AB-type monomer of polyhedral oligomeric silsesquioxane

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1. NMR spectra
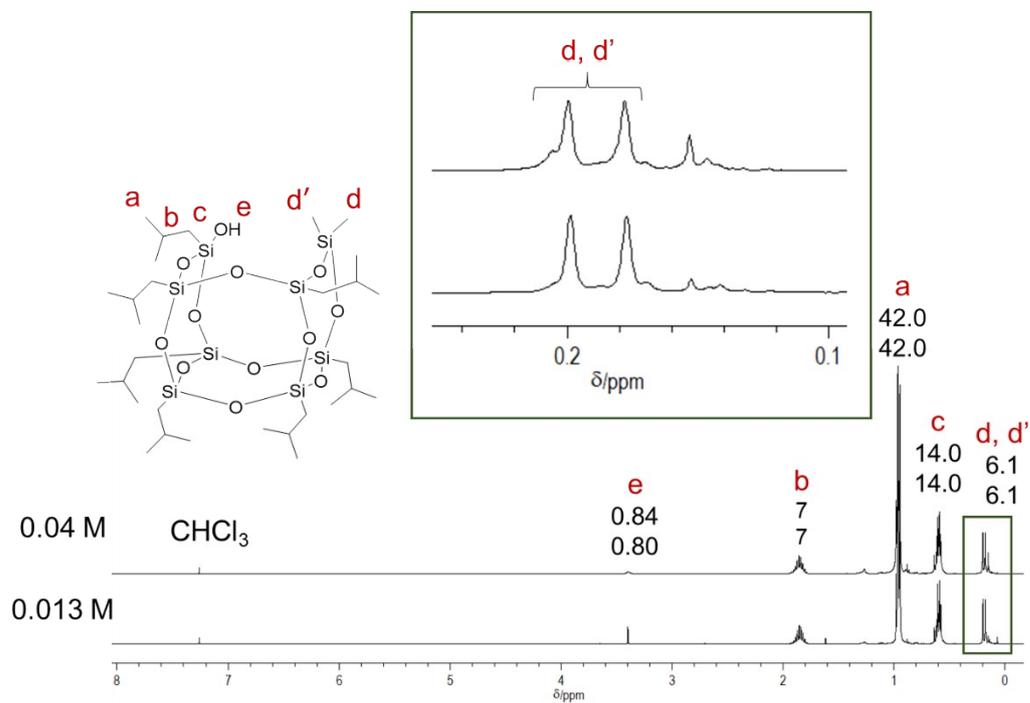
**Figure S1.** ^{1}H-NMR spectra (400 MHz) of **2** in CDCl$_3$.
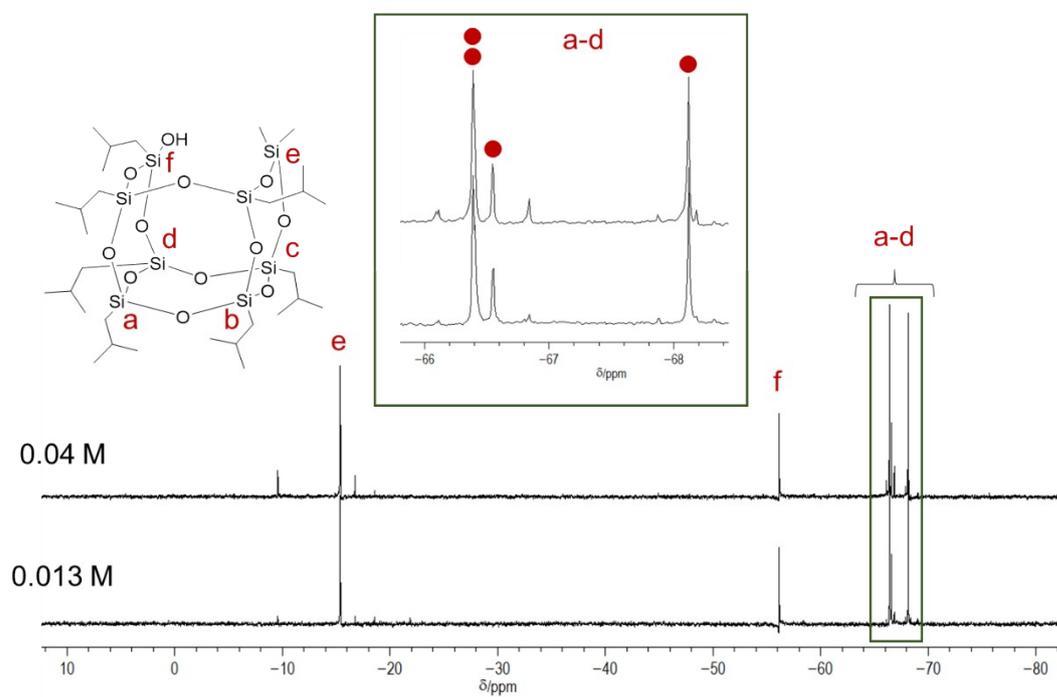
**Figure S2.** ^{29}Si-NMR spectra (80 MHz) of **2** in CDCl$_3$.
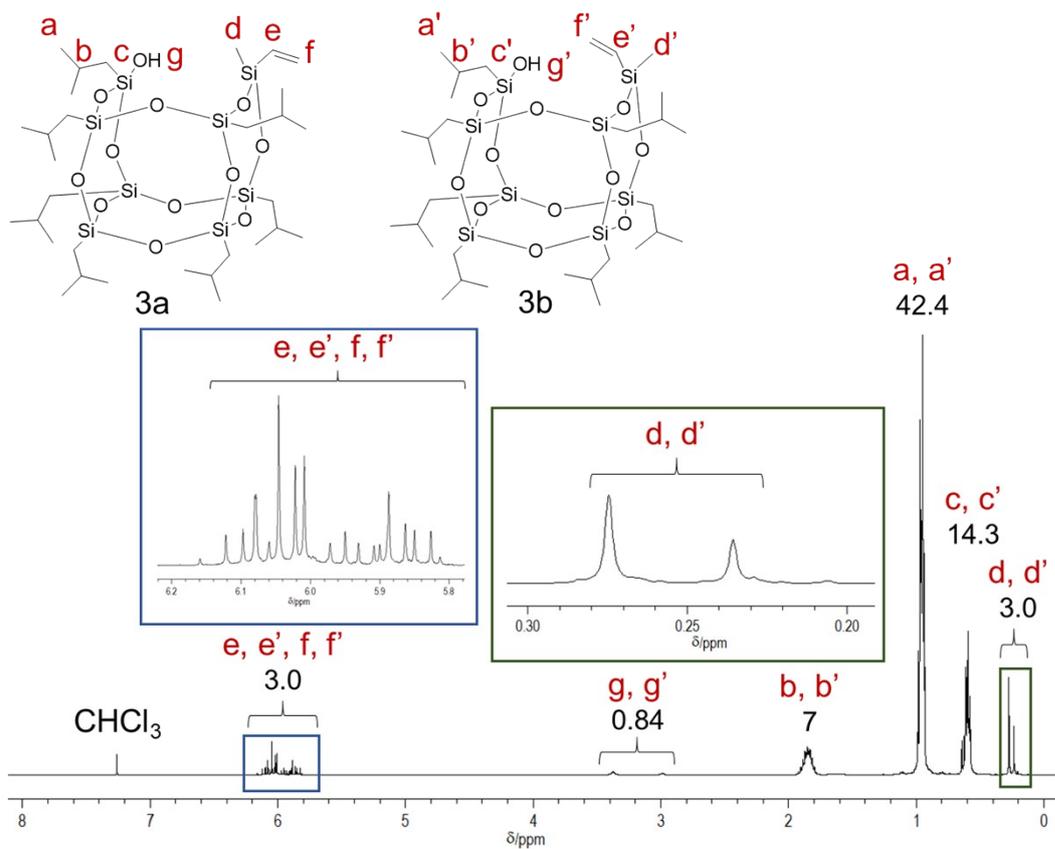
Figure S3. ^{1}H-NMR spectra (400 MHz) of **3** in CDCl$_3$.
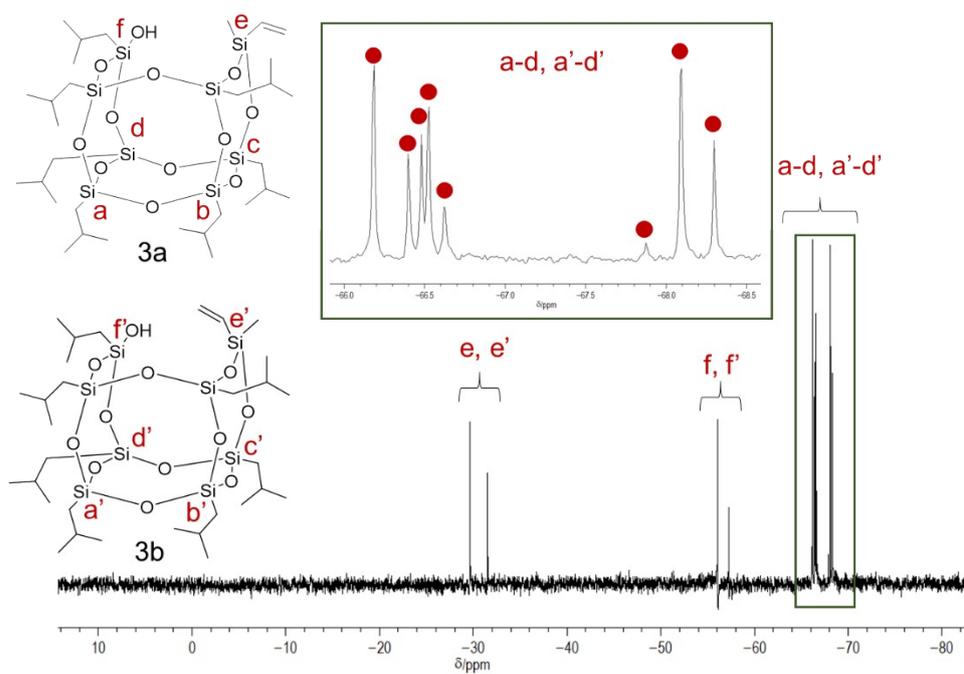
Figure S4. ^{29}Si-NMR spectra (80 MHz) of **3** in CDCl$_3$.
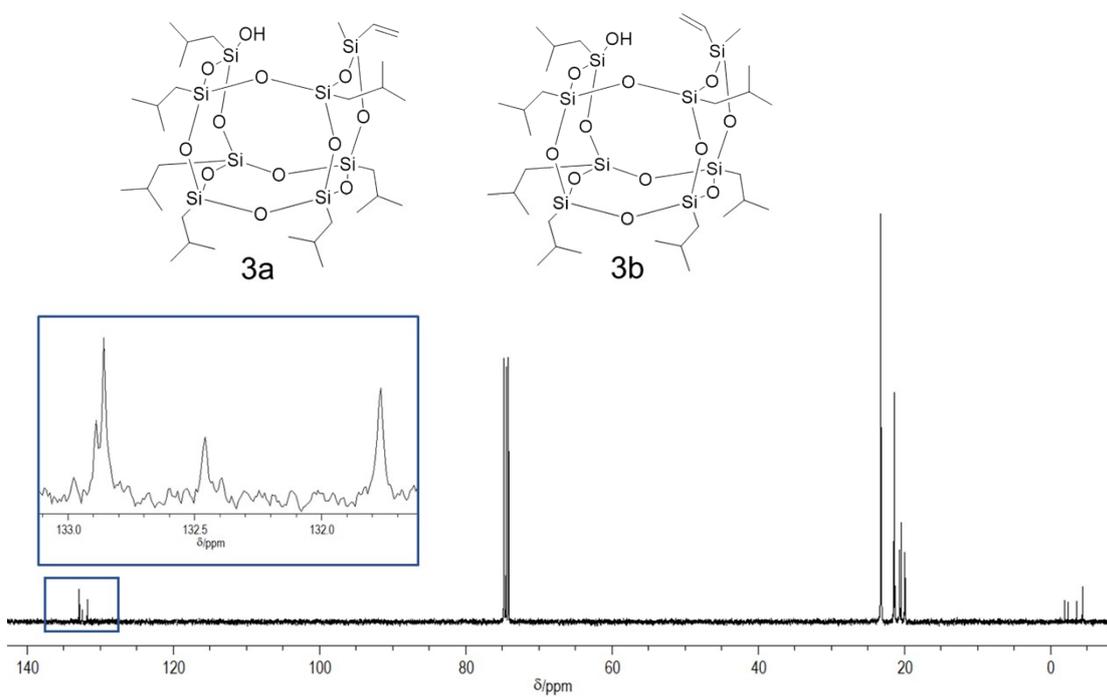
Figure S5. ^{13}C-NMR spectra (100 MHz) of **3** in CDCl$_3$.
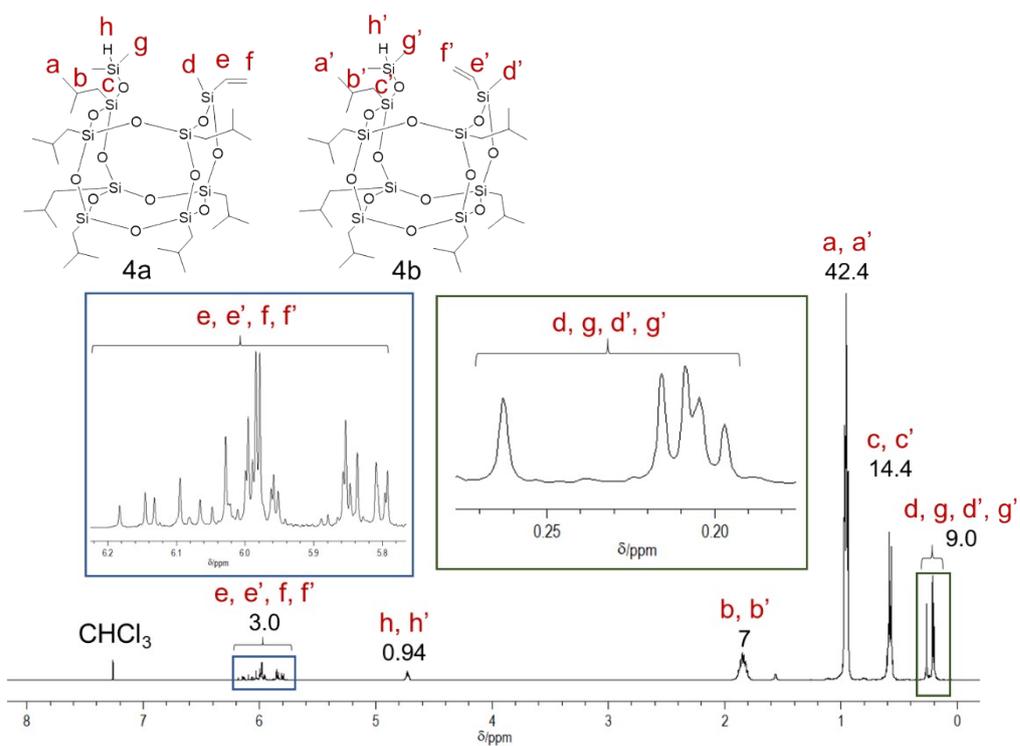
Figure S6. ^{1}H-NMR spectra (400 MHz) of **4** in CDCl$_3$.
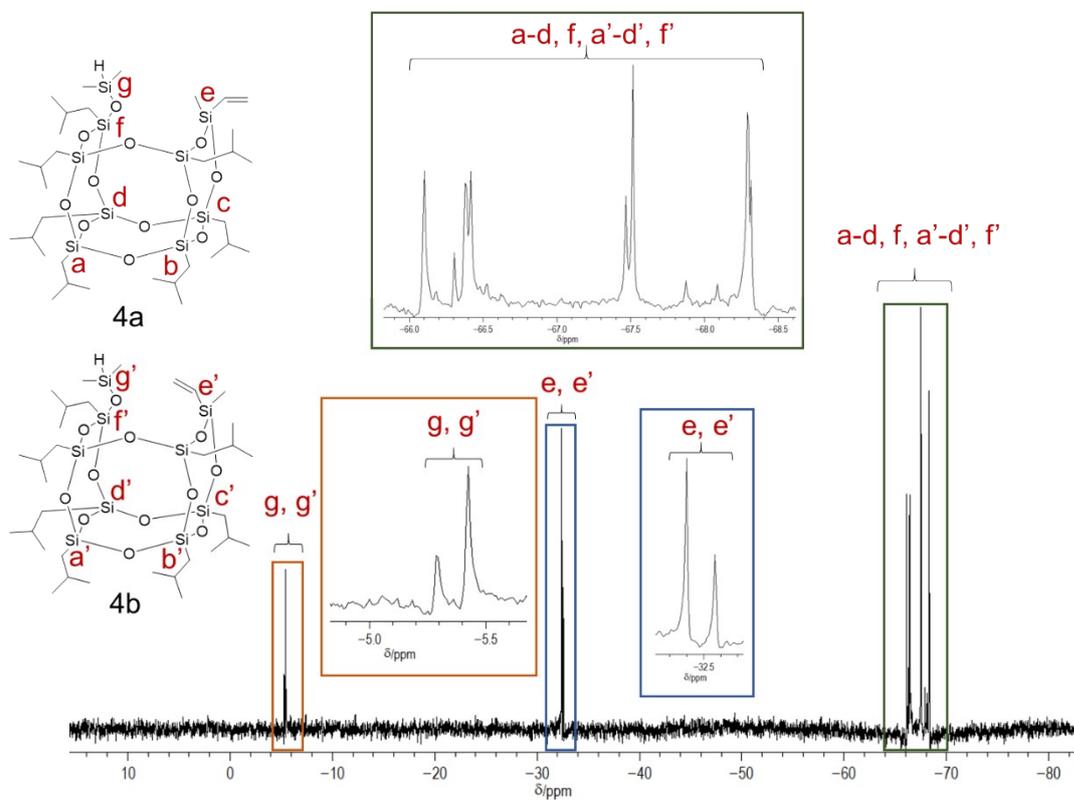
Figure S7. ^{29}Si-NMR spectra (80 MHz) of **4** in CDCl$_3$.
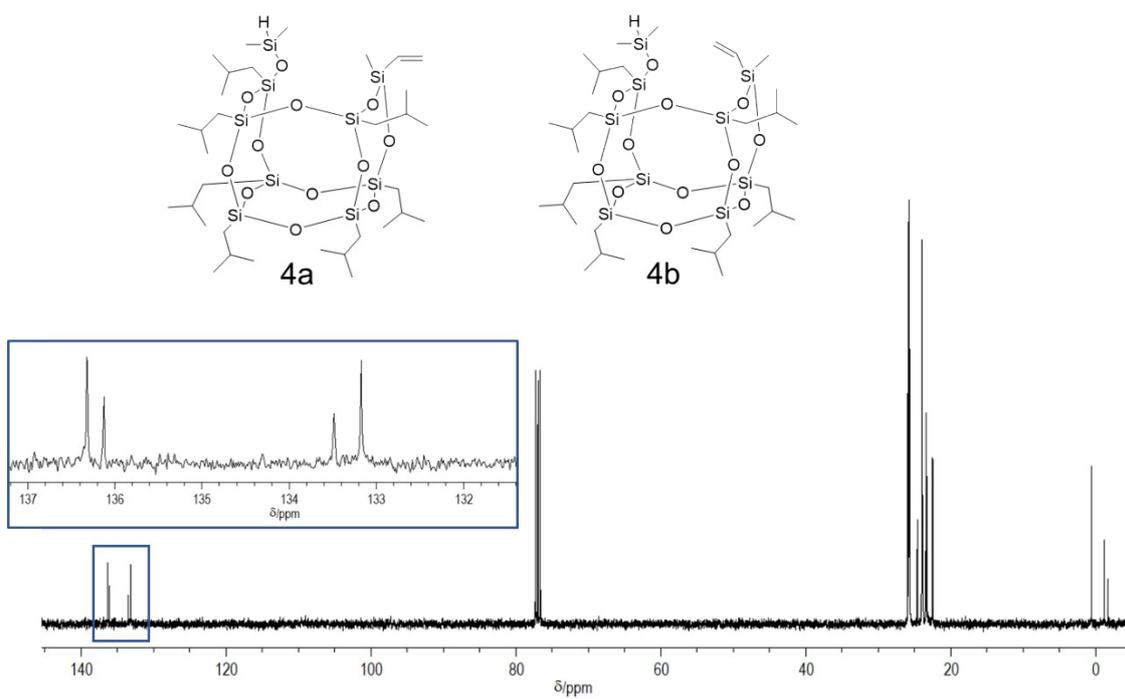
Figure S8. ^{13}C-NMR spectra (100 MHz) of **4** in CDCl$_3$.
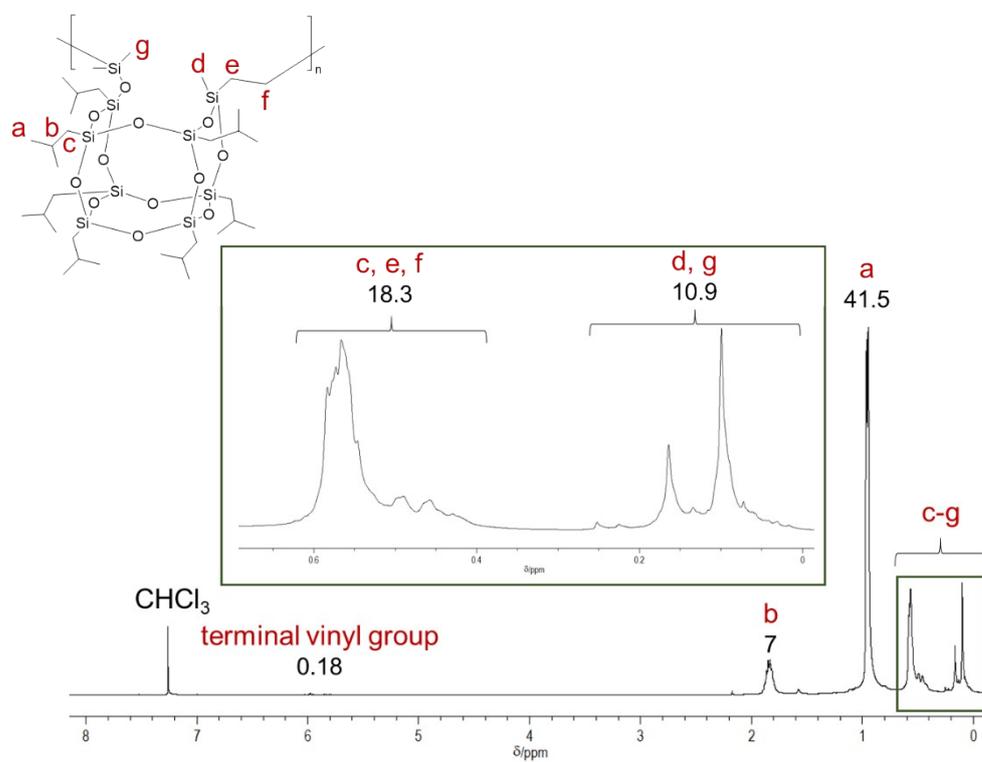
Figure S9. ^{1}H-NMR spectra (400 MHz) of **5** in CDCl$_3$.
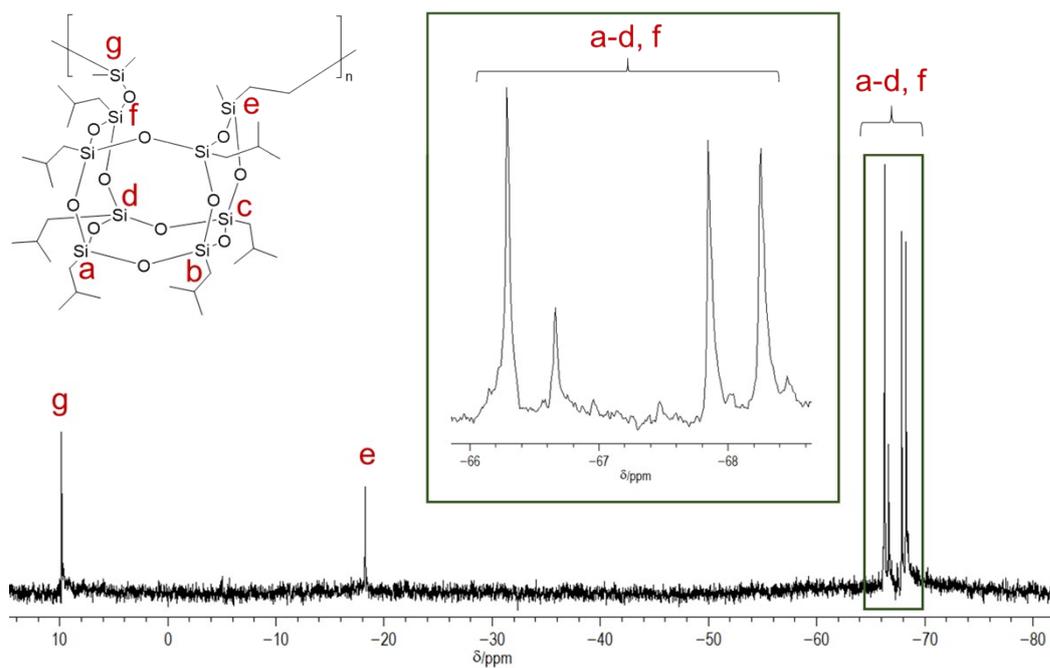
Figure S10. ^{29}Si-NMR spectra (80 MHz) of **5** in CDCl$_3$.
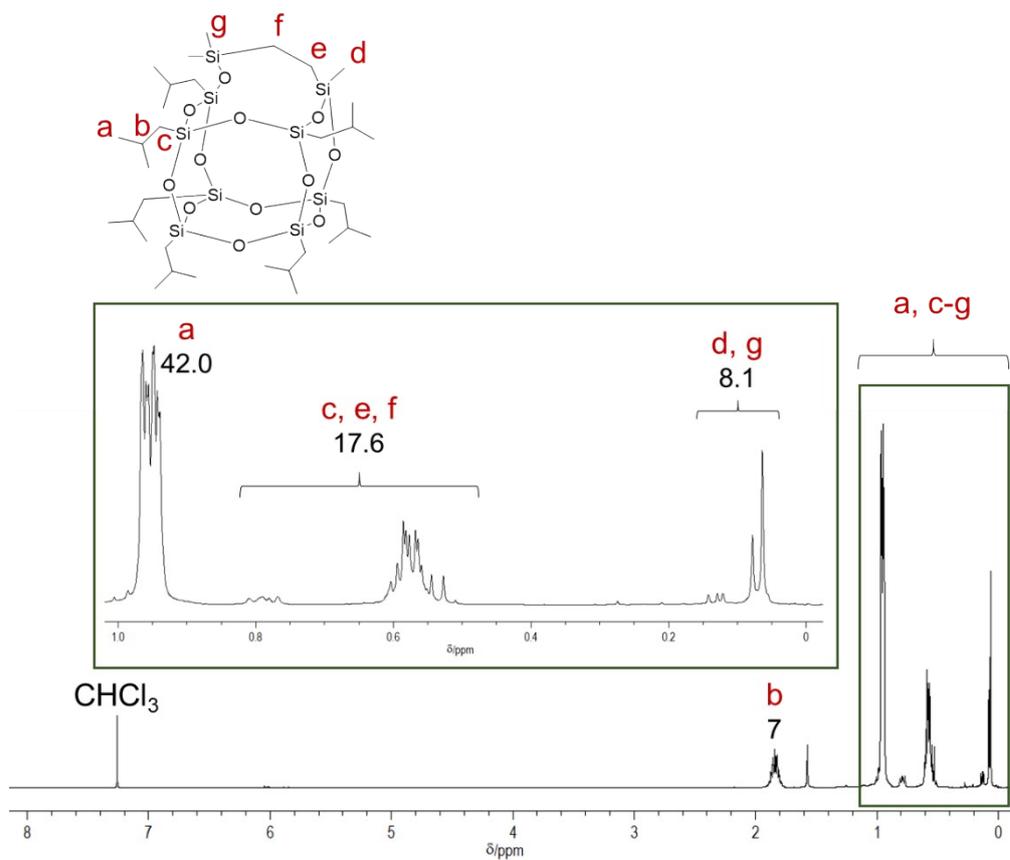
**Figure S11.** ^{1}H-NMR spectra (400 MHz) of **6** in CDCl$_3$.
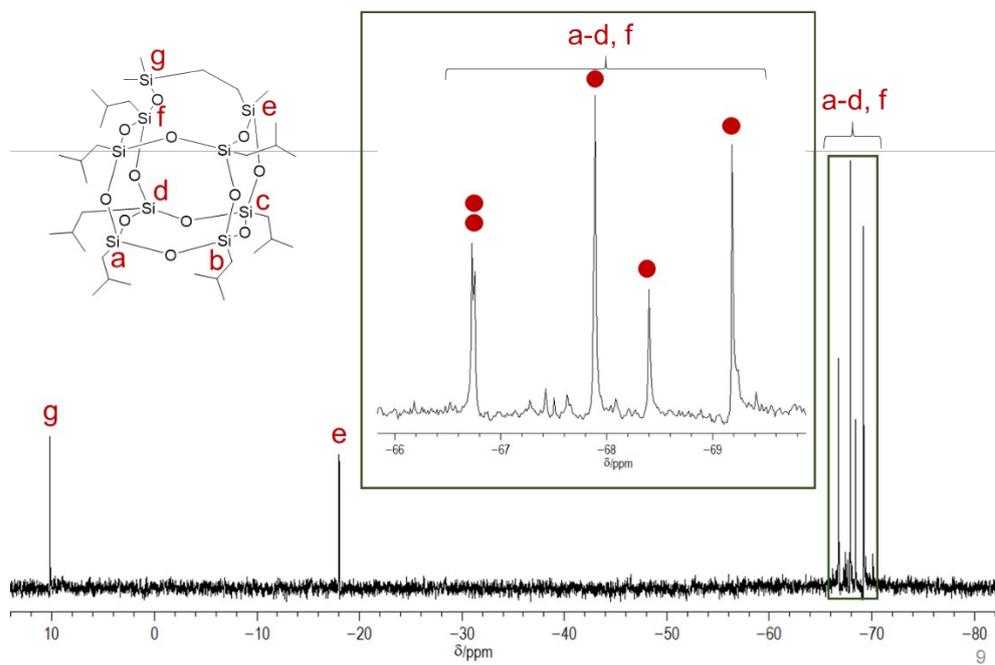
Figure S12. ^{29}Si-NMR spectra (80 MHz) of **6** in CDCl$_3$.
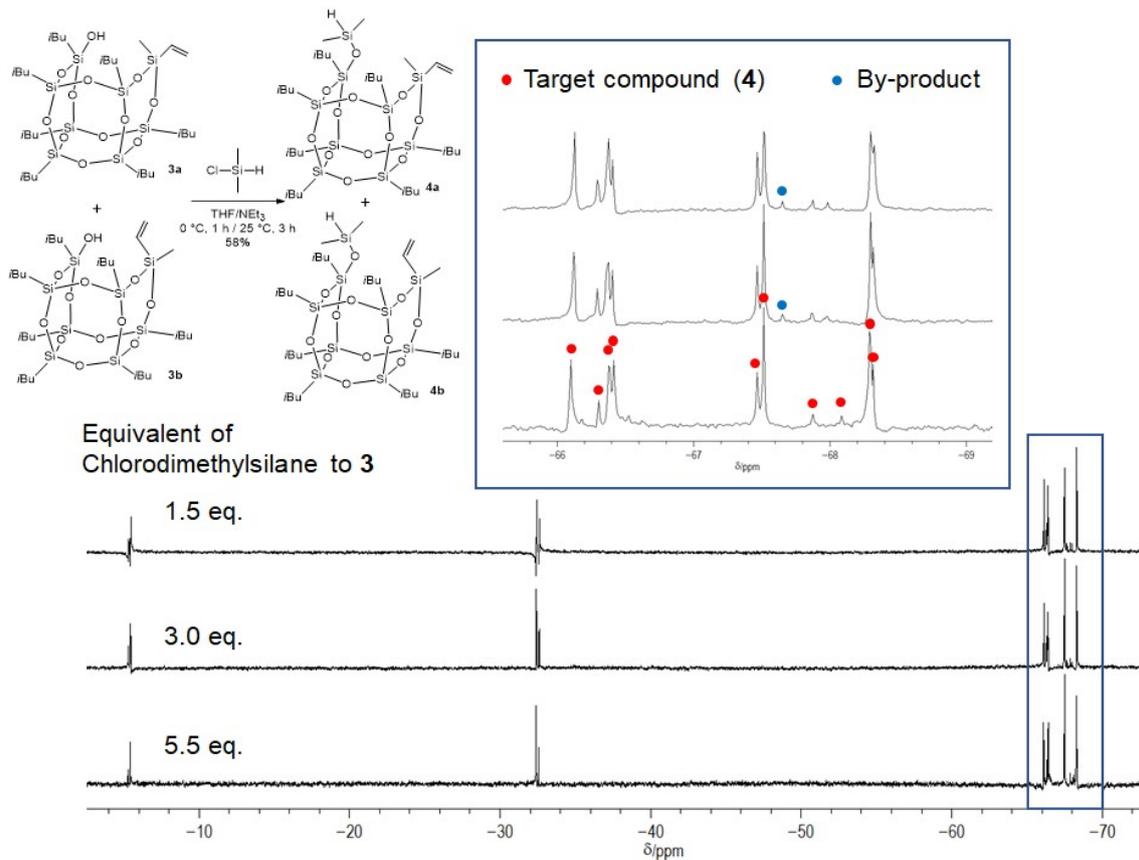
Figure S13. ^{29}Si-NMR spectra (80 MHz in CDCl$_3$) of crude products after the reaction of **3a/3b** with chlorodimethylsilane (1.5, 3.0, and 5.5 eq.). Red and blue dots indicate target compound **4a/4b** and by-products, respectively.
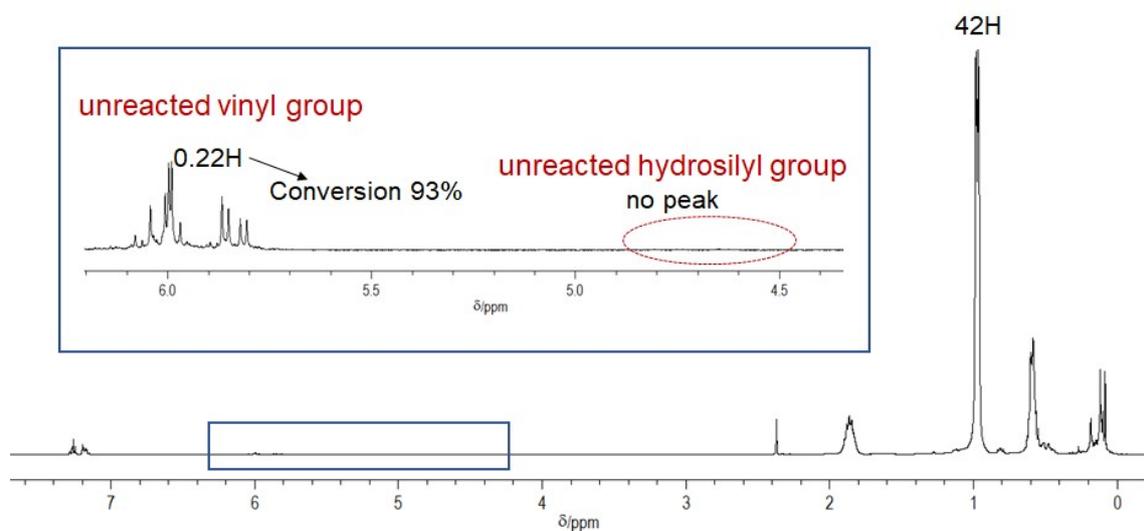
Figure S14. ^{1}H-NMR spectrum (400 MHz in CDCl$_3$) of crude product after hydrosilylation polymerization.
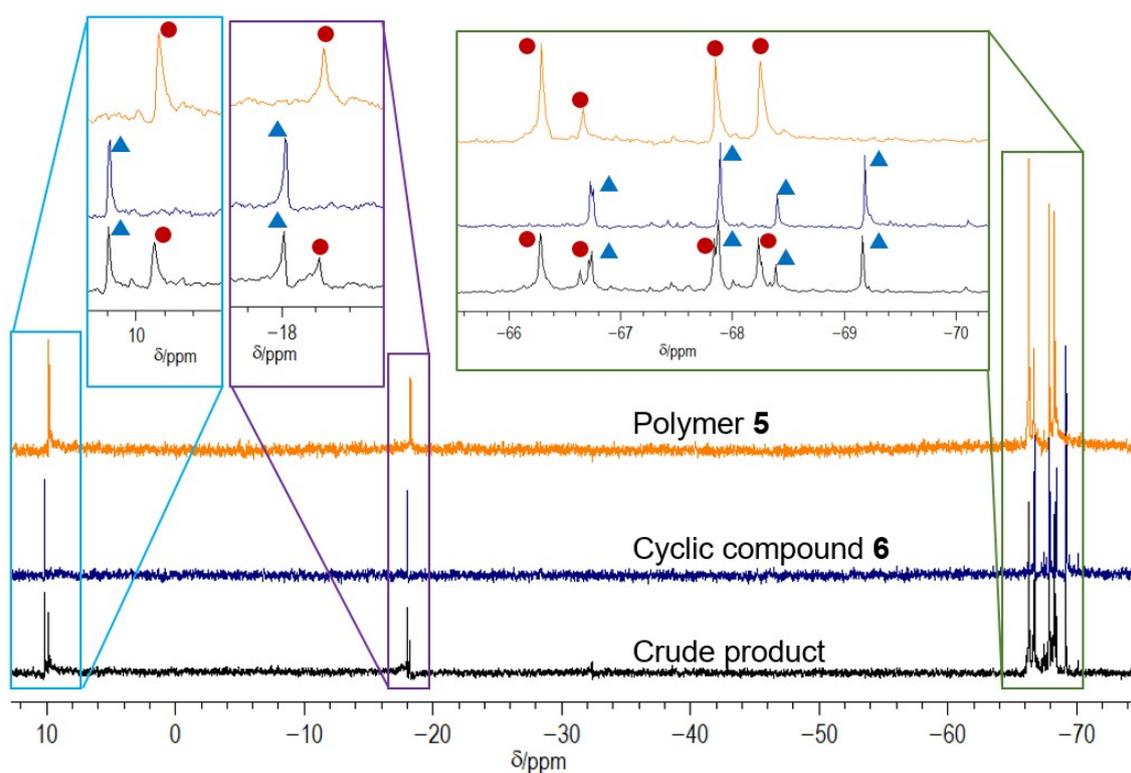
Figure S15. ^{29}Si-NMR spectra (80 MHz in CDCl$_3$) of polymer **5** (top), cyclic compound **6** (middle), and crude product after hydrosilylation polymerization (bottom).

2. MALDI-TOF-MS

C₃₀H₇₀O₁₂Si₈Na [M+Na]+
calculated: 869.2914, found: 869.2922

Figure S16. MALDI-TOF-MS spectrum of **2**. Matrix: DCTB (20 mg/mL in CHCl₃), cationizing agents: TFANa (1 mg/mL in THF).

C₃₃H₇₆O₁₂Si₉Na [M+Na]+
calculated: 939.3152, found: 939.3008

Figure S17. MALDI-TOF-MS spectrum of **4**. Matrix: DCTB (20 mg/mL in CHCl₃), cationizing agents: TFANa (1 mg/mL in THF).

C₃₃H₇₆O₁₂Si₉Na [M+Na]+
calculated: 939.3152, found: 939.3042

Figure S18. MALDI-TOF-MS spectrum of **6**. Matrix: DCTB (20 mg/mL in CHCl₃), cationizing agents: TFANa (1 mg/mL in THF).

2. MALDI-TOF-MS

$C_{30}H_{70}O_{12}Si_8Na$ [M+Na]+
calculated: 869.2914, found: 869.2922

Figure S16. MALDI-TOF-MS spectrum of **2**. Matrix: DCTB (20 mg/mL in CHCl₃), cationizing agents: TFANa (1 mg/mL in THF).

$C_{33}H_{76}O_{12}Si_9Na$ [M+Na]+
calculated: 939.3152, found: 939.3008

Figure S17. MALDI-TOF-MS spectrum of **4**. Matrix: DCTB (20 mg/mL in $CHCl_3$), cationizing agents: TFANa (1 mg/mL in THF).

$C_{33}H_{76}O_{12}Si_9Na$ [M+Na]+
calculated: 939.3152, found: 939.3042

Figure S18. MALDI-TOF-MS spectrum of **6**. Matrix: DCTB (20 mg/mL in $CHCl_3$), cationizing agents: TFANa (1 mg/mL in THF).

3. SEC traces

$M_n=900$
$M_w/M_n=1.11$

Elution volume [mL]
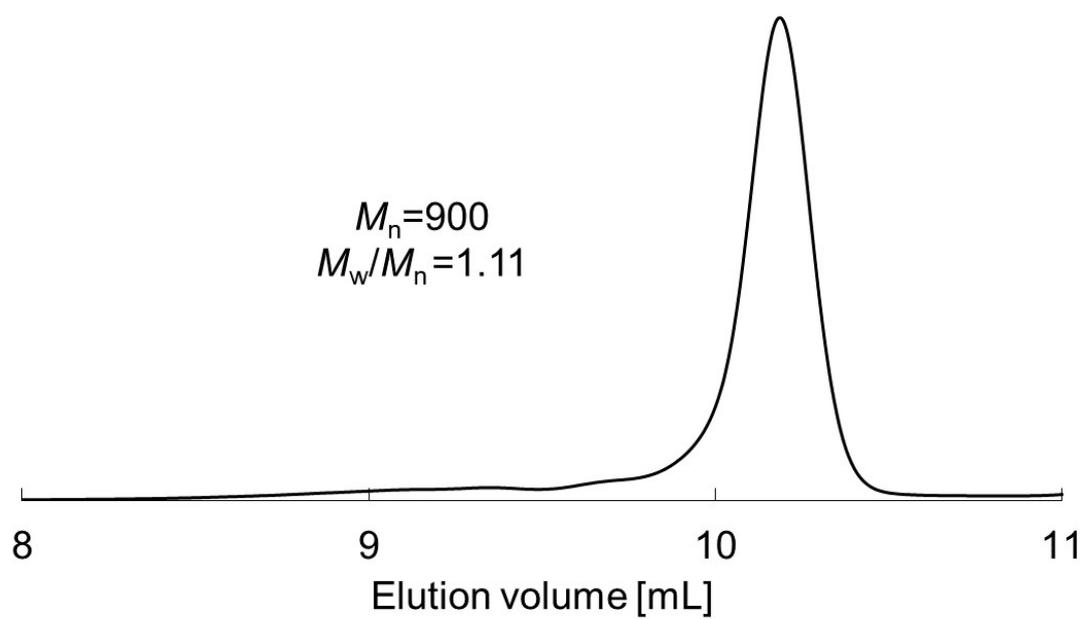
Figure S19. SEC traces (1 mL/min in THF, RI detector) of **2**.

M_n=1,100
M_w/M_n=1.03

Elution volume [mL]
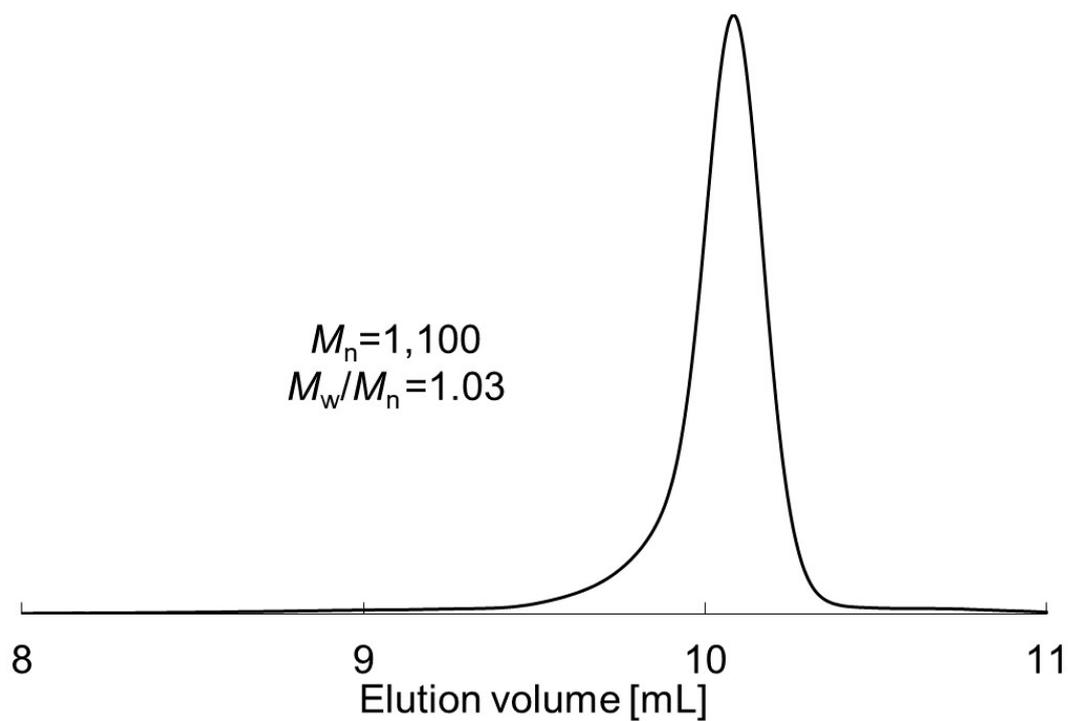
Figure S20. SEC traces (1 mL/min in THF, RI detector) of **3**.

M_n=1,100
M_w/M_n=1.03

Elution volume [mL]
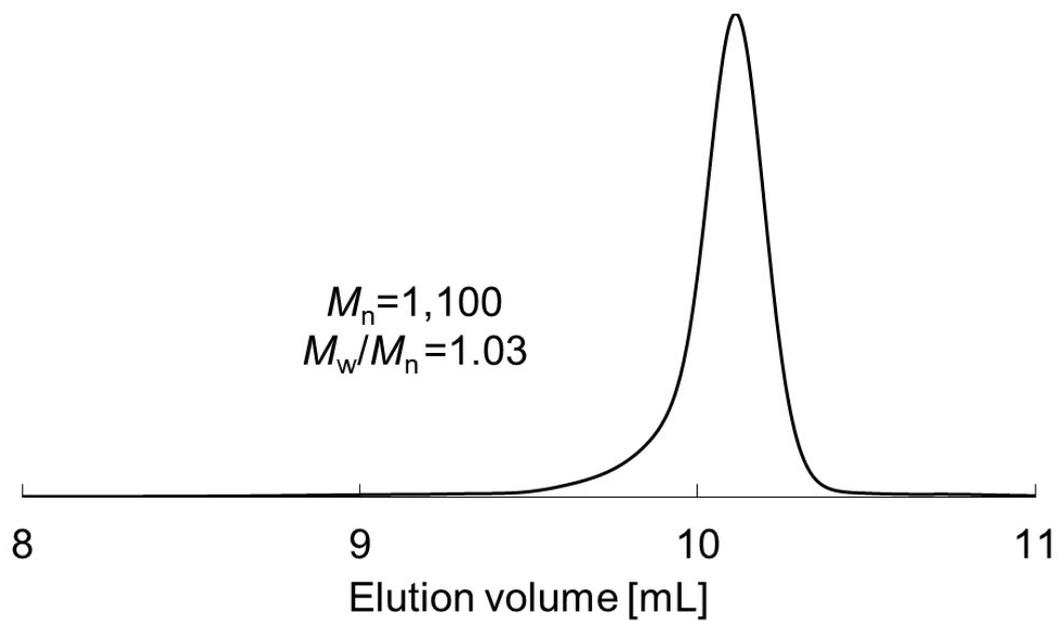
Figure S21. SEC traces (1 mL/min in THF, RI detector) of **4**.

M_n=13,700
M_w/M_n=1.30

Elution volume [mL]
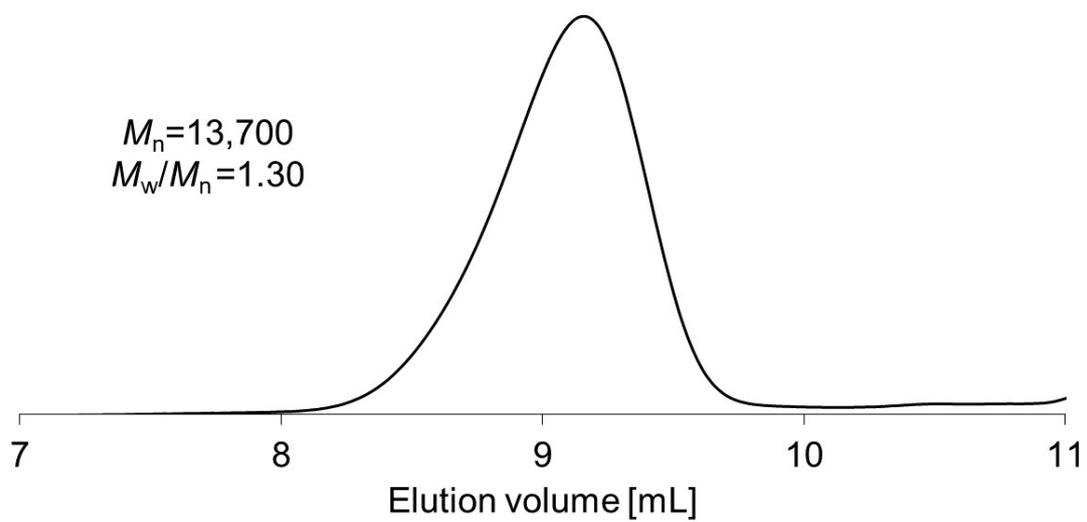
Figure S22. SEC traces (1 mL/min in THF, RI detector) of **5**.

M_n=900
M_w/M_n=1.08

Elution volume [mL]
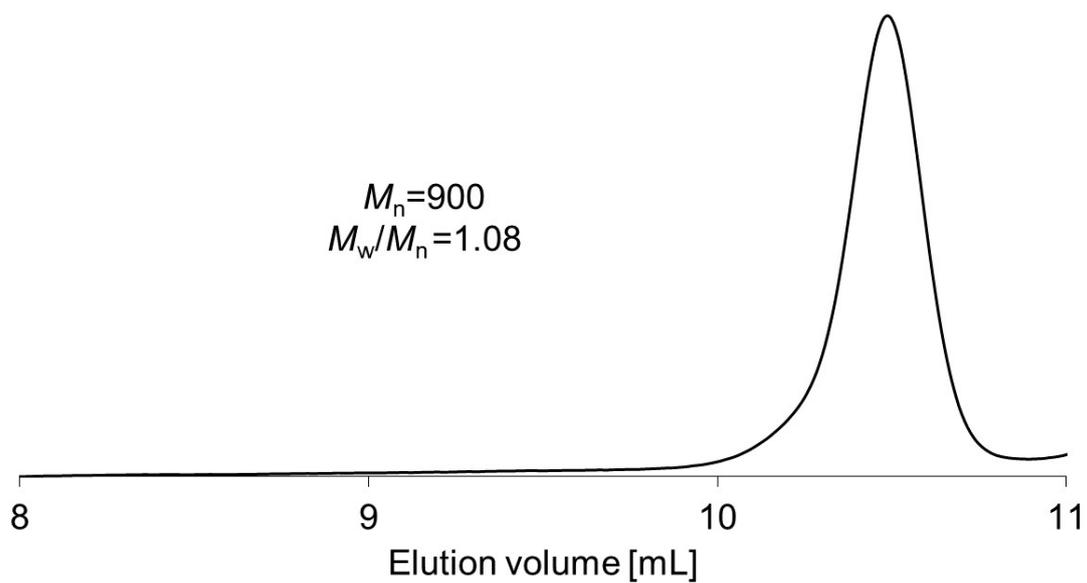
Figure S23. SEC traces (1 mL/min in THF, RI detector) of **6**.
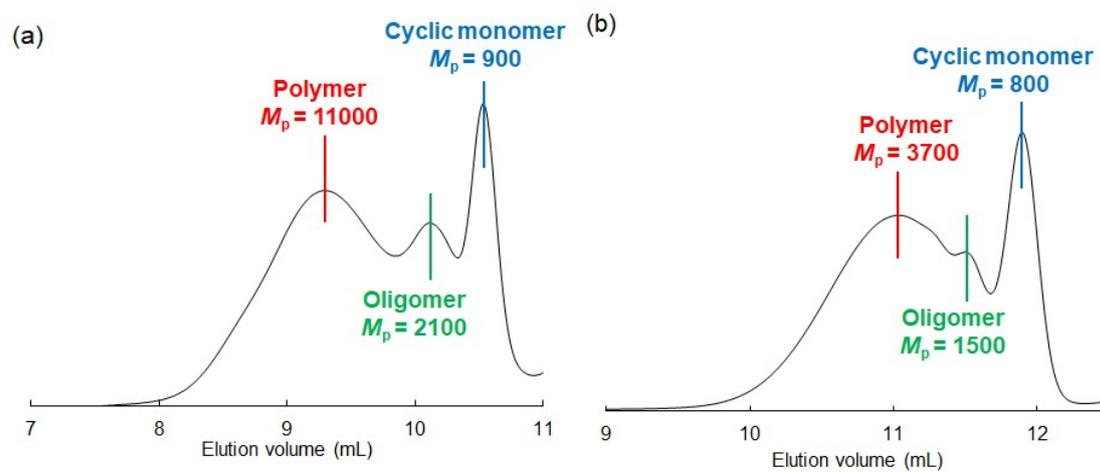
Figure S24. SEC traces (1 mL/min in THF, RI detector) of crude products obtained by using (a) the Karstedt catalyst and (b) Wilkinson catalyst.

4. Substrate scope
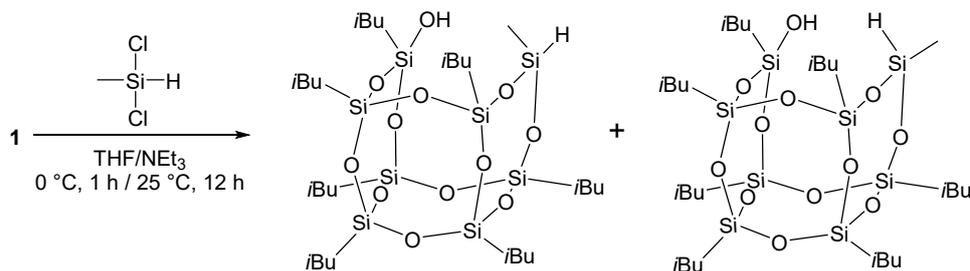
Scheme S1. Cyclization between **1** and dichloromethylsilane.
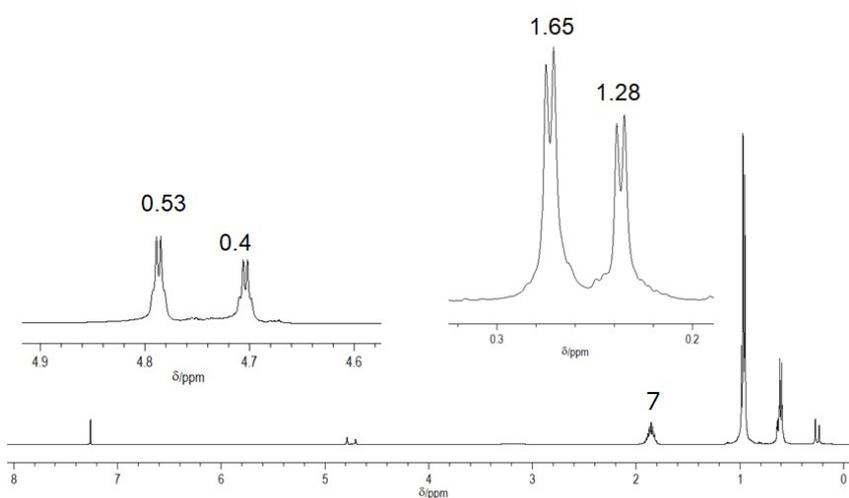
Figure S25. ¹H-NMR spectrum (400 MHz in CDCl₃) of the products of Scheme S1. The integral ratio of the two isomers was ca. 57/43.
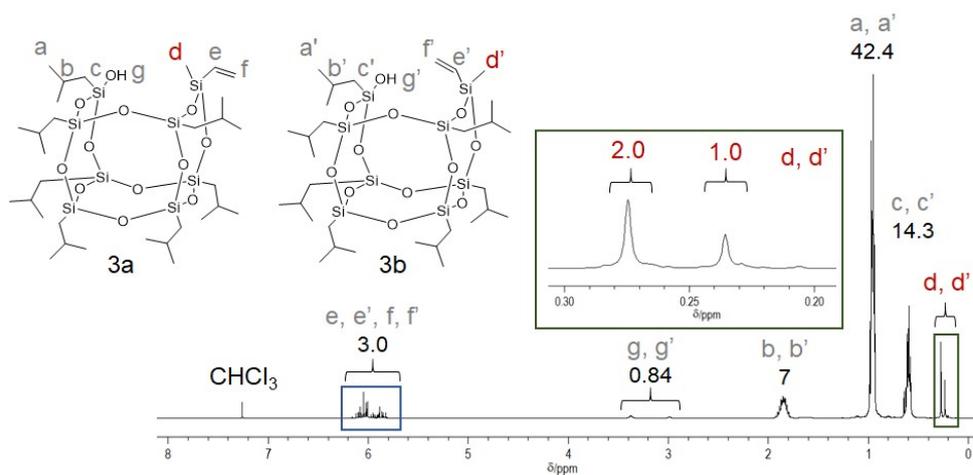
Figure S26. ¹H-NMR spectrum (400 MHz in CDCl₃) of **3a/3b**. The integral ratio of the two isomers was ca. 67/33, judging from the signals due to the methyl groups (d and d').
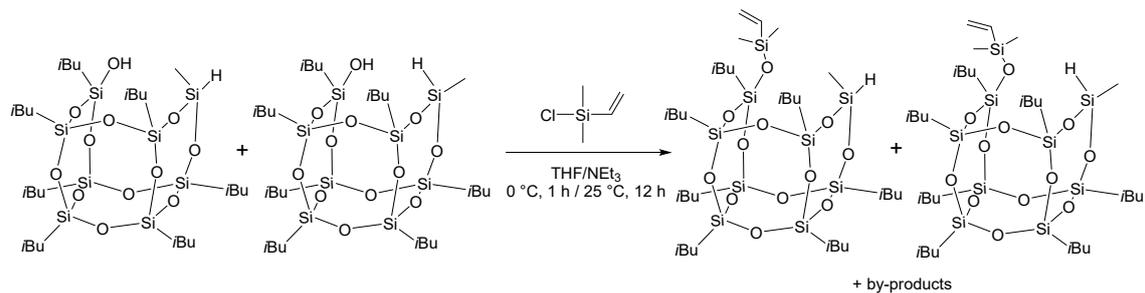
Scheme S2. Condensation of the product of Scheme S1 with chlorodimethylvinylsilane.
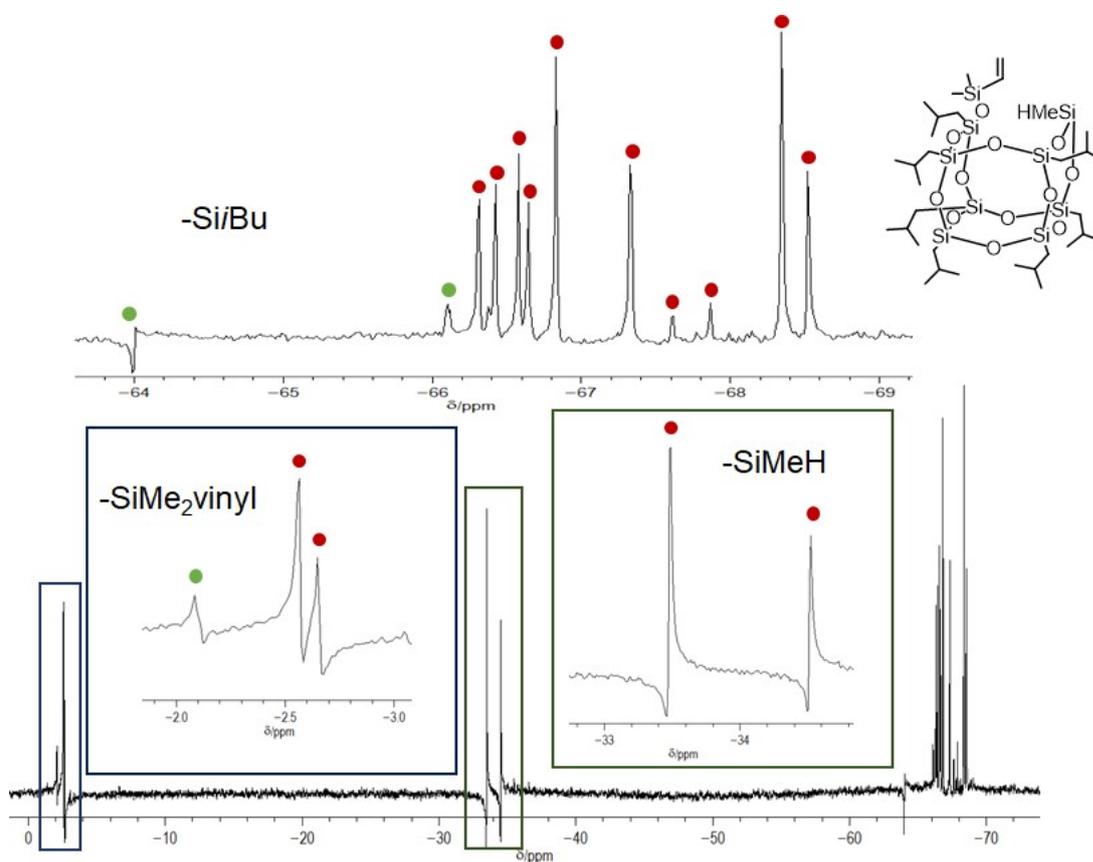
Figure S27. ^{29}Si-NMR (80 MHz in CDCl$_3$) of the product of Scheme S2. Red and green dots indicate the target compound and by-products, respectively.

5. DFT calculations

Cartesian coordinates in the structures optimized by DFT calculations
Optimized by B3LYP/6-31G(d)

Model of **4a**: E = -3987.2552 hartree

Number	Atom	X	Y	Z
1	Si	1.006626	-2.98195	-0.34827
2	Si	-2.67432	-0.87518	0.858919
3	O	-0.25217	-2.62237	-1.34802
4	Si	-1.30834	-1.49355	-1.92284
5	O	-0.48813	-0.13916	-2.36614
6	Si	0.647004	1.025939	-2.12929
7	O	2.116463	0.324405	-1.87198
8	Si	3.070312	-0.67233	-0.97142
9	O	2.342014	-2.14414	-0.82401
10	Si	0.131099	-1.36539	2.228928
11	Si	0.732956	2.907564	0.409324
12	Si	2.529588	0.731345	1.787407
13	O	-1.24073	-0.66467	1.646974
14	O	1.286746	-0.20595	2.321597
15	O	1.938802	2.182603	1.286882
16	C	-2.20228	-2.1796	-3.39988
17	C	0.742071	2.10748	-3.63844
18	C	-3.59933	-2.33251	1.565131
19	C	1.360194	-4.80279	-0.42189
20	C	4.718734	-0.8785	-1.79914
21	C	3.752044	1.004336	3.159087
22	O	0.209027	1.888989	-0.79574
23	O	0.608269	-2.56051	1.196571
24	O	3.283189	-0.02259	0.528583
25	O	-2.40179	-1.12496	-0.74938
26	H	-2.91856	-1.45086	-3.79424
27	H	-2.75276	-3.08865	-3.13527
28	H	-1.49711	-2.42942	-4.19971
29	H	1.03154	1.526058	-4.52029

30	H	-0.22696	2.575376	-3.84314
31	H	1.481884	2.902794	-3.49676
32	H	-4.54935	-2.48316	1.040601
33	H	-3.01571	-3.25551	1.469715
34	H	-3.82269	-2.1793	2.626772
35	H	1.628724	-5.10529	-1.43957
36	H	2.191872	-5.06335	0.241227
37	H	0.484197	-5.3835	-0.11413
38	H	4.602095	-1.32444	-2.79253
39	H	5.217459	0.089405	-1.91626
40	H	5.371943	-1.52907	-1.20805
41	H	4.577566	1.641702	2.824854
42	H	4.174505	0.053131	3.500024
43	H	3.272126	1.490756	4.014975
44	C	-0.15082	-2.09197	3.917205
45	H	-0.47581	-1.31844	4.62133
46	H	-0.9205	-2.87093	3.888695
47	H	0.769145	-2.5409	4.306878
48	C	-0.73207	3.269817	1.507594
49	H	-1.49981	3.842722	0.97482
50	H	-1.1883	2.334081	1.849332
51	H	-0.42947	3.849264	2.387078
52	O	-3.55326	0.489139	1.044789
53	Si	-4.41622	1.758186	0.398914
54	C	-3.70247	2.279638	-1.26071
55	H	-3.85809	1.502509	-2.01787
56	H	-4.17785	3.201223	-1.61959
57	H	-2.62384	2.455528	-1.18542
58	C	-6.22493	1.263157	0.236997
59	H	-6.83007	2.107159	-0.11727
60	H	-6.35161	0.439935	-0.47649
61	H	-6.6357	0.939302	1.20005
62	H	-4.30633	2.882134	1.370898
63	C	1.469075	4.441402	-0.36007
64	H	0.822971	5.068039	-0.98068
65	C	2.740663	4.827797	-0.19593

| 66 | H | 3.435203 | 4.251542 | 0.411721 |
| 67 | H | 3.144575 | 5.729273 | -0.65586 |

Model of **4b**: *E* = -3987.2544 hartree

Number	Atom	X	Y	Z
1	Si	-1.8097	-2.64859	-0.27932
2	Si	2.326065	-1.21416	-1.01194
3	O	-0.55427	-2.87481	0.764174
4	Si	0.734945	-2.18473	1.527868
5	O	0.279855	-0.76168	2.207818
6	Si	-0.56012	0.639885	2.369253
7	O	-2.14899	0.37358	2.013819
8	Si	-3.28016	-0.12075	0.922173
9	O	-2.91971	-1.64553	0.408024
10	Si	-0.46563	-0.71183	-2.39807
11	Si	-0.10147	3.051934	0.321707
12	Si	-2.33669	1.723841	-1.44393
13	O	0.99857	-0.4917	-1.67245
14	O	-1.33116	0.666044	-2.20767
15	O	-1.44018	2.841985	-0.6392
16	C	1.364565	-3.33892	2.840082
17	C	-0.41876	1.23904	4.123839
18	C	2.999117	-2.52048	-2.16035
19	C	-2.60277	-4.2834	-0.65905
20	C	-4.95763	-0.11888	1.717095
21	C	-3.42138	2.57612	-2.6875
22	O	0.059111	1.737667	1.317445
23	O	-1.23995	-1.97516	-1.67415
24	O	-3.28225	0.899012	-0.37228
25	O	1.934389	-1.9152	0.430671
26	C	-0.38739	4.599141	1.33649
27	H	2.224475	-2.90357	3.360308
28	H	1.678199	-4.29261	2.402445
29	H	0.586711	-3.5453	3.582931
30	H	-0.81482	0.495831	4.824152

31	H	0.62824	1.427694	4.384377
32	H	-0.97789	2.170094	4.267312
33	H	3.87705	-3.00889	-1.72324
34	H	2.25071	-3.29656	-2.35811
35	H	3.299415	-2.08413	-3.11944
36	H	-2.98496	-4.75078	0.254612
37	H	-3.44064	-4.1568	-1.35276
38	H	-1.88202	-4.96946	-1.11639
39	H	-4.98308	-0.80034	2.573988
40	H	-5.21803	0.884184	2.071194
41	H	-5.72559	-0.43829	1.004698
42	H	-4.08434	3.295625	-2.19538
43	H	-4.04366	1.852682	-3.22499
44	H	-2.81623	3.118621	-3.42159
45	H	0.438164	4.783022	2.032945
46	H	-1.30828	4.498349	1.922494
47	H	-0.50009	5.483599	0.699365
48	C	-0.26784	-1.07218	-4.21169
49	H	0.25152	-0.24925	-4.71456
50	H	0.310296	-1.98858	-4.37276
51	H	-1.24404	-1.20055	-4.69152
52	Si	4.53483	0.48976	0.396179
53	O	3.449193	-0.04734	-0.75579
54	C	5.694722	-0.91036	0.889055
55	H	6.280438	-1.26735	0.033352
56	H	6.400266	-0.57893	1.661254
57	H	5.135292	-1.76194	1.293307
58	C	5.482319	1.932676	-0.34345
59	H	6.227607	2.31355	0.365841
60	H	6.009033	1.635823	-1.25798
61	H	4.805277	2.756426	-0.59308
62	H	3.787806	0.942919	1.60339
63	C	1.424913	3.143581	-0.74164
64	H	1.757241	2.22748	-1.233
65	C	2.123046	4.267336	-0.95163
66	H	1.854045	5.216168	-0.48928

| 67 | H | 2.998598 | 4.299246 | -1.59958 |

Model of cyclic compound **6'**: *E* = -3987.2669 hartree

Number	Atom	X	Y	Z
1	Si	-2.69519	1.823702	0.537457
2	Si	1.772265	1.425692	1.332717
3	O	-1.5197	2.645403	-0.27175
4	Si	-0.00896	2.73305	-0.92589
5	O	0.137592	1.575682	-2.09751
6	Si	-0.06738	-0.05748	-2.20242
7	O	-1.67531	-0.41428	-2.26168
8	Si	-3.03611	-0.67833	-1.37161
9	O	-3.32257	0.640543	-0.42383
10	Si	-0.94286	0.014321	2.395032
11	Si	1.099143	-2.16684	-0.19094
12	Si	-1.6862	-2.62618	0.623674
13	O	0.571846	0.493766	1.973601
14	O	-1.28802	-1.44088	1.704175
15	O	-0.3049	-3.08798	-0.1843
16	C	0.242578	4.409465	-1.68309
17	C	0.662352	-0.64777	-3.81182
18	C	2.561837	2.419476	2.697891
19	C	-4.04713	2.994433	1.034788
20	C	-4.48668	-0.96755	-2.49235
21	C	-2.42222	-4.09269	1.494514
22	O	0.594098	-0.7012	-0.82881
23	O	-2.03846	1.134104	1.884309
24	O	-2.80038	-2.01577	-0.43002
25	O	1.127708	2.477959	0.237176
26	C	2.542073	-2.68898	-1.28692
27	H	1.236269	4.485587	-2.13707
28	H	0.153086	5.196146	-0.92648
29	H	-0.50358	4.598651	-2.46199
30	H	0.038398	-0.27631	-4.63256
31	H	1.679569	-0.28035	-3.97488

32	H	0.673368	-1.74123	-3.87397
33	H	3.357049	3.062548	2.304723
34	H	1.823916	3.061116	3.191992
35	H	3.002088	1.763309	3.45695
36	H	-4.49058	3.472478	0.154908
37	H	-4.84146	2.464335	1.570794
38	H	-3.65906	3.780978	1.690554
39	H	-4.65942	-0.0991	-3.13665
40	H	-4.31396	-1.83945	-3.13196
41	H	-5.397	-1.14713	-1.91059
42	H	-2.66239	-4.88407	0.776338
43	H	-3.34441	-3.81504	2.01578
44	H	-1.72218	-4.50356	2.229673
45	H	2.215533	-3.12868	-2.23846
46	H	3.103501	-3.47529	-0.76612
47	C	-1.05955	-0.15166	4.243809
48	H	-0.33122	-0.87881	4.619174
49	H	-0.86317	0.807744	4.734494
50	H	-2.05868	-0.48712	4.541861
51	C	3.476736	-1.4718	-1.5807
52	H	4.396952	-1.84444	-2.05952
53	H	3.000345	-0.84696	-2.34432
54	C	1.755737	-2.32231	1.569767
55	H	2.571959	-1.64606	1.81866
56	H	0.979872	-2.21276	2.326338
57	H	2.135765	-3.35189	1.636967
58	O	2.907658	0.478507	0.6279
59	Si	4.117015	-0.22657	-0.27724
60	C	4.989545	1.135993	-1.248
61	H	5.432076	1.87705	-0.57175
62	H	5.796039	0.73556	-1.87454
63	H	4.287929	1.664912	-1.90391
64	C	5.337469	-1.04182	0.909353
65	H	6.198316	-1.44334	0.359952
66	H	5.718813	-0.31479	1.636241
67	H	4.889203	-1.86862	1.470827

Model of cyclic compound **6**: E = -3987.2981 hartree

Number	Atom	X	Y	Z
1	Si	-2.15326	-2.40636	0.050163
2	Si	2.296953	-1.90521	-0.47949
3	O	-1.04775	-2.44876	1.273222
4	Si	0.279893	-1.74283	1.950897
5	O	0.049915	-0.11591	2.038045
6	Si	-0.84948	1.249773	2.241961
7	O	-2.383	0.971887	1.706162
8	Si	-3.36783	0.466451	0.48525
9	O	-3.20718	-1.16515	0.301014
10	Si	-0.30812	-1.26208	-2.2472
11	Si	0.384499	3.046087	-0.0863
12	Si	-1.71689	1.63547	-1.93788
13	O	1.17966	-1.3497	-1.55918
14	O	-0.78081	0.309158	-2.21535
15	O	-0.78532	2.800995	-1.24747
16	C	0.565345	-2.4737	3.636303
17	C	-0.91075	1.744256	4.033466
18	C	2.915402	-3.58323	-0.99663
19	C	-3.09061	-4.00789	0.002688
20	C	-5.13225	0.868116	0.898415
21	C	-2.43305	2.280702	-3.52652
22	O	-0.15464	2.449443	1.367977
23	O	-1.36937	-2.18309	-1.38423
24	O	-2.94472	1.218741	-0.9184
25	O	1.601882	-2.01992	1.015183
26	C	0.60529	4.89325	0.113743
27	H	1.441361	-2.02151	4.113549
28	H	0.737185	-3.55314	3.566814
29	H	-0.30025	-2.31099	4.28773
30	H	-1.37816	0.962594	4.642246
31	H	0.097085	1.922948	4.423374
32	H	-1.4912	2.664201	4.161232

33	H	3.656068	-3.96178	-0.28391
34	H	2.093934	-4.30682	-1.04528
35	H	3.388686	-3.53819	-1.98352
36	H	-3.61642	-4.17827	0.948096
37	H	-3.83282	-3.99972	-0.80252
38	H	-2.41279	-4.85117	-0.16678
39	H	-5.4357	0.377296	1.829164
40	H	-5.26407	1.948054	1.023486
41	H	-5.80453	0.532837	0.101606
42	H	-3.03962	3.173935	-3.34305
43	H	-3.07176	1.52926	-4.00315
44	H	-1.63828	2.549592	-4.23055
45	H	1.367586	5.121007	0.867829
46	H	-0.33258	5.361685	0.43203
47	H	0.912125	5.358769	-0.82987
48	C	-0.24347	-1.88058	-3.99946
49	H	0.462869	-1.29023	-4.59303
50	H	0.077365	-2.9274	-4.03294
51	H	-1.22758	-1.81358	-4.47585
52	Si	4.295306	0.57153	0.011536
53	C	1.936796	2.12232	-0.61156
54	H	1.592407	1.180147	-1.05605
55	H	2.409277	2.675899	-1.43601
56	C	2.972914	1.832164	0.503921
57	H	2.460435	1.435296	1.390751
58	H	3.459736	2.762937	0.830873
59	O	3.54506	-0.85581	-0.43264
60	C	5.432491	0.206568	1.470554
61	H	6.174376	-0.55851	1.212888
62	H	5.976864	1.1049	1.787623
63	H	4.862857	-0.15992	2.33268
64	C	5.294285	1.155649	-1.47552
65	H	5.841135	2.080043	-1.25116
66	H	6.02829	0.398984	-1.77649
67	H	4.646754	1.350325	-2.33804

Model of dimer **7a**: *E* = -7974.5547 hartree

Number	Atom	X	Y	Z
1	Si	-7.19714	-0.11331	1.856134
2	Si	-5.15579	2.784963	-0.72139
3	O	-7.5511	0.199025	0.277385
4	Si	-7.02064	0.309061	-1.28107
5	O	-6.07164	-0.98201	-1.63903
6	Si	-4.90615	-2.10164	-1.34005
7	O	-5.25231	-2.89624	0.064993
8	Si	-5.44809	-2.74603	1.695132
9	O	-6.64774	-1.65754	2.004936
10	Si	-4.52384	1.556897	2.11976
11	Si	-1.90708	-1.19956	-0.64426
12	Si	-2.79464	-1.14097	2.360605
13	O	-4.39979	2.073976	0.560018
14	O	-3.39218	0.395127	2.354618
15	O	-1.87989	-1.3715	1.01355
16	C	-8.47901	0.34146	-2.43158
17	C	-4.87254	-3.32724	-2.73838
18	C	-6.13954	4.266732	-0.15873
19	C	-8.72415	0.103203	2.889476
20	C	-5.90818	-4.39262	2.418254
21	C	-1.75467	-1.39849	3.878206
22	O	-3.47092	-1.32309	-1.18616
23	O	-6.03432	0.940992	2.366149
24	O	-4.04643	-2.21422	2.375294
25	O	-6.15758	1.701014	-1.46047
26	H	-8.15033	0.432696	-3.4724
27	H	-9.13551	1.18869	-2.20645
28	H	-9.06693	-0.57807	-2.34054
29	H	-5.84142	-3.82734	-2.84218
30	H	-4.64545	-2.82736	-3.6862
31	H	-4.11172	-4.09688	-2.56855
32	H	-6.65581	4.735673	-1.00373
33	H	-6.89855	3.981112	0.578828

34	H	-5.48877	5.020923	0.297644
35	H	-9.50951	-0.59063	2.571488
36	H	-8.50807	-0.08847	3.945832
37	H	-9.11445	1.122609	2.80109
38	H	-6.84526	-4.75892	1.985826
39	H	-5.1281	-5.13523	2.219896
40	H	-6.03936	-4.31821	3.502939
41	H	-1.30778	-2.3983	3.88076
42	H	-2.36291	-1.29669	4.783523
43	H	-0.94424	-0.66368	3.929236
44	C	-4.232	2.953665	3.312578
45	H	-3.23867	3.389988	3.161791
46	H	-4.97534	3.747473	3.181084
47	H	-4.29439	2.601234	4.347757
48	C	-1.27024	0.49815	-1.09862
49	H	-1.21445	0.617391	-2.18707
50	H	-1.94414	1.268895	-0.70904
51	H	-0.27047	0.666184	-0.68231
52	O	-4.00196	3.248996	-1.78536
53	Si	-3.49305	3.210811	-3.37251
54	C	-4.82942	3.909539	-4.49927
55	H	-5.05105	4.956313	-4.25896
56	H	-4.51665	3.866896	-5.55009
57	H	-5.75986	3.337921	-4.40493
58	C	-1.90769	4.213199	-3.4814
59	H	-1.50044	4.194537	-4.49989
60	H	-2.08246	5.260663	-3.20879
61	H	-1.14183	3.8161	-2.80583
62	H	-3.22122	1.798747	-3.76689
63	Si	1.709765	-3.93104	-1.63938
64	O	3.291128	-3.61697	-1.17765
65	C	1.622786	-4.02361	-3.52281
66	C	1.249818	-5.5885	-0.87162
67	Si	4.589146	-2.65929	-1.43483
68	H	2.273373	-4.81667	-3.91082
69	H	0.603752	-4.23505	-3.86913

70	H	1.941326	-3.07794	-3.9771
71	H	0.215645	-5.86848	-1.10659
72	H	1.902603	-6.38832	-1.24043
73	H	1.348088	-5.5556	0.219664
74	O	5.154011	-2.15378	0.033308
75	C	5.916588	-3.60011	-2.35026
76	O	4.109694	-1.35013	-2.3254
77	Si	6.455588	-1.50297	0.805638
78	H	5.55776	-3.92074	-3.33468
79	H	6.808672	-2.9821	-2.50404
80	H	6.215751	-4.49625	-1.79503
81	Si	4.478745	0.207809	-2.71216
82	O	5.8936	-0.58981	2.046413
83	O	7.300944	-0.56019	-0.25344
84	C	7.573379	-2.83627	1.46286
85	O	6.078714	0.476159	-2.40844
86	O	3.55939	1.23182	-1.81543
87	C	4.135366	0.496248	-4.51558
88	Si	5.577489	0.786241	2.893373
89	Si	7.28242	0.709228	-1.30764
90	H	7.031991	-3.48458	2.16025
91	H	7.961915	-3.4606	0.650916
92	H	8.428167	-2.40384	1.994111
93	Si	3.170642	2.074444	-0.45791
94	H	3.081981	0.303889	-4.74612
95	H	4.746227	-0.16439	-5.14005
96	H	4.360089	1.531316	-4.79424
97	O	3.94952	0.931549	3.076929
98	C	6.386783	0.719963	4.564564
99	O	6.160864	2.086804	2.062337
100	O	7.014636	2.110122	-0.48492
101	C	8.916307	0.813011	-2.18318
102	O	4.501863	2.874055	0.094745
103	C	1.844794	3.313392	-0.8618
104	O	2.662625	0.997633	0.677095
105	Si	2.514067	0.642081	2.293262

106	H	6.155138	1.619493	5.144826
107	H	7.475664	0.649701	4.469332
108	H	6.03683	-0.14939	5.131375
109	Si	6.061578	2.880249	0.619738
110	H	8.927225	1.653278	-2.88543
111	H	9.731224	0.958414	-1.46617
112	H	9.11808	-0.10406	-2.74676
113	H	2.190415	4.020811	-1.6233
114	H	0.946443	2.814718	-1.2411
115	H	1.564761	3.883844	0.030445
116	C	2.056624	-1.1613	2.440818
117	C	1.24453	1.78003	3.053328
118	C	6.65099	4.627748	0.82943
119	H	1.046711	-1.34508	2.057958
120	H	2.75937	-1.77906	1.87026
121	H	2.08517	-1.48314	3.488207
122	H	0.230285	1.763681	2.645362
123	C	1.496233	2.612279	4.071908
124	H	6.615548	5.1677	-0.12266
125	H	6.023727	5.164027	1.549325
126	H	7.683124	4.648643	1.194919
127	H	2.484973	2.676972	4.521417
128	H	0.734658	3.263829	4.499638
129	C	0.619307	-2.53835	-0.9757
130	H	0.71588	-2.53783	0.117702
131	H	1.060171	-1.58804	-1.30868
132	C	-0.87917	-2.60031	-1.36695
133	H	-1.32299	-3.55087	-1.03615
134	H	-0.99156	-2.57989	-2.46063

Model of dimer **7b**: E = -7974.5502 hartree

Number	Atom	X	Y	Z
1	Si	6.589056	-1.27758	-2.48015
2	Si	5.765564	2.590702	-0.60455
3	O	7.539118	-0.51122	-1.37344

4	Si	7.672083	0.192548	0.112989
5	O	6.931815	-0.74222	1.241275
6	Si	5.751754	-1.71782	1.83959
7	O	5.481118	-2.96099	0.788152
8	Si	5.016926	-3.39427	-0.73248
9	O	6.011004	-2.67757	-1.83591
10	Si	4.048745	0.603185	-2.35519
11	Si	2.731496	-0.64709	2.047697
12	Si	2.344601	-1.69858	-0.90708
13	O	4.558433	1.615103	-1.15867
14	O	2.895191	-0.37603	-1.72346
15	O	2.086395	-1.29716	0.662847
16	C	9.468097	0.383112	0.549049
17	C	6.313393	-2.4145	3.470082
18	C	6.474796	3.618329	-1.9912
19	C	7.587616	-1.66056	-3.99764
20	C	5.126271	-5.23878	-0.91286
21	C	0.76054	-2.29068	-1.67488
22	O	4.382841	-0.83254	2.008836
23	O	5.329459	-0.29142	-2.8856
24	O	3.468723	-2.90243	-0.9994
25	O	6.964009	1.679241	0.071603
26	C	2.027709	-1.60766	3.495528
27	H	9.582086	0.865999	1.525532
28	H	9.987595	0.995659	-0.19552
29	H	9.963856	-0.59249	0.592797
30	H	7.237539	-2.99023	3.351284
31	H	6.504223	-1.61149	4.190242
32	H	5.553518	-3.07897	3.895622
33	H	7.272643	4.27269	-1.62231
34	H	6.901315	2.983237	-2.77632
35	H	5.705701	4.252102	-2.4467
36	H	8.427983	-2.31886	-3.75322
37	H	6.970956	-2.16153	-4.75136
38	H	7.990974	-0.74436	-4.4417
39	H	6.152628	-5.58498	-0.75147

40	H	4.479503	-5.73928	-0.18446
41	H	4.815075	-5.55074	-1.91544
42	H	0.428332	-3.22176	-1.20285
43	H	0.895925	-2.48473	-2.74444
44	H	-0.0349	-1.54797	-1.55481
45	H	2.429963	-1.24665	4.449475
46	H	2.269736	-2.67331	3.40835
47	H	0.936629	-1.51628	3.530694
48	C	3.332254	1.55408	-3.78337
49	H	2.477309	2.155391	-3.45599
50	H	4.075471	2.228024	-4.22314
51	H	2.987103	0.873567	-4.56918
52	Si	5.405363	4.508837	1.880462
53	O	5.113152	3.548492	0.551226
54	C	3.793328	5.35862	2.337868
55	H	3.934718	6.039181	3.186532
56	H	3.404215	5.945551	1.498312
57	H	3.027847	4.625285	2.617744
58	C	6.086658	3.485418	3.302636
59	H	6.30691	4.117853	4.171771
60	H	5.372513	2.715069	3.616081
61	H	7.012644	2.978795	3.009113
62	H	6.416518	5.542161	1.50072
63	Si	-0.37548	1.658359	1.320808
64	O	-0.98298	0.099451	1.303493
65	C	0.196525	2.094731	-0.41979
66	C	-1.72666	2.839049	1.901618
67	Si	-2.22373	-0.95601	1.286766
68	H	0.610441	3.110542	-0.45527
69	H	0.971886	1.405492	-0.77068
70	H	-0.63996	2.046276	-1.12687
71	H	-1.3652	3.874803	1.925286
72	H	-2.6	2.80772	1.240475
73	H	-2.06619	2.579809	2.911412
74	O	-2.82867	-1.04201	-0.25501
75	C	-1.63166	-2.63134	1.849268

76	O	-3.40553	-0.41178	2.306894
77	Si	-3.94643	-1.83294	-1.1698
78	H	-1.3409	-2.60726	2.905218
79	H	-2.41811	-3.38613	1.735293
80	H	-0.759	-2.95047	1.269819
81	Si	-5.01693	-0.32789	2.612506
82	O	-4.80643	-0.69364	-1.98343
83	O	-4.94979	-2.69738	-0.18437
84	C	-3.11596	-2.99949	-2.35757
85	O	-5.7361	-1.76074	2.209684
86	O	-5.65408	0.875292	1.690582
87	C	-5.28195	-0.0013	4.423576
88	Si	-6.12832	-0.13945	-2.79864
89	Si	-6.17203	-2.70025	0.925411
90	H	-2.42283	-2.46141	-3.01283
91	H	-2.54567	-3.76491	-1.82041
92	H	-3.85399	-3.50954	-2.98657
93	Si	-6.88044	1.665772	0.930679
94	H	-4.81416	0.943552	4.720391
95	H	-4.84473	-0.80142	5.030388
96	H	-6.34973	0.057218	4.661384
97	O	-6.07842	1.503024	-2.77399
98	C	-6.14818	-0.73325	-4.5597
99	O	-7.49182	-0.67085	-2.03615
100	O	-7.54392	-2.09853	0.240251
101	C	-6.48789	-4.43667	1.501288
102	O	-7.94278	0.561475	0.320649
103	C	-7.77798	2.787807	2.111382
104	O	-6.24194	2.555293	-0.28752
105	Si	-5.63667	2.784385	-1.81183
106	H	-7.01429	-0.32761	-5.09345
107	H	-6.20425	-1.82623	-4.60789
108	H	-5.24408	-0.41288	-5.08835
109	Si	-8.20261	-0.8106	-0.55335
110	H	-7.29266	-4.45779	2.243737
111	H	-6.78222	-5.07656	0.662712

112	H	-5.59096	-4.86621	1.95991
113	H	-8.21592	2.220445	2.939961
114	H	-7.09529	3.533697	2.532484
115	H	-8.58844	3.319879	1.601766
116	C	-6.40912	4.327568	-2.53012
117	C	-3.77728	2.864249	-1.72131
118	C	-10.0262	-1.08557	-0.76319
119	H	-6.19	5.210771	-1.91993
120	H	-7.49789	4.210749	-2.57062
121	H	-6.05547	4.517713	-3.54943
122	H	-3.24761	1.974562	-1.37237
123	C	-3.05644	3.937439	-2.07031
124	H	-10.5186	-1.19144	0.209198
125	H	-10.4868	-0.24268	-1.28914
126	H	-10.2179	-1.99463	-1.34294
127	H	-3.52015	4.854355	-2.43143
128	H	-1.96895	3.957305	-2.01328
129	C	1.052535	1.741569	2.565652
130	H	1.144095	2.809691	2.820888
131	H	0.708401	1.260927	3.493197
132	C	2.4518	1.207996	2.170111
133	H	3.187003	1.540366	2.919723
134	H	2.790455	1.657854	1.227501