

# Electronic Supplementary Information (ESI)

## Symmetry driving: Synthesis of co-substituents octasilsesquioxane

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# Electronic Supplementary Information (ESI)

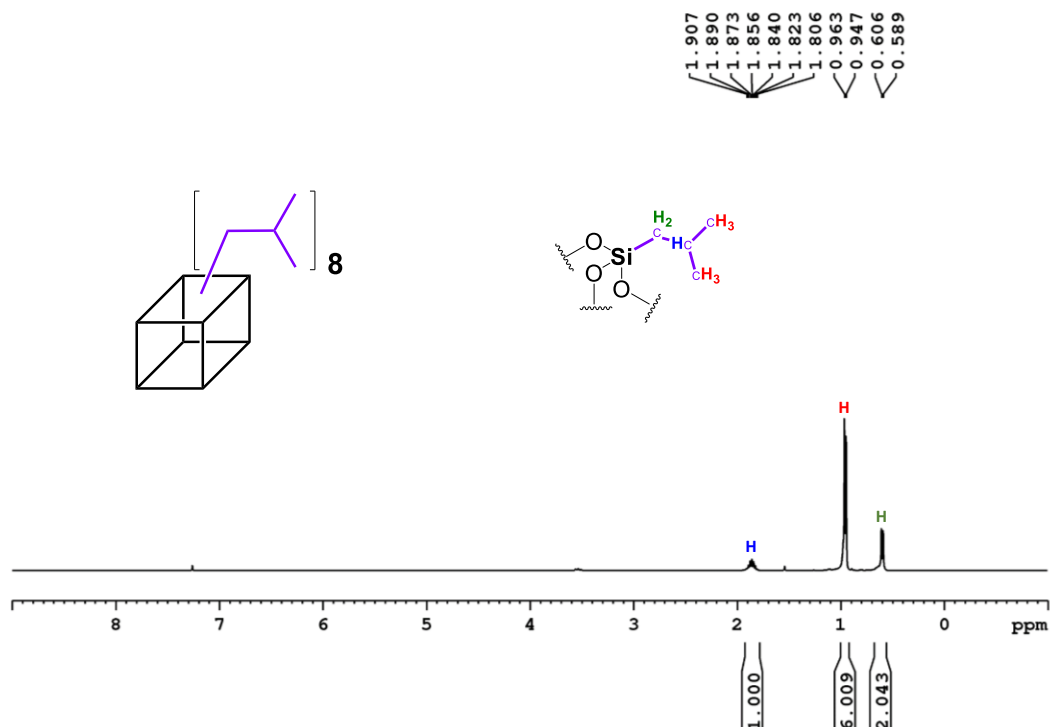


Figure S1 <sup>1</sup>H NMR spectrum of *i*-butyl T<sub>8</sub> in CDCl<sub>3</sub>.

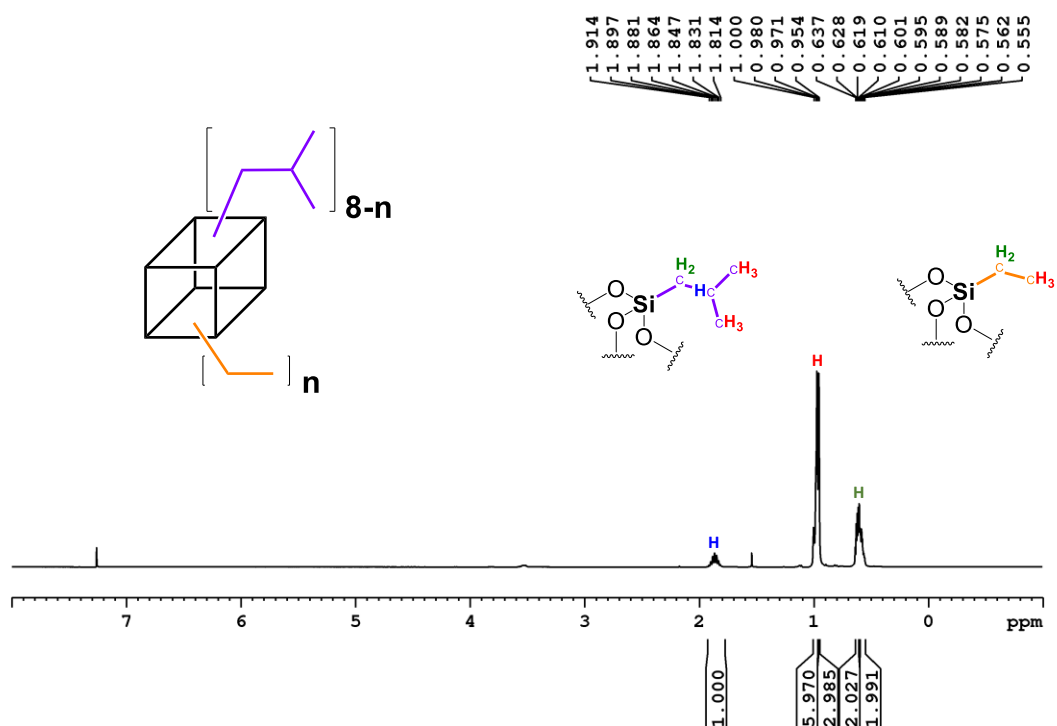


Figure S2 <sup>1</sup>H NMR spectrum of *i*-butyl-ethyl T<sub>8</sub> in CDCl<sub>3</sub>.

# Electronic Supplementary Information (ESI)

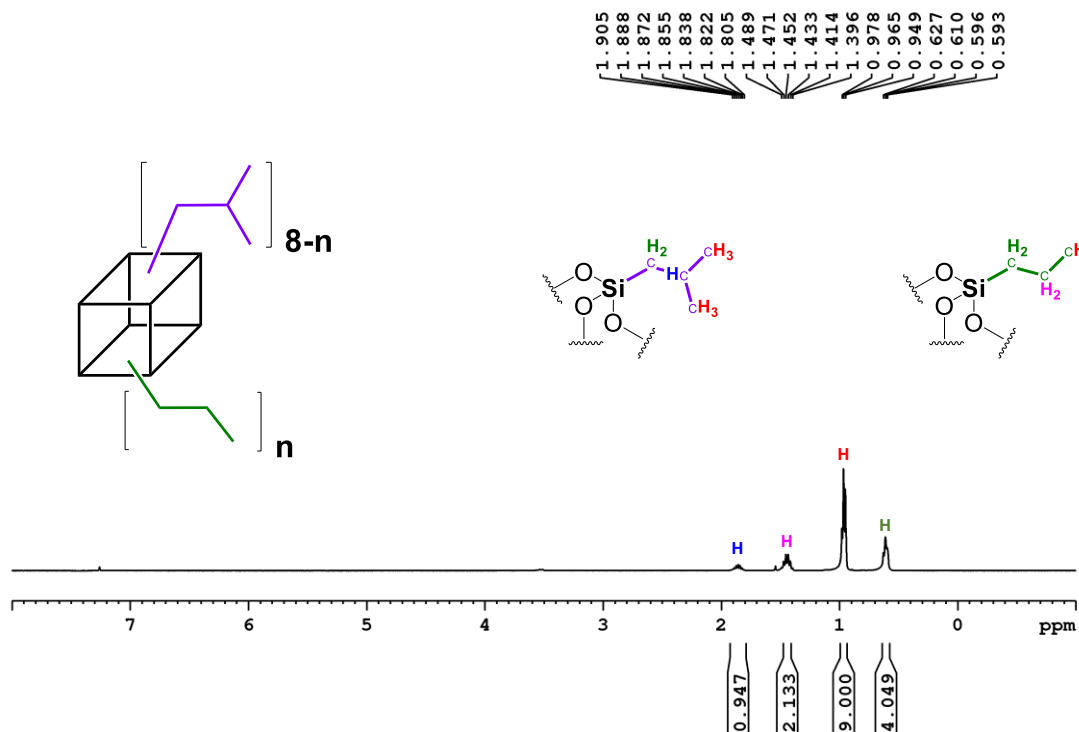


Figure S3  $^1\text{H}$  NMR spectrum of *i*-butyl-propyl  $\text{T}_8$  in  $\text{CDCl}_3$ .

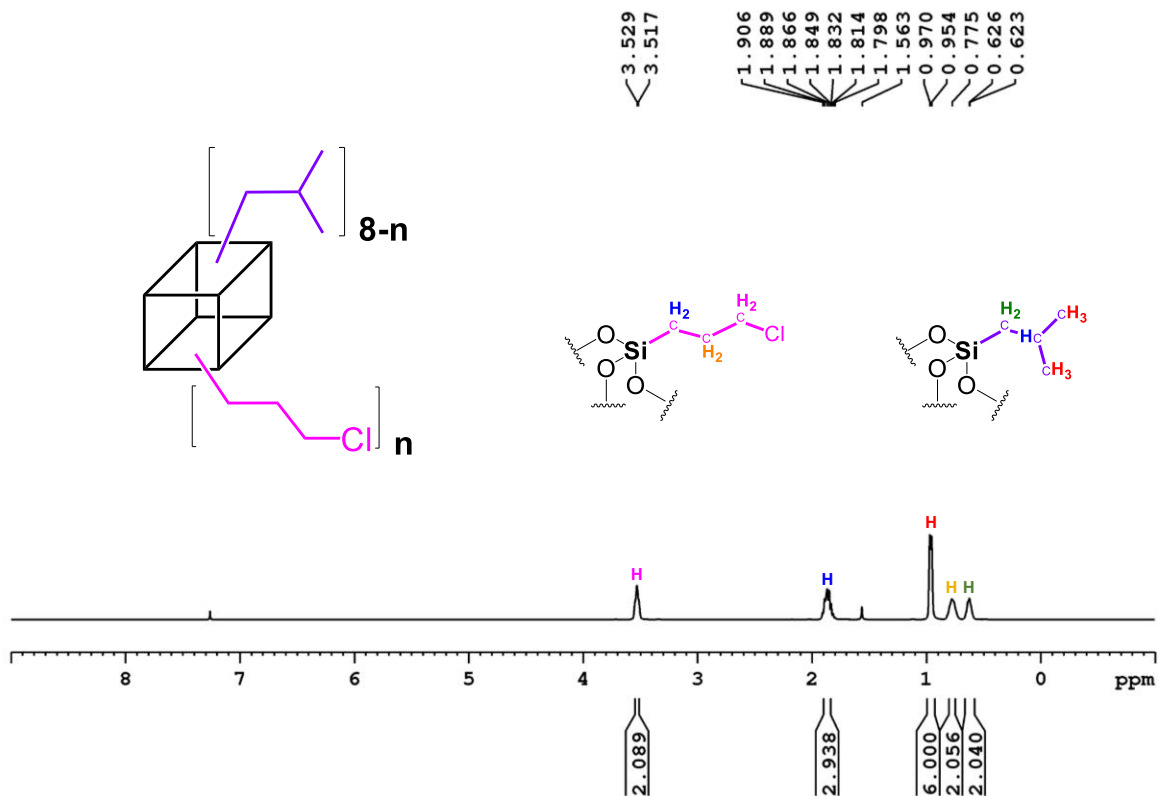


Figure S4  $^1\text{H}$  NMR spectrum of *i*-butyl-propyl chloride  $\text{T}_8$  in  $\text{CDCl}_3$ .

# Electronic Supplementary Information (ESI)

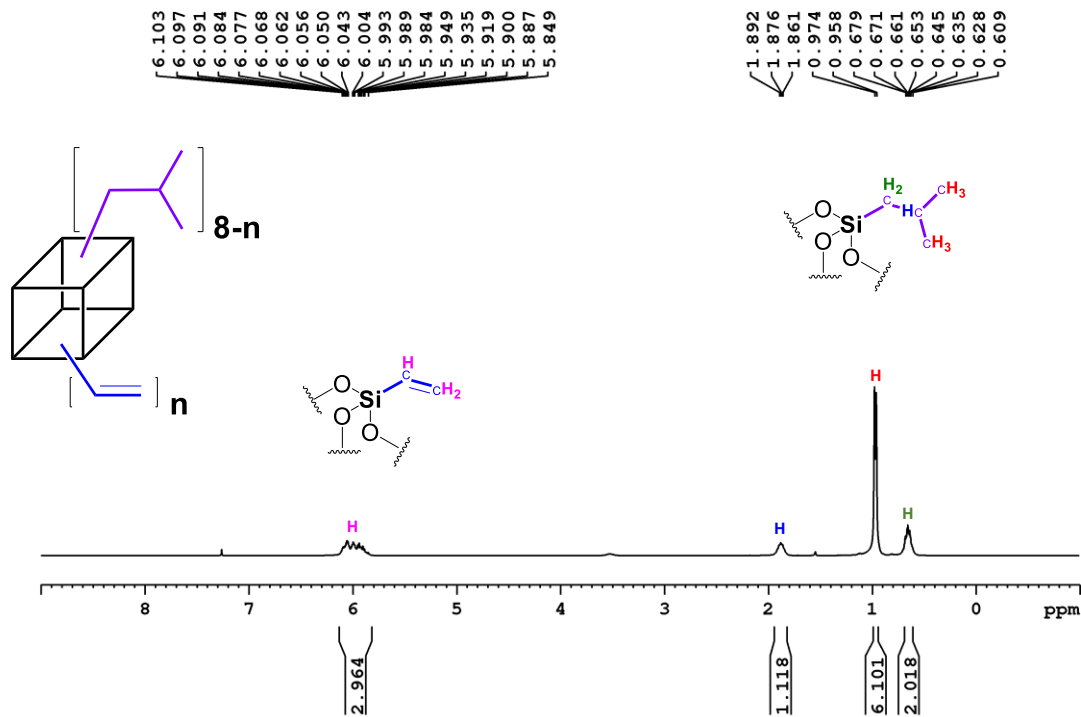


Figure S5  $^1\text{H}$  NMR spectrum of *i*-butyl-vinyl  $\text{T}_8$  in  $\text{CDCl}_3$ .

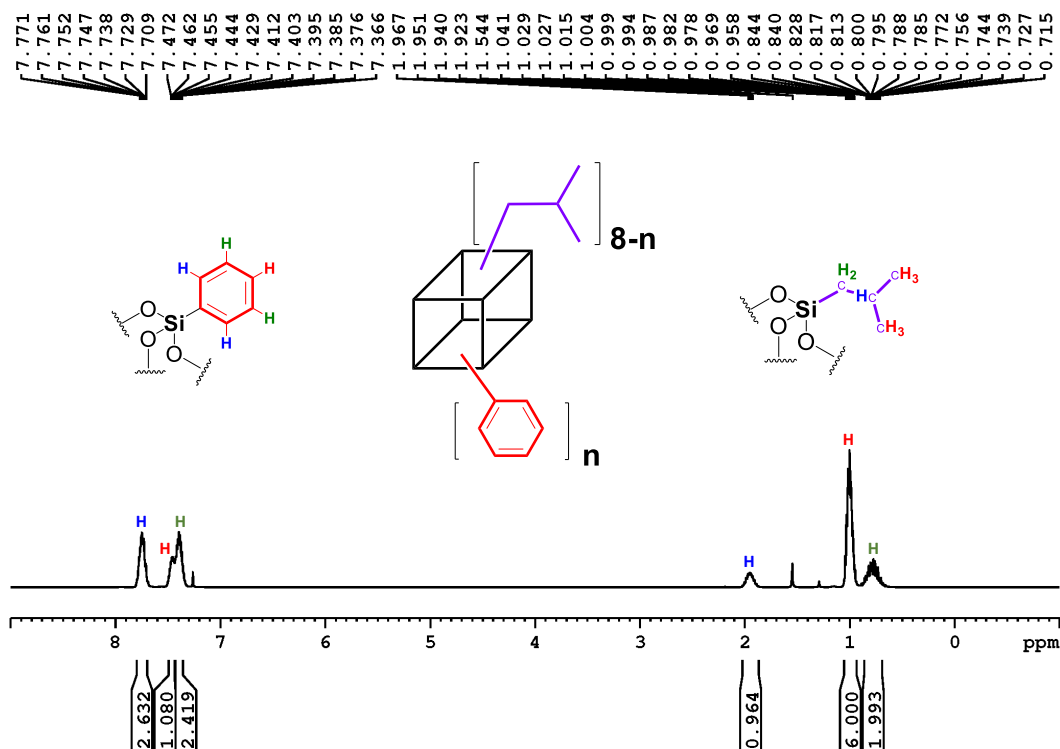


Figure S6  $^1\text{H}$  NMR spectra of *i*-butyl-phenyl  $\text{T}_8$  in  $\text{CDCl}_3$ .

# Electronic Supplementary Information (ESI)

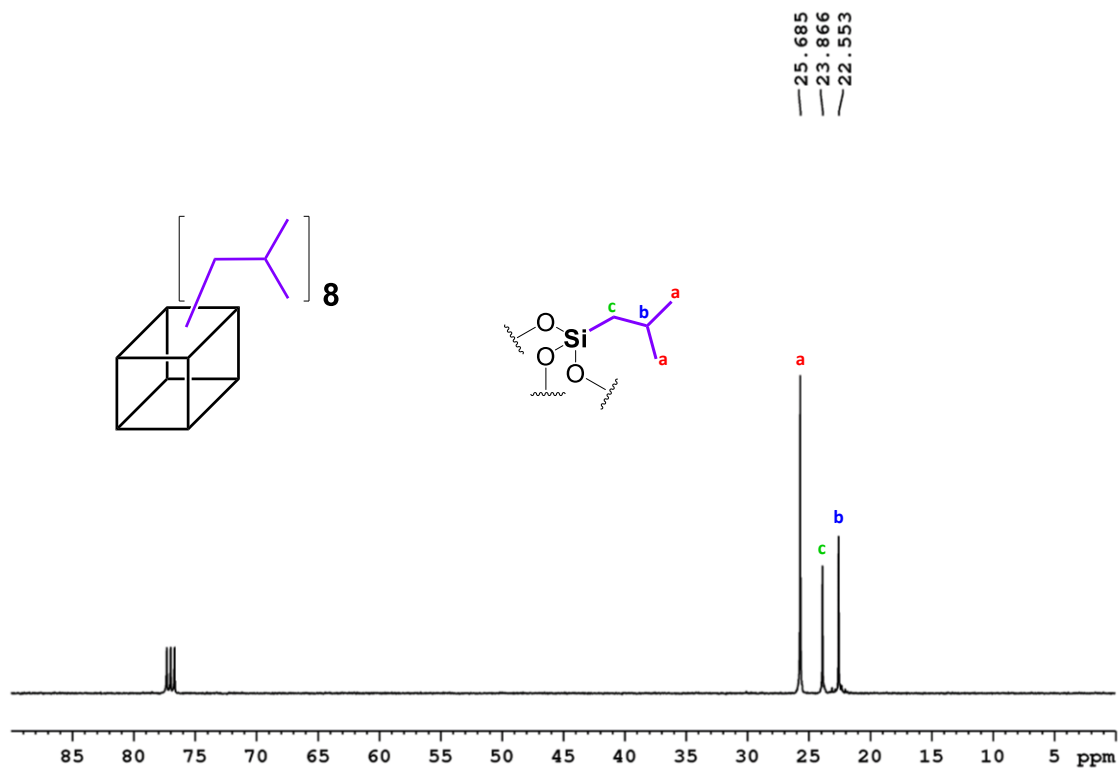


Figure S7 <sup>13</sup>C NMR spectrum of *i*-butyl T<sub>8</sub> in CDCl<sub>3</sub>.

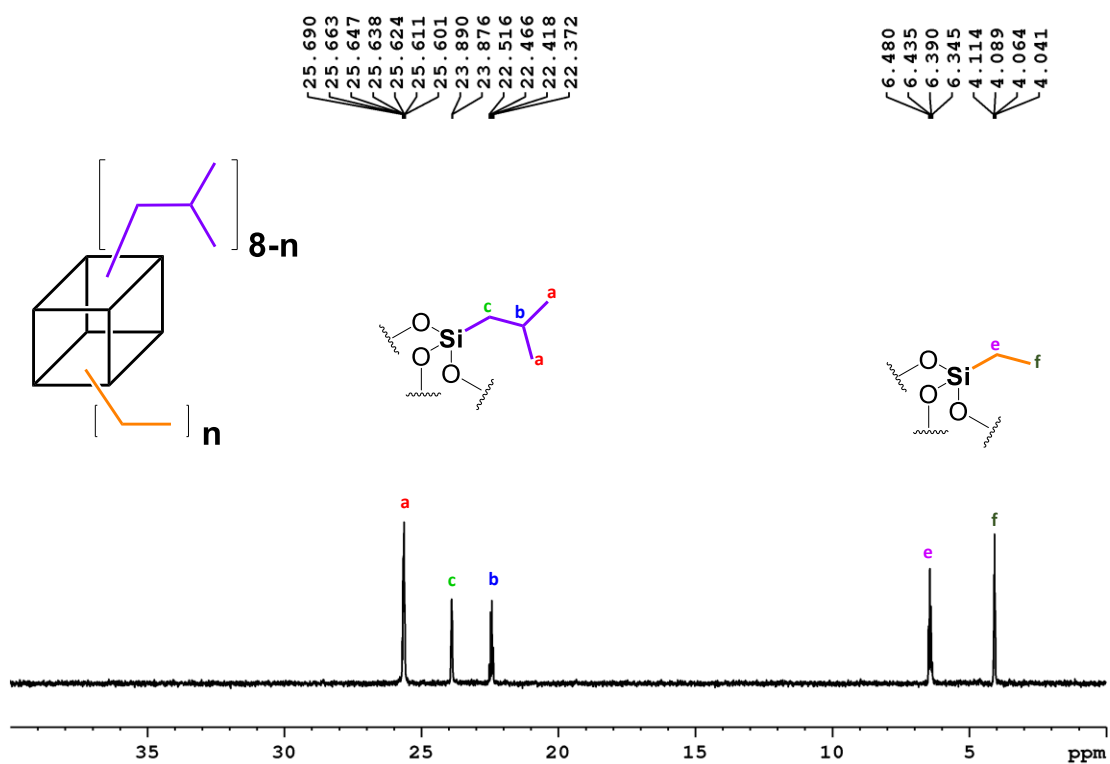


Figure S8 <sup>13</sup>C NMR spectrum of *i*-butyl-ethyl T<sub>8</sub> in CDCl<sub>3</sub>.

# Electronic Supplementary Information (ESI)

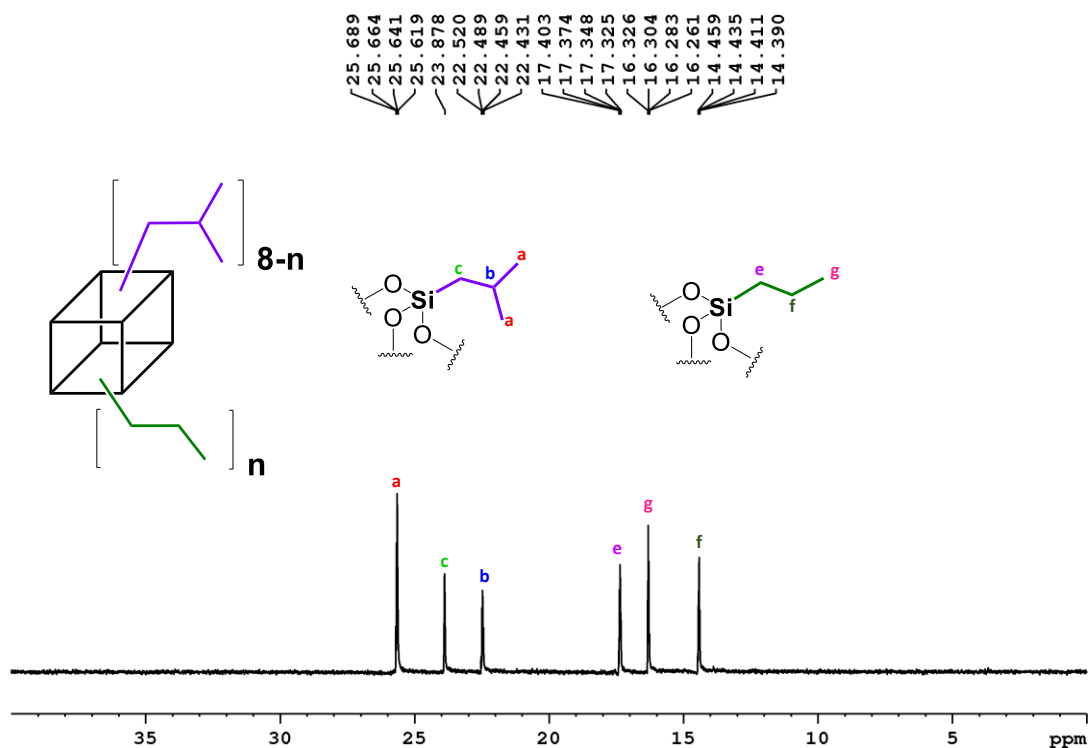


Figure S9  $^{13}\text{C}$  NMR spectrum of *i*-butyl-propyl  $\text{T}_8$  in  $\text{CDCl}_3$ .

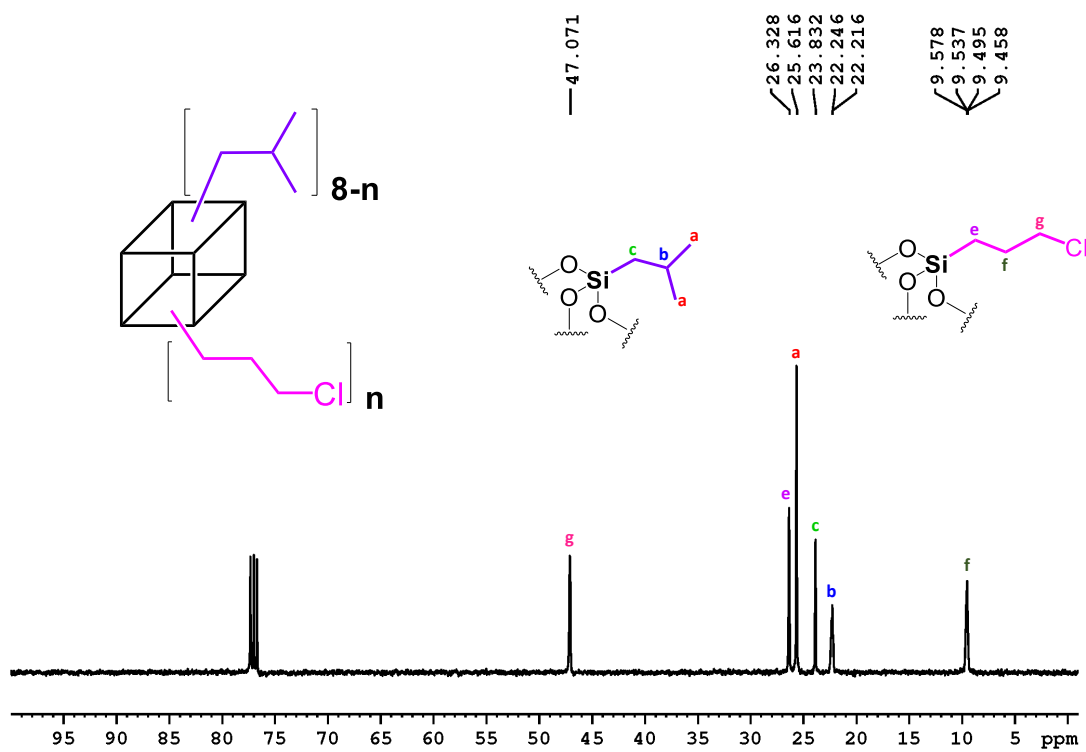


Figure S10  $^{13}\text{C}$  NMR spectrum of *i*-butyl-propyl chloride  $\text{T}_8$  in  $\text{CDCl}_3$ .

# Electronic Supplementary Information (ESI)

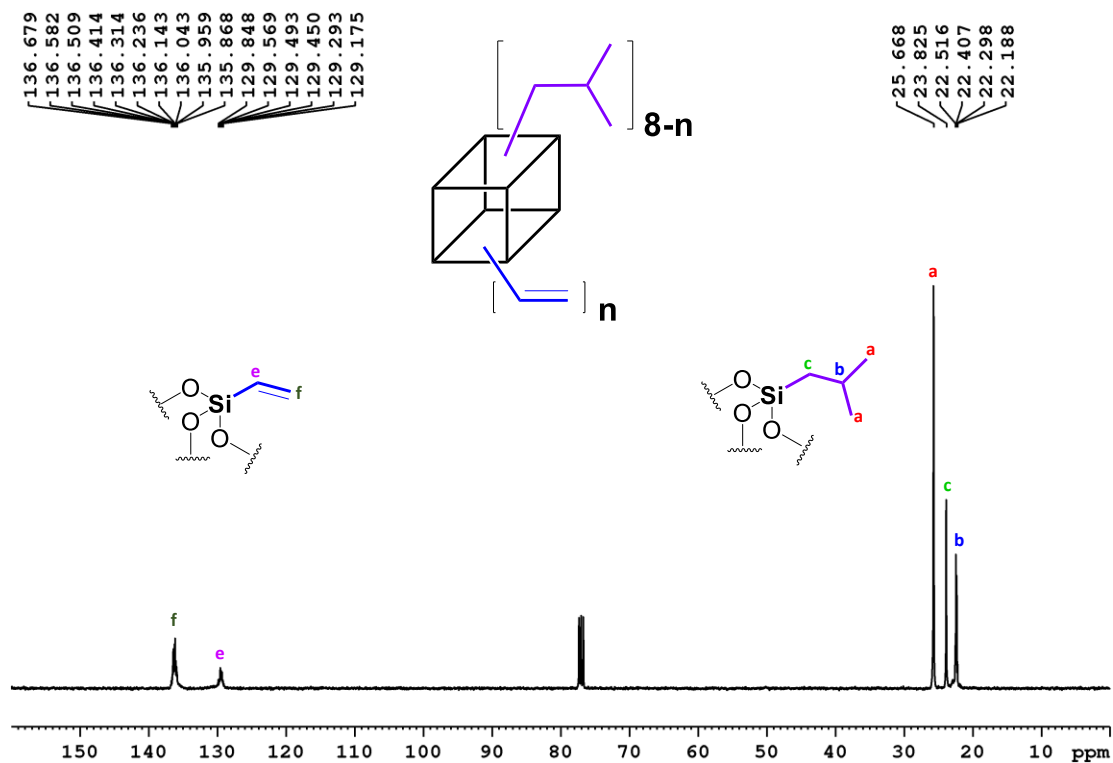


Figure S11 <sup>13</sup>C NMR spectrum of *i*-butyl-vinyl T<sub>8</sub> in CDCl<sub>3</sub>.

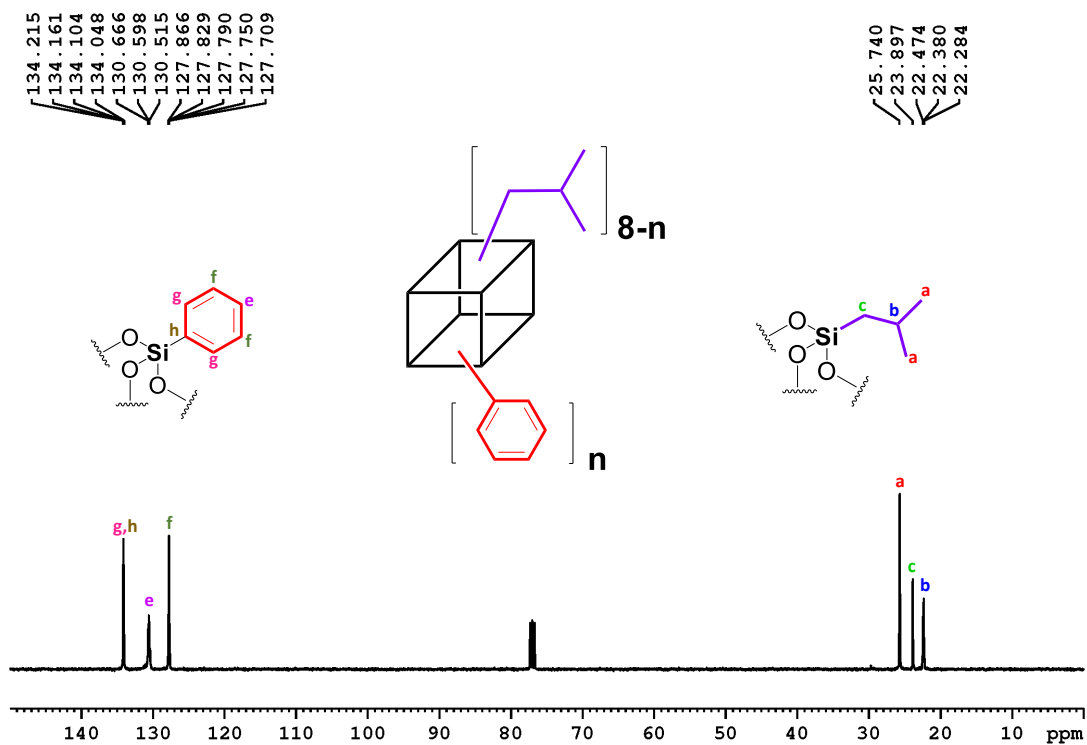


Figure S12 <sup>13</sup>C NMR spectrum of *i*-butyl-phenyl T<sub>8</sub> in CDCl<sub>3</sub>.

# Electronic Supplementary Information (ESI)

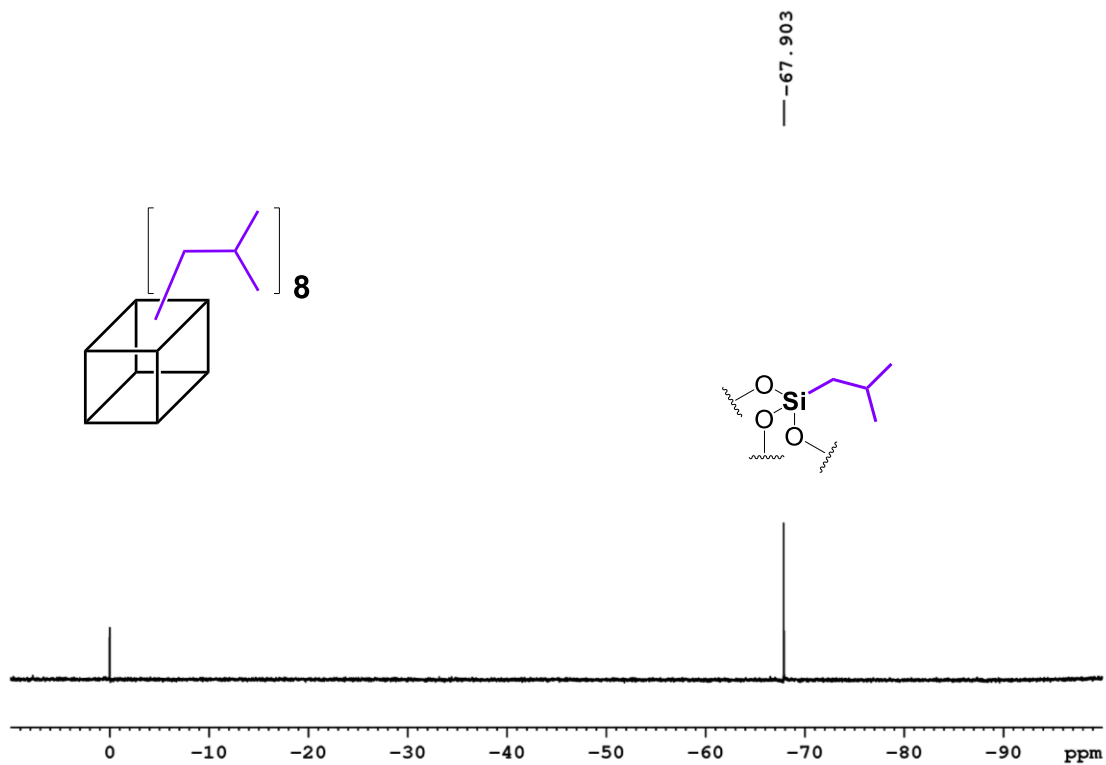


Figure S13 <sup>29</sup>Si NMR spectrum of *i*-butyl T<sub>8</sub> in CDCl<sub>3</sub>.

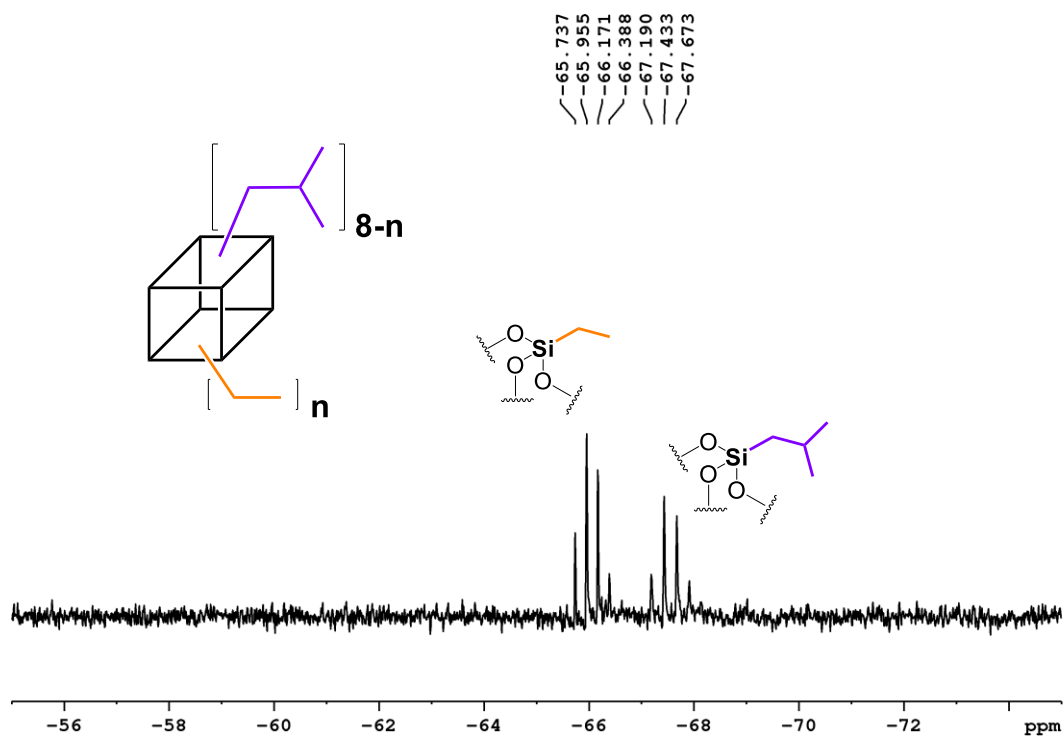


Figure S14 <sup>29</sup>Si NMR spectrum of *i*-butyl-ethyl T<sub>8</sub> in CDCl<sub>3</sub>.



# Electronic Supplementary Information (ESI)

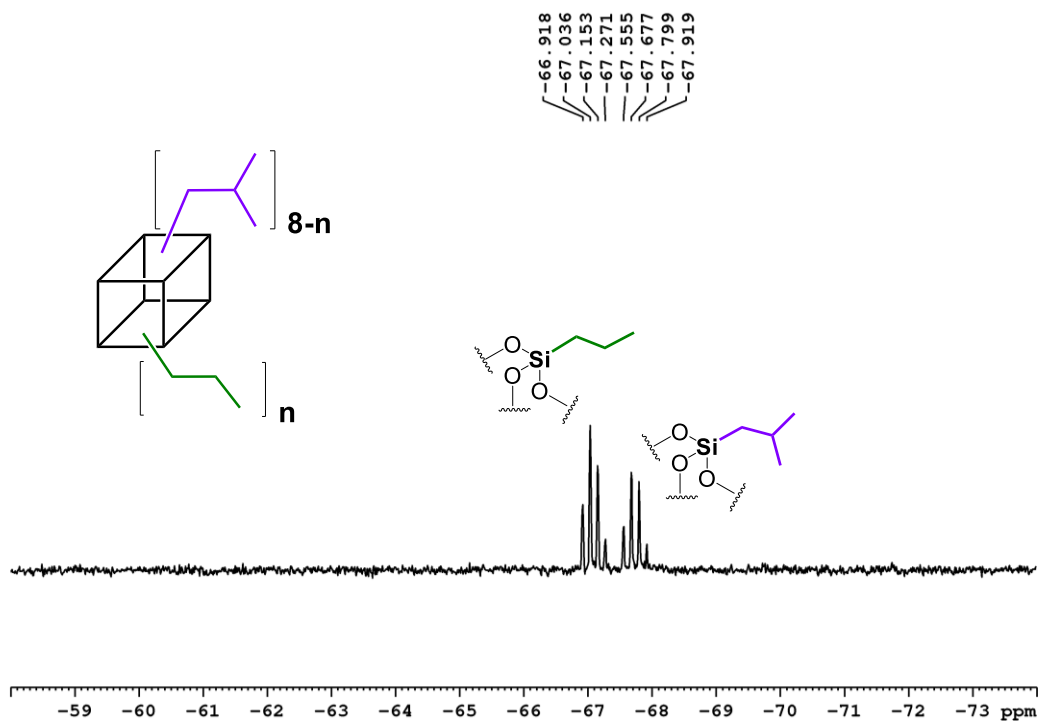


Figure S15  $^{29}\text{Si}$  NMR spectrum of *i*-butyl-propyl  $\text{T}_8$  in  $\text{CDCl}_3$ .

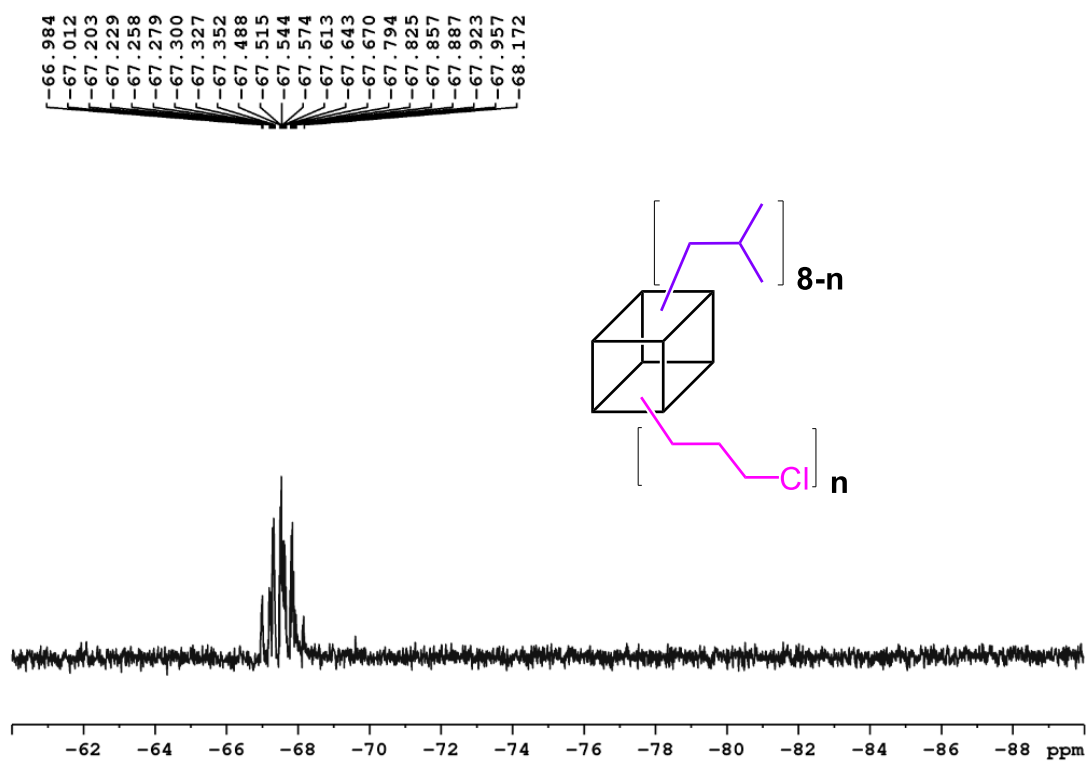


Figure S16  $^{29}\text{Si}$  NMR spectrum of *i*-butyl-propyl chloride  $\text{T}_8$  in  $\text{CDCl}_3$ .

# Electronic Supplementary Information (ESI)

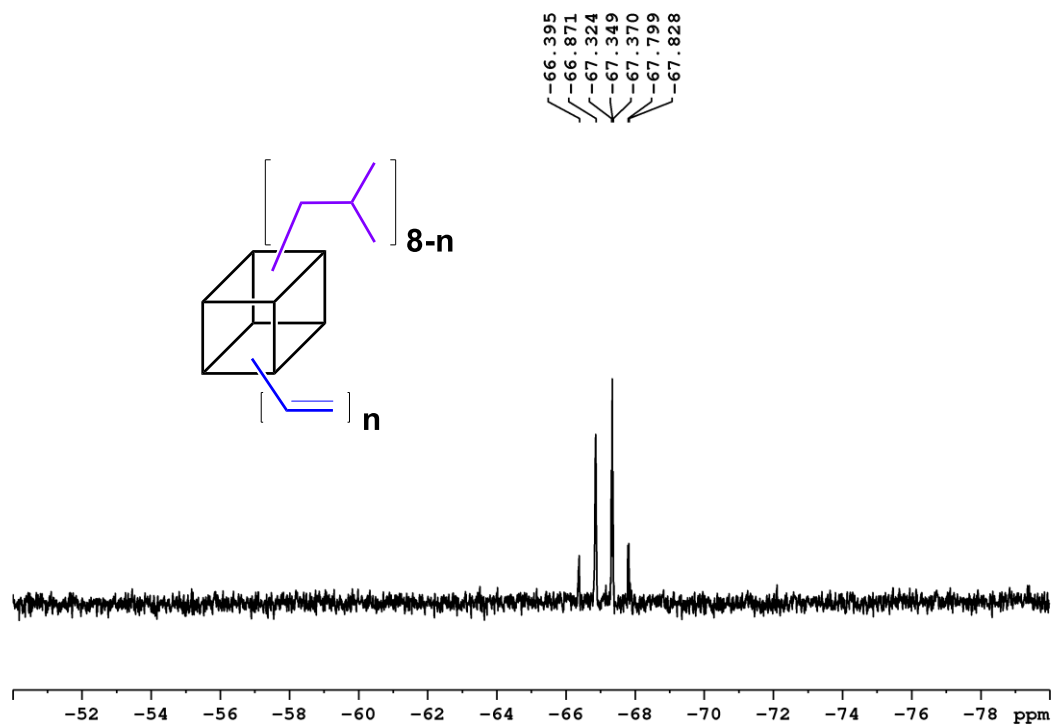


Figure S17 <sup>29</sup>Si NMR spectrum of *i*-butyl-vinyl T<sub>8</sub> in CDCl<sub>3</sub>.

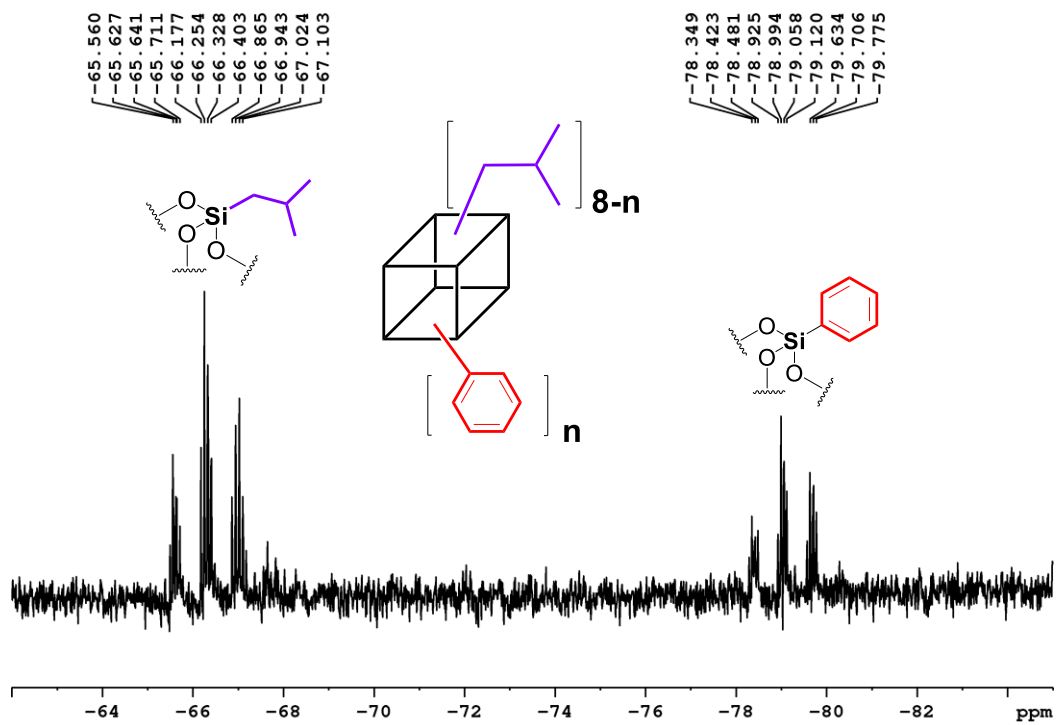
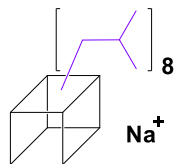
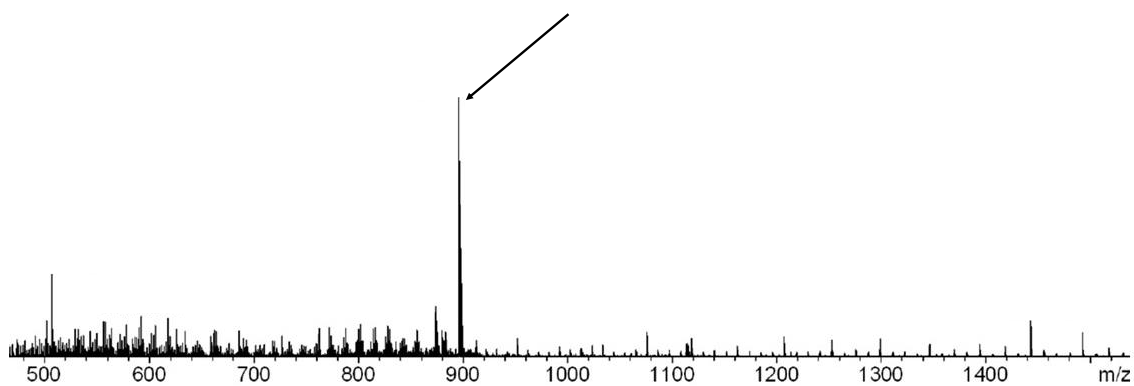


Figure S18 <sup>29</sup>Si NMR spectrum of *i*-butyl-phenyl T<sub>8</sub> in CDCl<sub>3</sub>.

# Electronic Supplementary Information (ESI)



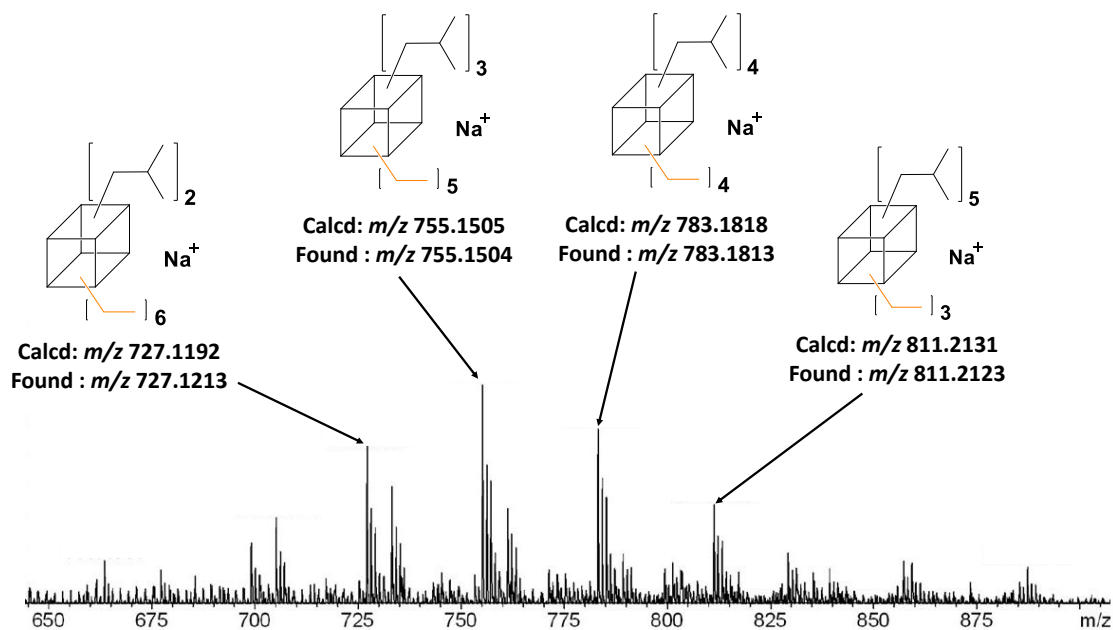
Calcd:  $m/z$  895.3070  
Found :  $m/z$  895.3072



#	$m/z$	I	I %	S/N	Res.
1	129.7569	3050	14.6	16.4	15725
2	144.9565	2829	13.6	15.2	15030
3	160.9967	2630	12.6	14.3	17666
4	233.5693	2630	12.6	15.4	22763
5	296.8383	4447	21.3	28.0	24163
6	296.9355	3059	14.6	19.2	19042
7	413.2676	6285	30.1	35.7	5001
8	419.0935	3217	15.4	17.8	30305
9	441.2977	3613	17.3	19.2	5005
10	507.3114	6868	32.9	32.9	4565
11	555.5093	3078	14.7	13.6	6041
12	557.5137	3051	14.6	13.5	4791
13	577.4819	2829	13.6	12.5	4320
14	591.4947	3499	16.8	15.8	5058
15	605.4999	2779	13.3	12.4	4833
16	617.5219	3311	15.9	15.0	5378
17	801.6871	2873	13.8	13.9	5046
18	827.7073	2715	13.0	13.3	5156
19	873.3322	3843	18.4	19.7	4951
20	874.3275	3124	15.0	15.8	5662
21	895.3072	20880	100.0	113.9	5299
22	896.3086	15829	75.8	86.1	5122
23	897.3086	12315	59.0	66.7	5352
24	898.3069	6106	29.2	32.5	5157
25	899.3106	2739	13.1	13.9	5220
26	1442.8367	3183	15.2	24.2	48906
27	1443.0690	2717	13.0	20.5	40664
28	2094.7278	2932	14.0	20.1	68883
29	2338.9265	5201	24.9	35.6	71446
30	2937.6458	3077	14.7	22.1	78011

**Figure S19** ESI-MS spectrum of *i*-butyl T<sub>8</sub>.

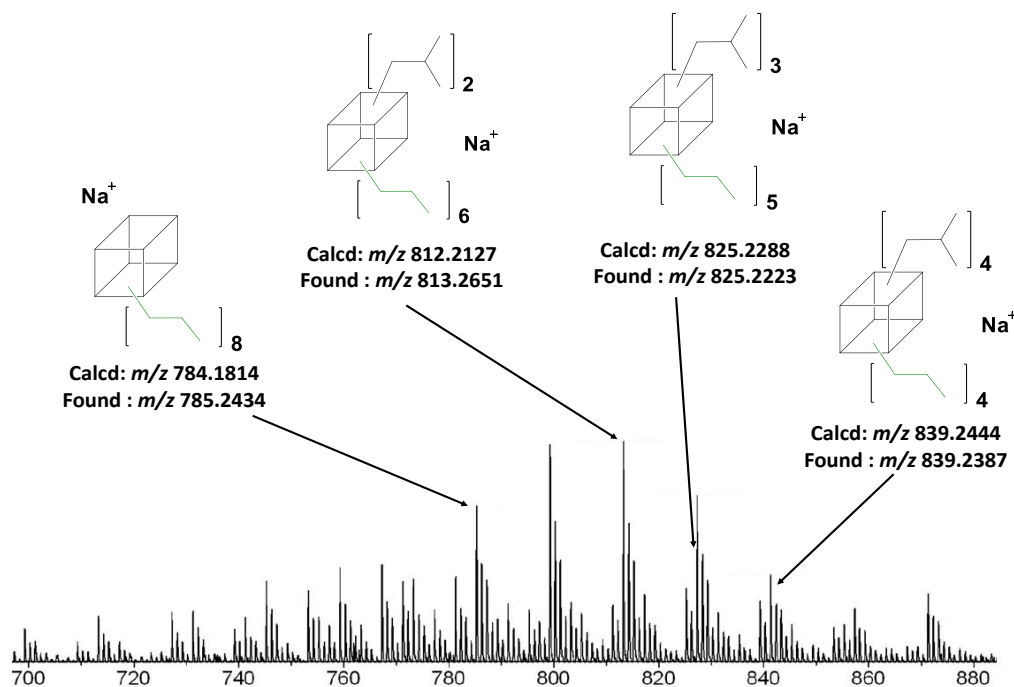
# Electronic Supplementary Information (ESI)



#	m/z	I	I%	S/N	Res.
1	145.0153	1543	21.7	25.3	14454
2	413.2648	5224	73.5	78.6	4848
3	441.2936	2746	38.6	37.0	4734
4	497.3645	1549	21.8	16.9	2699
5	699.0924	2110	29.7	16.5	4205
6	705.1394	2942	41.4	23.9	4830
7	706.1394	1873	26.3	14.3	5278
8	727.1213	5099	71.7	42.3	4758
9	728.1202	3234	45.5	25.9	5104
10	729.1221	2626	36.9	20.5	4463
11	733.1709	3916	55.1	31.7	4942
12	734.1664	2644	37.2	20.6	5494
13	735.1696	2063	29.0	15.5	4629
14	755.1504	7111	100.0	61.5	5051
15	756.1489	4575	64.3	38.7	5163
16	757.1509	4109	57.8	34.6	4810
17	758.1512	1738	24.4	13.1	4161
18	761.1985	3230	45.4	26.8	4790
19	762.1948	2438	34.3	19.6	5224
20	763.1978	2004	28.2	15.7	4861
21	783.1813	5730	80.6	51.6	5060
22	784.1801	4189	58.9	37.1	5464
23	785.1813	3496	49.2	30.6	4538
24	786.1866	1803	25.4	14.5	4767
25	789.2265	1806	25.4	14.6	4517
26	811.2123	3364	47.3	30.8	5230
27	812.2098	2366	33.3	20.9	5671
28	813.2131	2211	31.1	19.4	4804
29	829.2281	1838	25.9	16.3	4630
30	857.2553	1587	22.3	14.6	4978

Figure S20 ESI-MS spectrum of *i*-butyl-ethyl T<sub>8</sub>.

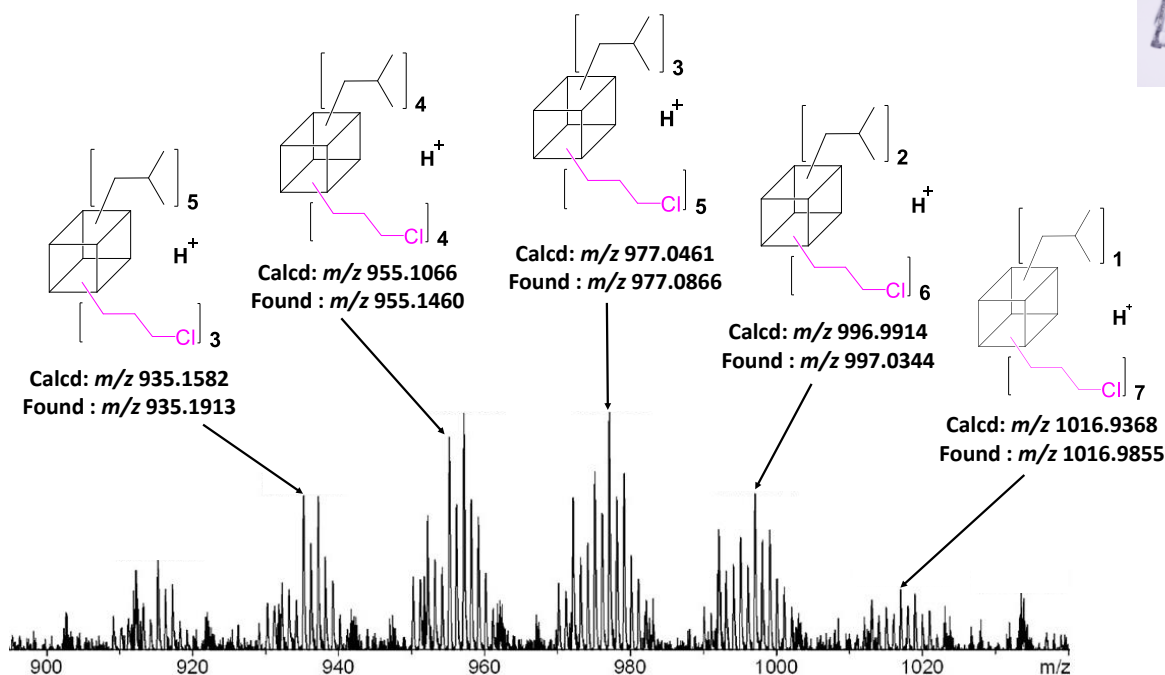
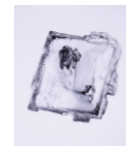
# Electronic Supplementary Information (ESI)



#	$m/z$	I	I %	S/N	Res.
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2	753.2203	5241	33.2	31.3	5366
3	759.2628	6893	43.6	42.1	4880
4	760.2670	4249	26.9	25.2	5110
5	767.2350	7109	45.0	43.8	5059
6	768.2358	4533	28.7	27.3	5238
7	771.2328	5932	37.5	36.4	4984
8	773.2662	6095	38.6	37.5	4664
9	781.2512	6248	39.5	38.9	5206
10	785.2434	11275	71.4	72.0	5305
11	786.2422	7184	45.5	45.2	5339
12	787.2578	5884	37.2	36.7	4401
13	791.2753	4331	27.4	26.6	4585
14	799.2538	15569	98.5	101.8	5239
15	800.2557	10125	64.1	65.6	5316
16	801.2579	7440	47.1	47.7	4893
17	803.2439	4319	27.3	26.9	4770
18	813.2651	15801	100.0	105.0	4810
19	814.2664	10032	63.5	66.0	4818
20	815.2666	7398	46.8	48.2	4752
21	817.2533	4592	29.1	29.2	4879
22	825.2223	5335	33.8	34.6	5176
23	827.2733	11963	75.7	80.4	4719
24	828.2774	7810	49.4	51.8	4931
25	829.2768	6019	38.1	39.5	4658
26	839.2387	4549	28.8	29.8	5308
27	841.2767	6408	40.6	42.8	4259
28	842.2815	4333	27.4	28.4	4479
29	871.2657	5039	31.9	34.6	5268
30	885.2805	5236	33.1	36.7	5134

Figure S21 ESI-MS spectrum of *i*-butyl-propyl T<sub>8</sub>.

# Electronic Supplementary Information (ESI)



#	$m/z$	I	I %	S/N	Res.
1	101.8815	3887	28.4	8.7	13995
2	129.7528	4658	34.0	10.5	16631
3	144.9590	4398	32.1	9.9	15956
4	195.5969	4224	30.8	9.8	20664
5	233.5678	4171	30.4	9.8	22868
6	296.8296	4567	33.3	11.2	21732
7	413.2635	13700	100.0	35.0	4402
8	532.0511	4170	30.4	10.2	35177
9	813.2830	5252	38.3	13.2	4911
10	935.1913	4823	35.2	11.2	4824
11	937.1920	4785	34.9	11.1	4800
12	952.1738	4246	31.0	9.9	6069
13	955.1460	6520	47.6	15.8	4769
14	956.1416	4556	33.3	10.8	4863
15	957.1419	7209	52.6	17.6	4494
16	958.1342	4693	34.3	11.1	4907
17	959.1329	4170	30.4	9.8	4639
18	972.1197	4746	34.6	11.5	5528
19	975.1076	5523	40.3	13.5	4738
20	976.1033	4299	31.4	10.3	4905
21	977.0866	7259	53.0	18.1	4635
22	978.0879	4784	34.9	11.6	4633
23	979.0830	5466	39.9	13.5	5282
24	997.0344	4879	35.6	12.2	4846
25	1442.8431	5032	36.7	14.8	52413
26	1863.9752	4206	30.7	11.9	60434
27	2035.7613	3859	28.2	10.3	64150
28	2338.9364	6212	45.3	16.2	70231
29	2339.1438	3885	28.4	10.0	37566
30	2937.6371	3853	28.1	9.6	78331

Figure S22 ESI-MS spectrum of *i*-butyl-propyl chloride T<sub>8</sub>.

# Electronic Supplementary Information (ESI)

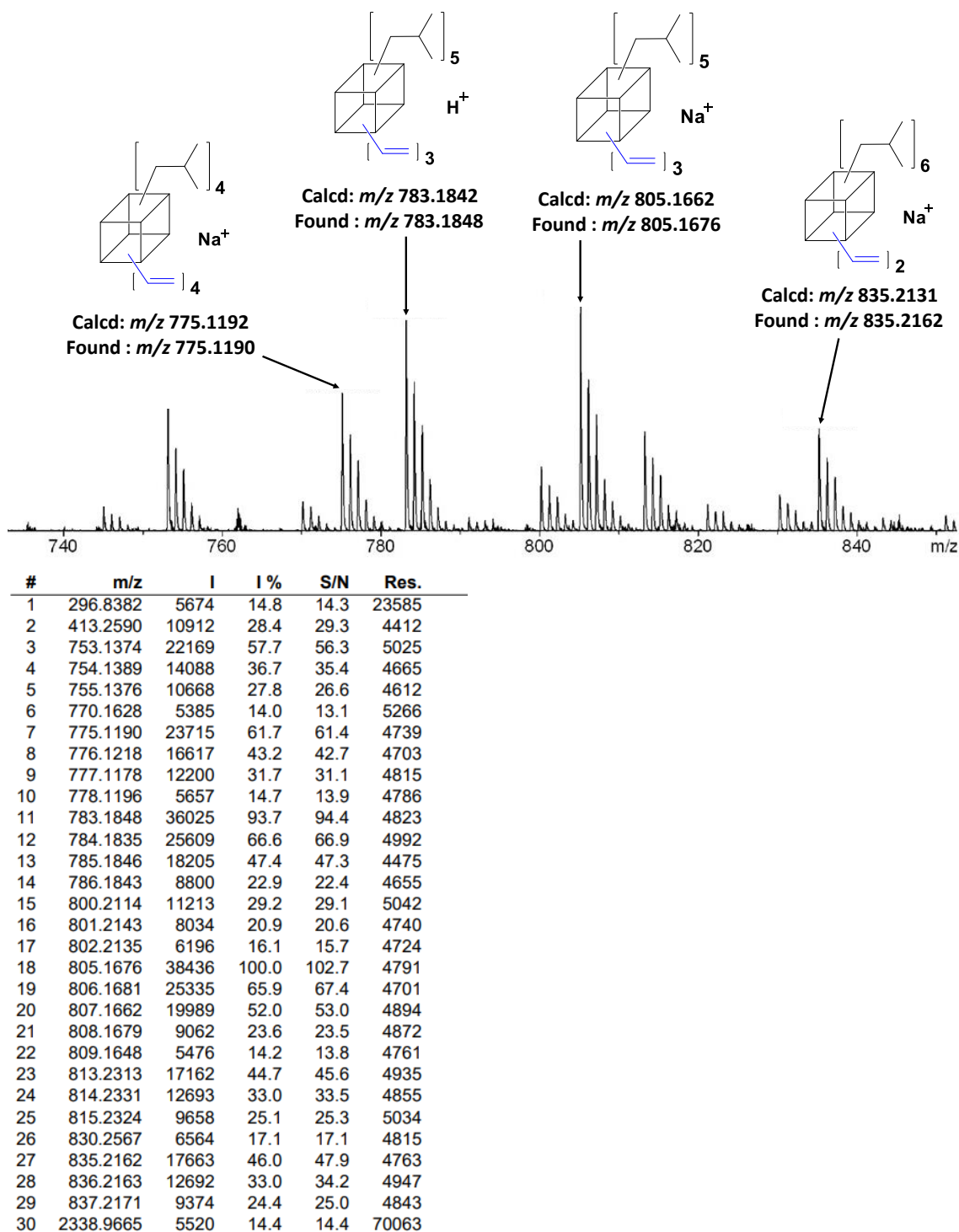
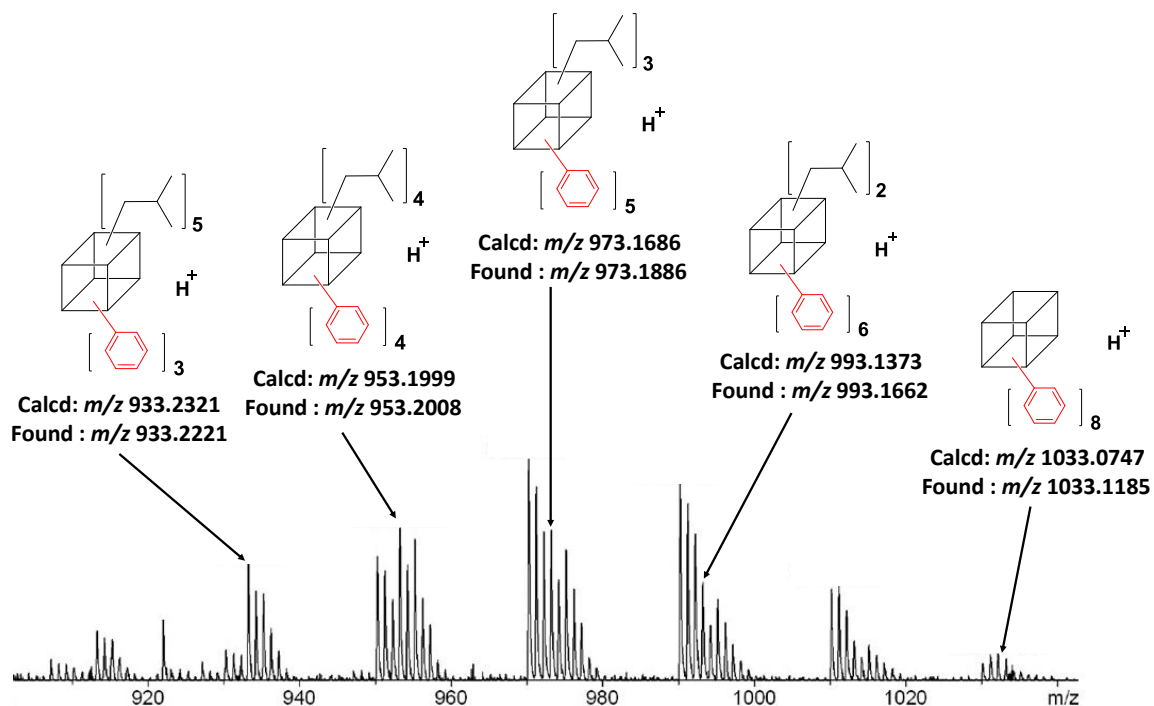
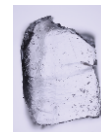


Figure S23 ESI-MS spectrum of *i*-butyl-vinyl T<sub>8</sub>.

# Electronic Supplementary Information (ESI)

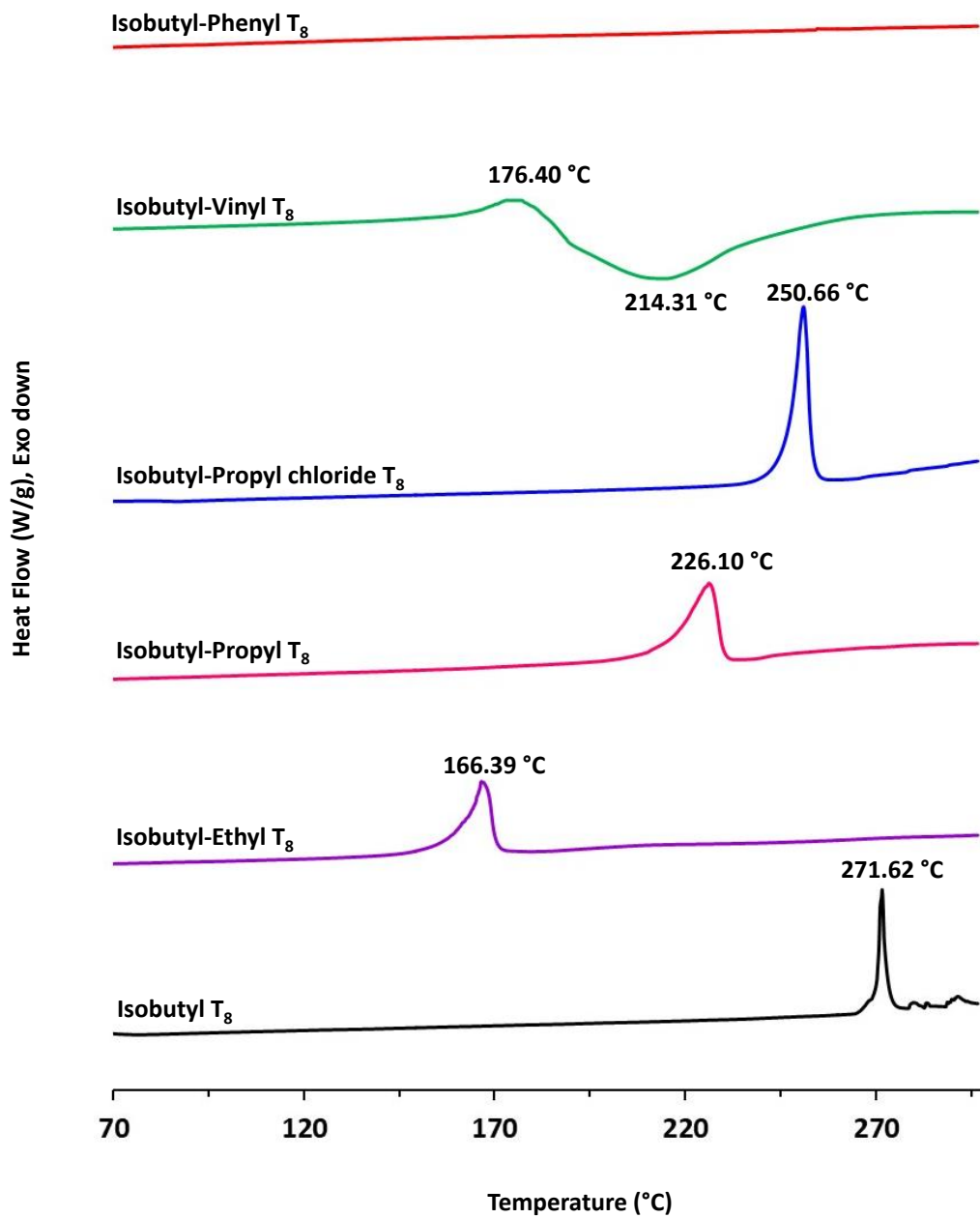


#	m/z	I	I %	S/N	Res.
1	413.2620	688	32.7	49.9	4146
2	875.1498	571	27.2	23.4	4685
3	922.0004	594	28.3	22.2	5516
4	933.2221	1131	53.8	43.1	5278
5	934.2261	872	41.5	32.9	5124
6	935.2198	843	40.1	31.8	4833
7	950.2470	1197	56.9	47.4	5025
8	951.2481	1058	50.3	41.8	5041
9	952.2387	793	37.7	30.9	4947
10	953.2008	1457	69.3	58.6	4451
11	954.2005	1112	52.9	44.3	4704
12	955.1965	1353	64.4	54.5	5413
13	956.1956	805	38.3	31.6	5143
14	970.2131	2102	100.0	88.7	5014
15	971.2119	1845	87.8	77.7	4956
16	972.2087	1423	67.7	59.6	4838
17	973.1886	1441	68.6	60.5	4576
18	974.1695	978	46.5	40.5	4772
19	975.1651	1257	59.8	52.8	5182
20	976.1722	896	42.6	37.1	5558
21	977.1627	568	27.0	22.8	5260
22	990.1813	1878	89.3	82.7	5235
23	991.1833	1692	80.5	74.5	4880
24	992.1842	1335	63.5	58.5	4597
25	993.1662	950	45.2	41.1	4391
26	995.1471	793	37.7	34.1	4751
27	996.1438	580	27.6	24.4	5122
28	1010.1555	887	42.2	39.9	5619
29	1011.1489	923	43.9	41.7	4900
30	1012.1470	687	32.7	30.6	5024

Figure S24 ESI-MS spectrum of *i*-butyl-phenyl Ts.

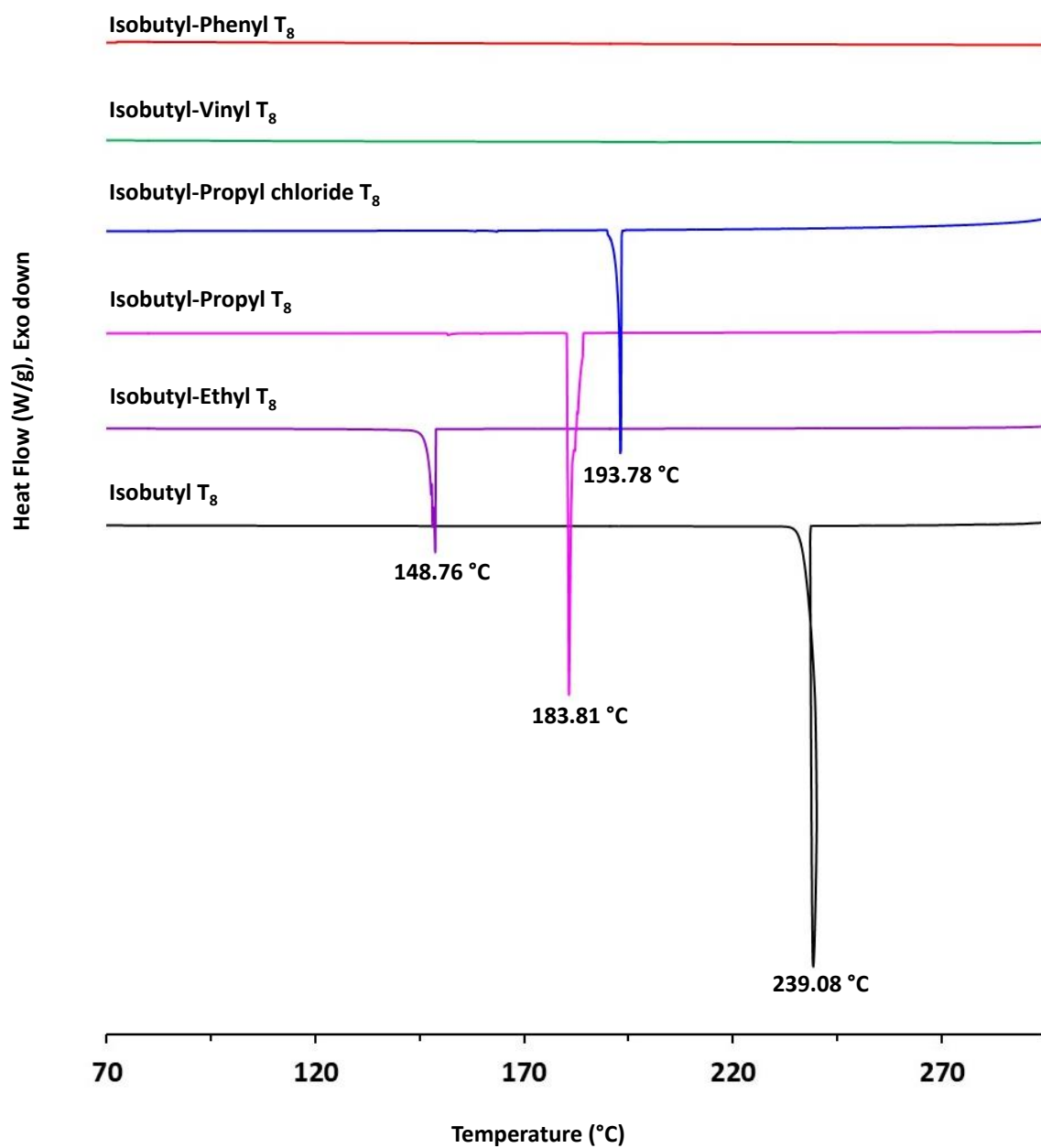


# Electronic Supplementary Information (ESI)



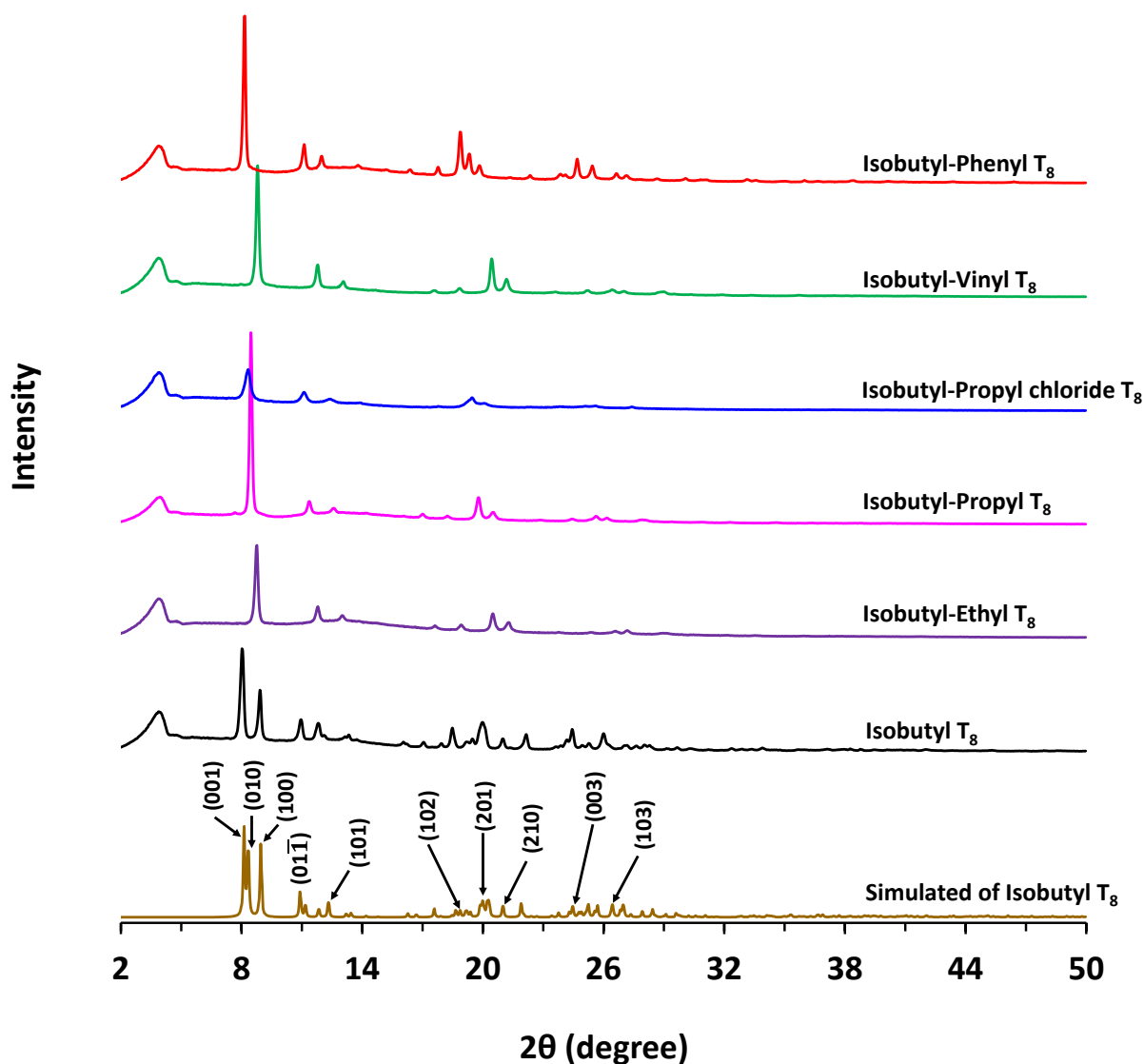
**Figure S25** DSC heating thermograms of *i*-butyl T<sub>8</sub> and mixed-substituent T<sub>8</sub>.

# Electronic Supplementary Information (ESI)



**Figure S26** DSC cooling thermograms of *i*-butyl T<sub>8</sub> and mixed-substituent T<sub>8</sub>.

# Electronic Supplementary Information (ESI)



**Figure S27** XRD patterns of mixed-substituent T<sub>8</sub>, *i*-butyl T<sub>8</sub>, and simulated of *i*-butyl T<sub>8</sub>. [1]

## Reference

[1] N. Prigyai, S. Chanmungkalakul, V. Ervithayasuporn, N. Yodsini, S. Jungstittiwong, N. Takeda, M. Unno, J. Boonmak, S. Kiatkamjornwong, Lithium-Templated Formation of Polyhedral Oligomeric Silsesquioxanes (POSS), *Inorg. Chem.*, 58 (2019) 15110-15117.