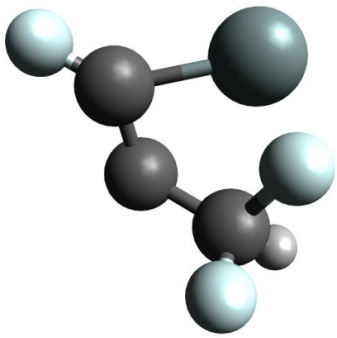
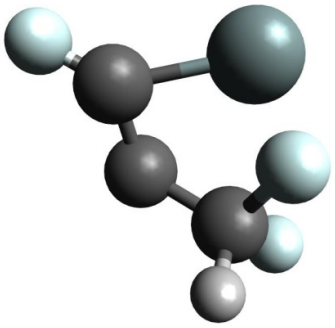
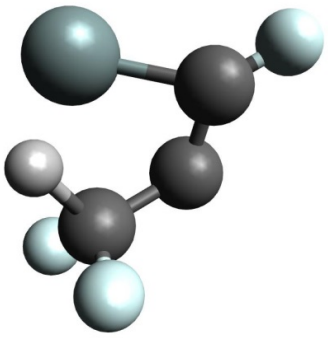
[i12c]				[i12d]			
							
-243.7 kJ mol^{-1}				-243.7 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-0.980308	2.921623	1.046459	Si	-0.980308	2.921623	1.046459
C	-1.407690	1.314359	0.084885	C	-1.407690	1.314359	0.084885
C	-0.359350	0.302722	0.082071	C	-0.359350	0.302722	0.082071
C	0.531367	-0.500595	0.106582	C	0.531367	-0.500595	0.106582
D	-2.336725	3.551344	0.727266	D	-2.336725	3.551344	0.727266
H	-1.671387	1.607227	-0.940700	D	-1.671387	1.607227	-0.940700
D	-2.336671	0.913777	0.513390	H	-2.336671	0.913777	0.513390
D	1.315662	-1.220461	0.122189	D	1.315662	-1.220461	0.122189
[i13a]				[i13b]			
							
-224.2 kJ mol^{-1}				-220.8 kJ mol^{-1}			
$C_s - {}^1A'$				$C_s - {}^1A'$			
Si	-1.688737	2.624682	0.616789	Si	-1.688737	2.624682	0.616789
C	-0.244907	1.218317	-0.220340	C	-0.244907	1.218317	-0.220340
C	1.218639	1.272651	-0.343790	C	1.218639	1.272651	-0.343790
C	-1.465384	0.927557	-0.237325	C	-1.465384	0.927557	-0.237325
H	-0.260660	3.204713	0.754427	D	-0.260660	3.204713	0.754427
D	1.524821	2.129620	-0.945098	D	1.524821	2.129620	-0.945098
D	1.687125	1.351436	0.638071	D	1.687125	1.351436	0.638071
D	1.564998	0.357273	-0.829223	H	1.564998	0.357273	-0.829223

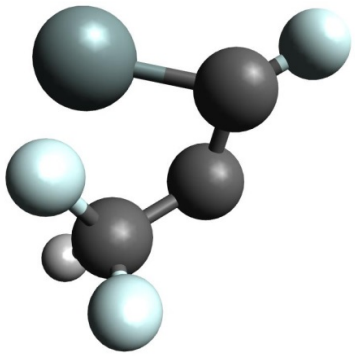
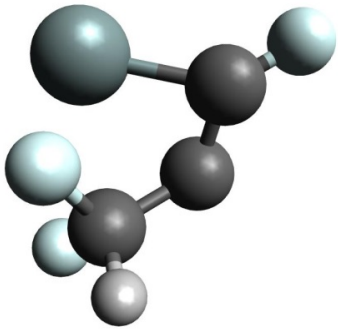
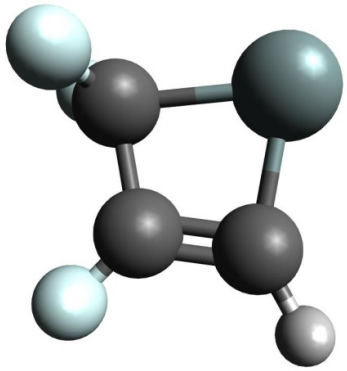
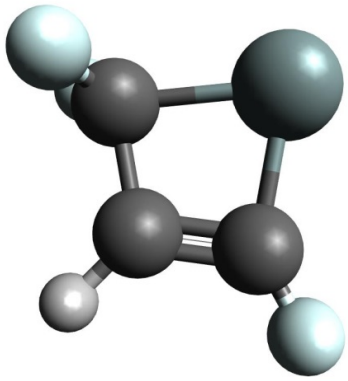
Transition States							
[i1a]→[i2a]				[i1a]→[i2e]			
							
-75.0 kJ mol^{-1}				-75.0 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	0.387656	1.918057	-0.868165	Si	-0.387656	1.918057	-0.868165
C	0.507204	-1.109474	-0.273582	C	-0.507204	-1.109474	-0.273582
C	-0.001009	0.171130	-0.093798	C	0.001009	0.171130	-0.093798
C	-0.892669	1.297958	0.108223	C	0.892669	1.297958	0.108223
D	1.347937	-1.296852	-0.939211	D	-1.347937	-1.296852	-0.939211
D	0.177136	-0.265142	0.972772	D	-0.177136	-0.265142	0.972772
D	0.170559	-1.954642	0.325094	D	-0.170559	-1.954642	0.325094
H	-1.765240	1.299326	0.746709	H	1.765240	1.299326	0.746709
[i1b]→[i2b]				[i1b]→[i2c]			
							
-76.5 kJ mol^{-1}				-74.7 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	0.387656	1.918057	-0.868165	Si	0.387656	1.918057	-0.868165
C	0.507204	-1.109474	-0.273582	C	0.507204	-1.109474	-0.273582
C	-0.001009	0.171130	-0.093798	C	-0.001009	0.171130	-0.093798
C	-0.892669	1.297958	0.108223	C	-0.892669	1.297958	0.108223
D	1.347937	-1.296852	-0.939211	D	1.347937	-1.296852	-0.939211
H	0.177136	-0.265142	0.972772	D	0.177136	-0.265142	0.972772
D	0.170559	-1.954642	0.325094	H	0.170559	-1.954642	0.325094
D	-1.765240	1.299326	0.746709	D	-1.765240	1.299326	0.746709

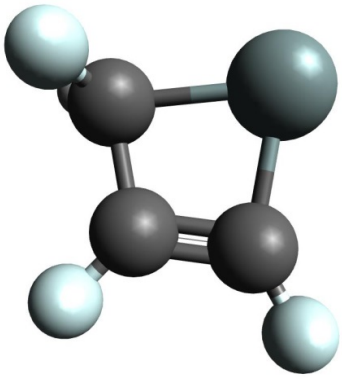
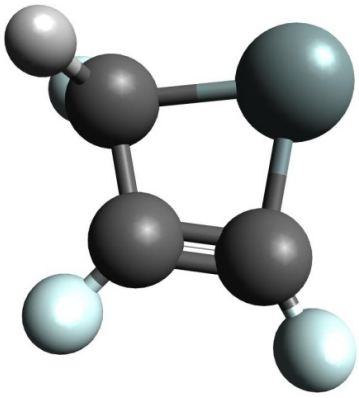
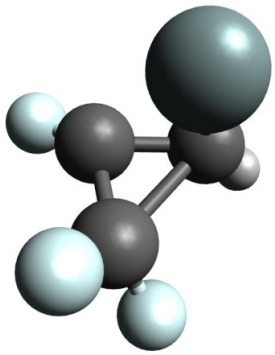
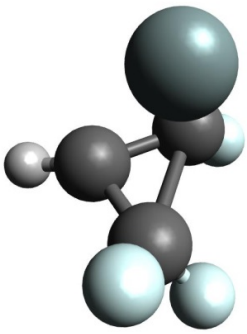
[i1b]→[i2d]				[i1b]→[i2f]			
							
-74.5 kJ mol^{-1}				-76.5 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	0.387656	1.918057	-0.868165	Si	-0.387656	1.918057	-0.868165
C	0.507204	-1.109474	-0.273582	C	-0.507204	-1.109474	-0.273582
C	-0.001009	0.171130	-0.093798	C	0.001009	0.171130	-0.093798
C	-0.892669	1.297958	0.108223	C	0.892669	1.297958	0.108223
H	1.347937	-1.296852	-0.939211	D	-1.347937	-1.296852	-0.939211
D	0.177136	-0.265142	0.972772	H	-0.177136	-0.265142	0.972772
D	0.170559	-1.954642	0.325094	D	-0.170559	-1.954642	0.325094
D	-1.765240	1.299326	0.746709	D	1.765240	1.299326	0.746709
[i1b]→[i2g]				[i1b]→[i2h]			
							
-74.7 kJ mol^{-1}				-74.5 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-0.387656	1.918057	-0.868165	Si	-0.387656	1.918057	-0.868165
C	-0.507204	-1.109474	-0.273582	C	-0.507204	-1.109474	-0.273582
C	0.001009	0.171130	-0.093798	C	0.001009	0.171130	-0.093798
C	0.892669	1.297958	0.108223	C	0.892669	1.297958	0.108223
D	-1.347937	-1.296852	-0.939211	H	-1.347937	-1.296852	-0.939211
D	-0.177136	-0.265142	0.972772	D	-0.177136	-0.265142	0.972772
H	-0.170559	-1.954642	0.325094	D	-0.170559	-1.954642	0.325094
D	1.765240	1.299326	0.746709	D	1.765240	1.299326	0.746709

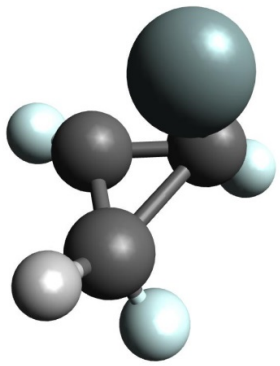
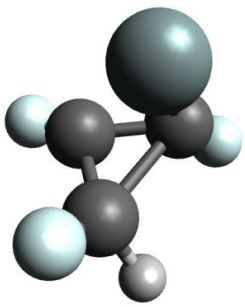
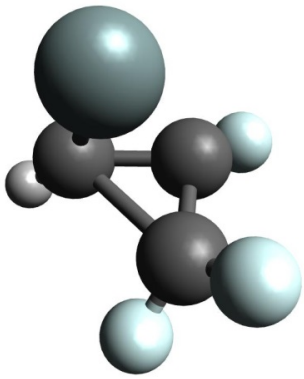
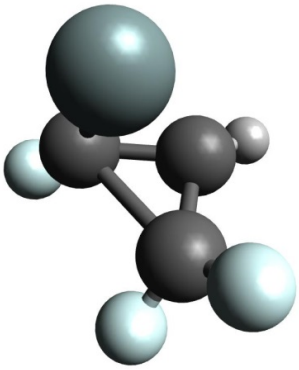
[i1a]→[i4a]				[i1b]→[i4b]			
							
-194.4 kJ mol^{-1}				-190.8 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-2.122577	1.493357	-0.465731	Si	-2.122577	1.493357	-0.465731
C	-3.577778	0.142016	0.174868	C	-3.577778	0.142016	0.174868
C	-2.426216	-0.379803	0.065365	C	-2.426216	-0.379803	0.065365
C	-1.341337	-1.393100	0.060616	C	-1.341337	-1.393100	0.060616
D	-1.737882	-2.337896	-0.315266	D	-1.737882	-2.337896	-0.315266
D	-0.507637	-1.078652	-0.566987	D	-0.507637	-1.078652	-0.566987
D	-0.973850	-1.547956	1.076886	H	-0.973850	-1.547956	1.076886
H	-3.309526	2.412152	-0.373543	D	-3.309526	2.412152	-0.373543
[i1a]→[i5a]				[i1b]→[i5b]			
							
-140.2 kJ mol^{-1}				-141.9 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	0.485782	2.153579	-0.469008	Si	0.485782	2.153579	-0.469008
C	0.332198	-1.132452	-0.095064	C	0.332198	-1.132452	-0.095064
C	0.161878	0.240941	-0.155304	C	0.161878	0.240941	-0.155304
C	-0.869881	1.190140	0.041691	C	-0.869881	1.190140	0.041691
D	1.058802	-0.010869	0.587659	H	1.058802	-0.010869	0.587659
D	-0.474833	-1.810179	0.181935	D	-0.474833	-1.810179	0.181935
D	1.295799	-1.572078	-0.331053	D	1.295799	-1.572078	-0.331053
H	-1.919433	1.016042	0.235748	D	-1.919433	1.016042	0.235748

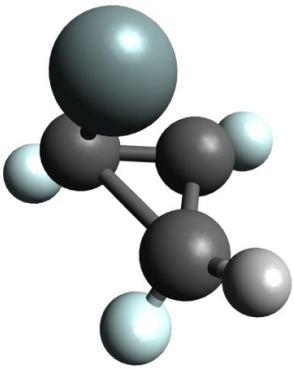
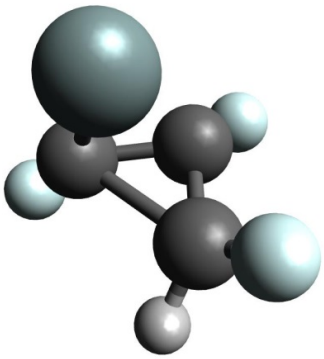
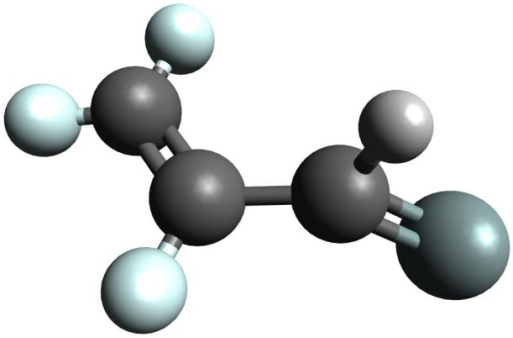
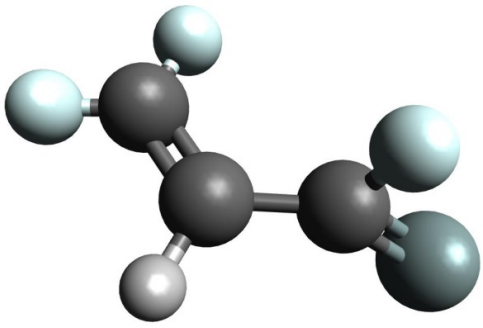
[i1b]→[i5c]				[i1b]→[i5d]			
							
-139.5 kJ mol^{-1}				-139.8 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	0.485782	2.153579	-0.469008	Si	0.485782	2.153579	-0.469008
C	0.332198	-1.132452	-0.095064	C	0.332198	-1.132452	-0.095064
C	0.161878	0.240941	-0.155304	C	0.161878	0.240941	-0.155304
C	-0.869881	1.190140	0.041691	C	-0.869881	1.190140	0.041691
D	1.058802	-0.010869	0.587659	D	1.058802	-0.010869	0.587659
D	-0.474833	-1.810179	0.181935	H	-0.474833	-1.810179	0.181935
H	1.295799	-1.572078	-0.331053	D	1.295799	-1.572078	-0.331053
D	-1.919433	1.016042	0.235748	D	-1.919433	1.016042	0.235748
[i1a]→[i6a]				[i1a]→[i6e]			
							
-122.9 kJ mol^{-1}				-122.9 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	0.778035	1.356341	0.013393	Si	-0.778035	1.356341	0.013393
C	-1.041349	0.972089	0.089159	C	1.041349	0.972089	0.089159
C	-0.726348	-0.144886	-0.571048	C	0.726348	-0.144886	-0.571048
C	0.465469	-0.839573	-0.180070	C	-0.465469	-0.839573	-0.180070
D	0.248932	-1.572742	0.597463	D	-0.248932	-1.572742	0.597463
D	1.180352	-1.204148	-0.916275	D	-1.180352	-1.204148	-0.916275
D	1.081984	-0.069503	0.844891	D	-1.081984	-0.069503	0.844891
H	-1.980789	1.508295	0.137363	H	1.980789	1.508295	0.137363

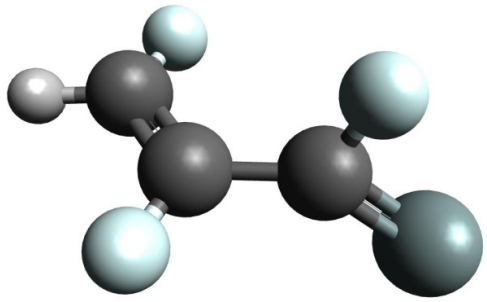
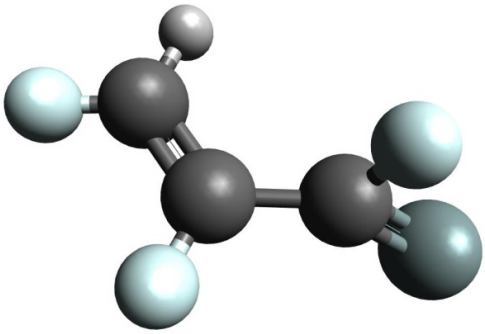
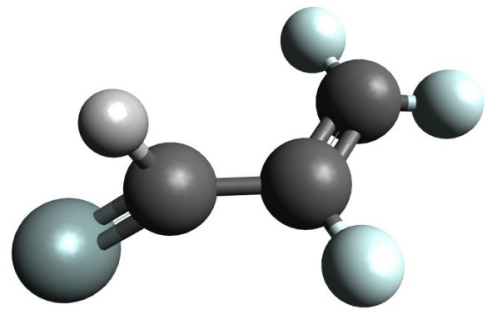
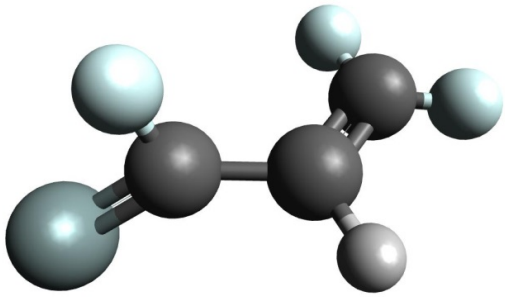
[i1b]→[i6b]				[i1b]→[i6c]			
							
-125.8 kJ mol^{-1}				-122.4 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	0.778035	1.356341	0.013393	Si	0.778035	1.356341	0.013393
C	-1.041349	0.972089	0.089159	C	-1.041349	0.972089	0.089159
C	-0.726348	-0.144886	-0.571048	C	-0.726348	-0.144886	-0.571048
C	0.465469	-0.839573	-0.180070	C	0.465469	-0.839573	-0.180070
D	0.248932	-1.572742	0.597463	D	0.248932	-1.572742	0.597463
D	1.180352	-1.204148	-0.916275	H	1.180352	-1.204148	-0.916275
H	1.081984	-0.069503	0.844891	D	1.081984	-0.069503	0.844891
D	-1.980789	1.508295	0.137363	D	-1.980789	1.508295	0.137363
[i1b]→[i6d]				[i1b]→[i6f]			
							
-122.4 kJ mol^{-1}				-125.8 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	0.778035	1.356341	0.013393	Si	-0.778035	1.356341	0.013393
C	-1.041349	0.972089	0.089159	C	1.041349	0.972089	0.089159
C	-0.726348	-0.144886	-0.571048	C	0.726348	-0.144886	-0.571048
C	0.465469	-0.839573	-0.180070	C	-0.465469	-0.839573	-0.180070
H	0.248932	-1.572742	0.597463	D	-0.248932	-1.572742	0.597463
D	1.180352	-1.204148	-0.916275	D	-1.180352	-1.204148	-0.916275
D	1.081984	-0.069503	0.844891	H	-1.081984	-0.069503	0.844891
D	-1.980789	1.508295	0.137363	D	1.980789	1.508295	0.137363

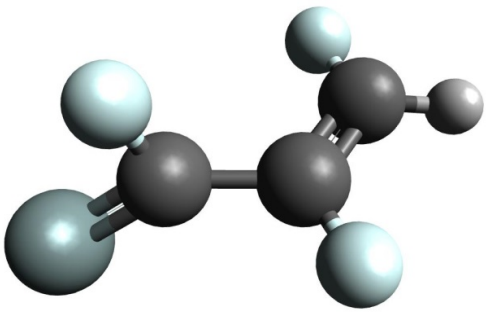
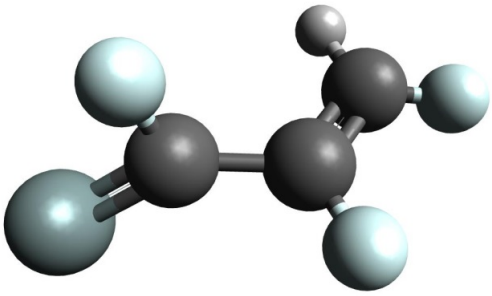
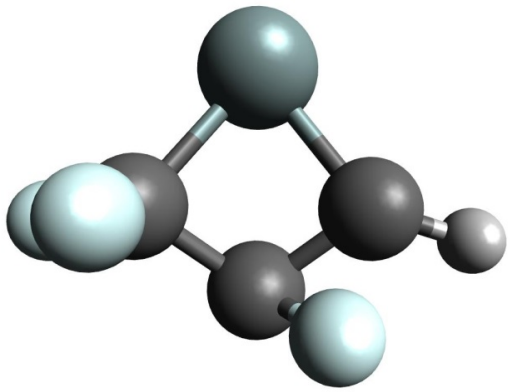
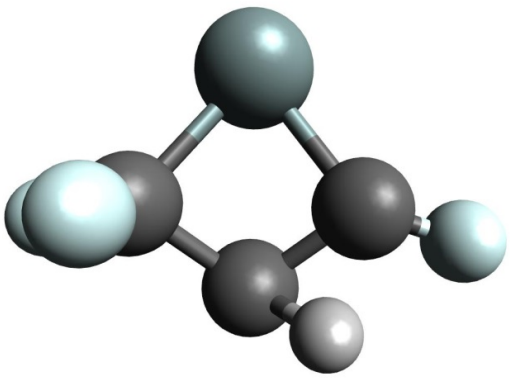
[i1b]→[i6g]				[i1b]→[i6h]			
							
-122.4 kJ mol^{-1}				-122.4 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-0.778035	1.356341	0.013393	Si	-0.778035	1.356341	0.013393
C	1.041349	0.972089	0.089159	C	1.041349	0.972089	0.089159
C	0.726348	-0.144886	-0.571048	C	0.726348	-0.144886	-0.571048
C	-0.465469	-0.839573	-0.180070	C	-0.465469	-0.839573	-0.180070
D	-0.248932	-1.572742	0.597463	H	-0.248932	-1.572742	0.597463
H	-1.180352	-1.204148	-0.916275	D	-1.180352	-1.204148	-0.916275
D	-1.081984	-0.069503	0.844891	D	-1.081984	-0.069503	0.844891
D	1.980789	1.508295	0.137363	D	1.980789	1.508295	0.137363
[i2a]→[i2e]				[i2b]→[i2f]			
							
-343.8 kJ mol^{-1}				-344.1 kJ mol^{-1}			
$C_s - {}^1A'$				$C_s - {}^1A'$			
Si	1.278722	2.298406	-0.055446	Si	1.278722	2.298406	-0.055446
C	-0.670175	2.114670	-0.122843	C	-0.670175	2.114670	-0.122843
C	0.931362	0.457675	0.076046	C	0.931362	0.457675	0.076046
C	-0.403313	0.629572	0.008121	C	-0.403313	0.629572	0.008121
D	-1.163674	2.406338	-1.054805	D	-1.163674	2.406338	-1.054805
D	-1.238437	2.548998	0.705255	D	-1.238437	2.548998	0.705255
D	-1.174293	-0.147915	0.038856	H	-1.174293	-0.147915	0.038856
H	1.448755	-0.490942	0.172710	D	1.448755	-0.490942	0.172710

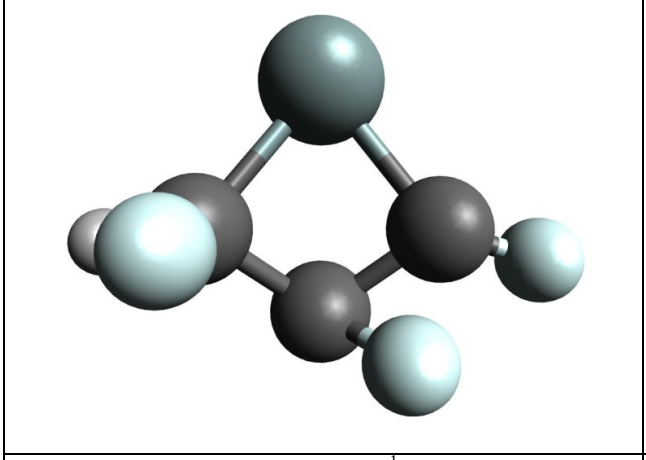
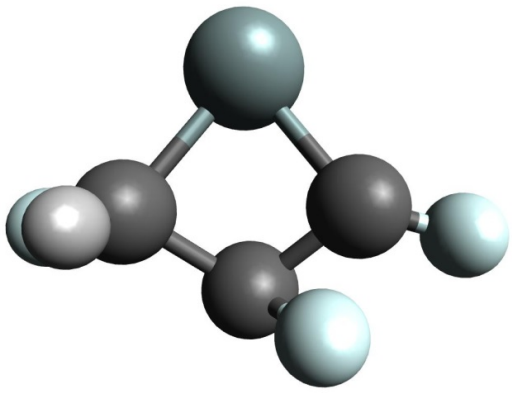
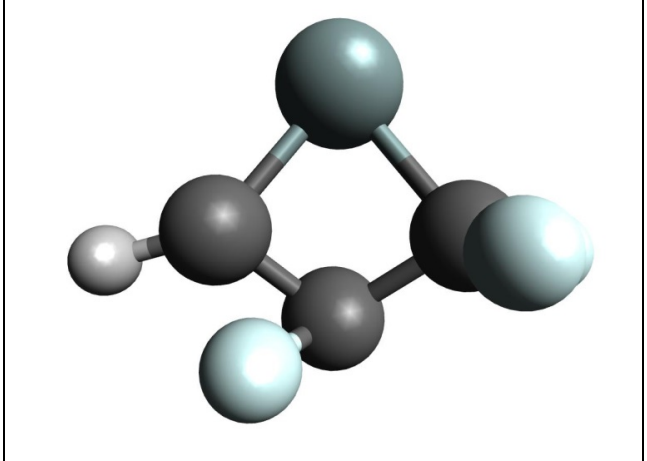
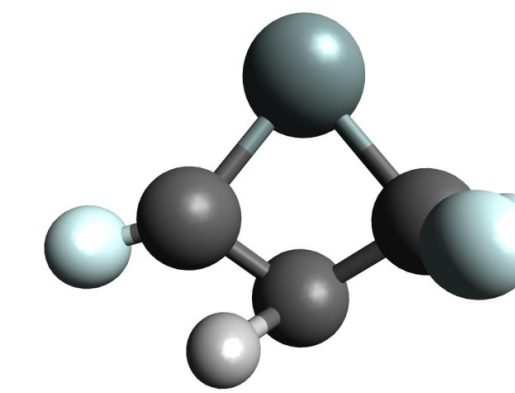
[i2c]→[i2h]				[i2d]→[i2g]			
							
-343.7 kJ mol^{-1}				-343.7 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	1.278722	2.298406	-0.055446	Si	1.278722	2.298406	-0.055446
C	-0.670175	2.114670	-0.122843	C	-0.670175	2.114670	-0.122843
C	0.931362	0.457675	0.076046	C	0.931362	0.457675	0.076046
C	-0.403313	0.629572	0.008121	C	-0.403313	0.629572	0.008121
H	-1.163674	2.406338	-1.054805	D	-1.163674	2.406338	-1.054805
D	-1.238437	2.548998	0.705255	H	-1.238437	2.548998	0.705255
D	-1.174293	-0.147915	0.038856	D	-1.174293	-0.147915	0.038856
D	1.448755	-0.490942	0.172710	D	1.448755	-0.490942	0.172710
[i2a]→[i3a]				[i2b]→[i3d]			
							
-187.7 kJ mol^{-1}				-187.3 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-2.150053	2.178667	0.625370	Si	-2.150053	2.178667	0.625370
C	-0.578457	1.585315	-0.456669	C	-0.578457	1.585315	-0.456669
C	-1.232877	0.355972	-0.039025	C	-1.232877	0.355972	-0.039025
C	-0.432102	1.821019	0.963102	C	-0.432102	1.821019	0.963102
H	0.445188	1.756078	1.604662	D	0.445188	1.756078	1.604662
D	0.020532	1.864829	-1.311772	H	0.020532	1.864829	-1.311772
D	-0.716789	-0.405155	0.544939	D	-0.716789	-0.405155	0.544939
D	-2.145988	-0.008539	-0.518207	D	-2.145988	-0.008539	-0.518207

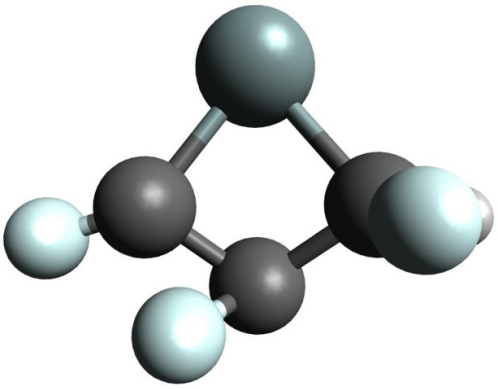
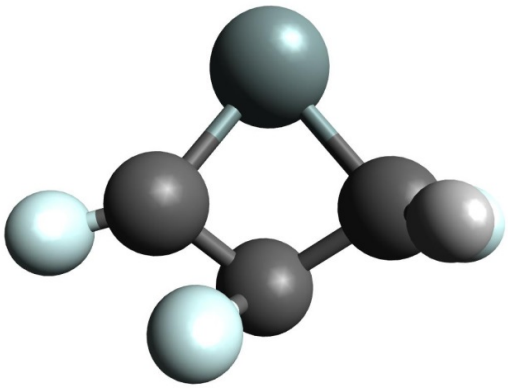
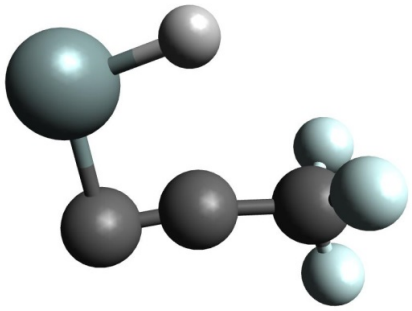
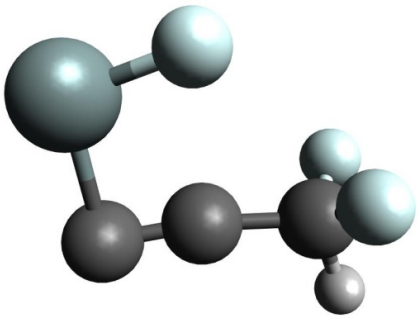
[i2c]→[i3c]				[i2d]→[i3b]			
							
-187.5 kJ mol^{-1}				-187.0 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-2.150053	2.178667	0.625370	Si	-2.150053	2.178667	0.625370
C	-0.578457	1.585315	-0.456669	C	-0.578457	1.585315	-0.456669
C	-1.232877	0.355972	-0.039025	C	-1.232877	0.355972	-0.039025
C	-0.432102	1.821019	0.963102	C	-0.432102	1.821019	0.963102
D	0.445188	1.756078	1.604662	D	0.445188	1.756078	1.604662
D	0.020532	1.864829	-1.311772	D	0.020532	1.864829	-1.311772
D	-0.716789	-0.405155	0.544939	H	-0.716789	-0.405155	0.544939
H	-2.145988	-0.008539	-0.518207	D	-2.145988	-0.008539	-0.518207
[i2e]→[i3d]				[i2f]→[i3a]			
							
-187.7 kJ mol^{-1}				-187.3 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	2.150053	2.178667	0.625370	Si	2.150053	2.178667	0.625370
C	0.578457	1.585315	-0.456669	C	0.578457	1.585315	-0.456669
C	1.232877	0.355972	-0.039025	C	1.232877	0.355972	-0.039025
C	0.432102	1.821019	0.963102	C	0.432102	1.821019	0.963102
H	-0.445188	1.756078	1.604662	D	-0.445188	1.756078	1.604662
D	-0.020532	1.864829	-1.311772	H	-0.020532	1.864829	-1.311772
D	0.716789	-0.405155	0.544939	D	0.716789	-0.405155	0.544939
D	2.145988	-0.008539	-0.518207	D	2.145988	-0.008539	-0.518207

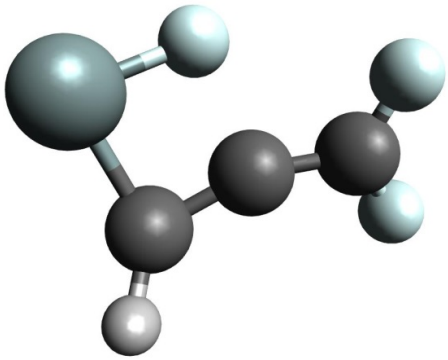
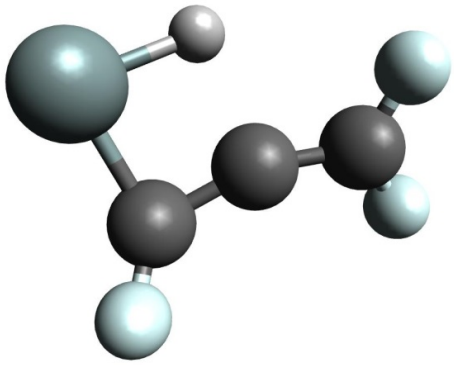
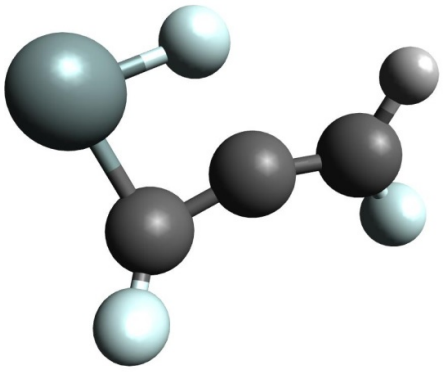
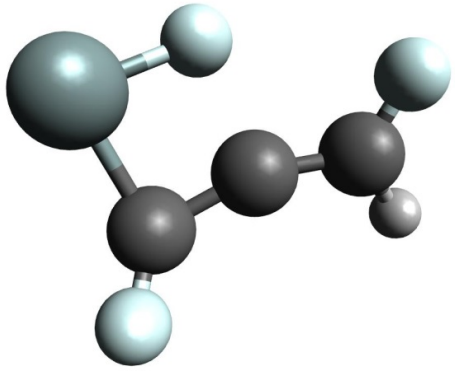
[i2g]→[i3c]				[i2h]→[i3b]			
							
-187.5 kJ mol^{-1}				-187.0 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	2.150053	2.178667	0.625370	Si	2.150053	2.178667	0.625370
C	0.578457	1.585315	-0.456669	C	0.578457	1.585315	-0.456669
C	1.232877	0.355972	-0.039025	C	1.232877	0.355972	-0.039025
C	0.432102	1.821019	0.963102	C	0.432102	1.821019	0.963102
D	-0.445188	1.756078	1.604662	D	-0.445188	1.756078	1.604662
D	-0.020532	1.864829	-1.311772	D	-0.020532	1.864829	-1.311772
D	0.716789	-0.405155	0.544939	H	0.716789	-0.405155	0.544939
H	2.145988	-0.008539	-0.518207	D	2.145988	-0.008539	-0.518207
[i2a]→[i5a]				[i2b]→[i5b]			
							
-294.0 kJ mol^{-1}				-292.4 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	0.342188	2.735051	-0.130811	Si	0.342188	2.735051	-0.130811
C	0.391241	-1.205372	-0.299825	C	0.391241	-1.205372	-0.299825
C	0.039692	-0.188254	0.478770	C	0.039692	-0.188254	0.478770
C	-0.308252	1.168082	-0.001663	C	-0.308252	1.168082	-0.001663
D	0.000480	-0.344895	1.555941	H	0.000480	-0.344895	1.555941
D	0.632717	-2.174234	0.123862	D	0.632717	-2.174234	0.123862
D	0.451087	-1.098752	-1.378354	D	0.451087	-1.098752	-1.378354
H	-1.322618	1.262237	-0.434147	D	-1.322618	1.262237	-0.434147

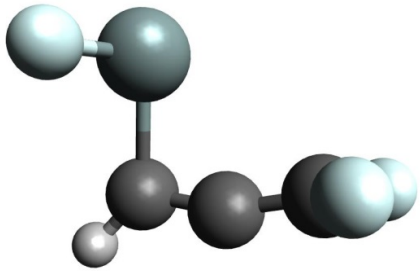
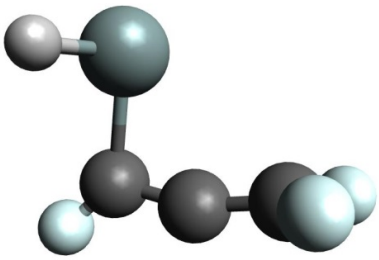
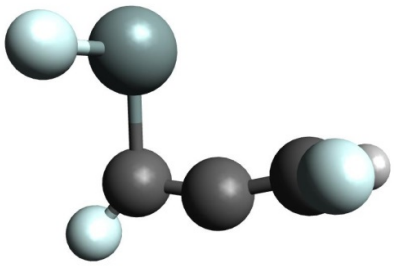
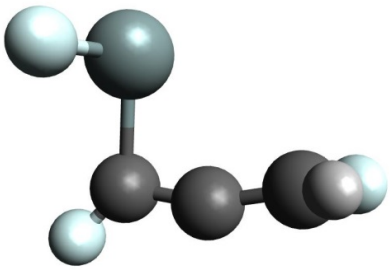
[i2c]→[i5c]				[i2d]→[i5d]			
							
-292.4 kJ mol^{-1}				-292.5 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	0.342188	2.735051	-0.130811	Si	0.342188	2.735051	-0.130811
C	0.391241	-1.205372	-0.299825	C	0.391241	-1.205372	-0.299825
C	0.039692	-0.188254	0.478770	C	0.039692	-0.188254	0.478770
C	-0.308252	1.168082	-0.001663	C	-0.308252	1.168082	-0.001663
D	0.000480	-0.344895	1.555941	D	0.000480	-0.344895	1.555941
H	0.632717	-2.174234	0.123862	D	0.632717	-2.174234	0.123862
D	0.451087	-1.098752	-1.378354	H	0.451087	-1.098752	-1.378354
D	-1.322618	1.262237	-0.434147	D	-1.322618	1.262237	-0.434147
[i2e]→[i5a]				[i2f]→[i5b]			
							
-294.0 kJ mol^{-1}				-292.4 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-0.342188	2.735051	-0.130811	Si	-0.342188	2.735051	-0.130811
C	-0.391241	-1.205372	-0.299825	C	-0.391241	-1.205372	-0.299825
C	-0.039692	-0.188254	0.478770	C	-0.039692	-0.188254	0.478770
C	0.308252	1.168082	-0.001663	C	0.308252	1.168082	-0.001663
D	-0.000480	-0.344895	1.555941	H	-0.000480	-0.344895	1.555941
D	-0.632717	-2.174234	0.123862	D	-0.632717	-2.174234	0.123862
D	-0.451087	-1.098752	-1.378354	D	-0.451087	-1.098752	-1.378354
H	1.322618	1.262237	-0.434147	D	1.322618	1.262237	-0.434147

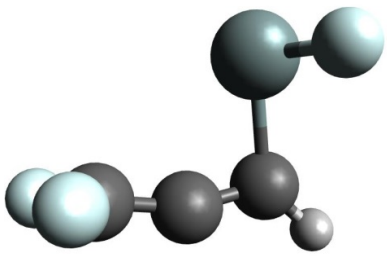
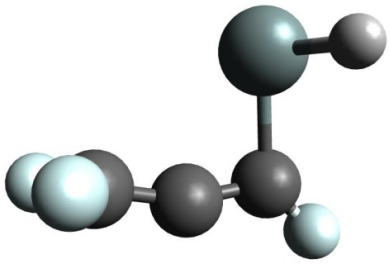
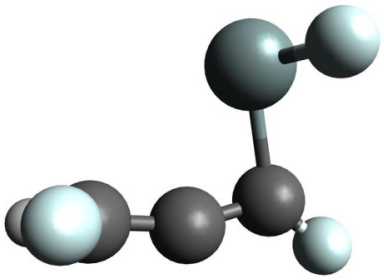
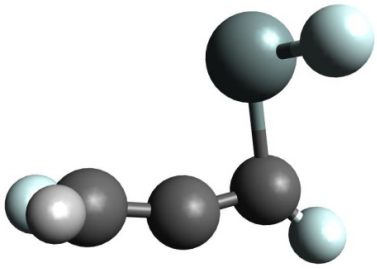
[i2g]→[i5c]				[i2h]→[i5d]			
							
-292.4 kJ mol^{-1}				-292.5 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-0.342188	2.735051	-0.130811	Si	-0.342188	2.735051	-0.130811
C	-0.391241	-1.205372	-0.299825	C	-0.391241	-1.205372	-0.299825
C	-0.039692	-0.188254	0.478770	C	-0.039692	-0.188254	0.478770
C	0.308252	1.168082	-0.001663	C	0.308252	1.168082	-0.001663
D	-0.000480	-0.344895	1.555941	D	-0.000480	-0.344895	1.555941
H	-0.632717	-2.174234	0.123862	D	-0.632717	-2.174234	0.123862
D	-0.451087	-1.098752	-1.378354	H	-0.451087	-1.098752	-1.378354
D	1.322618	1.262237	-0.434147	D	1.322618	1.262237	-0.434147
[i2a]→[i10d]				[i2b]→[i10c]			
							
-25.2 kJ mol^{-1}				-27.6 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	0.728857	1.050351	-1.035226	Si	0.728857	1.050351	-1.035226
C	0.745086	-0.738470	-0.340304	C	0.745086	-0.738470	-0.340304
C	0.053676	-0.073521	0.854344	C	0.053676	-0.073521	0.854344
C	-0.693567	0.957443	0.165361	C	-0.693567	0.957443	0.165361
D	1.677882	-1.260348	-0.131790	D	1.677882	-1.260348	-0.131790
D	0.063165	-1.398234	-0.873462	D	0.063165	-1.398234	-0.873462
D	-1.158678	-0.176597	0.686967	H	-1.158678	-0.176597	0.686967
H	-1.402374	1.604957	0.677393	D	-1.402374	1.604957	0.677393

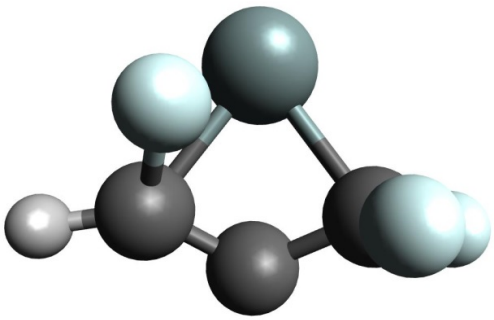
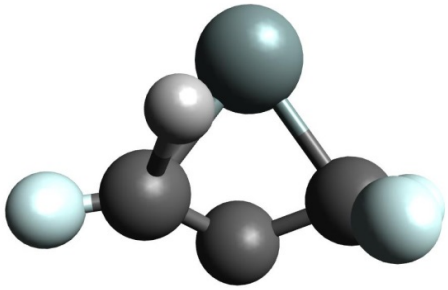
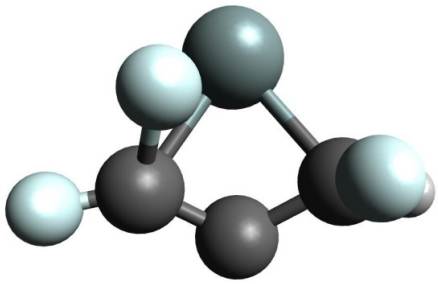
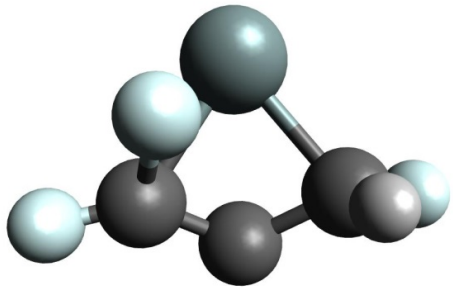
[i2c]→[i10b]				[i2d]→[i10a]			
							
-25.0 kJ mol^{-1}				-25.3 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	0.728857	1.050351	-1.035226	Si	0.728857	1.050351	-1.035226
C	0.745086	-0.738470	-0.340304	C	0.745086	-0.738470	-0.340304
C	0.053676	-0.073521	0.854344	C	0.053676	-0.073521	0.854344
C	-0.693567	0.957443	0.165361	C	-0.693567	0.957443	0.165361
H	1.677882	-1.260348	-0.131790	D	1.677882	-1.260348	-0.131790
D	0.063165	-1.398234	-0.873462	H	0.063165	-1.398234	-0.873462
D	-1.158678	-0.176597	0.686967	D	-1.158678	-0.176597	0.686967
D	-1.402374	1.604957	0.677393	D	-1.402374	1.604957	0.677393
[i2e]→[i10b]				[i2f]→[i10a]			
							
-25.2 kJ mol^{-1}				-27.6 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-0.728857	1.050351	-1.035226	Si	-0.728857	1.050351	-1.035226
C	-0.745086	-0.738470	-0.340304	C	-0.745086	-0.738470	-0.340304
C	-0.053676	-0.073521	0.854344	C	-0.053676	-0.073521	0.854344
C	0.693567	0.957443	0.165361	C	0.693567	0.957443	0.165361
D	-1.677882	-1.260348	-0.131790	D	-1.677882	-1.260348	-0.131790
D	-0.063165	-1.398234	-0.873462	D	-0.063165	-1.398234	-0.873462
D	1.158678	-0.176597	0.686967	H	1.158678	-0.176597	0.686967
H	1.402374	1.604957	0.677393	D	1.402374	1.604957	0.677393

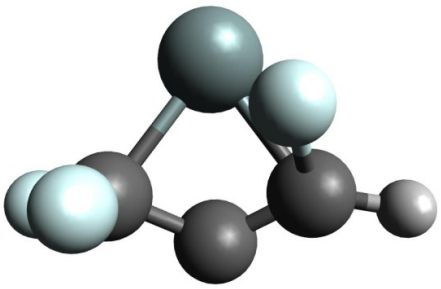
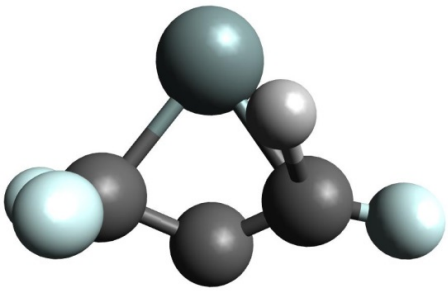
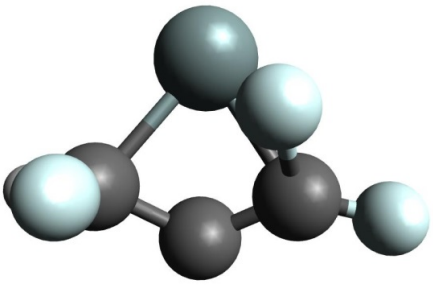
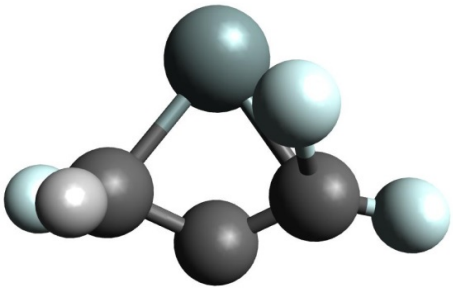
[i2g]→[i10d]				[i2h]→[i10c]			
							
-25.0 kJ mol^{-1}				-25.3 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-0.728857	1.050351	-1.035226	Si	-0.728857	1.050351	-1.035226
C	-0.745086	-0.738470	-0.340304	C	-0.745086	-0.738470	-0.340304
C	-0.053676	-0.073521	0.854344	C	-0.053676	-0.073521	0.854344
C	0.693567	0.957443	0.165361	C	0.693567	0.957443	0.165361
H	-1.677882	-1.260348	-0.131790	D	-1.677882	-1.260348	-0.131790
D	-0.063165	-1.398234	-0.873462	H	-0.063165	-1.398234	-0.873462
D	1.158678	-0.176597	0.686967	D	1.158678	-0.176597	0.686967
D	1.402374	1.604957	0.677393	D	1.402374	1.604957	0.677393
[i4a]→[i13a]				[i4b]→[i13b]			
							
-224.9 kJ mol^{-1}				-221.4 kJ mol^{-1}			
$C_s - {}^1A'$				$C_s - {}^1A'$			
Si	-1.742300	2.701762	0.558436	Si	-1.742300	2.701762	0.558436
C	-1.453027	0.995062	-0.232032	C	-1.453027	0.995062	-0.232032
C	-0.226982	1.212635	-0.272076	C	-0.226982	1.212635	-0.272076
C	1.233250	1.262100	-0.377354	C	1.233250	1.262100	-0.377354
H	-0.321943	3.146011	0.987967	D	-0.321943	3.146011	0.987967
D	1.549669	2.031502	-1.083304	D	1.549669	2.031502	-1.083304
D	1.675869	1.477113	0.596678	D	1.675869	1.477113	0.596678
D	1.597521	0.293445	-0.727392	H	1.597521	0.293445	-0.727392

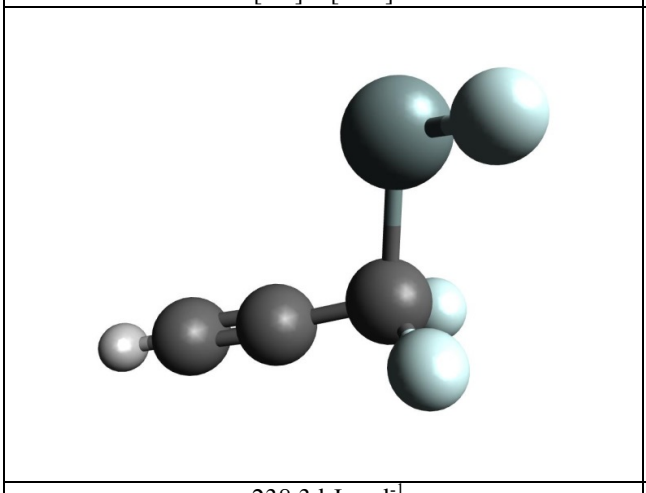
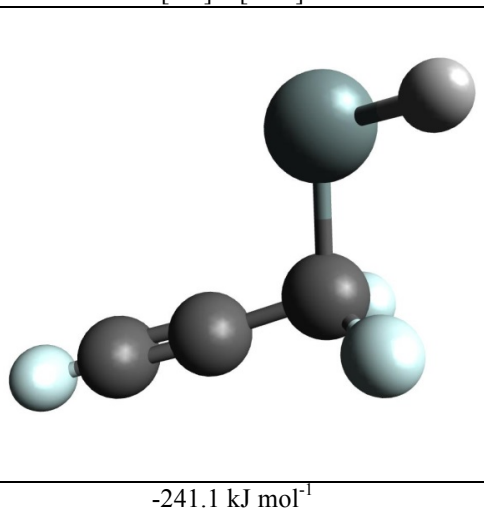
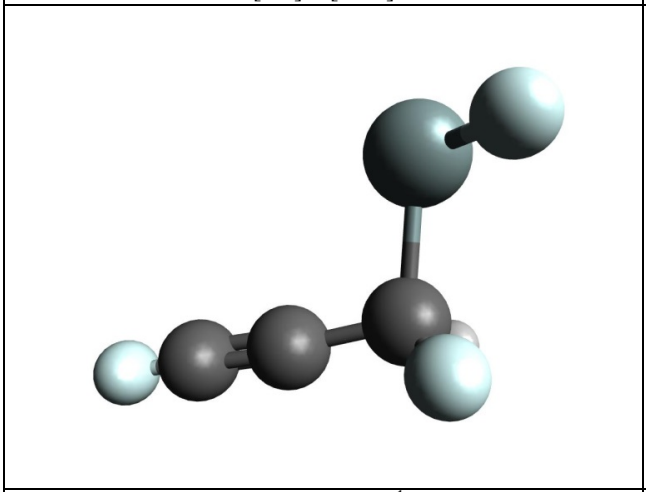
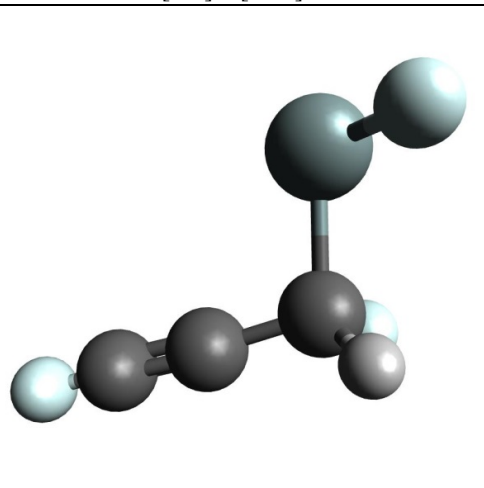
[i5a]→[i9a]				[i5b]→[i9b]			
							
-202.5 kJ mol^{-1}				-205.3 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-1.992862	2.228890	0.527181	Si	-1.992862	2.228890	0.527181
C	-1.168691	0.701841	0.088179	C	-1.168691	0.701841	0.088179
C	0.014708	1.354943	0.010861	C	0.014708	1.354943	0.010861
C	1.299058	1.583736	-0.198471	C	1.299058	1.583736	-0.198471
D	-0.660165	2.892930	0.016175	H	-0.660165	2.892930	0.016175
H	-1.325198	-0.327819	0.375544	D	-1.325198	-0.327819	0.375544
D	1.802093	2.476996	0.142678	D	1.802093	2.476996	0.142678
D	1.862043	0.843052	-0.756205	D	1.862043	0.843052	-0.756205
[i5c]→[i9d]				[i5d]→[i9c]			
							
-202.3 kJ mol^{-1}				-202.5 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-1.992862	2.228890	0.527181	Si	-1.992862	2.228890	0.527181
C	-1.168691	0.701841	0.088179	C	-1.168691	0.701841	0.088179
C	0.014708	1.354943	0.010861	C	0.014708	1.354943	0.010861
C	1.299058	1.583736	-0.198471	C	1.299058	1.583736	-0.198471
D	-0.660165	2.892930	0.016175	D	-0.660165	2.892930	0.016175
D	-1.325198	-0.327819	0.375544	D	-1.325198	-0.327819	0.375544
H	1.802093	2.476996	0.142678	D	1.802093	2.476996	0.142678
D	1.862043	0.843052	-0.756205	H	1.862043	0.843052	-0.756205

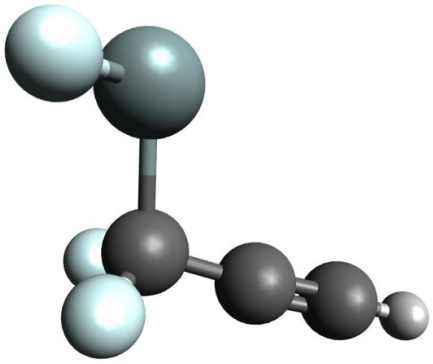
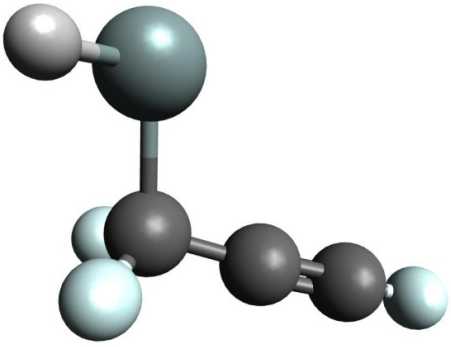
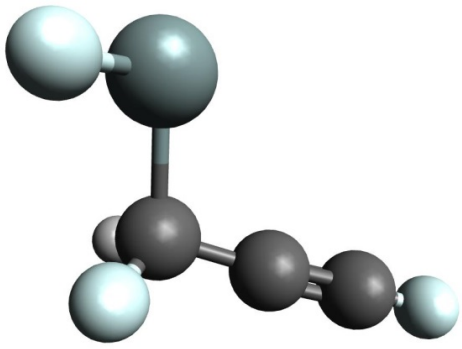
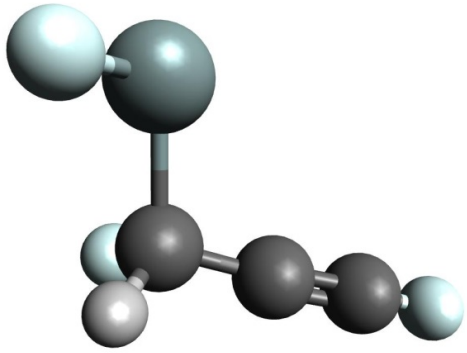
[i6a]→[i9a]				[i6b]→[i9b]			
							
-256.0 kJ mol^{-1}				-258.8 kJ mol^{-1}			
C_1 – ^{1}A				C_1 – ^{1}A			
Si	1.820646	2.497868	0.585175	Si	1.820646	2.497868	0.585175
C	1.254585	0.742483	0.074294	C	1.254585	0.742483	0.074294
C	0.032876	1.141174	-0.073976	C	0.032876	1.141174	-0.073976
C	-1.054450	1.887589	-0.083800	C	-1.054450	1.887589	-0.083800
D	2.460246	2.819309	-0.774176	H	2.460246	2.819309	-0.774176
H	1.690241	-0.197006	-0.235942	D	1.690241	-0.197006	-0.235942
D	-1.294651	2.500444	-0.946357	D	-1.294651	2.500444	-0.946357
D	-1.774537	1.839849	0.726578	D	-1.774537	1.839849	0.726578
[i6c]→[i9c]				[i6d]→[i9d]			
							
-255.8 kJ mol^{-1}				-255.7 kJ mol^{-1}			
C_1 – ^{1}A				C_1 – ^{1}A			
Si	1.820646	2.497868	0.585175	Si	1.820646	2.497868	0.585175
C	1.254585	0.742483	0.074294	C	1.254585	0.742483	0.074294
C	0.032876	1.141174	-0.073976	C	0.032876	1.141174	-0.073976
C	-1.054450	1.887589	-0.083800	C	-1.054450	1.887589	-0.083800
D	2.460246	2.819309	-0.774176	D	2.460246	2.819309	-0.774176
D	1.690241	-0.197006	-0.235942	D	1.690241	-0.197006	-0.235942
D	-1.294651	2.500444	-0.946357	H	-1.294651	2.500444	-0.946357
H	-1.774537	1.839849	0.726578	D	-1.774537	1.839849	0.726578

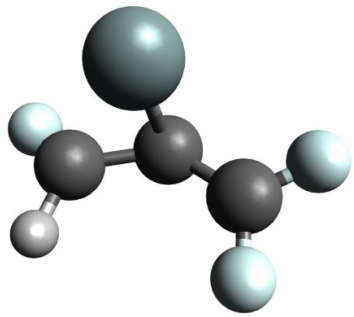
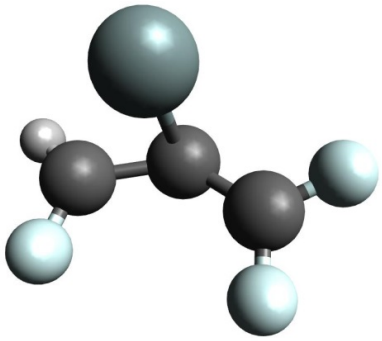
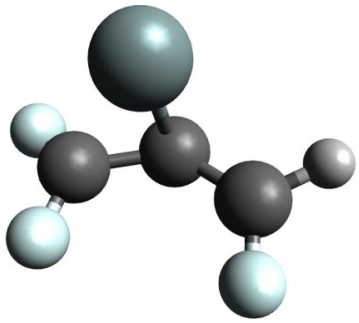
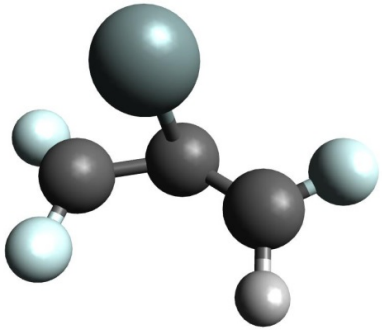
[i6e]→[i9a]				[i6f]→[i9b]			
							
-256.0 kJ mol^{-1}				-258.8 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-1.820646	2.497868	0.585175	Si	-1.820646	2.497868	0.585175
C	-1.254585	0.742483	0.074294	C	-1.254585	0.742483	0.074294
C	-0.032876	1.141174	-0.073976	C	-0.032876	1.141174	-0.073976
C	1.054450	1.887589	-0.083800	C	1.054450	1.887589	-0.083800
D	-2.460246	2.819309	-0.774176	H	-2.460246	2.819309	-0.774176
H	-1.690241	-0.197006	-0.235942	D	-1.690241	-0.197006	-0.235942
D	1.294651	2.500444	-0.946357	D	1.294651	2.500444	-0.946357
D	1.774537	1.839849	0.726578	D	1.774537	1.839849	0.726578
[i6g]→[i9d]				[i6h]→[i9c]			
							
-255.8 kJ mol^{-1}				-255.7 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-1.820646	2.497868	0.585175	Si	-1.820646	2.497868	0.585175
C	-1.254585	0.742483	0.074294	C	-1.254585	0.742483	0.074294
C	-0.032876	1.141174	-0.073976	C	-0.032876	1.141174	-0.073976
C	1.054450	1.887589	-0.083800	C	1.054450	1.887589	-0.083800
D	-2.460246	2.819309	-0.774176	D	-2.460246	2.819309	-0.774176
D	-1.690241	-0.197006	-0.235942	D	-1.690241	-0.197006	-0.235942
D	1.294651	2.500444	-0.946357	H	1.294651	2.500444	-0.946357
H	1.774537	1.839849	0.726578	D	1.774537	1.839849	0.726578

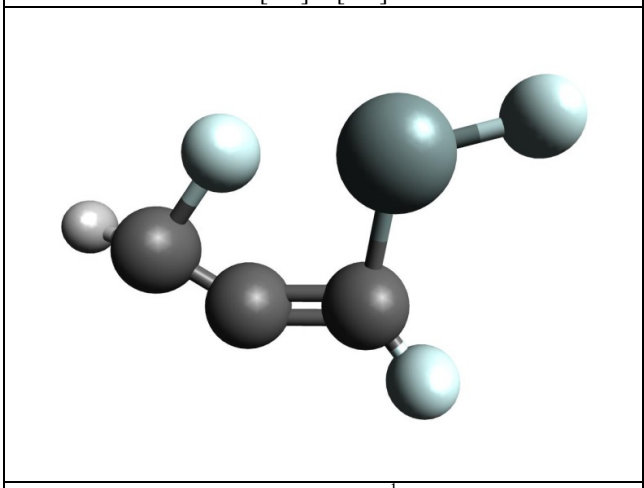
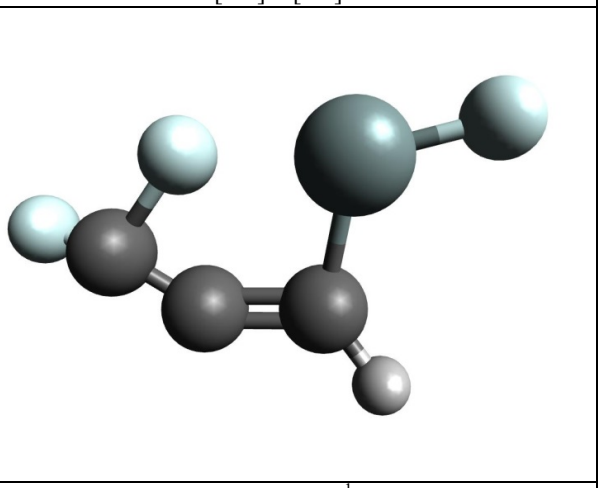
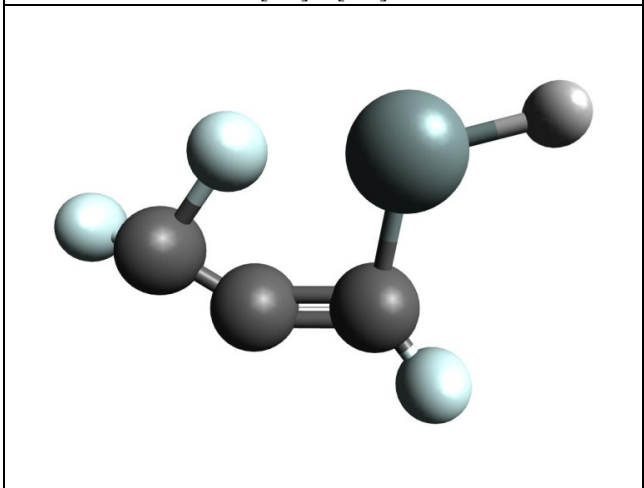
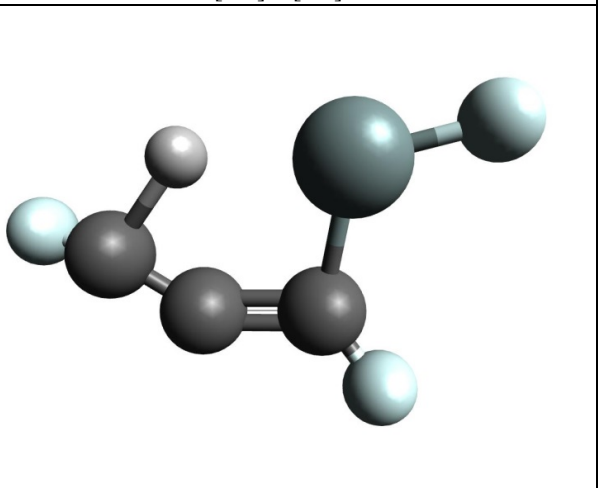
[i6a]→[i10b]				[i6b]→[i10a]			
							
-155.7 kJ mol^{-1}				-158.9 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	1.108893	2.428844	0.896755	Si	1.108893	2.428844	0.896755
C	1.254157	0.804122	-0.190514	C	1.254157	0.804122	-0.190514
C	-0.047399	0.766331	0.066469	C	-0.047399	0.766331	0.066469
C	-0.677368	2.066019	0.073662	C	-0.677368	2.066019	0.073662
H	2.054356	0.150676	-0.497980	D	2.054356	0.150676	-0.497980
D	1.608219	2.139909	-0.662094	H	1.608219	2.139909	-0.662094
D	-0.645862	2.587746	-0.883451	D	-0.645862	2.587746	-0.883451
D	-1.601289	2.227878	0.621898	D	-1.601289	2.227878	0.621898
[i6c]→[i10d]				[i6d]→[i10c]			
							
-155.4 kJ mol^{-1}				-155.7 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	1.108893	2.428844	0.896755	Si	1.108893	2.428844	0.896755
C	1.254157	0.804122	-0.190514	C	1.254157	0.804122	-0.190514
C	-0.047399	0.766331	0.066469	C	-0.047399	0.766331	0.066469
C	-0.677368	2.066019	0.073662	C	-0.677368	2.066019	0.073662
D	2.054356	0.150676	-0.497980	D	2.054356	0.150676	-0.497980
D	1.608219	2.139909	-0.662094	D	1.608219	2.139909	-0.662094
D	-0.645862	2.587746	-0.883451	H	-0.645862	2.587746	-0.883451
H	-1.601289	2.227878	0.621898	D	-1.601289	2.227878	0.621898

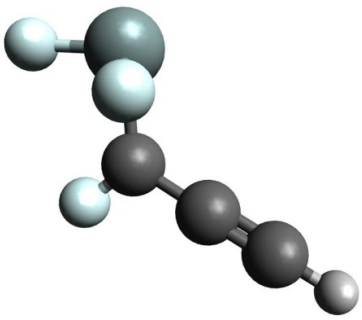
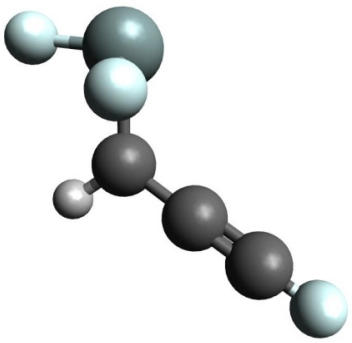
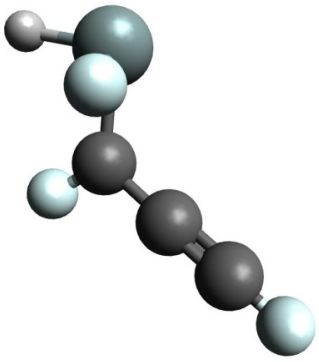
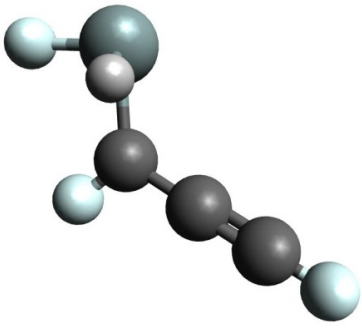
[i6e]→[i10d]				[i6f]→[i10c]			
							
-155.7 kJ mol^{-1}				-158.9 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-1.108893	2.428844	0.896755	Si	-1.108893	2.428844	0.896755
C	-1.254157	0.804122	-0.190514	C	-1.254157	0.804122	-0.190514
C	0.047399	0.766331	0.066469	C	0.047399	0.766331	0.066469
C	0.677368	2.066019	0.073662	C	0.677368	2.066019	0.073662
H	-2.054356	0.150676	-0.497980	D	-2.054356	0.150676	-0.497980
D	-1.608219	2.139909	-0.662094	H	-1.608219	2.139909	-0.662094
D	0.645862	2.587746	-0.883451	D	0.645862	2.587746	-0.883451
D	1.601289	2.227878	0.621898	D	1.601289	2.227878	0.621898
[i6g]→[i10b]				[i6h]→[i10a]			
							
-155.4 kJ mol^{-1}				-155.7 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-1.108893	2.428844	0.896755	Si	-1.108893	2.428844	0.896755
C	-1.254157	0.804122	-0.190514	C	-1.254157	0.804122	-0.190514
C	0.047399	0.766331	0.066469	C	0.047399	0.766331	0.066469
C	0.677368	2.066019	0.073662	C	0.677368	2.066019	0.073662
D	-2.054356	0.150676	-0.497980	D	-2.054356	0.150676	-0.497980
D	-1.608219	2.139909	-0.662094	D	-1.608219	2.139909	-0.662094
D	0.645862	2.587746	-0.883451	H	0.645862	2.587746	-0.883451
H	1.601289	2.227878	0.621898	D	1.601289	2.227878	0.621898

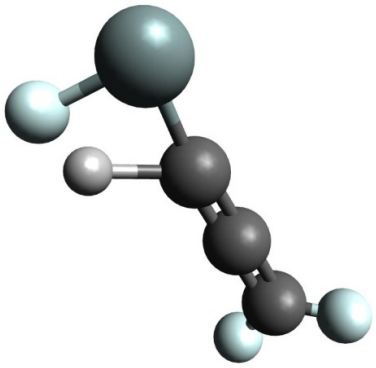
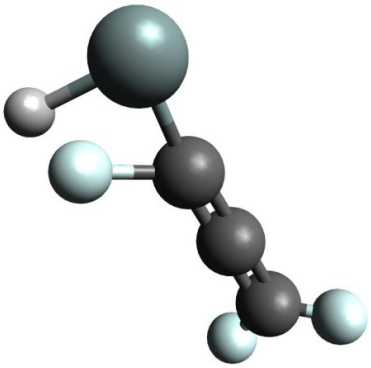
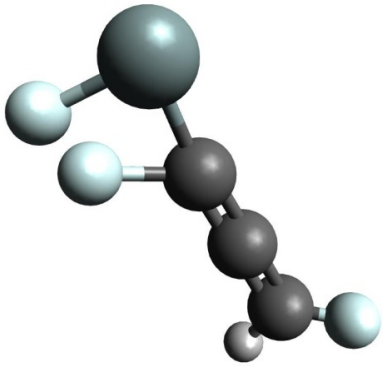
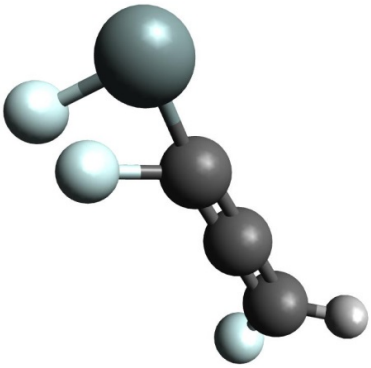
[i6a]→[i12a]				[i6b]→[i12b]			
							
-238.3 kJ mol^{-1}				-241.1 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	0.852609	1.635684	0.581065	Si	0.852609	1.635684	0.581065
C	-0.565860	0.423002	0.059391	C	-0.565860	0.423002	0.059391
C	0.001882	-0.919555	0.000234	C	0.001882	-0.919555	0.000234
C	0.544992	-1.989473	-0.037835	C	0.544992	-1.989473	-0.037835
D	0.555684	2.682867	-0.493235	H	0.555684	2.682867	-0.493235
D	-1.048992	0.683920	-0.883382	D	-1.048992	0.683920	-0.883382
D	-1.329382	0.463880	0.848535	D	-1.329382	0.463880	0.848535
H	1.001958	-2.950630	-0.071481	D	1.001958	-2.950630	-0.071481
[i6c]→[i12d]				[i6d]→[i12c]			
							
-237.7 kJ mol^{-1}				-237.4 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	0.852609	1.635684	0.581065	Si	0.852609	1.635684	0.581065
C	-0.565860	0.423002	0.059391	C	-0.565860	0.423002	0.059391
C	0.001882	-0.919555	0.000234	C	0.001882	-0.919555	0.000234
C	0.544992	-1.989473	-0.037835	C	0.544992	-1.989473	-0.037835
D	0.555684	2.682867	-0.493235	D	0.555684	2.682867	-0.493235
D	-1.048992	0.683920	-0.883382	H	-1.048992	0.683920	-0.883382
H	-1.329382	0.463880	0.848535	D	-1.329382	0.463880	0.848535
D	1.001958	-2.950630	-0.071481	D	1.001958	-2.950630	-0.071481

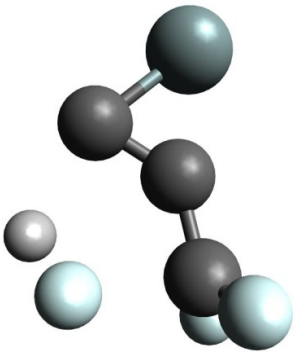
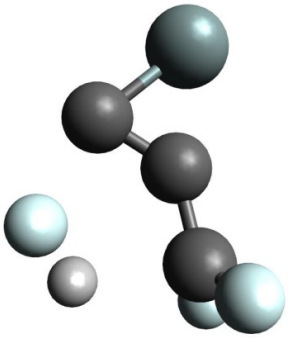
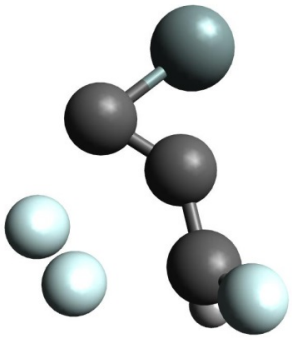
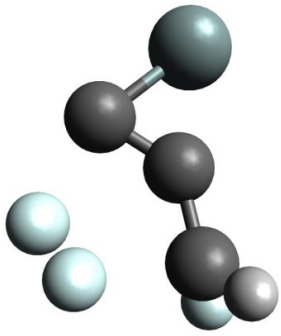
[i6e]→[i12a]				[i6f]→[i12b]			
							
-238.3 kJ mol^{-1}				-241.1 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-0.852609	1.635684	0.581065	Si	-0.852609	1.635684	0.581065
C	0.565860	0.423002	0.059391	C	0.565860	0.423002	0.059391
C	-0.001882	-0.919555	0.000234	C	-0.001882	-0.919555	0.000234
C	-0.544992	-1.989473	-0.037835	C	-0.544992	-1.989473	-0.037835
D	-0.555684	2.682867	-0.493235	H	-0.555684	2.682867	-0.493235
D	1.048992	0.683920	-0.883382	D	1.048992	0.683920	-0.883382
D	1.329382	0.463880	0.848535	D	1.329382	0.463880	0.848535
H	-1.001958	-2.950630	-0.071481	D	-1.001958	-2.950630	-0.071481
[i6g]→[i12c]				[i6h]→[i12d]			
							
-237.7 kJ mol^{-1}				-237.4 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-0.852609	1.635684	0.581065	Si	-0.852609	1.635684	0.581065
C	0.565860	0.423002	0.059391	C	0.565860	0.423002	0.059391
C	-0.001882	-0.919555	0.000234	C	-0.001882	-0.919555	0.000234
C	-0.544992	-1.989473	-0.037835	C	-0.544992	-1.989473	-0.037835
D	-0.555684	2.682867	-0.493235	D	-0.555684	2.682867	-0.493235
D	1.048992	0.683920	-0.883382	H	1.048992	0.683920	-0.883382
H	1.329382	0.463880	0.848535	D	1.329382	0.463880	0.848535
D	-1.001958	-2.950630	-0.071481	D	-1.001958	-2.950630	-0.071481

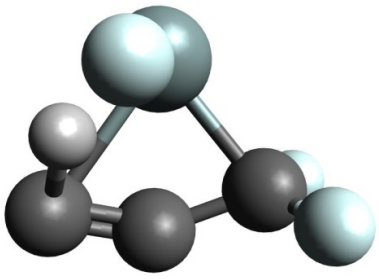
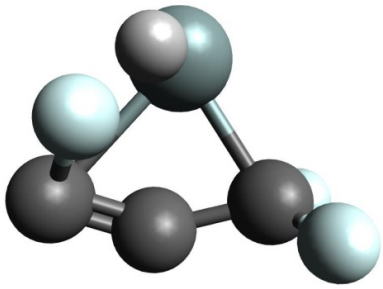
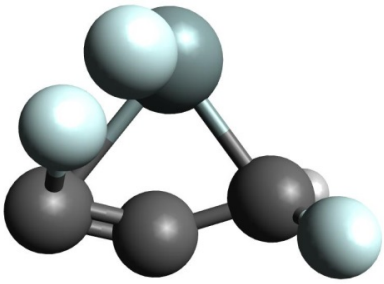
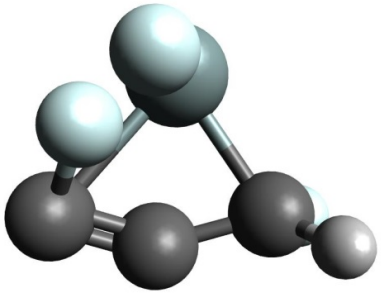
[i7a]→[i10a]				[i7b]→[i10b]			
							
-276.6 kJ mol^{-1}				-276.4 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-1.965407	2.054224	0.949023	Si	-1.965407	2.054224	0.949023
C	-2.941031	0.741834	-0.252682	C	-2.941031	0.741834	-0.252682
C	-1.529983	0.959789	-0.397630	C	-1.529983	0.959789	-0.397630
C	-0.519325	0.330323	0.274811	C	-0.519325	0.330323	0.274811
D	-3.585322	1.284613	-0.938932	H	-3.585322	1.284613	-0.938932
H	-3.363470	-0.192898	0.123519	D	-3.363470	-0.192898	0.123519
D	-0.582867	-0.703830	0.623728	D	-0.582867	-0.703830	0.623728
D	0.457528	0.798760	0.345200	D	0.457528	0.798760	0.345200
[i7c]→[i10d]				[i7d]→[i10c]			
							
-276.4 kJ mol^{-1}				-276.7 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-1.965407	2.054224	0.949023	Si	-1.965407	2.054224	0.949023
C	-2.941031	0.741834	-0.252682	C	-2.941031	0.741834	-0.252682
C	-1.529983	0.959789	-0.397630	C	-1.529983	0.959789	-0.397630
C	-0.519325	0.330323	0.274811	C	-0.519325	0.330323	0.274811
D	-3.585322	1.284613	-0.938932	D	-3.585322	1.284613	-0.938932
D	-3.363470	-0.192898	0.123519	D	-3.363470	-0.192898	0.123519
D	-0.582867	-0.703830	0.623728	H	-0.582867	-0.703830	0.623728
H	0.457528	0.798760	0.345200	D	0.457528	0.798760	0.345200

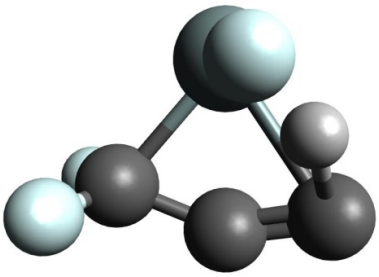
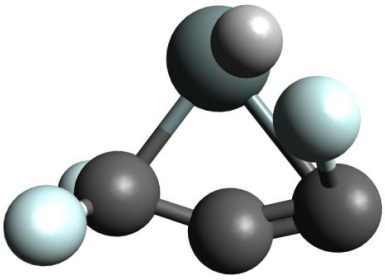
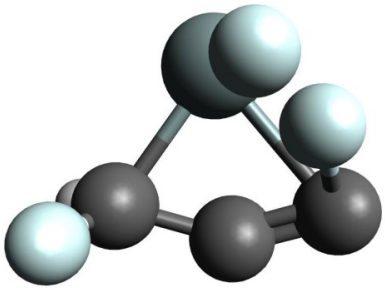
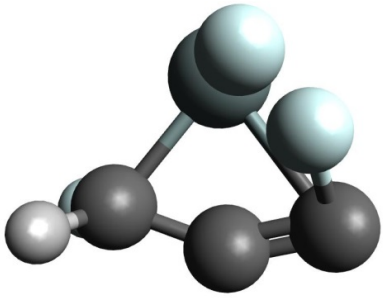
[i8a]→[i9d]				[i8b]→[i9a]			
							
-47.9 kJ mol^{-1}				-47.6 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	1.041061	0.917892	0.436916	Si	1.041061	0.917892	0.436916
C	0.760892	-0.738193	-0.161392	C	0.760892	-0.738193	-0.161392
C	-0.609128	-0.750344	-0.306514	C	-0.609128	-0.750344	-0.306514
C	-1.670823	-0.094074	-0.212414	C	-1.670823	-0.094074	-0.212414
D	2.501462	1.265763	0.648959	D	2.501462	1.265763	0.648959
D	-0.818889	0.943557	0.334551	D	-0.818889	0.943557	0.334551
D	1.411713	-1.596634	-0.075037	H	1.411713	-1.596634	-0.075037
H	-2.618347	0.185964	-0.624789	D	-2.618347	0.185964	-0.624789
[i8c]→[i9b]				[i8d]→[i9c]			
							
-50.0 kJ mol^{-1}				-51.4 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	1.041061	0.917892	0.436916	Si	1.041061	0.917892	0.436916
C	0.760892	-0.738193	-0.161392	C	0.760892	-0.738193	-0.161392
C	-0.609128	-0.750344	-0.306514	C	-0.609128	-0.750344	-0.306514
C	-1.670823	-0.094074	-0.212414	C	-1.670823	-0.094074	-0.212414
H	2.501462	1.265763	0.648959	D	2.501462	1.265763	0.648959
D	-0.818889	0.943557	0.334551	H	-0.818889	0.943557	0.334551
D	1.411713	-1.596634	-0.075037	D	1.411713	-1.596634	-0.075037
D	-2.618347	0.185964	-0.624789	D	-2.618347	0.185964	-0.624789

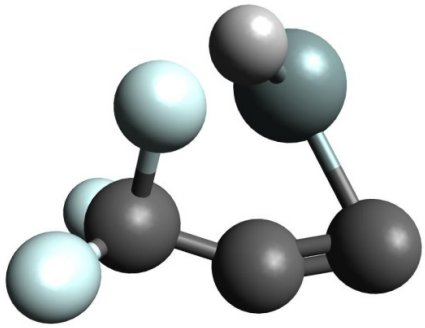
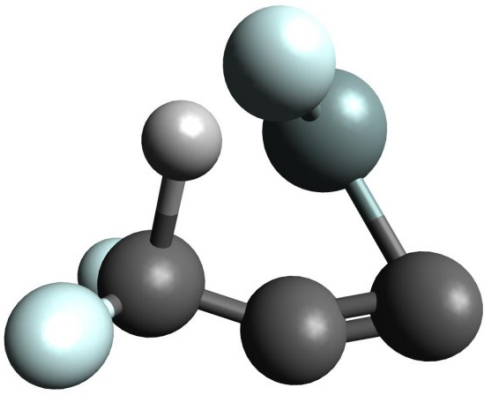
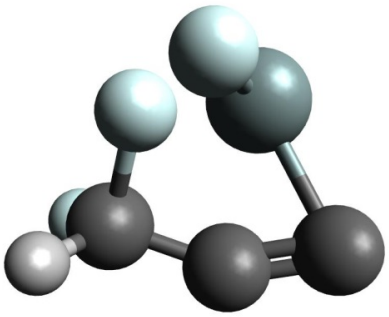
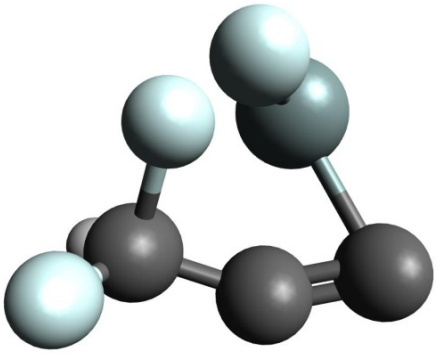
[i8a]→[i12a]				[i8b]→[i12c]			
							
-108.7 kJ mol^{-1}				-108.2 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-2.521663	2.463165	1.136938	Si	-2.521663	2.463165	1.136938
C	-0.857503	2.002660	0.565118	C	-0.857503	2.002660	0.565118
C	-0.462648	0.671903	0.277186	C	-0.462648	0.671903	0.277186
C	-0.127979	-0.463490	0.061318	C	-0.127979	-0.463490	0.061318
D	-0.053439	2.725894	0.410733	H	-0.053439	2.725894	0.410733
H	0.166755	-1.470185	-0.125512	D	0.166755	-1.470185	-0.125512
D	-2.334378	3.957638	1.028947	D	-2.334378	3.957638	1.028947
D	-2.405675	1.983846	-0.345689	D	-2.405675	1.983846	-0.345689
[i8c]→[i12b]				[i8d]→[i12d]			
							
-110.5 kJ mol^{-1}				-111.6 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-2.521663	2.463165	1.136938	Si	-2.521663	2.463165	1.136938
C	-0.857503	2.002660	0.565118	C	-0.857503	2.002660	0.565118
C	-0.462648	0.671903	0.277186	C	-0.462648	0.671903	0.277186
C	-0.127979	-0.463490	0.061318	C	-0.127979	-0.463490	0.061318
D	-0.053439	2.725894	0.410733	D	-0.053439	2.725894	0.410733
D	0.166755	-1.470185	-0.125512	D	0.166755	-1.470185	-0.125512
H	-2.334378	3.957638	1.028947	D	-2.334378	3.957638	1.028947
D	-2.405675	1.983846	-0.345689	H	-2.405675	1.983846	-0.345689

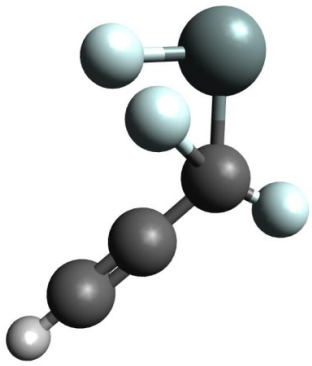
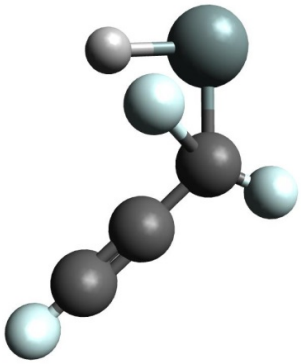
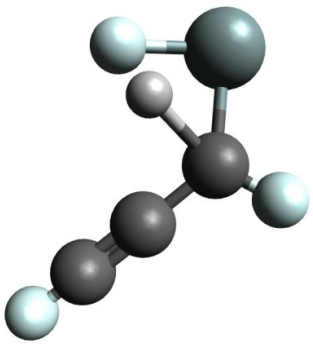
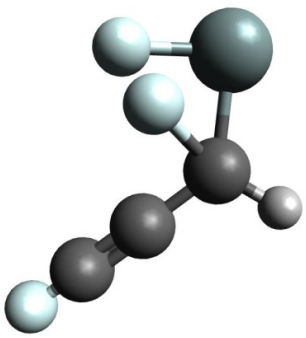
[i9a]→**p1a**				[i9b]→**p1a**			
							
-84.8 kJ mol^{-1}				-83.8 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-0.744770	2.157892	1.133843	Si	-0.744770	2.157892	1.133843
C	-0.117447	0.739329	0.301978	C	-0.117447	0.739329	0.301978
C	0.508868	-0.265289	-0.184605	C	0.508868	-0.265289	-0.184605
C	1.137912	-1.291212	-0.706981	C	1.137912	-1.291212	-0.706981
D	2.192710	-1.451493	-0.511820	D	2.192710	-1.451493	-0.511820
D	0.620937	-2.000203	-1.344227	D	0.620937	-2.000203	-1.344227
H	-1.537155	0.742156	0.712436	D	-1.537155	0.742156	0.712436
D	-2.215299	1.527879	0.692674	H	-2.215299	1.527879	0.692674
[i9c]→**p1b**				[i9d]→**p1b**			
							
-81.1 kJ mol^{-1}				-81.1 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-0.744770	2.157892	1.133843	Si	-0.744770	2.157892	1.133843
C	-0.117447	0.739329	0.301978	C	-0.117447	0.739329	0.301978
C	0.508868	-0.265289	-0.184605	C	0.508868	-0.265289	-0.184605
C	1.137912	-1.291212	-0.706981	C	1.137912	-1.291212	-0.706981
D	2.192710	-1.451493	-0.511820	H	2.192710	-1.451493	-0.511820
H	0.620937	-2.000203	-1.344227	D	0.620937	-2.000203	-1.344227
D	-1.537155	0.742156	0.712436	D	-1.537155	0.742156	0.712436
D	-2.215299	1.527879	0.692674	D	-2.215299	1.527879	0.692674

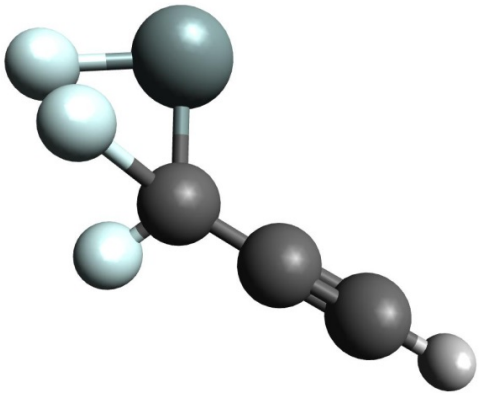
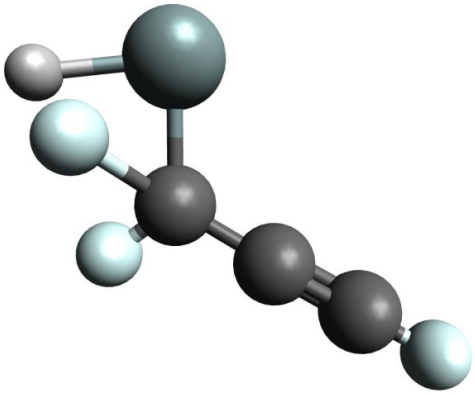
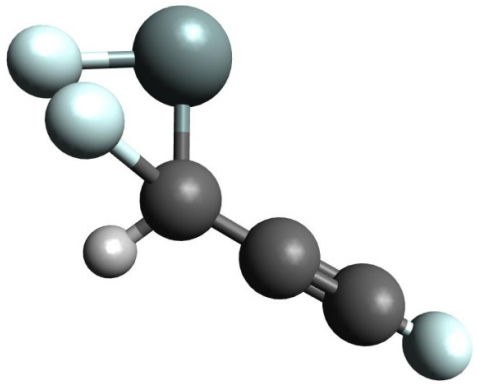
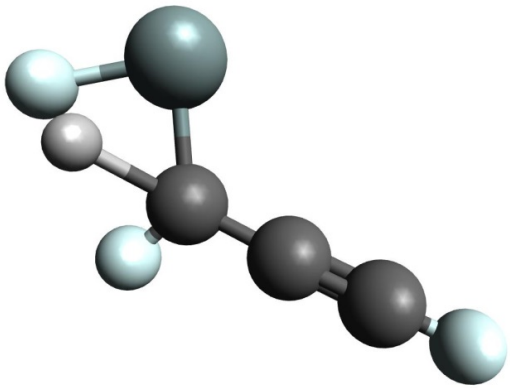
[i1a]→**p2a**				[i1b]→**p2a**			
							
10.8 kJ mol^{-1}				11.0 kJ mol^{-1}			
$C_s - {}^1A'$				$C_s - {}^1A'$			
Si	0.528665	2.400596	-0.746415	Si	0.528665	2.400596	-0.746415
C	0.638969	-0.741790	0.047537	C	0.638969	-0.741790	0.047537
C	0.334217	0.578629	-0.236986	C	0.334217	0.578629	-0.236986
C	-0.782728	1.293996	-0.211915	C	-0.782728	1.293996	-0.211915
D	1.142678	-0.981263	0.980498	D	1.142678	-0.981263	0.980498
D	0.810919	-1.435189	-0.771673	D	0.810919	-1.435189	-0.771673
H	-1.559747	-0.175915	0.315690	D	-1.559747	-0.175915	0.315690
D	-1.065292	-0.900941	0.410427	H	-1.065292	-0.900941	0.410427
[i1b]→**p2b**				[i1b]→**p2c**			
							
13.9 kJ mol^{-1}				13.9 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	0.528665	2.400596	-0.746415	Si	0.528665	2.400596	-0.746415
C	0.638969	-0.741790	0.047537	C	0.638969	-0.741790	0.047537
C	0.334217	0.578629	-0.236986	C	0.334217	0.578629	-0.236986
C	-0.782728	1.293996	-0.211915	C	-0.782728	1.293996	-0.211915
D	1.142678	-0.981263	0.980498	H	1.142678	-0.981263	0.980498
H	0.810919	-1.435189	-0.771673	D	0.810919	-1.435189	-0.771673
D	-1.559747	-0.175915	0.315690	D	-1.559747	-0.175915	0.315690
D	-1.065292	-0.900941	0.410427	D	-1.065292	-0.900941	0.410427

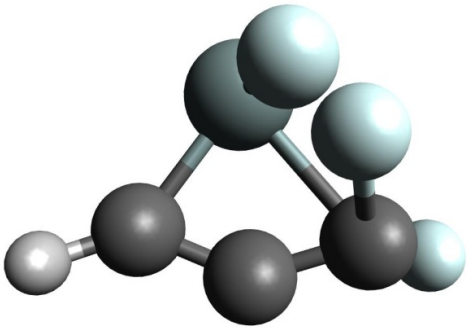
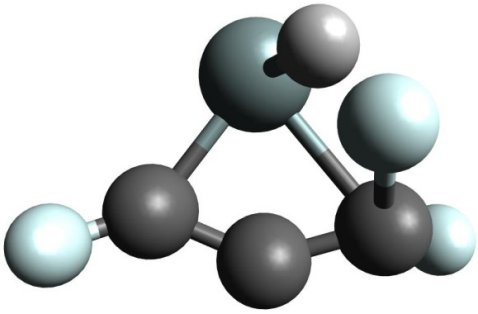
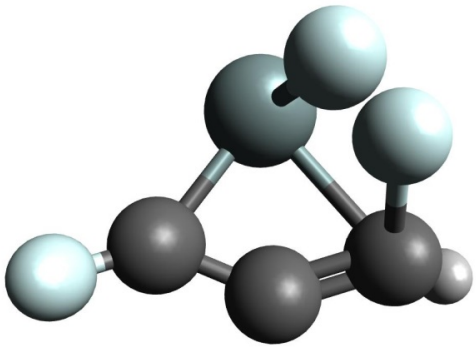
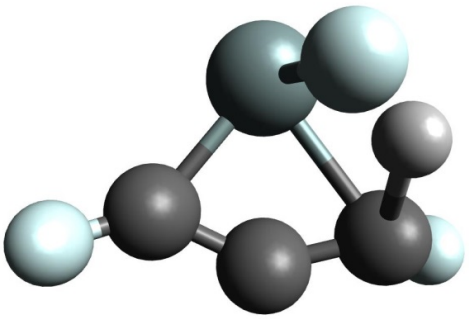
[i6a]→**p2a**				[i6b]→**p2a**			
							
-43.5 kJ mol^{-1}				-41.9 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	1.178923	2.205371	0.803390	Si	1.178923	2.205371	0.803390
C	-0.641206	2.137118	-0.050763	C	-0.641206	2.137118	-0.050763
C	-0.130702	0.814244	0.053579	C	-0.130702	0.814244	0.053579
C	0.888991	0.086553	0.200705	C	0.888991	0.086553	0.200705
D	-0.835280	2.504167	-1.054512	D	-0.835280	2.504167	-1.054512
D	-1.380706	2.457777	0.683302	D	-1.380706	2.457777	0.683302
H	1.725043	1.088245	-0.475804	D	1.725043	1.088245	-0.475804
D	1.923344	2.086626	-0.687100	H	1.923344	2.086626	-0.687100
[i6c]→**p2b**				[i6d]→**p2c**			
							
-39.4 kJ mol^{-1}				-39.4 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	1.178923	2.205371	0.803390	Si	1.178923	2.205371	0.803390
C	-0.641206	2.137118	-0.050763	C	-0.641206	2.137118	-0.050763
C	-0.130702	0.814244	0.053579	C	-0.130702	0.814244	0.053579
C	0.888991	0.086553	0.200705	C	0.888991	0.086553	0.200705
D	-0.835280	2.504167	-1.054512	H	-0.835280	2.504167	-1.054512
H	-1.380706	2.457777	0.683302	D	-1.380706	2.457777	0.683302
D	1.725043	1.088245	-0.475804	D	1.725043	1.088245	-0.475804
D	1.923344	2.086626	-0.687100	D	1.923344	2.086626	-0.687100

[i6e]→**p2a**				[i6f]→**p2a**			
							
-43.5 kJ mol^{-1}				-41.9 kJ mol^{-1}			
C_1 – ^{1}A				C_1 – ^{1}A			
Si	-1.178923	2.205371	0.803390	Si	-1.178923	2.205371	0.803390
C	0.641206	2.137118	-0.050763	C	0.641206	2.137118	-0.050763
C	0.130702	0.814244	0.053579	C	0.130702	0.814244	0.053579
C	-0.888991	0.086553	0.200705	C	-0.888991	0.086553	0.200705
D	0.835280	2.504167	-1.054512	D	0.835280	2.504167	-1.054512
D	1.380706	2.457777	0.683302	D	1.380706	2.457777	0.683302
H	-1.725043	1.088245	-0.475804	D	-1.725043	1.088245	-0.475804
D	-1.923344	2.086626	-0.687100	H	-1.923344	2.086626	-0.687100
[i6g]→**p2c**				[i6h]→**p2b**			
							
-39.4 kJ mol^{-1}				-39.4 kJ mol^{-1}			
C_1 – ^{1}A				C_1 – ^{1}A			
Si	-1.178923	2.205371	0.803390	Si	-1.178923	2.205371	0.803390
C	0.641206	2.137118	-0.050763	C	0.641206	2.137118	-0.050763
C	0.130702	0.814244	0.053579	C	0.130702	0.814244	0.053579
C	-0.888991	0.086553	0.200705	C	-0.888991	0.086553	0.200705
D	0.835280	2.504167	-1.054512	H	0.835280	2.504167	-1.054512
H	1.380706	2.457777	0.683302	D	1.380706	2.457777	0.683302
D	-1.725043	1.088245	-0.475804	D	-1.725043	1.088245	-0.475804
D	-1.923344	2.086626	-0.687100	D	-1.923344	2.086626	-0.687100

[i13a]→**p2a**				[i13b]→**p2a**			
							
-42.3 kJ mol^{-1}				-43.1 kJ mol^{-1}			
C_1 – ^{1}A				C_1 – ^{1}A			
Si	-0.830773	0.883817	0.953003	Si	-0.830773	0.883817	0.953003
C	-1.811287	-0.696687	0.301549	C	-1.811287	-0.696687	0.301549
C	-0.590983	-0.923847	0.102221	C	-0.590983	-0.923847	0.102221
C	0.749568	-0.461799	-0.040845	C	0.749568	-0.461799	-0.040845
D	1.185475	-0.546441	-1.038520	D	1.185475	-0.546441	-1.038520
D	1.455315	-0.696271	0.749183	D	1.455315	-0.696271	0.749183
D	0.271987	0.942873	-0.437740	H	0.271987	0.942873	-0.437740
H	-0.545547	1.525644	-0.576927	D	-0.545547	1.525644	-0.576927
[i13b]→**p2b**				[i13b]→**p2c**			
							
-39.9 kJ mol^{-1}				-39.7 kJ mol^{-1}			
C_1 – ^{1}A				C_1 – ^{1}A			
Si	-0.830773	0.883817	0.953003	Si	-0.830773	0.883817	0.953003
C	-1.811287	-0.696687	0.301549	C	-1.811287	-0.696687	0.301549
C	-0.590983	-0.923847	0.102221	C	-0.590983	-0.923847	0.102221
C	0.749568	-0.461799	-0.040845	C	0.749568	-0.461799	-0.040845
H	1.185475	-0.546441	-1.038520	D	1.185475	-0.546441	-1.038520
D	1.455315	-0.696271	0.749183	H	1.455315	-0.696271	0.749183
D	0.271987	0.942873	-0.437740	D	0.271987	0.942873	-0.437740
D	-0.545547	1.525644	-0.576927	D	-0.545547	1.525644	-0.576927

[i12a]→**p3a**				[i12b]→**p3c**			
							
-64.2 kJ mol^{-1}				-66.3 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-1.151997	1.718947	0.728726	Si	-1.151997	1.718947	0.728726
C	-0.793552	-0.036891	0.485201	C	-0.793552	-0.036891	0.485201
C	0.356363	-0.744575	0.018188	C	0.356363	-0.744575	0.018188
C	1.337204	-1.326892	-0.364743	C	1.337204	-1.326892	-0.364743
D	-1.597641	-0.704860	0.800559	D	-1.597641	-0.704860	0.800559
H	2.205962	-1.845464	-0.696218	D	2.205962	-1.845464	-0.696218
D	-0.463884	1.036474	-0.582223	D	-0.463884	1.036474	-0.582223
D	0.061553	1.931814	-0.358027	H	0.061553	1.931814	-0.358027
[i12c]→**p3c**				[i12d]→**p3b**			
							
-66.8 kJ mol^{-1}				-63.6 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-1.151997	1.718947	0.728726	Si	-1.151997	1.718947	0.728726
C	-0.793552	-0.036891	0.485201	C	-0.793552	-0.036891	0.485201
C	0.356363	-0.744575	0.018188	C	0.356363	-0.744575	0.018188
C	1.337204	-1.326892	-0.364743	C	1.337204	-1.326892	-0.364743
D	-1.597641	-0.704860	0.800559	H	-1.597641	-0.704860	0.800559
D	2.205962	-1.845464	-0.696218	D	2.205962	-1.845464	-0.696218
H	-0.463884	1.036474	-0.582223	D	-0.463884	1.036474	-0.582223
D	0.061553	1.931814	-0.358027	D	0.061553	1.931814	-0.358027

[i12a]→**p3a′**				[i12b]→**p3c′**			
							
-69.9 kJ mol^{-1}				-71.9 kJ mol^{-1}			
C_1 – ^{1}A				C_1 – ^{1}A			
Si	-1.555112	0.642765	0.911988	Si	-1.555112	0.642765	0.911988
C	0.049390	0.418870	0.114001	C	0.049390	0.418870	0.114001
C	0.581034	-0.893905	-0.073288	C	0.581034	-0.893905	-0.073288
C	1.006592	-2.011224	-0.207659	C	1.006592	-2.011224	-0.207659
D	0.726733	1.208649	-0.209397	D	0.726733	1.208649	-0.209397
H	1.387736	-2.997804	-0.330653	D	1.387736	-2.997804	-0.330653
D	-1.435106	2.141508	0.235326	H	-1.435106	2.141508	0.235326
D	-1.002771	1.445970	-0.426216	D	-1.002771	1.445970	-0.426216
[i12c]→**p3b′**				[i12d]→**p3c′**			
							
-69.2 kJ mol^{-1}				-72.6 kJ mol^{-1}			
C_1 – ^{1}A				C_1 – ^{1}A			
Si	-1.555112	0.642765	0.911988	Si	-1.555112	0.642765	0.911988
C	0.049390	0.418870	0.114001	C	0.049390	0.418870	0.114001
C	0.581034	-0.893905	-0.073288	C	0.581034	-0.893905	-0.073288
C	1.006592	-2.011224	-0.207659	C	1.006592	-2.011224	-0.207659
H	0.726733	1.208649	-0.209397	D	0.726733	1.208649	-0.209397
D	1.387736	-2.997804	-0.330653	D	1.387736	-2.997804	-0.330653
D	-1.435106	2.141508	0.235326	D	-1.435106	2.141508	0.235326
D	-1.002771	1.445970	-0.426216	H	-1.002771	1.445970	-0.426216

[i6a]→**p4a**				[i6b]→**p4b**			
							
-107.7 kJ mol^{-1}				-109.7 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	0.831125	0.640403	0.777373	Si	0.831125	0.640403	0.777373
C	-1.185225	0.266693	0.157410	C	-1.185225	0.266693	0.157410
C	-0.415827	-0.797532	0.102736	C	-0.415827	-0.797532	0.102736
C	0.854625	-1.135711	0.195070	C	0.854625	-1.135711	0.195070
D	-2.051331	0.445181	0.777573	D	-2.051331	0.445181	0.777573
H	1.482402	-1.878498	-0.264555	D	1.482402	-1.878498	-0.264555
D	-0.203090	1.162708	-0.807825	D	-0.203090	1.162708	-0.807825
D	0.676107	1.295027	-0.933420	H	0.676107	1.295027	-0.933420
[i6c]→**p4a**				[i6d]→**p4b**			
							
-107.7 kJ mol^{-1}				-110.6 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	0.831125	0.640403	0.777373	Si	0.831125	0.640403	0.777373
C	-1.185225	0.266693	0.157410	C	-1.185225	0.266693	0.157410
C	-0.415827	-0.797532	0.102736	C	-0.415827	-0.797532	0.102736
C	0.854625	-1.135711	0.195070	C	0.854625	-1.135711	0.195070
H	-2.051331	0.445181	0.777573	D	-2.051331	0.445181	0.777573
D	1.482402	-1.878498	-0.264555	D	1.482402	-1.878498	-0.264555
D	-0.203090	1.162708	-0.807825	H	-0.203090	1.162708	-0.807825
D	0.676107	1.295027	-0.933420	D	0.676107	1.295027	-0.933420

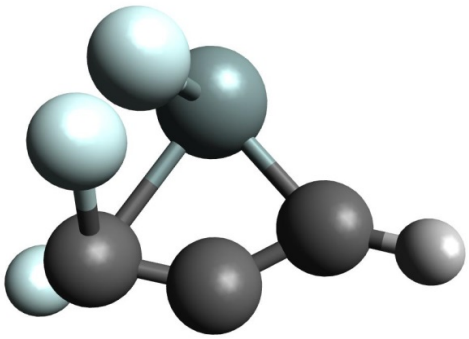
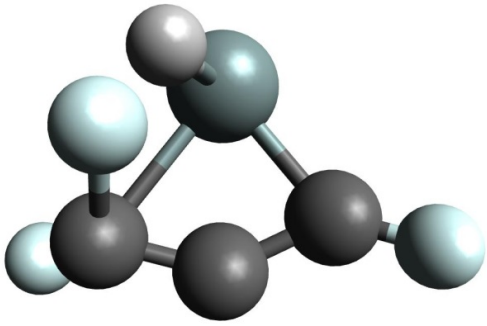
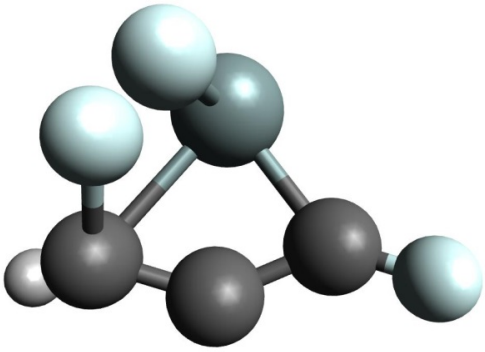
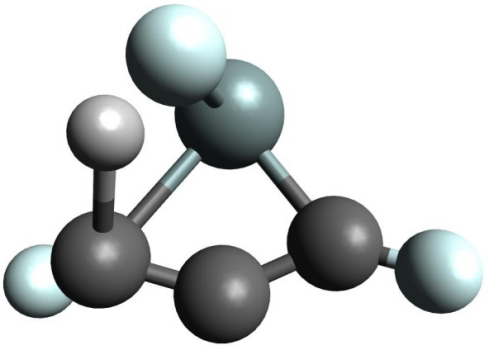
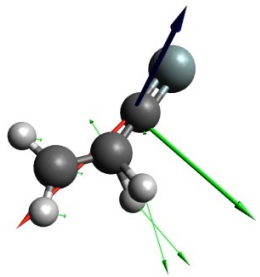
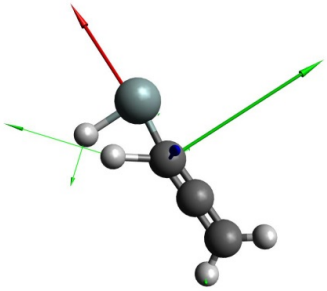
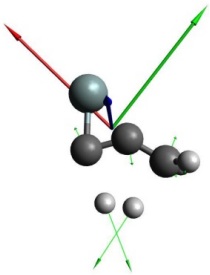
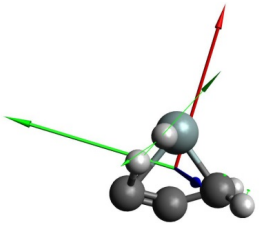
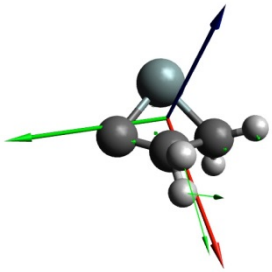
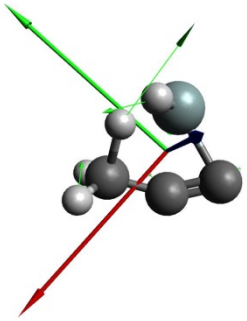
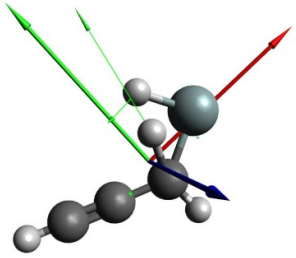
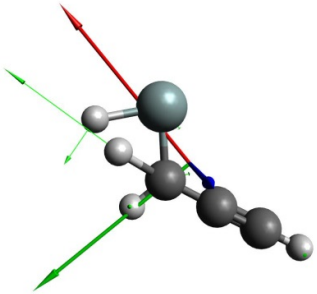
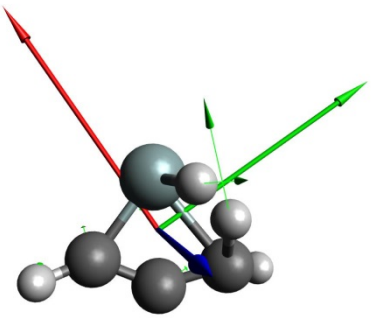
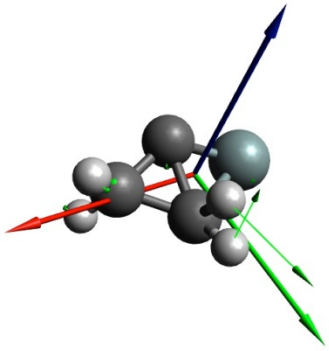
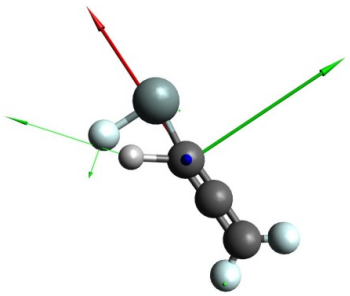
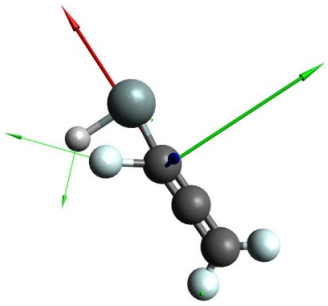
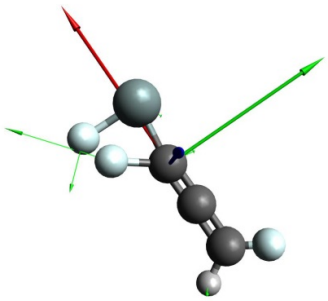
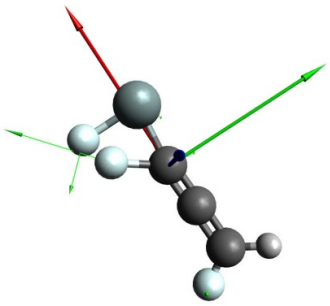
[i6e]→**p4a**				[i6f]→**p4b**			
							
-107.7 kJ mol^{-1}				-109.7 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-0.831125	0.640403	0.777373	Si	-0.831125	0.640403	0.777373
C	1.185225	0.266693	0.157410	C	1.185225	0.266693	0.157410
C	0.415827	-0.797532	0.102736	C	0.415827	-0.797532	0.102736
C	-0.854625	-1.135711	0.195070	C	-0.854625	-1.135711	0.195070
D	2.051331	0.445181	0.777573	D	2.051331	0.445181	0.777573
H	-1.482402	-1.878498	-0.264555	D	-1.482402	-1.878498	-0.264555
D	0.203090	1.162708	-0.807825	D	0.203090	1.162708	-0.807825
D	-0.676107	1.295027	-0.933420	H	-0.676107	1.295027	-0.933420
[i6g]→**p4a**				[i6h]→**p4b**			
							
-107.7 kJ mol^{-1}				-110.6 kJ mol^{-1}			
$C_1 - {}^1A$				$C_1 - {}^1A$			
Si	-0.831125	0.640403	0.777373	Si	-0.831125	0.640403	0.777373
C	1.185225	0.266693	0.157410	C	1.185225	0.266693	0.157410
C	0.415827	-0.797532	0.102736	C	0.415827	-0.797532	0.102736
C	-0.854625	-1.135711	0.195070	C	-0.854625	-1.135711	0.195070
H	2.051331	0.445181	0.777573	D	2.051331	0.445181	0.777573
D	-1.482402	-1.878498	-0.264555	D	-1.482402	-1.878498	-0.264555
D	0.203090	1.162708	-0.807825	H	0.203090	1.162708	-0.807825
D	-0.676107	1.295027	-0.933420	D	-0.676107	1.295027	-0.933420

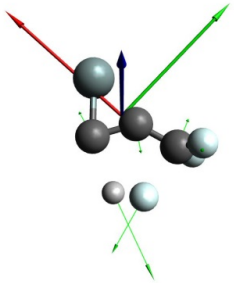
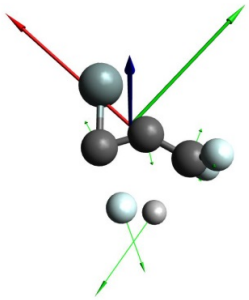
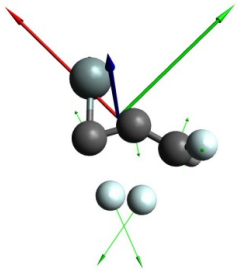
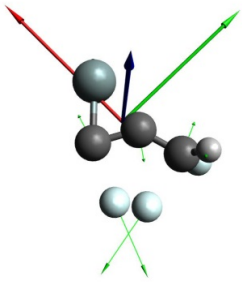
Table S3: Geometries of exit transition states for the emission of H_2/HD/D_2 and angles of emission relative to the three principal axes.

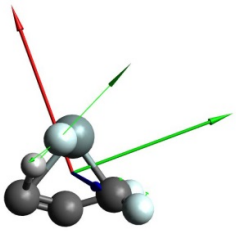
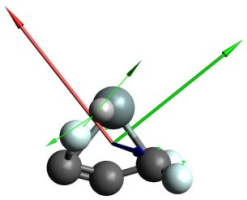
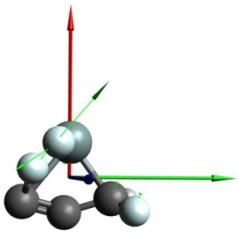
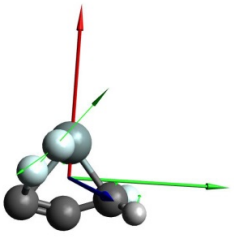
Transition State	Structure	I (amu a_0^2)	Θ(°)
[i5]→**p1**		35.6	111.4°
		704.3	158.6°
		736.8	90.1°
[i9]→**p1**		22.4	118.1°
		748.2	28.1°
		768.9	90.1°
[i1]→**p2**		90.8	128.3°
		418.3	141.7°
		496.9	90.0°
[i6]→**p2**		187.7	63.2°
		215.7	96.5°
		364.0	27.7°

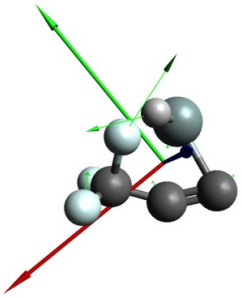
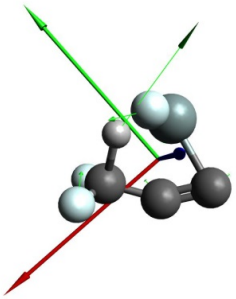
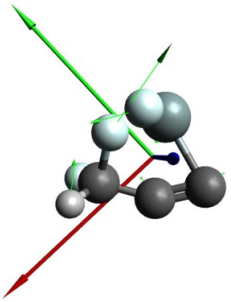
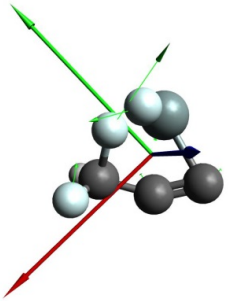
[i11]→**p2**		175.7	146.1º
		215.1	83.4º
		356.6	56.9º
[i13]→**p2**		171.1	109.3º
		238.0	80.4º
		373.2	21.7º
[i12]→**p3**		50.2	95.2º
		647.7	11.0º
		690.1	99.7º
[i12]→**p3′**		66.2	33.2º
		598.2	58.0º
		658.3	98.0º

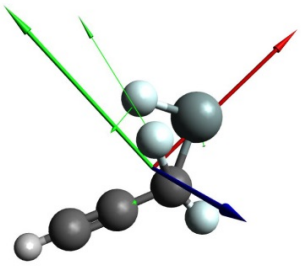
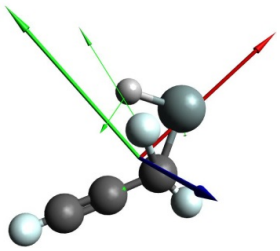
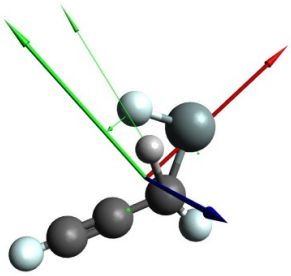
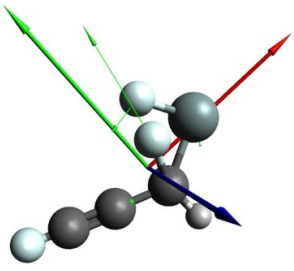
[i6]→**p4**		176.8	67.9º
		212.0	84.3º
		349.2	22.9º
[i11]→**p5**		89.0	107.6º
		341.2	65.3º
		395.7	31.1º

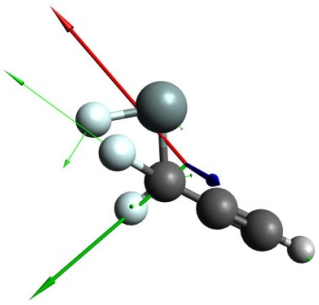
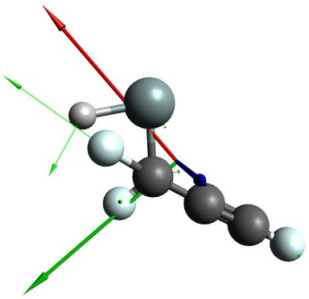
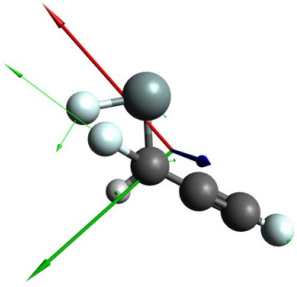
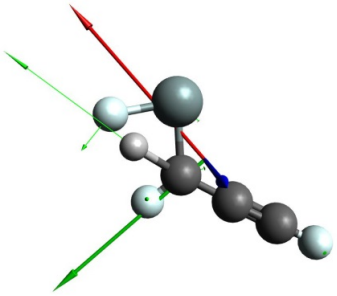
[i9a]→**p1a**		37.1	115.9º
		828.8	25.9º
		863.6	91.5º
[i9b]→**p1a**		34.5	121.4º
		820.3	31.4º
		851.5	89.8º
[i9c]→**p1b**		39.6	119.3º
		797.2	29.3º
		833.9	89.4º
[i9d]→**p1b**		39.0	117.9º
		798.2	27.9º
		834.4	88.9º

[i1a]→**p2a**		107.3	127.8º
		479.7	142.2º
		562.6	90.0º
[i1b]→**p2a**		113.0	127.4º
		470.7	142.6º
		559.4	90.0º
[i1b]→**p2b**		113.0	129.9º
		465.0	140.1º
		560.2	89.2º
[i1b]→**p2c**		113.0	129.9º
		465.0	140.1º
		560.2	90.8º

[i6a]→**p2a**		225.7	74.3º
		236.0	71.9º
		394.3	24.3º
[i6b]→**p2a**		224.2	78.7º
		230.1	61.5º
		395.3	31.0º
[i6c]→**p2b**		220.3	65.9º
		234.8	76.6º
		385.0	28.0º
[i6d]→**p2c**		221.4	63.6º
		231.7	82.0º
		387.0	27.8º

[i13a]→**p2a**		188.4	110.6º
		274.5	76.1º
		409.4	25.2º
[i13b]→**p2a**		192.1	104.7º
		278.9	77.3º
		408.6	19.6º
[i13b]→**p2b**		196.5	110.3º
		264.0	75.7º
		396.0	25.3º
[i13b]→**p2c**		192.9	106.4º
		268.0	73.8º
		400.9	23.4º

[i12a]→**p3a**		73.6	95.1º
		653.7	8.4º
		713.5	96.7º
[i12b]→**p3c**		66.5	93.0º
		692.6	8.8º
		746.0	98.2º
[i12c]→**p3c**		71.2	98.5º
		692.5	12.0º
		754.7	98.3º
[i12d]→**p3b**		64.2	95.8º
		695.3	9.0º
		746.0	96.8º

[i12a]→**p3a′**		87.9	31.9º
		625.2	59.0º
		701.9	96.7º
[i12b]→**p3c′**		86.2	28.7º
		646.4	62.4º
		721.8	97.1º
[i12c]→**p3b′**		78.4	30.7º
		665.6	60.2º
		733.4	96.9º
[i12d]→**p3c′**		84.1	34.6º
		657.3	56.5º
		734.1	97.7º

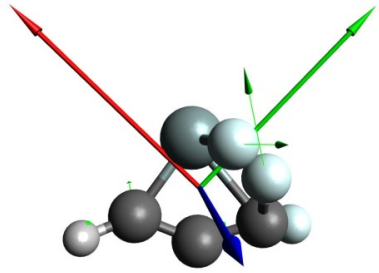
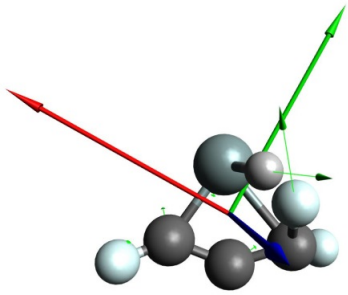
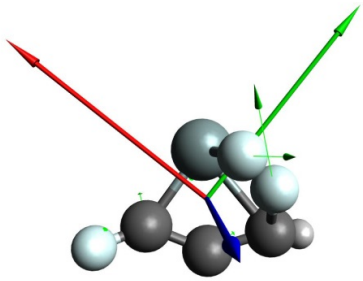
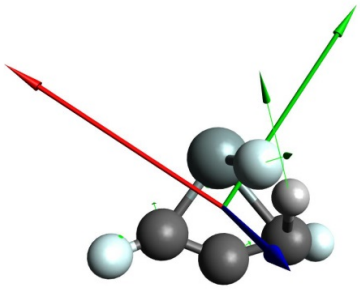
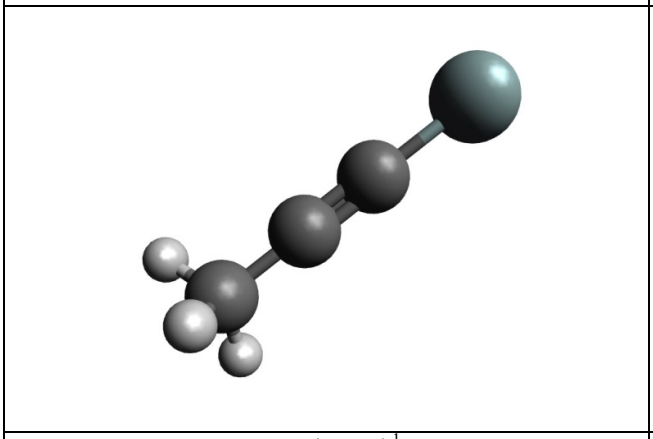
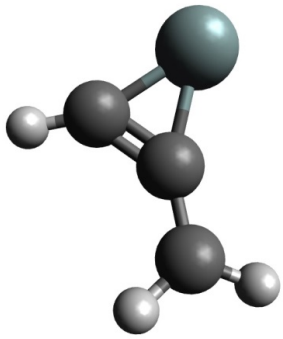
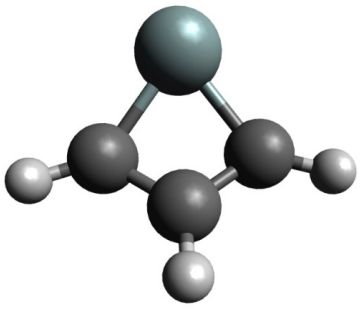
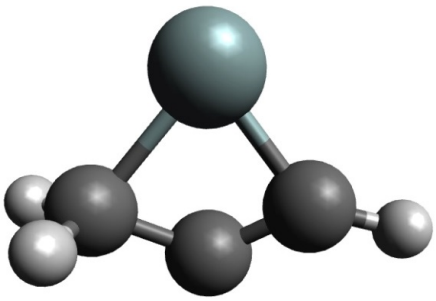
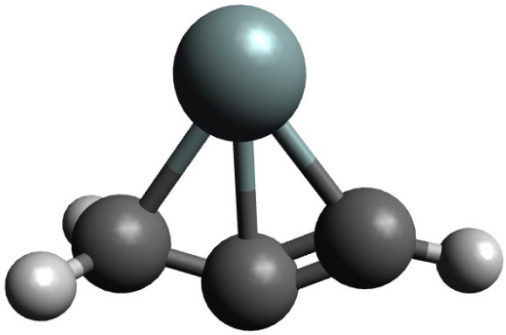
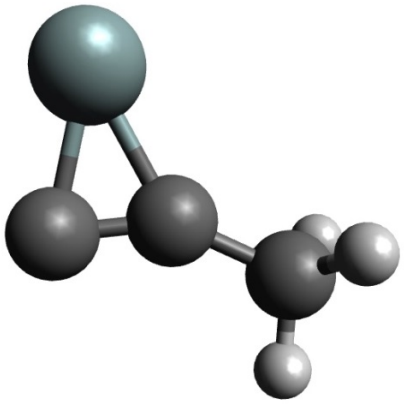
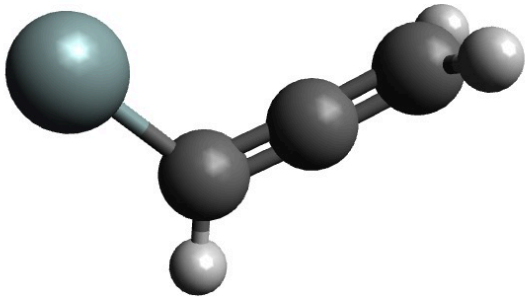
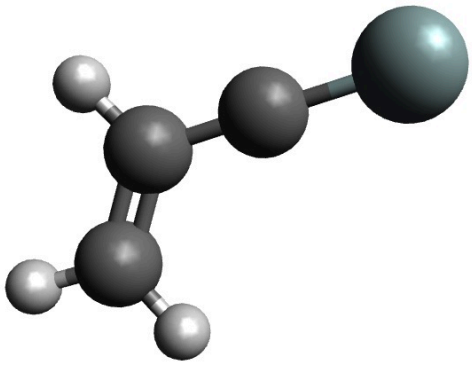
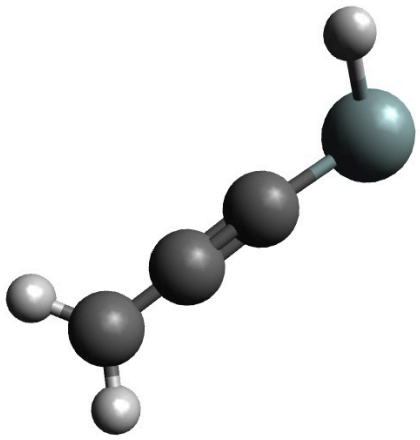
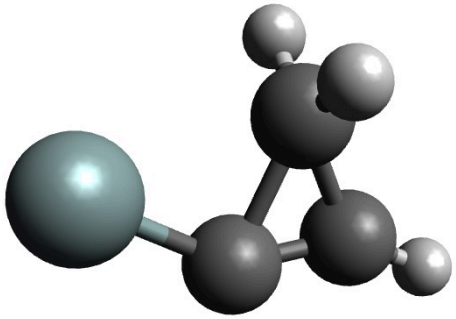
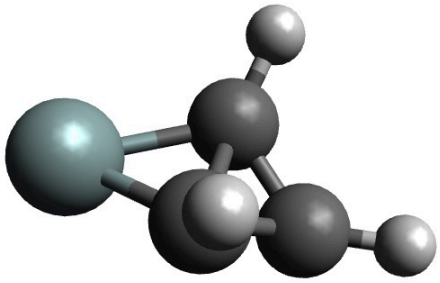
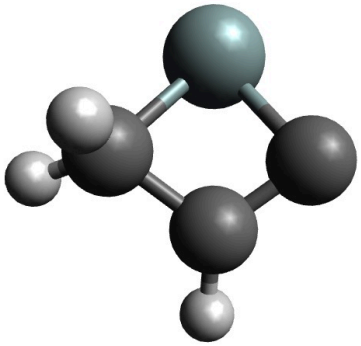
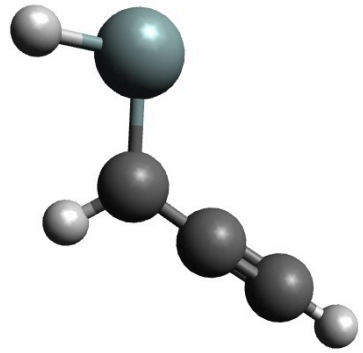
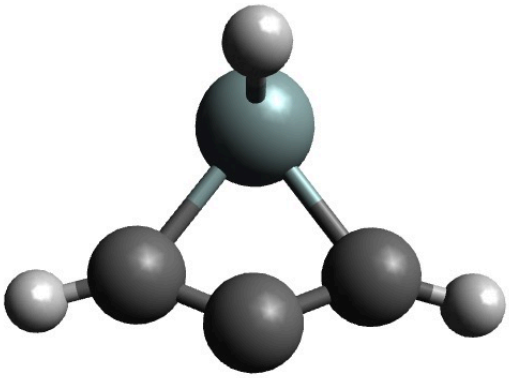
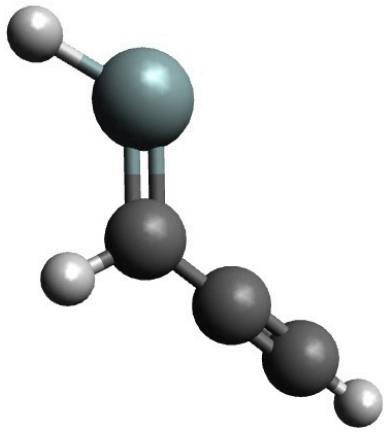
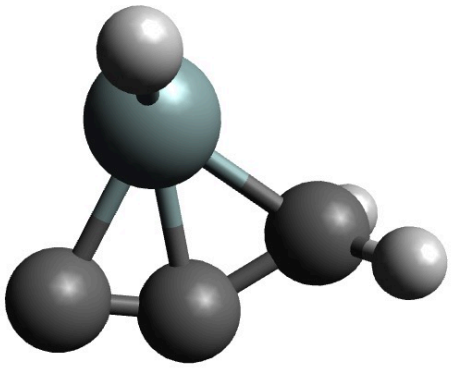
[i6a]→**p4a**		204.1	69.2º
		244.8	76.1º
		374.4	25.3º
[i6b]→**p4b**		206.1	71.0º
		241.3	73.8º
		390.5	25.4º
[i6c]→**p4a**		216.4	72.3º
		231.5	74.5º
		376.2	23.9º
[i6d]→**p4b**		210.3	70.7º
		242.8	76.8º
		389.9	23.7º

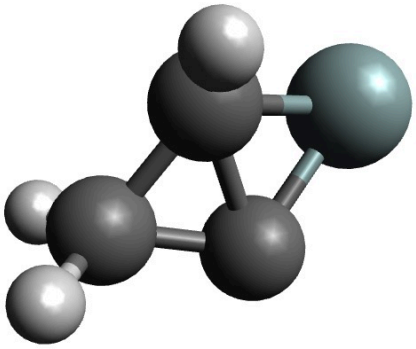
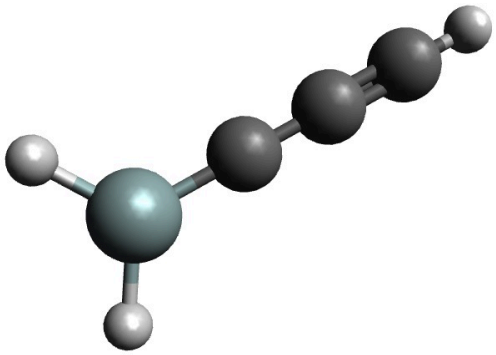
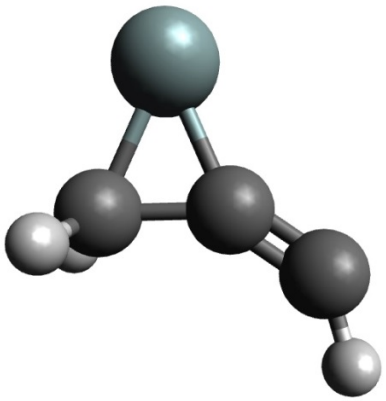
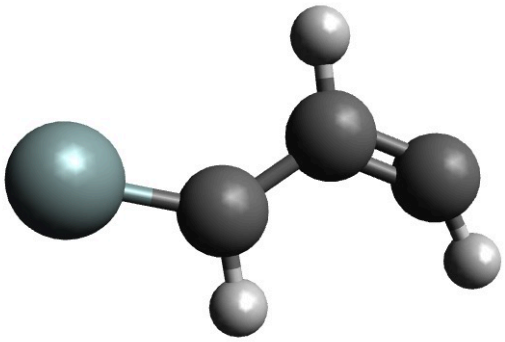
Table S4: Products relevant to the reaction of electronically excited atomic silicon with methylacetylene/allene to form atomic hydrogen and SiC_3H_3. Geometries were calculated at the ωB97X-V//cc-pVTZ level of theory; relative energies were calculated at the CCSD(T)//CBS level of theory.

SiC_3H_3 + H Products							
n1				**n2**			
							
-10.0 kJ mol^{-1}				3.9 kJ mol^{-1}			
C_{3v}-$^2A_1$				C_s – $^2A'$			
Si	2.256938	0.386814	-0.000054	Si	-1.648670	1.864824	-0.639004
C	0.452597	0.445576	0.001238	C	-3.059962	0.865119	-0.096199
C	-0.767469	0.480303	0.004880	C	-1.956341	0.083084	-0.283303
C	-2.224034	0.526369	0.004637	C	-1.616436	-1.271962	-0.143675
H	-2.643608	-0.348009	-0.498856	H	-2.264110	-1.960263	0.392886
H	-2.561104	1.418906	-0.528946	H	-0.692145	-1.662759	-0.553724
H	-2.617180	0.570276	1.023216	H	-4.087409	0.662816	0.185587
n3				**n4**			
							
7.0 kJ mol^{-1}				11.4 kJ mol^{-1}			
C_s – $^2A'$				C_1 – ^2A			
Si	1.265159	2.162075	-0.444465	Si	1.208012	2.089231	-0.448538
C	-0.607874	2.024234	-0.328499	C	-0.745936	2.116845	-0.093209
C	0.896654	0.500285	0.357941	C	0.910530	0.446506	0.329165
C	-0.395785	0.642838	-0.176604	C	-0.351043	0.718990	-0.018821
H	-1.518838	2.509970	-0.653582	H	-1.431207	2.427755	-0.878519
H	-1.060126	-0.160934	-0.504981	H	-0.968549	2.572982	0.868603
H	1.374406	-0.420749	0.666057	H	1.419426	-0.479092	0.553088

n5				**n6**			
							
11.5 kJ mol^{-1}				24.4 kJ mol^{-1}			
$C_s - {}^2A'$				$C_s - {}^2A'$			
Si	-0.357120	1.246352	-0.941397	Si	-1.573453	1.860263	-0.624254
C	-0.224659	-0.413295	0.358340	C	-3.053427	0.877832	-0.162194
C	-1.552969	-0.035456	0.272406	C	-2.014789	0.087378	-0.128936
C	0.911547	-0.089182	-0.083811	C	-1.441504	-1.261433	0.109938
H	-2.226882	-0.652993	-0.312865	H	-2.222907	-1.968179	0.399486
H	-1.995601	0.484661	1.115990	H	-0.947918	-1.627458	-0.792862
H	1.959706	-0.318373	-0.071805	H	-0.690455	-1.217933	0.901573
n7				**n8**			
							
33.1 kJ mol^{-1}				45.1 kJ mol^{-1}			
$C_s - {}^2A'$				$C_s - {}^2A'$			
Si	-2.187581	1.634287	1.295559	Si	-2.654104	0.750695	0.461772
C	0.051611	1.182614	-0.115557	C	0.054200	2.167105	0.127665
C	1.314261	1.492673	-0.038176	C	1.204947	1.500096	-0.166927
C	-1.232532	0.906849	-0.142409	C	-1.174983	1.525933	0.279596
H	1.718281	2.306210	-0.630132	H	0.101347	3.249863	0.248999
H	1.982839	0.942873	0.614082	H	2.148416	2.023473	-0.279824
H	-1.605409	0.188127	-0.870198	H	1.196132	0.423506	-0.294711

n9				**n10**			
							
62.1 kJ mol^{-1}				72.1 kJ mol^{-1}			
C_1-^{1}A				C_s – ^{2}A′			
Si	-2.291802	2.588971	1.004979	Si	1.258456	2.565463	1.003571
C	0.397110	1.552862	0.026512	C	-0.623501	1.956099	-0.193860
C	1.610713	1.062007	-0.294224	C	0.616569	1.034679	0.382244
C	-0.724745	2.021162	0.301926	C	-0.361129	0.485074	-0.277162
H	-2.437580	3.782829	0.074313	H	-0.481565	2.545990	-1.097167
H	2.447989	1.727500	-0.468446	H	-1.405388	2.291595	0.484508
H	1.769210	-0.006354	-0.382326	H	-0.795541	-0.412938	-0.675421
n11				**n12**			
							
80.2 kJ mol^{-1}				92.2 kJ mol^{-1}			
C_s – ^{2}A′				C_1-^{2}A			
Si	-2.574063	2.832638	0.123250	Si	1.209442	2.097470	-0.530517
C	-1.238260	1.527070	0.101728	C	-0.698444	2.114228	-0.082086
C	-2.654502	1.156447	0.943789	C	0.871270	0.519741	0.408493
C	-1.892585	0.264449	0.139078	C	-0.386726	0.642348	-0.077667
H	-1.517244	-0.732291	0.331673	H	-1.404686	2.446373	-0.846667
H	-2.823994	0.955161	2.000984	H	-0.946638	2.519689	0.893844
H	-0.211210	1.638921	0.447506	H	-1.011254	-0.121945	-0.542215

n13				**n14**			
							
95.3 kJ mol^{-1}				96.2 kJ mol^{-1}			
C_1-^{2}A				C_s – ^{2}A′			
Si	-0.985382	2.986144	1.021451	Si	1.266892	2.417929	0.545124
C	-1.112970	1.510143	-0.086940	C	-0.513422	2.108452	-0.345251
C	-0.249537	0.428763	0.000560	C	1.220128	0.475897	0.012334
C	0.510002	-0.511322	0.124227	C	0.113298	0.965102	-0.496432
H	-2.442307	3.405788	0.874610	H	2.016603	2.947139	-0.672214
H	-1.803839	1.493576	-0.929501	H	-1.434786	2.608535	-0.574972
H	1.175602	-1.336872	0.224343	H	1.790465	-0.429923	0.089828
n15				**n16**			
							
100.5 kJ mol^{-1}				103.4 kJ mol^{-1}			
C_s – ^{2}A′				C_1-^{2}A			
Si	-1.190224	2.801061	0.833141	Si	1.193399	2.298845	0.391243
C	-1.168840	1.085298	0.732883	C	-0.704840	2.116248	-0.023680
C	-0.098546	0.262454	0.301977	C	1.226452	0.404007	-0.057734
C	0.810323	-0.436603	-0.063699	C	0.069526	0.893913	-0.211514
H	-2.431565	3.480292	1.319383	H	1.934239	3.126046	-0.613101
H	-2.086989	0.582431	1.037028	H	-1.095714	2.589399	-0.921264
H	1.612611	-1.057174	-0.386591	H	-1.404169	2.114579	0.807277

n17				**n18**			
							
108.7 kJ mol^{-1}				117.5 kJ mol^{-1}			
C_1-^{2}A				C_{2v}-$^2A_1$			
Si	-2.464141	2.945399	0.274357	Si	-2.311951	2.797319	0.436930
C	-1.402738	1.539986	0.017239	C	-1.347058	1.427980	0.366860
C	-2.656658	1.177833	0.870404	C	-0.579950	0.339258	0.311177
C	-1.964943	0.185393	-0.030971	C	0.125545	-0.661917	0.259982
H	-1.409247	-0.612469	0.460416	H	-1.741994	4.155135	0.537058
H	-2.744651	0.954547	1.933667	H	-3.785613	2.721926	0.402298
H	-2.472267	-0.129035	-0.938397	H	0.738262	-1.531412	0.215476
n19				**n20**			
							
142.3 kJ mol^{-1}				162.9 kJ mol^{-1}			
$C_s - ^2A'$				$C_s - ^2A'$			
Si	0.043742	3.154114	-0.166368	Si	-2.830058	1.396545	0.563817
C	-0.724823	1.416847	-0.148213	C	0.020435	1.929632	0.104027
C	0.785745	1.448685	-0.065657	C	1.226258	1.487302	-0.182331
C	1.844977	0.723600	0.018307	C	-1.178048	1.088902	0.213717
H	-1.148970	1.007794	-1.064990	H	-0.107872	2.998903	0.273833
H	-1.249067	1.071020	0.742447	H	1.697174	0.537596	-0.400024
H	2.139985	-0.317762	0.070963	H	-1.007629	0.017638	0.036540

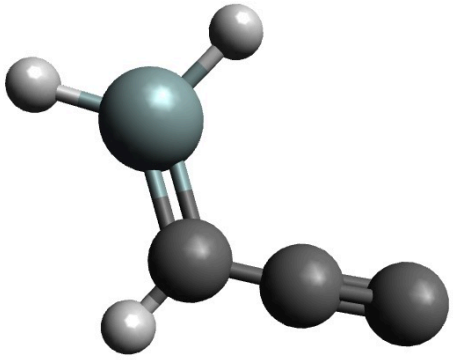
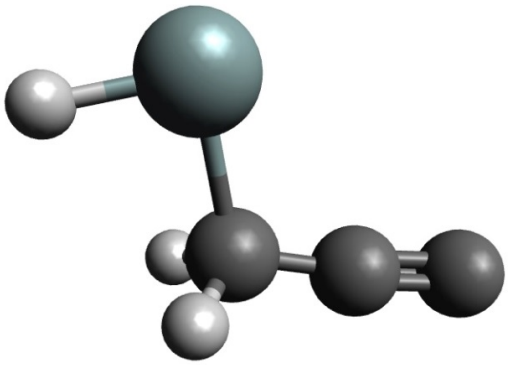
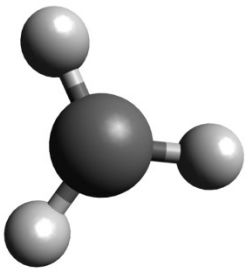
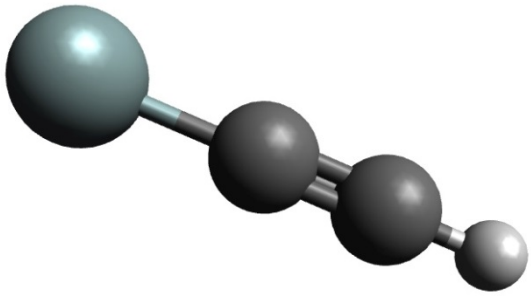
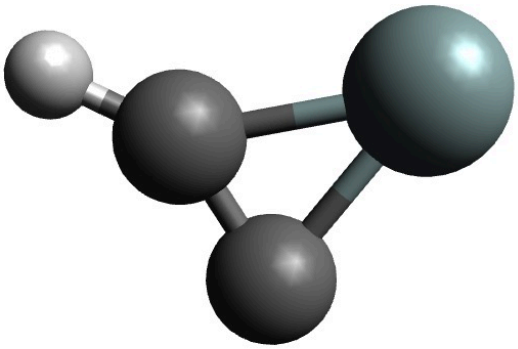
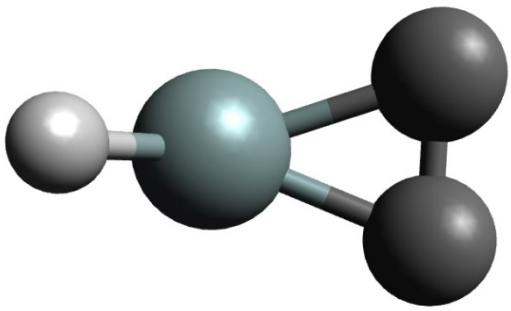
n21				n22			
							
221.1 kJ mol^{-1}				303.6 kJ mol^{-1}			
$C_s - {}^2A'$				$C_s - {}^2A'$			
Si	-2.111813	2.725963	0.436207	Si	-0.952202	2.895186	1.046884
C	-0.502023	2.028434	0.423706	C	-1.442045	1.273467	0.049434
C	-0.381293	0.665379	0.337252	C	-0.404343	0.306776	0.063506
C	-0.337798	-0.605402	0.255140	C	0.600189	-0.477548	0.149868
H	-2.333611	4.183554	0.526784	H	-2.310437	3.508799	0.720181
H	-3.302425	1.864084	0.355458	H	-1.683793	1.658231	-0.950735
H	0.387891	2.652209	0.482682	H	-2.368134	0.945547	0.540814

Table S5: Products relevant to the reaction of electronically excited atomic silicon with methylacetylene/allene to form methyl radical and SiC_2H. Geometries were calculated at the ωB97X-V//cc-pVTZ level of theory; relative energies were calculated at the CCSD(T)//CBS level of theory.

$SiC_2H + CH_3$ Products							
CH_3				**m1**			
							
--				-30.0 kJ mol^{-1}			
$D_{3h} - {}^2A''_2$				$C_{\infty v} - {}^2\Pi$			
C	-0.951849	0.641383	0.030228	Si	-2.442919	0.826756	0.000000
H	0.066970	0.283748	-0.012939	C	-0.664513	1.191684	0.000000
H	-1.461269	0.932347	-0.877290	C	0.527499	1.436282	0.000000
H	-1.461264	0.707991	0.980921	H	1.572824	1.650730	0.000000
m2				**m3**			
							
-5.0 kJ mol^{-1}				144.5 kJ mol^{-1}			
$C_s - {}^2A'$				$C_s - {}^2A'$			
Si	-0.263369	1.916480	0.123746	Si	-0.098748	1.527158	-0.929747
C	1.306779	2.912456	-0.144538	C	-0.713212	0.293539	0.287855
C	1.559669	1.640124	-0.007267	C	0.539217	0.390597	0.368126
H	1.692598	3.909459	-0.305242	H	-0.233597	3.003472	-0.658751

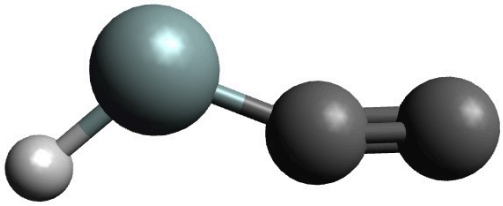
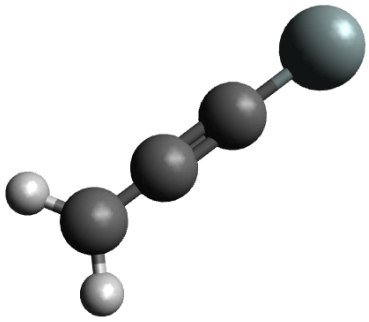
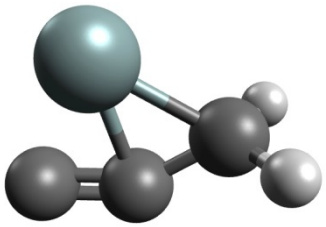
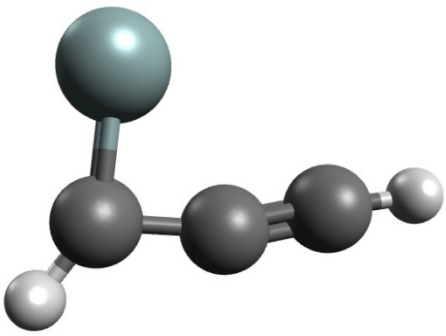
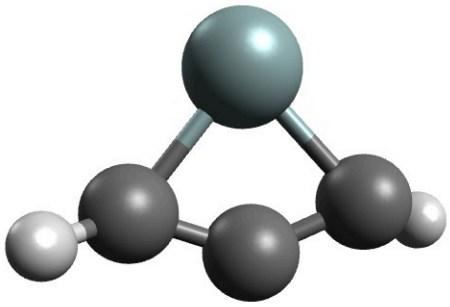
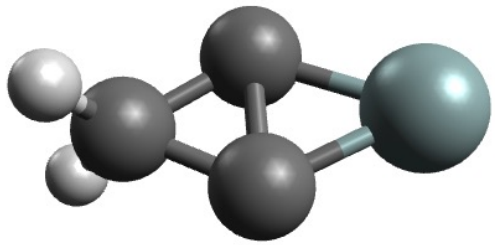
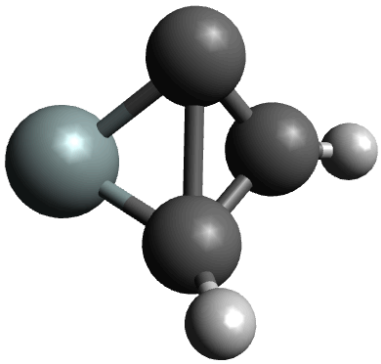
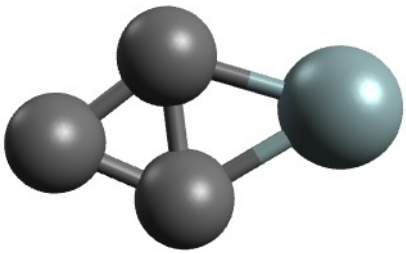
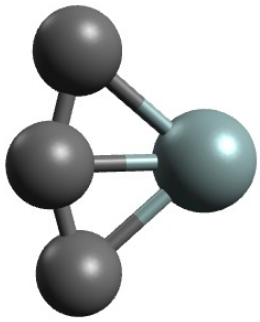
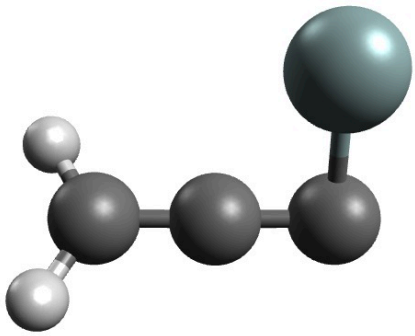
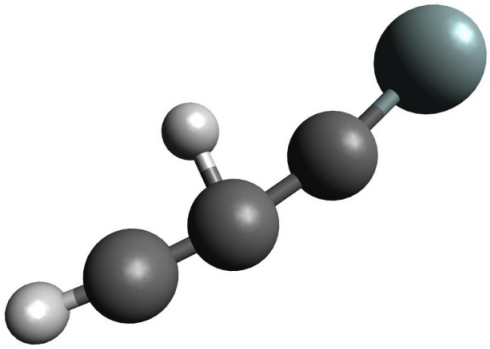
m4			
			
159.2 kJ mol^{-1}			
$C_s - {}^2A'$			
Si	-1.052457	2.186941	0.048100
C	0.478917	1.465532	0.044356
C	1.698811	1.296828	-0.287872
H	-2.136410	1.624032	0.921397

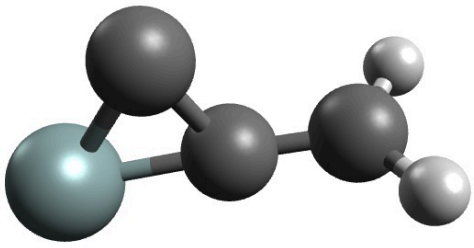
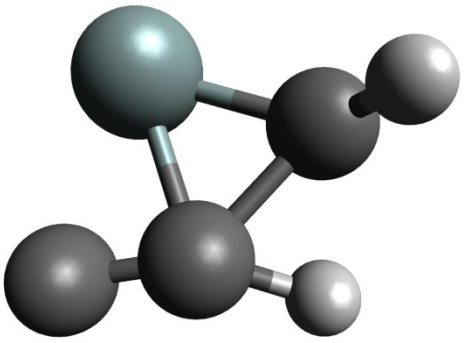
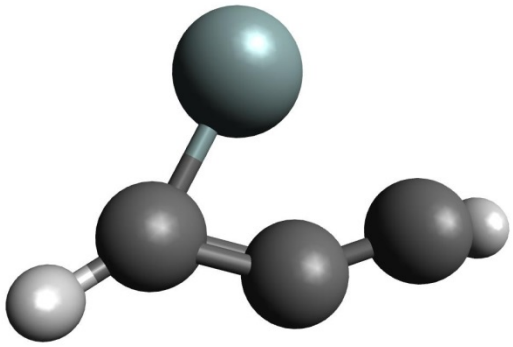
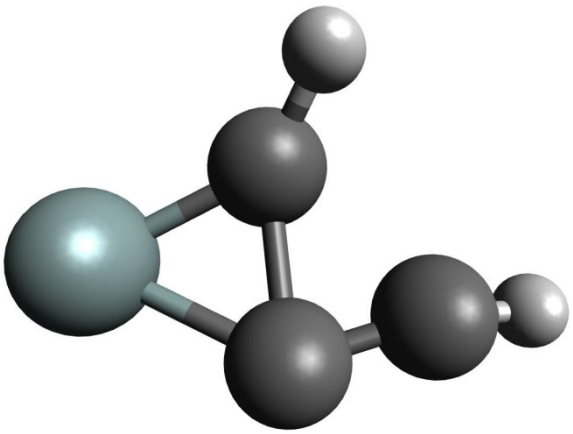
Table S6: Reactants, products, intermediates, and transition state structures relevant to the singlet SiC_3H_2 system. Geometries were calculated at the ωB97X-V//cc-pVTZ level of theory; relative energies were calculated at the CCSD(T)//CBS level of theory.

Reactants (SiC_3H_2)							
p1				**p2**			
							
0 kJ mol^{-1}				15.7 kJ mol^{-1}			
C_{2v} – $^1A_1$				C_s – $^1A'$			
Si	-2.667415	2.191276	0.000000	Si	-3.530077	0.607099	0.333008
C	-0.985018	2.220382	0.000000	C	-2.115964	1.751749	-0.167586
C	0.298405	2.242563	0.000000	C	-1.762971	0.449585	-0.634584
C	1.607796	2.265203	0.000000	C	-2.980050	2.474570	0.443216
H	2.142021	3.207971	0.000000	H	-0.954113	-0.065250	-0.122807
H	2.174299	1.341470	0.000000	H	-1.792019	0.273905	-1.706863
p3				**p4**			
							
26.2 kJ mol^{-1}				30.3 kJ mol^{-1}			
C_s – $^1A'$				C_s – $^1A'$			
Si	-1.497455	1.581760	-1.469801	Si	0.015583	1.421694	0.441321
C	-1.339958	2.070906	0.170228	C	-1.710909	1.657474	1.228824
C	0.014251	1.630794	0.108585	C	-1.833196	1.452865	-0.080188
C	1.093044	1.182725	-0.237854	C	-1.051473	1.232997	-1.134185
H	-1.794955	2.499942	1.048186	H	-2.213088	1.188068	2.060067
H	2.054975	0.801432	-0.489589	H	-1.030405	1.710504	-2.101157

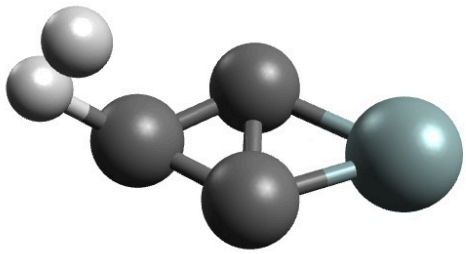
p5				**p6**			
							
51.0 kJ mol^{-1}				89.8 kJ mol^{-1}			
$C_{2v} - {}^1A_1$				$C_1 - {}^1A$			
Si	-0.153925	2.791130	0.597108	Si	0.000000	0.000000	0.000000
C	-0.701267	1.901637	-0.854814	C	0.000000	0.000000	1.806628
C	-1.470675	0.643621	-0.899626	C	-1.286808	0.627089	1.815653
C	-1.079103	1.277031	0.374194	C	-0.765193	1.502612	0.924959
H	-0.958764	-0.265564	-1.204780	H	0.697327	0.000000	2.637474
H	-2.515112	0.686694	-1.198739	H	-2.217623	0.494213	2.353974
Products (SiC_3)							
[1]				**[2]**			
							
327.1 kJ mol^{-1}				332.4 kJ mol^{-1}			
$C_{2v} - {}^1A_1$				$C_{2v} - {}^1A_1$			
Si	-3.475749	2.641607	0.512311	Si	-3.427362	1.625193	1.036789
C	-2.415184	1.166612	0.747246	C	-2.211335	0.501827	-0.133135
C	-2.016023	1.994725	-0.385703	C	-2.242047	1.804914	-0.422423
C	-1.293928	0.804610	-0.061731	C	-2.684682	3.045589	-0.204463

[3]			
			
394.5 kJ mol^{-1}			
$C_{\infty v}$-$^1\Pi$			
Si	-2.145893	0.448617	-0.269059
C	-0.515622	0.067722	0.114369
C	0.708771	-0.218171	0.402492
C	1.942409	-0.506338	0.693099

Transition States (SiC_3H_2)							
p1-p2				**p1-p3**			
							
73.7 kJ mol^{-1}				292.3 kJ mol^{-1}			
C_1-^1A				$C_s - {}^1A'$			
Si	-1.658581	1.905372	0.779310	Si	-2.507882	1.510190	-1.237408
C	-1.148281	2.429951	-0.785493	C	-1.349116	0.507922	-0.612484
C	0.093463	2.368595	-0.368703	C	-0.344930	-0.152986	0.049360
C	1.352227	2.282628	0.047174	C	0.577768	-0.599243	0.746176
H	2.023595	3.126519	-0.048111	H	-0.353452	0.864522	0.641182
H	1.729586	1.348340	0.442558	H	1.360507	-0.908868	1.399559

p2-p5				p2-p6			
							
216.6 kJ mol^{-1}				326.5 kJ mol^{-1}			
C_s-$^1A'$				C_s – $^1A'$			
Si	-1.747415	2.192117	0.631384	Si	-0.055032	1.783261	0.075704
C	-0.726407	2.290059	-0.882772	C	-1.168897	0.125688	-0.408579
C	0.016254	2.219441	0.409350	C	-1.787386	1.063113	0.218017
C	1.348831	2.236480	0.302214	C	-1.427514	2.444367	1.067918
H	1.899910	3.173627	0.295983	H	-2.035607	3.266860	0.681532
H	1.914855	1.315559	0.186033	H	-2.549883	1.381730	1.028390
p3-p4				**p3-p6**			
							
34.8 kJ mol^{-1}				190.5 kJ mol^{-1}			
C_1-^1A				C_s – $^1A'$			
Si	-1.069242	1.492753	-1.390925	Si	-1.913929	1.504303	-1.242424
C	-1.320148	1.984111	0.282526	C	-0.837758	2.188007	-0.048120
C	0.040325	1.733392	0.253700	C	-0.271626	0.758029	-0.566567
C	1.042599	1.415660	-0.447969	C	0.707158	1.171608	0.093043
H	-1.929010	2.506285	0.997954	H	-0.902898	2.598930	0.949658
H	1.756851	0.623631	-0.570277	H	1.716663	1.490465	0.251411

p5-[1]

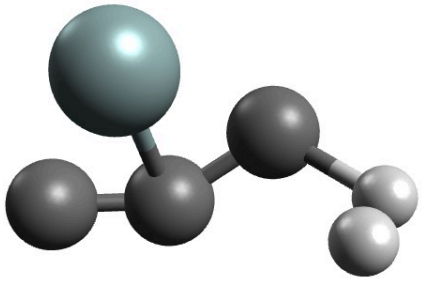


417.8 kJ mol^{-1}

C_s-$^1A'$

Si	-0.467866	3.174918	0.595550
C	-0.477089	2.021651	-0.792545
C	-0.673171	0.590493	-0.708054
C	-0.877286	1.422661	0.457992
H	-1.559940	-0.070334	-1.308318
H	-2.249902	0.491914	-1.259838

p2-[2]

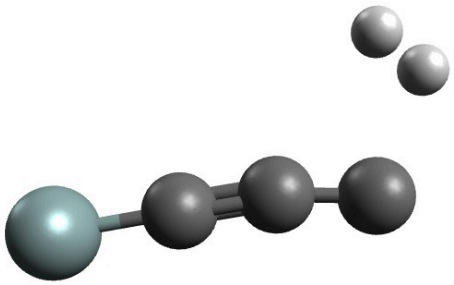


400.4 kJ mol^{-1}

C_1-^1A

Si	-3.654008	0.659771	0.202068
C	-3.156407	2.579324	0.092405
C	-2.151736	1.771052	-0.080262
C	-1.646692	0.497172	0.138953
H	-1.557132	-0.024346	-1.630107
H	-1.044179	-0.140306	-1.013032

p1-[3]

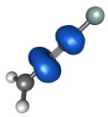
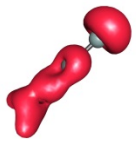
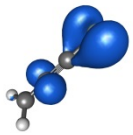
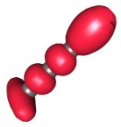
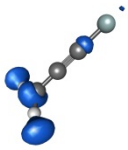
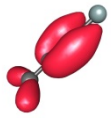
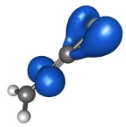
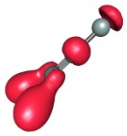
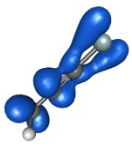
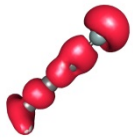


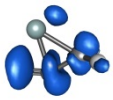
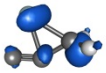
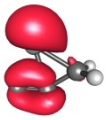
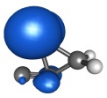
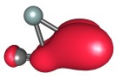
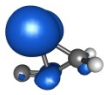
412.5 kJ mol^{-1}

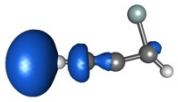
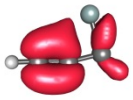
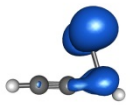
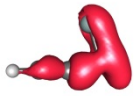
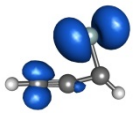
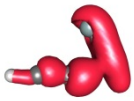
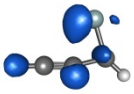
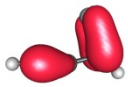
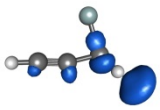
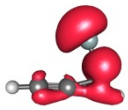
C_s-$^1A'$

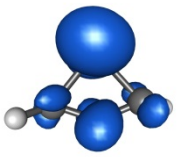
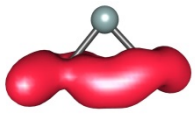
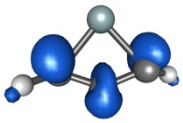
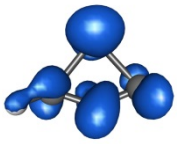
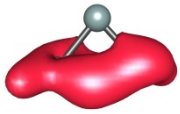
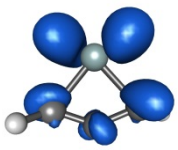
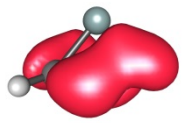
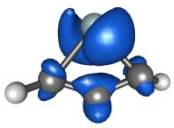
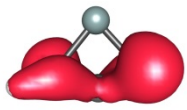
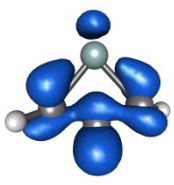
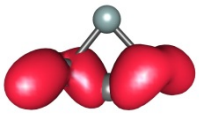
Si	-1.284546	0.614725	0.341830
C	0.280930	-0.071001	0.309093
C	1.457679	-0.594085	0.274620
C	2.575093	-1.242370	0.051990
H	3.725873	-0.775049	1.241686
H	3.408591	-0.262386	1.718808

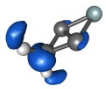
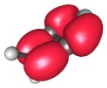
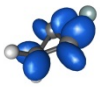
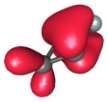
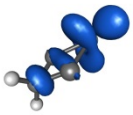
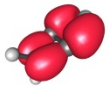
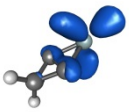
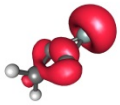
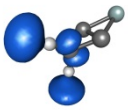
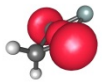
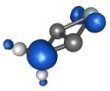
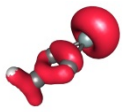
Table S7: Excited states of six SiC_3H_2 isomers **p1-p6** along with excitation energies (eV) in the region of a Lyman-α photon.

p1						
State	Excitation Energy	Oscillator Strength	Symmetry	Major Amplitudes	Attachment Density	Detachment Density
42	9.865	5.61×10^{-2}	$^1A_1$	$2b_2 \rightarrow 4b_2 = 0.300$ $2b_1 \rightarrow 5b_1 = -0.199$ $11a_1 \rightarrow 12a_1 = -0.440$ $11a_1 \rightarrow 13a_1 = -0.179$ $3b_2 \rightarrow 5b_2 = -0.277$ $3b_1 \rightarrow 5b_1 = -0.196$		
46	10.074	1.99×10^{-4}	$^1B_2$	$9a_1 \rightarrow 4b_2 = 0.225$ $10a_1 \rightarrow 4b_2 = 0.617$		
47	10.175	6.77×10^{-2}	$^1B_2$	$3b_2 \rightarrow 13a_1 = 0.675$		
50	10.430	0.177	$^1A_1$	$2b_2 \rightarrow 4b_2 = 0.546$ $11a_1 \rightarrow 12a_1 = 0.225$ $11a_1 \rightarrow 14a_1 = -0.190$ $3b_2 \rightarrow 5b_2 = 0.165$ $3b_1 \rightarrow 5b_1 = 0.161$		
52	10.544	2.45×10^{-2}	$^1B_1$	$10a_1 \rightarrow 4b_1 = 0.454$ $11a_1 \rightarrow 5b_1 = -0.440$ $3b_1 \rightarrow 6b_1 = -0.257$		

p2						
State	Excitation Energy	Oscillator Strength	Symmetry	Major Amplitudes	Attachment Density	Detachment Density
46	10.029	0.538	$^1A'$	12a′→17a′ = 0.375 3a″→5a″ = 0.313 13a′→17a′ = -0.369		
49	10.207	0.203	$^1A'$	13a′→18a′ = 0.633		
50	10.320	1.04×10^{-3}	$^1A''$	11a′→4a″ = -0.365 3a″→17a′ = -0.159 3a″→17a′ = 0.553		
51	10.436	0.235	$^1A'$	2a″→4a″ = 0.637		
52	10.588	0.182	$^1A''$	11a′→4a″ = 0.566 3a″→18a′ = 0.371		

p3						
State	Excitation Energy	Oscillator Strength	Symmetry	Major Amplitudes	Attachment Density	Detachment Density
48	9.879	1.30×10^{-2}	$^1A'$	13a′→18a′ = 0.574 14a′→18a′ = -0.343		
49	9.957	1.08×10^{-2}	$^1A''$	12a′→4a″ = 0.612 3a″→20a′ = -0.279		
50	10.007	0.178	$^1A'$	12a′→15a′ = 0.620		
51	10.220	1.81×10^{-2}	$^1A''$	3a″→21a′ = 0.650		
55	10.678	0.120	$^1A'$	14a′→18a′ = 0.195 14a′→19a′ = 0.580		

p4						
State	Excitation Energy	Oscillator Strength	Symmetry	Major Amplitudes	Attachment Density	Detachment Density
43	9.826	2.49×10^{-2}	^{1}A	5b→8b = 0.534 6b→9b = -0.237 6b→10b = -0.348		
44	9.889	0.895	^{1}B	7b→11a = 0.163 7b→12a = 0.560 9a→9b = 0.249 10a→10b = -0.177		
47	10.207	0.248	^{1}A	8a→11a = 0.169 5b→8b = 0.384 6b→9b = 0.231 6b→10b = 0.426 9a→11a = 0.164		
50	10.422	5.62×10^{-2}	^{1}A	6b→9b = 0.575 6b→10b = -0.320		
52	10.507	0.147	^{1}B	8a→8b = -0.168 5b→11a = -0.251 10a→12b = 0.602		
53	10.598	5.95×10^{-3}	^{1}B	5b→11a = 0.618 10a→12b = 0.259		

p5						
State	Excitation Energy	Oscillator Strength	Symmetry	Major Amplitudes	Attachment Density	Detachment Density
40	9.778	1.17×10^{-2}	$^1B_2$	$4b_2 \rightarrow 11a_1 = 0.621$ $4b_2 \rightarrow 12a_1 = -0.264$		
41	9.848	5.06×10^{-7}	$^1A_2$	$3b_1 \rightarrow 6b_2 = 0.678$		
42	9.909	1.32×10^{-2}	$^1B_2$	$4b_2 \rightarrow 11a_1 = 0.259$ $4b_2 \rightarrow 12a_1 = 0.636$		
44	10.025	0.499	$^1A_1$	$9a_1 \rightarrow 11a_1 = -0.155$ $9a_1 \rightarrow 12a_1 = 0.659$		
46	10.156	1.17×10^{-2}	$^1B_1$	$9a_1 \rightarrow 5b_1 = 0.208$ $10a_1 \rightarrow 5b_1 = 0.666$		
50	10.468	0.436	$^1A_1$	$9a_1 \rightarrow 11a_1 = 0.589$ $9a_1 \rightarrow 13a_1 = 0.154$ $3b_1 \rightarrow 5b_1 = 0.201$ $10a_1 \rightarrow 11a_1 = -0.155$ $10a_1 \rightarrow 13a_1 = -0.186$		

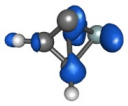
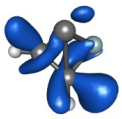
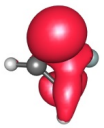
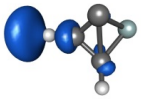
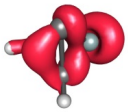
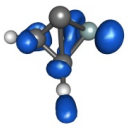
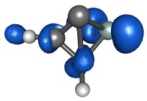
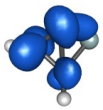
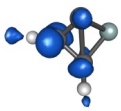
p6						
State	Excitation Energy	Oscillator Strength	Symmetry	Major Amplitudes	Attachment Density	Detachment Density
45	9.801	0.158	^{1}A	15a→22a = 0.554 16a→23a = 0.291 16a→24a = 0.195		
47	9.857	5.58×10^{-2}	^{1}A	17a→25a = 0.673		
49	9.991	4.45×10^{-2}	^{1}A	13a→18a = 0.167 15a→22a = -0.286 16a→22a = 0.162 16a→23a = 0.572		
51	10.154	4.37×10^{-2}	^{1}A	13a→18a = 0.410 15a→23a = 0.228 16a→22a = 0.160 16a→23a = -0.201 16a→24a = 0.382		
53	10.236	0.187	^{1}A	13a→18a = -0.451 15a→23a = 0.367 16a→24a = 0.259		
54	10.292	2.07×10^{-2}	^{1}A	13a→19a = 0.573 15a→23a = 0.321		
57	10.338	5.44×10^{-2}	^{1}A	13a→19a = 0.317 15a→23a = -0.403 16a→24a = 0.381		

Table S8: Products relevant to the photodissociation of SiC_3H_2 to form atomic hydrogen and SiC_3H. Geometries were calculated at the ωB97X-V//cc-pVTZ level of theory; relative energies were calculated at the CCSD(T)//CBS level of theory.

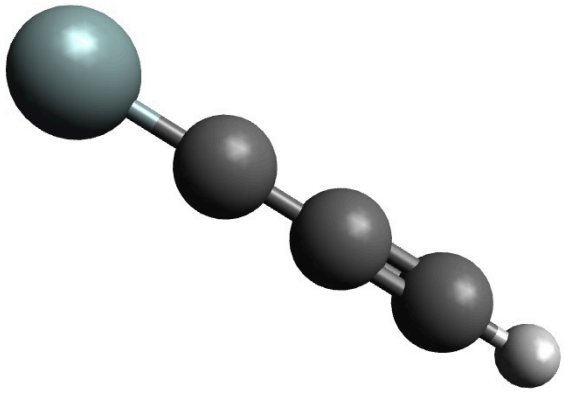
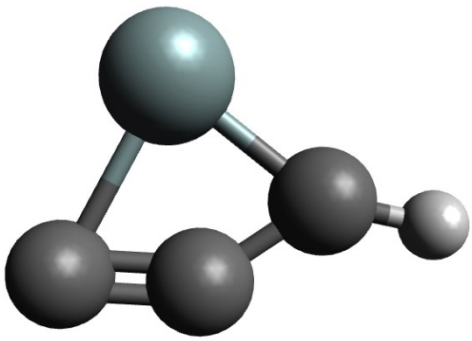
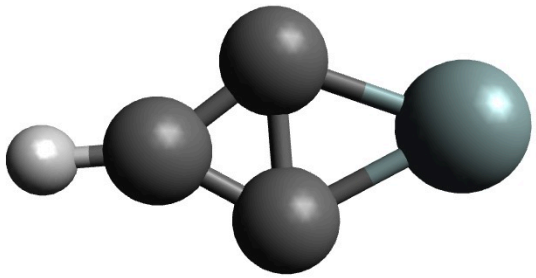
SiC_3H + H Products							
1				**2**			
							
386.9 kJ mol^{-1}				399.7 kJ mol^{-1}			
$C_{\infty v}$ – $^2\Pi$				C_s – $^2A'$			
Si	-0.151031	2.995567	0.000000	Si	0.160190	2.314648	0.000000
C	-0.284810	1.318339	0.000000	C	1.981786	2.002412	0.000000
C	-0.391670	-0.020999	0.000000	C	1.341367	0.789581	0.000000
C	-0.488903	-1.239734	0.000000	C	0.164322	0.230650	0.000000
H	-0.573593	-2.301281	0.000000	H	3.012843	2.311956	0.000000
3							
							
409.7 kJ mol^{-1}							
C_{2v}-$^2A_1$							
Si	0.375572	2.261711	0.000000				
C	-0.388292	0.542499	0.000000				
C	1.102760	0.526660	0.000000				
C	0.345057	-0.611559	0.000000				
H	0.333627	-1.686713	0.000000				

Table S9: Tunneling-corrected RRKM reaction rate constants, transition state imaginary frequencies, and reaction path degeneracies for the silicon–methylacetylene, silicon–allene, and silicon–D3-methylacetlyene systems.

Reaction	k_f (s^{-1})	k_b (s^{-1})	ω_b (cm^{-1})	Forward Reaction Path Degeneracy	Backward Reaction Path Degeneracy
[i1]→[i2]	3.74×10^{6}	5.64×10^{7}	1235	2	1
[i1]→[i4]	1.37×10^{11}	5.67×10^{10}	168	2	2
[i1]→[i5]	3.44×10^{8}	2.88×10^{9}	1399	2	2
[i1]→[i6]	6.03×10^{7}	1.39×10^{9}	1018	2	1
[i2]→[i5]	8.55×10^{12}	4.76×10^{12}	190	1	2
[i2]→[i10]	2.78×10^{5}	1.52×10^{6}	1207	1	2
[i4]→[i13]	1.45×10^{11}	6.54×10^{12}	203	2	2
[i5]→[i9]	1.04×10^{11}	2.38×10^{11}	883	2	2
[i6]→[i9]	4.62×10^{12}	3.83×10^{12}	240	1	2
[i6]→[i10]	1.16×10^{10}	4.13×10^{10}	989	1	2
[i6]→[i12]	3.73×10^{12}	3.22×10^{12}	217	1	2
[i7]→[i10]	7.49×10^{11}	3.28×10^{12}	124	2	2
[i8]→[i9]	2.05×10^{7}	5.54×10^{7}	1532	2	2
[i8]→[i12]	2.11×10^{9}	5.95×10^{9}	1082	2	2
[i9]→**p1**	1.36×10^{9}		1470	2	
[i1]→**p2**	4.81×10^{2}		1225	1	
[i6]→**p2**	8.41×10^{6}		1429	1	
[i13]→**p2**	1.09×10^{7}		1399	2	
[i12]→**p3**	1.65×10^{8}		1475	2	
[i12]→**p3′**	2.49×10^{8}		1424	2	
[i6]→**p4**	1.97×10^{9}		908	1	
[i1]→**n2**	1.47×10^{5}			1	
[i13]→**n6**	1.39×10^{5}			1	
[i1]→**n6**	6.58×10^{3}			1	
[i2]→**n3**	4.94×10^{5}			1	
[i2]→**n4**	7.54×10^{4}			1	
[i4]→**n1**	4.11×10^{6}			1	
[i6]→**n4**	2.32×10^{5}			1	
[i1]→**m2**	5.40×10^{5}			1	

Reaction	k_f (s^{-1})	k_b (s^{-1})	ω_b (cm^{-1})	Forward Reaction Path Degeneracy	Backward Reaction Path Degeneracy
[i1a]→[i2a]	1.28×10^{6}	1.93×10^{7}	977	1	1
[i1b]→[i2b]	1.56×10^{6}	2.33×10^{7}	1184	1	1
[i1b]→[i2c]	1.34×10^{6}	1.99×10^{7}	1006	1	1
[i1b]→[i2d]	1.35×10^{6}	2.01×10^{7}	1000	1	1
[i1a]→[i2e]	1.28×10^{6}	1.93×10^{7}	977	1	1
[i1b]→[i2f]	1.56×10^{6}	2.33×10^{7}	1184	1	1
[i1b]→[i2g]	1.34×10^{6}	1.99×10^{7}	1006	1	1
[i1b]→[i2h]	1.35×10^{6}	2.01×10^{7}	1000	1	1
[i1a]→[i4a]	9.67×10^{10}	4.35×10^{10}	166	2	2
[i1b]→[i4b]	9.27×10^{10}	5.44×10^{10}	152	2	2
[i1a]→[i5a]	1.49×10^{8}	1.48×10^{9}	1063	2	2
[i1b]→[i5b]	2.00×10^{8}	1.93×10^{9}	1371	2	2
[i1b]→[i5c]	1.57×10^{8}	1.58×10^{9}	1075	2	2
[i1b]→[i5d]	1.53×10^{8}	1.51×10^{9}	1078	2	2
[i1a]→[i6a]	2.58×10^{7}	6.60×10^{8}	801	1	1
[i1b]→[i6b]	3.44×10^{7}	8.92×10^{8}	993	1	1
[i1b]→[i6c]	2.50×10^{7}	6.49×10^{8}	803	1	1
[i1b]→[i6d]	2.53×10^{7}	6.55×10^{8}	816	1	1
[i1a]→[i6e]	2.58×10^{7}	6.60×10^{8}	801	1	1
[i1b]→[i6f]	3.44×10^{7}	8.92×10^{8}	993	1	1
[i1b]→[i6g]	2.50×10^{7}	6.49×10^{8}	803	1	1
[i1b]→[i6h]	2.53×10^{7}	6.55×10^{8}	816	1	1
[i2a]→[i2e]	3.64×10^{12}	3.64×10^{12}	227	1	1
[i2b]→[i2f]	3.98×10^{12}	3.98×10^{12}	249	1	1
[i2c]→[i2h]	3.65×10^{12}	3.68×10^{12}	229	1	1
[i2d]→[i2g]	3.68×10^{12}	3.65×10^{12}	229	1	1
[i2a]→[i3a]	9.68×10^{9}	1.04×10^{11}	587	1	1
[i2b]→[i3d]	8.81×10^{9}	9.40×10^{10}	551	1	1
[i2c]→[i3c]	9.22×10^{9}	1.02×10^{11}	589	1	1
[i2d]→[i3b]	9.12×10^{9}	1.01×10^{11}	566	1	1
[i2e]→[i3d]	9.68×10^{9}	1.04×10^{11}	587	1	1
[i2f]→[i3a]	8.81×10^{9}	9.40×10^{10}	551	1	1
[i2g]→[i3c]	9.22×10^{9}	1.02×10^{11}	589	1	1
[i2d]→[i3b]	9.12×10^{9}	1.01×10^{11}	566	1	1
[i2a]→[i5a]	6.86×10^{12}	4.52×10^{12}	177	1	1
[i2b]→[i5b]	6.17×10^{12}	3.98×10^{12}	161	1	1
[i2c]→[i5c]	5.79×10^{12}	3.93×10^{12}	155	1	1
[i2d]→[i5d]	6.08×10^{12}	4.00×10^{12}	160	1	1
[i2e]→[i5a]	6.86×10^{12}	4.52×10^{12}	177	1	1
[i2f]→[i5b]	6.17×10^{12}	3.98×10^{12}	161	1	1
[i2g]→[i5c]	5.79×10^{12}	3.93×10^{12}	155	1	1

[i2h]→[i5d]	6.08×10^{12}	4.00×10^{12}	160	1	1
[i2a]→[i10d]	5.41×10^{4}	3.34×10^{5}	912	1	1
[i2b]→[i10c]	9.27×10^{4}	5.70×10^{5}	1195	1	1
[i2c]→[i10b]	5.41×10^{4}	3.34×10^{5}	903	1	1
[i2d]→[i10a]	5.28×10^{4}	3.26×10^{5}	903	1	1
[i2e]→[i10b]	5.41×10^{4}	3.34×10^{5}	912	1	1
[i2f]→[i10a]	9.27×10^{4}	5.70×10^{5}	1195	1	1
[i2g]→[i10d]	5.41×10^{4}	3.34×10^{5}	903	1	1
[i2h]→[i10c]	5.28×10^{4}	3.26×10^{5}	903	1	1
[i4a]→[i13a]	1.16×10^{11}	6.46×10^{12}	202	2	2
[i4b]→[i13b]	1.28×10^{11}	5.47×10^{12}	171	2	2
[i5a]→[i9a]	7.40×10^{10}	7.21×10^{10}	706	2	2
[i5b]→[i9b]	8.26×10^{10}	8.19×10^{10}	832	2	2
[i5c]→[i9d]	7.22×10^{10}	6.91×10^{10}	706	2	2
[i5d]→[i9c]	7.01×10^{10}	6.89×10^{10}	716	2	2
[i6a]→[i9a]	3.40×10^{12}	1.29×10^{12}	199	1	1
[i6b]→[i9b]	4.04×10^{12}	1.49×10^{12}	224	1	1
[i6c]→[i9c]	3.61×10^{12}	1.34×10^{12}	205	1	1
[i6d]→[i9d]	3.47×10^{12}	1.29×10^{12}	197	1	1
[i6e]→[i9a]	3.40×10^{12}	1.29×10^{12}	199	1	1
[i6f]→[i9b]	4.04×10^{12}	1.49×10^{12}	224	1	1
[i6g]→[i9d]	3.61×10^{12}	1.34×10^{12}	205	1	1
[i6h]→[i9c]	3.47×10^{12}	1.29×10^{12}	197	1	1
[i6a]→[i10b]	6.54×10^{9}	2.39×10^{10}	795	1	1
[i6b]→[i10a]	8.57×10^{9}	3.05×10^{10}	980	1	1
[i6c]→[i10d]	6.42×10^{9}	2.26×10^{10}	794	1	1
[i6d]→[i10c]	6.65×10^{9}	2.36×10^{10}	794	1	1
[i6e]→[i10d]	6.54×10^{9}	2.39×10^{10}	795	1	1
[i6f]→[i10c]	8.57×10^{9}	3.05×10^{10}	980	1	1
[i6g]→[i10b]	6.42×10^{9}	2.26×10^{10}	794	1	1
[i6h]→[i10a]	6.65×10^{9}	2.36×10^{10}	794	1	1
[i6a]→[i12a]	2.39×10^{12}	2.39×10^{12}	163	1	1
[i6b]→[i12b]	3.32×10^{12}	3.10×10^{12}	213	1	1
[i6c]→[i12d]	2.52×10^{12}	2.39×10^{12}	163	1	1
[i6d]→[i12c]	2.42×10^{12}	2.29×10^{12}	163	1	1
[i6e]→[i12a]	2.39×10^{12}	2.39×10^{12}	163	1	1
[i6f]→[i12b]	3.32×10^{12}	3.10×10^{12}	213	1	1
[i6g]→[i12c]	2.52×10^{12}	2.39×10^{12}	163	1	1
[i6h]→[i12d]	2.42×10^{12}	2.29×10^{12}	163	1	1
[i7a]→[i10a]	6.96×10^{11}	3.07×10^{12}	116	2	2
[i7b]→[i10b]	7.04×10^{11}	3.09×10^{12}	116	2	2
[i7c]→[i10d]	6.86×10^{11}	3.08×10^{12}	117	2	2
[i7d]→[i10c]	7.29×10^{11}	3.21×10^{12}	123	2	2
[i8a]→[i9d]	4.65×10^{6}	5.06×10^{6}	1134	2	2
[i8b]→[i9c]	7.22×10^{6}	8.24×10^{6}	1498	2	2

[i8c]→[i9b]	5.32×10^{6}	5.90×10^{6}	1148	2	2
[i8d]→[i9a]	4.54×10^{6}	5.21×10^{6}	1134	2	2
[i8a]→[i12a]	8.84×10^{8}	2.51×10^{9}	789	2	2
[i8b]→[i12c]	8.48×10^{8}	2.46×10^{9}	811	2	2
[i8c]→[i12b]	8.72×10^{8}	2.45×10^{9}	794	2	2
[i8d]→[i12d]	1.23×10^{9}	3.63×10^{9}	1058	2	2
[i9a]→**p1a**	2.29×10^{8}		1403	2	
[i9b]→**p1a**	1.84×10^{8}		1118	2	
[i9c]→**p1b**	1.43×10^{8}		1064	2	
[i9d]→**p1b**	1.44×10^{8}		1064	2	
[i1a]→**p2a**	4.83×10^{1}		1104	1	
[i1b]→**p2a**	4.93×10^{1}		1105	1	
[i1b]→**p2b**	1.42×10^{1}		980	1	
[i1b]→**p2c**	1.42×10^{1}		980	1	
[i6a]→**p2a**	2.67×10^{6}		1372	1	
[i6b]→**p2a**	2.12×10^{6}		1080	1	
[i6c]→**p2b**	1.57×10^{6}		1032	1	
[i6d]→**p2c**	1.58×10^{6}		1032	1	
[i6e]→**p2a**	2.67×10^{6}		1372	1	
[i6f]→**p2a**	2.12×10^{6}		1080	1	
[i6g]→**p2c**	1.57×10^{6}		1032	1	
[i6h]→**p2b**	1.58×10^{6}		1032	1	
[i13a]→**p2a**	3.10×10^{6}		1067	2	
[i13b]→**p2a**	4.78×10^{6}		1327	2	
[i13b]→**p2b**	2.65×10^{6}		1030	2	
[i13b]→**p2c**	2.65×10^{6}		1024	2	
[i12a]→**p3a**	4.26×10^{7}		1060	2	
[i12b]→**p3c**	5.00×10^{7}		1111	2	
[i12c]→**p3c**	6.76×10^{7}		1409	2	
[i12d]→**p3b**	4.61×10^{7}		1076	2	
[i12a]→**p3a′**	7.47×10^{7}		1023	2	
[i12b]→**p3c′**	8.62×10^{7}		1071	2	
[i12c]→**p3b′**	7.30×10^{7}		1034	2	
[i12d]→**p3c′**	1.19×10^{8}		1364	2	
[i6a]→**p4a**	7.46×10^{8}		675	1	
[i6b]→**p4b**	8.81×10^{8}		720	1	
[i6c]→**p4a**	7.71×10^{8}		679	1	
[i6d]→**p4b**	1.05×10^{9}		837	1	
[i6e]→**p4a**	7.46×10^{8}		675	1	
[i6f]→**p4b**	8.81×10^{8}		720	1	
[i6g]→**p4a**	7.71×10^{8}		679	1	
[i6h]→**p4b**	1.05×10^{9}		837	1	

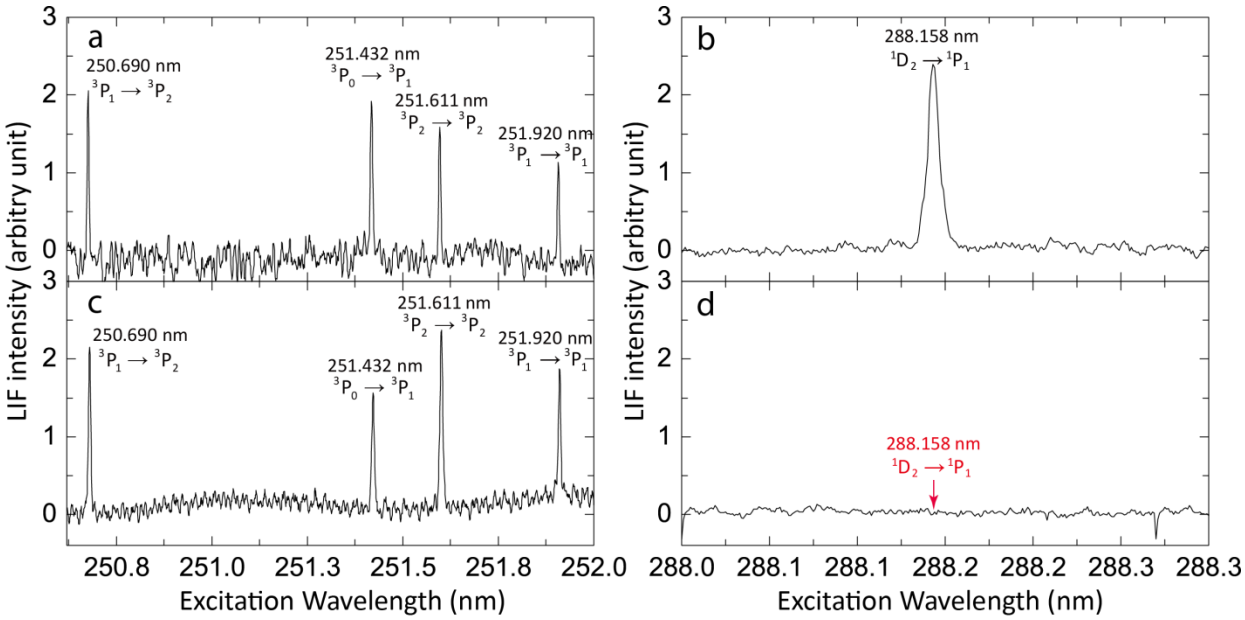


Fig. S1. Laser-induced fluorescence (LIF) detection of atomic silicon species in the photolysis source of disilane ((a) & (b)) and in the ablation source of the silicon rod ((c) & (d)), respectively. Relevant atomic transitions are noted in the figure.

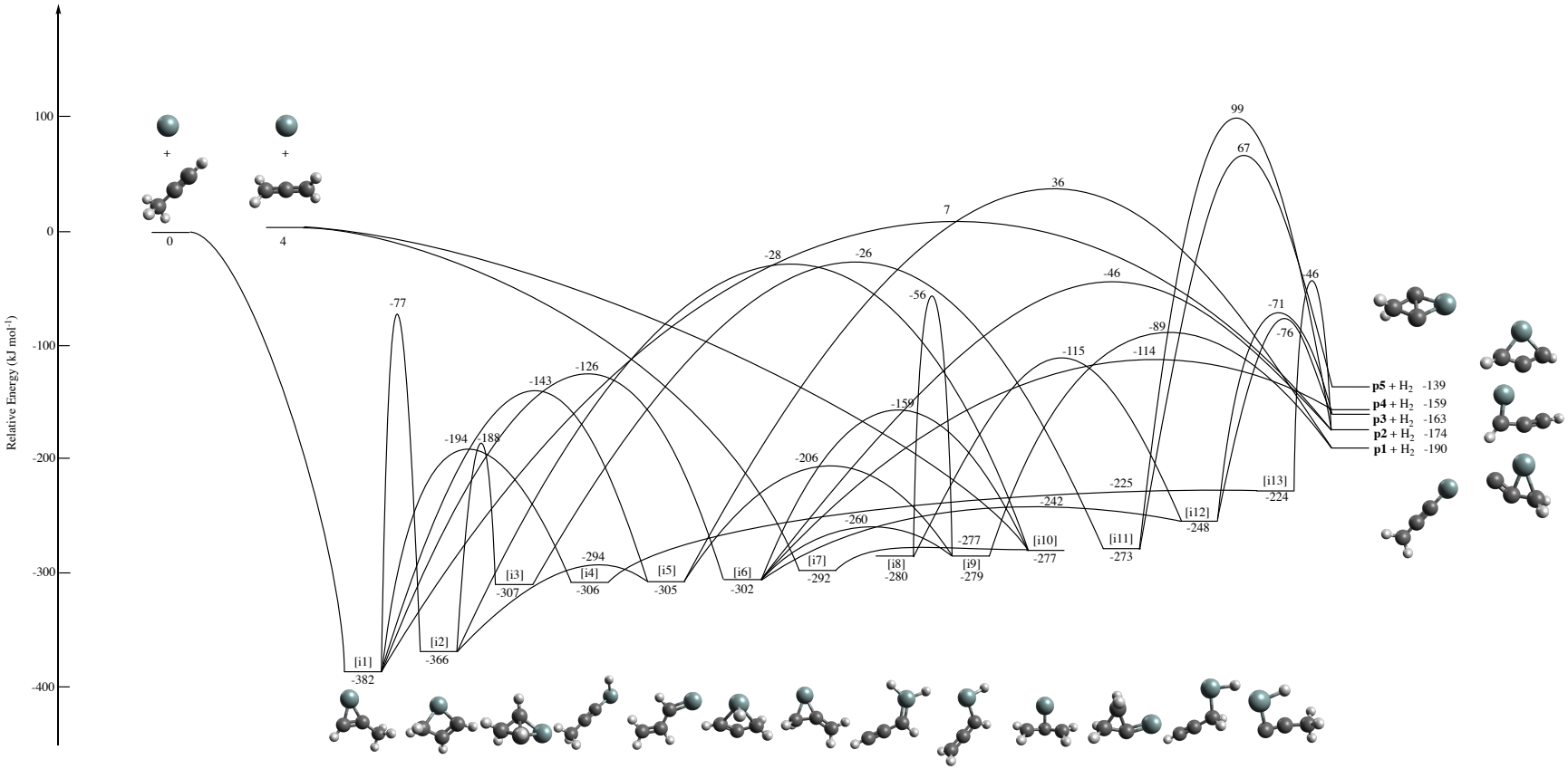


Fig. S2. Complete potential energy surfaces involved in the reactions of electronically excited silicon atoms (Si(^{1}D)) with allene and methylacetylene. Relative energies are given in units of kJ mol^{-1}. Colors of the atoms: silicon (green), carbon (black) and hydrogen (light grey).

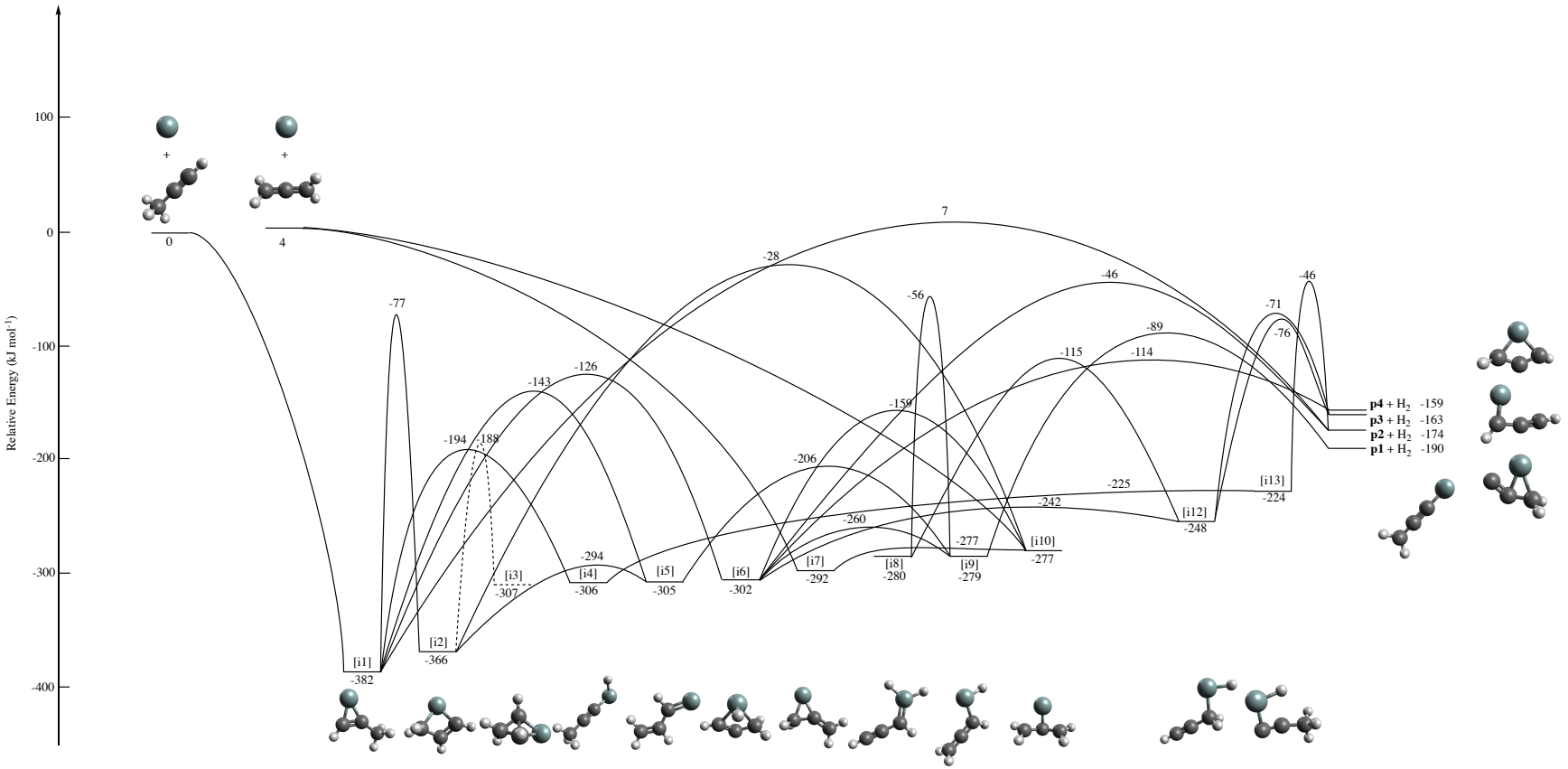


Fig. S3. Pathways exploited in the RRKM calculations to determine the branching ratios in the reactions of electronically excited silicon atoms (Si(^{1}D)) with methylacetylene, allene, and D3-methylacetylene. Relative energies are given in units of kJ mol^{-1}. Colors of the atoms: silicon (green), carbon (black) and hydrogen (light grey).