Electronic Supplementary Material (ESI) for Polymer Chemistry.

Supporting Information

Effect of polycyclosilane microstructure on thermal properties

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1. Supplemental Figures

Figure S1. ^{29}Si INEPT+ NMR spectrum (79 MHz, Benzene-d_6) of *lin*-poly(**1,3Si$_6$**). The family of doublets (δ -109.8 to -117.0, $^1J_{SiH}$ = 160.1 Hz) were assigned to *Si*H internal resonances. The triplet (δ -97.3, $^1J_{SiH}$ = 172.3 Hz) was assigned to *Si*H$_2$ end groups, consistent with assignment of *lin*-poly(**1,3Si$_6$**) to a linear polymer of **1,3Si6**. The experimentally measured coupling constants were consistent with typical one-bond coupling constants between silicon and proton.

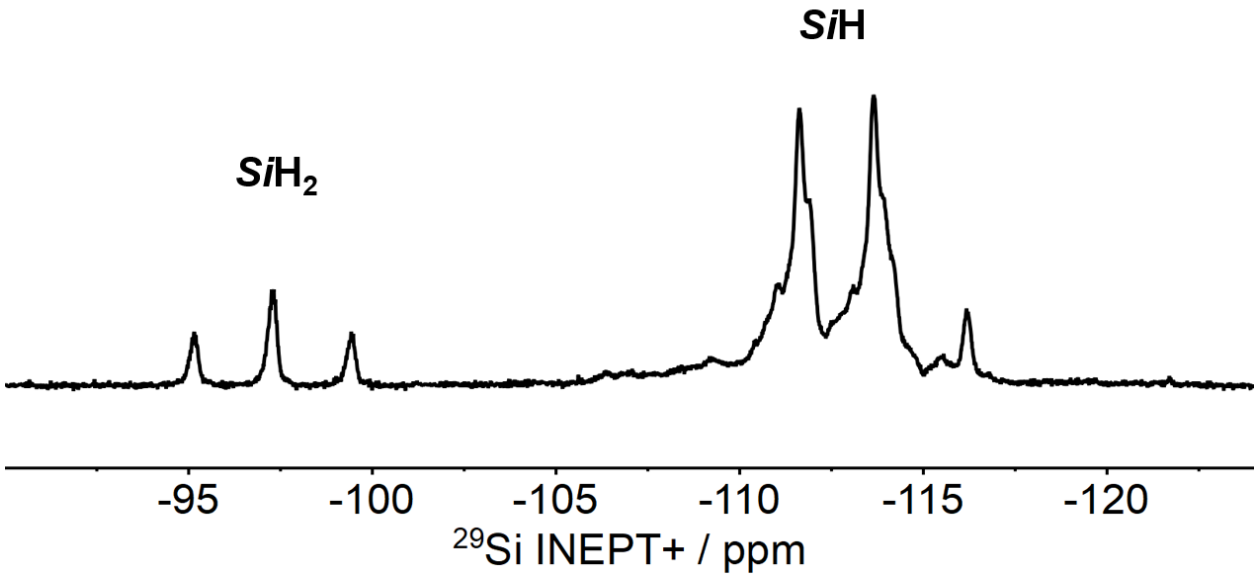


Figure S2. The second cooling cycle of DSC measurement of *lin*-poly(**1,3Si$_6$**). Cooling rate: 3 °C min^{-1}. No phase transition was observed.

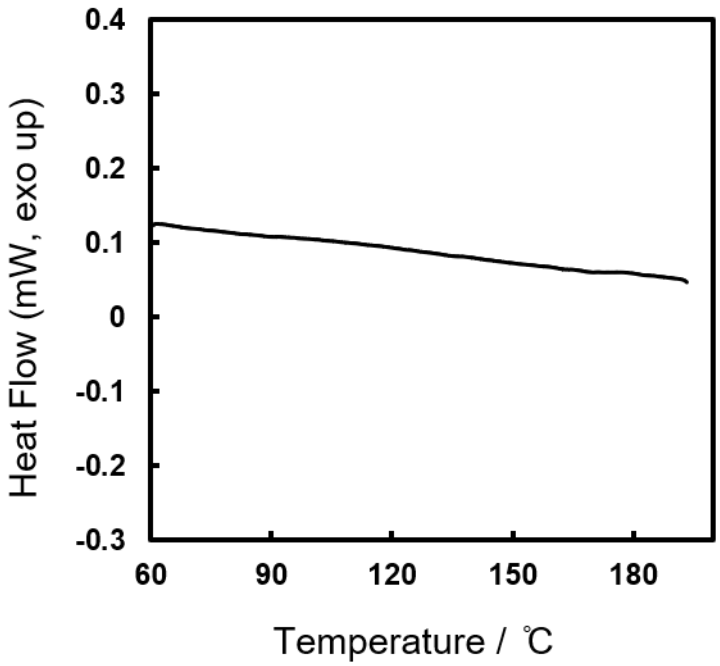
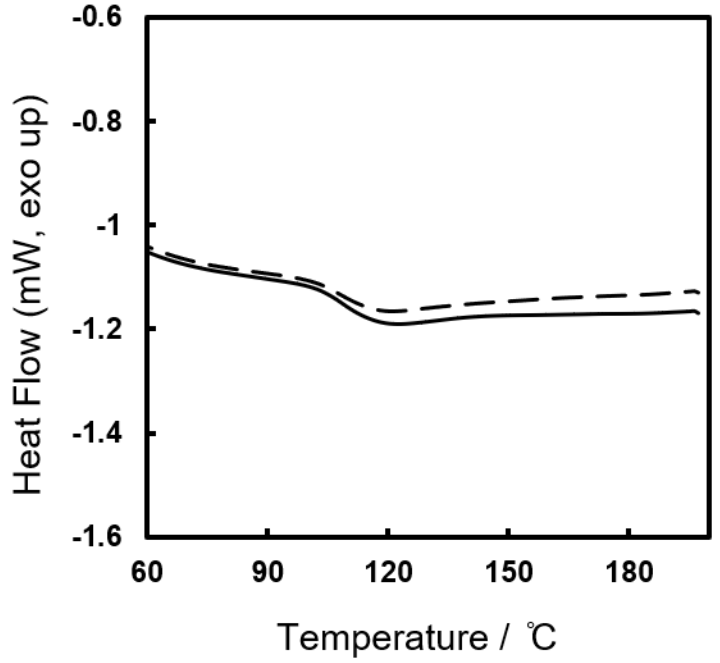


Figure S3. The overlay of the second (solid line) and third (dotted line) heating cycle of DSC measurement of *lin*-poly(**1,3Si$_6$**). Heating rate: 20 °C min^{-1}.



NMR Spectra

Figure S4. ^{1}H NMR Spectrum (400 MHz, Benzene-d_6) of *lin*-poly(**1,3Si$_6$**).

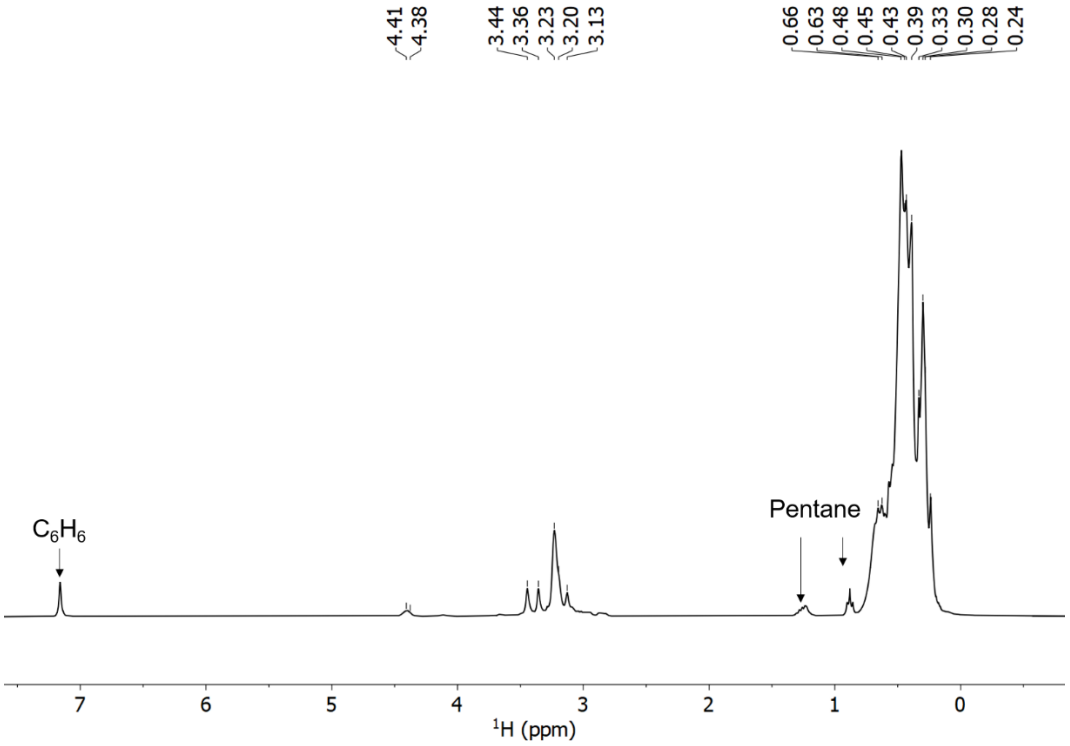


Figure S5. ^{29}Si {^{1}H} NMR Spectrum (79 MHz, Benzene-d_6) of *lin*-poly(**1,3Si$_6$**). $^{1}J_{Si\text{-}H}$ = 120 Hz.

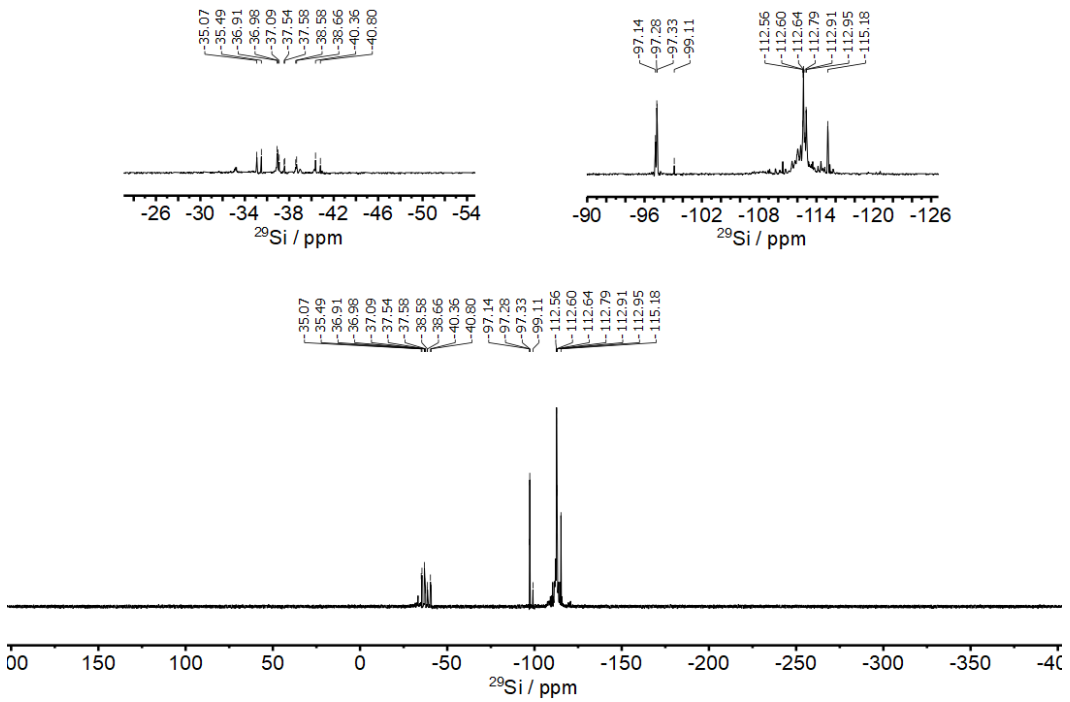


Figure S6. ^{13}C {^{1}H} NMR Spectrum (101 MHz, Benzene-d_6) of *lin*-poly(**1,3Si$_6$**).

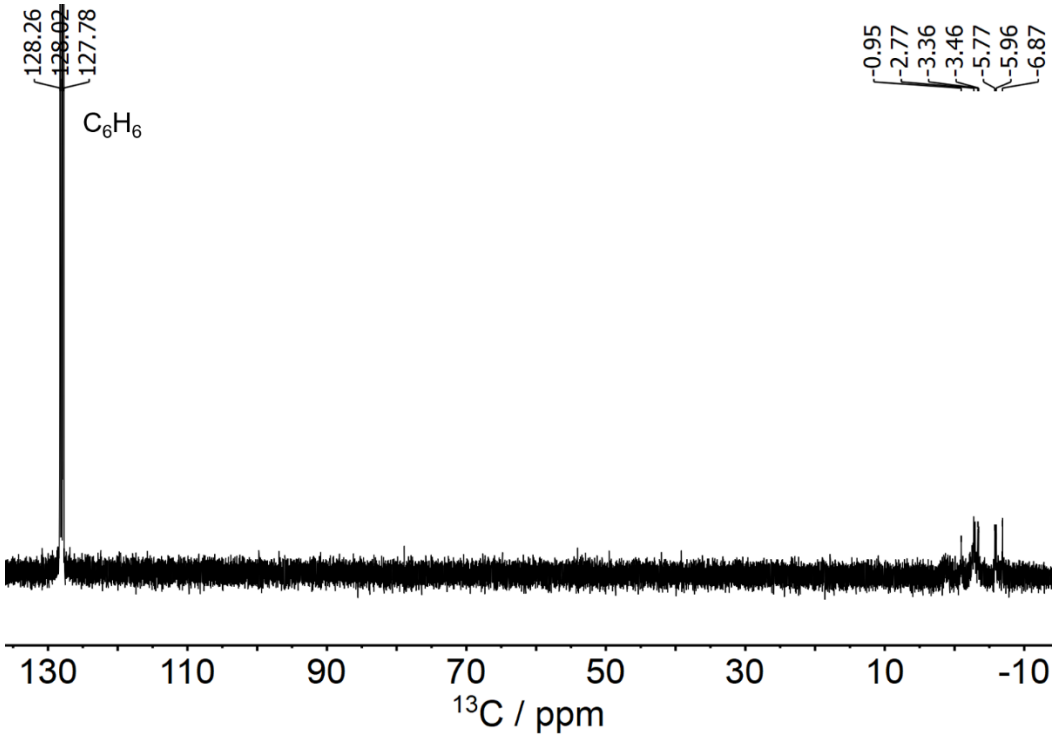


Figure S7. ^{1}H- ^{29}Si HSQC NMR spectrum (400 MHz, Benzene-d_6) of *lin*-poly(**1,3Si$_6$**). $^{1}J_{Si\text{-}H}$ = 120 Hz.

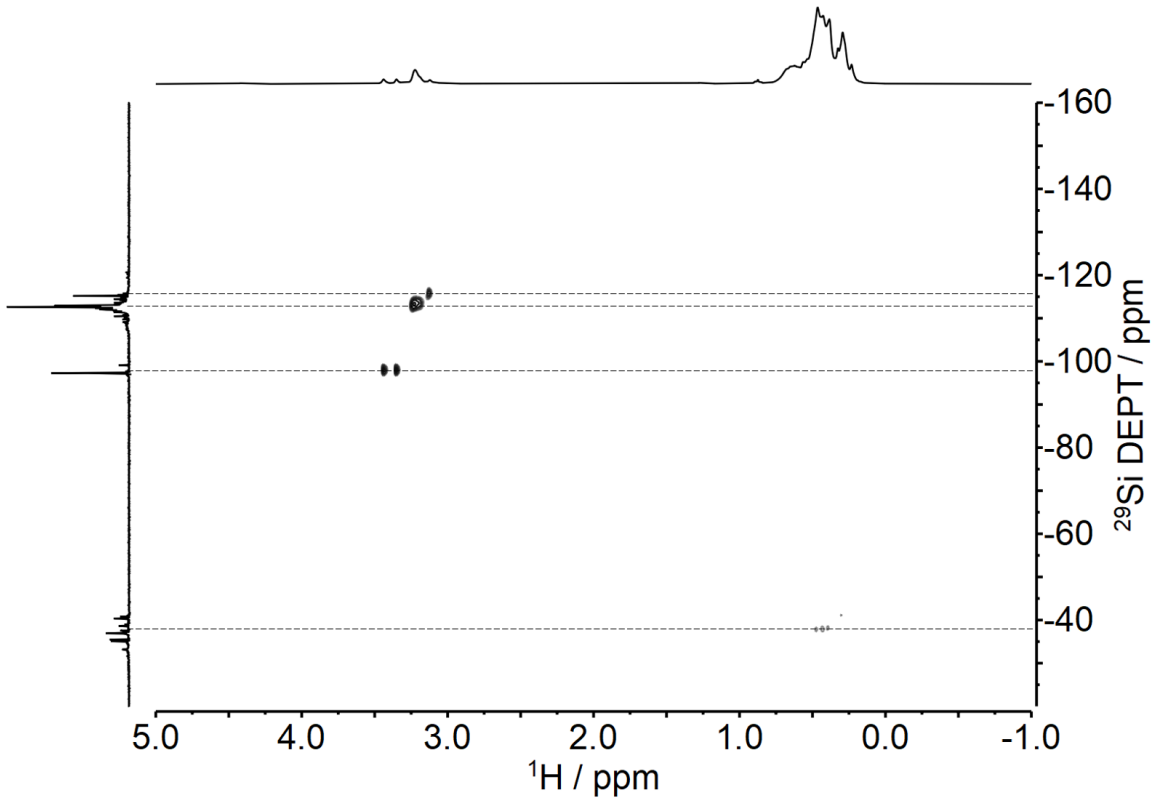


Figure S8. ^{1}H NMR Spectrum (400 MHz, Benzene-d_6) of *cyc*-poly(**1,3Si$_6$**) (Cp_2ZrMe_2 synthesis).

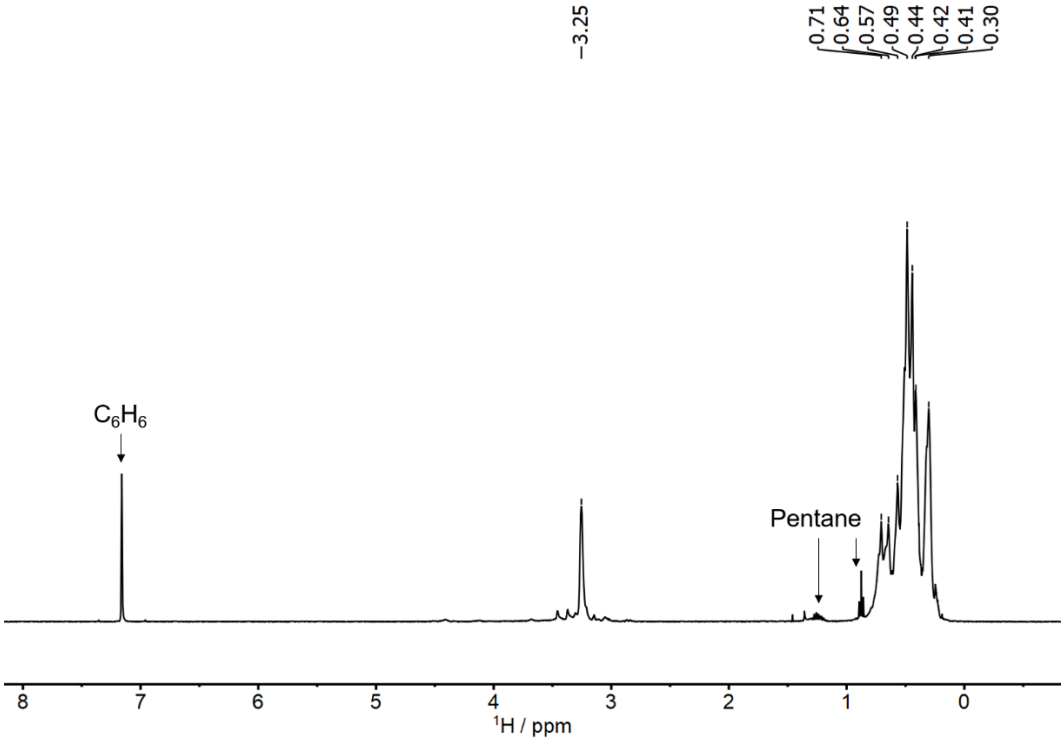


Figure S9. ^{29}Si {^{1}H} NMR Spectrum (79 MHz, Benzene-d_6) of *cyc*-poly(**1,3Si$_6$**) (Cp_2ZrMe_2 synthesis). $^{1}J_{Si\text{-}H}$ = 120 Hz.

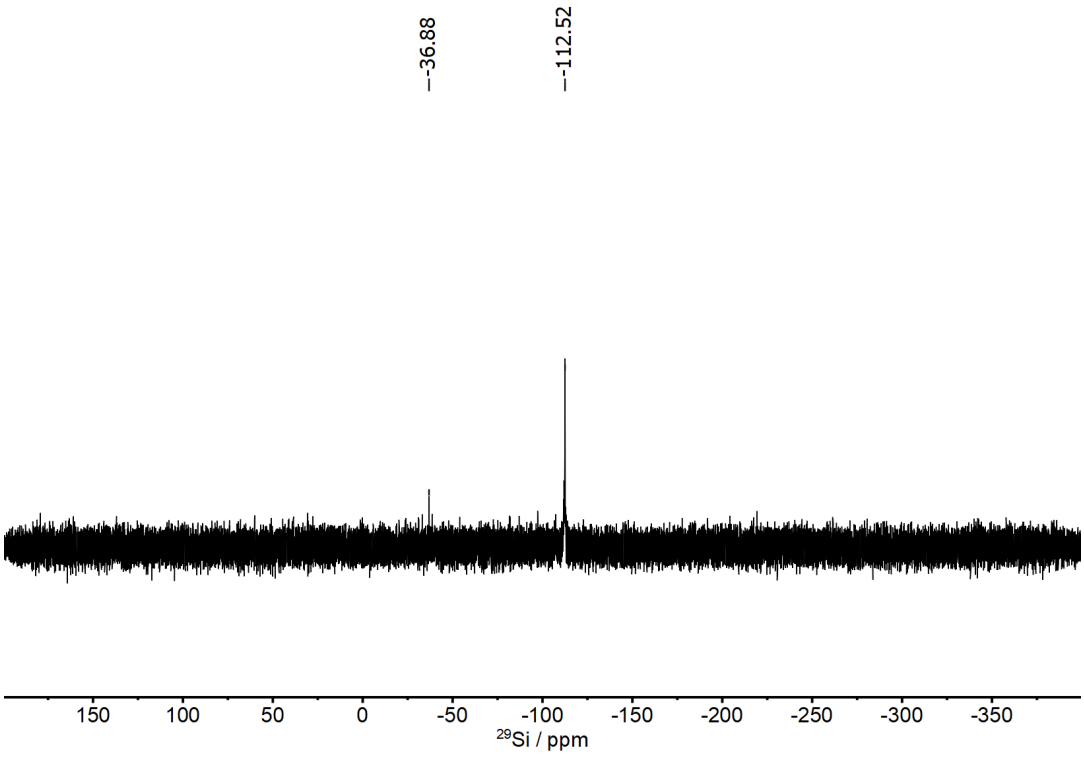


Figure S10. ^{1}H NMR Spectrum (400 MHz, Benzene-d_6) of *lin*-poly(**1,4Si$_6$**).

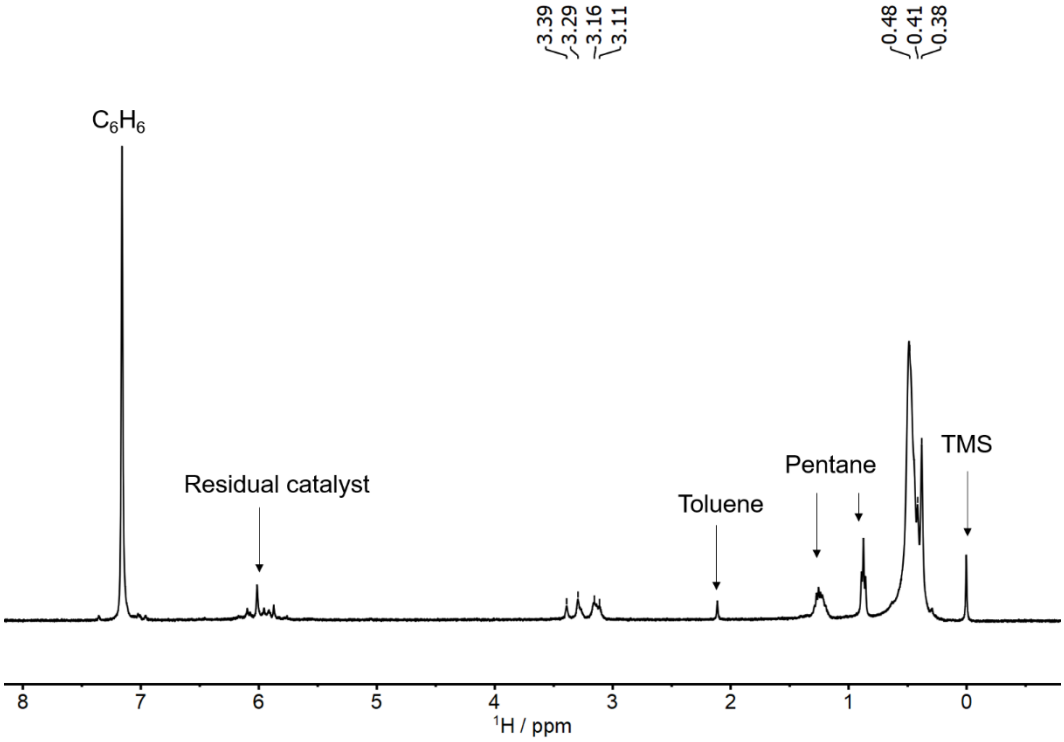


Figure S11. ^{29}Si {^{1}H} NMR Spectrum (79 MHz, Benzene-d_6) of *lin*-poly(**1,4Si$_6$**). $^{1}J_{Si-H}$ = 120 Hz.

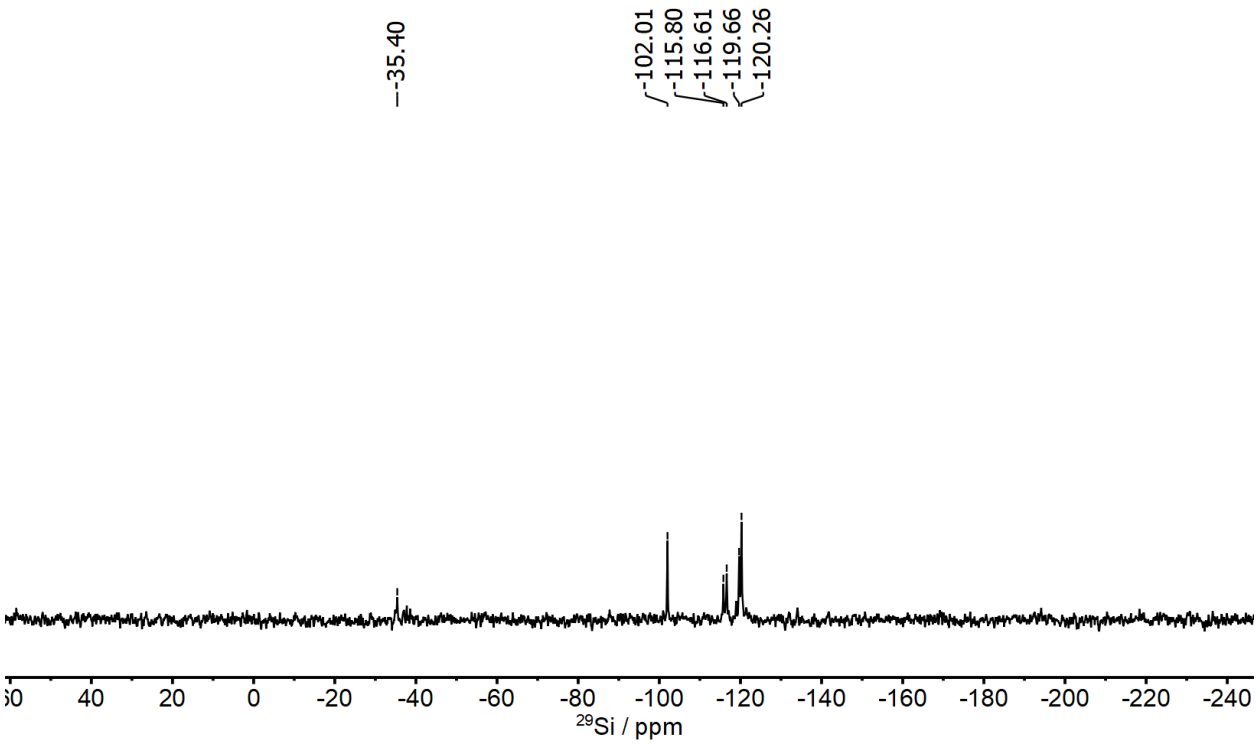


Figure S12. ^{1}H NMR Spectrum (400 MHz, Benzene-d_6) of *cyc*-poly(**1,3Si$_6$**) (Cp_2ZrCl_2 synthesis).

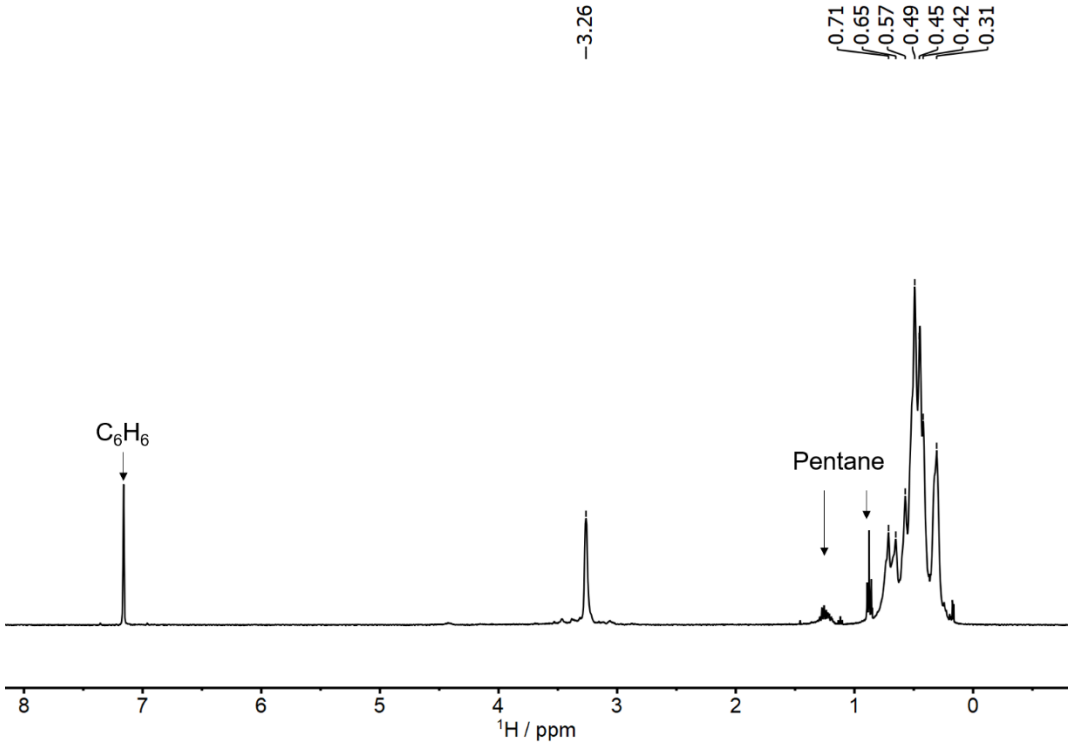
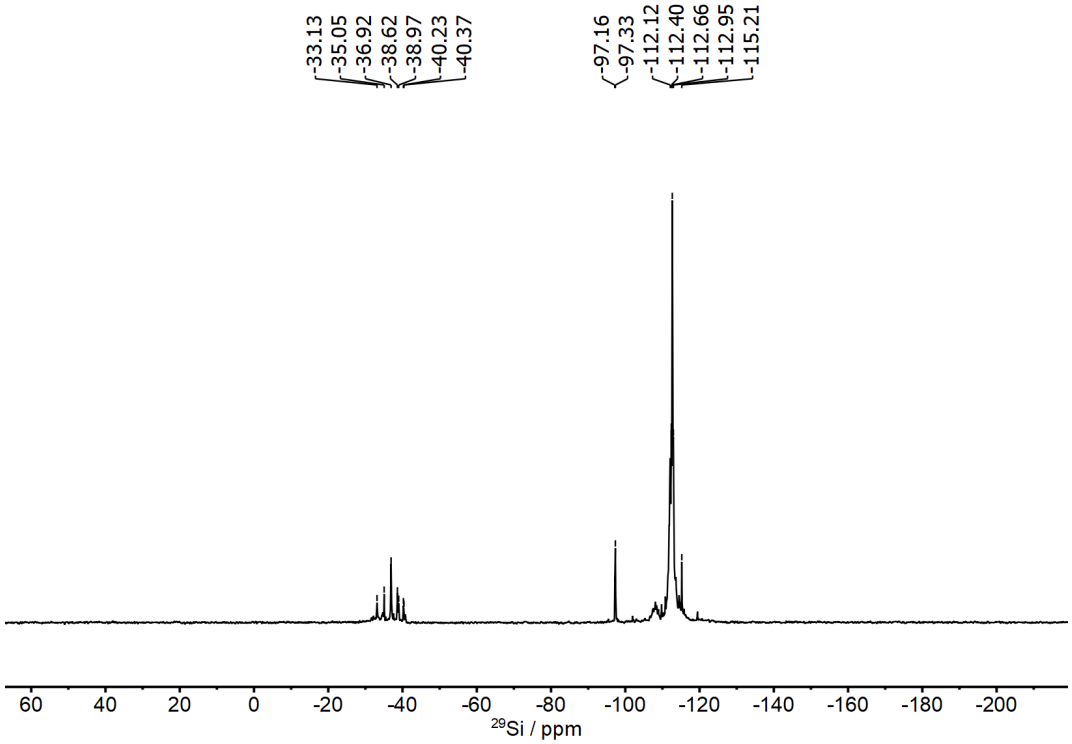
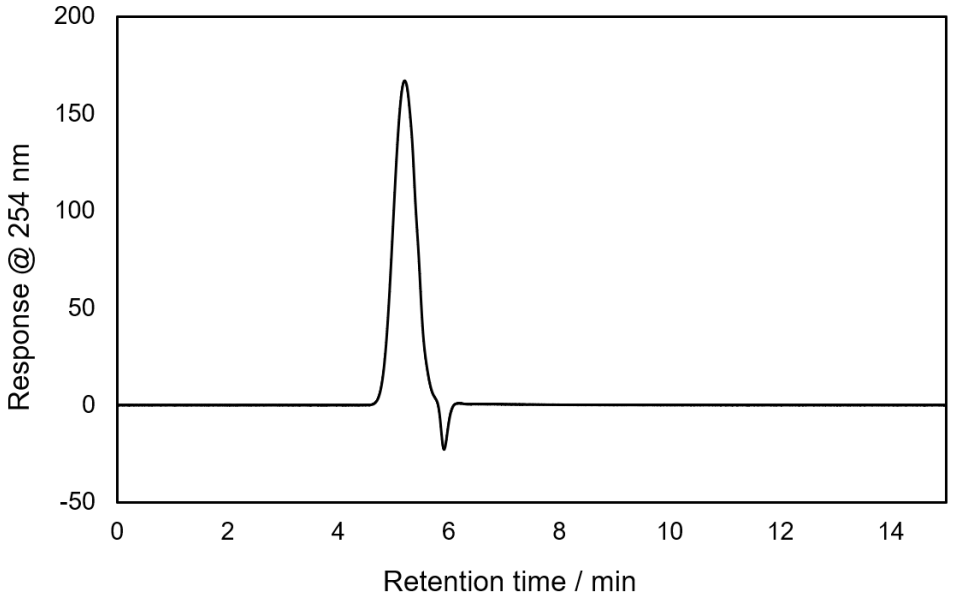


Figure S13. ^{29}Si {^{1}H} NMR Spectrum (79 MHz, Benzene-d_6) of *cyc*-poly(**1,3Si$_6$**) (Cp_2ZrCl_2 synthesis). $^{1}J_{Si-H}$ = 120 Hz.



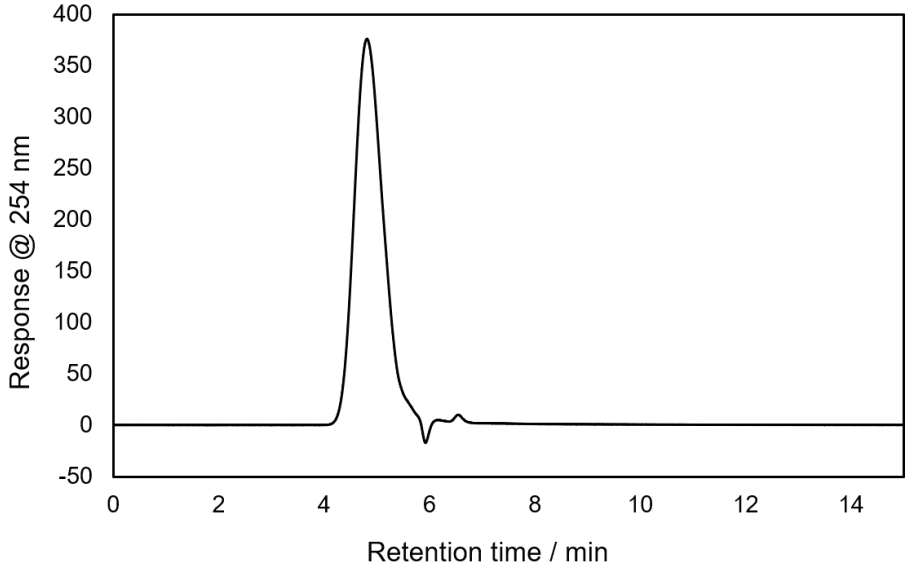
2. Gel Permeation Chromatography

2.1 *lin*-poly(**1,3Si$_6$**)



Peak No.	M_n	M_w	M_w / M_n
1	1770	2390	1.35

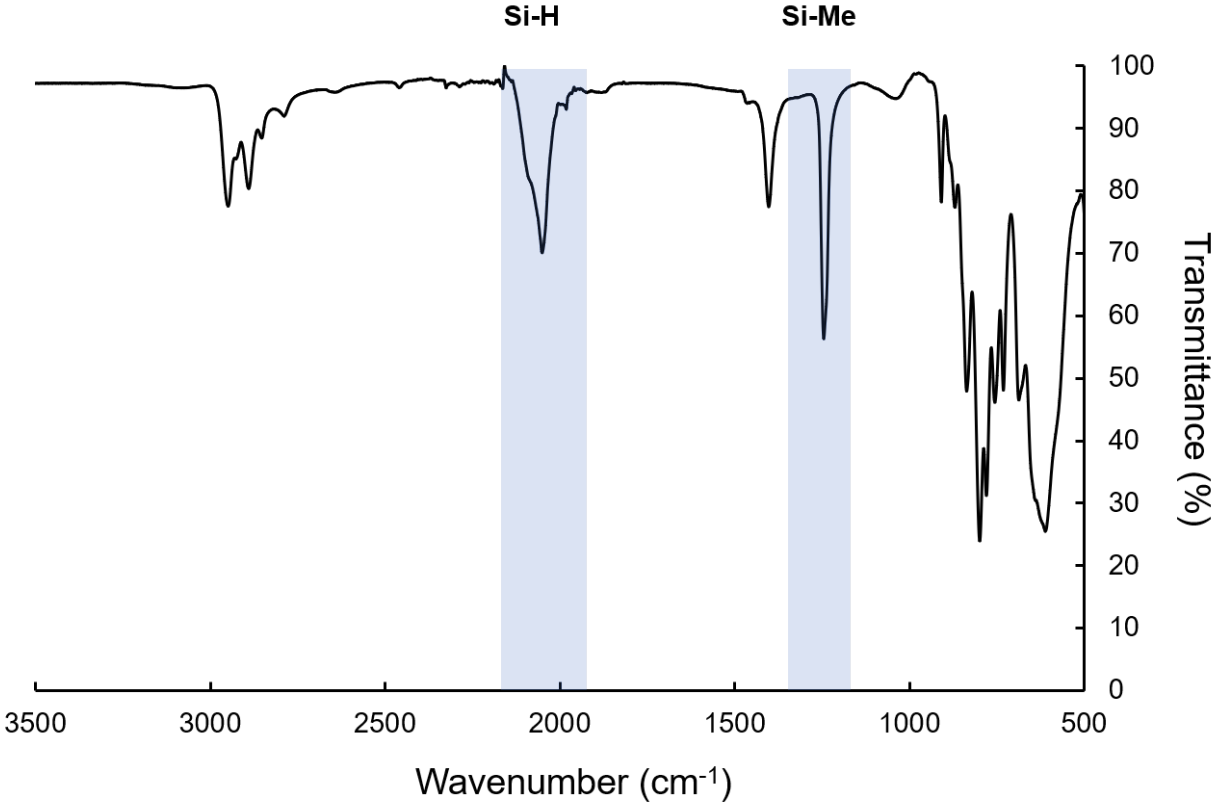
2.2 *cyc*-poly(**1,3Si$_6$**) (Cp_2ZrMe_2 synthesis)



Peak No.	M_n	M_w	M_w / M_n
1	3840	7270	1.90

3. ATR-FTIR Spectroscopy

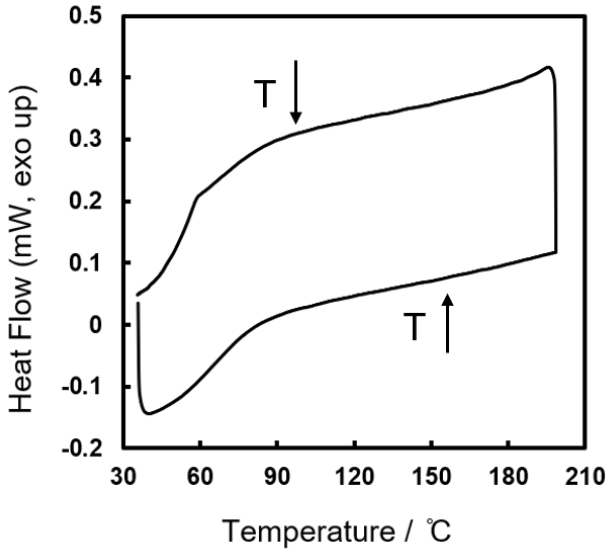
3.1 ATR-FTIR spectrum of *lin*-poly(**1,3Si$_6$**)



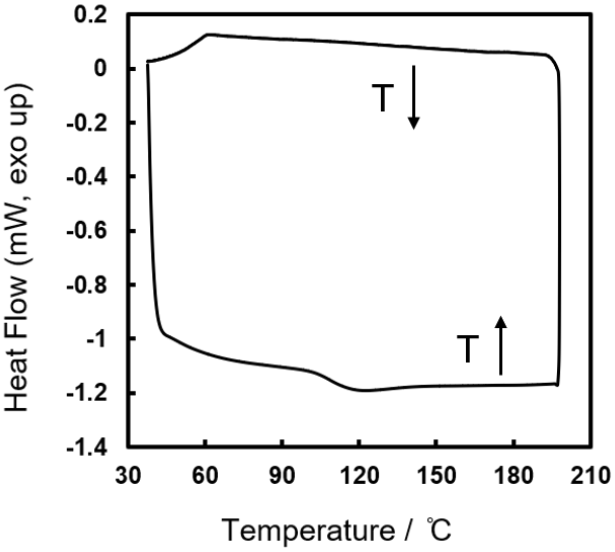
4. Differential scanning calorimetry

Differential scanning calorimetry (DSC) was conducted using a TA Instruments DSC Q20 V24.11 Build 124 and processing was performed using Universal V4.5A (TA Instruments). Samples were sealed in hermetic aluminum pans, heated from 35 to 200 °C (3 °C min^{-1} for *lin*-poly(**1,4Si$_6$**) and 20 °C min^{-1} for *cyc*-poly(**1,3Si$_6$**) and *lin*-poly(**1,3Si$_6$**)), and cooled from 200 to 35 °C (3 °C min^{-1}), for three cycles under a purge gas of nitrogen (25 mL min^{-1}). Phase transition temperature were calculated from the second heating cycle. The second heating and cooling cycles are shown.

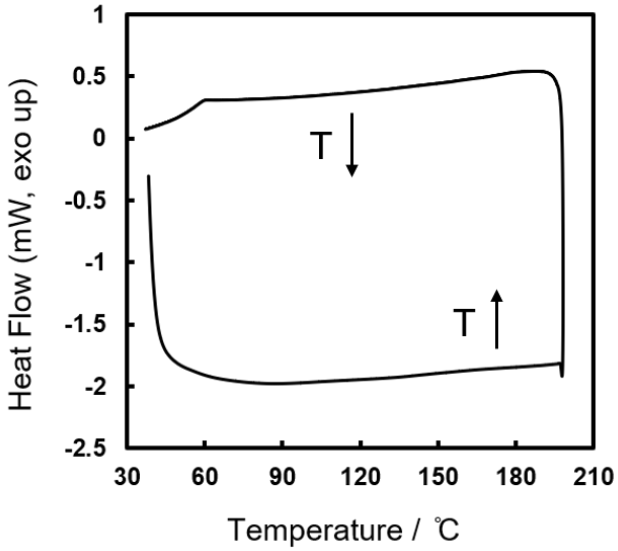
7.1 *lin*-poly(**1,4Si$_6$**)



7.2 *cyc*-poly(**1,3Si$_6$**)



7.3 *lin*-poly(**1,3Si$_6$**)



5. Computational Methods

All the DFT calculations are performed with the Gaussian 09 package. Geometries were optimized using the B3LYP functional with the 6-31G(d) basis. No symmetry restrictions were applied to geometry optimization. Homolytic bond dissociation energies (BDEs) are calculated as follows: BDE = $\sum E_{rs} - E_{cs}$, where $\sum E_{rs}$ is the sum of energy of all radical species, and E_{cs} is the energy of the closed shell species. Hydrogens in optimized structures are omitted for clarity.

Table S1. Calculated energy of closed shell and radical species of **1,4Si$_6$**. Radical species are generated by homolytic bond dissociation as labeled on the left column.

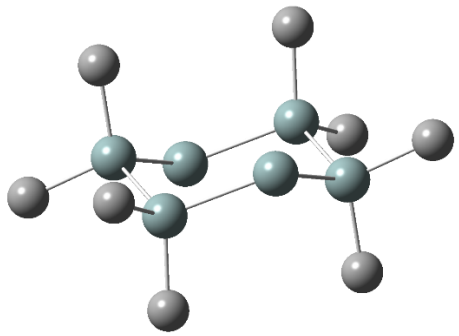
Closed Shell Energies (E_h)	-2058.79738594
Radical Species Energies (E_h)	
Si(1)-H^a	-2058.15686167
Si(1)-H^e	-2058.15931009
Si(2)-Me^a	-2018.83157300
Si(2)-Me^e	-2018.83335389
Si(1)-Si(2)	-2058.68840089
Si(2)-Si(2)	-2058.68886887

Table S2. Calculated energy of closed shell and radical species of *lin*-(**1,4Si$_6$**)$_3$. Radical species are generated by homolytic bond dissociation as labeled on the left column.

Closed Shell Energies (E_h)	-6174.01411855
Radical Species Energies (E_h)	
Si(1)-H^a	-6173.37304659
Si(1)-H^e	-6173.37569970
Si(4)-H^e	-6173.37738920
Si(6)-Me^a	-6134.05889350
Si(6)-Me^e	-6134.05908879
Si(2)-Si(3)	-6173.91376417
Si(3)-Si(4)	-6173.91906634
Si(4)-Si(5)	-4115.76713951 (dimer)
	-2058.15941768 (monomer)

6.1 **1,4Si$_6$** and its radical species

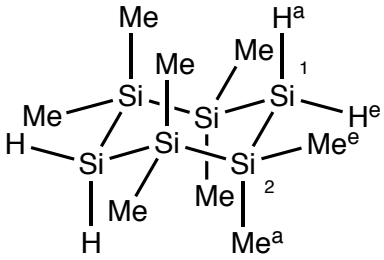
1,4Si$_6$ (charge = 0, multiplicity = 1)



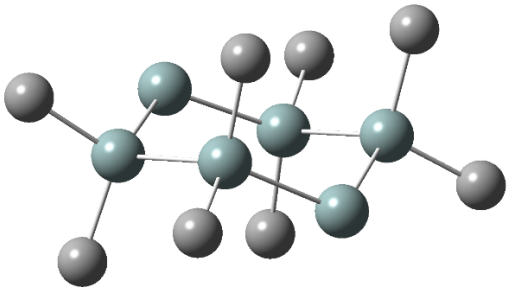
E(RB3LYP) = -2058.79738594 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-2.569659	-0.637739	-0.356331
2	14	0	-3.444674	0.444823	1.565310
3	14	0	-5.801826	0.218408	1.586254
4	1	0	-6.359925	0.921230	2.789080
5	1	0	-6.354401	0.956059	0.403474
6	14	0	-6.615051	-2.004916	1.516256
7	14	0	-5.740036	-3.087478	-0.405385
8	14	0	-3.382885	-2.861063	-0.426328
9	1	0	-2.824786	-3.563885	-1.629155
10	1	0	-2.830309	-3.598714	0.756452
11	6	0	-3.107866	0.296597	-1.932811
12	1	0	-2.709979	1.318702	-1.931222
13	1	0	-2.733556	-0.203925	-2.833797
14	1	0	-4.198159	0.365518	-2.017209
15	6	0	-0.660109	-0.667459	-0.298452
16	1	0	-0.251011	-1.165590	-1.185521

17	1	0	-0.251895	0.350374	-0.269797
18	1	0	-0.291955	-1.202598	0.583814
19	6	0	-6.188827	-4.945224	-0.393908
20	1	0	-7.276495	-5.087715	-0.404310
21	1	0	-5.778485	-5.450660	-1.276307
22	1	0	-5.791974	-5.450396	0.493717
23	6	0	-6.471320	-2.303662	-1.985783
24	1	0	-6.054680	-2.772750	-2.885036
25	1	0	-7.559841	-2.435198	-2.016176
26	1	0	-6.265214	-1.229134	-2.043101
27	6	0	-8.524601	-1.975196	1.458377
28	1	0	-8.932816	-2.993030	1.429722
29	1	0	-8.933700	-1.477065	2.345446
30	1	0	-8.892756	-1.440057	0.576111
31	6	0	-6.076844	-2.939252	3.092736
32	1	0	-6.451155	-2.438731	3.993723
33	1	0	-6.474731	-3.961357	3.091147
34	1	0	-4.986551	-3.008174	3.177135
35	6	0	-2.713390	-0.338994	3.145708
36	1	0	-1.624869	-0.207457	3.176101
37	1	0	-3.130030	0.130095	4.044961
38	1	0	-2.919497	-1.413521	3.203027
39	6	0	-2.995884	2.302569	1.553833
40	1	0	-3.406225	2.808004	2.436232
41	1	0	-1.908215	2.445060	1.564235
42	1	0	-3.392737	2.807741	0.666208



Si(1)-H[a] dissociated radical (charge = 0, multiplicity = 2)

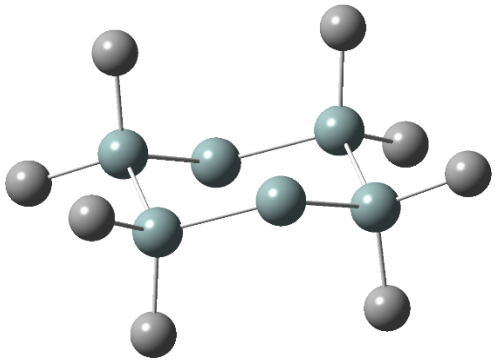


E(UB3LYP) = -2058.15686167 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-2.562477	-0.647836	-0.335273
2	14	0	-3.402079	0.457964	1.588572
3	14	0	-5.731075	0.111982	1.686254
4	1	0	-6.406101	0.965249	2.723273
5	14	0	-6.633225	-2.060017	1.548211
6	14	0	-5.743970	-3.092292	-0.393546
7	14	0	-3.386644	-2.868134	-0.388715
8	1	0	-2.817950	-3.580955	-1.580858
9	1	0	-2.847279	-3.598878	0.804354
10	6	0	-3.104805	0.279928	-1.913514
11	1	0	-2.693149	1.296487	-1.925460
12	1	0	-2.747613	-0.233602	-2.814158
13	1	0	-4.195055	0.362070	-1.984707
14	6	0	-0.652720	-0.692392	-0.290035

15	1	0	-0.253782	-1.198694	-1.177088
16	1	0	-0.235684	0.322136	-0.269760
17	1	0	-0.283039	-1.225712	0.592692
18	6	0	-6.195165	-4.949062	-0.430599
19	1	0	-7.283114	-5.088959	-0.447821
20	1	0	-5.783305	-5.431697	-1.324929
21	1	0	-5.802012	-5.478343	0.444523
22	6	0	-6.463364	-2.267728	-1.957657
23	1	0	-6.037078	-2.708971	-2.866464
24	1	0	-7.551167	-2.401101	-2.001574
25	1	0	-6.259290	-1.191560	-1.979404
26	6	0	-8.536598	-1.939649	1.449016
27	1	0	-8.987008	-2.938743	1.398391
28	1	0	-8.941629	-1.436289	2.334920
29	1	0	-8.861684	-1.377321	0.567120
30	6	0	-6.184438	-3.090562	3.095450
31	1	0	-6.566202	-2.616906	4.007329
32	1	0	-6.624220	-4.093847	3.028454
33	1	0	-5.100658	-3.206256	3.205188
34	6	0	-2.544828	-0.230274	3.153744
35	1	0	-1.463217	-0.048937	3.110638
36	1	0	-2.930548	0.254942	4.057845
37	1	0	-2.700174	-1.309446	3.259740
38	6	0	-3.058014	2.334832	1.504377
39	1	0	-3.476003	2.846639	2.379367
40	1	0	-1.978992	2.532300	1.486986
41	1	0	-3.499162	2.787815	0.610077

Si(1)-H^{e} dissociated radical (charge = 0, multiplicity = 2)

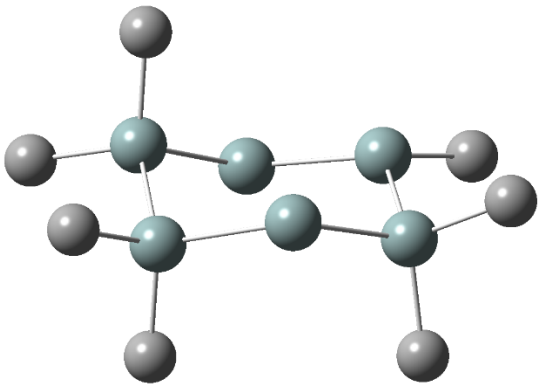


E(UB3LYP) = -2058.15931009 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-2.559998	-0.647007	-0.347115
2	14	0	-3.435971	0.458887	1.569234
3	14	0	-5.775149	0.171354	1.588668
4	1	0	-6.398297	0.989970	0.491356
5	14	0	-6.627592	-2.024390	1.527075
6	14	0	-5.745744	-3.093625	-0.406798
7	14	0	-3.388322	-2.865825	-0.404892
8	1	0	-2.823427	-3.574420	-1.601243
9	1	0	-2.845375	-3.601760	0.783424
10	6	0	-3.092718	0.283486	-1.926951
11	1	0	-2.683101	1.300919	-1.933491
12	1	0	-2.726846	-0.227328	-2.825648
13	1	0	-4.182443	0.363277	-2.006647
14	6	0	-0.649428	-0.689760	-0.292255
15	1	0	-0.246614	-1.196781	-1.177374
16	1	0	-0.234625	0.325563	-0.271516
17	1	0	-0.283185	-1.221686	0.592667
18	6	0	-6.197097	-4.951806	-0.428628

19	1	0	-7.284934	-5.091502	-0.448876
20	1	0	-5.781317	-5.441837	-1.317350
21	1	0	-5.806951	-5.472879	0.452679
22	6	0	-6.467590	-2.283702	-1.977281
23	1	0	-6.045110	-2.737520	-2.881653
24	1	0	-7.555880	-2.414377	-2.017035
25	1	0	-6.260005	-1.208702	-2.012538
26	6	0	-8.534737	-1.975438	1.465830
27	1	0	-8.950903	-2.989354	1.419717
28	1	0	-8.939223	-1.488144	2.360698
29	1	0	-8.895808	-1.422699	0.591715
30	6	0	-6.088581	-2.974055	3.091570
31	1	0	-6.475710	-2.490694	3.996135
32	1	0	-6.471355	-4.001688	3.071170
33	1	0	-4.997831	-3.027985	3.181223
34	6	0	-2.681435	-0.295153	3.151032
35	1	0	-1.591855	-0.169007	3.158795
36	1	0	-3.081649	0.195297	4.046009
37	1	0	-2.892309	-1.367125	3.234078
38	6	0	-3.020245	2.321721	1.522462
39	1	0	-3.420959	2.831124	2.406696
40	1	0	-1.934953	2.480902	1.508267
41	1	0	-3.443723	2.806757	0.636142

Si(2)-Me[a] dissociated radical (charge = 0, multiplicity = 2)

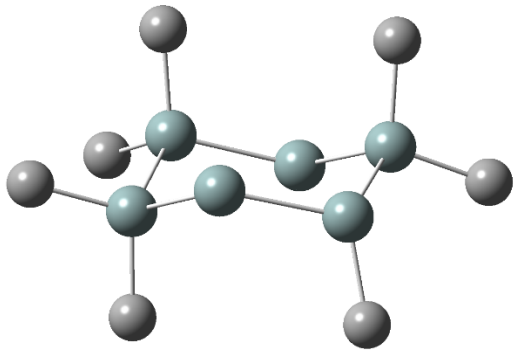


E(UB3LYP) = -2018.83157300 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-2.583903	-0.649939	-0.426802
2	14	0	-3.628982	0.512195	1.341123
3	14	0	-5.960535	0.259839	1.519456
4	1	0	-6.412706	0.940495	2.775678
5	1	0	-6.670030	0.976298	0.407070
6	14	0	-6.622662	-2.011982	1.531712
7	14	0	-5.785946	-3.050832	-0.429023
8	14	0	-3.426469	-2.861994	-0.452566
9	1	0	-2.878399	-3.573256	-1.654903
10	1	0	-2.876804	-3.593623	0.733319
11	6	0	-2.916968	0.181983	-2.116288
12	1	0	-2.529138	1.207484	-2.129343
13	1	0	-2.421562	-0.373976	-2.922080
14	1	0	-3.987025	0.225401	-2.346125
15	6	0	-0.697000	-0.677751	-0.144790
16	1	0	-0.194157	-1.222627	-0.952885
17	1	0	-0.287259	0.339532	-0.123785
18	1	0	-0.440173	-1.165330	0.801468

19	6	0	-6.265794	-4.899727	-0.477595
20	1	0	-7.355779	-5.022945	-0.482191
21	1	0	-5.872262	-5.380301	-1.381248
22	1	0	-5.869711	-5.442715	0.387744
23	6	0	-6.511566	-2.199493	-1.976739
24	1	0	-6.111772	-2.646400	-2.894761
25	1	0	-7.602865	-2.306419	-2.003449
26	1	0	-6.283801	-1.127809	-1.998668
27	6	0	-8.529281	-2.116294	1.590910
28	1	0	-8.864921	-3.160476	1.608489
29	1	0	-8.919611	-1.626598	2.491058
30	1	0	-8.987254	-1.630798	0.721959
31	6	0	-5.910783	-2.856115	3.087380
32	1	0	-6.288256	-2.377090	3.998618
33	1	0	-6.195765	-3.914604	3.124759
34	1	0	-4.816694	-2.803138	3.110801
35	6	0	-3.036219	2.318350	1.580002
36	1	0	-3.431158	2.735224	2.512719
37	1	0	-1.942668	2.370755	1.621565
38	1	0	-3.375254	2.958795	0.756045

Si(2)-Me^{e} dissociated radical (charge = 0, multiplicity = 2)

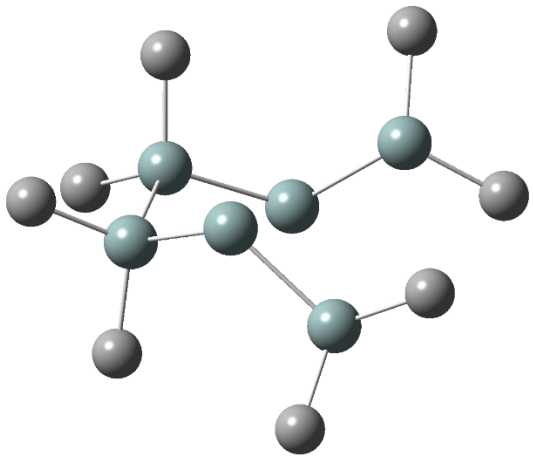


E(UB3LYP) = -2018.83335389 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-2.560124	-0.689025	-0.372079
2	14	0	-3.502819	0.378703	1.509856
3	14	0	-5.846935	0.196682	1.590758
4	1	0	-6.365423	0.888841	2.814146
5	1	0	-6.416786	0.935322	0.419999
6	14	0	-6.631745	-2.043904	1.521334
7	14	0	-5.772836	-3.078695	-0.434483
8	14	0	-3.410560	-2.903702	-0.449284
9	1	0	-2.861838	-3.631977	-1.642536
10	1	0	-2.877732	-3.635862	0.745376
11	6	0	-3.041970	0.250740	-1.959092
12	1	0	-2.617981	1.261721	-1.948095
13	1	0	-2.661861	-0.264403	-2.849411
14	1	0	-4.128093	0.346942	-2.065660
15	6	0	-0.659086	-0.729268	-0.228960
16	1	0	-0.216305	-1.233434	-1.096220
17	1	0	-0.250294	0.287492	-0.186521
18	1	0	-0.333354	-1.263421	0.670143
19	6	0	-6.255027	-4.927465	-0.481671
20	1	0	-7.345092	-5.049586	-0.494253
21	1	0	-5.855381	-5.410461	-1.381341
22	1	0	-5.865928	-5.469069	0.387696
23	6	0	-6.488512	-2.231395	-1.988626
24	1	0	-6.084455	-2.682692	-2.902623
25	1	0	-7.579850	-2.336107	-2.020775

26	1	0	-6.257472	-1.160692	-2.013788
27	6	0	-8.542699	-2.063940	1.515371
28	1	0	-8.924390	-3.092147	1.488071
29	1	0	-8.940547	-1.584910	2.417895
30	1	0	-8.948791	-1.531557	0.648197
31	6	0	-6.018015	-2.966313	3.075979
32	1	0	-6.393391	-2.490023	3.989556
33	1	0	-6.367495	-4.005932	3.075726
34	1	0	-4.923856	-2.984290	3.132949
35	6	0	-2.684603	-0.155402	3.158597
36	1	0	-1.607809	0.045788	3.140290
37	1	0	-3.115570	0.392125	4.003718
38	1	0	-2.821234	-1.227817	3.347683

Si(2)-Si(2) dissociated radical (charge = 0, multiplicity = 3)



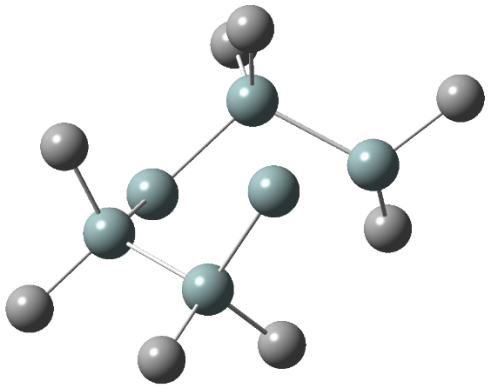
E(UB3LYP) = -2058.68886887 E_h

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

1	14	0	-2.486994	-0.799159	-1.543249
2	14	0	-3.630160	0.520909	2.848114
3	14	0	-5.722437	0.249924	1.794674
4	1	0	-6.783239	1.002802	2.548484
5	1	0	-5.650697	0.902830	0.450614
6	14	0	-6.425039	-2.002627	1.565812
7	14	0	-5.673539	-2.952117	-0.473798
8	14	0	-3.317829	-2.839407	-0.703030
9	1	0	-2.881315	-3.975327	-1.586664
10	1	0	-2.663389	-3.093488	0.618161
11	6	0	-2.904126	-0.532145	-3.385051
12	1	0	-2.574720	0.459698	-3.716247
13	1	0	-2.401632	-1.278200	-4.015401
14	1	0	-3.981081	-0.607172	-3.568076
15	6	0	-0.611811	-0.593399	-1.264683
16	1	0	-0.043111	-1.337362	-1.838598
17	1	0	-0.278128	0.401073	-1.583940
18	1	0	-0.354122	-0.714529	-0.207571
19	6	0	-6.180966	-4.794808	-0.530569
20	1	0	-7.269569	-4.908200	-0.456337
21	1	0	-5.860634	-5.255948	-1.472376
22	1	0	-5.727896	-5.364461	0.288614
23	6	0	-6.501815	-2.059931	-1.944935
24	1	0	-6.184680	-2.494793	-2.900532
25	1	0	-7.593572	-2.148285	-1.887952
26	1	0	-6.254731	-0.992521	-1.960756
27	6	0	-8.336204	-2.039681	1.598524
28	1	0	-8.714516	-3.065293	1.507528
29	1	0	-8.715951	-1.625774	2.540253
30	1	0	-8.765035	-1.449896	0.780504

31	6	0	-5.778311	-3.026009	3.042204
32	1	0	-6.139995	-2.618260	3.994038
33	1	0	-6.120712	-4.065878	2.976969
34	1	0	-4.683061	-3.036855	3.074902
35	6	0	-3.713306	0.236616	4.732433
36	1	0	-2.711967	0.286876	5.175981
37	1	0	-4.333398	1.000565	5.220446
38	1	0	-4.137352	-0.744384	4.971410
39	6	0	-2.818837	2.204733	2.473575
40	1	0	-3.411456	3.031526	2.887559
41	1	0	-1.815829	2.258972	2.913142
42	1	0	-2.725754	2.363624	1.394257

Si(1)-Si(2) dissociated radical (charge = 0, multiplicity = 3)



E(UB3LYP) = -2058.68840089 E_h

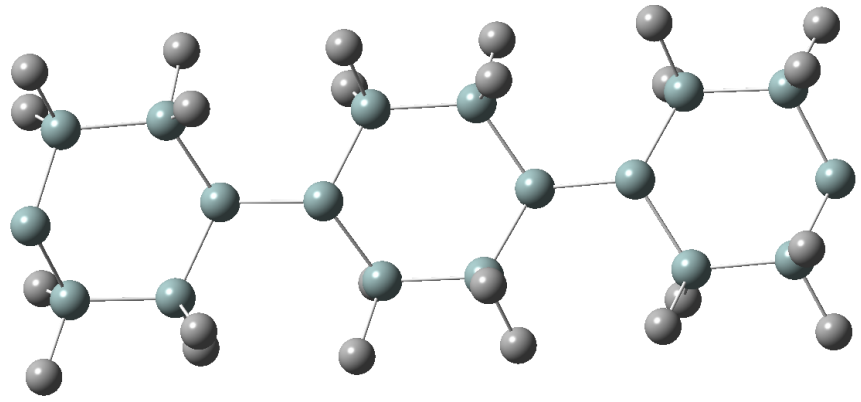
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-2.524417	-0.583065	-0.134458

2	14	0	-2.548274	0.295425	2.057123
3	14	0	-7.539103	0.330929	0.520647
4	1	0	-8.170028	1.219458	1.547101
5	1	0	-8.325293	0.473807	-0.744181
6	14	0	-7.150796	-1.890146	1.208987
7	14	0	-5.831808	-3.009590	-0.419803
8	14	0	-3.498717	-2.745171	-0.099703
9	1	0	-2.837424	-3.564346	-1.170946
10	1	0	-3.122538	-3.417768	1.185581
11	6	0	-3.483497	0.584351	-1.297851
12	1	0	-2.998505	1.566905	-1.347408
13	1	0	-3.519870	0.182050	-2.317461
14	1	0	-4.513755	0.737545	-0.956748
15	6	0	-0.740320	-0.762354	-0.806478
16	1	0	-0.750135	-1.188997	-1.817036
17	1	0	-0.239502	0.212159	-0.856945
18	1	0	-0.135027	-1.419821	-0.172759
19	6	0	-6.198405	-4.883221	-0.313740
20	1	0	-7.259734	-5.087240	-0.500839
21	1	0	-5.614837	-5.434625	-1.060534
22	1	0	-5.946601	-5.291457	0.671580
23	6	0	-6.301922	-2.412239	-2.171149
24	1	0	-5.725781	-2.951580	-2.932612
25	1	0	-7.365357	-2.589033	-2.372922
26	1	0	-6.111469	-1.341475	-2.303059
27	6	0	-8.825193	-2.798826	1.391911
28	1	0	-8.663801	-3.835243	1.714241
29	1	0	-9.456686	-2.307433	2.141039
30	1	0	-9.380682	-2.821858	0.448004
31	6	0	-6.298827	-1.842344	2.911661

32	1	0	-6.941928	-1.358851	3.656599
33	1	0	-6.080965	-2.856901	3.266999
34	1	0	-5.354005	-1.288005	2.871826
35	6	0	-1.429918	-0.660293	3.271904
36	1	0	-0.367823	-0.514409	3.032559
37	1	0	-1.587367	-0.315249	4.300573
38	1	0	-1.636758	-1.735333	3.242775
39	6	0	-2.161129	2.162342	2.158942
40	1	0	-2.325740	2.536529	3.176357
41	1	0	-1.114941	2.369084	1.895567
42	1	0	-2.800043	2.740531	1.483086

5.2 *lin*-(**1,4Si$_6$**)$_3$ and its radical species

lin-(**1,4Si$_6$**)$_3$ (charge = 0, multiplicity = 1)



E(RB3LYP) = -6174.01411855 E_h

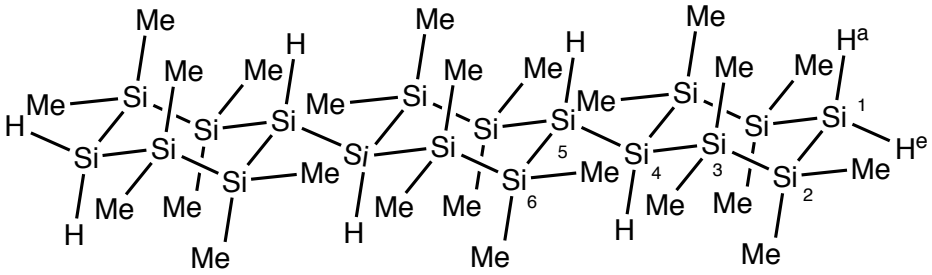
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.848100	3.133600	9.954000
2	14	0	0.948700	2.553400	8.540300
3	1	0	2.205000	2.493300	9.355700

4	1	0	1.185600	3.617500	7.509500
5	14	0	0.606800	0.463000	7.502900
6	6	0	-0.516500	4.832100	10.767200
7	1	0	-0.422100	5.614200	10.004300
8	1	0	0.408700	4.824800	11.353700
9	1	0	-1.337600	5.117400	11.436500
10	6	0	-2.459900	3.279400	8.939400
11	1	0	-3.290600	3.597200	9.581300
12	1	0	-2.745400	2.330000	8.473500
13	1	0	-2.354800	4.024000	8.141200
14	6	0	-0.921100	0.560000	6.360500
15	1	0	-0.811900	1.368100	5.627400
16	1	0	-1.845400	0.740500	6.920000
17	1	0	-1.046100	-0.377300	5.805000
18	6	0	2.119100	0.024700	6.418300
19	1	0	1.990200	-0.951900	5.935400
20	1	0	3.041400	-0.011200	7.008200
21	1	0	2.257600	0.771600	5.627300
22	14	0	0.317600	-1.274700	9.103200
23	14	0	-1.083600	1.515800	11.676600
24	6	0	-0.465700	-2.715600	8.114400
25	1	0	-0.664000	-3.600300	8.726200
26	1	0	-1.419600	-2.400800	7.675600
27	1	0	0.193400	-3.021300	7.291800
28	6	0	2.052100	-1.765200	9.735100
29	1	0	2.687800	-2.100400	8.906700
30	1	0	2.550100	-0.912300	10.210900
31	1	0	2.005700	-2.574100	10.471900
32	6	0	0.354300	1.798100	12.902600
33	1	0	0.331100	1.088600	13.735800

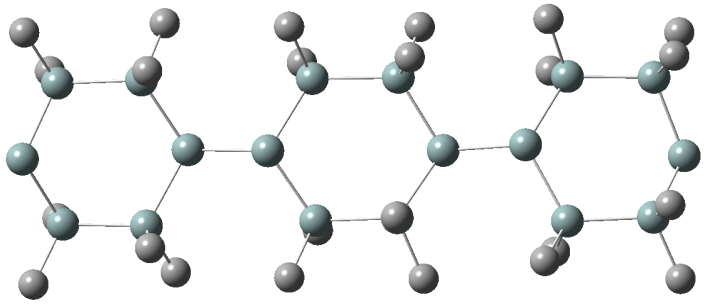
34	1	0	1.321500	1.686600	12.398400
35	1	0	0.314800	2.810800	13.322100
36	6	0	-2.767900	1.897900	12.504700
37	1	0	-2.763600	2.902100	12.947100
38	1	0	-3.570700	1.866600	11.759100
39	1	0	-3.028600	1.187600	13.295000
40	14	0	-1.093700	-0.763200	10.965900
41	1	0	-2.494700	-1.012400	10.480000
42	14	0	-1.039400	-4.566800	12.119500
43	14	0	-1.125700	-6.246000	13.820300
44	14	0	-2.138400	-5.722400	15.908600
45	1	0	-3.624200	-5.823400	15.705200
46	14	0	-1.707000	-3.458700	16.491000
47	14	0	-2.054300	-1.889100	14.734900
48	14	0	-0.746400	-2.299200	12.790500
49	1	0	0.689400	-2.148000	13.207700
50	6	0	-2.644900	-4.676200	11.087000
51	1	0	-2.619400	-3.980400	10.240900
52	1	0	-2.789200	-5.686600	10.686700
53	1	0	-3.526400	-4.428000	11.689900
54	6	0	-3.904600	-1.863300	14.259200
55	1	0	-4.232900	-2.832700	13.866400
56	1	0	-4.528400	-1.631100	15.130900
57	1	0	-4.110900	-1.107900	13.491800
58	6	0	-2.906600	-2.866300	17.862000
59	1	0	-2.840900	-3.469000	18.771700
60	1	0	-2.691400	-1.826900	18.139000
61	1	0	-3.944900	-2.908900	17.512800
62	6	0	-2.103100	-7.663100	12.980600
63	1	0	-1.593600	-8.008300	12.072000

64	1	0	-2.236300	-8.529600	13.634600
65	1	0	-3.099900	-7.313800	12.689600
66	6	0	0.672300	-6.803500	14.155800
67	1	0	0.714700	-7.608500	14.897400
68	1	0	1.152100	-7.165300	13.238800
69	1	0	1.275900	-5.972600	14.540300
70	6	0	0.436100	-5.143500	11.042900
71	1	0	0.283600	-6.175000	10.700400
72	1	0	0.580900	-4.520800	10.155800
73	1	0	1.367800	-5.121100	11.619000
74	6	0	-1.601900	-0.220800	15.559300
75	1	0	-1.747500	0.634400	14.894500
76	1	0	-2.223800	-0.056100	16.448000
77	1	0	-0.554400	-0.215500	15.881800
78	6	0	0.097100	-3.286400	17.097300
79	1	0	0.306000	-2.258600	17.418400
80	1	0	0.307200	-3.948800	17.944500
81	1	0	0.807400	-3.533900	16.299800
82	14	0	-1.568300	-7.336700	17.606200
83	1	0	-0.067200	-7.326100	17.692700
84	14	0	-2.317000	-6.692100	19.783300
85	14	0	-2.129400	-8.380400	21.444700
86	14	0	-3.092900	-10.393100	20.684200
87	1	0	-3.055600	-11.443600	21.754400
88	1	0	-4.545300	-10.153200	20.401700
89	14	0	-2.053800	-11.175300	18.718100
90	14	0	-2.149100	-9.567800	16.965800
91	6	0	-2.921700	-12.772300	18.125400
92	1	0	-2.463500	-13.154600	17.204900
93	1	0	-2.844200	-13.557600	18.887000

94	1	0	-3.985800	-12.603400	17.927700
95	6	0	-3.910200	-9.575100	16.227600
96	1	0	-3.999400	-8.877800	15.387000
97	1	0	-4.177800	-10.575100	15.865600
98	1	0	-4.654200	-9.283300	16.978000
99	6	0	-0.896000	-10.223400	15.675800
100	1	0	-1.177600	-11.233800	15.352500
101	1	0	-0.827900	-9.598300	14.781400
102	1	0	0.106500	-10.283600	16.114500
103	6	0	-0.227300	-11.606600	19.078700
104	1	0	-0.148000	-12.346100	19.884400
105	1	0	0.248500	-12.034600	18.187700
106	1	0	0.355200	-10.727100	19.374300
107	6	0	-3.033300	-7.789700	23.022400
108	1	0	-2.930100	-8.529800	23.825000
109	1	0	-2.617500	-6.842300	23.386800
110	1	0	-4.103500	-7.641100	22.841700
111	6	0	-0.292600	-8.653800	21.891500
112	1	0	0.142300	-7.733500	22.300100
113	1	0	-0.183300	-9.437600	22.650500
114	1	0	0.305700	-8.945100	21.021400
115	6	0	-1.220900	-5.257600	20.420200
116	1	0	-1.188200	-4.406300	19.735000
117	1	0	-1.587800	-4.892700	21.388000
118	1	0	-0.190500	-5.602600	20.564800
119	6	0	-4.146300	-6.149000	19.698800
120	1	0	-4.792900	-6.994000	19.434600
121	1	0	-4.484600	-5.764500	20.668700
122	1	0	-4.306400	-5.363400	18.952600



Si(1)-H[a] dissociated radical (charge = 0, multiplicity = 2)



E(UB3LYP) = -6173.37304659 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.897227	3.143234	9.958021
2	14	0	0.870825	2.531058	8.540819
3	1	0	1.331312	3.626779	7.620464
4	14	0	0.624216	0.446989	7.488996
5	6	0	-0.541088	4.841213	10.758649
6	1	0	-0.437476	5.617079	9.990715
7	1	0	0.383402	4.826080	11.345712
8	1	0	-1.359800	5.139902	11.425170
9	6	0	-2.530697	3.295029	8.972920
10	1	0	-3.354218	3.590121	9.635506
11	1	0	-2.808453	2.350031	8.493376
12	1	0	-2.443631	4.055250	8.187874
13	6	0	-0.860357	0.482775	6.282076

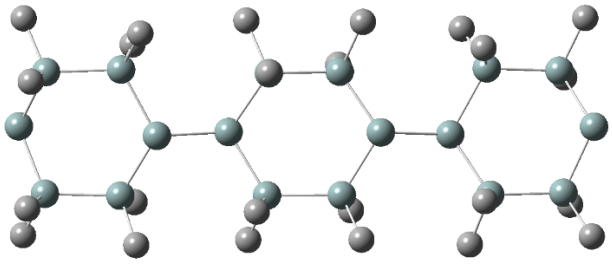
14	1	0	-0.725699	1.261400	5.522251
15	1	0	-1.805316	0.680831	6.799604
16	1	0	-0.956443	-0.479174	5.762988
17	6	0	2.187260	0.043416	6.466805
18	1	0	2.095351	-0.935153	5.979253
19	1	0	3.086156	0.025499	7.092067
20	1	0	2.340493	0.793125	5.681298
21	14	0	0.315438	-1.275001	9.102967
22	14	0	-1.108195	1.518638	11.676584
23	6	0	-0.469508	-2.717670	8.117631
24	1	0	-0.676101	-3.597653	8.733345
25	1	0	-1.419071	-2.401006	7.671039
26	1	0	0.193004	-3.032099	7.300971
27	6	0	2.044691	-1.769845	9.745017
28	1	0	2.684616	-2.108231	8.921183
29	1	0	2.541262	-0.917085	10.222509
30	1	0	1.991192	-2.577239	10.482931
31	6	0	0.330401	1.812918	12.898131
32	1	0	0.320883	1.097237	13.726368
33	1	0	1.296222	1.718588	12.387891
34	1	0	0.278413	2.821979	13.324912
35	6	0	-2.793000	1.884418	12.510842
36	1	0	-2.799017	2.891852	12.946127
37	1	0	-3.599434	1.837724	11.769958
38	1	0	-3.040325	1.177022	13.307907
39	14	0	-1.102010	-0.758843	10.960669
40	1	0	-2.500952	-1.015031	10.472559
41	14	0	-1.049333	-4.562864	12.116405
42	14	0	-1.137013	-6.242936	13.816462
43	14	0	-2.138956	-5.717501	15.909489

44	1	0	-3.625976	-5.813521	15.712822
45	14	0	-1.697159	-3.455568	16.490071
46	14	0	-2.050921	-1.885203	14.735896
47	14	0	-0.751025	-2.295041	12.785763
48	1	0	0.686360	-2.145850	13.198193
49	6	0	-2.656651	-4.668888	11.086383
50	1	0	-2.631531	-3.972707	10.240527
51	1	0	-2.803631	-5.678839	10.685881
52	1	0	-3.536547	-4.419298	11.691015
53	6	0	-3.903332	-1.860447	14.268068
54	1	0	-4.232447	-2.830324	13.877034
55	1	0	-4.523649	-1.628636	15.142347
56	1	0	-4.113782	-1.105626	13.501425
57	6	0	-2.887227	-2.859967	17.867936
58	1	0	-2.820126	-3.465046	18.776012
59	1	0	-2.665575	-1.822254	18.146122
60	1	0	-3.927389	-2.896828	17.523734
61	6	0	-2.123726	-7.655148	12.979479
62	1	0	-1.619007	-8.002267	12.068880
63	1	0	-2.258727	-8.521284	13.633496
64	1	0	-3.119873	-7.300932	12.692126
65	6	0	0.660090	-6.807478	14.145012
66	1	0	0.702619	-7.610975	14.888201
67	1	0	1.134355	-7.173136	13.226698
68	1	0	1.268813	-5.978226	14.524957
69	6	0	0.423943	-5.143741	11.038879
70	1	0	0.267206	-6.174116	10.694757
71	1	0	0.572014	-4.520412	10.152965
72	1	0	1.355469	-5.126252	11.615463
73	6	0	-1.595008	-0.217849	15.560385

74	1	0	-1.742585	0.638630	14.897642
75	1	0	-2.213235	-0.054279	16.451759
76	1	0	-0.546212	-0.213619	15.878724
77	6	0	0.110676	-3.289464	17.086715
78	1	0	0.325160	-2.262368	17.406234
79	1	0	0.322586	-3.952322	17.933105
80	1	0	0.815902	-3.540131	16.285649
81	14	0	-1.566488	-7.334750	17.603294
82	1	0	-0.065023	-7.328806	17.683788
83	14	0	-2.304584	-6.689886	19.783842
84	14	0	-2.117350	-8.380776	21.442811
85	14	0	-3.088132	-10.390322	20.683158
86	1	0	-3.049763	-11.441954	21.752245
87	1	0	-4.540904	-10.146729	20.405891
88	14	0	-2.057711	-11.172972	18.712720
89	14	0	-2.156749	-9.563409	16.962777
90	6	0	-2.931140	-12.767726	18.121820
91	1	0	-2.476363	-13.150668	17.199903
92	1	0	-2.853427	-13.553512	18.882878
93	1	0	-3.995348	-12.596175	17.927110
94	6	0	-3.921422	-9.564591	16.233125
95	1	0	-4.013548	-8.863887	15.395737
96	1	0	-4.192577	-10.562763	15.868623
97	1	0	-4.661167	-9.274431	16.988364
98	6	0	-0.911923	-10.220620	15.665604
99	1	0	-1.198782	-11.229163	15.341157
100	1	0	-0.845601	-9.593627	14.772452
101	1	0	0.092400	-10.285679	16.099519
102	6	0	-0.230895	-11.608416	19.066198
103	1	0	-0.150331	-12.349536	19.870356

104	1	0	0.240939	-12.035780	18.172872
105	1	0	0.354338	-10.730613	19.361406
106	6	0	-3.015584	-7.789261	23.023452
107	1	0	-2.912217	-8.530415	23.825127
108	1	0	-2.596348	-6.843287	23.387710
109	1	0	-4.085825	-7.637700	22.845762
110	6	0	-0.280155	-8.659263	21.884895
111	1	0	0.158061	-7.740383	22.293195
112	1	0	-0.171015	-9.443844	22.643084
113	1	0	0.315505	-8.951418	21.013238
114	6	0	-1.200984	-5.260113	20.418590
115	1	0	-1.168440	-4.407442	19.734964
116	1	0	-1.562619	-4.895861	21.388604
117	1	0	-0.171147	-5.608716	20.558134
118	6	0	-4.132071	-6.139829	19.706605
119	1	0	-4.783070	-6.982395	19.445345
120	1	0	-4.464934	-5.753589	20.677669
121	1	0	-4.292175	-5.353935	18.960661

Si(1)-H^{e} dissociated radical (charge = 0, multiplicity = 2)



E(UB3LYP) = -6173.37569970 E_h

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

1	14	0	-0.856206	3.144317	9.960147
2	14	0	0.914921	2.536780	8.544028
3	1	0	2.217217	2.560774	9.296391
4	14	0	0.612720	0.459763	7.492902
5	6	0	-0.511555	4.832638	10.785027
6	1	0	-0.429138	5.621867	10.028457
7	1	0	0.422151	4.818854	11.357607
8	1	0	-1.322952	5.109687	11.469492
9	6	0	-2.472348	3.293439	8.955769
10	1	0	-3.305286	3.585745	9.606738
11	1	0	-2.746075	2.350420	8.469932
12	1	0	-2.377023	4.056188	8.174069
13	6	0	-0.906289	0.541062	6.340256
14	1	0	-0.782949	1.329503	5.588662
15	1	0	-1.831468	0.746001	6.890058
16	1	0	-1.038224	-0.409194	5.809006
17	6	0	2.139414	0.021250	6.431518
18	1	0	2.023995	-0.964320	5.963571
19	1	0	3.055758	0.003536	7.031267
20	1	0	2.277384	0.756960	5.630385
21	14	0	0.311886	-1.279759	9.100992
22	14	0	-1.094466	1.511867	11.679027
23	6	0	-0.465746	-2.725073	8.112374
24	1	0	-0.664381	-3.608287	8.726467
25	1	0	-1.418549	-2.413379	7.669362
26	1	0	0.197550	-3.031384	7.293400
27	6	0	2.046613	-1.762490	9.736465
28	1	0	2.683606	-2.102498	8.911083
29	1	0	2.541238	-0.904391	10.206200

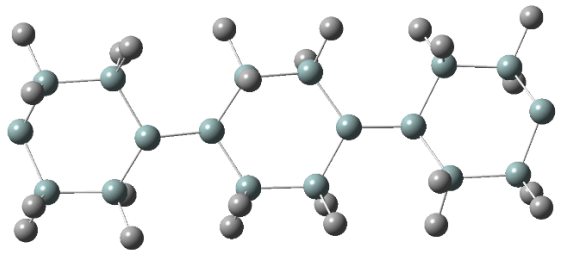
30	1	0	2.000885	-2.566069	10.479083
31	6	0	0.344766	1.792775	12.902653
32	1	0	0.327340	1.075841	13.729685
33	1	0	1.310274	1.690307	12.393697
34	1	0	0.300933	2.801537	13.330952
35	6	0	-2.778205	1.891678	12.511545
36	1	0	-2.772129	2.894392	12.957316
37	1	0	-3.582566	1.863000	11.767597
38	1	0	-3.036881	1.178501	13.300075
39	14	0	-1.102782	-0.763876	10.959535
40	1	0	-2.503891	-1.017352	10.476519
41	14	0	-1.040109	-4.566367	12.117645
42	14	0	-1.127095	-6.245545	13.818560
43	14	0	-2.138540	-5.721576	15.907368
44	1	0	-3.624466	-5.821948	15.704741
45	14	0	-1.705382	-3.458045	16.488515
46	14	0	-2.055215	-1.888135	14.733140
47	14	0	-0.750049	-2.297473	12.786407
48	1	0	0.686298	-2.143198	13.200441
49	6	0	-2.644492	-4.677946	11.083674
50	1	0	-2.619831	-3.981649	10.237890
51	1	0	-2.786812	-5.688392	10.682739
52	1	0	-3.526784	-4.431680	11.686157
53	6	0	-3.906224	-1.863706	14.259869
54	1	0	-4.233947	-2.833467	13.867396
55	1	0	-4.529116	-1.632487	15.132478
56	1	0	-4.114675	-1.108574	13.492961
57	6	0	-2.902655	-2.864883	17.861188
58	1	0	-2.835883	-3.467730	18.770763
59	1	0	-2.686487	-1.825650	18.137977

60	1	0	-3.941491	-2.907010	17.513613
61	6	0	-2.105853	-7.661753	12.979013
62	1	0	-1.596751	-8.007483	12.070319
63	1	0	-2.239647	-8.528029	13.633101
64	1	0	-3.102390	-7.311556	12.688133
65	6	0	0.670588	-6.804379	14.153377
66	1	0	0.712565	-7.609285	14.895102
67	1	0	1.149777	-7.166775	13.236312
68	1	0	1.275131	-5.973994	14.537474
69	6	0	0.437615	-5.142230	11.043545
70	1	0	0.285896	-6.173671	10.700376
71	1	0	0.584609	-4.519402	10.157040
72	1	0	1.368056	-5.120082	11.621721
73	6	0	-1.602412	-0.220728	15.559372
74	1	0	-1.748121	0.636144	14.896718
75	1	0	-2.223607	-0.057800	16.448805
76	1	0	-0.554708	-0.216231	15.881249
77	6	0	0.099661	-3.286641	17.092248
78	1	0	0.309847	-2.258904	17.412534
79	1	0	0.310331	-3.948768	17.939503
80	1	0	0.808786	-3.535231	16.293975
81	14	0	-1.567875	-7.335729	17.604772
82	1	0	-0.066673	-7.326205	17.689606
83	14	0	-2.313886	-6.690187	19.782450
84	14	0	-2.126495	-8.378583	21.443847
85	14	0	-3.092371	-10.390451	20.684227
86	1	0	-3.055096	-11.440862	21.754540
87	1	0	-4.544775	-10.149315	20.402966
88	14	0	-2.055434	-11.173705	18.717429
89	14	0	-2.151200	-9.566410	16.965073

90	6	0	-2.924927	-12.770262	18.125596
91	1	0	-2.467085	-13.153340	17.205255
92	1	0	-2.848074	-13.555254	18.887560
93	1	0	-3.988861	-12.600493	17.927861
94	6	0	-3.912970	-9.572073	16.228531
95	1	0	-4.002623	-8.873902	15.388765
96	1	0	-4.181383	-10.571630	15.865819
97	1	0	-4.656105	-9.280686	16.979967
98	6	0	-0.899808	-10.222863	15.673836
99	1	0	-1.182835	-11.232729	15.350145
100	1	0	-0.831493	-9.597399	14.779734
101	1	0	0.102926	-10.284599	16.111887
102	6	0	-0.229080	-11.606409	19.076732
103	1	0	-0.149961	-12.346247	19.882215
104	1	0	0.245876	-12.034544	18.185425
105	1	0	0.354294	-10.727508	19.372354
106	6	0	-3.028841	-7.786710	23.021998
107	1	0	-2.925856	-8.526741	23.824758
108	1	0	-2.611921	-6.839608	23.385984
109	1	0	-4.098987	-7.637133	22.842029
110	6	0	-0.289674	-8.653441	21.889597
111	1	0	0.146241	-7.733450	22.297840
112	1	0	-0.180583	-9.437139	22.648702
113	1	0	0.308013	-8.945402	21.019264
114	6	0	-1.215851	-5.256672	20.418299
115	1	0	-1.183233	-4.405181	19.733241
116	1	0	-1.581356	-4.891627	21.386557
117	1	0	-0.185605	-5.602548	20.561601
118	6	0	-4.142750	-6.145585	19.699525
119	1	0	-4.790368	-6.990238	19.436596

120	1	0	-4.479724	-5.760107	20.669470
121	1	0	-4.303054	-5.360384	18.952903

Si(4)-H dissociated radical (charge = 0, multiplicity = 2)



E(UB3LYP) = 12 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-1.389025	3.019528	9.805204
2	14	0	0.486642	2.703877	8.410357
3	1	0	1.727227	2.933247	9.219416
4	1	0	0.522376	3.726572	7.313444
5	14	0	0.542512	0.530373	7.498111
6	6	0	-1.414266	4.814582	10.463190
7	1	0	-1.480036	5.528783	9.633564
8	1	0	-0.507886	5.048674	11.032537
9	1	0	-2.277590	4.985154	11.118110
10	6	0	-3.004109	2.726120	8.829411
11	1	0	-3.877118	2.917002	9.465529
12	1	0	-3.081898	1.696928	8.462162
13	1	0	-3.071855	3.397040	7.964724
14	6	0	-0.890318	0.349441	6.246393
15	1	0	-0.824064	1.115589	5.464576

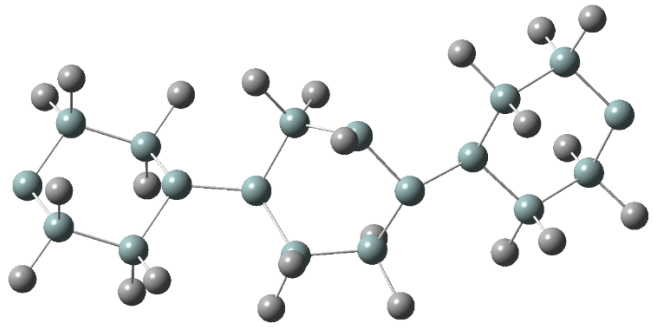
16	1	0	-1.871799	0.445488	6.723547
17	1	0	-0.853441	-0.630249	5.755106
18	6	0	2.181369	0.264402	6.550148
19	1	0	2.228220	-0.742644	6.117201
20	1	0	3.050297	0.389046	7.205372
21	1	0	2.275909	0.984538	5.728468
22	14	0	0.373563	-1.173006	9.155083
23	14	0	-1.238022	1.523481	11.642980
24	6	0	-0.217850	-2.712526	8.182283
25	1	0	-0.325821	-3.599195	8.813178
26	1	0	-1.190146	-2.519357	7.715151
27	1	0	0.491926	-2.958617	7.382050
28	6	0	2.119673	-1.482469	9.864156
29	1	0	2.829739	-1.728537	9.065471
30	1	0	2.498528	-0.594739	10.384005
31	1	0	2.120325	-2.309800	10.582434
32	6	0	0.331804	1.977926	12.631457
33	1	0	0.492433	1.306364	13.481446
34	1	0	1.222097	1.925999	11.993907
35	1	0	0.265037	3.001231	13.021034
36	6	0	-2.805208	1.835915	12.695125
37	1	0	-2.848806	2.886553	13.008792
38	1	0	-3.707401	1.627489	12.108279
39	1	0	-2.848800	1.219462	13.597790
40	14	0	-1.139555	-0.760302	10.961119
41	1	0	-2.504679	-1.058234	10.398440
42	14	0	-0.847080	-4.590748	12.130254
43	14	0	-0.967593	-6.246270	13.853797
44	14	0	-1.939031	-5.679744	15.952547
45	1	0	-3.428812	-5.654127	15.759378

46	14	0	-1.297243	-3.466904	16.546508
47	14	0	-1.750042	-1.844274	14.865637
48	14	0	-0.774167	-2.306319	12.761500
49	6	0	-2.352245	-4.837509	10.971987
50	1	0	-2.324979	-4.134020	10.132643
51	1	0	-2.372867	-5.854106	10.560811
52	1	0	-3.293431	-4.672379	11.508561
53	6	0	-3.647583	-1.674884	14.683870
54	1	0	-4.099117	-2.616525	14.352084
55	1	0	-4.108298	-1.400487	15.641500
56	1	0	-3.910679	-0.903802	13.951307
57	6	0	-2.288700	-2.797134	18.041591
58	1	0	-2.165152	-3.402106	18.943357
59	1	0	-1.965094	-1.776903	18.282936
60	1	0	-3.359663	-2.758347	17.811723
61	6	0	-1.972677	-7.649470	13.026207
62	1	0	-1.479603	-7.991713	12.107466
63	1	0	-2.095768	-8.518069	13.678434
64	1	0	-2.972535	-7.295097	12.752589
65	6	0	0.814266	-6.854302	14.189981
66	1	0	0.826910	-7.670472	14.920851
67	1	0	1.290064	-7.217681	13.271533
68	1	0	1.440035	-6.048046	14.590739
69	6	0	0.742476	-5.071724	11.175739
70	1	0	0.679331	-6.108182	10.819889
71	1	0	0.918454	-4.434832	10.304267
72	1	0	1.622078	-4.996704	11.824366
73	6	0	-1.057738	-0.217647	15.599242
74	1	0	-1.217338	0.639683	14.939356
75	1	0	-1.543277	0.008295	16.556802

76	1	0	0.019629	-0.299498	15.782407
77	6	0	0.566197	-3.445053	16.965421
78	1	0	0.892550	-2.438706	17.254724
79	1	0	0.799769	-4.122731	17.795007
80	1	0	1.170978	-3.754618	16.104995
81	14	0	-1.492747	-7.368602	17.615217
82	1	0	0.005013	-7.464079	17.708057
83	14	0	-2.197051	-6.692733	19.793554
84	14	0	-2.371979	-8.411622	21.424908
85	14	0	-3.526869	-10.263698	20.530919
86	1	0	-3.737706	-11.319263	21.576049
87	1	0	-4.898575	-9.821142	20.119188
88	14	0	-2.420975	-11.160491	18.651150
89	14	0	-2.218203	-9.540347	16.922905
90	6	0	-3.414457	-12.641397	17.961379
91	1	0	-2.925976	-13.067139	17.076107
92	1	0	-3.493678	-13.436183	18.712784
93	1	0	-4.430771	-12.348265	17.676848
94	6	0	-3.925999	-9.402568	16.077056
95	1	0	-3.916796	-8.694591	15.241493
96	1	0	-4.247531	-10.376426	15.688076
97	1	0	-4.687655	-9.062836	16.788815
98	6	0	-0.933063	-10.282139	15.711864
99	1	0	-1.279124	-11.252465	15.333118
100	1	0	-0.734098	-9.642100	14.847698
101	1	0	0.021449	-10.448217	16.224536
102	6	0	-0.697240	-11.805587	19.162499
103	1	0	-0.778613	-12.541355	19.971501
104	1	0	-0.204621	-12.297648	18.315339
105	1	0	-0.039250	-11.001085	19.508298

106	6	0	-3.327484	-7.713320	22.926754
107	1	0	-3.408189	-8.468276	23.718031
108	1	0	-2.814874	-6.840493	23.349831
109	1	0	-4.342839	-7.407386	22.652410
110	6	0	-0.643053	-8.946675	22.035101
111	1	0	-0.131320	-8.106338	22.519550
112	1	0	-0.720111	-9.755987	22.770966
113	1	0	-0.004272	-9.298414	21.217845
114	6	0	-0.897428	-5.464834	20.480234
115	1	0	-0.660362	-4.657496	19.780746
116	1	0	-1.247442	-5.006397	21.413822
117	1	0	0.038849	-5.991210	20.699107
118	6	0	-3.920012	-5.874562	19.679931
119	1	0	-4.680251	-6.614304	19.402150
120	1	0	-4.213571	-5.446349	20.646167
121	1	0	-3.950434	-5.073443	18.934739

Si(6)-Me[a] dissociated radical (charge = 0, multiplicity = 2)



E(UB3LYP) = -6134.05889350 E_h

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

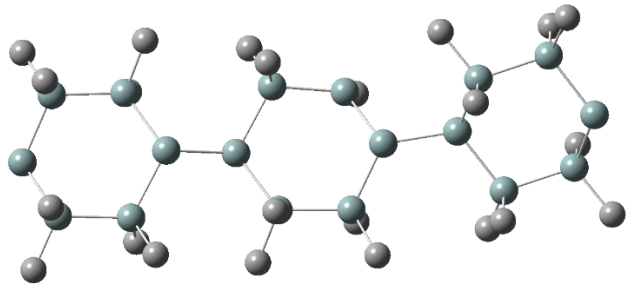
1	14	0	0.710202	2.702833	10.968946
2	14	0	0.594593	2.492830	8.617206
3	1	0	1.933257	2.043229	8.114360
4	1	0	0.365499	3.837532	7.991715
5	14	0	-1.042737	0.969674	7.849378
6	6	0	2.193633	3.813582	11.436762
7	1	0	2.081278	4.815800	11.006064
8	1	0	3.138287	3.397017	11.070108
9	1	0	2.274334	3.925480	12.525175
10	6	0	-0.884992	3.524579	11.622569
11	1	0	-0.824013	3.678113	12.706935
12	1	0	-1.770793	2.911157	11.423638
13	1	0	-1.043081	4.504729	11.157218
14	6	0	-2.783667	1.634918	8.264713
15	1	0	-2.946054	2.619640	7.810423
16	1	0	-2.934596	1.734333	9.345141
17	1	0	-3.558945	0.960194	7.881467
18	6	0	-0.903289	0.803231	5.949870
19	1	0	-1.653911	0.105817	5.557813
20	1	0	0.085031	0.438442	5.649014
21	1	0	-1.063255	1.772518	5.462487
22	14	0	-0.732429	-1.161560	8.856617
23	14	0	0.954841	0.554646	11.948709
24	6	0	-2.146362	-2.296820	8.250279
25	1	0	-2.008035	-3.328264	8.592219
26	1	0	-3.122559	-1.951562	8.608983
27	1	0	-2.180974	-2.315109	7.153718
28	6	0	0.920153	-1.907110	8.257144
29	1	0	0.894315	-2.059016	7.170988

30	1	0	1.770008	-1.252505	8.478223
31	1	0	1.119281	-2.879289	8.722390
32	6	0	2.647559	-0.199549	11.488023
33	1	0	2.757120	-1.200512	11.922341
34	1	0	2.785682	-0.287270	10.405213
35	1	0	3.462323	0.423065	11.877674
36	6	0	0.929558	0.748542	13.849708
37	1	0	1.728681	1.425121	14.177640
38	1	0	-0.021190	1.156267	14.210472
39	1	0	1.092392	-0.217497	14.341060
40	14	0	-0.788742	-0.900267	11.224070
41	1	0	-2.084465	-0.182487	11.478896
42	14	0	-1.326194	-4.966670	11.759495
43	14	0	-1.051426	-6.583271	13.483184
44	14	0	-2.715958	-6.338187	15.180031
45	1	0	-3.896067	-7.163628	14.748254
46	14	0	-3.511234	-4.112962	15.241697
47	14	0	-1.980044	-2.405915	14.697102
48	14	0	-0.804032	-2.824676	12.646156
49	1	0	0.632403	-2.984016	13.067863
50	6	0	-3.095179	-5.068494	11.051383
51	1	0	-3.257410	-4.331840	10.257017
52	1	0	-3.278339	-6.062660	10.625304
53	1	0	-3.850213	-4.897472	11.825200
54	6	0	-2.936361	-0.756485	14.642044
55	1	0	-3.701873	-0.753974	13.858647
56	1	0	-3.433227	-0.571343	15.602002
57	1	0	-2.260321	0.083247	14.444894
58	6	0	-5.240813	-3.922583	14.432903
59	1	0	-5.940836	-4.654792	14.849954

60	1	0	-5.644841	-2.921877	14.622986
61	1	0	-5.214293	-4.071188	13.346442
62	6	0	-1.209750	-8.313777	12.681306
63	1	0	-0.432579	-8.460449	11.920917
64	1	0	-1.111996	-9.120674	13.416102
65	1	0	-2.183719	-8.430795	12.192654
66	6	0	0.696950	-6.382520	14.221929
67	1	0	0.896221	-7.130944	14.995710
68	1	0	1.459594	-6.497296	13.441670
69	1	0	0.831632	-5.391715	14.670021
70	6	0	-0.097562	-5.403001	10.359516
71	1	0	-0.284642	-6.414379	9.977902
72	1	0	-0.189800	-4.709083	9.516373
73	1	0	0.939810	-5.363739	10.710630
74	6	0	-0.690128	-2.330143	16.102177
75	1	0	0.058748	-1.552842	15.912834
76	1	0	-1.177301	-2.105689	17.058341
77	1	0	-0.162027	-3.284109	16.212815
78	14	0	-2.118186	-7.118962	17.360954
79	1	0	-0.964679	-6.264995	17.806443
80	14	0	-3.886270	-6.756223	18.923853
81	14	0	-3.246026	-7.400433	21.119669
82	14	0	-2.499362	-9.640769	21.136557
83	1	0	-2.099704	-10.047671	22.524410
84	1	0	-3.646451	-10.533589	20.770865
85	14	0	-0.728251	-10.031987	19.625052
86	14	0	-1.360562	-9.381370	17.428379
87	6	0	-0.280963	-11.890969	19.623308
88	1	0	0.542336	-12.099591	18.928882
89	1	0	0.036332	-12.214728	20.621905

90	1	0	-1.135165	-12.510474	19.328311
91	6	0	-2.739412	-10.537290	16.787905
92	1	0	-3.043583	-10.266811	15.769712
93	1	0	-2.391491	-11.577326	16.766365
94	1	0	-3.631850	-10.499427	17.422401
95	6	0	0.184767	-9.640616	16.332764
96	1	0	0.519677	-10.683908	16.391951
97	1	0	-0.015535	-9.418420	15.279954
98	1	0	1.017364	-9.005984	16.656523
99	6	0	0.817364	-9.050991	20.168611
100	1	0	1.135719	-9.346832	21.175390
101	1	0	1.655013	-9.240212	19.486295
102	1	0	0.634951	-7.970875	20.179775
103	6	0	-4.739271	-7.217990	22.299376
104	1	0	-4.460456	-7.492331	23.323909
105	1	0	-5.102392	-6.183130	22.318741
106	1	0	-5.572965	-7.861585	21.997270
107	6	0	-1.852663	-6.251660	21.741581
108	1	0	-2.204764	-5.214298	21.796456
109	1	0	-1.518529	-6.542322	22.744670
110	1	0	-0.980626	-6.270710	21.078566
111	6	0	-4.372547	-4.910996	19.010874
112	1	0	-4.730756	-4.541346	18.043362
113	1	0	-5.172785	-4.761635	19.747139
114	1	0	-3.522629	-4.285523	19.305979
115	6	0	-5.423337	-7.751178	18.381672
116	1	0	-5.230416	-8.829542	18.365096
117	1	0	-6.258562	-7.573525	19.070077
118	1	0	-5.750065	-7.456107	17.377379

Si(6)-Me^{e} dissociated radical (charge = 0, multiplicity = 2)



E(UB3LYP) = -6134.05908879 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.496714	3.142268	10.307288
2	14	0	0.414996	2.477347	8.237192
3	1	0	1.879938	2.214326	8.414804
4	1	0	0.320987	3.588549	7.233665
5	14	0	-0.611985	0.520632	7.417316
6	6	0	0.393890	4.714113	10.932950
7	1	0	0.254044	5.542237	10.227751
8	1	0	1.471100	4.550135	11.045205
9	1	0	-0.002087	5.033526	11.904871
10	6	0	-2.346671	3.567456	10.093879
11	1	0	-2.762944	3.950941	11.033157
12	1	0	-2.940597	2.695614	9.798743
13	1	0	-2.486067	4.341124	9.329414
14	6	0	-2.462451	0.845086	7.071365
15	1	0	-2.591839	1.666299	6.356330
16	1	0	-3.014354	1.104352	7.981414
17	1	0	-2.933523	-0.046964	6.640674

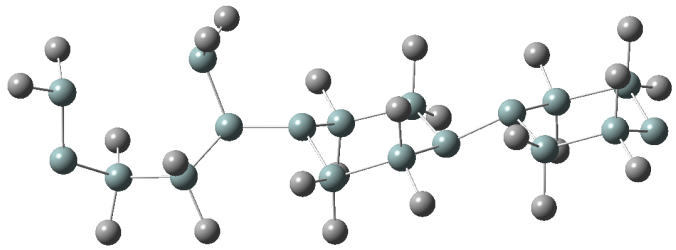
18	6	0	0.210223	0.008488	5.768527
19	1	0	-0.237054	-0.909991	5.368857
20	1	0	1.284708	-0.165311	5.891565
21	1	0	0.083758	0.795284	5.015068
22	14	0	-0.377757	-1.270647	8.961992
23	14	0	-0.238845	1.429041	11.935393
24	6	0	-1.556915	-2.626530	8.300537
25	1	0	-1.550750	-3.539016	8.902782
26	1	0	-2.587694	-2.254465	8.275732
27	1	0	-1.280493	-2.904808	7.275445
28	6	0	1.435688	-1.867103	8.881841
29	1	0	1.690620	-2.204485	7.869815
30	1	0	2.124766	-1.055294	9.143342
31	1	0	1.628124	-2.696822	9.570478
32	6	0	1.598384	1.367552	12.453736
33	1	0	1.776365	0.612856	13.227782
34	1	0	2.240678	1.122855	11.599642
35	1	0	1.926337	2.336876	12.848285
36	6	0	-1.318850	1.997387	13.410377
37	1	0	-0.982694	2.975860	13.776631
38	1	0	-2.365372	2.101050	13.101050
39	1	0	-1.292863	1.301517	14.253341
40	14	0	-0.933952	-0.747314	11.229720
41	1	0	-2.436440	-0.725414	11.281401
42	14	0	-0.917641	-4.658604	12.101564
43	14	0	-0.615304	-6.403013	13.697608
44	14	0	-1.605196	-5.822739	15.774589
45	1	0	-3.027814	-5.460851	15.454661
46	14	0	-0.570156	-3.835437	16.477822
47	14	0	-0.810486	-1.976079	15.046852

48	14	0	-0.239034	-2.467439	12.773530
49	1	0	1.263735	-2.482544	12.737015
50	6	0	-2.761740	-4.621599	11.605434
51	1	0	-2.959483	-3.869173	10.834024
52	1	0	-3.083274	-5.594731	11.215011
53	1	0	-3.394730	-4.384753	12.468589
54	6	0	-2.628401	-1.404617	15.131563
55	1	0	-3.305693	-2.218922	14.848792
56	1	0	-2.889704	-1.094842	16.150278
57	1	0	-2.824369	-0.562384	14.458872
58	6	0	-1.419132	-7.965332	12.936343
59	1	0	-0.996059	-8.181295	11.947193
60	1	0	-1.252247	-8.847221	13.564890
61	1	0	-2.501199	-7.839991	12.816923
62	6	0	1.249949	-6.744836	13.921841
63	1	0	1.428642	-7.539143	14.655722
64	1	0	1.696195	-7.065313	12.972680
65	1	0	1.790253	-5.853009	14.257610
66	6	0	0.152168	-5.227192	10.617565
67	1	0	-0.184976	-6.205120	10.251148
68	1	0	0.119971	-4.529857	9.776437
69	1	0	1.200965	-5.329467	10.919779
70	6	0	0.355901	-0.642219	15.763880
71	1	0	0.358014	0.283108	15.180767
72	1	0	0.057526	-0.391047	16.789226
73	1	0	1.386184	-1.014153	15.798370
74	6	0	1.234656	-4.118105	17.057027
75	1	0	1.641717	-3.207908	17.511361
76	1	0	1.280530	-4.918074	17.804088
77	1	0	1.892421	-4.398729	16.224723

78	14	0	-1.688280	-7.357183	17.599825
79	1	0	-0.482825	-7.036365	18.438966
80	14	0	-3.604231	-6.814044	18.904267
81	14	0	-3.600041	-8.019930	20.947981
82	14	0	-3.394844	-10.330481	20.487337
83	1	0	-3.386721	-11.112336	21.768238
84	1	0	-4.621479	-10.781944	19.753227
85	14	0	-1.499735	-10.896973	19.191478
86	14	0	-1.507729	-9.684289	17.148134
87	6	0	-1.520708	-12.771808	18.818455
88	1	0	-0.650720	-13.063404	18.217103
89	1	0	-1.493688	-13.353924	19.747445
90	1	0	-2.422714	-13.063098	18.269070
91	6	0	-2.952474	-10.289960	16.056281
92	1	0	-2.976776	-9.765314	15.094226
93	1	0	-2.851916	-11.362104	15.847110
94	1	0	-3.921842	-10.137495	16.543748
95	6	0	0.136970	-10.054921	16.245065
96	1	0	0.244505	-11.131247	16.060549
97	1	0	0.190266	-9.546040	15.276324
98	1	0	0.998461	-9.730688	16.839803
99	6	0	0.092740	-10.502949	20.169770
100	1	0	0.115769	-11.049758	21.120009
101	1	0	0.981192	-10.795739	19.596926
102	1	0	0.181293	-9.434624	20.396206
103	6	0	-5.226900	-7.703230	21.900130
104	1	0	-5.238733	-8.255401	22.847536
105	1	0	-5.344233	-6.637796	22.133939
106	1	0	-6.101005	-8.018281	21.319662
107	6	0	-2.144831	-7.451225	22.046071

108	1	0	-2.249804	-6.391141	22.307470
109	1	0	-2.110991	-8.022436	22.981449
110	1	0	-1.179580	-7.574559	21.542596
111	6	0	-3.633143	-4.940130	19.272068
112	1	0	-3.668269	-4.356421	18.344885
113	1	0	-4.516404	-4.677345	19.867900
114	1	0	-2.744637	-4.622810	19.828841
115	6	0	-5.179235	-7.246125	17.914218
116	1	0	-5.259232	-8.320743	17.715483
117	1	0	-6.076365	-6.944164	18.468575
118	1	0	-5.193093	-6.723957	16.950197

Si(2)-Si(3) dissociated radical (charge = 0, multiplicity = 3)



E(UB3LYP) = -6173.91376417 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-1.639123	2.031408	8.866302
2	14	0	0.005651	3.690091	8.463108
3	1	0	-0.031470	4.690710	9.577170
4	1	0	-0.395277	4.459703	7.234345
5	14	0	2.243055	2.971417	8.284040
6	6	0	-3.338845	2.905692	8.821013

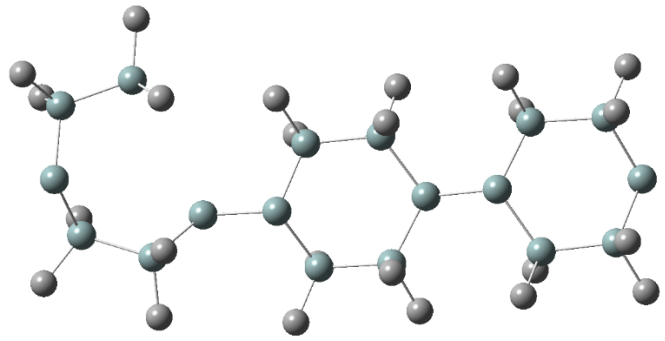
7	1	0	-3.510152	3.363747	7.839586
8	1	0	-3.412803	3.696522	9.575559
9	1	0	-4.151927	2.192400	9.003655
10	6	0	-1.614088	0.748786	7.455333
11	1	0	-2.429678	0.025993	7.576842
12	1	0	-0.675127	0.184893	7.431599
13	1	0	-1.742898	1.238811	6.482630
14	6	0	2.557713	1.755233	6.851364
15	1	0	2.364284	2.228145	5.879080
16	1	0	1.917959	0.869985	6.931071
17	1	0	3.600760	1.417356	6.855644
18	6	0	3.465482	4.431847	8.180030
19	1	0	4.501655	4.075582	8.221155
20	1	0	3.315958	5.133366	9.007273
21	1	0	3.339257	4.986348	7.240438
22	14	0	1.054511	-1.707808	9.674679
23	14	0	-1.326682	1.048504	11.023078
24	6	0	1.217787	-3.476059	8.978727
25	1	0	1.286306	-4.212406	9.790644
26	1	0	0.361762	-3.743437	8.351126
27	1	0	2.125832	-3.566439	8.370455
28	6	0	2.585848	-1.320880	10.742437
29	1	0	3.505103	-1.470298	10.163685
30	1	0	2.580572	-0.287253	11.103251
31	1	0	2.630623	-1.984374	11.616740
32	6	0	0.157609	1.853737	11.910290
33	1	0	0.343056	1.393556	12.887707
34	1	0	1.074128	1.766907	11.315626
35	1	0	-0.026231	2.922527	12.074572
36	6	0	-2.896366	1.390439	12.057213

37	1	0	-3.094294	2.467553	12.117673
38	1	0	-3.781178	0.914430	11.619700
39	1	0	-2.785205	1.015584	13.080545
40	14	0	-0.983619	-1.292707	10.789698
41	1	0	-2.058864	-1.760606	9.850791
42	14	0	-2.487243	-4.618867	12.163704
43	14	0	-2.274452	-6.373707	13.760189
44	14	0	-2.373184	-5.714658	16.055699
45	1	0	-3.830466	-5.502458	16.358082
46	14	0	-1.324959	-3.608586	16.470012
47	14	0	-1.761290	-1.942600	14.828503
48	14	0	-1.135144	-2.747433	12.691840
49	1	0	0.259260	-3.274832	12.893401
50	6	0	-4.314124	-4.078732	12.026121
51	1	0	-4.428586	-3.275084	11.288777
52	1	0	-4.936277	-4.920364	11.697678
53	1	0	-4.717166	-3.719171	12.978604
54	6	0	-3.610981	-1.471459	14.911027
55	1	0	-4.258267	-2.348443	14.802955
56	1	0	-3.838454	-1.011940	15.880983
57	1	0	-3.889207	-0.753178	14.131750
58	6	0	-2.008502	-2.839836	18.085697
59	1	0	-1.861175	-3.475744	18.962562
60	1	0	-1.518888	-1.878825	18.288504
61	1	0	-3.084020	-2.650072	17.991904
62	6	0	-3.727924	-7.554803	13.361574
63	1	0	-3.665315	-7.899503	12.321465
64	1	0	-3.750352	-8.440463	14.002526
65	1	0	-4.685519	-7.035240	13.481246
66	6	0	-0.608301	-7.249513	13.431167

67	1	0	-0.447817	-8.093662	14.110622
68	1	0	-0.565056	-7.632534	12.404356
69	1	0	0.230596	-6.555856	13.562296
70	6	0	-1.987759	-5.334695	10.462478
71	1	0	-2.598782	-6.210528	10.210453
72	1	0	-2.136370	-4.587553	9.673696
73	1	0	-0.936306	-5.640196	10.439603
74	6	0	-0.737387	-0.401253	15.314802
75	1	0	-0.966641	0.448958	14.662143
76	1	0	-0.956804	-0.093636	16.344768
77	1	0	0.338909	-0.595078	15.245550
78	6	0	0.565407	-3.844354	16.602151
79	1	0	1.059941	-2.899276	16.857412
80	1	0	0.832179	-4.579695	17.368987
81	1	0	0.984083	-4.190715	15.650273
82	14	0	-1.634359	-7.458130	17.549729
83	1	0	-0.190044	-7.710097	17.216573
84	14	0	-1.653457	-6.772771	19.841043
85	14	0	-1.362111	-8.514803	21.431387
86	14	0	-2.822948	-10.305856	20.970944
87	1	0	-2.704947	-11.377025	22.014507
88	1	0	-4.234645	-9.809172	21.056594
89	14	0	-2.455810	-11.193860	18.818224
90	14	0	-2.758460	-9.531394	17.145939
91	6	0	-3.694372	-12.612328	18.486719
92	1	0	-3.551171	-13.040582	17.486828
93	1	0	-3.560309	-13.419917	19.216475
94	1	0	-4.731221	-12.266337	18.559351
95	6	0	-4.633866	-9.211599	16.971233
96	1	0	-4.851313	-8.465373	16.199274

97	1	0	-5.163346	-10.134342	16.704751
98	1	0	-5.059380	-8.845908	17.913173
99	6	0	-2.075640	-10.337192	15.549099
100	1	0	-2.602099	-11.277623	15.341479
101	1	0	-2.177934	-9.699868	14.666659
102	1	0	-1.011275	-10.572160	15.664944
103	6	0	-0.692593	-11.920398	18.708155
104	1	0	-0.528025	-12.673878	19.487598
105	1	0	-0.538340	-12.408033	17.738015
106	1	0	0.079206	-11.150984	18.819129
107	6	0	-1.730267	-7.805905	23.168929
108	1	0	-1.569344	-8.570004	23.938995
109	1	0	-1.072946	-6.958154	23.399007
110	1	0	-2.766608	-7.460893	23.253570
111	6	0	0.447795	-9.124869	21.423452
112	1	0	1.129054	-8.308061	21.691371
113	1	0	0.594000	-9.931041	22.152246
114	1	0	0.752994	-9.502715	20.441700
115	6	0	-0.199469	-5.571559	20.171031
116	1	0	-0.208392	-4.694974	19.518036
117	1	0	-0.228786	-5.213342	21.208025
118	1	0	0.758564	-6.083625	20.024267
119	6	0	-3.320253	-5.920770	20.226092
120	1	0	-4.149924	-6.633130	20.145921
121	1	0	-3.327023	-5.518624	21.246515
122	1	0	-3.527576	-5.093623	19.538791

Si(3)-Si(4) dissociated radical (charge = 0, multiplicity = 3)



E(UB3LYP) = -6173.91906634 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-1.125970	3.172216	9.521424
2	14	0	0.397611	2.457348	7.870532
3	1	0	1.787300	2.526801	8.428120
4	1	0	0.383975	3.390782	6.696089
5	14	0	-0.046717	0.246733	7.185005
6	6	0	-0.699051	4.955345	10.064312
7	1	0	-0.769524	5.644077	9.213789
8	1	0	0.318552	5.022957	10.464299
9	1	0	-1.390197	5.311296	10.838316
10	6	0	-2.897637	3.190425	8.807033
11	1	0	-3.604650	3.590273	9.544003
12	1	0	-3.242402	2.189483	8.525653
13	1	0	-2.954509	3.826056	7.915284
14	6	0	-1.786320	0.153043	6.401711
15	1	0	-1.885210	0.866691	5.575109
16	1	0	-2.578070	0.370410	7.126847
17	1	0	-1.971611	-0.849575	5.997890
18	6	0	1.220310	-0.292088	5.857898

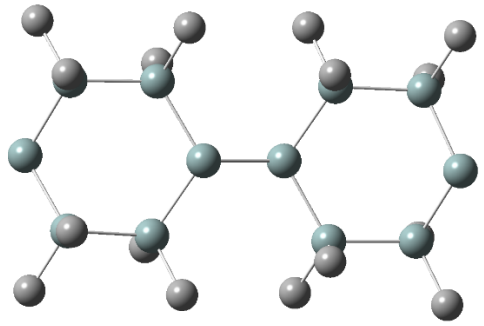
19	1	0	1.039195	-1.324407	5.533817
20	1	0	2.248215	-0.232192	6.231966
21	1	0	1.149403	0.351531	4.972772
22	14	0	0.107404	-1.258416	9.018570
23	14	0	-1.019516	1.765092	11.434299
24	6	0	-0.652116	-2.892812	8.373501
25	1	0	-0.647855	-3.688537	9.123244
26	1	0	-1.692497	-2.735432	8.066377
27	1	0	-0.098721	-3.256603	7.498439
28	6	0	1.961172	-1.498167	9.412061
29	1	0	2.502656	-1.865743	8.531842
30	1	0	2.421937	-0.549472	9.711281
31	1	0	2.119100	-2.213420	10.226565
32	6	0	0.576438	2.229687	12.377299
33	1	0	0.717367	1.626801	13.280144
34	1	0	1.458284	2.084225	11.742205
35	1	0	0.556917	3.284279	12.678119
36	6	0	-2.572074	2.215189	12.460730
37	1	0	-2.543780	3.269354	12.764757
38	1	0	-3.476499	2.067622	11.859164
39	1	0	-2.680623	1.611107	13.366213
40	14	0	-1.045803	-0.585972	11.002167
41	1	0	-2.490976	-0.917639	10.751779
42	14	0	-0.562680	-4.240072	12.528828
43	14	0	-0.374746	-5.663210	14.430831
44	14	0	-1.575844	-4.892057	16.317915
45	1	0	-3.037365	-4.911858	15.975252
46	14	0	-0.972062	-2.649716	16.788796
47	14	0	-1.480761	-1.232911	14.947922
48	14	0	-0.390342	-1.885774	12.924614

49	1	0	1.070893	-1.605834	13.138544
50	6	0	-2.245472	-4.603829	11.699119
51	1	0	-2.380610	-4.025826	10.778461
52	1	0	-2.333123	-5.666898	11.444217
53	1	0	-3.076537	-4.354433	12.369377
54	6	0	-3.371749	-1.233529	14.679907
55	1	0	-3.735536	-2.238487	14.436166
56	1	0	-3.894753	-0.902724	15.585441
57	1	0	-3.666685	-0.567091	13.861397
58	6	0	-1.934865	-2.019818	18.315327
59	1	0	-1.703598	-2.633149	19.194420
60	1	0	-1.666834	-0.982939	18.552928
61	1	0	-3.018293	-2.058344	18.155275
62	6	0	-1.036281	-7.382974	13.919150
63	1	0	-0.489265	-7.778420	13.054121
64	1	0	-0.920123	-8.096481	14.744617
65	1	0	-2.099267	-7.343424	13.656711
66	6	0	1.465157	-5.868840	14.899997
67	1	0	1.575185	-6.565897	15.739259
68	1	0	2.035624	-6.273191	14.054900
69	1	0	1.929091	-4.920311	15.191187
70	6	0	0.865429	-4.826969	11.395767
71	1	0	0.761389	-5.897627	11.177558
72	1	0	0.906699	-4.298753	10.439401
73	1	0	1.830186	-4.684134	11.895602
74	6	0	-0.914877	0.501737	15.528227
75	1	0	-1.110699	1.288251	14.794792
76	1	0	-1.438051	0.774874	16.453428
77	1	0	0.160186	0.507781	15.742659
78	6	0	0.891141	-2.546826	17.189704

79	1	0	1.166777	-1.522327	17.468632
80	1	0	1.152444	-3.201873	18.029103
81	1	0	1.511111	-2.834483	16.333643
82	14	0	-1.298837	-6.363851	18.124582
83	1	0	0.091949	-6.272220	18.680100
84	14	0	-2.907977	-6.666291	19.818559
85	14	0	-2.392164	-8.639217	21.047912
86	14	0	-3.399601	-10.592680	20.146724
87	1	0	-3.736448	-11.465214	21.322511
88	1	0	-4.726183	-10.233070	19.551176
89	14	0	-2.242011	-11.990320	18.622557
90	14	0	-2.048667	-11.004812	16.484635
91	6	0	-3.219082	-13.635206	18.526332
92	1	0	-2.725708	-14.342950	17.848986
93	1	0	-3.284051	-14.105478	19.515204
94	1	0	-4.240230	-13.477108	18.162270
95	6	0	-3.641629	-10.159053	15.863239
96	1	0	-3.460899	-9.650277	14.909323
97	1	0	-4.446723	-10.889363	15.705183
98	1	0	-4.002777	-9.411585	16.577522
99	6	0	-1.428345	-12.230956	15.156487
100	1	0	-2.179095	-13.004290	14.944205
101	1	0	-1.217874	-11.707469	14.216331
102	1	0	-0.507222	-12.733422	15.471168
103	6	0	-0.498802	-12.393168	19.287050
104	1	0	-0.556175	-12.870754	20.272729
105	1	0	0.020911	-13.085981	18.613803
106	1	0	0.118419	-11.493775	19.381878
107	6	0	-3.093499	-8.442849	22.816402
108	1	0	-2.856561	-9.322729	23.426174

109	1	0	-2.666786	-7.563372	23.313644
110	1	0	-4.183475	-8.328451	22.809951
111	6	0	-0.501276	-8.856019	21.186555
112	1	0	-0.047575	-7.993888	21.690448
113	1	0	-0.246427	-9.751219	21.766281
114	1	0	-0.032500	-8.946815	20.200586
115	6	0	-2.911291	-5.186697	21.033536
116	1	0	-3.161859	-4.255142	20.512989
117	1	0	-3.655179	-5.339691	21.825688
118	1	0	-1.934795	-5.051653	21.511724
119	6	0	-4.631178	-6.765057	19.010480
120	1	0	-4.698838	-7.591474	18.295053
121	1	0	-5.408824	-6.916869	19.768823
122	1	0	-4.863021	-5.837029	18.474582

Si(4)-Si(5) dissociated dimer radical (charge = 0, multiplicity = 2)



E(UB3LYP) = -4115.76713951 E_h

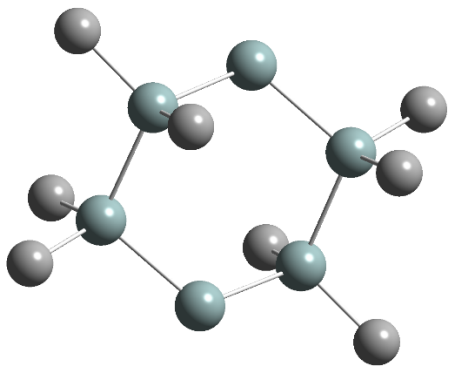
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.669829	3.145642	9.998197
2	14	0	0.794816	2.491810	8.270884

3	1	0	2.186075	2.388137	8.818080
4	1	0	0.853277	3.545127	7.204492
5	14	0	0.178817	0.404175	7.365543
6	6	0	-0.047846	4.766781	10.799307
7	1	0	-0.005450	5.573139	10.057209
8	1	0	0.956051	4.648994	11.221786
9	1	0	-0.716725	5.092625	11.605788
10	6	0	-2.400128	3.489806	9.264569
11	1	0	-3.083625	3.852646	10.041615
12	1	0	-2.848676	2.596056	8.817510
13	1	0	-2.345300	4.259717	8.485554
14	6	0	-1.577733	0.497358	6.619929
15	1	0	-1.644301	1.284133	5.859066
16	1	0	-2.338880	0.701884	7.380877
17	1	0	-1.839171	-0.452581	6.137692
18	6	0	1.384395	-0.080034	5.962056
19	1	0	1.122217	-1.055711	5.534578
20	1	0	2.419090	-0.135242	6.318101
21	1	0	1.350035	0.658049	5.151624
22	14	0	0.255217	-1.278710	9.041476
23	14	0	-0.813904	1.501714	11.711031
24	6	0	-0.431942	-2.838952	8.170394
25	1	0	-0.454020	-3.723009	8.812766
26	1	0	-1.454796	-2.660659	7.818714
27	1	0	0.181942	-3.081893	7.293652
28	6	0	2.082265	-1.547701	9.529614
29	1	0	2.678121	-1.845336	8.658103
30	1	0	2.520595	-0.625989	9.929832
31	1	0	2.194323	-2.325383	10.293190
32	6	0	0.752253	1.661081	12.794036

33	1	0	0.742628	0.952303	13.629073
34	1	0	1.657737	1.466650	12.207101
35	1	0	0.838435	2.671776	13.210934
36	6	0	-2.361394	2.020708	12.712569
37	1	0	-2.253153	3.052516	13.070999
38	1	0	-3.255957	1.982925	12.080268
39	1	0	-2.546469	1.387100	13.583924
40	14	0	-1.028927	-0.771170	10.993124
41	1	0	-2.465431	-0.930434	10.578356
42	14	0	-0.803036	-4.599759	12.079309
43	14	0	-0.939514	-6.228072	13.814668
44	14	0	-2.618819	-5.622203	15.337877
45	1	0	-3.968520	-5.666153	14.676038
46	14	0	-2.264708	-3.530098	16.340429
47	14	0	-2.062817	-1.814748	14.692974
48	14	0	-0.683791	-2.327397	12.806528
49	1	0	0.732442	-2.122344	13.266856
50	6	0	-2.350950	-4.825990	10.983821
51	1	0	-2.371569	-4.113961	10.152235
52	1	0	-2.388542	-5.837793	10.562321
53	1	0	-3.264866	-4.676832	11.570703
54	6	0	-3.826740	-1.407892	14.085018
55	1	0	-4.297760	-2.290102	13.635916
56	1	0	-4.461273	-1.079768	14.917054
57	1	0	-3.824883	-0.614147	13.330570
58	6	0	-3.731075	-3.078860	17.478480
59	1	0	-3.820377	-3.802705	18.297116
60	1	0	-3.593423	-2.085908	17.924179
61	1	0	-4.679790	-3.073724	16.931139
62	6	0	-1.334880	-7.915377	13.010193

63	1	0	-0.564026	-8.194755	12.281283
64	1	0	-1.376707	-8.704620	13.770089
65	1	0	-2.299243	-7.899305	12.490947
66	6	0	0.733262	-6.382054	14.720916
67	1	0	0.686968	-7.160254	15.491799
68	1	0	1.529837	-6.656032	14.018594
69	1	0	1.027933	-5.446711	15.209297
70	6	0	0.784430	-5.055610	11.108441
71	1	0	0.712906	-6.078947	10.718506
72	1	0	0.980010	-4.391972	10.261415
73	1	0	1.657879	-5.013158	11.769377
74	6	0	-1.324196	-0.323911	15.643055
75	1	0	-1.197651	0.565162	15.018971
76	1	0	-1.971725	-0.048887	16.485471
77	1	0	-0.340591	-0.582582	16.051267
78	6	0	-0.682403	-3.587283	17.406479
79	1	0	-0.524290	-2.627623	17.913247
80	1	0	-0.758945	-4.363062	18.177226
81	1	0	0.210816	-3.798109	16.808084

Si(4)-Si(5) dissociated monomer radical (charge = 0, multiplicity = 2)



E(UB3LYP) = -2058.15941768 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.862114	3.188792	9.950872
2	14	0	0.880150	2.525404	8.489163
3	1	0	2.156684	2.457911	9.272907
4	1	0	1.102860	3.594291	7.459558
5	14	0	0.560952	0.443752	7.405534
6	6	0	-0.410287	4.861924	10.759025
7	1	0	-0.272095	5.636936	9.995465
8	1	0	0.517789	4.793904	11.337268
9	1	0	-1.205448	5.198279	11.435854
10	6	0	-2.476681	3.422338	8.959529
11	1	0	-3.288903	3.760454	9.614482
12	1	0	-2.800755	2.491867	8.480811
13	1	0	-2.347323	4.176515	8.174083
14	6	0	-0.987982	0.525481	6.293169
15	1	0	-0.896909	1.327696	5.551210
16	1	0	-1.898081	0.708126	6.875014
17	1	0	-1.124184	-0.416947	5.748966
18	6	0	2.075410	0.065228	6.301766
19	1	0	1.955457	-0.895926	5.786859
20	1	0	2.999485	0.020065	6.888442
21	1	0	2.202988	0.840520	5.536652
22	14	0	0.281337	-1.252517	9.050982
23	14	0	-1.166930	1.512987	11.613042
24	6	0	-0.204236	-2.907801	8.232724
25	1	0	-0.319503	-3.695381	8.986566
26	1	0	-1.150680	-2.825652	7.687116

27	1	0	0.566475	-3.234165	7.523489
28	6	0	1.916063	-1.497005	10.003849
29	1	0	2.717464	-1.813559	9.325170
30	1	0	2.242985	-0.574080	10.495676
31	1	0	1.806836	-2.267655	10.775733
32	6	0	0.355355	1.470550	12.762186
33	1	0	0.245663	0.694967	13.529064
34	1	0	1.278396	1.265795	12.208216
35	1	0	0.481617	2.432385	13.273917
36	6	0	-2.718242	1.891241	12.659218
37	1	0	-2.629928	2.869102	13.148539
38	1	0	-3.624280	1.903617	12.043567
39	1	0	-2.855671	1.136599	13.442448
40	14	0	-1.412329	-0.572769	10.543532
41	1	0	-2.751506	-0.645069	9.863038

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