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Modification of H-Terminated Silicon Surface by Organic Sulfide Molecules: Mechanism and Origin of Reactivity

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S1: Energy profiles for the four reactions present in Scheme 2 in the paper

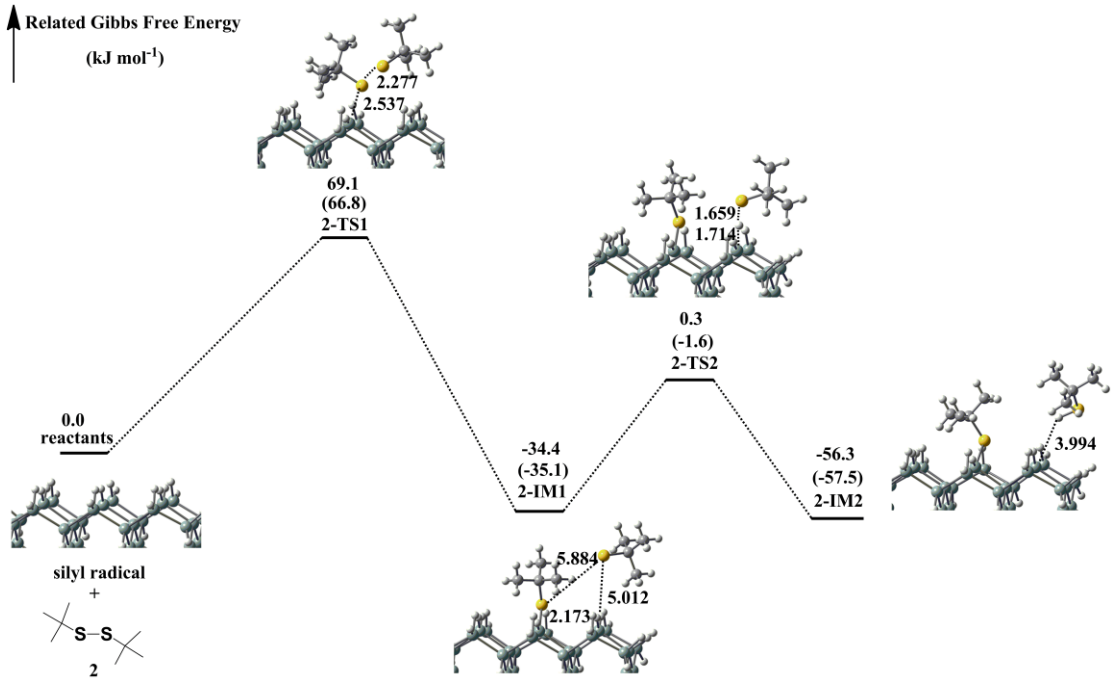


Figure S1 Energy profile in dichloromethane for the Si-S bond formation reactions between di-*t*-butyldisulfide (**2**) and the silyl radical, the results calculated in the solvent acetonitrile are given in the parenthesis.

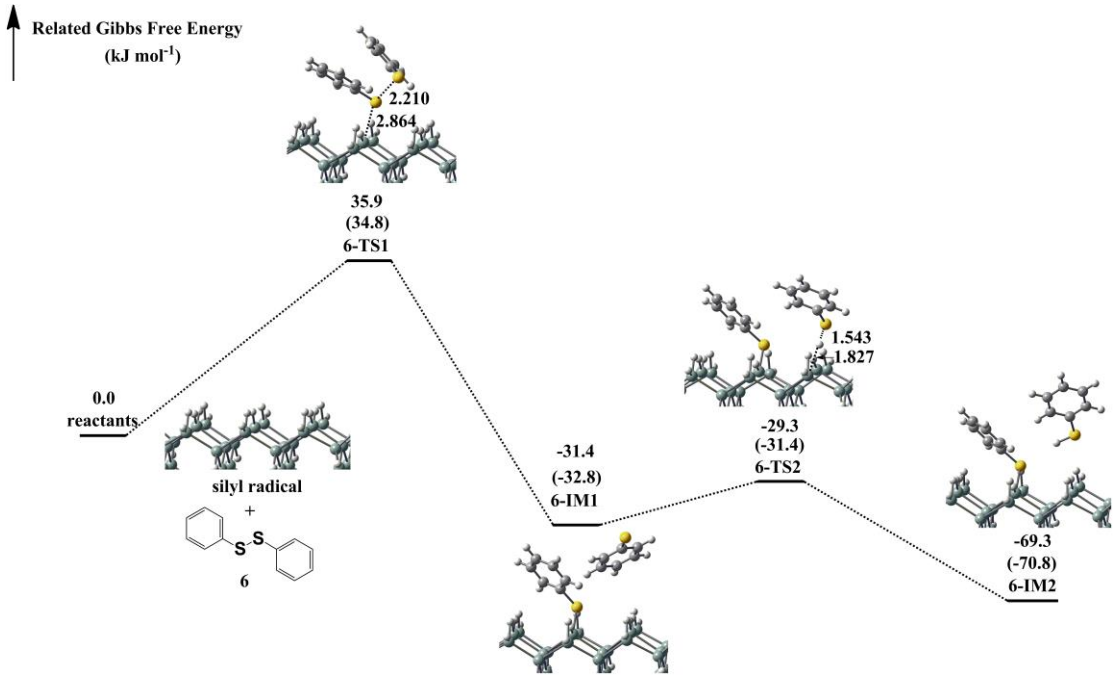


Figure S2 Energy profile in dichloromethane for the Si-S bond formation reactions between di-phenyl disulfide (**6**) and the silyl radical, the results calculated in the solvent acetonitrile are given in the parenthesis.

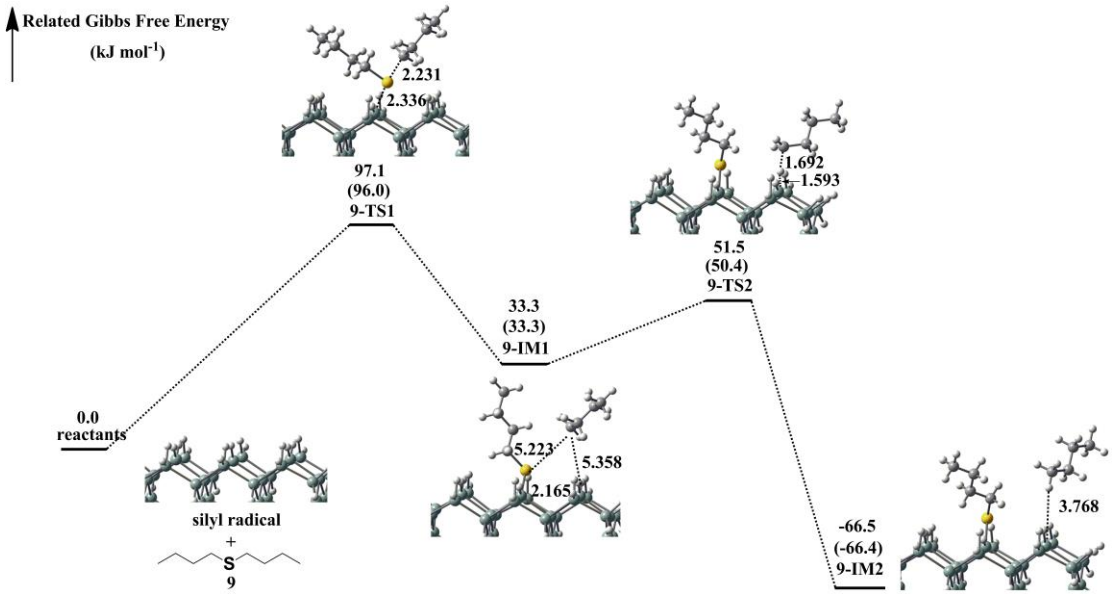


Figure S3 Energy profile in dichloromethane for the Si-S bond formation reactions between di-*n*-butyl sulfide (**9**) and the silyl radical, the results calculated in the solvent acetonitrile are given in the parenthesis.

S2: Choice of the cluster

Firstly, five clusters, deriving from the Si(100) surface, was designed to simulate the H-terminated Si(100)surface. All the five clusters were derived from the diamond-type silicon cubic crystal structure cutting out along the [100] direction and saturating all of the surface silicon dangling bonds with hydrogen atoms on both the top and bottom faces of the slab. The bulk is large enough for us to cut all the five clusters. Then, the clusters were cut from this H-terminated Si(100) surface, and the dangling bonds resulting from the truncation of the bulk were saturated by hydrogen atoms to maintain the sp^3 hybridization of the Si atoms. Fully geometry optimization was performed on these clusters. The optimized geometries are shown in Figure S4. The calculated key structural parameters and the HOMO-LUMO gap of the clusters are presented in the Table S1. As shown in Table S1, the calculated structural parameters of the five clusters are quite in similar. The differences in the average Si-Si bond lengths of Si1-Si2, Si2-Si3, Si3-Si4, Si4-Si5, Si1-Si6, Si6-Si7, Si7-Si8, Si8-Si5 bonds in the five clusters are all lower than 0.007 Å. The differences in the angles and dihedral angles are lower than 3 and 7 °, respectively. On the other hand, the differences in the calculated HOMO-LUMO gaps are lower than 0.022 eV. All the mentioned differences are acceptable. Therefore, considering the computational cost, the cluster $Si_{35}H_{48}$ (cluster1) was chosen to simulate the H-terminated Si(100)surface.

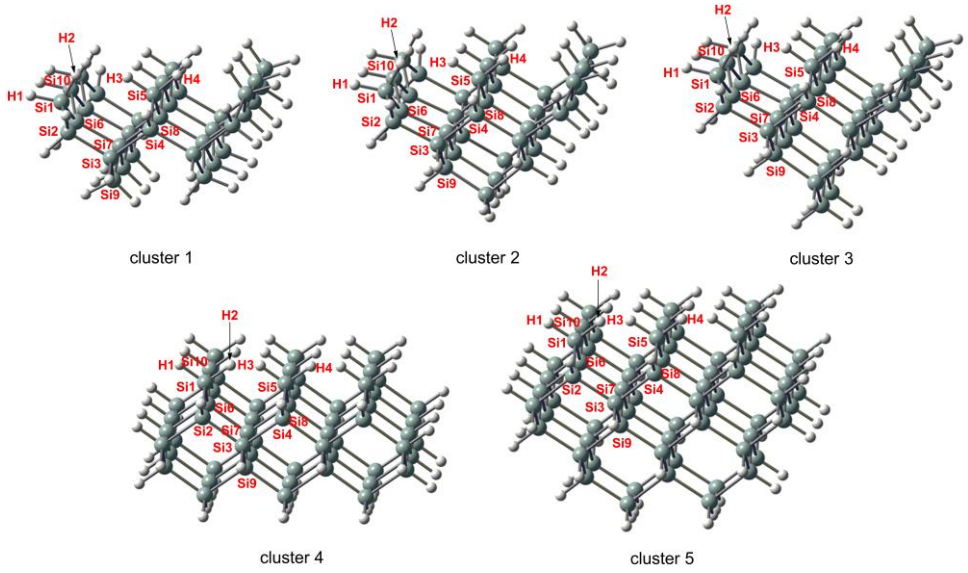


Figure S4 The optimized geometries of the clusters.

Table S1 calculated structural parameters and the HOMO-LUMO gap of the clusters.

Species	Cluster1	Cluster2	Cluster3	Cluster4	Cluster5
The average Si-Si bond length of the Si1-Si2, Si2-Si3, Si3-Si4, Si4-Si5, Si1-Si6, Si6-Si7, Si7-Si8, Si8-Si5 bonds (Å)	2.372	2.370	2.371	2.375	2.377
The average Si-H bond length of the Si1-H1, Si1-H2, Si5-H3, Si5-H4,bonds (Å)	1.490	1.490	1.490	1.489	1.489
The Si1-Si2-Si3 angle ( )	114.3	113.1	113.7	112.3	113.2
The Si2-Si3-Si4 angle ( )	112.3	114.1	114.1	115.2	113.9
The Si3-Si4-Si5 angle ( )	108.9	108.8	109.6	107.7	108.4
The Si1-Si9-Si5 angle ( )	58.6	59.1	59.2	56.4	56.2
The Si1-Si6-Si10 angle ( )	112.2	110.1	111.8	108.5	110.5
The H1-Si1-H2 angle ( )	107.1	107.2	107.2	107.1	107
The H3-Si5-H4 angle ( )	107.1	107.2	107.1	106.9	106.7
The Si4-Si3-Si2-Si1 dihedral angle ( )	71.9	72.2	70.4	65.7	65.4
The HOMO-LUMO band gap (e)	0.180	0.178	0.171	0.170	0.158

S3: Energy summary

Table S2 Energies of the species involved in the reaction between di-*n*-butyldisulfide and the silyl radical.

Species	G_c (a.u.)[a]	$E_{sp\ (solvent1)}$ (a.u.)[b]	$G_{(solvent1)}$ (a.u.)[c]	$\Delta G_{(solvent1)}$ (kJ	$E_{sp\ (solvent2)}$ (a.u.)[b]	$G_{(solvent2)}$ (a.u.)[c]	$\Delta G_{(solvent2)}$ (kJ mol^{-1})[d]

				mol^{-1})^{d}			
1	0.20561	-1112.00681	-1111.80120	-	-1112.00490	-1111.79929	-
radical	0.33647	-10160.28104	-10159.94457	-	-10160.27543	-10159.93896	-
1 + radical	0.54208	-11272.28785	-11271.74577	**0.0**	-11272.28033	-11271.73825	**0.0**
1a-TS1	0.56020	-11272.29029	-11271.73009	**41.2**	-11272.28320	-11271.72300	**40.0**
1a-IM1	0.55833	-11272.31887	-11271.76054	**-38.8**	-11272.31159	-11271.75326	**-39.4**
1a-TS2	0.55639	-11272.30707	-11271.75068	**-12.9**	-11272.30026	-11271.74387	**-14.8**
1a-IM2	0.55652	-11272.32613	-11271.76961	**-62.6**	-11272.31899	-11271.76246	**-63.6**
1b-TS1	0.56112	-11272.28639	-11271.72527	**53.8**	-11272.27931	-11271.71819	**52.7**
1b-IM1	0.55468	-11272.31427	-11271.75960	**-36.3**	-11272.30685	-11271.75217	**-36.6**
1b-TS2	0.55785	-11272.30427	-11271.74642	**-1.7**	-11272.29797	-11271.74011	**-4.9**
1b-IM2	0.55815	-11272.31597	-11271.75782	**-31.6**	-11272.30904	-11271.75089	**-33.2**

a: G_c is the thermal correction to Gibbs free energy calculated at the B3LYP/[6-31G(d,p),6-31G] level;

b: E_{sp} is the single-point energies calculated at the M06-2X/6-311++G(d,p) level in the solvent based on the optimized structures; the solvent1 and solvent2 are dichloromethane and acetonitrile, respectively.

c: G is the Gibbs free energy corrected by G_c, $G_{gas}= E_{sp}+ G_c$;

d: ΔG is the relative Gibbs free energy in kJ mol^{-1}.

Table S3 Energies of the species involved in the reaction between di-*t*-butyldisulfide and the silyl radical as well as those discussed in the steric effect section.

Species	G_c **(a.u.)**^{a}	$E_{sp\ (solvent1)}$ **(a.u.)**^{b}	$G_{(solvent1)}$ **(a.u.)**^{c}	$\Delta G_{(solvent1)}$ **(kJ mol^{-1})**^{d}	$E_{sp\ (solvent2)}$ **(a.u.)**^{b}	$G_{(solvent2)}$ **(a.u.)**^{c}	$\Delta G_{(solvent2)}$ **(kJ mol^{-1})**^{d}
2	0.20670	-1112.01845	-1111.81174	-	-1112.01690	-1111.81019	-
2 + radical	0.54317	-11272.29948	-11271.75631	**0.0**	-11272.29233	-11271.74916	**0.0**
2-TS1	0.56435	-11272.29434	-11271.72999	**69.1**	-11272.28807	-11271.72372	**66.8**
2-IM1	0.55448	-11272.32389	-11271.76941	**-34.4**	-11272.31701	-11271.76253	**-35.1**
2-TS2	0.56092	-11272.31712	-11271.75620	**0.3**	-11272.31070	-11271.74978	**-1.6**
2-IM2	0.55538	-11272.33313	-11271.77775	**-56.3**	-11272.32643	-11271.77105	**-57.5**

a: G_c is the thermal correction to Gibbs free energy calculated at the B3LYP/[6-31G(d,p),6-31G] level;

b: E_{sp} is the single-point energies calculated at the M06-2X/6-311++G(d,p) level in the solvent based on the optimized structures; the solvent1 and solvent2 are dichloromethane and acetonitrile, respectively.

c: G is the Gibbs free energy corrected by G_c, $G_{gas}= E_{sp}+ G_c$;

d: ΔG is the relative Gibbs free energy in kJ mol^{-1}.

Table S4 Energies of the species discussed in the steric effect section.

Species	G_c **(a.u.)**^{a}	$E_{sp\ (solvent1)}$ **(a.u.)**^{b}	$G_{(solvent1)}$ **(a.u.)**^{c}	$\Delta G_{(solvent1)}$ **(kJ**	$E_{sp\ (solvent2)}$ **(a.u.)**^{b}	$G_{(solvent2)}$ **(a.u.)**^{c}	$\Delta G_{(solvent2)}$ **(kJ mol^{-1})**^{d}

				mol^{-1})^{d}			
3	0.20577	-1112.01153	-1111.80576	-	-1112.00977	-1111.80400	-
3 + radical	0.54224	-11272.29257	-11271.75033	**0.0**	-11272.28521	-11271.74297	**0.0**
3-TS1	0.56394	-11272.29392	-11271.72998	**53.4**	-11272.28715	-11271.72321	**51.9**
4	0.20301	-1112.00916	-1111.80615	-	-1112.00740	-1111.80439	-
4 + radical	0.53948	-11272.29019	-11271.75071	**0.0**	-11272.28283	-11271.74335	**0.0**
4-TS1	0.56289	-11272.29317	-11271.73028	**53.6**	-11272.28622	-11271.72333	**52.6**
5	0.25754	-1190.62296	-1190.36542	-	-1190.62104	-1190.36350	-
5 + radical	0.59401	-11350.90400	-11350.30999	**0.0**	-11350.89647	-11350.30246	**0.0**
5-TS1	0.61675	-11350.90666	-11350.28991	**52.7**	-11350.89971	-11350.28295	**51.2**

a: G_c is the thermal correction to Gibbs free energy calculated at the B3LYP/[6-31G(d,p),6-31G] level;

b: E_{sp} is the single-point energies calculated at the M06-2X/6-311++G(d,p) level in the solvent based on the optimized structures; the solvent1 and solvent2 are dichloromethane and acetonitrile, respectively.

c: G is the Gibbs free energy corrected by G_c, $G_{gas}= E_{sp}+ G_c$;

d: ΔG is the relative Gibbs free energy in kJ mol^{-1}.

Table S5 Energies of the species involved in the reaction between di-phenyl disulfide and the silyl radical as well as those in the electronic effect section.

Species	G_c **(a.u.)**^{a}	$E_{sp\ (solvent1)}$ **(a.u.)**^{b}	$G_{(solvent1)}$ **(a.u.)**^{c}	$\Delta G_{(solvent1)}$ **(kJ mol^{-1})**^{d}	$E_{sp\ (solvent2)}$ **(a.u.)**^{b}	$G_{(solvent2)}$ **(a.u.)**^{c}	$\Delta G_{(solvent2)}$ **(kJ mol^{-1})**^{d}
6	0.14133	-1259.60291	-1259.46158	-	-1259.60081	-1259.45948	-
6 + radical	0.47780	-11419.88395	-11419.40615	**0.0**	-11419.87625	-11419.39844	**0.0**
6-TS1	0.49643	-11419.88889	-11419.39246	**35.9**	-11419.88164	-11419.38521	**34.8**
6-IM1	0.49300	-11419.91109	-11419.41809	**-31.4**	-11419.90393	-11419.41093	**-32.8**
6-TS2	0.49523	-11419.91255	-11419.41732	**-29.3**	-11419.90562	-11419.41039	**-31.4**
6-IM2	0.49404	-11419.92659	-11419.43255	**-69.3**	-11419.91946	-11419.42542	**-70.8**
7	0.19992	-1488.63347	-1488.43354	-	-1488.63219	-1488.43226	-
7 + radical	0.53639	-11648.91451	-11648.37811	**0.0**	-11648.90762	-11648.37123	**0.0**
7-TS1	0.55576	-11648.92051	-11648.36475	**35.1**	-11648.91419	-11648.35843	**33.6**
8	0.13902	-1668.58522	-1668.44620	-	-1668.58415	-1668.44513	-
8 + radical	0.47549	-11828.86626	-11828.39077	**0.0**	-11828.85958	-11828.38409	**0.0**
8-TS1	0.49334	-11828.86906	-11828.37572	**35.1**	-11828.86264	-11828.36930	**39.5**

a: G_c is the thermal correction to Gibbs free energy calculated at the B3LYP/[6-31G(d,p),6-31G] level;

b: E_{sp} is the single-point energies calculated at the M06-2X/6-311++G(d,p) level in the solvent based on the optimized structures; the solvent1 and solvent2 are dichloromethane and acetonitrile, respectively.

c: G is the Gibbs free energy corrected by G_c, $G_{gas}= E_{sp}+ G_c$;

d: ΔG is the relative Gibbs free energy in kJ mol^{-1}.

Table S6 Energies of the species involved in the reaction between di-*n*-butylsulfide and the silyl radical.

Species	G_c **(a.u.)**[a]	$E_{sp\ (solvent1)}$ **(a.u.)**[b]	$G_{(solvent1)}$ **(a.u.)**[c]	$\Delta G_{(solvent1)}$ **(kJ mol^{-1})**[d]	$E_{sp\ (solvent2)}$ **(a.u.)**[b]	$G_{(solvent2)}$ **(a.u.)**[c]	$\Delta G_{(solvent2)}$ **(kJ mol^{-1})**[d]
9	0.20674	-713.81362	-713.60688	-	-713.81181	-713.60507	-
9 + radical	0.54321	-10874.09466	-10873.55144	**0.0**	-10874.08725	-10873.54403	**0.0**
9-TS1	0.56326	-10874.07770	-10873.51445	**97.1**	-10874.07072	-10873.50747	**96.0**
9-IM1	0.55708	-10874.09585	-10873.53877	**33.3**	-10874.08844	-10873.53136	**33.3**
9-TS2	0.55600	-10874.08796	-10873.53197	**51.1**	-10874.08084	-10873.52485	**50.4**
9-IM2	0.55706	-10874.13384	-10873.57677	**-66.5**	-10874.12637	-10873.56931	**-66.4**

a: G_c is the thermal correction to Gibbs free energy calculated at the B3LYP/[6-31G(d,p),6-31G] level;

b: E_{sp} is the single-point energies calculated at the M06-2X/6-311++G(d,p) level in the solvent based on the optimized structures; the solvent1 and solvent2 are dichloromethane and acetonitrile, respectively.

c: G is the Gibbs free energy corrected by G_c, $G_{gas}= E_{sp}+ G_c$;

d: ΔG is the relative Gibbs free energy in kJ mol^{-1}.

Table S7 Energies of the species discussed in the section of the effect of the substrate with different dissociating S-X bond.

Species	G_c **(a.u.)**[a]	$E_{sp\ (solvent1)}$ **(a.u.)**[b]	$G_{(solvent1)}$ **(a.u.)**[c]	$\Delta G_{(solvent1)}$ **(kJ mol^{-1})**[d]	$E_{sp\ (solvent2)}$ **(a.u.)**[b]	$G_{(solvent2)}$ **(a.u.)**[c]	$\Delta G_{(solvent2)}$ **(kJ mol^{-1})**[d]
10	0.21284	-1055.76544	-1055.55261		-1055.76351	-1055.55067	-
10 + radical	0.54931	-11216.04648	-11215.49717		-11216.03895	-11215.48964	**0.0**
10-TS1	0.56940	-11216.04644	-11215.47703	**52.9**	-11216.03925	-11215.46985	**52.0**
11	0.21981	-1004.52312	-1004.30331	-	-1004.52098	-1004.30117	-
11 + radical	0.55628	-11164.80415	-11164.24787	**0.0**	-11164.79641	-11164.24013	**0.0**
11-TS1	0.57677	-11164.78443	-11164.20766	**105.6**	-11164.77716	-11164.20039	**104.3**
12	0.18230	-749.69838	-749.51608	-	-749.69708	-749.51478	-
12 + radical	0.51877	-10909.97942	-10909.46065	**0.0**	-10909.97252	-10909.45375	**0.0**
12-TS1	0.53947	-10909.98226	-10909.44279	**46.9**	-10909.97557	-10909.43610	**46.3**
13	0.19534	-729.84080	-729.64546	-	-729.83940	-729.64406	-
13 + radical	0.53181	-10890.12184	-10889.59003	**0.0**	-10890.11483	-10889.58302	**0.0**
13-TS1	0.55234	-10890.11700	-10889.56466	**66.6**	-10890.11027	-10889.55793	**65.9**

a: G_c is the thermal correction to Gibbs free energy calculated at the B3LYP/[6-31G(d,p),6-31G] level;

b: E_{sp} is the single-point energies calculated at the M06-2X/6-311++G(d,p) level in the solvent

based on the optimized structures; the solvent1 and solvent2 are dichloromethane and acetonitrile, respectively.

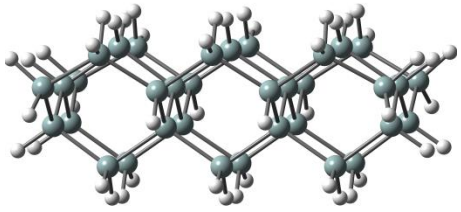
c: G is the Gibbs free energy corrected by G_c, $G_{gas} = E_{sp} + G_c$;

d: ΔG is the relative Gibbs free energy in kJ mol^{-1}.

S4: Cartesian coordinates and 3D structures of the reactants, products, intermediates and transition states involved in the reaction

S5.1 Reaction between di-*n*-butyldisulfide and the silyl radical

Radical



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	3.922663	-4.433979	-1.650833
2	14	0	1.978581	-2.012733	0.919824
3	14	0	5.887492	-2.004624	0.862397
4	14	0	-5.887673	-2.003803	0.862956
5	14	0	-3.923478	-4.434272	-1.649816
6	14	0	-0.000439	-4.281150	-1.692310
7	14	0	-1.978719	-2.012370	0.920031
8	14	0	3.923497	4.432233	-1.646844
9	14	0	3.874705	-0.005367	-1.792429
10	14	0	5.889381	1.999022	0.861107
11	14	0	1.978757	2.005462	0.914405
12	14	0	1.964926	-0.010850	-0.400127
13	14	0	-3.922666	4.431935	-1.647887
14	14	0	0.000446	4.355364	-1.651866
15	14	0	-3.874726	-0.005818	-1.792417
16	14	0	-1.978617	2.005825	0.914187
17	14	0	-5.889209	1.999861	0.860566
18	14	0	-5.828784	-0.002600	-0.455365
19	14	0	-0.000007	-0.059697	-1.685417
20	14	0	-1.964935	-0.010623	-0.400129
21	14	0	5.828774	-0.003081	-0.455393
22	1	0	3.920504	-5.878674	-2.022349
23	1	0	3.894078	-3.652910	-2.917047

24	1	0	7.131193	-1.983592	1.718558
25	1	0	-7.131258	-1.982391	1.719274
26	1	0	-3.921487	-5.879232	-2.020305
27	1	0	-3.894969	-3.654106	-2.916590
28	1	0	-0.000557	-5.658215	-2.270343
29	1	0	-0.000516	-3.322678	-2.831932
30	1	0	3.885529	3.647894	-2.910765
31	1	0	3.924613	5.875982	-2.022004
32	1	0	3.863389	-1.202572	-2.677064
33	1	0	3.855678	1.195821	-2.671785
34	1	0	7.133162	1.977399	1.717109
35	1	0	-3.884611	3.646698	-2.911244
36	1	0	-3.923631	5.875417	-2.024065
37	1	0	0.000539	3.472196	-2.849830
38	1	0	0.000556	5.765253	-2.143486
39	1	0	-3.863458	-1.203824	-2.675971
40	1	0	-3.855683	1.194570	-2.672860
41	1	0	-7.133098	1.978659	1.716420
42	1	0	-7.047250	-0.003465	-1.349940
43	1	0	0.000052	0.970055	-2.769379
44	1	0	7.047238	-0.003757	-1.349968
45	14	0	-3.959931	-2.199423	2.263607
46	1	0	-3.959280	-3.569611	2.891205
47	1	0	-3.971891	-1.191268	3.377605
48	14	0	-0.000014	-2.191521	2.273246
49	1	0	-0.000123	-3.558139	2.908639
50	1	0	0.000171	-1.179492	3.384567
51	14	0	-3.961977	2.194592	2.261450
52	1	0	-3.972247	1.183117	3.372454
53	1	0	-3.960524	3.563462	2.892458
54	14	0	0.000011	2.175812	2.267666
55	1	0	-0.000185	1.160280	3.375634
56	1	0	0.000113	3.540329	2.907802
57	14	0	3.959876	-2.200094	2.263235
58	1	0	3.972032	-1.191892	3.377189
59	1	0	3.959134	-3.570256	2.890881
60	14	0	3.962038	2.193915	2.261824
61	1	0	3.960711	3.562807	2.892790
62	1	0	3.972120	1.182483	3.372867
63	14	0	-5.950430	3.967135	-0.504063
64	1	0	-7.079653	3.870896	-1.498657
65	1	0	-6.259899	5.128329	0.407538
66	14	0	-1.966982	4.020590	-0.379937
67	1	0	-1.945388	5.081863	0.676187

68	14	0	1.967534	4.020393	-0.379469
69	1	0	1.945621	5.081492	0.676824
70	14	0	5.951173	3.966493	-0.503217
71	1	0	6.261228	5.127464	0.408466
72	1	0	7.080228	3.869907	-1.497970
73	14	0	5.947921	-3.972905	-0.500853
74	1	0	7.080194	-3.879821	-1.492299
75	1	0	6.252558	-5.133913	0.412638
76	14	0	1.960658	-4.013550	-0.395263
77	1	0	1.911822	-5.092451	0.641857
78	14	0	-1.961208	-4.013355	-0.394810
79	1	0	-1.912065	-5.092080	0.642480
80	14	0	-5.948645	-3.972257	-0.500024
81	1	0	-6.253858	-5.133054	0.413542
82	1	0	-7.080760	-3.878823	-1.491618

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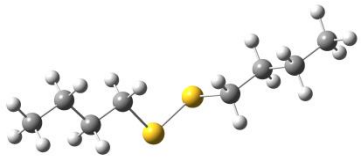

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	1	0	-1.930833	-0.262683	-1.427031
3	1	0	-1.390294	0.959875	-0.259842
4	16	0	-0.905955	-1.298290	0.511296
5	16	0	0.905948	-1.298276	-0.511332
6	6	0	1.896870	-0.004238	0.365236
7	1	0	1.390326	0.959817	0.259990
8	1	0	1.930880	-0.262845	1.427064
9	6	0	3.304210	0.055222	-0.233704
10	1	0	3.782511	-0.928454	-0.143329
11	1	0	3.238856	0.272695	-1.307717
12	6	0	4.182000	1.115487	0.448256
13	1	0	3.697396	2.097072	0.361929
14	1	0	4.243160	0.898075	1.522686
15	6	0	-3.304198	0.055256	0.233731
16	1	0	-3.238874	0.272690	1.307754
17	1	0	-3.782481	-0.928424	0.143308
18	6	0	-4.181989	1.115529	-0.448215
19	1	0	-3.697434	2.097129	-0.361791

20	1	0	-4.243069	0.898184	-1.522662
21	6	0	-5.593415	1.187058	0.142003
22	1	0	-5.564830	1.435190	1.208828
23	1	0	-6.196186	1.949747	-0.361076
24	1	0	-6.115067	0.229081	0.039193
25	6	0	5.593382	1.187122	-0.142054
26	1	0	6.196147	1.949817	0.361023
27	1	0	6.115091	0.229166	-0.039326
28	1	0	5.564713	1.435306	-1.208864

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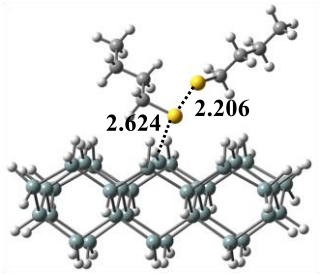

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3	14	0	5.397504	-0.339690	-3.059684
4	14	0	-6.177844	1.419830	-1.849603
5	14	0	-3.674642	4.509967	-1.352868
6	14	0	0.176092	3.877771	-1.689406
7	14	0	-2.329746	0.830494	-2.279450
8	14	0	3.436483	-4.234203	2.652483
9	14	0	3.759092	-0.393139	0.455512
10	14	0	5.083219	-3.752231	-0.975505
11	14	0	1.242098	-3.136623	-0.540886
12	14	0	1.616090	-0.760121	-0.478902
13	14	0	-4.222319	-2.851404	3.585638
14	14	0	-0.418447	-3.669044	3.095955
15	14	0	-3.883856	0.900254	1.237277
16	14	0	-2.636169	-2.506047	-0.087017
17	14	0	-6.465919	-1.878695	0.405073
18	14	0	-6.037759	0.478344	0.349519
19	14	0	-0.069143	0.156851	0.907099
20	14	0	-2.217424	-0.130843	-0.085867
21	14	0	5.426592	-1.381637	-0.902763

22	1	0	4.243616	4.717620	-2.445978
23	1	0	4.146694	3.279816	-0.531409
24	1	0	6.467749	-0.963026	-3.923624
25	1	0	-7.541573	1.117228	-2.423020
26	1	0	-3.523328	5.911563	-1.841785
27	1	0	-3.477043	4.539919	0.122835
28	1	0	0.362215	5.309207	-2.073546
29	1	0	0.284080	3.802675	-0.207561
30	1	0	3.684920	-2.923475	3.310178
31	1	0	3.406294	-5.270736	3.725230
32	1	0	4.023279	1.067433	0.571145
33	1	0	3.816962	-0.974272	1.822828
34	1	0	6.141707	-4.372795	-1.856081
35	1	0	-3.872344	-1.523771	4.159873
36	1	0	-4.260715	-3.824310	4.716073
37	1	0	-0.109077	-2.408182	3.822619
38	1	0	-0.485227	-4.756032	4.118608
39	1	0	-3.644804	2.371181	1.287133
40	1	0	-3.808899	0.404670	2.639865
41	1	0	-7.843869	-2.132818	-0.158185
42	1	0	-7.074640	1.161417	1.212092
43	1	0	-0.132157	-0.732274	2.105265
44	1	0	6.784896	-1.129896	-0.288001
45	16	0	1.091479	2.098509	2.236890
46	16	0	2.595810	2.274280	3.840304
47	6	0	-0.385946	2.853457	3.066908
48	1	0	-0.579200	2.284447	3.980644
49	1	0	-1.213211	2.672804	2.374240
50	6	0	-0.235861	4.346134	3.353953
51	1	0	0.625967	4.502292	4.013519
52	1	0	-0.025108	4.876859	2.417225
53	6	0	-1.494905	4.931416	4.013042
54	1	0	-2.359149	4.772077	3.354677
55	1	0	-1.709089	4.381492	4.939046
56	6	0	-1.356739	6.425079	4.325104
57	1	0	-2.264314	6.817330	4.794606
58	1	0	-0.520833	6.611053	5.008748
59	1	0	-1.175716	7.005888	3.413793
60	6	0	3.673603	3.619794	3.177415
61	1	0	3.966326	3.353845	2.157564
62	1	0	3.098657	4.549626	3.139523
63	6	0	4.910467	3.778891	4.068580
64	1	0	4.599232	4.007647	5.096011
65	1	0	5.455026	2.827351	4.111011

66	6	0	5.846684	4.886220	3.559308
67	1	0	5.294282	5.833924	3.509416
68	1	0	6.152832	4.655680	2.530427
69	6	0	7.089331	5.062176	4.437948
70	1	0	7.738432	5.855044	4.052827
71	1	0	6.814700	5.326253	5.465359
72	1	0	7.679342	4.139813	4.479929
73	14	0	-4.487075	0.543813	-3.294914
74	1	0	-4.494757	1.340833	-4.574589
75	1	0	-4.748552	-0.890303	-3.658165
76	14	0	-0.600890	-0.034275	-3.702352
77	1	0	-0.600144	0.773080	-4.975361
78	1	0	-0.855208	-1.465934	-4.081622
79	14	0	-4.839575	-3.082276	-0.867390
80	1	0	-4.993468	-2.831240	-2.340813
81	1	0	-5.041711	-4.558311	-0.636867
82	14	0	-0.957254	-3.671522	-1.350876
83	1	0	-1.090264	-3.406314	-2.824309
84	1	0	-1.171099	-5.149205	-1.143133
85	14	0	3.268304	-0.593175	-4.111813
86	1	0	3.015013	-2.016847	-4.519782
87	1	0	3.244190	0.244416	-5.364926
88	14	0	2.914387	-4.303891	-1.817120
89	1	0	2.689775	-5.782477	-1.626604
90	1	0	2.793587	-4.017613	-3.287306
91	14	0	-6.397017	-2.740170	2.639678
92	1	0	-7.297418	-1.922657	3.531746
93	1	0	-6.968733	-4.135362	2.595155
94	14	0	-2.548921	-3.552138	2.067712
95	1	0	-2.892277	-4.971708	1.735867
96	14	0	1.322071	-4.227675	1.590635
97	1	0	1.064849	-5.655057	1.217029
98	14	0	5.248211	-4.735814	1.202231
99	1	0	5.303063	-6.230936	1.008863
100	1	0	6.545611	-4.326639	1.853237
101	14	0	1.897326	2.606224	-2.699487
102	1	0	1.821283	2.923959	-4.160988
103	14	0	5.829475	2.013211	-2.924246
104	1	0	7.085089	2.262216	-2.126268
105	1	0	6.095440	2.499692	-4.327197
106	14	0	-1.985290	3.197722	-2.365110
107	1	0	-2.075060	3.492753	-3.830124
108	14	0	-5.889989	3.797462	-1.820522
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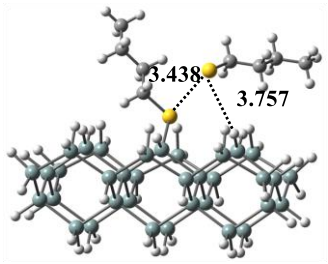

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	14	0	-5.507703	-0.143295	-2.807092
4	14	0	6.096520	-1.812450	-1.764257
5	14	0	3.573057	-4.723149	-0.616289
6	14	0	-0.281857	-4.351731	-1.290872
7	14	0	2.226993	-1.262082	-2.120386
8	14	0	-3.310617	4.488466	2.221352
9	14	0	-3.731849	0.371313	0.604546
10	14	0	-5.130069	3.515577	-1.217383
11	14	0	-1.269604	2.957544	-0.891704
12	14	0	-1.638289	0.617875	-0.467976
13	14	0	4.425682	3.385145	2.911064
14	14	0	0.580608	4.068280	2.524845
15	14	0	3.978761	-0.717540	1.275637
16	14	0	2.617313	2.395725	-0.541459
17	14	0	6.481841	1.863773	-0.180976
18	14	0	6.077386	-0.463486	0.215145
19	14	0	0.120053	-0.025100	0.990283
20	14	0	2.228348	0.057981	-0.116208
21	14	0	-5.450989	1.177297	-0.810380
22	1	0	-4.362597	-5.086196	-1.572933
23	1	0	-4.164476	-3.405882	0.127055
24	1	0	-6.603385	0.372347	-3.709254
25	1	0	7.431404	-1.654972	-2.452268
26	1	0	3.414389	-6.193237	-0.815409
27	1	0	3.393325	-4.453380	0.836036
28	1	0	-0.430607	-5.723920	-1.862673
29	1	0	-0.432889	-4.468423	0.180810

30	1	0	-3.506589	3.271547	3.053359
31	1	0	-3.234639	5.655643	3.147354
32	1	0	-3.975819	-1.065608	0.892640
33	1	0	-3.740439	1.120278	1.887043
34	1	0	-6.229212	4.012712	-2.125691
35	1	0	4.129343	2.182276	3.735719
36	1	0	4.518137	4.547254	3.841783
37	1	0	0.337882	2.939187	3.463110
38	1	0	0.686664	5.307831	3.351016
39	1	0	3.764532	-2.155733	1.596869
40	1	0	3.964838	0.025419	2.566569
41	1	0	7.817024	2.018051	-0.868917
42	1	0	7.157911	-0.973994	1.140774
43	1	0	0.185197	0.995749	2.076294
44	1	0	-6.782194	1.011683	-0.113075
45	16	0	-0.368775	-1.911461	1.954086
46	16	0	-2.749473	-1.491562	4.398690
47	6	0	0.780544	-1.912441	3.417206
48	1	0	0.460730	-1.114109	4.091453
49	1	0	1.792962	-1.695299	3.067652
50	6	0	0.742530	-3.268465	4.122683
51	1	0	-0.286730	-3.481151	4.434351
52	1	0	1.037975	-4.056464	3.418700
53	6	0	1.665716	-3.298251	5.350324
54	1	0	2.692983	-3.063106	5.040896
55	1	0	1.364946	-2.505723	6.047739
56	6	0	1.645315	-4.650253	6.071079
57	1	0	2.310543	-4.647059	6.940438
58	1	0	0.637268	-4.895027	6.423792
59	1	0	1.969453	-5.458904	5.406343
60	6	0	-3.731218	-3.003195	4.125532
61	1	0	-3.224542	-3.532675	3.306383
62	1	0	-3.623659	-3.642420	5.010735
63	6	0	-5.206410	-2.770773	3.785812
64	1	0	-5.684082	-2.219280	4.605656
65	1	0	-5.271987	-2.126223	2.901016
66	6	0	-5.966181	-4.081319	3.534321
67	1	0	-5.882249	-4.727877	4.418577
68	1	0	-5.483882	-4.626923	2.711622
69	6	0	-7.445242	-3.858390	3.202445
70	1	0	-7.962323	-4.807265	3.026862
71	1	0	-7.961779	-3.344006	4.020652
72	1	0	-7.560596	-3.244769	2.301874
73	14	0	-3.008691	3.935099	-2.232587

74	1	0	-2.766846	5.422502	-2.257371
75	1	0	-2.959669	3.447617	-3.652744
76	14	0	-3.417366	-0.057786	-3.962911
77	1	0	-3.170834	1.291157	-4.576872
78	1	0	-3.441331	-1.065593	-5.083019
79	14	0	0.877527	3.360672	-1.886956
80	1	0	0.934247	2.875330	-3.307868
81	1	0	1.097102	4.851432	-1.912497
82	14	0	0.467251	-0.605605	-3.613033
83	1	0	0.425472	-1.606142	-4.739120
84	1	0	0.720983	0.744264	-4.221864
85	14	0	4.763549	2.823764	-1.535594
86	1	0	4.828338	2.334743	-2.954419
87	1	0	4.952165	4.318847	-1.563978
88	14	0	4.344206	-1.172244	-3.257980
89	1	0	4.283926	-2.169549	-4.386149
90	1	0	4.598619	0.178240	-3.865294
91	14	0	5.782887	-4.133969	-1.256571
92	1	0	6.136695	-4.909308	-2.501105
93	1	0	6.752796	-4.556897	-0.181901
94	14	0	1.896295	-3.621531	-1.867826
95	1	0	2.093256	-4.089513	-3.277058
96	14	0	-2.028241	-3.054004	-2.230405
97	1	0	-2.080350	-3.480065	-3.665246
98	14	0	-5.952863	-2.450301	-2.335887
99	1	0	-7.172633	-2.567827	-1.456417
100	1	0	-6.288903	-3.115785	-3.647185
101	14	0	-5.197466	4.787255	0.811354
102	1	0	-5.275127	6.242353	0.421445
103	1	0	-6.456465	4.466587	1.576777
104	14	0	-1.255777	4.355342	1.056002
105	1	0	-1.050945	5.711064	0.453668
106	14	0	2.649193	3.796691	1.403290
107	1	0	2.943184	5.138783	0.807859
108	14	0	6.539240	3.109515	1.864510
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110	1	0	7.089478	4.475166	1.537256

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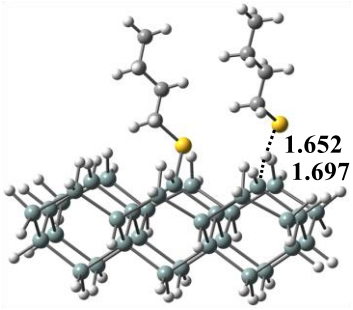

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	14	0	-5.310196	-1.060424	-3.066855
4	14	0	6.299595	-1.760054	-1.272485
5	14	0	3.900854	-4.636321	0.181654
6	14	0	0.063493	-4.592227	-0.666728
7	14	0	2.431025	-1.535109	-1.884111
8	14	0	-3.659168	4.479603	1.265734
9	14	0	-3.745901	0.163219	0.325103
10	14	0	-5.257371	2.797193	-2.023429
11	14	0	-1.384756	2.553387	-1.468884
12	14	0	-1.615604	0.275114	-0.700508
13	14	0	4.072812	3.962627	2.454639
14	14	0	0.225134	4.329324	1.794079
15	14	0	3.956181	-0.369274	1.471640
16	14	0	2.516401	2.337139	-0.879651
17	14	0	6.376460	2.123321	-0.261952
18	14	0	6.090765	-0.137117	0.478195
19	14	0	0.104653	0.029038	0.910966
20	14	0	2.251530	0.071024	-0.108878
21	14	0	-5.452491	0.523006	-1.274733
22	1	0	-3.937646	-5.686215	-1.081432
23	1	0	-3.938283	-3.726899	0.317268
24	1	0	-6.381895	-0.720831	-4.075093
25	1	0	7.658744	-1.610978	-1.913293
26	1	0	3.843753	-6.127003	0.197676
27	1	0	3.631252	-4.169837	1.568814
28	1	0	0.026987	-6.062216	-0.929029
29	1	0	-0.160682	-4.387651	0.785560
30	1	0	-3.819732	3.467421	2.344458
31	1	0	-3.686230	5.822248	1.916487
32	1	0	-4.147457	-1.171745	1.292304

33	1	0	-3.819746	1.255598	1.339109
34	1	0	-6.338215	3.075531	-3.041689
35	1	0	3.798355	2.880007	3.438326
36	1	0	4.043617	5.254341	3.200376
37	1	0	0.004989	3.360048	2.902467
38	1	0	0.210071	5.692942	2.403280
39	1	0	3.804350	-1.753733	1.999493
40	1	0	3.824851	0.557483	2.630505
41	1	0	7.736085	2.255886	-0.905130
42	1	0	7.151938	-0.425357	1.515389
43	1	0	0.050033	1.242011	1.779594
44	1	0	-6.798526	0.372255	-0.608201
45	16	0	-0.352967	-1.650754	2.202298
46	16	0	-4.913400	-2.014285	2.488866
47	6	0	0.671534	-1.280233	3.709534
48	1	0	0.522540	-0.231187	3.982397
49	1	0	1.726351	-1.425944	3.461863
50	6	0	0.262569	-2.202363	4.860433
51	1	0	-0.801871	-2.056429	5.083593
52	1	0	0.374691	-3.248355	4.548625
53	6	0	1.094656	-1.950689	6.127127
54	1	0	2.158433	-2.097565	5.898100
55	1	0	0.988754	-0.900018	6.428705
56	6	0	0.690321	-2.861251	7.291160
57	1	0	1.297017	-2.661653	8.180065
58	1	0	-0.360275	-2.712306	7.564603
59	1	0	0.817852	-3.917858	7.030871
60	6	0	-4.216059	-1.054740	3.894261
61	1	0	-3.125285	-1.137325	3.867835
62	1	0	-4.488695	-0.000899	3.780017
63	6	0	-4.764641	-1.597173	5.220929
64	1	0	-5.860272	-1.538707	5.213933
65	1	0	-4.509295	-2.660285	5.314816
66	6	0	-4.218301	-0.829382	6.434467
67	1	0	-4.468594	0.235072	6.333479
68	1	0	-3.121205	-0.886376	6.436588
69	6	0	-4.761585	-1.360304	7.764988
70	1	0	-4.358461	-0.797328	8.613039
71	1	0	-5.853987	-1.284957	7.804467
72	1	0	-4.498045	-2.414216	7.908602
73	14	0	-3.171102	-0.978800	-4.129268
74	1	0	-2.969173	0.293425	-4.901957
75	1	0	-3.079099	-2.119294	-5.110085
76	14	0	-3.116469	3.210642	-3.002329

77	1	0	-2.967911	4.695261	-3.216015
78	1	0	-2.969036	2.546433	-4.341054
79	14	0	0.716592	-1.218269	-3.531821
80	1	0	0.799952	-2.362707	-4.508603
81	1	0	0.916308	0.050337	-4.311399
82	14	0	0.785521	2.962525	-2.424365
83	1	0	0.947152	2.284973	-3.755260
84	1	0	0.901013	4.447014	-2.658100
85	14	0	4.597739	-1.469331	-2.924420
86	1	0	4.663572	-2.622623	-3.892127
87	1	0	4.800872	-0.207931	-3.714898
88	14	0	4.685273	2.752198	-1.829993
89	1	0	4.859233	2.058280	-3.150645
90	1	0	4.790242	4.234741	-2.080065
91	14	0	6.253023	3.673648	1.560182
92	1	0	7.199096	3.254096	2.656947
93	1	0	6.734175	5.006999	1.045006
94	14	0	2.362820	4.021135	0.820689
95	1	0	2.607988	5.272260	0.035274
96	14	0	-1.546969	4.244006	0.224526
97	1	0	-1.379584	5.488103	-0.592391
98	14	0	-5.508415	4.354170	-0.219864
99	1	0	-5.703173	5.715691	-0.839469
100	1	0	-6.759790	4.041048	0.560786
101	14	0	-5.627248	-3.322893	-2.350646
102	1	0	-6.906965	-3.439596	-1.563260
103	1	0	-5.796233	-4.150544	-3.600423
104	14	0	-1.690573	-3.627826	-1.933342
105	1	0	-1.588838	-4.262019	-3.286013
106	14	0	2.223357	-3.845848	-1.286612
107	1	0	2.506213	-4.509523	-2.599198
108	14	0	6.102467	-3.997905	-0.438596
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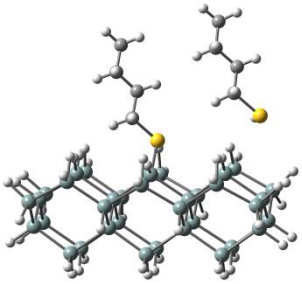
1a-IM2



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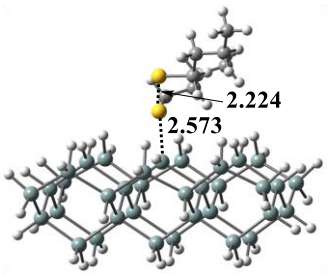
4	14	0	-6.303353	1.510073	-1.646054
5	14	0	-3.802876	4.603580	-1.138071
6	14	0	0.015559	4.178332	-1.917828
7	14	0	-2.456731	0.973666	-2.207208
8	14	0	3.481629	-4.154539	2.385217
9	14	0	3.696503	-0.228973	0.293361
10	14	0	5.024809	-3.563775	-1.259297
11	14	0	1.178333	-3.017966	-0.721001
12	14	0	1.552889	-0.637745	-0.604827
13	14	0	-4.160656	-2.941172	3.577001
14	14	0	-0.367550	-3.701372	2.947732
15	14	0	-3.930167	0.903830	1.358796
16	14	0	-2.677520	-2.434651	-0.124034
17	14	0	-6.503290	-1.869709	0.501400
18	14	0	-6.102095	0.491793	0.512981
19	14	0	-0.108626	0.162039	0.880962
20	14	0	-2.287454	-0.058874	-0.045891
21	14	0	5.345294	-1.184904	-1.104644
22	1	0	4.065020	4.906667	-2.267750
23	1	0	3.954774	3.279132	-0.509940
24	1	0	6.304284	-0.672164	-4.141996
25	1	0	-7.679527	1.215612	-2.193435
26	1	0	-3.692644	6.026745	-1.572525
27	1	0	-3.530899	4.569817	0.324752
28	1	0	0.112198	5.474992	-2.653686
29	1	0	0.221343	4.470407	-0.477450
30	1	0	3.724665	-2.850512	3.058851
31	1	0	3.487683	-5.206437	3.444021
32	1	0	5.649431	2.888395	1.283375
33	1	0	3.763140	-0.804148	1.669444
34	1	0	6.062809	-4.148475	-2.190132
35	1	0	-3.800639	-1.635074	4.193375
36	1	0	-4.156547	-3.958973	4.667786
37	1	0	-0.059106	-2.466720	3.720211
38	1	0	-0.392081	-4.829063	3.926899
39	1	0	-3.706013	2.373267	1.458569
40	1	0	-3.808180	0.350477	2.736246
41	1	0	-7.891681	-2.125014	-0.034669

42	1	0	-7.118419	1.134585	1.429113
43	1	0	-0.098753	-0.720196	2.085322
44	1	0	6.718054	-0.948830	-0.522728
45	16	0	0.484727	2.130032	1.576618
46	16	0	6.026736	1.836049	2.037929
47	6	0	-0.525096	2.340725	3.123234
48	1	0	-0.423880	1.436208	3.730413
49	1	0	-1.576227	2.453588	2.844477
50	6	0	-0.045553	3.569412	3.898942
51	1	0	1.013100	3.443561	4.159773
52	1	0	-0.105078	4.454854	3.253517
53	6	0	-0.867207	3.806631	5.175085
54	1	0	-1.925332	3.927338	4.907876
55	1	0	-0.812828	2.915034	5.813919
56	6	0	-0.395290	5.032234	5.964108
57	1	0	-0.996106	5.177891	6.867339
58	1	0	0.650634	4.926260	6.273588
59	1	0	-0.471595	5.944564	5.362164
60	6	0	4.966964	2.218773	3.498301
61	1	0	3.919547	2.214849	3.181823
62	1	0	5.109206	1.359825	4.162016
63	6	0	5.334308	3.521119	4.211145
64	1	0	6.395691	3.495082	4.486276
65	1	0	5.215963	4.362471	3.515220
66	6	0	4.478126	3.769490	5.462030
67	1	0	4.591151	2.923537	6.153394
68	1	0	3.416936	3.791979	5.178406
69	6	0	4.842667	5.071678	6.182445
70	1	0	4.219945	5.223625	7.069904
71	1	0	5.889014	5.064050	6.507364
72	1	0	4.706286	5.939115	5.527011
73	14	0	2.841329	-4.118088	-2.063092
74	1	0	2.637411	-5.602969	-1.899701
75	1	0	2.678517	-3.801690	-3.522878
76	14	0	3.100191	-0.347178	-4.246441
77	1	0	2.860878	-1.768188	-4.672310
78	1	0	3.034797	0.509724	-5.484661
79	14	0	-1.040947	-3.558872	-1.478148
80	1	0	-1.226679	-3.253284	-2.937773
81	1	0	-1.245282	-5.041815	-1.300204
82	14	0	-0.782295	0.155574	-3.720718
83	1	0	-0.845498	0.997695	-4.969149
84	1	0	-1.041634	-1.267591	-4.126882
85	14	0	-4.896261	-3.005114	-0.854523

86	1	0	-5.098953	-2.717289	-2.314803
87	1	0	-5.062881	-4.490198	-0.659101
88	14	0	-4.645630	0.687299	-3.158989
89	1	0	-4.698042	1.512412	-4.419115
90	1	0	-4.905595	-0.740575	-3.547143
91	14	0	-6.363468	-2.808436	2.701132
92	1	0	-7.239287	-2.027800	3.648777
93	1	0	-6.928833	-4.204777	2.625296
94	14	0	-2.526817	-3.565878	1.984475
95	1	0	-2.866356	-4.973480	1.602603
96	14	0	1.342168	-4.165703	1.376667
97	1	0	1.104622	-5.587276	0.969426
98	14	0	5.258639	-4.610959	0.880550
99	1	0	5.312591	-6.100901	0.650169
100	1	0	6.569511	-4.211953	1.509841
101	14	0	5.656076	2.261301	-3.010110
102	1	0	6.930706	2.490271	-2.236691
103	1	0	5.871200	2.825546	-4.392461
104	14	0	1.745380	2.800292	-2.769076
105	1	0	1.761291	3.085371	-4.239542
106	14	0	-2.169019	3.350271	-2.300961
107	1	0	-2.433521	3.614892	-3.751232
108	14	0	-6.031411	3.887410	-1.532613
109	1	0	-6.483775	4.450206	-2.856915
110	1	0	-6.942798	4.458535	-0.475278

1b-TS1



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3	14	0	5.082201	2.731314	-2.488843
4	14	0	-6.434461	1.798477	-0.247637
5	14	0	-4.107302	3.950388	2.223124
6	14	0	-0.287227	4.283686	1.376546

7	14	0	-2.609484	2.109530	-1.018309
8	14	0	3.943561	-4.116520	-0.644318
9	14	0	3.749119	0.252314	0.190595
10	14	0	5.316356	-1.218745	-3.050440
11	14	0	1.469703	-1.501173	-2.413750
12	14	0	1.593657	0.269319	-0.778581
13	14	0	-3.747239	-4.796346	0.630658
14	14	0	0.081753	-4.596275	-0.178893
15	14	0	-3.876019	-0.461639	1.586552
16	14	0	-2.423664	-1.816849	-1.733382
17	14	0	-6.252088	-2.131104	-1.006659
18	14	0	-6.041391	-0.394838	0.631743
19	14	0	-0.061861	-0.351779	0.814777
20	14	0	-2.247390	-0.069405	-0.080819
21	14	0	5.399573	0.584515	-1.473376
22	1	0	3.547418	6.072236	1.212207
23	1	0	3.780096	3.753106	1.774235
24	1	0	6.118843	2.917855	-3.570885
25	1	0	-7.819461	1.847522	-0.847430
26	1	0	-4.109520	5.304048	2.850437
27	1	0	-3.741905	2.973408	3.284831
28	1	0	-0.254099	5.567508	2.137691
29	1	0	0.032862	3.201688	2.346381
30	1	0	4.050451	-3.494103	0.703919
31	1	0	4.111273	-5.587780	-0.462135
32	1	0	3.843071	1.328927	1.216188
33	1	0	3.991870	-1.042104	0.884771
34	1	0	6.384023	-0.993381	-4.094528
35	1	0	-3.495297	-4.224958	1.980438
36	1	0	-3.620022	-6.278448	0.744190
37	1	0	0.293196	-4.212677	1.242407
38	1	0	0.197418	-6.084378	-0.249535
39	1	0	-3.771729	0.575251	2.650216
40	1	0	-3.641644	-1.784865	2.224009
41	1	0	-7.633071	-2.058863	-1.613765
42	1	0	-7.072709	-0.649978	1.707300
43	1	0	0.076572	-1.838738	0.793431
44	1	0	6.768108	0.577532	-0.830859
45	16	0	0.325437	-0.657856	3.339676
46	16	0	1.019896	-2.100850	4.882813
47	6	0	0.331747	0.942989	4.266034
48	1	0	-0.177257	0.734632	5.210596
49	1	0	-0.310936	1.608130	3.682950
50	6	0	1.711109	1.553454	4.497939

51	1	0	2.342885	0.824102	5.018490
52	1	0	2.190534	1.755084	3.531731
53	6	0	1.641422	2.845080	5.327760
54	1	0	0.994726	3.571588	4.818479
55	1	0	1.160637	2.629780	6.291251
56	6	0	3.020376	3.467484	5.569736
57	1	0	2.944218	4.382844	6.165055
58	1	0	3.679013	2.775102	6.106162
59	1	0	3.510225	3.724574	4.623731
60	6	0	2.824530	-2.247321	4.526449
61	1	0	2.945413	-2.517815	3.473756
62	1	0	3.307051	-1.279903	4.690944
63	6	0	3.440144	-3.320262	5.431884
64	1	0	3.280189	-3.051234	6.483966
65	1	0	2.923391	-4.274760	5.271318
66	6	0	4.944565	-3.499985	5.173223
67	1	0	5.456437	-2.540359	5.324847
68	1	0	5.100561	-3.767215	4.119750
69	6	0	5.576966	-4.566502	6.072963
70	1	0	6.646449	-4.676157	5.866770
71	1	0	5.466655	-4.308154	7.132135
72	1	0	5.106252	-5.544006	5.919932
73	14	0	-4.823469	2.361271	-1.919520
74	1	0	-4.993988	3.812044	-2.291590
75	1	0	-5.012018	1.550953	-3.170223
76	14	0	-0.966583	2.647592	-2.683166
77	1	0	-1.159326	4.091537	-3.069966
78	1	0	-1.141801	1.823821	-3.927224
79	14	0	-4.609534	-1.931676	-2.733089
80	1	0	-4.879151	-0.755774	-3.629046
81	1	0	-4.660607	-3.171807	-3.588661
82	14	0	-0.714965	-1.616026	-3.413471
83	1	0	-0.967714	-0.454237	-4.332994
84	1	0	-0.757928	-2.866481	-4.254400
85	14	0	2.896489	2.948444	-3.431953
86	1	0	2.732252	2.113941	-4.669955
87	1	0	2.690104	4.388191	-3.828175
88	14	0	3.175087	-1.349671	-4.105198
89	1	0	3.118911	-2.611583	-4.927723
90	1	0	2.945165	-0.194169	-5.037478
91	14	0	-5.973464	-4.299264	-0.026721
92	1	0	-6.898368	-4.450862	1.154722
93	1	0	-6.403976	-5.311996	-1.058471
94	14	0	-2.106499	-4.041839	-0.898088

95	1	0	-2.317322	-4.860679	-2.134586
96	14	0	1.797820	-3.716039	-1.555587
97	1	0	1.746824	-4.536152	-2.807821
98	14	0	5.725668	-3.334423	-2.004134
99	1	0	5.959190	-4.338096	-3.105613
100	1	0	6.994740	-3.266593	-1.191777
101	14	0	1.396607	4.294148	-0.279326
102	1	0	1.113471	5.461201	-1.172540
103	14	0	5.326206	4.512759	-0.907696
104	1	0	6.626957	4.368641	-0.158469
105	1	0	5.405225	5.800079	-1.689649
106	14	0	-2.463239	3.935367	0.521377
107	1	0	-2.758302	5.123416	-0.340248
108	14	0	-6.304042	3.486312	1.448488
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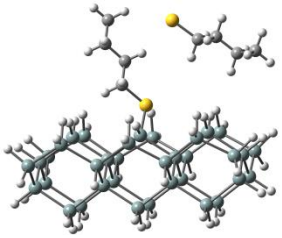

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3	14	0	-5.060665	-1.659892	-3.224092
4	14	0	6.471468	-1.529745	-0.879833
5	14	0	4.155991	-4.398002	0.725900
6	14	0	0.388605	-4.709086	-0.352554
7	14	0	2.632896	-1.584734	-1.684570
8	14	0	-3.910129	4.204610	0.753021
9	14	0	-3.706177	-0.194927	0.097323
10	14	0	-5.274453	2.269809	-2.478745
11	14	0	-1.424962	2.318902	-1.784805
12	14	0	-1.562083	0.107299	-0.852842
13	14	0	3.788869	4.370407	2.197285
14	14	0	-0.049793	4.406731	1.397270
15	14	0	3.928439	-0.033085	1.611405

16	14	0	2.448754	2.358571	-1.023275
17	14	0	6.289015	2.430223	-0.256865
18	14	0	6.090725	0.239139	0.689847
19	14	0	0.084132	0.044773	0.851217
20	14	0	2.273530	0.153903	-0.069993
21	14	0	-5.363696	0.052747	-1.575364
22	1	0	-3.525188	-6.019161	-0.805604
23	1	0	-3.710380	-3.999701	0.477238
24	1	0	-6.105617	-1.488032	-4.300693
25	1	0	7.851303	-1.367540	-1.471340
26	1	0	4.180745	-5.882285	0.874705
27	1	0	3.783473	-3.828987	2.049425
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29	1	0	0.084738	-4.526005	1.087884
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31	1	0	-4.061537	5.538627	1.403206
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33	1	0	-3.924516	0.793280	1.189604
34	1	0	-6.335449	2.403765	-3.544805
35	1	0	3.550215	3.370328	3.273126
36	1	0	3.654375	5.722327	2.813240
37	1	0	-0.253001	3.498436	2.558809
38	1	0	-0.172554	5.803557	1.911213
39	1	0	3.840547	-1.372258	2.257020
40	1	0	3.687054	0.981548	2.674406
41	1	0	7.663466	2.575305	-0.864918
42	1	0	7.115849	0.115399	1.793776
43	1	0	-0.080198	1.282947	1.669363
44	1	0	-6.729748	-0.137787	-0.956159
45	16	0	-0.360125	-1.627388	2.154029
46	16	0	-3.278476	-0.907857	6.710753
47	6	0	0.596527	-1.217304	3.696105
48	1	0	0.324141	-0.205732	4.011354
49	1	0	1.663694	-1.231781	3.459540
50	6	0	0.277958	-2.234024	4.794294
51	1	0	-0.796600	-2.215054	5.011775
52	1	0	0.514266	-3.243738	4.435181
53	6	0	1.062036	-1.951063	6.084853
54	1	0	2.138828	-1.958483	5.868222
55	1	0	0.825319	-0.938395	6.437016
56	6	0	0.751805	-2.961980	7.193513
57	1	0	1.320983	-2.740888	8.102161
58	1	0	-0.312460	-2.945798	7.451504
59	1	0	1.004691	-3.981833	6.882038

60	6	0	-4.407957	-1.013870	5.290178
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62	1	0	-4.685321	-2.074298	5.202296
63	6	0	-5.647279	-0.119111	5.362911
64	1	0	-6.212260	-0.361064	6.271590
65	1	0	-5.330492	0.925972	5.467386
66	6	0	-6.553168	-0.266137	4.131876
67	1	0	-6.858594	-1.316211	4.027360
68	1	0	-5.978234	-0.024677	3.227279
69	6	0	-7.797814	0.624702	4.200078
70	1	0	-8.425146	0.501561	3.311567
71	1	0	-8.409631	0.383044	5.076439
72	1	0	-7.523530	1.683197	4.270531
73	14	0	4.842761	-1.493340	-2.628583
74	1	0	5.018052	-2.727643	-3.474966
75	1	0	5.020414	-0.302855	-3.527576
76	14	0	0.987260	-1.519071	-3.430584
77	1	0	1.175877	-2.745701	-4.285230
78	1	0	1.160267	-0.321091	-4.320804
79	14	0	4.627820	2.811031	-1.932231
80	1	0	4.890771	2.009828	-3.175116
81	1	0	4.658781	4.267753	-2.317661
82	14	0	0.758651	2.758217	-2.684483
83	1	0	1.010502	1.972266	-3.939925
84	1	0	0.816033	4.219429	-3.048593
85	14	0	-2.882848	-1.554907	-4.205220
86	1	0	-2.725025	-0.349044	-5.087518
87	1	0	-2.684668	-2.774177	-5.068103
88	14	0	-3.130346	2.739204	-3.425087
89	1	0	-3.066007	4.204112	-3.773042
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91	14	0	6.011710	4.140443	1.396583
92	1	0	6.944430	3.894645	2.555632
93	1	0	6.425847	5.444708	0.762391
94	14	0	2.135454	4.168479	0.517164
95	1	0	2.324130	5.362012	-0.367224
96	14	0	-1.755369	4.103151	-0.217757
97	1	0	-1.661430	5.307513	-1.102737
98	14	0	-5.681455	3.932306	-0.803516
99	1	0	-5.891742	5.244052	-1.517611
100	1	0	-6.959442	3.619116	-0.066639
101	14	0	-1.371719	-3.890533	-1.711952
102	1	0	-1.218975	-4.629017	-3.006233
103	14	0	-5.300043	-3.850614	-2.284553

104	1	0	-6.594496	-3.937733	-1.515331
105	1	0	-5.405581	-4.817173	-3.437733
106	14	0	2.526010	-3.844401	-0.895140
107	1	0	2.934457	-4.592778	-2.126677
108	14	0	6.349726	-3.685894	0.159143
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110	1	0	7.223806	-3.710334	1.387896

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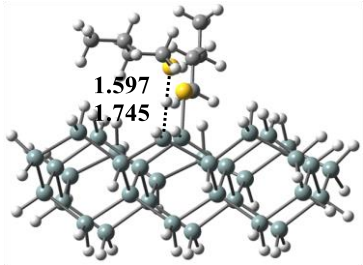

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3	14	0	-6.416726	-1.052669	-0.955010
4	14	0	4.985404	-3.903030	-1.306186
5	14	0	2.658937	-5.411173	1.581351
6	14	0	-1.216348	-4.829134	1.460771
7	14	0	1.181342	-2.957098	-1.235714
8	14	0	-2.841778	5.061636	0.106179
9	14	0	-3.826736	0.876655	1.188415
10	14	0	-5.484314	2.742879	-1.807377
11	14	0	-1.701642	1.772146	-1.935189
12	14	0	-2.058763	0.138767	-0.196146
13	14	0	4.738643	3.133620	0.054048
14	14	0	0.985814	4.264853	-0.235743
15	14	0	3.697814	-1.069749	1.030901
16	14	0	2.158613	0.819729	-1.999629
17	14	0	5.955723	-0.091800	-1.986662
18	14	0	5.496640	-1.771665	-0.339594
19	14	0	0.019622	0.246094	0.959719
20	14	0	1.747697	-0.823313	-0.282346
21	14	0	-5.804314	1.097230	-0.094853
22	1	0	-5.193466	-4.722346	2.557505
23	1	0	-4.444983	-2.474309	2.935704
24	1	0	-7.687200	-0.915236	-1.759424

25	1	0	6.130555	-4.319436	-2.198091
26	1	0	2.368500	-6.730771	2.213675
27	1	0	2.826432	-4.423211	2.682257
28	1	0	-1.575566	-6.258497	1.696290
29	1	0	-1.003767	-4.222817	2.800486
30	1	0	-2.880334	4.522197	1.489397
31	1	0	-2.483568	6.507325	0.193779
32	1	0	-4.053098	-0.111234	2.279117
33	1	0	-3.472400	2.175989	1.817311
34	1	0	-6.755522	2.852867	-2.615171
35	1	0	4.533196	2.598694	1.424522
36	1	0	5.106389	4.573859	0.180965
37	1	0	0.934530	4.117979	1.502635
38	1	0	1.345967	5.711466	-0.382504
39	1	0	3.455173	-2.079808	2.097618
40	1	0	4.038090	0.217921	1.691558
41	1	0	7.114668	-0.555950	-2.836331
42	1	0	6.737041	-1.936331	0.508543
43	1	0	0.379217	1.689174	0.825199
44	1	0	-6.927967	1.574567	0.796539
45	16	0	0.055955	0.182467	3.120808
46	16	0	0.848776	4.270268	3.089859
47	6	0	-0.352826	-1.540101	3.655128
48	1	0	0.368044	-2.234718	3.215615
49	1	0	-1.351702	-1.802109	3.295406
50	6	0	-0.298157	-1.608627	5.184781
51	1	0	0.698963	-1.299645	5.523076
52	1	0	-1.006442	-0.882488	5.603280
53	6	0	-0.614303	-3.008728	5.730509
54	1	0	-1.610675	-3.318351	5.388176
55	1	0	0.093365	-3.733892	5.307386
56	6	0	-0.556800	-3.070716	7.260445
57	1	0	-0.787486	-4.076512	7.625589
58	1	0	0.438732	-2.801795	7.630862
59	1	0	-1.276144	-2.378727	7.712394
60	6	0	1.304362	6.050419	3.154343
61	1	0	0.723342	6.591114	2.399426
62	1	0	0.935126	6.390427	4.129195
63	6	0	2.799994	6.342532	3.015139
64	1	0	3.349883	5.765547	3.768724
65	1	0	3.150888	5.984162	2.038355
66	6	0	3.125832	7.836448	3.158558
67	1	0	2.771367	8.192660	4.135504
68	1	0	2.564387	8.406010	2.405494

69	6	0	4.621492	8.137233	3.016806
70	1	0	4.825222	9.207590	3.123906
71	1	0	5.205412	7.608975	3.778872
72	1	0	4.997541	7.823103	2.036579
73	14	0	2.972554	-3.815079	-2.592583
74	1	0	2.592418	-5.217168	-2.993061
75	1	0	3.153185	-3.019696	-3.853328
76	14	0	-0.856060	-2.864004	-2.499983
77	1	0	-1.219081	-4.273267	-2.890988
78	1	0	-0.699118	-2.071910	-3.766000
79	14	0	4.055676	0.302235	-3.385477
80	1	0	3.792678	-0.852299	-4.309559
81	1	0	4.329625	1.511046	-4.242710
82	14	0	0.190862	1.233760	-3.324913
83	1	0	-0.102180	0.096261	-4.262305
84	1	0	0.473783	2.446835	-4.173702
85	14	0	-4.687028	-1.936258	-2.346477
86	1	0	-4.554965	-1.157702	-3.623774
87	1	0	-5.032270	-3.355483	-2.716366
88	14	0	-3.667089	2.183277	-3.260036
89	1	0	-3.377207	3.372652	-4.139134
90	1	0	-3.999059	1.030089	-4.163824
91	14	0	6.548537	2.000286	-0.981777
92	1	0	7.658175	1.788639	0.017076
93	1	0	7.099281	2.879355	-2.076812
94	14	0	2.740178	3.005006	-1.203339
95	1	0	3.051576	3.721429	-2.483349
96	14	0	-1.169502	3.981597	-1.170604
97	1	0	-1.122981	4.743851	-2.460904
98	14	0	-4.996682	4.894679	-0.874267
99	1	0	-5.093802	5.899233	-1.995227
100	1	0	-6.049460	5.260125	0.141604
101	14	0	-3.069125	-3.818350	0.386618
102	1	0	-3.559720	-4.864529	-0.565470
103	14	0	-6.819875	-2.631302	0.802250
104	1	0	-7.748278	-2.029988	1.826991
105	1	0	-7.536139	-3.810725	0.193293
106	14	0	0.809381	-4.813065	0.234705
107	1	0	0.659262	-5.929826	-0.750879
108	14	0	4.689728	-5.591628	0.365988
109	1	0	4.702738	-6.927725	-0.333480
110	1	0	5.854716	-5.579768	1.323107

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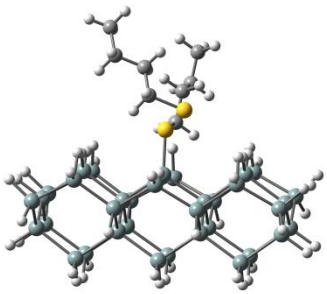

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	14	0	-6.038401	-2.144152	-0.986808
4	14	0	5.702266	-2.861244	-1.215877
5	14	0	3.677396	-4.513966	1.824939
6	14	0	-0.235177	-4.640765	1.706424
7	14	0	1.787996	-2.642137	-1.184789
8	14	0	-3.679157	4.585527	-0.422622
9	14	0	-3.863456	0.385189	0.980048
10	14	0	-5.831827	1.680610	-2.133379
11	14	0	-1.935291	1.431261	-2.218938
12	14	0	-1.984700	-0.112766	-0.366033
13	14	0	4.137195	4.095490	-0.469325
14	14	0	0.238869	4.349035	-0.585216
15	14	0	3.901344	-0.140399	0.881506
16	14	0	2.032184	1.187117	-2.265372
17	14	0	5.930237	0.992652	-2.251972
18	14	0	5.803156	-0.591106	-0.456640
19	14	0	0.038645	0.460155	0.746281
20	14	0	1.941443	-0.369055	-0.420877
21	14	0	-5.843665	0.141322	-0.296314
22	1	0	-4.179649	-5.225954	2.803647
23	1	0	-3.876321	-2.853837	2.984138
24	1	0	-7.305623	-2.306424	-1.791621
25	1	0	6.911033	-3.142333	-2.076089
26	1	0	3.636508	-5.807170	2.567737
27	1	0	3.649004	-3.423561	2.837747
28	1	0	-0.325182	-6.071924	2.120104
29	1	0	-0.139973	-3.847830	2.960518
30	1	0	-3.659872	4.138394	0.993820
31	1	0	-3.599578	6.074360	-0.431702
32	1	0	-3.906312	-0.540400	2.146065
33	1	0	-3.755706	1.770686	1.508953

34	1	0	-7.097363	1.475812	-2.931591
35	1	0	4.050983	3.642501	0.946193
36	1	0	4.238530	5.583961	-0.449049
37	1	0	-0.890826	3.408798	3.177592
38	1	0	0.337600	5.840614	-0.494846
39	1	0	3.854991	-1.096627	2.021897
40	1	0	3.986695	1.233081	1.446347
41	1	0	7.154138	0.679010	-3.079383
42	1	0	7.051068	-0.441227	0.383321
43	1	0	0.155265	1.930677	0.493565
44	1	0	-7.037000	0.462515	0.574237
45	16	0	0.055872	0.622330	2.911221
46	16	0	-0.979040	4.748234	3.029912
47	6	0	-0.342500	-1.027332	3.647523
48	1	0	0.495753	-1.704132	3.466912
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50	6	0	-0.590186	-0.864896	5.149828
51	1	0	0.295928	-0.415720	5.616516
52	1	0	-1.415932	-0.159516	5.305870
53	6	0	-0.913577	-2.198089	5.840666
54	1	0	-1.797284	-2.647383	5.368297
55	1	0	-0.087806	-2.903255	5.678560
56	6	0	-1.163283	-2.036825	7.343757
57	1	0	-1.395930	-2.998176	7.812436
58	1	0	-0.283690	-1.623496	7.849865
59	1	0	-2.003838	-1.360498	7.535129
60	6	0	0.734078	5.146936	3.582961
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62	1	0	0.811073	6.231590	3.455037
63	6	0	1.042265	4.749049	5.027321
64	1	0	0.303806	5.209554	5.694970
65	1	0	0.925623	3.662736	5.136163
66	6	0	2.460108	5.156530	5.455012
67	1	0	2.574224	6.243334	5.343853
68	1	0	3.190904	4.701690	4.772959
69	6	0	2.785849	4.752594	6.896765
70	1	0	3.799905	5.056011	7.176326
71	1	0	2.091546	5.218131	7.605336
72	1	0	2.714743	3.667101	7.029072
73	14	0	3.715458	-3.265534	-2.483647
74	1	0	3.607595	-4.743958	-2.755621
75	1	0	3.748949	-2.565722	-3.811881
76	14	0	-0.227536	-3.030312	-2.428422
77	1	0	-0.328002	-4.511592	-2.687470

78	1	0	-0.215191	-2.340566	-3.762167
79	14	0	3.984743	0.906942	-3.639553
80	1	0	3.937005	-0.351986	-4.457675
81	1	0	4.028578	2.066949	-4.600572
82	14	0	0.021719	1.118078	-3.587015
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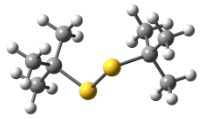
84	1	0	0.081471	2.277934	-4.547593
85	14	0	-4.165127	-2.804025	-2.316758
86	1	0	-4.169755	-2.126295	-3.656818
87	1	0	-4.242188	-4.289117	-2.560426
88	14	0	-3.934259	1.349257	-3.551230
89	1	0	-3.868347	2.490413	-4.533402
90	1	0	-4.037865	0.079049	-4.346529
91	14	0	6.126544	3.236593	-1.437654
92	1	0	7.258315	3.320262	-0.444305
93	1	0	6.503540	4.104818	-2.612019
94	14	0	2.172850	3.501093	-1.644575
95	1	0	2.316926	4.163587	-2.983081
96	14	0	-1.805729	3.745280	-1.597589
97	1	0	-1.866224	4.415212	-2.938671
98	14	0	-5.752621	3.956274	-1.391638
99	1	0	-6.012180	4.820339	-2.600487
100	1	0	-6.874027	4.211538	-0.416018
101	14	0	-2.237840	-4.119876	0.554903
102	1	0	-2.499651	-5.324499	-0.294467
103	14	0	-6.152129	-3.640807	0.881338
104	1	0	-7.197736	-3.168157	1.859504
105	1	0	-6.607788	-4.979804	0.357465
106	14	0	1.756261	-4.390824	0.452518
107	1	0	1.811227	-5.606377	-0.419491
108	14	0	5.712857	-4.413617	0.608634
109	1	0	5.985051	-5.781754	0.035208
110	1	0	6.847116	-4.093475	1.549200

S5.2Reaction between di-*t*-butyldisulfide and the silyl radical

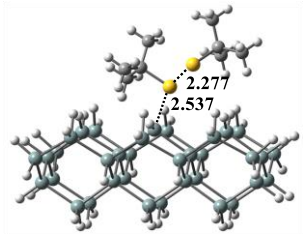
2



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-2.178249	0.191643	0.063042
2	16	0	-0.778850	-0.830970	-0.693730
3	16	0	0.778849	-0.830814	0.693916
4	6	0	2.178248	0.191628	-0.063085
5	6	0	-3.281390	0.093288	-1.003411
6	1	0	-3.566673	-0.946143	-1.192588
7	1	0	-4.171635	0.627693	-0.652434
8	1	0	-2.968501	0.544479	-1.950030
9	6	0	-2.633292	-0.456798	1.375476
10	1	0	-2.944457	-1.493112	1.218360
11	1	0	-1.830428	-0.446727	2.118188
12	1	0	-3.482546	0.100391	1.790185
13	6	0	-1.769498	1.647440	0.290808
14	1	0	-0.936639	1.716423	0.995336
15	1	0	-1.477339	2.134521	-0.643670
16	1	0	-2.614331	2.204077	0.715071
17	6	0	3.281401	0.093489	1.003377
18	1	0	4.171646	0.627809	0.652276
19	1	0	2.968526	0.544885	1.949904
20	1	0	3.566673	-0.945905	1.192772
21	6	0	1.769509	1.647382	-0.291151
22	1	0	0.936644	1.716226	-0.995685
23	1	0	1.477364	2.134660	0.643228
24	1	0	2.614343	2.203921	-0.715539
25	6	0	2.633273	-0.457091	-1.375387
26	1	0	3.482527	0.100004	-1.790223
27	1	0	2.944432	-1.493375	-1.218057
28	1	0	1.830401	-0.447170	-2.118093

2-TS1



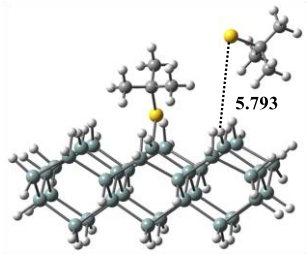
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-3.877095	-4.321231	-0.427428
2	14	0	-1.528507	-1.607367	-2.206014
3	14	0	-5.400003	-1.469620	-2.814405
4	14	0	6.253523	-1.887022	-1.209291

5	14	0	3.925931	-4.604102	0.666884
6	14	0	0.017751	-4.415355	0.143735
7	14	0	2.362426	-1.767492	-1.681324
8	14	0	-3.723711	4.466643	0.931263
9	14	0	-3.830421	0.077159	0.396157
10	14	0	-5.353302	2.502666	-2.191070
11	14	0	-1.478966	2.329179	-1.621443
12	14	0	-1.680770	0.162045	-0.589703
13	14	0	4.077676	4.191717	1.947919
14	14	0	0.190488	4.451119	1.387761
15	14	0	4.012532	-0.216602	1.429478
16	14	0	2.424785	2.176405	-1.104364
17	14	0	6.319287	2.112296	-0.661444
18	14	0	6.097501	-0.055728	0.325468
19	14	0	0.049568	0.049448	1.053791
20	14	0	2.191611	0.005259	-0.071795
21	14	0	-5.533765	0.317868	-1.227649
22	1	0	-3.976370	-5.800080	-0.255738
23	1	0	-4.016173	-3.712788	0.923117
24	1	0	-6.480526	-1.298698	-3.855367
25	1	0	7.586106	-1.832563	-1.917437
26	1	0	3.890283	-6.087526	0.823994
27	1	0	3.714535	-4.018583	2.019064
28	1	0	-0.078701	-5.872333	0.456791
29	1	0	-0.142361	-3.677166	1.424878
30	1	0	-3.867590	3.516081	2.065611
31	1	0	-3.774949	5.846353	1.497524
32	1	0	-4.016575	-1.217975	1.103817
33	1	0	-3.968748	1.168997	1.392485
34	1	0	-6.444827	2.689449	-3.217893
35	1	0	3.872350	3.223283	3.059737
36	1	0	4.060977	5.557852	2.547546
37	1	0	0.006719	3.614747	2.604277
38	1	0	0.187389	5.876238	1.836289
39	1	0	3.969354	-1.541247	2.105687
40	1	0	3.921741	0.816658	2.498646
41	1	0	7.649627	2.203489	-1.369803
42	1	0	7.194081	-0.218295	1.353848
43	1	0	0.068510	1.427365	1.627112
44	1	0	-6.876399	0.224661	-0.537885
45	16	0	-1.020246	-0.942310	3.130025
46	16	0	-2.621449	0.112497	4.358500
47	6	0	0.420023	-1.177477	4.372378
48	6	0	1.380059	-2.192210	3.740652

49	1	0	1.780927	-1.846216	2.787338
50	1	0	2.226427	-2.348079	4.420625
51	1	0	0.890400	-3.155767	3.578619
52	6	0	-0.144623	-1.761750	5.671164
53	1	0	0.692496	-1.962064	6.350415
54	1	0	-0.824509	-1.064116	6.161722
55	1	0	-0.668144	-2.705914	5.494834
56	6	0	1.095591	0.170556	4.640516
57	1	0	1.899562	0.035517	5.374194
58	1	0	1.538574	0.595209	3.735876
59	1	0	0.382211	0.892321	5.047601
60	6	0	-3.973762	-1.096911	4.926363
61	6	0	-3.869943	-1.256338	6.450846
62	1	0	-4.707160	-1.865673	6.815222
63	1	0	-2.941698	-1.753570	6.742427
64	1	0	-3.913761	-0.288094	6.958286
65	6	0	-5.301818	-0.414535	4.556642
66	1	0	-5.402087	-0.301086	3.474614
67	1	0	-6.139770	-1.022689	4.920465
68	1	0	-5.385640	0.576704	5.012998
69	6	0	-3.860279	-2.456252	4.231838
70	1	0	-2.919516	-2.959323	4.469934
71	1	0	-4.681508	-3.098880	4.571931
72	1	0	-3.930343	-2.363923	3.145353
73	14	0	4.483564	-1.818367	-2.810271
74	1	0	4.524488	-3.084063	-3.628123
75	1	0	4.632724	-0.663914	-3.759888
76	14	0	4.541259	2.520360	-2.199923
77	1	0	4.674237	1.677979	-3.437291
78	1	0	4.594273	3.964110	-2.630954
79	14	0	0.602062	-1.657371	-3.303962
80	1	0	0.661091	-2.912540	-4.136426
81	1	0	0.779208	-0.492940	-4.236489
82	14	0	0.659045	2.623971	-2.664876
83	1	0	0.794486	1.800194	-3.914598
84	1	0	0.773532	4.070960	-3.071703
85	14	0	-3.259836	-1.511936	-3.870770
86	1	0	-3.069192	-0.349186	-4.802492
87	1	0	-3.149064	-2.770808	-4.692586
88	14	0	-3.217893	2.804410	-3.215206
89	1	0	-3.072707	4.250672	-3.615011
90	1	0	-3.072865	1.979162	-4.462669
91	14	0	6.226947	3.838767	0.998815
92	1	0	7.221451	3.548695	2.095130

93	1	0	6.666593	5.118384	0.331864
94	14	0	2.302505	4.044851	0.390746
95	1	0	2.511791	5.198281	-0.541470
96	14	0	-1.621036	4.188884	-0.118112
97	1	0	-1.497967	5.349470	-1.057148
98	14	0	-5.576770	4.223025	-0.537159
99	1	0	-5.762719	5.521983	-1.281880
100	1	0	-6.830833	3.996979	0.270131
101	14	0	-5.692903	-3.613676	-1.785147
102	1	0	-6.960936	-3.628767	-0.968458
103	1	0	-5.872599	-4.618033	-2.896409
104	14	0	-1.743420	-3.817824	-1.317061
105	1	0	-1.592320	-4.684463	-2.528370
106	14	0	2.156023	-3.969869	-0.771302
107	1	0	2.283550	-4.848696	-1.976359
108	14	0	6.094178	-4.007915	-0.102668
109	1	0	6.540172	-5.052809	-1.095322
110	1	0	7.060607	-4.060742	1.054203

2-IM1



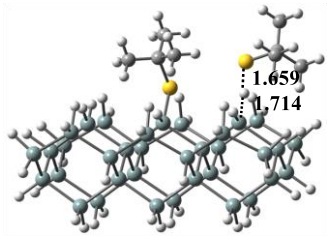
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-4.163123	-3.310514	-1.506281
2	14	0	-1.275853	-0.740895	-2.565470
3	14	0	-5.011518	0.170759	-3.318079
4	14	0	6.190453	-2.563975	-0.991159
5	14	0	3.290087	-5.147950	0.013488
6	14	0	-0.424068	-4.402609	-1.016964
7	14	0	2.461585	-1.658804	-1.789668
8	14	0	-2.817979	4.929409	1.582602
9	14	0	-3.512367	0.762339	0.209293
10	14	0	-4.396286	3.881896	-1.945575
11	14	0	-0.664317	2.965695	-1.199984
12	14	0	-1.311535	0.712472	-0.654717
13	14	0	4.610474	3.061708	3.182002

14	14	0	0.943630	4.129836	2.317290
15	14	0	3.883098	-1.081734	1.756645
16	14	0	3.087805	2.034389	-0.397753
17	14	0	6.801330	1.124978	0.440447
18	14	0	6.095122	-1.114968	0.914087
19	14	0	0.211012	-0.013717	1.016861
20	14	0	2.404863	-0.214340	0.126605
21	14	0	-5.003426	1.625847	-1.415109
22	1	0	-4.519903	-4.751961	-1.653153
23	1	0	-4.291545	-2.969190	-0.064242
24	1	0	-5.959814	0.727637	-4.353169
25	1	0	7.600236	-2.564570	-1.532380
26	1	0	2.997558	-6.602763	-0.142012
27	1	0	3.003355	-4.786625	1.427380
28	1	0	-0.678926	-5.802472	-1.471191
29	1	0	-0.707087	-4.348847	0.438795
30	1	0	-3.220086	3.807114	2.473381
31	1	0	-2.704365	6.149300	2.433949
32	1	0	-3.943889	-0.608157	0.594445
33	1	0	-3.559103	1.606296	1.435088
34	1	0	-5.348787	4.410389	-2.991410
35	1	0	4.085238	1.954953	4.026817
36	1	0	4.728378	4.265860	4.054828
37	1	0	0.478214	3.101637	3.288944
38	1	0	1.098319	5.404162	3.080482
39	1	0	3.474190	-2.460746	2.136693
40	1	0	3.827403	-0.243577	2.985905
41	1	0	8.212321	1.090073	-0.096439
42	1	0	7.019750	-1.676160	1.970436
43	1	0	0.278939	1.087226	2.018310
44	1	0	-6.402945	1.647496	-0.842726
45	16	0	-0.483884	-1.791862	2.053712
46	16	0	-5.568246	-2.569180	4.911254
47	6	0	-0.684337	-1.347175	3.894325
48	6	0	0.659249	-0.919526	4.494299
49	1	0	1.033412	0.003344	4.042337
50	1	0	0.535865	-0.733976	5.568557
51	1	0	1.415376	-1.698926	4.367937
52	6	0	-1.157905	-2.665193	4.527849
53	1	0	-1.289377	-2.515544	5.605998
54	1	0	-2.117997	-2.986796	4.115078
55	1	0	-0.425741	-3.464846	4.383022
56	6	0	-1.749333	-0.260450	4.076723
57	1	0	-1.894175	-0.070887	5.147593

58	1	0	-1.453640	0.684495	3.612504
59	1	0	-2.708527	-0.573452	3.656299
60	6	0	-6.901180	-2.899635	3.672225
61	6	0	-8.229927	-3.188153	4.389447
62	1	0	-9.023472	-3.362248	3.651926
63	1	0	-8.155176	-4.080604	5.018123
64	1	0	-8.525933	-2.349207	5.024644
65	6	0	-7.013803	-1.608512	2.832581
66	1	0	-6.077934	-1.384381	2.312475
67	1	0	-7.797837	-1.746197	2.077685
68	1	0	-7.287886	-0.747698	3.449693
69	6	0	-6.493864	-4.082308	2.777435
70	1	0	-6.369644	-4.999056	3.362145
71	1	0	-7.274303	-4.266710	2.028427
72	1	0	-5.554654	-3.878997	2.256468
73	14	0	-2.824230	-0.028225	-4.260324
74	1	0	-2.383800	1.249101	-4.917589
75	1	0	-2.849009	-1.096915	-5.322423
76	14	0	-2.154787	4.016632	-2.766244
77	1	0	-1.763567	5.469432	-2.854805
78	1	0	-2.028972	3.429635	-4.143144
79	14	0	0.930980	-0.931932	-3.488564
80	1	0	0.892777	-1.993044	-4.557936
81	1	0	1.379882	0.345256	-4.140516
82	14	0	1.607287	3.077869	-1.977650
83	1	0	1.753190	2.490756	-3.352970
84	1	0	1.988413	4.533216	-2.066956
85	14	0	4.678924	-1.850210	-2.699167
86	1	0	4.633729	-2.905986	-3.773715
87	1	0	5.130340	-0.571436	-3.346246
88	14	0	5.364937	2.172336	-1.157657
89	1	0	5.532449	1.585628	-2.530231
90	1	0	5.722440	3.634026	-1.243748
91	14	0	-5.737835	-2.040253	-2.749595
92	1	0	-7.042437	-1.970921	-1.994851
93	1	0	-6.017325	-2.762195	-4.044279
94	14	0	-1.927674	-3.021126	-2.218329
95	1	0	-1.892959	-3.544695	-3.621362
96	14	0	1.861491	-3.952819	-1.444011
97	1	0	2.118700	-4.523398	-2.804713
98	14	0	5.599618	-4.815811	-0.426131
99	1	0	5.991892	-5.684054	-1.595625
100	1	0	6.412564	-5.276426	0.757718
101	14	0	6.780699	2.494105	2.405617

102	1	0	7.553046	1.818855	3.510872
103	1	0	7.511465	3.770351	2.070244
104	14	0	3.073100	3.558346	1.453905
105	1	0	3.578160	4.818382	0.821823
106	14	0	-0.689640	4.498630	0.643540
107	1	0	-0.281714	5.781257	-0.012734
108	14	0	-4.524965	5.304657	-0.023054
109	1	0	-4.414928	6.727948	-0.509967
110	1	0	-5.875939	5.163957	0.632197

2-TS2



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-3.808858	-4.205589	-0.218668
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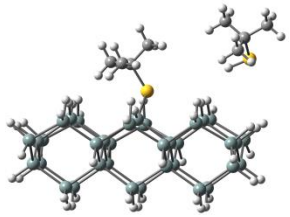
3	14	0	-5.210052	-1.370912	-2.675389
4	14	0	6.376190	-2.146241	-0.823707
5	14	0	3.914371	-4.696705	1.057778
6	14	0	0.068709	-4.657969	0.236780
7	14	0	2.512865	-1.886202	-1.427932
8	14	0	-3.386071	4.768408	0.693966
9	14	0	-3.606211	0.376617	0.488450
10	14	0	-5.019599	2.608145	-2.289861
11	14	0	-1.165496	2.328696	-1.655004
12	14	0	-1.469446	0.213553	-0.525782
13	14	0	4.318773	4.129977	2.060846
14	14	0	0.483678	4.520146	1.313301
15	14	0	4.094003	-0.288054	1.715245
16	14	0	2.722349	2.077515	-1.007468
17	14	0	6.575611	1.839003	-0.352756
18	14	0	6.222522	-0.291844	0.682656
19	14	0	0.242428	0.134044	1.121589
20	14	0	2.386103	-0.035461	0.097654
21	14	0	-5.292853	0.495379	-1.176002
22	1	0	-3.974889	-5.669989	0.013691
23	1	0	-3.914849	-3.514539	1.091000

24	1	0	-6.279555	-1.165711	-3.722001
25	1	0	7.732366	-2.126888	-1.487473
26	1	0	3.806115	-6.164743	1.300785
27	1	0	3.686282	-4.013683	2.359419
28	1	0	-0.015937	-6.148464	0.190756
29	1	0	-0.136924	-4.242207	1.646280
30	1	0	-3.597872	3.974151	1.933861
31	1	0	-3.368760	6.206722	1.091452
32	1	0	-3.999549	-0.712417	1.752550
33	1	0	-3.627114	1.668649	1.233467
34	1	0	-6.088652	2.743143	-3.349113
35	1	0	4.002728	3.228157	3.201810
36	1	0	4.338278	5.523529	2.593466
37	1	0	0.217076	3.721640	2.541299
38	1	0	0.512434	5.954092	1.729761
39	1	0	3.901194	-1.553312	2.473530
40	1	0	4.035975	0.832979	2.692958
41	1	0	7.938789	1.852934	-1.002061
42	1	0	7.281108	-0.466725	1.747861
43	1	0	0.226096	1.466557	1.786840
44	1	0	-6.652791	0.516082	-0.518194
45	16	0	-0.229769	-1.357620	2.623097
46	16	0	-4.297215	-1.416435	3.224737
47	6	0	-0.073088	-0.543733	4.339702
48	6	0	1.360708	-0.062520	4.579634
49	1	0	1.634871	0.750647	3.901253
50	1	0	1.449362	0.321949	5.603453
51	1	0	2.080586	-0.875796	4.456586
52	6	0	-0.423467	-1.691848	5.300044
53	1	0	-0.366017	-1.324957	6.331768
54	1	0	-1.438474	-2.059268	5.125905
55	1	0	0.274052	-2.528247	5.197567
56	6	0	-1.077679	0.602508	4.495515
57	1	0	-1.013406	0.997710	5.517391
58	1	0	-0.861775	1.428189	3.811869
59	1	0	-2.100294	0.258619	4.321601
60	6	0	-6.057617	-0.879085	3.541662
61	6	0	-6.393135	-1.465156	4.927464
62	1	0	-7.424409	-1.198968	5.190557
63	1	0	-6.314597	-2.556337	4.931832
64	1	0	-5.731867	-1.066482	5.702304
65	6	0	-6.164185	0.652502	3.582841
66	1	0	-5.918919	1.100381	2.615327
67	1	0	-7.190727	0.948043	3.833886

68	1	0	-5.491119	1.075835	4.333236
69	6	0	-7.001701	-1.466073	2.482339
70	1	0	-6.930294	-2.556523	2.451228
71	1	0	-8.039723	-1.194933	2.713813
72	1	0	-6.774186	-1.079806	1.484837
73	14	0	-2.860160	2.794601	-3.294736
74	1	0	-2.665249	4.223338	-3.734201
75	1	0	-2.724014	1.928063	-4.513877
76	14	0	-3.072453	-1.518334	-3.729783
77	1	0	-2.837281	-0.387121	-4.689438
78	1	0	-3.013321	-2.800246	-4.519595
79	14	0	1.019943	2.522166	-2.641440
80	1	0	1.181499	3.952628	-3.088250
81	1	0	1.167906	1.654351	-3.858956
82	14	0	0.794282	-1.769233	-3.097012
83	1	0	0.833751	-3.050095	-3.889796
84	1	0	1.024117	-0.639285	-4.059886
85	14	0	4.902851	2.296592	-1.996535
86	1	0	5.060305	1.427022	-3.211512
87	1	0	5.047009	3.728341	-2.445151
88	14	0	4.665584	-2.036571	-2.487884
89	1	0	4.682147	-3.314679	-3.285958
90	1	0	4.896392	-0.903537	-3.447224
91	14	0	6.122279	-4.240459	0.312517
92	1	0	6.530029	-5.321324	-0.657554
93	1	0	7.077597	-4.309814	1.477569
94	14	0	2.243966	-4.077615	-0.497616
95	1	0	2.488578	-4.936351	-1.700288
96	14	0	-1.668271	-3.835282	-1.147987
97	1	0	-1.599438	-4.665545	-2.392447
98	14	0	-5.589507	-3.481618	-1.609730
99	1	0	-6.873489	-3.435038	-0.820274
100	1	0	-5.790999	-4.484461	-2.718572
101	14	0	-5.231973	4.446401	-0.768081
102	1	0	-5.394100	5.691100	-1.604596
103	1	0	-6.493773	4.294685	0.044286
104	14	0	-1.274412	4.273557	-0.255244
105	1	0	-1.039229	5.366074	-1.252268
106	14	0	2.617026	3.999796	0.421789
107	1	0	2.910252	5.113091	-0.535821
108	14	0	6.491126	3.625620	1.242983
109	1	0	7.407824	3.325236	2.402166
110	1	0	7.032985	4.855913	0.558638

2-IM2



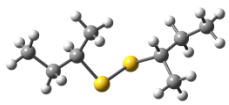
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-3.822514	-3.778684	-0.783567
2	14	0	-1.173878	-1.279477	-2.394467
3	14	0	-4.996701	-0.825663	-3.187715
4	14	0	6.435052	-2.195806	-0.700311
5	14	0	3.780072	-4.876227	0.689250
6	14	0	0.001183	-4.600479	-0.343964
7	14	0	2.622269	-1.755617	-1.542000
8	14	0	-3.226731	4.692285	0.985055
9	14	0	-3.515514	0.346597	0.146161
10	14	0	-4.696512	3.095389	-2.369186
11	14	0	-0.888486	2.637957	-1.555187
12	14	0	-1.330564	0.424832	-0.714366
13	14	0	4.359610	3.767315	2.719689
14	14	0	0.601023	4.392851	1.773221
15	14	0	4.035833	-0.586112	1.850959
16	14	0	2.912044	2.126011	-0.650133
17	14	0	6.714027	1.707142	0.211579
18	14	0	6.235991	-0.506344	0.986505
19	14	0	0.221310	0.083847	1.047007
20	14	0	2.436715	-0.090574	0.179393
21	14	0	-5.106594	0.884585	-1.511996
22	1	0	-4.065939	-5.230654	-0.540387
23	1	0	-3.928084	-3.080479	0.526131
24	1	0	-5.993250	-0.516837	-4.279277
25	1	0	7.833149	-2.154961	-1.269382
26	1	0	3.629558	-6.359922	0.735086
27	1	0	3.462256	-4.360916	2.048760
28	1	0	-0.137770	-6.061437	-0.623868
29	1	0	-0.250240	-4.401837	1.105057
30	1	0	-3.528381	3.625425	1.977602
31	1	0	-3.236830	5.992936	1.716554
32	1	0	-5.627030	-2.258548	2.315248
33	1	0	-3.668064	1.182384	1.375051

34	1	0	-5.690478	3.394356	-3.467992
35	1	0	3.953743	2.729821	3.706971
36	1	0	4.365762	5.077231	3.433545
37	1	0	0.227666	3.482798	2.890770
38	1	0	0.647155	5.774719	2.338111
39	1	0	3.791178	-1.953436	2.384422
40	1	0	3.892458	0.362039	2.991049
41	1	0	8.116394	1.738821	-0.346948
42	1	0	7.206445	-0.835140	2.097815
43	1	0	0.219788	1.333863	1.856825
44	1	0	-6.492102	0.876490	-0.912363
45	16	0	-0.684861	-1.501342	2.217528
46	16	0	-6.957114	-2.311037	2.535655
47	6	0	-0.114804	-1.479425	4.035685
48	6	0	1.018863	-2.496341	4.212595
49	1	0	1.910632	-2.207861	3.651958
50	1	0	1.292989	-2.560423	5.273302
51	1	0	0.714120	-3.492110	3.879471
52	6	0	-1.359064	-1.933069	4.817071
53	1	0	-1.104415	-2.024751	5.879824
54	1	0	-2.175370	-1.212259	4.719980
55	1	0	-1.716243	-2.908131	4.472275
56	6	0	0.316961	-0.084520	4.491828
57	1	0	0.549029	-0.115732	5.563308
58	1	0	1.217064	0.258381	3.973539
59	1	0	-0.473475	0.655052	4.338214
60	6	0	-6.973326	-1.242265	4.073347
61	6	0	-8.442577	-1.200323	4.522452
62	1	0	-8.532709	-0.584206	5.424257
63	1	0	-9.083286	-0.764034	3.749998
64	1	0	-8.817588	-2.201133	4.757161
65	6	0	-6.097691	-1.879770	5.161157
66	1	0	-5.051202	-1.941010	4.844414
67	1	0	-6.135440	-1.273441	6.075153
68	1	0	-6.439138	-2.889643	5.403625
69	6	0	-6.476587	0.170018	3.734600
70	1	0	-7.090383	0.627405	2.954128
71	1	0	-6.521055	0.807909	4.626672
72	1	0	-5.438573	0.155220	3.386509
73	14	0	5.158404	2.374073	-1.472893
74	1	0	5.368812	1.625242	-2.757723
75	1	0	5.360823	3.838608	-1.765726
76	14	0	4.845872	-1.857752	-2.452595
77	1	0	4.891127	-3.047101	-3.377138

78	1	0	5.170627	-0.641107	-3.271906
79	14	0	-2.475642	3.312578	-3.228001
80	1	0	-2.220288	4.768223	-3.525466
81	1	0	-2.292861	2.552565	-4.510790
82	14	0	-2.803540	-0.956311	-4.133062
83	1	0	-2.489204	0.252423	-4.969075
84	1	0	-2.736434	-2.159162	-5.038622
85	14	0	1.037737	-1.404116	-3.310076
86	1	0	1.377803	-0.193702	-4.133053
87	1	0	1.101409	-2.601469	-4.222942
88	14	0	1.369147	2.828514	-2.353518
89	1	0	1.646663	4.282573	-2.638187
90	1	0	1.572786	2.073446	-3.636539
91	14	0	6.049011	-4.389422	0.183926
92	1	0	6.523759	-5.372368	-0.857052
93	1	0	6.898318	-4.602426	1.411912
94	14	0	2.233472	-4.024875	-0.884980
95	1	0	2.528542	-4.753402	-2.159702
96	14	0	-1.643140	-3.511259	-1.658538
97	1	0	-1.634263	-4.257793	-2.957379
98	14	0	-5.502131	-2.971491	-2.251818
99	1	0	-6.831408	-2.923822	-1.545143
100	1	0	-5.637068	-3.942379	-3.398722
101	14	0	6.570977	3.315608	1.981387
102	1	0	7.412271	2.867937	3.150168
103	1	0	7.172954	4.599600	1.467986
104	14	0	2.771362	3.887123	0.970700
105	1	0	3.167020	5.082429	0.160224
106	14	0	-1.061789	4.376712	0.085260
107	1	0	-0.787236	5.602660	-0.729884
108	14	0	-4.943259	4.745349	-0.652509
109	1	0	-4.927020	6.099223	-1.317286
110	1	0	-6.286170	4.596262	0.017176

S5.3 Structures involved in the steric effect section

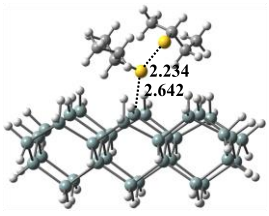
3



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.982968	0.068422	0.219758

2	1	0	1.484218	0.981101	0.563165
3	16	0	0.811798	-0.771728	-0.973969
4	16	0	-0.910939	-1.178273	0.118625
5	6	0	-2.072813	0.235481	-0.263891
6	1	0	-2.181238	0.245347	-1.354034
7	6	0	-3.418254	-0.159448	0.371268
8	1	0	-3.667960	-1.182601	0.066132
9	1	0	-3.309506	-0.177090	1.463451
10	6	0	3.211023	0.452254	-0.625315
11	1	0	2.876091	1.007415	-1.509757
12	1	0	3.690928	-0.463120	-0.994956
13	6	0	-4.574057	0.771741	-0.017700
14	1	0	-5.514270	0.412947	0.412516
15	1	0	-4.417832	1.793493	0.340969
16	1	0	-4.700716	0.813138	-1.105131
17	6	0	-1.535644	1.581985	0.211383
18	1	0	-1.405763	1.591189	1.298725
19	1	0	-0.573419	1.803371	-0.257697
20	1	0	-2.223618	2.389932	-0.060720
21	6	0	2.308330	-0.823577	1.414732
22	1	0	1.396222	-1.122559	1.937670
23	1	0	2.833682	-1.729169	1.094061
24	1	0	2.942000	-0.290426	2.131824
25	6	0	4.238380	1.300079	0.136364
26	1	0	4.671836	0.756785	0.981014
27	1	0	5.060308	1.589320	-0.525966
28	1	0	3.785693	2.219322	0.524644

3-TS1



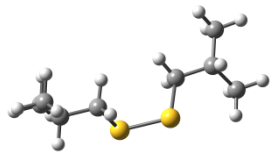
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-4.453742	-3.808461	-0.884697
2	14	0	-1.938641	-0.991801	-2.293473
3	14	0	-5.809519	-0.410577	-2.498820
4	14	0	5.813414	-2.148652	-1.900760
5	14	0	3.319963	-4.791062	-0.165993

6	14	0	-0.557943	-4.231320	-0.476842
7	14	0	1.944601	-1.573144	-2.102563
8	14	0	-3.234114	4.510388	2.084059
9	14	0	-3.836124	0.289899	0.796007
10	14	0	-5.390354	3.302983	-1.087424
11	14	0	-1.514985	2.779335	-1.091372
12	14	0	-1.809779	0.487276	-0.408259
13	14	0	4.558331	3.725216	2.014010
14	14	0	0.681988	4.294854	1.961259
15	14	0	3.912014	-0.562141	1.062048
16	14	0	2.407463	2.258685	-1.067963
17	14	0	6.286156	1.732566	-0.996238
18	14	0	5.926002	-0.491081	-0.177229
19	14	0	0.051629	0.027723	0.986642
20	14	0	2.060660	0.001379	-0.296773
21	14	0	-5.654262	0.982298	-0.553559
22	1	0	-4.661786	-5.279514	-1.024422
23	1	0	-4.496995	-3.495646	0.568142
24	1	0	-6.931608	0.095377	-3.373618
25	1	0	7.107092	-2.137338	-2.679437
26	1	0	3.127816	-6.270390	-0.135678
27	1	0	3.242935	-4.309423	1.240435
28	1	0	-0.768793	-5.705900	-0.369642
29	1	0	-0.588213	-3.677673	0.903408
30	1	0	-3.294510	3.341983	3.002942
31	1	0	-3.102262	5.732985	2.929027
32	1	0	-4.029498	-1.127101	1.206481
33	1	0	-3.786456	1.120461	2.028774
34	1	0	-6.577295	3.755008	-1.904464
35	1	0	4.374089	2.660082	3.037366
36	1	0	4.728804	5.013339	2.747219
37	1	0	0.582540	3.304008	3.067367
38	1	0	0.842180	5.635683	2.600397
39	1	0	3.730530	-1.926234	1.633243
40	1	0	3.996189	0.379255	2.214062
41	1	0	7.547745	1.743546	-1.826135
42	1	0	7.080274	-0.840120	0.734583
43	1	0	0.198917	1.269481	1.805736
44	1	0	-6.941828	0.826620	0.223400
45	16	0	-0.530734	-1.446690	3.100174
46	16	0	-2.057298	-1.682580	4.714296
47	6	0	1.511247	-2.102725	4.929303
48	1	0	1.694597	-2.979615	4.303584
49	1	0	2.457848	-1.822720	5.402933

50	1	0	0.805869	-2.376122	5.718310
51	6	0	0.708362	0.341374	4.922382
52	1	0	0.241666	1.086362	4.269767
53	1	0	-0.019088	0.110604	5.708597
54	6	0	-1.353414	-4.410736	5.054922
55	1	0	-1.704321	-5.442082	5.166163
56	1	0	-0.591275	-4.398606	4.269650
57	1	0	-0.885839	-4.112695	5.996447
58	6	0	-3.250019	-3.879962	3.403880
59	1	0	-2.535021	-3.857314	2.572118
60	1	0	-4.003945	-3.116086	3.187203
61	6	0	0.978692	-0.931998	4.105990
62	1	0	1.699431	-0.702000	3.313246
63	6	0	-2.516704	-3.486549	4.696467
64	1	0	-3.243757	-3.491297	5.522454
65	6	0	1.974149	0.945089	5.547313
66	1	0	1.731780	1.883788	6.055183
67	1	0	2.428121	0.280673	6.288734
68	1	0	2.730900	1.167394	4.786261
69	6	0	-3.926287	-5.256220	3.468800
70	1	0	-4.496889	-5.442176	2.553457
71	1	0	-3.202758	-6.070318	3.574249
72	1	0	-4.624741	-5.316660	4.311625
73	14	0	5.494156	-4.353749	-1.017697
74	1	0	5.762068	-5.320865	-2.144057
75	1	0	6.517418	-4.632494	0.054691
76	14	0	1.567130	-3.841235	-1.439629
77	1	0	1.572065	-4.574973	-2.744752
78	14	0	-2.313717	-3.292278	-1.754315
79	1	0	-2.256994	-3.961202	-3.092525
80	14	0	-6.262017	-2.695450	-1.944707
81	1	0	-7.485200	-2.791128	-1.067721
82	1	0	-6.582775	-3.412007	-3.232652
83	14	0	6.553545	3.291608	0.802982
84	1	0	7.625571	2.811031	1.748604
85	1	0	7.039539	4.587314	0.202895
86	14	0	2.623779	3.902715	0.662578
87	1	0	2.818642	5.159748	-0.128175
88	14	0	-1.322134	4.357716	0.700889
89	1	0	-1.261894	5.659517	-0.037184
90	14	0	-5.272855	4.669523	0.876795
91	1	0	-5.446440	6.100155	0.430619
92	1	0	-6.428671	4.350415	1.791546
93	14	0	4.449703	2.511519	-2.314592

94	1	0	4.383008	1.815904	-3.644750
95	1	0	4.649303	3.981548	-2.583558
96	14	0	0.526343	3.068061	-2.326777
97	1	0	0.448386	2.437428	-3.688825
98	1	0	0.725950	4.548152	-2.532103
99	14	0	-3.380867	3.662876	-2.329643
100	1	0	-3.159632	5.146227	-2.480574
101	1	0	-3.471588	3.079536	-3.711427
102	14	0	-3.770074	-0.435906	-3.745260
103	1	0	-3.530708	0.857209	-4.471281
104	1	0	-3.860305	-1.524201	-4.784673
105	14	0	0.103295	-1.067458	-3.553577
106	1	0	-0.019128	-2.183342	-4.559231
107	1	0	0.336759	0.203209	-4.320835
108	14	0	3.981423	-1.714413	-3.370530
109	1	0	3.836363	-2.876181	-4.319854
110	1	0	4.211654	-0.482450	-4.199257

4



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.937351	0.063704	-0.534556
2	1	0	1.517303	1.074928	-0.505553
3	1	0	1.873247	-0.307861	-1.560429
4	16	0	0.894262	-1.050481	0.519376
5	16	0	-0.931380	-1.067154	-0.475165
6	6	0	-1.814602	0.399296	0.237506
7	1	0	-1.827532	0.292608	1.326611
8	1	0	-1.240798	1.295421	-0.015328
9	6	0	-3.245479	0.507524	-0.317654
10	1	0	-3.183872	0.487331	-1.415046
11	6	0	3.397688	0.076194	-0.051921
12	1	0	3.744122	-0.965771	-0.008352
13	6	0	4.266744	0.820550	-1.078424
14	1	0	5.318116	0.814522	-0.772401
15	1	0	4.202491	0.360595	-2.069954
16	1	0	3.954420	1.867453	-1.171963
17	6	0	3.548953	0.695707	1.345298

18	1	0	3.214138	1.740068	1.344596
19	1	0	2.963097	0.159085	2.097072
20	1	0	4.596666	0.681935	1.662979
21	6	0	-4.139659	-0.654392	0.138926
22	1	0	-5.146122	-0.555516	-0.280678
23	1	0	-3.739305	-1.624017	-0.169520
24	1	0	-4.232410	-0.664750	1.231564
25	6	0	-3.849841	1.860013	0.093585
26	1	0	-3.246857	2.698718	-0.269964
27	1	0	-4.860662	1.972328	-0.312185
28	1	0	-3.919069	1.943506	1.184621

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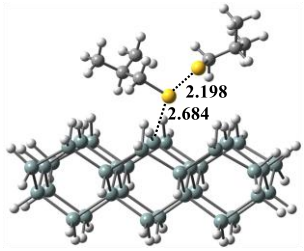

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-4.235679	-3.434741	-1.558830
2	14	0	-1.692954	-0.474822	-2.522684
3	14	0	-5.551619	0.146021	-2.830021
4	14	0	6.035016	-1.723549	-1.884446
5	14	0	3.487104	-4.687993	-0.951989
6	14	0	-0.365595	-4.038746	-1.270618
7	14	0	2.178468	-1.104165	-2.220817
8	14	0	-3.301576	4.434945	2.462572
9	14	0	-3.775316	0.427488	0.593637
10	14	0	-5.118463	3.705289	-1.036267
11	14	0	-1.270130	3.069080	-0.727332
12	14	0	-1.665313	0.712815	-0.436305
13	14	0	4.406306	3.146495	3.123828
14	14	0	0.577323	3.922139	2.759877
15	14	0	3.896286	-0.833477	1.203784
16	14	0	2.615734	2.434348	-0.402193
17	14	0	6.463194	1.817225	-0.046552
18	14	0	6.011600	-0.522875	0.190036
19	14	0	0.068228	-0.085653	0.966568
20	14	0	2.175543	0.078785	-0.134898
21	14	0	-5.479603	1.353679	-0.762888

22	1	0	-4.459526	-4.872245	-1.891771
23	1	0	-4.281675	-3.320474	-0.075154
24	1	0	-6.640431	0.720105	-3.704837
25	1	0	7.376340	-1.528525	-2.550254
26	1	0	3.300246	-6.130563	-1.284297
27	1	0	3.334913	-4.556371	0.522979
28	1	0	-0.581028	-5.493552	-1.531753
29	1	0	-0.444998	-3.836373	0.200444
30	1	0	-3.523293	3.169227	3.212186
31	1	0	-3.216975	5.536279	3.465481
32	1	0	-4.043419	-1.023447	0.775903
33	1	0	-3.785119	1.072386	1.933211
34	1	0	-6.209498	4.270620	-1.914142
35	1	0	4.089216	1.884394	3.846695
36	1	0	4.503462	4.227600	4.147228
37	1	0	0.308612	2.739024	3.621614
38	1	0	0.698004	5.101759	3.668581
39	1	0	3.662634	-2.292648	1.386879
40	1	0	3.878441	-0.215219	2.559450
41	1	0	7.808959	1.986039	-0.710374
42	1	0	7.079757	-1.116072	1.080476
43	1	0	0.174437	0.891748	2.092585
44	1	0	-6.815023	1.170864	-0.077844
45	16	0	-1.037870	-1.920688	2.583551
46	16	0	-2.806960	-2.216019	3.853868
47	6	0	0.355882	-2.060891	3.809010
48	1	0	-0.121394	-2.045938	4.792921
49	1	0	0.944984	-1.144577	3.709423
50	6	0	1.246580	-3.302159	3.643321
51	1	0	1.641209	-3.300021	2.618555
52	6	0	-3.345416	-3.917286	3.366230
53	1	0	-3.194607	-4.007043	2.287021
54	1	0	-2.705314	-4.650694	3.867294
55	6	0	-4.824124	-4.167039	3.713651
56	1	0	-5.416476	-3.381875	3.225186
57	6	0	2.437728	-3.186765	4.610301
58	1	0	3.114621	-4.039064	4.492046
59	1	0	3.015419	-2.273417	4.433947
60	1	0	2.098018	-3.174250	5.652880
61	6	0	-5.256657	-5.524241	3.134724
62	1	0	-4.679111	-6.344266	3.577866
63	1	0	-6.314749	-5.713327	3.344342
64	1	0	-5.117371	-5.562460	2.049168
65	6	0	0.485736	-4.614812	3.862533

66	1	0	0.063081	-4.659057	4.873820
67	1	0	-0.332480	-4.727855	3.146008
68	1	0	1.155911	-5.472202	3.742954
69	6	0	-5.089612	-4.105736	5.225172
70	1	0	-4.501711	-4.864826	5.755473
71	1	0	-4.831694	-3.128933	5.646620
72	1	0	-6.146895	-4.292328	5.439943
73	14	0	-5.175094	4.853586	1.065314
74	1	0	-5.225065	6.331153	0.765411
75	1	0	-6.444227	4.509528	1.803783
76	14	0	-1.241768	4.341737	1.302297
77	1	0	-1.009934	5.731627	0.794565
78	14	0	2.650169	3.694641	1.636022
79	1	0	2.970733	5.071825	1.142367
80	14	0	6.525308	2.925637	2.076161
81	1	0	7.476543	2.210076	3.002298
82	1	0	7.088552	4.305148	1.842217
83	14	0	-6.023563	-2.178060	-2.488497
84	1	0	-7.247200	-2.335787	-1.620935
85	1	0	-6.359986	-2.767512	-3.835755
86	14	0	-2.089216	-2.829238	-2.349772
87	1	0	-2.057109	-3.268759	-3.780779
88	14	0	1.790265	-3.459471	-2.051667
89	1	0	1.841864	-3.902378	-3.480940
90	14	0	5.698888	-4.074000	-1.560839
91	1	0	6.035436	-4.752875	-2.865257
92	1	0	6.666824	-4.596430	-0.528901
93	14	0	-2.986959	4.151501	-2.018754
94	1	0	-2.729398	5.635865	-1.964762
95	1	0	-2.940379	3.740551	-3.463434
96	14	0	0.889292	3.503471	-1.684847
97	1	0	0.947943	3.112231	-3.134906
98	1	0	1.125542	4.990695	-1.614111
99	14	0	4.778587	2.899714	-1.350372
100	1	0	4.852753	2.503136	-2.797852
101	1	0	4.998911	4.389463	-1.278347
102	14	0	-3.458332	0.263574	-3.976940
103	1	0	-3.195280	1.639836	-4.519070
104	1	0	-3.497492	-0.682688	-5.149765
105	14	0	0.416416	-0.342320	-3.661054
106	1	0	0.357380	-1.263111	-4.852867
107	1	0	0.682311	1.043208	-4.178298
108	14	0	4.298082	-0.971794	-3.344653
109	1	0	4.236897	-1.896144	-4.533788

110	1	0	4.566686	0.412094	-3.864024

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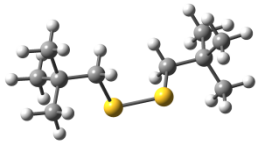

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.865162	0.271810	-0.450109
2	1	0	1.374086	1.234173	-0.276386
3	1	0	1.780718	0.028949	-1.513004
4	16	0	0.921024	-1.029194	0.482204
5	16	0	-0.921020	-1.029164	-0.482259
6	6	0	-1.865185	0.271724	0.450189
7	1	0	-1.780793	0.028719	1.513056
8	1	0	-1.374087	1.234102	0.276618
9	6	0	-3.354052	0.362611	0.038941
10	6	0	3.354050	0.362616	-0.038920
11	6	0	3.982569	1.485985	-0.890203
12	1	0	5.044031	1.602612	-0.645418
13	1	0	3.908684	1.264436	-1.960525
14	1	0	3.490456	2.448058	-0.709382
15	6	0	3.491574	0.725072	1.452562
16	1	0	2.967490	1.659632	1.682126
17	1	0	3.081437	-0.055265	2.100957
18	1	0	4.546063	0.858617	1.717244
19	6	0	-4.088281	-0.960139	0.330795
20	1	0	-5.153811	-0.864052	0.095481
21	1	0	-3.687168	-1.787836	-0.261162
22	1	0	-4.001292	-1.234287	1.387896
23	6	0	-3.982556	1.485974	0.890244
24	1	0	-3.490377	2.448027	0.709500
25	1	0	-5.043997	1.602675	0.645401
26	1	0	-3.908747	1.264367	1.960559
27	6	0	-3.491491	0.725138	-1.452531
28	1	0	-4.545962	0.858727	-1.717259
29	1	0	-2.967366	1.659692	-1.682027
30	1	0	-3.081346	-0.055184	-2.100940
31	6	0	4.088200	-0.960157	-0.330864
32	1	0	4.001169	-1.234245	-1.387977
33	1	0	5.153742	-0.864141	-0.095572

34	1	0	3.687057	-1.787864	0.261061

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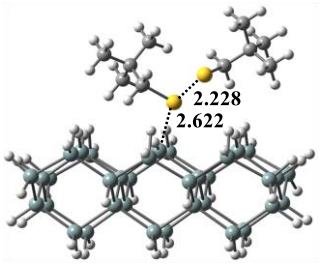


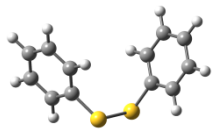
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-3.927008	-3.407913	-2.193433
2	14	0	-1.424258	-0.336021	-2.807549
3	14	0	-5.268420	0.208720	-3.331839
4	14	0	6.289874	-1.422978	-1.832532
5	14	0	3.806622	-4.543492	-1.333033
6	14	0	-0.058803	-3.891753	-1.658284
7	14	0	2.440543	-0.889701	-2.330749
8	14	0	-3.473986	4.204384	2.373269
9	14	0	-3.726102	0.331215	0.227890
10	14	0	-5.029040	3.655394	-1.289391
11	14	0	-1.195376	3.068729	-0.741685
12	14	0	-1.554406	0.689918	-0.641425
13	14	0	4.177912	2.902498	3.498271
14	14	0	0.382979	3.712304	2.915451
15	14	0	3.941762	-0.890690	1.193198
16	14	0	2.674036	2.481191	-0.193742
17	14	0	6.503480	1.920355	0.378313
18	14	0	6.105329	-0.441106	0.345679
19	14	0	0.104409	-0.171105	0.823464
20	14	0	2.272174	0.102634	-0.154744
21	14	0	-5.360214	1.284570	-1.194366
22	1	0	-4.093816	-4.830659	-2.611303
23	1	0	-4.069855	-3.371408	-0.711884
24	1	0	-6.318133	0.808404	-4.236683
25	1	0	7.658888	-1.119384	-2.392756
26	1	0	3.684535	-5.944827	-1.830876
27	1	0	3.592445	-4.582494	0.139002
28	1	0	-0.243400	-5.354469	-1.896072
29	1	0	-0.193293	-3.657839	-0.195423
30	1	0	-3.724663	2.900921	3.044475

31	1	0	-3.482064	5.256835	3.430941
32	1	0	-3.984551	-1.129209	0.352755
33	1	0	-3.836218	0.937588	1.579351
34	1	0	-6.066663	4.261652	-2.204128
35	1	0	3.828667	1.574280	4.072553
36	1	0	4.180978	3.881217	4.624343
37	1	0	0.068477	2.476985	3.683460
38	1	0	0.424635	4.834841	3.900557
39	1	0	3.740368	-2.365878	1.231313
40	1	0	3.833609	-0.405588	2.598425
41	1	0	7.889364	2.188172	-0.158332
42	1	0	7.131124	-1.101434	1.238833
43	1	0	0.156238	0.807791	1.952185
44	1	0	-6.732423	1.032614	-0.611184
45	16	0	-1.046723	-1.950108	2.368552
46	16	0	-2.849461	-1.852090	3.673685
47	6	0	0.283310	-2.072595	3.668254
48	1	0	-0.099774	-1.531062	4.536977
49	1	0	1.122349	-1.498777	3.264079
50	6	0	0.766440	-3.486418	4.070538
51	6	0	-3.792771	-3.328671	3.081274
52	1	0	-3.852169	-3.269968	1.990394
53	1	0	-3.226760	-4.226328	3.347180
54	6	0	-5.223100	-3.421524	3.673849
55	6	0	1.880698	-3.268287	5.119086
56	1	0	2.282613	-4.231745	5.450015
57	1	0	2.711331	-2.683779	4.708213
58	1	0	1.501536	-2.743530	6.003048
59	6	0	-5.848548	-4.713677	3.106308
60	1	0	-5.270736	-5.598600	3.395491
61	1	0	-6.868145	-4.841903	3.485721
62	1	0	-5.899598	-4.685588	2.012248
63	6	0	-0.361803	-4.318470	4.703866
64	1	0	-0.826555	-3.796116	5.546119
65	1	0	-1.143943	-4.546271	3.974551
66	1	0	0.035947	-5.271252	5.070066
67	6	0	-5.175158	-3.517104	5.210969
68	1	0	-4.558739	-4.362563	5.536548
69	1	0	-4.762086	-2.608481	5.660800
70	1	0	-6.182750	-3.661236	5.615798
71	6	0	1.344795	-4.238774	2.860253
72	1	0	2.180017	-3.691743	2.410461
73	1	0	1.717114	-5.222370	3.166040
74	1	0	0.585143	-4.392835	2.087874

75	6	0	-6.080410	-2.215339	3.246667
76	1	0	-6.123579	-2.129198	2.155269
77	1	0	-7.105997	-2.328162	3.614623
78	1	0	-5.682646	-1.275917	3.641317
79	14	0	6.373933	2.807840	2.600245
80	1	0	7.264934	2.013209	3.522012
81	1	0	6.927783	4.210126	2.552184
82	14	0	2.534875	3.573081	1.934606
83	1	0	2.885264	4.985959	1.582273
84	14	0	-1.335135	4.205943	1.361993
85	1	0	-1.090971	5.628331	0.961435
86	14	0	-5.254149	4.666192	0.870992
87	1	0	-5.318475	6.158031	0.656098
88	1	0	-6.562854	4.253758	1.496954
89	14	0	-5.686106	-2.145121	-3.169041
90	1	0	-6.960684	-2.392247	-2.401070
91	1	0	-5.910690	-2.656008	-4.570584
92	14	0	-1.752856	-2.706368	-2.807222
93	1	0	-1.606824	-3.069290	-4.252489
94	14	0	2.107322	-3.258828	-2.364955
95	1	0	2.187140	-3.591130	-3.822569
96	14	0	6.020435	-3.802677	-1.768791
97	1	0	6.439204	-4.330186	-3.118609
98	1	0	6.956564	-4.404105	-0.750625
99	14	0	-2.841199	4.202332	-2.081559
100	1	0	-2.626692	5.684733	-1.910417
101	1	0	-2.680594	3.891678	-3.542965
102	14	0	1.015016	3.610563	-1.512980
103	1	0	1.182481	3.323412	-2.978674
104	1	0	1.210924	5.093335	-1.324446
105	14	0	4.883442	3.074655	-0.944834
106	1	0	5.068665	2.796465	-2.409760
107	1	0	5.057540	4.558187	-0.740935
108	14	0	-3.111102	0.457871	-4.323547
109	1	0	-2.853594	1.874836	-4.751496
110	1	0	-3.040507	-0.404133	-5.558290
111	14	0	0.739746	-0.063831	-3.807069
112	1	0	0.773865	-0.891797	-5.066270
113	1	0	0.991233	1.363395	-4.204512
114	14	0	4.610376	-0.595584	-3.317381
115	1	0	4.645854	-1.416810	-4.581314
116	1	0	4.856364	0.834812	-3.705580

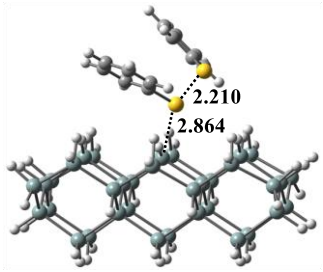
S5.4 reaction between di-phenyldisulfide and the silyl radical

6



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.687843	-1.692127	-0.805307
2	16	0	-0.687842	-1.692127	0.805307
3	6	0	-1.855417	-0.389672	0.398211
4	6	0	-1.713300	0.875203	0.984438
5	6	0	-2.935010	-0.645006	-0.458494
6	6	0	-2.645724	1.877373	0.712174
7	1	0	-0.877670	1.064785	1.649967
8	6	0	-3.859673	0.361978	-0.730720
9	1	0	-3.042384	-1.628151	-0.905011
10	6	0	-3.716793	1.622769	-0.145703
11	1	0	-2.534103	2.856114	1.169576
12	1	0	-4.695098	0.161573	-1.395154
13	1	0	-4.441402	2.403832	-0.356580
14	6	0	1.855417	-0.389672	-0.398210
15	6	0	1.713299	0.875204	-0.984438
16	6	0	2.935011	-0.645005	0.458493
17	6	0	2.645723	1.877374	-0.712173
18	1	0	0.877668	1.064785	-1.649965
19	6	0	3.859674	0.361978	0.730719
20	1	0	3.042385	-1.628151	0.905010
21	6	0	3.716793	1.622770	0.145703
22	1	0	2.534101	2.856115	-1.169574
23	1	0	4.695100	0.161573	1.395152
24	1	0	4.441402	2.403833	0.356580

6-TS1



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3	14	0	5.974240	0.043961	-2.380318
4	14	0	-5.763570	0.832836	-2.741580
5	14	0	-3.610731	4.104802	-1.885941
6	14	0	0.293553	3.775384	-1.687512
7	14	0	-1.857807	0.562990	-2.648999
8	14	0	3.573328	-3.975294	3.061823
9	14	0	3.866831	-0.112844	0.873333
10	14	0	5.675496	-3.360895	-0.295473
11	14	0	1.775669	-3.102550	-0.431625
12	14	0	1.930596	-0.700592	-0.349682
13	14	0	-4.234568	-3.357500	2.888358
14	14	0	-0.336990	-3.800356	2.940429
15	14	0	-3.882734	0.459344	0.637389
16	14	0	-2.174312	-2.817630	-0.522847
17	14	0	-6.073164	-2.517904	-0.573993
18	14	0	-5.843479	-0.132661	-0.549661
19	14	0	-0.014480	0.010450	0.780141
20	14	0	-1.981745	-0.414126	-0.463514
21	14	0	5.787386	-0.967953	-0.216835
22	1	0	4.335223	4.986118	-2.036723
23	1	0	4.124703	3.575680	-0.109299
24	1	0	7.198912	-0.502335	-3.074771
25	1	0	-7.008011	0.431214	-3.496946
26	1	0	-3.510222	5.520283	-2.347213
27	1	0	-3.623515	4.129214	-0.397785
28	1	0	0.404121	5.231779	-1.998670
29	1	0	0.227762	3.633532	-0.210056
30	1	0	3.596736	-2.637972	3.713868
31	1	0	3.481345	-4.994593	4.147473
32	1	0	3.972304	1.367071	0.972470
33	1	0	3.780823	-0.659036	2.254656
34	1	0	6.902619	-3.883963	-1.003409
35	1	0	-4.092186	-2.017367	3.518462
36	1	0	-4.344227	-4.354959	3.992784
37	1	0	-0.252183	-2.520780	3.695736
38	1	0	-0.442298	-4.893603	3.953389
39	1	0	-3.779726	1.941802	0.721068
40	1	0	-3.957036	-0.066018	2.027000
41	1	0	-7.328767	-2.876528	-1.332703

42	1	0	-7.050263	0.438070	0.160511
43	1	0	-0.125250	-0.823683	2.013190
44	1	0	7.021293	-0.593904	0.572473
45	16	0	0.707117	2.206260	2.471603
46	16	0	2.128985	3.505896	3.555331
47	14	0	-3.827915	0.120702	-3.949906
48	1	0	-3.726145	0.936559	-5.213310
49	1	0	-3.917516	-1.323697	-4.353937
50	14	0	0.107162	-0.145078	-3.833919
51	1	0	0.201097	0.670372	-5.098013
52	1	0	0.023037	-1.589851	-4.239113
53	14	0	-4.189038	-3.565315	-1.606529
54	1	0	-4.156349	-3.313302	-3.087467
55	1	0	-4.292377	-5.055458	-1.403645
56	14	0	-0.237247	-3.822194	-1.531596
57	1	0	-0.190390	-3.566557	-3.011859
58	1	0	-0.347909	-5.313277	-1.339536
59	14	0	4.040960	-0.387635	-3.717207
60	1	0	3.963547	-1.825975	-4.144859
61	1	0	4.123965	0.449716	-4.967948
62	14	0	3.713791	-4.115655	-1.434870
63	1	0	3.595911	-5.608251	-1.258591
64	1	0	3.782497	-3.841272	-2.910535
65	14	0	-6.251662	-3.420432	1.637367
66	1	0	-7.341305	-2.707530	2.398614
67	1	0	-6.680371	-4.859936	1.497628
68	14	0	-2.303961	-3.876205	1.623466
69	1	0	-2.456736	-5.318049	1.247793
70	14	0	1.646703	-4.181289	1.704299
71	1	0	1.586471	-5.626984	1.318015
72	14	0	5.616391	-4.312774	1.902101
73	1	0	5.838968	-5.797250	1.752718
74	1	0	6.759350	-3.774297	2.725317
75	14	0	2.221944	2.687099	-2.520446
76	1	0	2.282273	3.013066	-3.980710
77	14	0	6.191977	2.426128	-2.248099
78	1	0	7.316461	2.793422	-1.312954
79	1	0	6.583111	2.910600	-3.622268
80	14	0	-1.696211	2.951314	-2.663589
81	1	0	-1.610136	3.265406	-4.125058
82	14	0	-5.676537	3.224870	-2.657142
83	1	0	-5.918056	3.729309	-4.058094
84	1	0	-6.798879	3.752314	-1.798543
85	6	0	-0.597612	1.946156	3.679029

86	6	0	-1.761804	2.724923	3.614732
87	6	0	-0.460018	0.972777	4.678733
88	6	0	-2.782932	2.525683	4.546506
89	1	0	-1.859676	3.479424	2.841221
90	6	0	-1.482203	0.782793	5.607753
91	1	0	0.444607	0.375384	4.724372
92	6	0	-2.644075	1.556831	5.542220
93	1	0	-3.684566	3.129009	4.493962
94	1	0	-1.372889	0.028688	6.381649
95	1	0	-3.439369	1.403941	6.265886
96	6	0	1.509424	5.149627	3.247782
97	6	0	1.999727	5.898082	2.165373
98	6	0	0.560040	5.718581	4.112451
99	6	0	1.541599	7.197443	1.950932
100	1	0	2.738883	5.456658	1.504459
101	6	0	0.105718	7.018488	3.891185
102	1	0	0.189299	5.140032	4.952157
103	6	0	0.593780	7.758312	2.811290
104	1	0	1.925481	7.773147	1.113712
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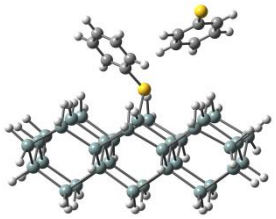
106	1	0	0.239376	8.771034	2.642325

6-IM1



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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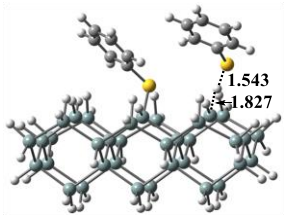
3	14	0	5.439511	-1.200199	-2.808239
4	14	0	-5.789340	2.253849	-2.113806
5	14	0	-2.861033	4.897527	-1.350699
6	14	0	0.889284	3.857451	-1.876878
7	14	0	-2.046699	1.103962	-2.368017
8	14	0	2.613744	-4.821147	2.697172
9	14	0	3.610651	-1.029223	0.603699
10	14	0	4.530668	-4.547362	-0.805859
11	14	0	0.795591	-3.401397	-0.605748

12	14	0	1.505762	-1.107163	-0.472394
13	14	0	-4.844568	-2.476461	3.200513
14	14	0	-1.161480	-3.794267	2.914739
15	14	0	-3.813640	1.281773	1.066071
16	14	0	-2.963546	-2.220329	-0.343509
17	14	0	-6.697185	-1.077142	-0.067245
18	14	0	-5.938981	1.192545	0.028811
19	14	0	-0.125698	-0.052360	0.886284
20	14	0	-2.231419	0.070443	-0.209336
21	14	0	5.192844	-2.249131	-0.667741
22	1	0	5.033256	3.963888	-2.177944
23	1	0	4.588529	2.532234	-0.295999
24	1	0	6.446558	-1.979791	-3.619841
25	1	0	-7.141004	2.203009	-2.785043
26	1	0	-2.491644	6.286632	-1.750964
27	1	0	-2.706121	4.813339	0.127544
28	1	0	1.244322	5.137052	-2.561428
29	1	0	1.040360	4.082856	-0.417671
30	1	0	2.997670	-3.553464	3.375193
31	1	0	2.370158	-5.836421	3.762803
32	1	0	4.064173	0.379791	0.733058
33	1	0	3.497494	-1.602435	1.972422
34	1	0	5.543481	-5.299209	-1.635977
35	1	0	-4.354920	-1.233865	3.856064
36	1	0	-5.092704	-3.477896	4.278164
37	1	0	-0.736423	-2.613060	3.714373
38	1	0	-1.439374	-4.896483	3.883458
39	1	0	-3.390686	2.703698	1.168201
40	1	0	-3.893128	0.727070	2.443836
41	1	0	-8.050849	-1.114607	-0.735146
42	1	0	-6.927750	1.974710	0.863333
43	1	0	-0.315879	-0.926523	2.077131
44	1	0	6.534501	-2.200509	0.026868
45	16	0	0.722775	1.809663	1.650489
46	16	0	4.887155	3.459646	5.025234
47	14	0	-4.166644	1.180744	-3.501708
48	1	0	-3.976497	2.006564	-4.748025
49	1	0	-4.620702	-0.185200	-3.932476
50	14	0	-0.413325	0.019863	-3.753275
51	1	0	-0.242552	0.857781	-4.994070
52	1	0	-0.865215	-1.344531	-4.191672
53	14	0	-5.164802	-2.449825	-1.282437
54	1	0	-5.179211	-2.141424	-2.752440
55	1	0	-5.571941	-3.891879	-1.119244

56	14	0	-1.404498	-3.594954	-1.549940
57	1	0	-1.409319	-3.284567	-3.019973
58	1	0	-1.846310	-5.027101	-1.391844
59	14	0	3.359519	-1.128426	-3.984825
60	1	0	2.917964	-2.494560	-4.428476
61	1	0	3.532366	-0.286265	-5.222426
62	14	0	2.366067	-4.780386	-1.792442
63	1	0	1.914562	-6.209880	-1.637367
64	1	0	2.383140	-4.469701	-3.261960
65	14	0	-6.910714	-2.030574	2.119852
66	1	0	-7.753788	-1.132936	2.990292
67	1	0	-7.659209	-3.331311	1.968909
68	14	0	-3.180668	-3.346415	1.761878
69	1	0	-3.684724	-4.691847	1.340014
70	14	0	0.593005	-4.527415	1.502479
71	1	0	0.185993	-5.902966	1.072339
72	14	0	4.423893	-5.569760	1.357559
73	1	0	4.276376	-7.055755	1.145330
74	1	0	5.721385	-5.353929	2.094936
75	14	0	2.433068	2.230520	-2.641672
76	1	0	2.539335	2.477264	-4.115229
77	14	0	6.215114	1.058235	-2.614468
78	1	0	7.452468	1.099766	-1.753320
79	1	0	6.624986	1.501354	-3.997150
80	14	0	-1.370753	3.401563	-2.416023
81	1	0	-1.490631	3.708271	-3.877122
82	14	0	-5.141276	4.552392	-1.916759
83	1	0	-5.399108	5.203463	-3.252734
84	1	0	-6.021978	5.248197	-0.909366
85	6	0	-0.152891	2.060512	3.209670
86	6	0	-1.046082	3.133199	3.331072
87	6	0	0.119504	1.252033	4.321970
88	6	0	-1.669727	3.385532	4.555057
89	1	0	-1.248642	3.763892	2.471684
90	6	0	-0.515117	1.505184	5.538385
91	1	0	0.827996	0.434875	4.233717
92	6	0	-1.409797	2.570939	5.658179
93	1	0	-2.360489	4.219191	4.642212
94	1	0	-0.301860	0.872910	6.395369
95	1	0	-1.897800	2.768044	6.608024
96	6	0	4.720762	4.442681	3.561519
97	6	0	5.854991	5.017886	2.965723
98	6	0	3.454445	4.651511	2.991802
99	6	0	5.716105	5.791532	1.813640

100	1	0	6.838414	4.862576	3.398897
101	6	0	3.333533	5.429603	1.840456
102	1	0	2.570998	4.209897	3.442180
103	6	0	4.458714	6.003018	1.244924
104	1	0	6.600619	6.232247	1.362289
105	1	0	2.348809	5.584371	1.409101
106	1	0	4.356602	6.609638	0.350476

6-TS2



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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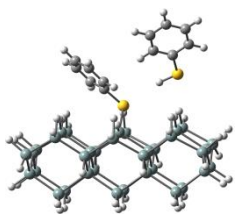
4	14	0	-6.402825	1.938601	-0.659780
5	14	0	-4.191650	4.138215	1.878781
6	14	0	-0.344475	4.586598	1.223771
7	14	0	-2.522436	2.162732	-1.189697
8	14	0	3.863478	-4.338094	-0.604837
9	14	0	3.713914	-0.020231	0.321363
10	14	0	5.367803	-1.388267	-2.881402
11	14	0	1.487938	-1.570079	-2.357706
12	14	0	1.606342	0.208620	-0.726177
13	14	0	-3.881208	-4.657874	0.600356
14	14	0	-0.018947	-4.572108	-0.104201
15	14	0	-4.011173	-0.288387	1.400066
16	14	0	-2.419341	-1.788814	-1.801758
17	14	0	-6.283699	-2.032151	-1.243327
18	14	0	-6.117214	-0.228243	0.321966
19	14	0	-0.139605	-0.291859	0.796547
20	14	0	-2.280652	-0.005066	-0.187942
21	14	0	5.448997	0.367220	-1.240548
22	1	0	3.614824	5.796604	1.542390
23	1	0	3.662503	3.422992	1.915317
24	1	0	6.352955	2.719704	-3.223218
25	1	0	-7.743519	1.992115	-1.352574

26	1	0	-4.220030	5.512040	2.460075
27	1	0	-3.910693	3.196131	2.996607
28	1	0	-0.378041	6.043484	1.550709
29	1	0	-0.138886	3.849558	2.495536
30	1	0	3.987873	-3.841285	0.791223
31	1	0	3.952146	-5.827032	-0.553270
32	1	0	4.145954	0.796048	1.897574
33	1	0	3.824738	-1.421795	0.821815
34	1	0	6.461461	-1.162096	-3.899536
35	1	0	-3.670236	-4.023697	1.929407
36	1	0	-3.780627	-6.133888	0.793348
37	1	0	0.169689	-4.116544	1.300466
38	1	0	0.060568	-6.063578	-0.087755
39	1	0	-3.957224	0.812862	2.397004
40	1	0	-3.838141	-1.574476	2.126634
41	1	0	-7.633536	-1.974374	-1.917519
42	1	0	-7.205131	-0.412433	1.355684
43	1	0	-0.018618	-1.744464	1.103655
44	1	0	6.783790	0.277306	-0.540146
45	16	0	0.251571	0.761979	2.666892
46	16	0	4.829449	1.128578	3.239939
47	14	0	-4.671552	2.413584	-2.237196
48	1	0	-4.793362	3.852297	-2.668925
49	1	0	-4.795944	1.563220	-3.469686
50	14	0	-0.775336	2.623293	-2.769031
51	1	0	-0.912006	4.063168	-3.192100
52	1	0	-0.900129	1.779920	-4.006086
53	14	0	-4.558794	-1.907223	-2.892223
54	1	0	-4.770699	-0.758026	-3.836164
55	1	0	-4.575283	-3.173774	-3.708771
56	14	0	-0.662107	-1.655649	-3.435294
57	1	0	-0.863352	-0.502896	-4.377512
58	1	0	-0.705685	-2.919952	-4.254791
59	14	0	3.133977	2.835137	-3.279541
60	1	0	3.012600	1.995992	-4.519616
61	1	0	2.995580	4.276450	-3.697136
62	14	0	3.250260	-1.451257	-3.988536
63	1	0	3.176774	-2.715805	-4.805661
64	1	0	3.067383	-0.295908	-4.930368
65	14	0	-6.072706	-4.161012	-0.165290
66	1	0	-7.043530	-4.253110	0.985114
67	1	0	-6.474813	-5.212539	-1.169111
68	14	0	-2.175111	-3.997282	-0.899388
69	1	0	-2.368424	-4.849169	-2.115772

70	14	0	1.737239	-3.792089	-1.489366
71	1	0	1.616168	-4.607715	-2.739707
72	14	0	5.693959	-3.545351	-1.893437
73	1	0	5.930821	-4.515893	-3.023732
74	1	0	6.941911	-3.539945	-1.046935
75	14	0	1.487953	4.262714	-0.242761
76	1	0	1.410413	5.399009	-1.214921
77	14	0	5.437622	4.299457	-0.581779
78	1	0	6.696109	4.119551	0.227225
79	1	0	5.578614	5.592159	-1.346295
80	14	0	-2.450433	4.053107	0.279982
81	1	0	-2.743205	5.171331	-0.672420
82	14	0	-6.345663	3.675732	0.990697
83	1	0	-6.861119	4.929792	0.329595
84	1	0	-7.295736	3.346603	2.114803
85	6	0	-0.678965	-0.190527	3.887176
86	6	0	-1.701893	0.443296	4.604296
87	6	0	-0.333417	-1.515006	4.191022
88	6	0	-2.377265	-0.247295	5.612783
89	1	0	-1.963585	1.470646	4.373317
90	6	0	-1.023372	-2.202255	5.190793
91	1	0	0.474152	-2.000247	3.652723
92	6	0	-2.044385	-1.570926	5.904714
93	1	0	-3.167601	0.251604	6.166159
94	1	0	-0.756302	-3.231031	5.415189
95	1	0	-2.575136	-2.106886	6.685914
96	6	0	4.694367	-0.459140	4.031920
97	6	0	3.516233	-0.814228	4.711642
98	6	0	5.781206	-1.349991	4.023929
99	6	0	3.429149	-2.042111	5.366464
100	1	0	2.679808	-0.123504	4.720795
101	6	0	5.688691	-2.574752	4.684528
102	1	0	6.691550	-1.071341	3.503095
103	6	0	4.513695	-2.923654	5.355074
104	1	0	2.514605	-2.306442	5.889666
105	1	0	6.534107	-3.256762	4.675928
106	1	0	4.444849	-3.877747	5.869799

6-IM2



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	3.706797	4.287742	0.312842
2	14	0	1.326107	2.184428	-2.091586
3	14	0	5.187720	2.269970	-2.796082
4	14	0	-6.369299	1.957853	-0.556082
5	14	0	-3.989572	4.296234	1.680505
6	14	0	-0.182202	4.615952	0.797623
7	14	0	-2.522841	2.080358	-1.330303
8	14	0	3.793007	-4.393459	-0.587286
9	14	0	3.748790	0.009721	-0.033073
10	14	0	5.201286	-1.723931	-3.211762
11	14	0	1.347907	-1.812100	-2.477550
12	14	0	1.601863	0.071433	-0.992804
13	14	0	-3.871259	-4.577986	1.013906
14	14	0	-0.060838	-4.611547	0.081687
15	14	0	-3.879905	-0.150114	1.516382
16	14	0	-2.513885	-1.906535	-1.662891
17	14	0	-6.341288	-2.037742	-0.852129
18	14	0	-6.049236	-0.133098	0.569550
19	14	0	-0.049794	-0.279694	0.667041
20	14	0	-2.248236	-0.016536	-0.192438
21	14	0	5.405965	0.145503	-1.710855
22	1	0	3.817405	5.624531	0.965936
23	1	0	3.838119	3.255797	1.375440
24	1	0	6.235274	2.383267	-3.877720
25	1	0	-7.747707	1.977546	-1.172352
26	1	0	-3.962842	5.707735	2.163281
27	1	0	-3.660199	3.429972	2.845456
28	1	0	-0.166769	6.095691	0.999819
29	1	0	0.058999	3.987341	2.120961
30	1	0	3.981117	-3.689668	0.709382
31	1	0	3.887232	-5.857996	-0.317323
32	1	0	3.187324	1.067278	3.435656
33	1	0	3.919451	-1.208372	0.811976
34	1	0	6.239347	-1.599427	-4.303557
35	1	0	-3.569456	-3.852722	2.277754
36	1	0	-3.778058	-6.037645	1.307947
37	1	0	0.209699	-4.065647	1.440499
38	1	0	-0.000734	-6.099466	0.196034
39	1	0	-3.745879	1.023456	2.418177
40	1	0	-3.678471	-1.379887	2.328472

41	1	0	-7.728803	-1.996567	-1.446245
42	1	0	-7.071949	-0.221997	1.679434
43	1	0	0.061360	-1.705456	1.084155
44	1	0	6.775936	0.079728	-1.078163
45	16	0	0.492800	0.915781	2.416749
46	16	0	4.502460	1.173723	3.717212
47	14	0	-4.729227	2.290666	-2.262967
48	1	0	-4.858485	3.698665	-2.784680
49	1	0	-4.936439	1.360695	-3.424511
50	14	0	-0.866463	2.403862	-3.037729
51	1	0	-1.011815	3.812454	-3.553418
52	1	0	-1.073094	1.476538	-4.201754
53	14	0	-4.720015	-2.056676	-2.606966
54	1	0	-4.973660	-0.971081	-3.613595
55	1	0	-4.804686	-3.375091	-3.332137
56	14	0	-0.865493	-1.929848	-3.412268
57	1	0	-1.108911	-0.841016	-4.418651
58	1	0	-0.991205	-3.247109	-4.134137
59	14	0	3.017718	2.527058	-3.766473
60	1	0	2.825292	1.616030	-4.945969
61	1	0	2.873329	3.942585	-4.263198
62	14	0	3.025254	-1.824435	-4.199162
63	1	0	2.895925	-3.132907	-4.936344
64	1	0	2.807429	-0.722494	-5.196511
65	14	0	-6.098042	-4.095806	0.348853
66	1	0	-7.000044	-4.096451	1.557369
67	1	0	-6.573339	-5.201846	-0.559840
68	14	0	-2.250674	-4.053061	-0.627024
69	1	0	-2.526956	-4.980223	-1.770163
70	14	0	1.630689	-3.955803	-1.441289
71	1	0	1.465040	-4.880466	-2.607831
72	14	0	5.546957	-3.800038	-2.070815
73	1	0	5.664527	-4.875033	-3.122481
74	1	0	6.855865	-3.764423	-1.323428
75	14	0	1.580557	4.123322	-0.707334
76	1	0	1.527289	5.222824	-1.722829
77	14	0	5.491076	4.059173	-1.234222
78	1	0	6.791144	3.874026	-0.493985
79	1	0	5.606739	5.338531	-2.025041
80	14	0	-2.342022	4.064649	-0.000616
81	1	0	-2.666382	5.121341	-1.011045
82	14	0	-6.196577	3.812942	0.950257
83	1	0	-6.729320	5.023797	0.225577
84	1	0	-7.086381	3.587538	2.146959

85	6	0	-0.460148	0.185612	3.766504
86	6	0	-1.340650	1.004195	4.485759
87	6	0	-0.269751	-1.146862	4.159255
88	6	0	-2.028378	0.489408	5.586331
89	1	0	-1.483074	2.036605	4.183988
90	6	0	-0.972827	-1.656992	5.252014
91	1	0	0.425193	-1.778754	3.615996
92	6	0	-1.851235	-0.841442	5.968543
93	1	0	-2.707370	1.130859	6.140499
94	1	0	-0.826052	-2.692310	5.545868
95	1	0	-2.391922	-1.240274	6.821574
96	6	0	4.568611	-0.096239	4.974329
97	6	0	3.416887	-0.672406	5.526426
98	6	0	5.830532	-0.503842	5.428810
99	6	0	3.532877	-1.647960	6.517097
100	1	0	2.432467	-0.361824	5.189824
101	6	0	5.934824	-1.473933	6.424880
102	1	0	6.728085	-0.066231	5.001110
103	6	0	4.788477	-2.052819	6.972913
104	1	0	2.631648	-2.087838	6.935223
105	1	0	6.918533	-1.780811	6.768939
106	1	0	4.873173	-2.810561	7.745934

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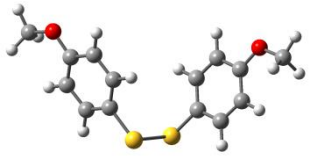
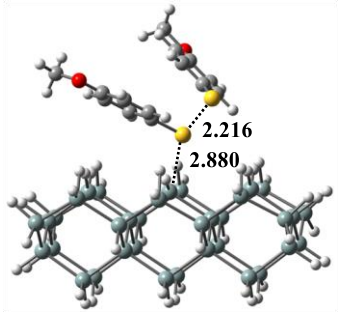


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.616472	2.229922	0.868246
2	16	0	-0.616527	2.230043	-0.868106
3	6	0	-1.824879	0.945267	-0.574197
4	6	0	-3.034539	1.237181	0.064747
5	6	0	-1.592818	-0.366225	-1.024657
6	6	0	-3.999653	0.249262	0.261713
7	1	0	-3.222815	2.247427	0.413526
8	6	0	-2.545362	-1.356706	-0.832794
9	1	0	-0.659899	-0.601141	-1.526303
10	6	0	-3.755053	-1.055743	-0.186806
11	1	0	-4.927723	0.504531	0.758720
12	1	0	-2.380385	-2.372736	-1.175710

13	6	0	1.824832	0.945190	0.574176
14	6	0	3.034477	1.237157	-0.064772
15	6	0	1.592782	-0.366340	1.024533
16	6	0	3.999602	0.249263	-0.261803
17	1	0	3.222730	2.247420	-0.413514
18	6	0	2.545345	-1.356793	0.832614
19	1	0	0.659856	-0.601309	1.526140
20	6	0	3.755045	-1.055760	0.186678
21	1	0	4.927618	0.504556	-0.758902
22	1	0	2.380378	-2.372854	1.175444
23	8	0	4.622444	-2.096194	0.047017
24	8	0	-4.622420	-2.096208	-0.047190
25	6	0	5.865673	-1.858442	-0.597696
26	1	0	6.389641	-2.814999	-0.600476
27	1	0	5.726158	-1.519945	-1.631955
28	1	0	6.467380	-1.118688	-0.055063
29	6	0	-5.865444	-1.858656	0.598005
30	1	0	-6.389225	-2.815310	0.601016
31	1	0	-5.725585	-1.520098	1.632200
32	1	0	-6.467493	-1.119022	0.055588

7-TS1



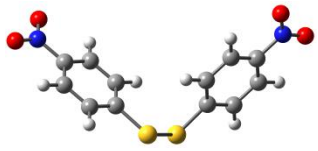
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	3.936219	3.608716	-2.055801
2	14	0	2.459169	-0.107983	-2.472556
3	14	0	6.309464	0.375503	-1.950948
4	14	0	-5.278221	-1.038296	-3.451639
5	14	0	-3.786007	2.671849	-3.078710
6	14	0	0.074392	3.100636	-2.533207
7	14	0	-1.417428	-0.577657	-2.981552
8	14	0	3.955464	-2.920619	3.976112
9	14	0	3.881028	0.454907	1.077025
10	14	0	6.323017	-2.563551	0.763144

11	14	0	2.479548	-3.056683	0.233681
12	14	0	2.225040	-0.693498	-0.159271
13	14	0	-3.763659	-3.817235	2.986335
14	14	0	0.111105	-3.497055	3.472999
15	14	0	-3.768028	-0.460644	0.068620
16	14	0	-1.420566	-3.521775	-0.268361
17	14	0	-5.279651	-3.966723	-0.720254
18	14	0	-5.451529	-1.612680	-1.132580
19	14	0	0.071963	-0.137022	0.628630
20	14	0	-1.630381	-1.152455	-0.664163
21	14	0	6.031588	-0.220128	0.352943
22	1	0	3.879233	4.920426	-2.765677
23	1	0	3.673738	3.877999	-0.616282
24	1	0	7.678811	-0.065989	-2.410239
25	1	0	-6.345766	-1.777346	-4.223099
26	1	0	-3.867505	3.973324	-3.804456
27	1	0	-3.967113	2.968971	-1.631148
28	1	0	-0.008662	4.456727	-3.153267
29	1	0	-0.139290	3.257015	-1.071453
30	1	0	3.681111	-1.504484	4.340417
31	1	0	3.898267	-3.719900	5.234730
32	1	0	3.728475	1.921079	0.881603
33	1	0	3.724094	0.167114	2.528330
34	1	0	7.695854	-2.974373	0.286118
35	1	0	-3.924619	-2.381902	3.342891
36	1	0	-3.840634	-4.599717	4.254440
37	1	0	-0.113169	-2.106246	3.952742
38	1	0	0.058053	-4.382343	4.675380
39	1	0	-3.926409	1.000729	-0.161964
40	1	0	-3.923296	-0.708618	1.527367
41	1	0	-6.358288	-4.677842	-1.502564
42	1	0	-6.811122	-1.159689	-0.648332
43	1	0	-0.050726	-0.722854	1.996352
44	1	0	7.084975	0.517915	1.147454
45	16	0	0.185886	2.457154	1.873538
46	16	0	1.247971	4.093204	2.925433
47	14	0	-3.126065	-1.590756	-4.332502
48	1	0	-3.012594	-1.008683	-5.718409
49	1	0	-2.937509	-3.076431	-4.453558
50	14	0	0.760339	-1.127898	-3.828383
51	1	0	0.873974	-0.559267	-5.219546
52	1	0	0.952315	-2.614396	-3.936670
53	14	0	-3.136367	-4.812952	-1.356659
54	1	0	-2.963905	-4.828999	-2.849395

55	1	0	-3.017592	-6.236472	-0.874140
56	14	0	0.763169	-4.325485	-0.873251
57	1	0	0.957701	-4.348048	-2.363622
58	1	0	0.868545	-5.749420	-0.388973
59	14	0	4.640206	-0.641922	-3.325808
60	1	0	4.842092	-2.125921	-3.445940
61	1	0	4.738333	-0.060659	-4.713117
62	14	0	4.665109	-3.869197	-0.360461
63	1	0	4.768598	-5.294942	0.118653
64	1	0	4.875915	-3.879005	-1.848319
65	14	0	-5.573346	-4.481065	1.600834
66	1	0	-6.852306	-3.860238	2.105391
67	1	0	-5.735993	-5.976807	1.709651
68	14	0	-1.633287	-4.182738	2.025209
69	1	0	-1.491892	-5.671036	1.934044
70	14	0	2.269109	-3.726621	2.525167
71	1	0	2.494946	-5.204795	2.439152
72	14	0	6.153489	-3.084800	3.094403
73	1	0	6.632212	-4.504542	3.270591
74	1	0	7.083860	-2.202947	3.888747
75	14	0	2.233674	2.228066	-2.947912
76	1	0	2.420123	2.276736	-4.433111
77	14	0	6.133064	2.739639	-2.294229
78	1	0	7.066935	3.469465	-1.361736
79	1	0	6.604345	3.020300	-3.699690
80	14	0	-1.636810	1.757552	-3.461772
81	1	0	-1.448214	1.806202	-4.946558
82	14	0	-5.585508	1.309529	-3.817525
83	1	0	-5.752373	1.509470	-5.303515
84	1	0	-6.865651	1.771113	-3.165905
85	6	0	-1.323836	2.269988	2.813986
86	6	0	-2.494930	2.904191	2.383338
87	6	0	-1.358632	1.496006	3.988418
88	6	0	-3.687188	2.772129	3.099419
89	1	0	-2.475870	3.506517	1.481054
90	6	0	-2.536371	1.361272	4.706683
91	1	0	-0.455034	1.004003	4.333025
92	6	0	-3.710679	1.997543	4.266899
93	1	0	-4.579350	3.271164	2.740525
94	1	0	-2.579331	0.766911	5.613346
95	6	0	0.547281	5.570079	2.233703
96	6	0	1.133487	6.191955	1.113665
97	6	0	-0.582276	6.160642	2.818251
98	6	0	0.604439	7.365277	0.599521

99	1	0	2.010122	5.745444	0.655272
100	6	0	-1.121746	7.342023	2.308762
101	1	0	-1.039629	5.691357	3.683257
102	6	0	-0.528235	7.949599	1.193411
103	1	0	1.048593	7.856351	-0.260050
104	1	0	-1.991411	7.777818	2.786051
105	8	0	-4.809513	1.800627	5.042334
106	6	0	-6.035621	2.399794	4.647408
107	1	0	-6.361626	2.040438	3.663333
108	1	0	-6.769077	2.104947	5.398906
109	1	0	-5.961527	3.494380	4.625257
110	8	0	-0.966560	9.099812	0.616144
111	6	0	-2.101294	9.748811	1.172359
112	1	0	-1.922987	10.052764	2.211401
113	1	0	-2.268116	10.636933	0.561523
114	1	0	-2.992338	9.109758	1.131613

8



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-0.681324	2.327840	-0.780333
2	16	0	0.681753	2.328012	0.779558
3	6	0	1.933910	1.109287	0.353549
4	6	0	1.794297	0.147587	-0.652346
5	6	0	3.099622	1.152752	1.135083
6	6	0	2.815546	-0.770499	-0.878561
7	1	0	0.898829	0.118002	-1.262364
8	6	0	4.117929	0.233221	0.917117
9	1	0	3.213602	1.906585	1.908216
10	6	0	3.961734	-0.718313	-0.089656
11	1	0	2.734797	-1.525078	-1.650867
12	1	0	5.027415	0.245335	1.504254
13	6	0	-1.933659	1.109436	-0.353942
14	6	0	-1.796211	0.150961	0.655323
15	6	0	-3.097361	1.149859	-1.138652
16	6	0	-2.817649	-0.766837	0.881836
17	1	0	-0.902233	0.123696	1.267657
18	6	0	-4.115854	0.230638	-0.920316

19	1	0	-3.209604	1.901010	-1.914649
20	6	0	-3.961871	-0.717617	0.089897
21	1	0	-2.738548	-1.518914	1.656748
22	1	0	-5.023801	0.240444	-1.509875
23	7	0	-5.037337	-1.689892	0.326535
24	7	0	5.036975	-1.690948	-0.325898
25	8	0	-6.035896	-1.621134	-0.389942
26	8	0	-4.873661	-2.514029	1.225872
27	8	0	6.037308	-1.619511	0.387833
28	8	0	4.871325	-2.518034	-1.222161

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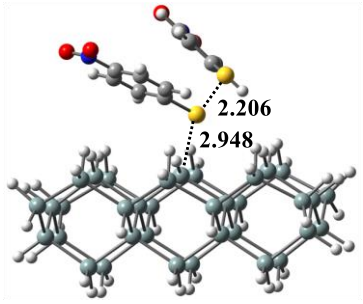

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3	14	0	6.271161	1.541833	-1.722792
4	14	0	-4.809447	-1.857996	-3.795863
5	14	0	-4.024593	2.036742	-3.261360
6	14	0	-0.333809	3.092639	-2.468886
7	14	0	-1.111771	-0.745391	-3.142251
8	14	0	4.355998	-2.410031	3.948795
9	14	0	3.774929	1.021659	1.195188
10	14	0	6.717684	-1.505161	0.843705
11	14	0	3.036239	-2.636146	0.151166
12	14	0	2.401236	-0.334376	-0.169619
13	14	0	-3.078834	-4.517869	2.649665
14	14	0	0.682518	-3.598046	3.285974
15	14	0	-3.567723	-1.141720	-0.188988
16	14	0	-0.709176	-3.744019	-0.504082
17	14	0	-4.422504	-4.816045	-1.115721
18	14	0	-4.979361	-2.517569	-1.498777
19	14	0	0.155392	-0.227664	0.538950
20	14	0	-1.319801	-1.436489	-0.856062

21	14	0	6.033888	0.771035	0.534090
22	1	0	3.072438	5.601236	-2.447103
23	1	0	2.966674	4.426867	-0.360179
24	1	0	7.713406	1.387671	-2.141737
25	1	0	-5.693219	-2.757991	-4.625329
26	1	0	-4.296060	3.331671	-3.949463
27	1	0	-4.312264	2.238241	-1.814430
28	1	0	-0.650182	4.460123	-2.977588
29	1	0	-0.621106	3.081735	-1.009687
30	1	0	3.832333	-1.076966	4.353050
31	1	0	4.395802	-3.260126	5.173722
32	1	0	3.369391	2.446964	1.063694
33	1	0	3.608417	0.631438	2.621383
34	1	0	8.153091	-1.645414	0.397215
35	1	0	-3.479737	-3.136068	3.028592
36	1	0	-3.063181	-5.334931	3.896981
37	1	0	0.218316	-2.278597	3.796884
38	1	0	0.746226	-4.517957	4.460614
39	1	0	-3.954201	0.285982	-0.360178
40	1	0	-3.718538	-1.475058	1.253282
41	1	0	-5.333041	-5.679607	-1.954985
42	1	0	-6.411657	-2.308951	-1.064455
43	1	0	0.074845	-0.840249	1.898297
44	1	0	6.908413	1.637839	1.410583
45	16	0	-0.192418	2.342956	1.940308
46	16	0	0.386925	4.193550	2.992576
47	14	0	-2.559850	-1.999972	-4.591785
48	1	0	-2.490719	-1.358076	-5.953438
49	1	0	-2.102601	-3.423237	-4.740094
50	14	0	1.161829	-0.858606	-3.908300
51	1	0	1.218117	-0.211496	-5.267986
52	1	0	1.628339	-2.278166	-4.066482
53	14	0	-2.147127	-5.266657	-1.691735
54	1	0	-1.920444	-5.202077	-3.175420
55	1	0	-1.797533	-6.660771	-1.238569
56	14	0	1.596412	-4.130056	-1.063167
57	1	0	1.828448	-4.049622	-2.545569
58	1	0	1.936132	-5.532907	-0.630118
59	14	0	4.872731	0.313522	-3.222262
60	1	0	5.353570	-1.097507	-3.409677
61	1	0	4.904388	0.985461	-4.570894
62	14	0	5.346868	-3.015952	-0.403368
63	1	0	5.686246	-4.427114	0.002445
64	1	0	5.584843	-2.899667	-1.882031

65	14	0	-4.706646	-5.430514	1.182462
66	1	0	-6.085566	-5.040433	1.649668
67	1	0	-4.619863	-6.934359	1.252560
68	14	0	-0.885843	-4.506242	1.761390
69	1	0	-0.500423	-5.947046	1.628387
70	14	0	2.875122	-3.425513	2.408118
71	1	0	3.347983	-4.839703	2.271950
72	14	0	6.574768	-2.165386	3.141777
73	1	0	7.277941	-3.493316	3.269274
74	1	0	7.320975	-1.180844	4.005944
75	14	0	1.964807	2.666931	-2.829495
76	1	0	2.192918	2.824537	-4.300462
77	14	0	5.672157	3.849893	-1.949541
78	1	0	6.407160	4.677789	-0.926260
79	1	0	6.145258	4.299147	-3.309187
80	14	0	-1.732199	1.529043	-3.558066
81	1	0	-1.470608	1.675826	-5.024398
82	14	0	-5.517499	0.406238	-4.127160
83	1	0	-5.643735	0.619736	-5.614524
84	1	0	-6.886115	0.611063	-3.529240
85	6	0	-1.558090	1.760783	2.953874
86	6	0	-2.877114	2.017813	2.549893
87	6	0	-1.310787	1.052238	4.139832
88	6	0	-3.946031	1.569386	3.323509
89	1	0	-3.061368	2.565572	1.632356
90	6	0	-2.371818	0.602982	4.919805
91	1	0	-0.289111	0.857493	4.446671
92	6	0	-3.673258	0.869265	4.496263
93	1	0	-4.974147	1.751938	3.036765
94	1	0	-2.212006	0.053071	5.838779
95	6	0	-0.697734	5.419989	2.281504
96	6	0	-0.298445	6.137418	1.140659
97	6	0	-1.936162	5.699775	2.884508
98	6	0	-1.126541	7.117022	0.601825
99	1	0	0.662329	5.924600	0.684285
100	6	0	-2.771234	6.678011	2.352549
101	1	0	-2.236213	5.152683	3.771496
102	6	0	-2.352224	7.368962	1.216913
103	1	0	-0.843187	7.685050	-0.275393
104	1	0	-3.729534	6.915433	2.797385
105	7	0	-4.800333	0.391958	5.318060
106	8	0	-5.937394	0.651642	4.928282
107	8	0	-4.531493	-0.235170	6.341052
108	7	0	-3.233919	8.403344	0.648598

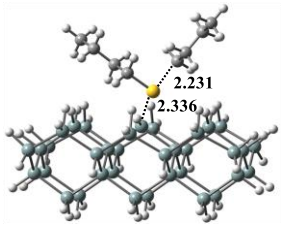
109	8	0	-4.312509	8.600380	1.206405
110	8	0	-2.836828	9.003621	-0.348900

S5.5 Reaction between di-*n*-butylsulfide and the silyl radical

9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.405296	0.439714	-0.000126
2	1	0	1.328157	1.080300	-0.886350
3	1	0	1.328078	1.080507	0.885942
4	6	0	2.740440	-0.308831	0.000023
5	1	0	2.789662	-0.964108	0.879081
6	1	0	2.789762	-0.964280	-0.878901
7	6	0	3.947393	0.639598	0.000004
8	1	0	3.892567	1.297299	-0.877866
9	1	0	3.892462	1.297473	0.877736
10	6	0	5.287685	-0.101796	0.000157
11	1	0	6.129916	0.597462	0.000136
12	1	0	5.386262	-0.741814	0.884026
13	1	0	5.386366	-0.741991	-0.883573
14	16	0	-0.000002	-0.744116	-0.000057
15	6	0	-1.405294	0.439707	-0.000099
16	1	0	-1.328094	1.080473	0.885992
17	1	0	-1.328155	1.080332	-0.886297
18	6	0	-2.740441	-0.308837	0.000010
19	1	0	-2.789673	-0.964145	0.879046
20	1	0	-2.789751	-0.964262	-0.878934
21	6	0	-3.947388	0.639592	0.000003
22	1	0	-3.892465	1.297443	0.877755
23	1	0	-3.892548	1.297325	-0.877844
24	6	0	-5.287683	-0.101787	0.000116
25	1	0	-5.386283	-0.741835	0.883962
26	1	0	-6.129907	0.597479	0.000107
27	1	0	-5.386365	-0.741956	-0.883634

9-TS1



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3	14	0	-5.721546	-1.621795	-2.213033
4	14	0	4.063612	-4.361929	0.068763
5	14	0	0.158904	-4.533352	-0.194561
6	14	0	2.118666	-1.471468	-1.920824
7	14	0	-4.034839	4.210989	1.621254
8	14	0	-3.888565	-0.161123	0.873237
9	14	0	-5.829221	2.305813	-1.417167
10	14	0	-1.917189	2.373997	-1.266143
11	14	0	-1.896606	0.145276	-0.365149
12	14	0	3.789029	4.317652	2.011510
13	14	0	-0.119926	4.395877	1.739086
14	14	0	3.890362	-0.049720	1.196925
15	14	0	2.028183	2.431050	-1.076431
16	14	0	5.932813	2.532829	-0.868393
17	14	0	5.886341	0.289254	-0.029391
18	14	0	-0.025632	0.035713	1.084384
19	14	0	1.990782	0.187213	-0.191632
20	14	0	-5.780336	0.080869	-0.528674
21	1	0	-3.765843	-5.975206	-0.088938
22	1	0	-3.768516	-3.956678	1.204622
23	1	0	-6.925687	-1.465345	-3.110704
24	1	0	4.119307	-5.851128	0.142235
25	1	0	3.927726	-3.860850	1.464148
26	1	0	0.180740	-6.025659	-0.258410
27	1	0	0.115302	-4.145683	1.238470
28	1	0	-4.013815	3.178943	2.693090
29	1	0	-4.101494	5.541960	2.292330
30	1	0	-3.908331	-1.516608	1.488721
31	1	0	-3.953246	0.830943	1.981141
32	1	0	-7.031120	2.445610	-2.320737
33	1	0	3.704994	3.268699	3.064200
34	1	0	3.739350	5.638939	2.702845

35	1	0	-0.167878	3.471217	2.904151
36	1	0	-0.165309	5.784964	2.287276
37	1	0	3.912565	-1.408960	1.806018
38	1	0	3.816193	0.926027	2.320903
39	1	0	7.208915	2.731653	-1.651042
40	1	0	7.071475	0.112362	0.892616
41	1	0	-0.039447	1.321467	1.846344
42	1	0	-7.037098	-0.117610	0.288198
43	16	0	-0.571256	-1.517735	2.740852
44	6	0	0.780675	-1.157549	3.964818
45	1	0	0.285623	-0.857036	4.892728
46	1	0	1.338625	-0.288997	3.604786
47	6	0	1.711817	-2.347833	4.197063
48	1	0	1.122458	-3.218644	4.511175
49	1	0	2.187690	-2.625924	3.249245
50	6	0	2.787552	-2.049284	5.252208
51	1	0	3.384009	-1.185772	4.928643
52	1	0	2.303908	-1.750755	6.192283
53	6	0	3.713099	-3.243087	5.508821
54	1	0	4.472910	-3.002448	6.259110
55	1	0	3.150074	-4.110650	5.871017
56	1	0	4.232560	-3.544879	4.592677
57	6	0	-1.951800	-2.364059	4.276163
58	1	0	-2.583228	-2.959437	3.618003
59	1	0	-1.260343	-2.985649	4.846951
60	6	0	-2.659658	-1.279189	5.044905
61	1	0	-1.932123	-0.635743	5.558066
62	1	0	-3.208858	-0.632483	4.349528
63	6	0	-3.645592	-1.841027	6.093640
64	1	0	-3.101228	-2.488524	6.793292
65	1	0	-4.379260	-2.483060	5.589536
66	6	0	-4.372357	-0.737093	6.869671
67	1	0	-5.067620	-1.158595	7.602780
68	1	0	-3.663537	-0.099846	7.410562
69	1	0	-4.948003	-0.093014	6.195564
70	14	0	-3.724776	-1.472319	-3.516488
71	1	0	-3.722310	-0.249893	-4.389932
72	1	0	-3.648375	-2.674169	-4.422833
73	14	0	-5.775544	-3.823059	-1.268029
74	1	0	-6.930450	-3.942255	-0.305244
75	1	0	-6.042846	-4.784970	-2.398921
76	14	0	-1.800212	-3.813700	-1.313307
77	1	0	-1.811613	-4.566866	-2.607860
78	14	0	2.156977	-3.751743	-1.192153

79	1	0	2.279417	-4.494090	-2.486746
80	14	0	6.119304	-3.589546	-0.832596
81	1	0	6.526476	-4.517827	-1.949650
82	1	0	7.194431	-3.669818	0.222179
83	14	0	6.033732	-1.376547	-1.745806
84	1	0	7.297097	-1.146676	-2.540504
85	14	0	5.882126	4.142289	0.904940
86	1	0	6.962345	3.831052	1.910489
87	1	0	6.214544	5.483524	0.300143
88	14	0	1.924245	4.177244	0.562994
89	1	0	2.004087	5.405771	-0.289818
90	14	0	-2.031095	4.125024	0.366682
91	1	0	-2.057391	5.348573	-0.496465
92	14	0	-6.004805	3.942672	0.323411
93	1	0	-6.325451	5.261725	-0.334388
94	1	0	-7.163564	3.608147	1.229183
95	14	0	-3.839451	2.809462	-2.643529
96	1	0	-3.839196	4.281331	-2.969246
97	1	0	-3.780425	2.062272	-3.945794
98	14	0	4.047647	2.968780	-2.271161
99	1	0	4.142466	2.228913	-3.575324
100	1	0	4.014673	4.441856	-2.590853
101	14	0	4.142810	-1.296639	-3.204821
102	1	0	4.197540	-2.489946	-4.124284
103	1	0	4.156393	-0.065890	-4.066098
104	14	0	0.207068	-1.380516	-3.367804
105	1	0	0.261858	-2.575680	-4.284414
106	1	0	0.217721	-0.152033	-4.232893
107	14	0	0.110589	2.865846	-2.457963
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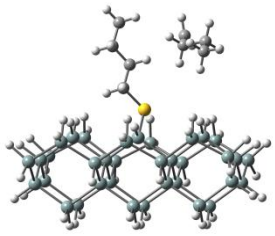
9-IM1



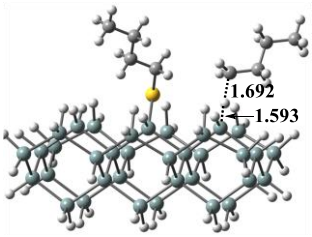
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	3.568292	4.690976	0.750557

2	14	0	1.479237	2.296135	-1.713437
3	14	0	5.367083	2.560508	-2.125144
4	14	0	-4.150779	4.005289	1.756580
5	14	0	-0.344354	4.672884	1.043248
6	14	0	-2.410680	2.007381	-1.247470
7	14	0	4.091680	-4.157709	0.075113
8	14	0	3.816617	0.245672	0.585437
9	14	0	5.659623	-1.421586	-2.402173
10	14	0	1.767255	-1.684004	-2.082913
11	14	0	1.762600	0.197293	-0.584691
12	14	0	-3.685730	-4.807563	0.709415
13	14	0	0.199924	-4.567637	0.288393
14	14	0	-3.885450	-0.424889	1.379360
15	14	0	-2.150903	-1.963254	-1.699820
16	14	0	-6.034848	-2.261058	-1.293396
17	14	0	-5.968880	-0.435905	0.258105
18	14	0	-0.009654	-0.222290	0.930688
19	14	0	-2.117352	-0.112782	-0.159724
20	14	0	5.601447	0.484035	-0.950894
21	1	0	3.544259	6.097364	1.247968
22	1	0	3.704516	3.802845	1.935706
23	1	0	6.491333	2.679964	-3.126343
24	1	0	-4.221427	5.383080	2.324610
25	1	0	-3.843437	3.080340	2.880787
26	1	0	-0.445362	6.156928	1.183548
27	1	0	-0.119517	4.114802	2.399388
28	1	0	4.092066	-3.457115	1.388030
29	1	0	4.231135	-5.616841	0.352915
30	1	0	3.829377	1.379174	1.547306
31	1	0	3.984816	-1.013297	1.361363
32	1	0	6.807713	-1.265928	-3.370551
33	1	0	-3.564878	-4.152510	2.040120
34	1	0	-3.559116	-6.277851	0.927827
35	1	0	0.265605	-3.998543	1.662157
36	1	0	0.329544	-6.049094	0.424824
37	1	0	-3.877155	0.671324	2.387567
38	1	0	-3.690283	-1.702621	2.118953
39	1	0	-7.355047	-2.228527	-2.025515
40	1	0	-7.074068	-0.647816	1.267470
41	1	0	0.141027	-1.628253	1.409499
42	1	0	6.909851	0.527125	-0.194835
43	16	0	0.257553	1.044558	2.666450
44	6	0	-0.703048	0.144811	3.981918
45	1	0	-0.498667	-0.925885	3.887715

46	1	0	-1.770077	0.310175	3.808909
47	6	0	-0.294090	0.651107	5.366601
48	1	0	0.779857	0.483211	5.513622
49	1	0	-0.455308	1.735320	5.422715
50	6	0	-1.077869	-0.043502	6.490635
51	1	0	-2.152889	0.133741	6.352870
52	1	0	-0.933723	-1.129608	6.414711
53	6	0	-0.650718	0.431497	7.883306
54	1	0	-1.215187	-0.080996	8.668898
55	1	0	0.414127	0.237700	8.052657
56	1	0	-0.815568	1.508238	8.002650
57	6	0	3.396681	-0.412605	6.578227
58	1	0	3.591625	0.512883	6.044949
59	1	0	3.311655	-0.353254	7.659393
60	6	0	3.554654	-1.731196	5.898413
61	1	0	2.925544	-2.486895	6.389284
62	1	0	3.209069	-1.661976	4.857781
63	6	0	5.015512	-2.254194	5.887745
64	1	0	5.374402	-2.331990	6.921708
65	1	0	5.656036	-1.512049	5.395269
66	6	0	5.152595	-3.608823	5.185614
67	1	0	6.190685	-3.957050	5.192729
68	1	0	4.541329	-4.374424	5.677089
69	1	0	4.828900	-3.548561	4.140109
70	14	0	3.270304	2.692758	-3.266665
71	1	0	3.210891	1.750344	-4.435238
72	1	0	3.101178	4.090163	-3.804816
73	14	0	5.476035	4.435479	-0.638982
74	1	0	6.717241	4.340448	0.212388
75	1	0	5.617743	5.671974	-1.491071
76	14	0	1.522490	4.275581	-0.361322
77	1	0	1.432261	5.335113	-1.416291
78	14	0	-2.417049	3.954372	0.149595
79	1	0	-2.782765	5.013149	-0.845139
80	14	0	-6.287342	3.472972	0.866509
81	1	0	-6.833902	4.701357	0.182549
82	1	0	-7.236568	3.133472	1.988309
83	14	0	-6.290131	1.709900	-0.757559
84	1	0	-7.625085	1.719600	-1.463179
85	14	0	-5.843996	-4.371325	-0.176937
86	1	0	-6.870866	-4.466347	0.923317
87	1	0	-6.172994	-5.443843	-1.184973
88	14	0	-1.907945	-4.126735	-0.695674
89	1	0	-1.977253	-5.032073	-1.886246

90	14	0	2.024275	-3.820229	-1.023481
91	1	0	2.048352	-4.745196	-2.200979
92	14	0	5.979055	-3.459509	-1.183769
93	1	0	6.302612	-4.535966	-2.189579
94	1	0	7.174135	-3.330978	-0.273082
95	14	0	3.615164	-1.646830	-3.620798
96	1	0	3.623434	-2.972017	-4.338795
97	1	0	3.461432	-0.572920	-4.659948
98	14	0	-4.241840	-2.146541	-2.870868
99	1	0	-4.431184	-1.026426	-3.853566
100	1	0	-4.209799	-3.434265	-3.653596
101	14	0	-4.551580	2.178944	-2.329076
102	1	0	-4.699781	3.601408	-2.803791
103	1	0	-4.647795	1.290168	-3.536893
104	14	0	-0.647205	2.435607	-2.817890
105	1	0	-0.811097	3.846698	-3.320808
106	1	0	-0.727407	1.522854	-4.008836
107	14	0	-0.320411	-1.877634	-3.255249
108	1	0	-0.494949	-0.779093	-4.265366
109	1	0	-0.303096	-3.182540	-4.009112

9-TS2



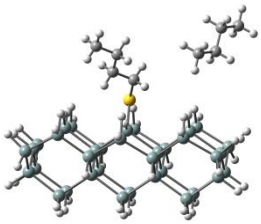
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-4.168309	-4.044034	0.200909
2	14	0	-1.671284	-1.697735	-1.864598
3	14	0	-5.534242	-1.261612	-2.321576
4	14	0	6.067744	-2.533647	-0.843752
5	14	0	3.542618	-4.809311	1.288881
6	14	0	-0.311828	-4.629603	0.570908
7	14	0	2.208100	-2.123792	-1.377906
8	14	0	-3.237364	4.909994	0.654262
9	14	0	-3.696454	0.489875	0.697557
10	14	0	-5.156755	2.700155	-2.111244
11	14	0	-1.283327	2.267643	-1.706831
12	14	0	-1.639049	0.240714	-0.448817

13	14	0	4.491084	4.035392	1.568545
14	14	0	0.641849	4.535780	1.031014
15	14	0	3.965256	-0.381519	1.603949
16	14	0	2.615169	1.853792	-1.257671
17	14	0	6.475147	1.445204	-0.750120
18	14	0	6.054924	-0.553055	0.504000
19	14	0	0.160289	0.163247	1.098333
20	14	0	2.239087	-0.161401	0.004310
21	14	0	-5.452112	0.656348	-0.888199
22	1	0	-4.390575	-5.483797	0.523108
23	1	0	-4.184869	-3.301615	1.488913
24	1	0	-6.639036	-1.057853	-3.331094
25	1	0	7.402617	-2.637505	-1.542292
26	1	0	3.369117	-6.250213	1.635077
27	1	0	3.376793	-4.027504	2.543150
28	1	0	-0.473504	-6.111729	0.656792
29	1	0	-0.452189	-4.087734	1.946084
30	1	0	-3.390582	4.174314	1.938523
31	1	0	-3.131270	6.360129	0.991280
32	1	0	-3.989850	-0.505842	1.905552
33	1	0	-3.623054	1.817173	1.380290
34	1	0	-6.277347	2.851076	-3.113702
35	1	0	4.207852	3.231860	2.788878
36	1	0	4.597655	5.461201	1.994888
37	1	0	0.418022	3.816138	2.315323
38	1	0	0.761432	5.986455	1.365525
39	1	0	3.737888	-1.591028	2.438458
40	1	0	3.965804	0.799481	2.510923
41	1	0	7.800576	1.304349	-1.459978
42	1	0	7.152795	-0.685847	1.534916
43	1	0	0.222805	1.512344	1.731139
44	1	0	-6.778649	0.746612	-0.167647
45	16	0	-0.136093	-1.207395	2.765217
46	6	0	-0.580564	-0.055534	4.155716
47	1	0	-1.141326	-0.688337	4.850937
48	1	0	-1.271600	0.705033	3.781239
49	6	0	0.621580	0.580512	4.852444
50	1	0	1.305589	-0.210403	5.183371
51	1	0	1.179445	1.193617	4.133455
52	6	0	0.207821	1.448069	6.051499
53	1	0	-0.485091	2.230281	5.713452
54	1	0	-0.351961	0.832999	6.768972
55	6	0	1.405175	2.094425	6.756111
56	1	0	1.084414	2.703662	7.607092

57	1	0	2.099915	1.335274	7.132228
58	1	0	1.963186	2.743990	6.072615
59	6	0	-4.386595	-1.076224	3.448169
60	1	0	-3.750352	-1.959195	3.429001
61	1	0	-3.987698	-0.248829	4.033646
62	6	0	-5.874715	-1.269974	3.441801
63	1	0	-6.376961	-0.320251	3.212214
64	1	0	-6.158134	-1.973383	2.647443
65	6	0	-6.422624	-1.802627	4.787390
66	1	0	-6.144480	-1.106303	5.588839
67	1	0	-5.930184	-2.754625	5.022657
68	6	0	-7.942822	-1.994432	4.771021
69	1	0	-8.305672	-2.371440	5.732721
70	1	0	-8.459421	-1.049844	4.566762
71	1	0	-8.243715	-2.709874	3.997519
72	14	0	6.585737	3.369873	0.671076
73	1	0	7.560771	3.125470	1.795306
74	1	0	7.134989	4.507633	-0.152813
75	14	0	2.688347	3.865936	0.045305
76	1	0	2.963465	4.899145	-1.003137
77	14	0	-1.218969	4.285358	-0.412160
78	1	0	-1.008271	5.317875	-1.476246
79	14	0	-5.189429	4.610251	-0.665597
80	1	0	-5.353709	5.827162	-1.542042
81	1	0	-6.397841	4.551976	0.235385
82	14	0	-5.981790	-3.288318	-1.129315
83	1	0	-7.204318	-3.120939	-0.261474
84	1	0	-6.307755	-4.348663	-2.151140
85	14	0	-2.048643	-3.817601	-0.817101
86	1	0	-2.070365	-4.735876	-1.999768
87	14	0	1.863907	-4.221097	-0.269764
88	1	0	2.024574	-5.181232	-1.407941
89	14	0	5.749870	-4.513916	0.466651
90	1	0	6.088819	-5.687869	-0.417985
91	1	0	6.727479	-4.529641	1.614949
92	14	0	-3.059898	2.732263	-3.259331
93	1	0	-2.828883	4.121073	-3.798320
94	1	0	-3.046776	1.789775	-4.428934
95	14	0	0.844832	2.283186	-2.825830
96	1	0	0.880182	1.323273	-3.981157
97	1	0	1.062671	3.666068	-3.384516
98	14	0	4.753525	1.866251	-2.354452
99	1	0	4.802932	0.894234	-3.498653
100	1	0	4.958388	3.246459	-2.924469

101	14	0	-3.461557	-1.593313	-3.464936
102	1	0	-3.217881	-0.538864	-4.506689
103	1	0	-3.510582	-2.922908	-4.173283
104	14	0	0.427455	-2.026345	-2.984609
105	1	0	0.366638	-3.359375	-3.685088
106	1	0	0.681123	-0.980936	-4.033388
107	14	0	4.319421	-2.476555	-2.473611
108	1	0	4.251303	-3.817418	-3.158099
109	1	0	4.581695	-1.443952	-3.533102

9-IM2



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-4.216634	-3.759899	-0.278106
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3	14	0	-5.427224	-0.937102	-2.824407
4	14	0	6.074123	-2.544069	-0.876548
5	14	0	3.427046	-5.009359	0.851275
6	14	0	-0.390936	-4.567082	0.100490
7	14	0	2.251854	-2.014097	-1.562915
8	14	0	-3.222562	4.795120	0.821079
9	14	0	-3.712646	0.413715	0.325743
10	14	0	-4.960689	3.018612	-2.303848
11	14	0	-1.122367	2.476117	-1.697722
12	14	0	-1.578674	0.349948	-0.652366
13	14	0	4.399689	3.740690	2.171795
14	14	0	0.635040	4.444850	1.368953
15	14	0	3.846813	-0.651407	1.681342
16	14	0	2.728744	1.920720	-1.006613
17	14	0	6.533713	1.383531	-0.265056
18	14	0	6.000987	-0.742979	0.702523
19	14	0	0.099351	0.106792	1.005050
20	14	0	2.232189	-0.202300	0.013241
21	14	0	-5.383757	0.887398	-1.271387
22	1	0	-4.490020	-5.189585	0.051529
23	1	0	-4.249903	-2.992872	0.996306

24	1	0	-6.477872	-0.667188	-3.874780
25	1	0	7.443940	-2.577187	-1.511198
26	1	0	3.213337	-6.477836	1.005244
27	1	0	3.223171	-4.389035	2.187407
28	1	0	-0.613702	-6.043511	0.115700
29	1	0	-0.526578	-4.081651	1.497279
30	1	0	-3.481597	3.808639	1.905126
31	1	0	-3.147931	6.142288	1.458129
32	1	0	-4.676839	-0.501955	3.851709
33	1	0	-3.776593	1.333316	1.502905
34	1	0	-6.014857	3.272127	-3.356933
35	1	0	3.992829	2.807938	3.257773
36	1	0	4.493475	5.103250	2.771990
37	1	0	0.305842	3.647680	2.582946
38	1	0	0.759507	5.866536	1.809255
39	1	0	3.543423	-1.948790	2.341434
40	1	0	3.811060	0.408298	2.726590
41	1	0	7.908653	1.306439	-0.884458
42	1	0	7.024938	-1.028567	1.777386
43	1	0	0.165288	1.421070	1.706511
44	1	0	-6.729579	0.961274	-0.588614
45	16	0	-0.382088	-1.323375	2.573194
46	6	0	-0.841542	-0.203964	3.986888
47	1	0	-1.508787	-0.816152	4.601589
48	1	0	-1.434419	0.630107	3.601629
49	6	0	0.352188	0.289274	4.802791
50	1	0	0.927924	-0.574781	5.156485
51	1	0	1.025137	0.866200	4.155713
52	6	0	-0.075802	1.155873	5.997572
53	1	0	-0.652314	2.017090	5.634214
54	1	0	-0.757396	0.580662	6.638477
55	6	0	1.114079	1.649468	6.827107
56	1	0	0.783321	2.264559	7.669997
57	1	0	1.689691	0.809792	7.232365
58	1	0	1.795992	2.255174	6.219788
59	6	0	-5.084399	-0.900362	4.787101
60	1	0	-4.249427	-1.313880	5.365277
61	1	0	-5.494056	-0.058722	5.357495
62	6	0	-6.153361	-1.965734	4.524665
63	1	0	-6.961249	-1.532795	3.918835
64	1	0	-5.722735	-2.775570	3.919816
65	6	0	-6.748708	-2.556972	5.808952
66	1	0	-7.178533	-1.746170	6.413315
67	1	0	-5.940408	-2.989317	6.414877

68	6	0	-7.817770	-3.622250	5.546517
69	1	0	-8.222509	-4.024087	6.481243
70	1	0	-8.655168	-3.209874	4.972011
71	1	0	-7.407775	-4.461974	4.973746
72	14	0	5.673487	-4.662955	0.166327
73	1	0	6.036906	-5.727342	-0.838734
74	1	0	6.595447	-4.836256	1.347102
75	14	0	1.813720	-4.197364	-0.677214
76	1	0	1.957633	-5.048614	-1.900821
77	14	0	-2.073389	-3.617206	-1.267311
78	1	0	-2.131996	-4.487545	-2.484869
79	14	0	-5.949977	-2.986671	-1.702556
80	1	0	-7.225918	-2.823636	-0.915287
81	1	0	-6.211148	-4.031366	-2.758788
82	14	0	6.550379	3.127001	1.377824
83	1	0	7.425068	2.729733	2.540040
84	1	0	7.183258	4.338309	0.739709
85	14	0	2.736299	3.794639	0.490637
86	1	0	3.130332	4.913385	-0.423568
87	14	0	-1.136711	4.346794	-0.199290
88	1	0	-0.889942	5.496105	-1.127053
89	14	0	-5.046820	4.789120	-0.695085
90	1	0	-5.042355	6.092296	-1.454359
91	1	0	-6.345300	4.724482	0.068855
92	14	0	4.943790	2.007526	-1.937720
93	1	0	5.069935	1.160511	-3.172108
94	1	0	5.204038	3.435949	-2.342007
95	14	0	1.087349	2.541096	-2.651006
96	1	0	1.188703	1.693170	-3.887780
97	1	0	1.371323	3.964631	-3.057452
98	14	0	-2.793610	3.084581	-3.314645
99	1	0	-2.512128	4.502954	-3.740514
100	1	0	-2.723293	2.224005	-4.544115
101	14	0	4.414763	-2.281588	-2.576123
102	1	0	4.367185	-3.541877	-3.401271
103	1	0	4.740446	-1.147869	-3.506744
104	14	0	0.564494	-1.744914	-3.248126
105	1	0	0.528155	-3.008249	-4.068925
106	1	0	0.883907	-0.612089	-4.182483
107	14	0	-3.299209	-1.223269	-3.876681
108	1	0	-2.992757	-0.099802	-4.826273
109	1	0	-3.329961	-2.497007	-4.681935

S3.6 Structures involved in the discussions on the effect of the S-X bond in the substrate on the reactivity

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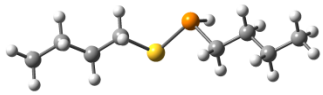
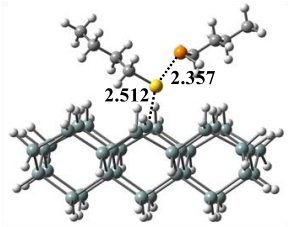


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.083219	0.147551	-0.315795
2	1	0	-1.750556	1.189276	-0.237219
3	1	0	-2.072879	-0.113077	-1.379168
4	6	0	-3.495098	-0.005350	0.269332
5	1	0	-3.810994	-1.055615	0.200248
6	1	0	-3.482086	0.239708	1.340135
7	6	0	-4.533741	0.877546	-0.437818
8	1	0	-4.221193	1.927845	-0.366931
9	1	0	-4.544198	0.634455	-1.508592
10	16	0	0.877660	-0.868573	-0.680093
11	6	0	2.111453	-0.003129	0.398259
12	1	0	1.755727	1.011105	0.602999
13	1	0	2.178765	-0.539567	1.348816
14	6	0	3.471768	0.038124	-0.299641
15	1	0	3.371105	0.541940	-1.269586
16	1	0	3.802059	-0.986139	-0.514311
17	6	0	4.536612	0.756427	0.542042
18	1	0	4.199736	1.779195	0.757577
19	1	0	4.629757	0.254652	1.514383
20	6	0	5.905252	0.802248	-0.143902
21	1	0	5.849910	1.327206	-1.104118
22	1	0	6.644130	1.319764	0.476160
23	1	0	6.283856	-0.206912	-0.340699
24	15	0	-0.829191	-0.887801	0.625971
25	1	0	-1.320270	-2.156753	0.206061
26	6	0	-5.944377	0.721297	0.137819
27	1	0	-5.971729	0.990300	1.199764
28	1	0	-6.661755	1.361401	-0.385606
29	1	0	-6.295962	-0.312888	0.050236

10-TS1

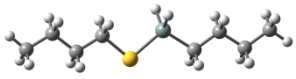


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.467568	3.252034	-1.496808
2	14	0	1.864621	0.334457	-2.440825
3	14	0	5.713144	-0.407518	-2.563669
4	14	0	-5.835776	1.826631	-2.168111
5	14	0	-3.235084	4.701894	-1.110934
6	14	0	0.610228	3.967891	-1.332156
7	14	0	-1.991391	1.080387	-2.316429
8	14	0	3.082129	-4.412892	2.782226
9	14	0	3.768090	-0.507388	0.789851
10	14	0	5.130167	-3.863773	-0.621861
11	14	0	1.282722	-3.148768	-0.574919
12	14	0	1.703586	-0.791978	-0.327332
13	14	0	-4.629889	-3.081225	2.920130
14	14	0	-0.808573	-3.922907	2.804100
15	14	0	-3.888229	0.864135	1.027114
16	14	0	-2.607060	-2.432204	-0.498754
17	14	0	-6.448999	-1.709934	-0.373837
18	14	0	-5.953063	0.618537	-0.102410
19	14	0	-0.078859	0.034030	0.995701
20	14	0	-2.123487	-0.087252	-0.225669
21	14	0	5.524487	-1.507127	-0.443321
22	1	0	4.741737	4.671864	-1.865141
23	1	0	4.470995	3.181090	-0.009731
24	1	0	6.815374	-1.062372	-3.361547
25	1	0	-7.149584	1.679902	-2.898085
26	1	0	-2.991828	6.140093	-1.425059
27	1	0	-3.143359	4.555385	0.367663
28	1	0	0.873136	5.406785	-1.634294
29	1	0	0.648232	3.805982	0.144763
30	1	0	3.265450	-3.114008	3.484763
31	1	0	2.925040	-5.463294	3.829980
32	1	0	4.049878	0.946655	0.949582
33	1	0	3.707409	-1.097933	2.154888
34	1	0	6.261454	-4.487895	-1.403599

35	1	0	-4.327677	-1.829824	3.667284
36	1	0	-4.817081	-4.162361	3.931091
37	1	0	-0.587339	-2.744012	3.685215
38	1	0	-1.002948	-5.102111	3.700718
39	1	0	-3.619443	2.311604	1.256570
40	1	0	-3.962084	0.221039	2.369681
41	1	0	-7.756523	-1.842776	-1.117555
42	1	0	-7.053565	1.232722	0.732707
43	1	0	-0.261383	-0.997478	2.062106
44	1	0	6.827699	-1.309623	0.297464
45	16	0	0.741398	1.842680	2.534139
46	6	0	-0.701508	1.841001	3.707544
47	1	0	-0.346926	1.426158	4.654542
48	1	0	-1.434175	1.142468	3.294092
49	6	0	-1.320596	3.224683	3.898124
50	1	0	-0.558117	3.916772	4.277606
51	1	0	-1.640627	3.614496	2.924070
52	6	0	-2.511653	3.197072	4.868345
53	1	0	-3.274414	2.505036	4.487314
54	1	0	-2.184404	2.790840	5.834686
55	6	0	-3.134463	4.581073	5.078654
56	1	0	-3.980247	4.534709	5.771909
57	1	0	-2.403546	5.285424	5.491508
58	1	0	-3.500006	4.998644	4.133921
59	6	0	3.055713	4.061425	3.088704
60	1	0	3.142434	3.782282	2.033322
61	1	0	2.334102	4.884932	3.144435
62	6	0	4.421256	4.513989	3.633535
63	1	0	4.332993	4.765665	4.699009
64	1	0	5.134027	3.680417	3.573215
65	14	0	-4.057459	1.016586	-3.543626
66	1	0	-3.907021	1.937999	-4.727153
67	1	0	-4.349442	-0.356821	-4.078518
68	14	0	-0.196101	0.242622	-3.669586
69	1	0	-0.056082	1.142396	-4.870640
70	1	0	-0.481524	-1.142121	-4.178585
71	14	0	-4.720516	-2.845223	-1.573560
72	1	0	-4.696789	-2.448075	-3.022388
73	1	0	-4.992812	-4.327165	-1.516078
74	14	0	-0.826082	-3.559724	-1.652861
75	1	0	-0.784507	-3.194444	-3.110123
76	1	0	-1.094579	-5.041001	-1.571910
77	14	0	3.664152	-0.511775	-3.790015
78	1	0	3.382029	-1.899161	-4.292391

79	1	0	3.783767	0.387697	-4.993766
80	14	0	3.053090	-4.310891	-1.716521
81	1	0	2.765010	-5.787533	-1.622806
82	1	0	3.108975	-3.955943	-3.175449
83	14	0	-6.672574	-2.810066	1.742262
84	1	0	-7.661470	-2.067927	2.605959
85	1	0	-7.254516	-4.176168	1.477083
86	14	0	-2.798370	-3.671136	1.544284
87	1	0	-3.111689	-5.047554	1.044217
88	14	0	1.106671	-4.364055	1.482680
89	1	0	0.919627	-5.768560	0.997363
90	14	0	5.039511	-4.907133	1.533215
91	1	0	5.097812	-6.397817	1.309854
92	1	0	6.261178	-4.532796	2.334579
93	14	0	2.326927	2.680558	-2.328529
94	1	0	2.349737	3.072191	-3.773319
95	14	0	6.245746	1.915549	-2.326120
96	1	0	7.453731	2.084782	-1.439062
97	1	0	6.625758	2.427892	-3.693018
98	14	0	-1.539630	3.425260	-2.156011
99	1	0	-1.546119	3.853780	-3.590604
100	14	0	-5.439184	4.162280	-1.811034
101	1	0	-5.703445	4.862818	-3.120638
102	1	0	-6.430693	4.705245	-0.812567
103	6	0	4.991378	5.722230	2.874242
104	1	0	4.277864	6.554860	2.934404
105	1	0	5.077417	5.469828	1.808996
106	6	0	6.354544	6.173764	3.407676
107	1	0	7.097188	5.371798	3.328706
108	1	0	6.734824	7.034751	2.848655
109	1	0	6.291698	6.463383	4.462732
110	15	0	2.330410	2.645412	4.079591
111	1	0	3.307670	1.672566	3.723006

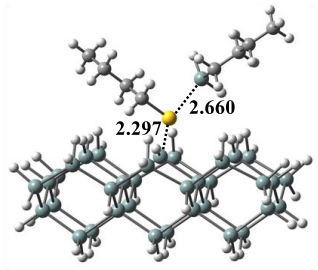
11



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.370700	-0.499047	0.000017
2	1	0	2.354005	-1.158975	0.877076
3	1	0	2.354017	-1.158816	-0.877162

4	6	0	3.661229	0.343450	0.000102
5	1	0	3.673397	1.004658	-0.877263
6	1	0	3.673378	1.004516	0.877573
7	6	0	4.938289	-0.508771	0.000048
8	1	0	4.928494	-1.169413	0.877319
9	1	0	4.928507	-1.169282	-0.877323
10	16	0	-0.899425	-0.802619	-0.000095
11	6	0	-2.305304	0.411479	0.000005
12	1	0	-2.220456	1.047236	0.886774
13	1	0	-2.220407	1.047439	-0.886613
14	6	0	-3.643661	-0.329082	-0.000115
15	1	0	-3.695479	-0.983845	0.878799
16	1	0	-3.695428	-0.983650	-0.879179
17	6	0	-4.842423	0.629938	-0.000044
18	1	0	-4.782683	1.287205	0.877787
19	1	0	-4.782633	1.287397	-0.877728
20	6	0	-6.188216	-0.101394	-0.000163
21	1	0	-6.291811	-0.740719	0.883529
22	1	0	-7.024793	0.604478	-0.000111
23	1	0	-6.291759	-0.740527	-0.883999
24	14	0	0.790834	0.537660	0.000101
25	1	0	0.742234	1.425105	1.198050
26	1	0	0.742289	1.425383	-1.197645
27	6	0	6.220928	0.327830	0.000120
28	1	0	6.273271	0.973665	0.883921
29	1	0	7.112439	-0.307409	0.000080
30	1	0	6.273286	0.973795	-0.883586

11-TS1



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-3.804005	-4.287744	-1.151496
2	14	0	-1.518987	-1.269566	-2.505243
3	14	0	-5.401621	-1.123497	-3.031673
4	14	0	3.947860	-4.496681	0.042826

5	14	0	0.088523	-4.497060	-0.697140
6	14	0	2.364202	-1.405236	-1.953283
7	14	0	-3.830009	4.215837	1.509327
8	14	0	-3.817632	-0.079619	0.353459
9	14	0	-5.460606	2.691771	-1.823041
10	14	0	-1.574603	2.564250	-1.377088
11	14	0	-1.715209	0.267978	-0.670926
12	14	0	3.943251	4.072244	2.430661
13	14	0	0.070585	4.305719	1.891800
14	14	0	3.901793	-0.248823	1.388664
15	14	0	2.347525	2.447797	-0.889257
16	14	0	6.223396	2.343208	-0.366222
17	14	0	6.011409	0.072059	0.366594
18	14	0	0.024496	0.022051	0.918457
19	14	0	2.151912	0.162054	-0.147905
20	14	0	-5.560883	0.386726	-1.178441
21	1	0	-3.865713	-5.775804	-1.239271
22	1	0	-3.939365	-3.922272	0.283782
23	1	0	-6.497025	-0.797684	-4.018705
24	1	0	3.932630	-5.988452	0.030803
25	1	0	3.687801	-4.066374	1.443690
26	1	0	0.071063	-5.977382	-0.893963
27	1	0	-0.120778	-4.233382	0.748900
28	1	0	-3.910500	3.079282	2.466783
29	1	0	-3.904151	5.472819	2.309542
30	1	0	-3.926049	-1.491507	0.810559
31	1	0	-3.952703	0.790785	1.554295
32	1	0	-6.582943	2.976276	-2.792444
33	1	0	3.740271	2.963319	3.402663
34	1	0	3.888373	5.348632	3.201070
35	1	0	-0.078990	3.313691	2.991620
36	1	0	0.025452	5.658833	2.523292
37	1	0	3.812803	-1.648424	1.889485
38	1	0	3.761437	0.645835	2.572396
39	1	0	7.564818	2.510570	-1.039104
40	1	0	7.098089	-0.191629	1.384037
41	1	0	-0.044774	1.250432	1.765505
42	1	0	-6.892285	0.151891	-0.501753
43	16	0	-0.538770	-1.644245	2.395947
44	6	0	0.605555	-1.220868	3.807643
45	1	0	-0.020956	-0.857337	4.627175
46	1	0	1.233337	-0.385960	3.484349
47	6	0	1.465260	-2.406177	4.247012
48	1	0	0.816255	-3.244275	4.528441

49	1	0	2.066831	-2.751609	3.397820
50	6	0	2.383454	-2.047325	5.425468
51	1	0	3.032710	-1.209128	5.138837
52	1	0	1.774470	-1.688537	6.266244
53	6	0	3.245072	-3.228416	5.884119
54	1	0	3.892651	-2.946036	6.720247
55	1	0	2.623381	-4.068611	6.212814
56	1	0	3.886600	-3.588743	5.072404
57	6	0	-3.380391	-1.420807	4.789854
58	1	0	-2.759662	-0.998018	5.591443
59	1	0	-3.539543	-0.606713	4.070921
60	6	0	-4.734196	-1.882056	5.369405
61	1	0	-4.574638	-2.703104	6.081441
62	1	0	-5.357328	-2.295051	4.564858
63	6	0	-5.503449	-0.751952	6.071622
64	1	0	-4.882400	-0.343453	6.880309
65	1	0	-5.658574	0.071473	5.361502
66	14	0	-3.276946	-0.960111	-4.114284
67	1	0	-3.124543	0.333074	-4.863601
68	1	0	-3.166570	-2.077715	-5.119649
69	14	0	-5.652170	-3.406886	-2.353091
70	1	0	-6.907985	-3.564729	-1.533031
71	1	0	-5.838515	-4.222468	-3.608220
72	14	0	-1.693975	-3.598306	-1.970727
73	1	0	-1.568407	-4.225901	-3.324531
74	14	0	2.220420	-3.725256	-1.377530
75	1	0	2.474888	-4.380733	-2.699847
76	14	0	6.121359	-3.782617	-0.594961
77	1	0	6.605442	-4.676478	-1.709477
78	1	0	7.071344	-3.966855	0.562004
79	14	0	6.245271	-1.529351	-1.401183
80	1	0	7.590720	-1.337376	-2.059352
81	14	0	6.104765	3.877020	1.469281
82	1	0	7.100411	3.487147	2.532747
83	1	0	6.518537	5.230887	0.948898
84	14	0	2.185488	4.093354	0.847133
85	1	0	2.362223	5.367839	0.080768
86	14	0	-1.750668	4.182614	0.382602
87	1	0	-1.695921	5.470028	-0.380685
88	14	0	-5.708952	4.152528	0.060122
89	1	0	-5.938050	5.542164	-0.479907
90	1	0	-6.940811	3.774740	0.843999
91	14	0	-3.364846	3.211659	-2.847871
92	1	0	-3.275440	4.704541	-3.034899

93	1	0	-3.237507	2.579771	-4.204861
94	14	0	4.479867	2.945830	-1.886896
95	1	0	4.643210	2.274517	-3.220851
96	1	0	4.542901	4.434103	-2.119041
97	14	0	4.512117	-1.270346	-3.024881
98	1	0	4.595181	-2.411785	-4.005662
99	1	0	4.668703	0.003907	-3.805273
100	14	0	0.622287	-1.110263	-3.575330
101	1	0	0.721408	-2.234327	-4.574312
102	1	0	0.779388	0.177455	-4.333319
103	14	0	0.556748	3.055634	-2.373149
104	1	0	0.700995	2.410652	-3.722693
105	1	0	0.626156	4.546977	-2.580673
106	14	0	-2.394234	-2.790792	3.917846
107	1	0	-3.185592	-3.399415	2.813509
108	1	0	-2.030901	-3.878052	4.883431
109	6	0	-6.853294	-1.204458	6.637577
110	1	0	-7.377509	-0.378436	7.129251
111	1	0	-7.506530	-1.587934	5.845502
112	1	0	-6.726552	-2.004202	7.376202

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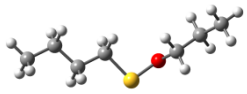

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-0.028218	-1.280695	-0.211072
2	8	0	-1.491013	-0.809255	0.498734
3	6	0	2.500741	-0.195951	-0.157348
4	1	0	2.502277	-0.273196	-1.252545
5	1	0	2.843388	-1.166588	0.224286
6	6	0	3.487861	0.897761	0.275894
7	1	0	3.482968	0.975535	1.370994
8	1	0	3.140250	1.868581	-0.101421
9	6	0	4.915230	0.638482	-0.214463
10	1	0	5.596229	1.432834	0.107033
11	1	0	5.302595	-0.309655	0.174829
12	1	0	4.955715	0.587839	-1.308254
13	6	0	1.075717	0.074772	0.337526
14	1	0	1.042781	0.119830	1.430466
15	1	0	0.706661	1.026065	-0.060347

16	6	0	-2.317910	0.029646	-0.327373
17	1	0	-2.541365	-0.479326	-1.274638
18	1	0	-1.792220	0.965391	-0.567305
19	6	0	-3.594912	0.316958	0.450997
20	1	0	-3.327936	0.798265	1.399011
21	1	0	-4.069390	-0.637545	0.706023
22	6	0	-4.566981	1.200054	-0.338051
23	1	0	-4.868076	0.723222	-1.277392
24	1	0	-5.474965	1.395403	0.239999
25	1	0	-4.117806	2.168170	-0.586562

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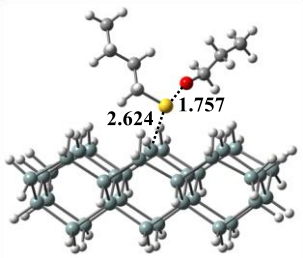

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-4.021070	-4.128170	-0.800731
2	14	0	-1.822731	-1.114037	-2.293221
3	14	0	-5.729533	-0.891464	-2.455837
4	14	0	6.008350	-1.574362	-1.899198
5	14	0	3.797896	-4.589599	-0.451401
6	14	0	-0.103359	-4.335042	-0.650648
7	14	0	2.105194	-1.343802	-2.122145
8	14	0	-3.678386	4.274115	2.082104
9	14	0	-3.837109	0.033293	0.800806
10	14	0	-5.569795	2.901709	-1.175799
11	14	0	-1.665986	2.662984	-1.008533
12	14	0	-1.815633	0.342864	-0.388255
13	14	0	4.130022	3.788788	2.484003
14	14	0	0.238510	4.145811	2.225042
15	14	0	3.908984	-0.443305	1.157328
16	14	0	2.276492	2.435773	-0.819127
17	14	0	6.172308	2.200382	-0.574920
18	14	0	5.947618	-0.115126	0.000364
19	14	0	0.036326	-0.119133	1.009291
20	14	0	2.069507	0.110805	-0.218636
21	14	0	-5.686126	0.586304	-0.570606

22	1	0	-4.119322	-5.612454	-0.917691
23	1	0	-4.016222	-3.806595	0.652933
24	1	0	-6.908296	-0.537780	-3.331162
25	1	0	7.300222	-1.346184	-2.647326
26	1	0	3.731387	-6.075187	-0.573640
27	1	0	3.693645	-4.265405	0.997848
28	1	0	-0.188981	-5.825377	-0.699584
29	1	0	-0.139706	-3.936576	0.781831
30	1	0	-3.745144	3.116598	3.014378
31	1	0	-3.653904	5.511817	2.914917
32	1	0	-3.962204	-1.388116	1.227068
33	1	0	-3.843571	0.873584	2.027938
34	1	0	-6.749445	3.236909	-2.057168
35	1	0	3.957351	2.626427	3.397533
36	1	0	4.169576	5.014146	3.334244
37	1	0	0.125409	3.065599	3.242450
38	1	0	0.280965	5.439862	2.970451
39	1	0	3.802231	-1.865175	1.593310
40	1	0	3.886897	0.386484	2.394925
41	1	0	7.471264	2.387231	-1.322286
42	1	0	7.102404	-0.483245	0.904267
43	1	0	0.088172	1.014334	1.984281
44	1	0	-6.966176	0.375809	0.206425
45	16	0	-0.842707	-1.792946	2.829253
46	6	0	0.545691	-1.508975	3.998887
47	1	0	0.382117	-0.530687	4.462263
48	1	0	1.443342	-1.442889	3.376502
49	6	0	0.684337	-2.612922	5.046631
50	1	0	-0.253056	-2.688415	5.608030
51	1	0	0.838410	-3.575404	4.543002
52	6	0	1.844958	-2.343227	6.017099
53	1	0	2.781644	-2.251904	5.451109
54	1	0	1.688954	-1.374463	6.509814
55	6	0	1.991729	-3.439679	7.077031
56	1	0	2.821933	-3.224773	7.757060
57	1	0	1.081556	-3.531325	7.680120
58	1	0	2.183073	-4.414688	6.615170
59	6	0	-2.949447	-2.885217	4.065641
60	1	0	-3.434642	-3.009501	3.087521
61	1	0	-2.362925	-3.793295	4.266969
62	6	0	-3.998628	-2.665145	5.149760
63	1	0	-3.488497	-2.507950	6.107445
64	1	0	-4.541522	-1.739485	4.927120
65	14	0	4.157106	-1.192093	-3.363685

66	1	0	4.139735	-2.282783	-4.404198
67	1	0	4.281070	0.117704	-4.089365
68	14	0	0.216342	-0.960719	-3.554860
69	1	0	0.195534	-2.051440	-4.594998
70	1	0	0.325070	0.349011	-4.283828
71	14	0	4.349739	2.944860	-1.930928
72	1	0	4.404568	2.348565	-3.308955
73	1	0	4.443271	4.442043	-2.082191
74	14	0	0.399603	3.150557	-2.137837
75	1	0	0.430716	2.554725	-3.517352
76	1	0	0.490411	4.646982	-2.295888
77	14	0	-3.713186	-0.747442	-3.731162
78	1	0	-3.610737	0.555662	-4.472191
79	1	0	-3.716544	-1.850207	-4.758837
80	14	0	-3.536595	3.398968	-2.329754
81	1	0	-3.425603	4.894053	-2.487056
82	1	0	-3.519799	2.799193	-3.707437
83	14	0	6.217079	3.596769	1.370008
84	1	0	7.264139	3.101260	2.335893
85	1	0	6.645360	4.971982	0.921781
86	14	0	2.273428	3.962727	1.027977
87	1	0	2.435821	5.283654	0.341118
88	14	0	-1.672962	4.199783	0.829308
89	1	0	-1.598880	5.521897	0.129448
90	14	0	-5.645254	4.320511	0.753131
91	1	0	-5.854917	5.731248	0.261688
92	1	0	-6.839259	3.968327	1.604730
93	14	0	-1.980452	-3.448288	-1.785930
94	1	0	-1.967621	-4.078928	-3.143821
95	14	0	-5.960193	-3.181997	-1.792441
96	1	0	-7.128097	-3.333069	-0.849913
97	1	0	-6.290263	-3.973428	-3.033582
98	14	0	1.952162	-3.678930	-1.618443
99	1	0	1.986972	-4.310435	-2.975474
100	14	0	5.915786	-3.879333	-1.254846
101	1	0	6.259430	-4.697324	-2.474780
102	1	0	6.970907	-4.169362	-0.216930
103	6	0	-4.974249	-3.842832	5.255260
104	1	0	-4.453320	-4.774579	5.502417
105	1	0	-5.719074	-3.662687	6.036066
106	1	0	-5.511979	-4.002153	4.314111
107	8	0	-2.094251	-1.730621	4.060716

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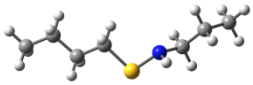

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.511104	-0.098021	-0.340517
2	1	0	2.862605	-0.895934	-1.016406
3	1	0	2.094698	0.690894	-0.976702
4	6	0	3.692389	0.449003	0.464440
5	1	0	3.332217	1.254725	1.114568
6	1	0	4.072616	-0.339285	1.129661
7	6	0	4.830194	0.952028	-0.428887
8	1	0	5.663282	1.333214	0.169541
9	1	0	5.219046	0.152123	-1.068682
10	1	0	4.492312	1.763870	-1.082503
11	16	0	0.001428	-1.139156	-0.200635
12	6	0	-1.212010	0.105444	0.398837
13	1	0	-1.234054	0.065769	1.492198
14	1	0	-0.860239	1.097918	0.100403
15	6	0	-2.595176	-0.184359	-0.188541
16	1	0	-2.906129	-1.201130	0.086229
17	1	0	-2.540257	-0.163212	-1.284890
18	6	0	-3.657080	0.817261	0.287755
19	1	0	-3.711917	0.792832	1.384189
20	1	0	-3.340599	1.834404	0.020945
21	6	0	-5.043620	0.541350	-0.301269
22	1	0	-5.400582	-0.456891	-0.024038
23	1	0	-5.780180	1.268690	0.054937
24	1	0	-5.026535	0.593469	-1.395664
25	7	0	1.442662	-0.543825	0.564401
26	1	0	1.787419	-1.254418	1.204666

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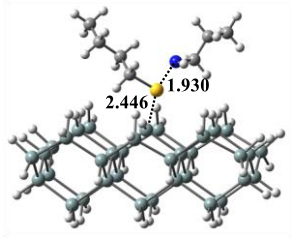

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	14	0	-4.138267	-4.096911	-0.754942
2	14	0	-1.948833	-1.048481	-2.202873
3	14	0	-5.861564	-0.801433	-2.259209
4	14	0	5.882201	-1.546039	-2.045468
5	14	0	3.689869	-4.542928	-0.513921
6	14	0	-0.221442	-4.337217	-0.694724
7	14	0	1.973282	-1.297620	-2.135979
8	14	0	-3.628818	4.221475	2.359374
9	14	0	-3.862943	0.010067	0.961032
10	14	0	-5.671361	2.939786	-0.843884
11	14	0	-1.764822	2.704887	-0.857026
12	14	0	-1.878932	0.373173	-0.272416
13	14	0	4.192332	3.850644	2.366921
14	14	0	0.293943	4.194417	2.294816
15	14	0	3.905098	-0.386763	1.070103
16	14	0	2.184103	2.478318	-0.843009
17	14	0	6.087611	2.251420	-0.777778
18	14	0	5.894380	-0.058304	-0.169071
19	14	0	0.018016	-0.042729	1.085621
20	14	0	2.004966	0.154999	-0.228457
21	14	0	-5.762435	0.603604	-0.320321
22	1	0	-4.244349	-5.576498	-0.915564
23	1	0	-4.107545	-3.818117	0.706811
24	1	0	-7.057884	-0.401646	-3.089615
25	1	0	7.149359	-1.340079	-2.840676
26	1	0	3.622529	-6.029482	-0.623329
27	1	0	3.613937	-4.206974	0.934291
28	1	0	-0.309057	-5.821778	-0.833263
29	1	0	-0.243658	-4.021143	0.757059
30	1	0	-3.636281	3.027198	3.247868
31	1	0	-3.577877	5.424130	3.240832
32	1	0	-3.962978	-1.426857	1.341217
33	1	0	-3.834626	0.793366	2.228016
34	1	0	-6.890061	3.302685	-1.658542
35	1	0	4.068564	2.693173	3.294467
36	1	0	4.265425	5.081633	3.206747
37	1	0	0.242028	3.133811	3.337843
38	1	0	0.360929	5.502403	3.013835
39	1	0	3.823913	-1.806602	1.515997
40	1	0	3.931986	0.449176	2.303824
41	1	0	7.349573	2.433831	-1.586946
42	1	0	7.083590	-0.409236	0.696207
43	1	0	0.094454	1.154877	1.978867
44	1	0	-7.012114	0.357371	0.494426

45	16	0	-0.555891	-1.708820	2.781952
46	6	0	0.875878	-1.396061	3.910709
47	1	0	0.506098	-0.746352	4.709440
48	1	0	1.623232	-0.838273	3.340649
49	6	0	1.467756	-2.686764	4.474159
50	1	0	0.665930	-3.260193	4.951428
51	1	0	1.857544	-3.297597	3.650262
52	6	0	2.585499	-2.412703	5.491938
53	1	0	3.376541	-1.815739	5.018196
54	1	0	2.187411	-1.798590	6.310740
55	6	0	3.189566	-3.699359	6.064201
56	1	0	3.979557	-3.479724	6.789428
57	1	0	2.427982	-4.301555	6.572080
58	1	0	3.626626	-4.317875	5.272334
59	6	0	-2.638460	-3.256178	3.908628
60	1	0	-3.305864	-2.993217	3.072656
61	1	0	-2.051182	-4.124569	3.588798
62	6	0	-3.488696	-3.626972	5.132538
63	1	0	-2.819943	-3.892320	5.959339
64	1	0	-4.053900	-2.743727	5.460193
65	14	0	3.984466	-1.156667	-3.445479
66	1	0	3.923846	-2.246296	-4.485308
67	1	0	4.091058	0.153014	-4.174223
68	14	0	0.054308	-0.883906	-3.516958
69	1	0	0.000507	-1.958600	-4.572273
70	1	0	0.151696	0.436347	-4.228213
71	14	0	4.202421	2.988836	-2.049723
72	1	0	4.195598	2.390871	-3.428094
73	1	0	4.285929	4.485989	-2.207224
74	14	0	0.249960	3.210893	-2.067055
75	1	0	0.217940	2.640495	-3.457198
76	1	0	0.333441	4.710081	-2.200880
77	14	0	-3.874817	-0.625889	-3.577228
78	1	0	-3.783152	0.698309	-4.281065
79	1	0	-3.911462	-1.697146	-4.636968
80	14	0	-3.692391	3.473966	-2.072964
81	1	0	-3.588874	4.973178	-2.189488
82	1	0	-3.740005	2.916253	-3.467264
83	14	0	6.224372	3.660265	1.154987
84	1	0	7.317846	3.172246	2.071930
85	1	0	6.626076	5.034300	0.679492
86	14	0	2.268150	4.009162	0.999372
87	1	0	2.391105	5.329045	0.302320
88	14	0	-1.691142	4.214138	1.002952

89	1	0	-1.686420	5.547077	0.320098
90	14	0	-5.661006	4.291342	1.133209
91	1	0	-5.906319	5.715690	0.701444
92	1	0	-6.807600	3.898917	2.031214
93	14	0	-2.113786	-3.395448	-1.758364
94	1	0	-2.137129	-3.977173	-3.137830
95	14	0	-6.092035	-3.114520	-1.680015
96	1	0	-7.245761	-3.296983	-0.725651
97	1	0	-6.445105	-3.854941	-2.945919
98	14	0	1.825020	-3.638219	-1.654465
99	1	0	1.859345	-4.248828	-3.021215
100	14	0	5.792039	-3.841612	-1.366691
101	1	0	6.110763	-4.675934	-2.582412
102	1	0	6.867580	-4.120059	-0.346670
103	6	0	-4.458479	-4.777636	4.841435
104	1	0	-3.920554	-5.684466	4.543863
105	1	0	-5.056220	-5.020626	5.725333
106	1	0	-5.150011	-4.520865	4.031437
107	7	0	-1.698012	-2.186964	4.262187
108	1	0	-2.229264	-1.335395	4.461548
