Supporting Information

Synthesis and Characterization of Sulfide/Sulfone-Containing 18-8-18-Membered-Ring Ladder-Type Siloxanes

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1. Experimental data

1-1 General information

Unless specifically stated, all reagents were commercially obtained and when necessary, purified prior to use. Toluene was dried using mBRAUN purification system. Precursors bis(4-methoxybenzyl)sulfane (**1**) and bis(3-methoxybenzyl)sulfane (**4**) were prepared according to reported methods.[1] All reactions were conducted under argon atmosphere utilizing standard Schlenk technique. Flash column chromatography was performed over silica (100-200 mesh). The Fourier transformation nuclear magnetic resonance (NMR) spectra were obtained using a JEOL JNM-ECA 600 NMR instrument, with ^{1}H at 600.17 MHz, ^{13}C at 150.91 MHz, ^{29}Si at 119.24 MHz. For ^{1}H NMR, chemical shifts are reported as δ units (ppm) relative to $SiMe_4$ (TMS), with residual solvent peaks serving as the standard. For ^{13}C NMR and ^{29}Si NMR, chemical shifts are reported as δ units (ppm) relative to $SiMe_4$ (TMS), with residual solvent peaks serving as the standard, and spectra were obtained with complete proton decoupling. MALDI-TOF mass analysis were carried out with a Shimadzu AXIMA Performance instrument using 2,5-dihydroxybenzoic acid (dithranol) as the matrix. IR spectra were measured with a Shimadzu FTIR-8400S. TGA was conducted under a nitrogen flow (250 mL min^{-1}) with a heating rate of 10 ˚C min^{-1}. All samples were measured with temperatures ranging from 50 to 1000 ˚C, where they remained for 5 min. The weight loss and heating rate were continuously recorded throughout the experiment. Thin layer chromatography was performed using Silica.

1-2 Single-crystal crystallography studies

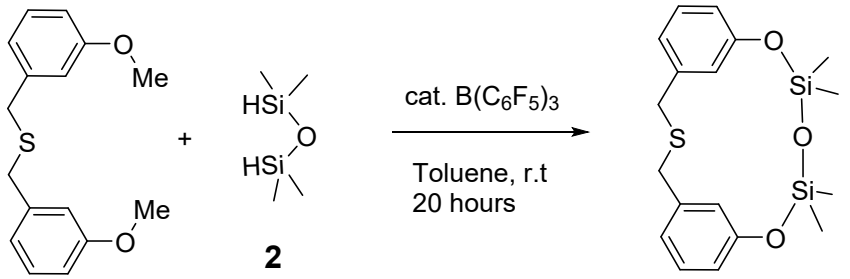
Single crystals of **7** and **9** suitable for X-ray structural analysis were obtained by slow recrystallization from dichloromethane/hexane after seven days. The colorless needle-shaped crystal was immersed in a drop of oil and mounted on a MicroMount. The intensity data were collected on a Rigaku VariMax with an XtaLab P200 diffractometer with multi-layer mirror monochromated Mo *Kα* radiation (λ= 0.71075 Å). The structures were solved using SHELXT,[2] and refined by full-matrix least-squares procedures on F^2 for all reflections (SHELXL-2014/7).[3] All the non-hydrogen atoms were refined anisotropically. All hydrogens were placed using AFIX instructions. All calculations were carried out using Yadokari-XG2009.[4] Crystallographic data of

7 and **9** have been deposited with Cambridge Crystallographic Data Centre: Deposition numbers CCDC-2254813 and 2254814, respectively. Copies of the data can be obtained free of charge via http://www.ccde.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge, CB2 1EZ, U.K.; Fax: +44 1223 336033; e-mail: deposit@ccdc.cam.ac.uk).

1-3 The Piers-Rubinsztajn reaction between bis(4-methoxybenzyl)sulfane (1) and 1,1,3,3-tetramethyldisiloxane (2)

To a 50 mL Schlenk flask was added bis(4-methoxybenzyl)sulfane (**1**) (0.274 g, 1 mmol), dry toluene (18 mL) and 1,1,3,3-tetramethyldisiloxane (**2**) (0.18 mL, 1 mmol). And then tris(pentafluorophenyl)borane (26 mg, 0.05 mmol) was added. The mixture was stirred at room temperature for 20 hours before the addition of 0.3 g of basic alumina. The resulting mixture was filtered and concentrated on the rotavapor to give a crude product, which was purified by column chromatography (silica gel, hexane : EtOAc = 50 : 1) to give the partially substituted compound **3** (30 mg) and linear oligomers.

1-4 Synthesis of cyclic compound (5)



4 **2** **5**

To a 50 mL Schlenk flask was added tris(pentafluorophenyl)borane (14.6 mg, 0.029 mmol, 5 mol%), dry toluene (15 mL) and bis(3-methoxybenzyl)sulfane (**4**) (0.157 g, 0.57 mmol). To this mixture, a solution of 1,1,3,3-tetramethyldisiloxane (**2**) (0.103 mL, 0.58 mmol) in 5 mL of dry toluene was added dropwise over 20 minutes. The reaction mixture was stirred at room temperature for 20 hours before the addition of 0.3 g of basic alumina. The resulting mixture was filtered and concentrated on the rotavapor to give a yellow oil, which was purified by column chromatography

(silica gel, hexane : EtOAc = 20 : 1) to give a white solid (0.11 g, 51% yield).

^{1}H NMR (600.17 MHz, CDCl) δ 7.25 (t, *J* = 7.8 Hz, 2H), 7.13 (d, *J* = 8.4 Hz, 2H), 6.75 (d, *J* = 8.4 Hz, 2H), 6.71 (s, 2H), 3.39 (s, 4H), 0.29 (s, 12H) ppm;

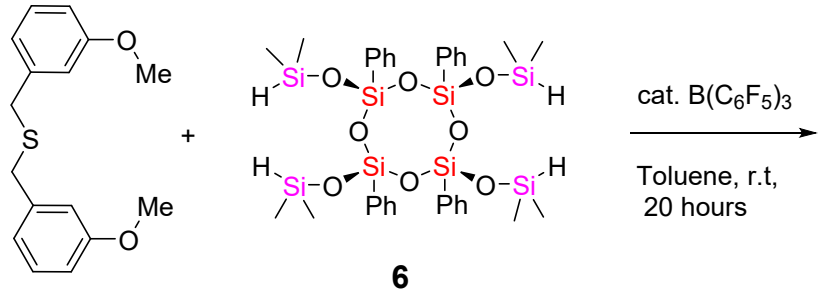
^{13}C NMR (150.91 MHz, $CDCl_3$) δ 153.78, 139.58, 130.16, 122.56, 121.62, 118.72, 33.85, −0.54 ppm;

^{29}Si NMR (119.24 MHz, $CDCl_3$) δ −12.35 (D-unit silicon) ppm;

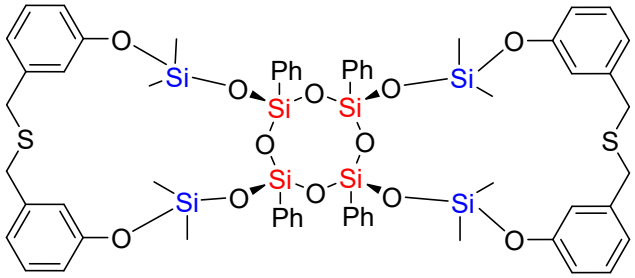
MALDI-TOF MS (m/z): 377.16 ($[M+H]^+$, calcd 377.10);

Elemental analysis: Calcd for $C_{18}H_{24}O_3SSi_2$: C, 57.41; H, 6.42. Found: C, 57.37; H, 6.39.

1-5 Synthesis of Ladder-type siloxane-based compound (7)



4 **6**



7

To a 50 mL Schlenk flask was added tris(pentafluorophenyl)borane (12 mg, 0.023 mmol, 5 mol%), dry toluene (15 mL) and bis(3-methoxybenzyl)sulfane (**4**) (0.24 g, 0.89 mmol). To this mixture, a solution of all-*cis*-cyclotetrasiloxane (**6**) (0.35 g, 0.45 mmol) in 5 mL of dry toluene was added dropwise over 20 minutes. The reaction mixture was stirred at room temperature for 20 hours before the addition of 0.3 g of basic alumina. The resulting mixture was filtered and concentrated on the rotavapor to give a yellow oil, which was purified by column chromatography (silica gel, hexane : EtOAc = 20 : 1) to give a white solid (0.18 g, 32% yield).

^{1}H NMR (600.17 MHz, $CDCl_3$) δ 7.22 (t, J = 7.8 Hz, 4H), 7.12-7.17 (m, 12H), 6.99 (t, J = 7.8 Hz, 12H), 6.71 (s, 4H), 6.65 (d, J = 7.8 Hz, 4H), 3.28-3.33 (ABq, J = 14.4 Hz, 8H), 0.46 (s, 12H), 0.28 (s, 12H) ppm;

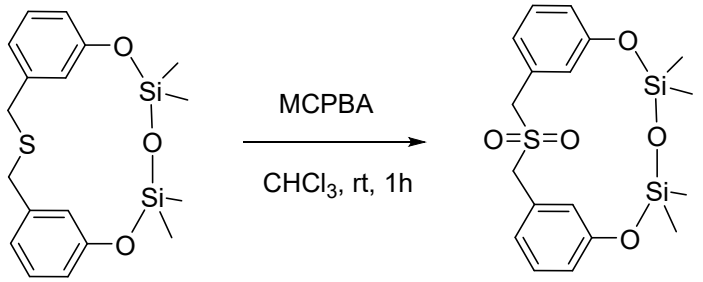
^{13}C NMR (150.91 MHz, $CDCl_3$) δ 134.06, 130.18, 129.74, 127.57, 122.44, 121.12, 118.53, 34.38, 0.03, −0.28 ppm;

^{29}Si NMR (119.24 MHz, $CDCl_3$) δ −11.18 (D-unit silicon), −79.08 (T-unit silicon) ppm;

MALDI-TOF MS (m/z): 1291.22 ([M+Na]$^+$, calcd 1291.85); 1307.79 ([M+K]$^+$, calcd 1307.19);

Elemental analysis: Calcd for $C_{60}H_{68}O_{12}S_2Si_8$: C, 56.75; H, 5.40. Found: C, 56.23; H, 5.41.

1-6 Synthesis of cyclic compound (8)



5 **8**

To a 30 mL flask was added **5** (37 mg, 0.1 mmol) and $CHCl_3$ (5 mL). The mixture was cooled down to 0 ˚C, and then *m*-chloroperoxybenzoic acid (69 mg, 0.40 mmol) was added at 0 °C. The mixture was stirred at 0 °C for 5 minutes, then at room temperature for 40 minutes. The mixture was quenched by saturated $Na_2S_2O_3$ (15 mL), and the organic phase was washed with saturated $NaHCO_3$ for 5 times, dried over anhydrous Na_2SO_4 for 1 hour, and concentrated under vacuum to give a white solid, which was purified by column chromatography (silica gel, hexane : EtOAc = from 10 : 1 to 1 : 1) to give a white solid (40 mg, 99% yield).

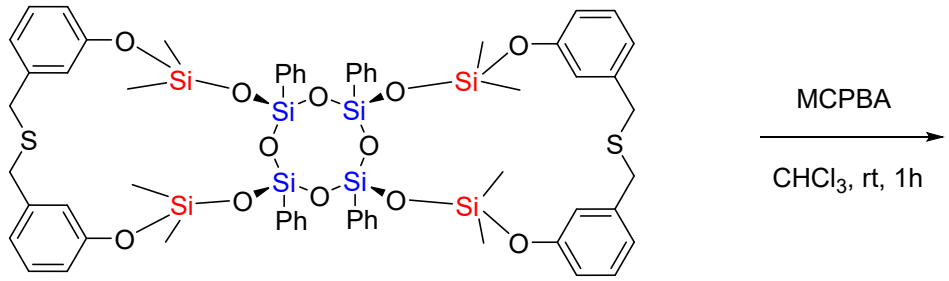
^{1}H NMR (600.17 MHz, $CDCl_3$) δ 7.32-7.35 (m, 4H), 6.90-6.91 (m, 2H), 6.79 (s, 2H), 3.94 (s, 4H), 0.29 (s, 12H) ppm;

^{13}C NMR (150.91 MHz, $CDCl_3$) δ 154.47, 130.81, 129.52, 124.18, 122.02, 120.99, 56.80, −0.64 ppm;

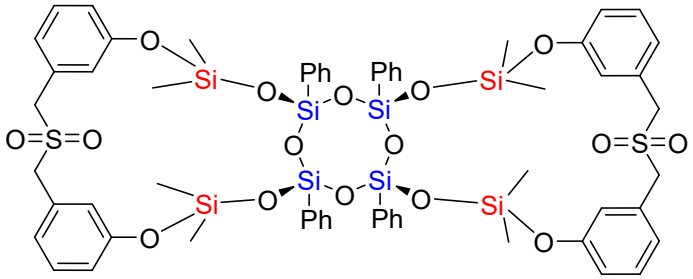
^{29}Si NMR (119.24 MHz, $CDCl_3$) δ −11.51 (D-unit silicon) ppm;

MALDI-TOF MS (m/z): 431.95 ([M+Na]$^+$, calcd 431.08); 447.92 ([M+K]$^+$, calcd 447.05);
Elemental analysis: Calcd for $C_{18}H_{24}O_5SSi_2$: C, 52.91; H, 5.92. Found: C, 53.25; H, 6.04.

1-7 Synthesis of Ladder-type siloxane-based compound (9)



7



9

To a 30 mL flask was added **7** (38 mg, 0.03 mmol) and $CHCl_3$ (5 mL). The mixture was cooled down to 0 ˚C, and then *m*-chloroperoxybenzoic acid (36 mg, 0.21 mmol) was added at 0 ºC. The mixture was stirred at 0 ºC for 15 minutes, then at room temperature for one hour. The mixture was quenched by saturated $Na_2S_2O_3$ (15 mL), and the organic phase was washed with saturated $NaHCO_3$ for 5 times, dried over anhydrous Na_2SO_4 for 1 hour, and concentrated under vacuum to give a white solid, which was purified by column chromatograph (hexane : EtOAc = from 10 : 1 to 1 : 1) to give a white solid (36 mg, 89% yield).

^{1}H NMR (600.17 MHz, $CDCl_3$) δ 7.20-7.24 (m, 8H), 7.15 (d, J = 7.8 Hz, 4H), 7.06 (d, J = 7.8 Hz, 8H), 6.98 (t, J = 7.8 Hz, 8H), 6.79 (d, J = 7.2 Hz, 4H), 6.69 (s, 4H), 3.67-3.77(ABq, J = 14.4 Hz, 8H), 0.50 (s, 12H), 0.29 (s, 12H) ppm;

^{13}C NMR (150.91 MHz, $CDCl_3$) δ 154.26, 133.86, 131.14, 130.47, 130.28, 129.71, 127.73, 124.42,

122.45, 120.56, 56.94, 0.14, −0.36 ppm;

^{29}Si NMR (119.24 MHz, $CDCl_3$) δ −10.54 (D-unit silicon), −78.98 (T-unit silicon) ppm;

MALDI-TOF MS (m/z): 1355.99 ($[M+Na]^+$, calcd 1355.20), 1371.89 ($[M+K]^+$, calcd 1371.17);

Elemental analysis: Calcd for $C_{60}H_{68}O_{16}S_2Si_8$: C, 54.02; H, 5.14. Found: C, 53.49; H, 5.27.

References

1 W. Yang, Y. Li, J. Zhu, W. Liu, J. Ke and C. He, Lewis acid-assisted Ir(III) reductive elimination enables construction of seven-membered-ring sulfoxides, *Chem. Sci.*, 2020, **11**, 10149-10158.

2 G. M. Sheldrick, SHELXT - integrated space-group and crystal-structure determination, *Acta Crystallogr., Sect. A: Found. Adv.*, 2015, **71**, 3–8.

3 G. M. Sheldrick, Crystal structure refinement with SHELXL, *Acta Crystallogr., Sect. C: Struct. Chem*., 2015, **71**, 3–8.

4 C. Kabuto, S. Akine, T. Nemoto, E. Kwon, Release of software (Yadokari-XG 2009) for crystal structure analyses. *J. Cryst. Soc. Jpn.*, 2009, **51**, 218-224.

2. NMR spectra for compounds 3, 5, 7, 8 and 9.

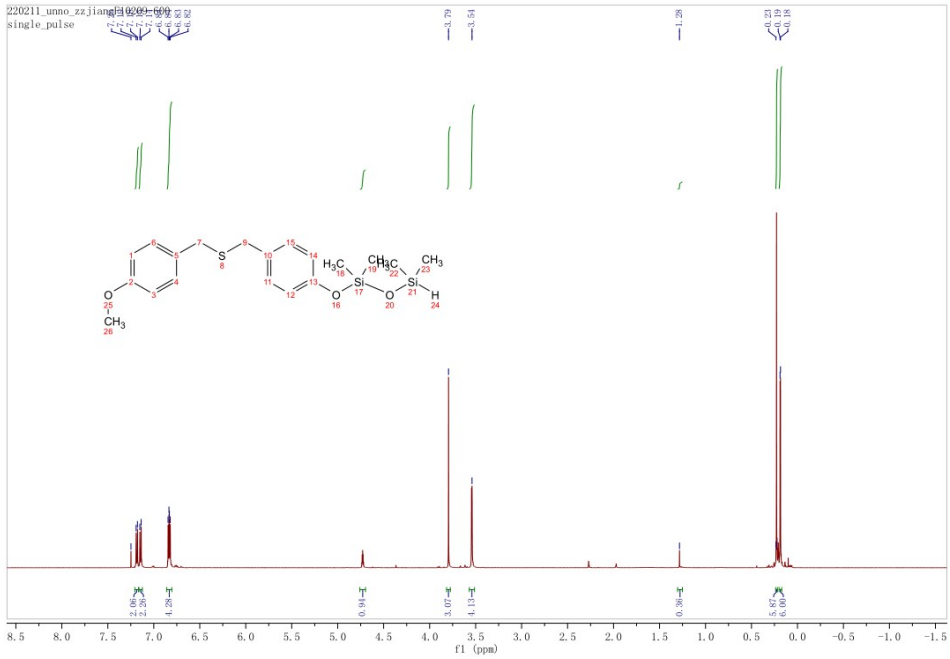


Figure S1: ^{1}H NMR spectrum of compound **3.**

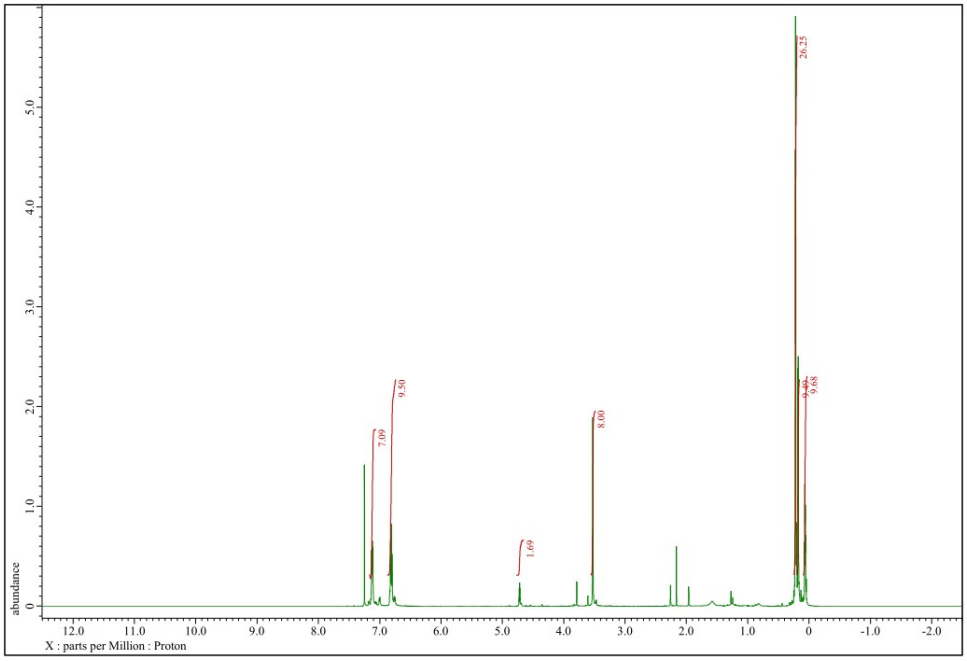


Figure S2: ^{1}H NMR spectrum of the obtained linear oligomers**.**

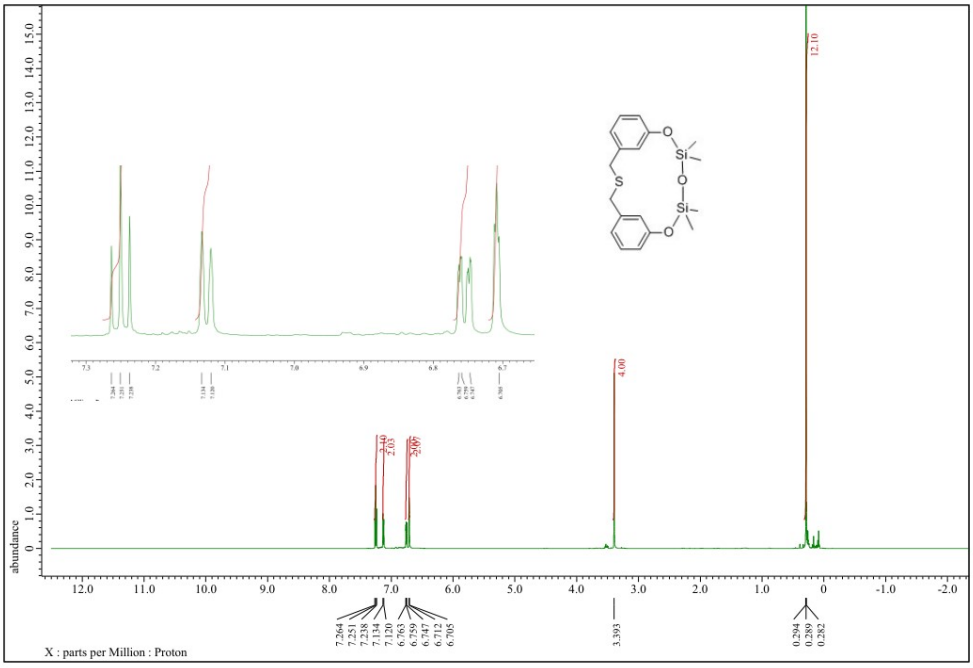


Figure S3: ^{1}H NMR spectrum of compound **5**.

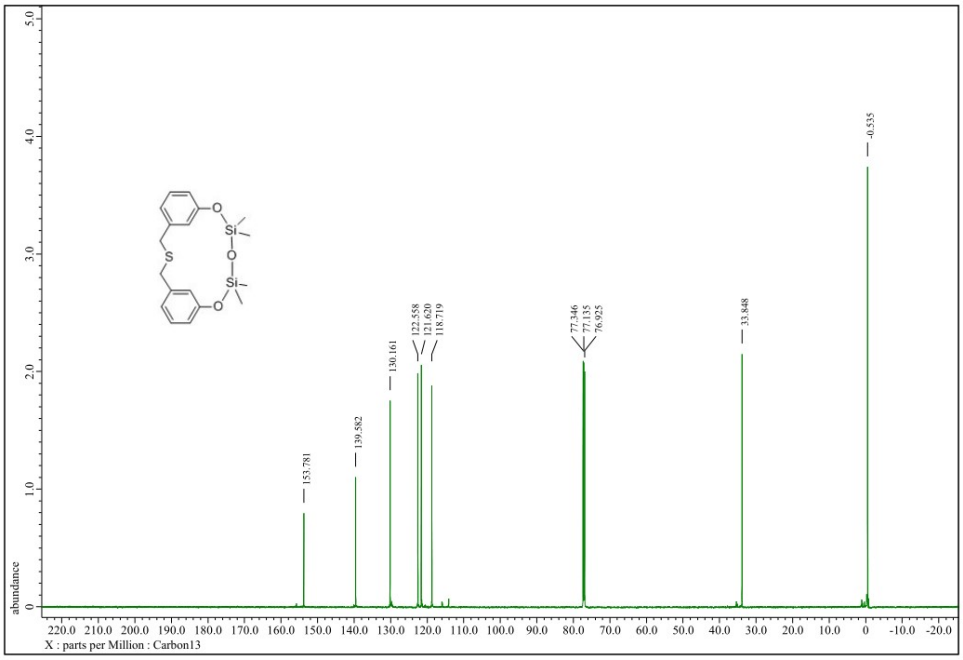


Figure S4: ^{13}C NMR spectrum of compound **5**.

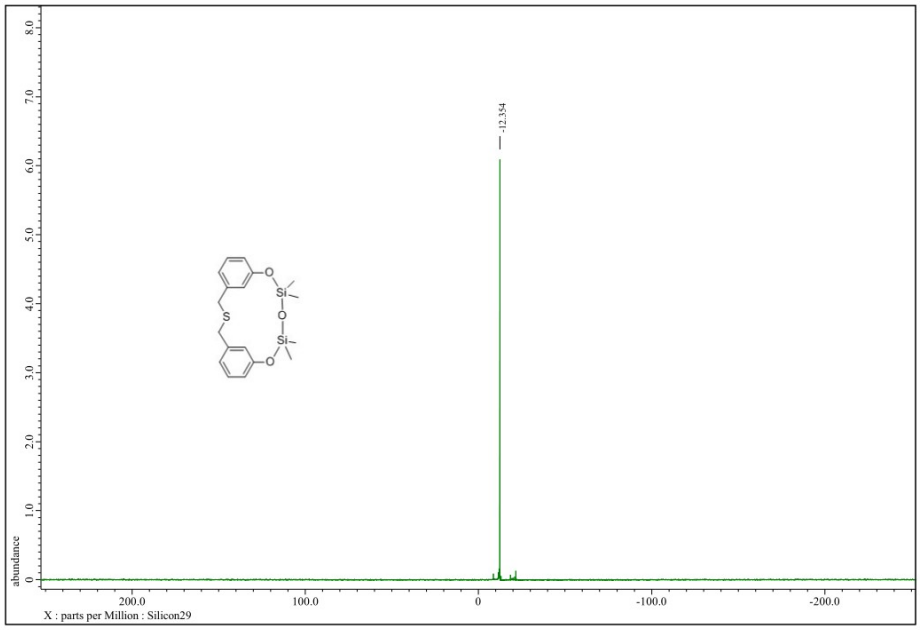


Figure S5: ^{29}Si NMR spectrum of compound **5**.

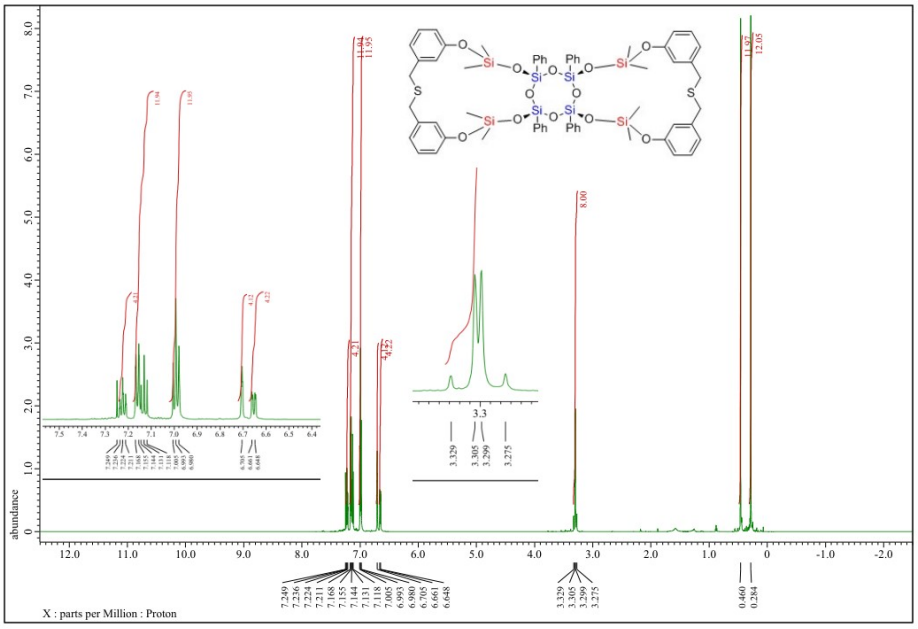


Figure S6: ^{1}H NMR spectrum of compound **7.**

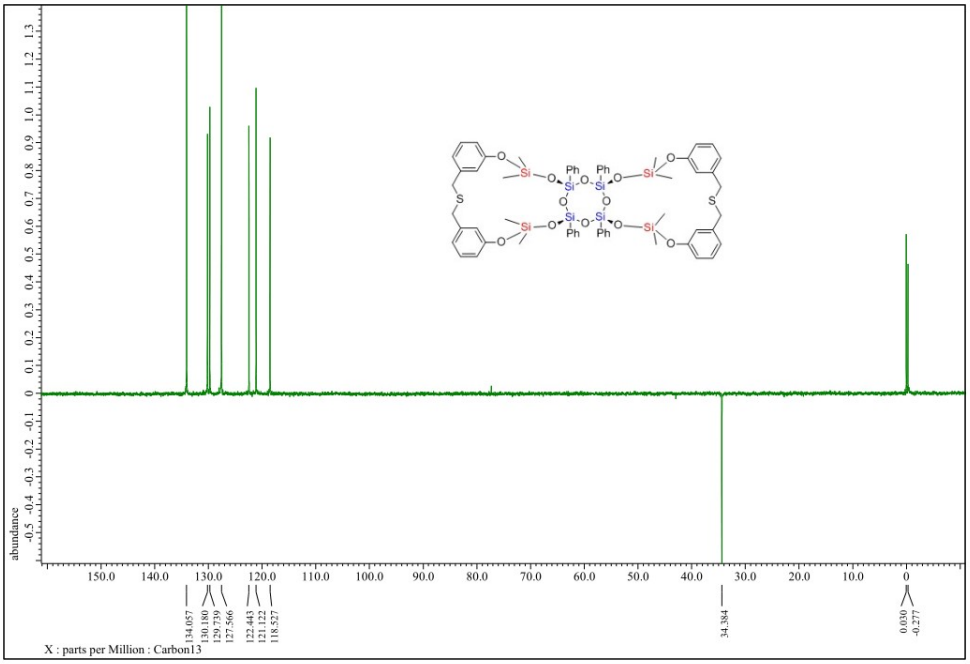


Figure S7: ^{13}C NMR spectrum of compound **7**.

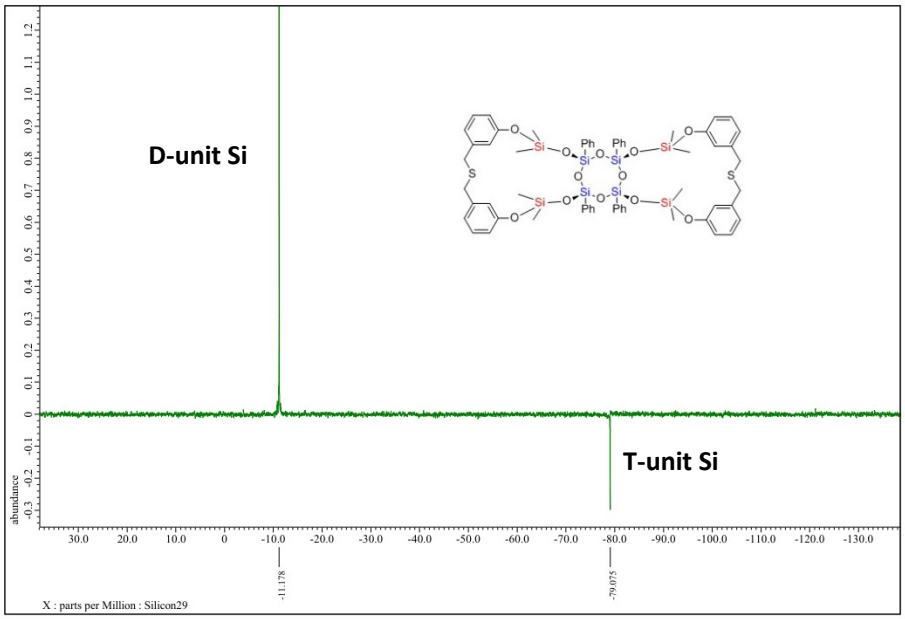


Figure S8: ^{29}Si NMR spectrum of compound **7**.

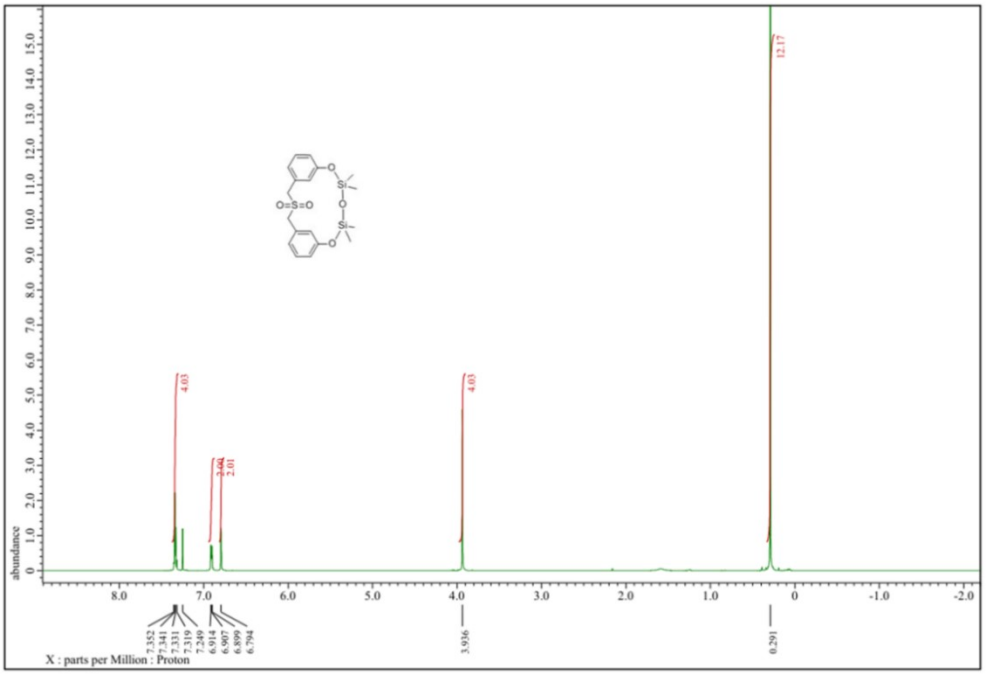


Figure S9: ^{1}H NMR spectrum of compound **8**.

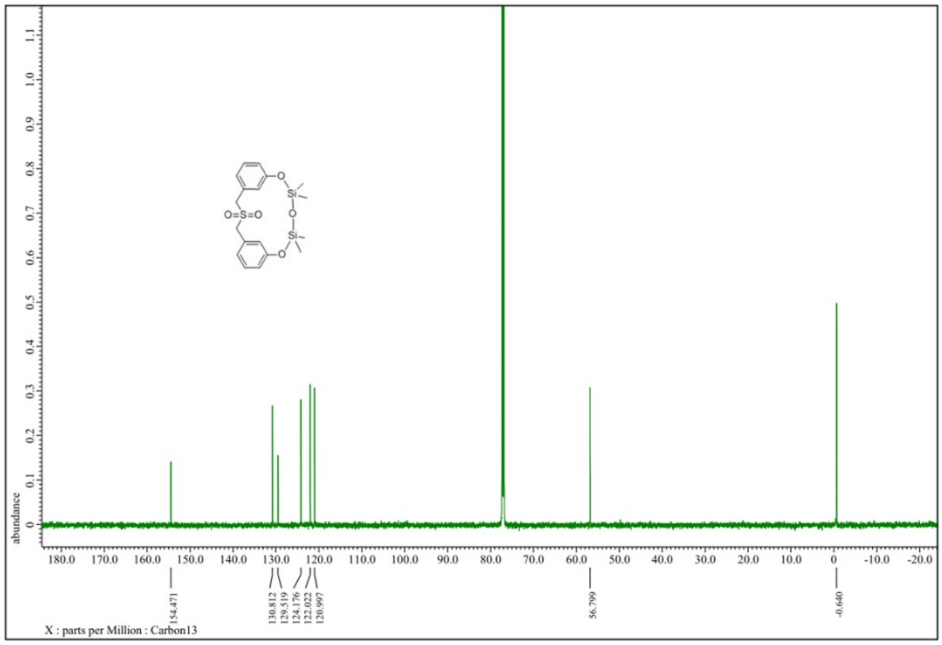


Figure S10: ^{13}C NMR spectrum of compound **8**.

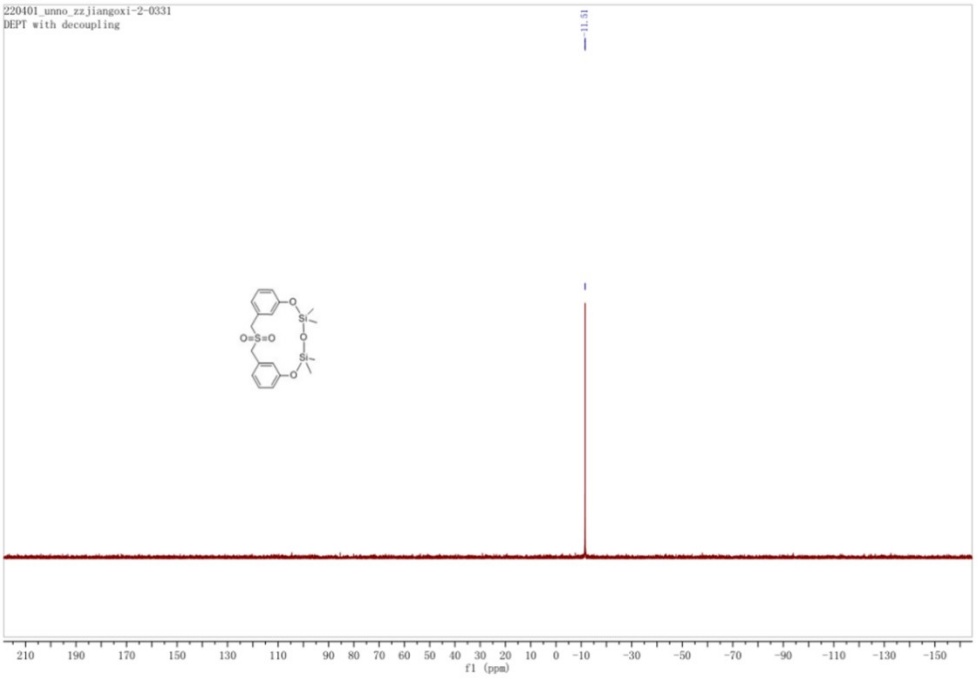


Figure S11: ^{29}Si NMR spectrum of compound **8**.

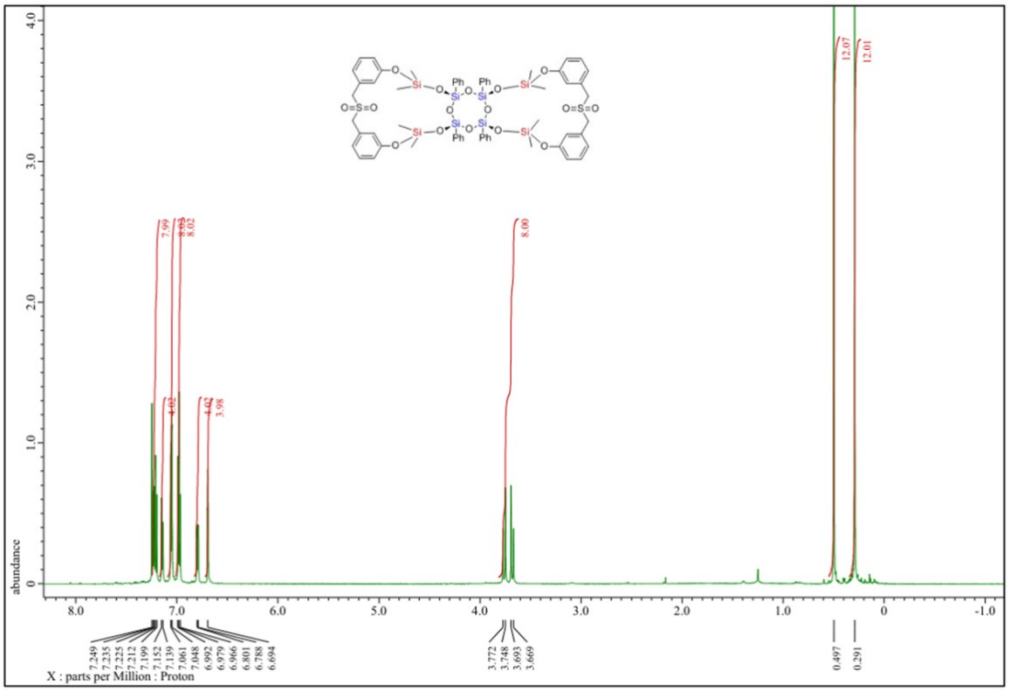


Figure S12: ^{1}H NMR spectrum of compound **9**.

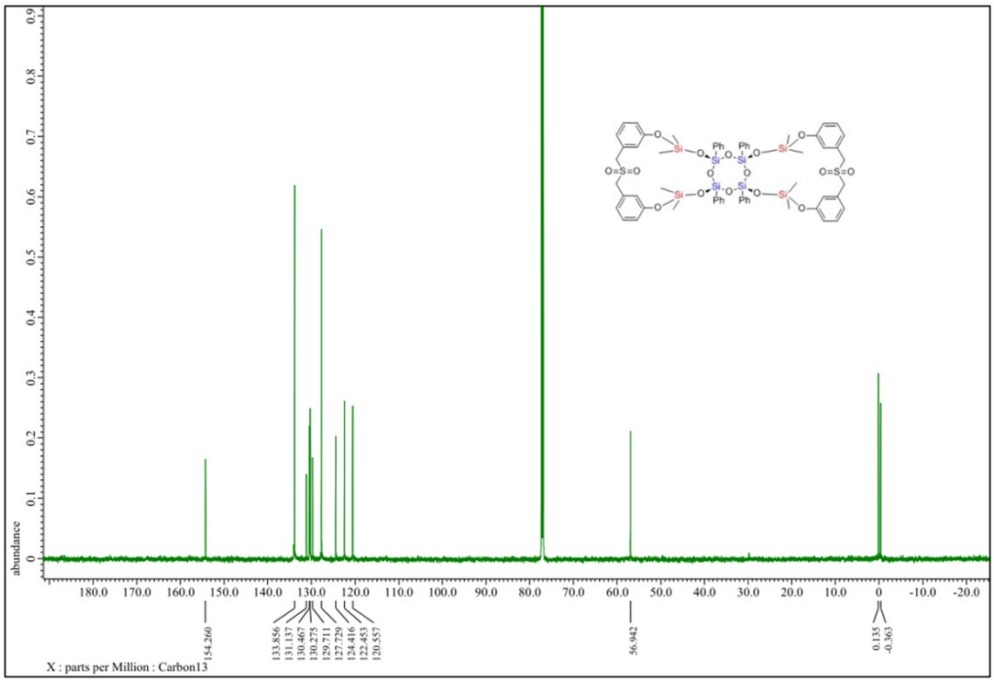


Figure S13: ^{13}C NMR spectrum of compound **9**.

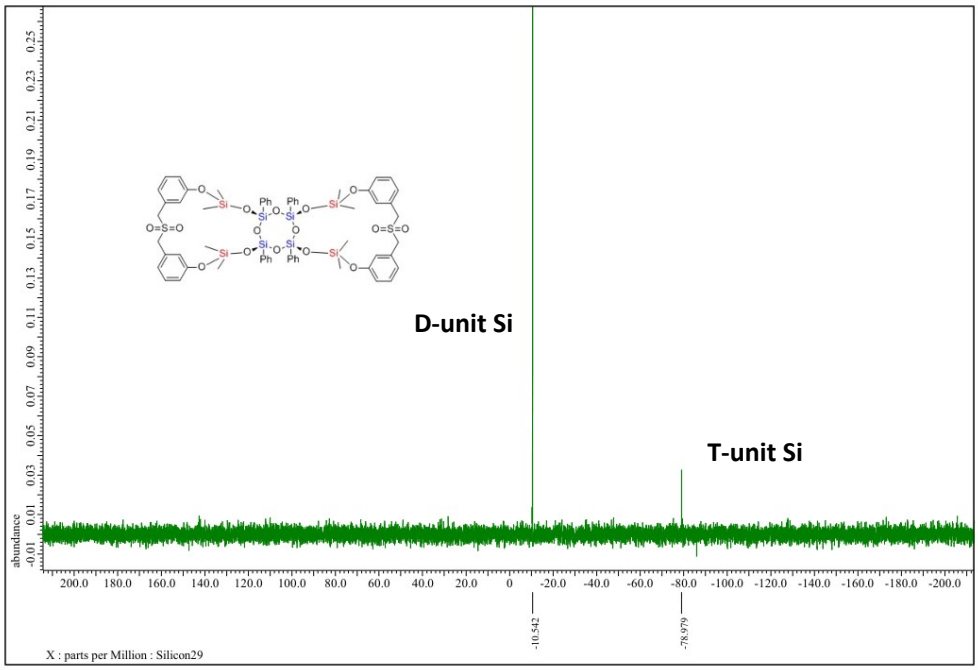


Figure S14: ^{29}Si NMR spectrum of compound **9**.

3. Infrared spectra for compounds 5, 7, 8 and 9

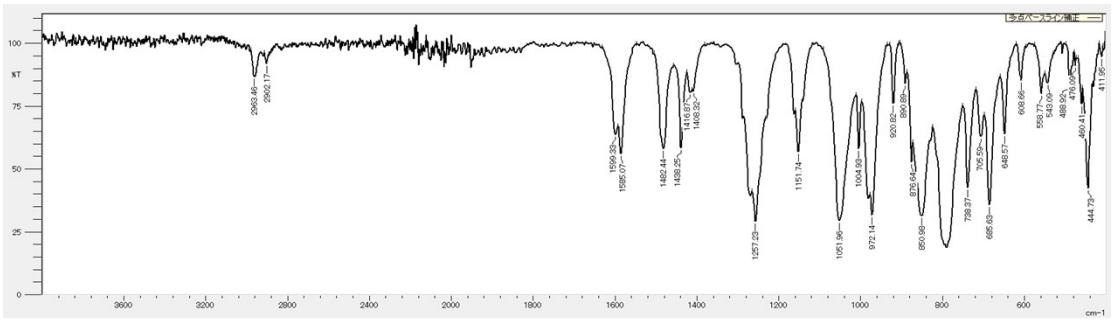


Figure S15: Infrared spectrum for **5**.

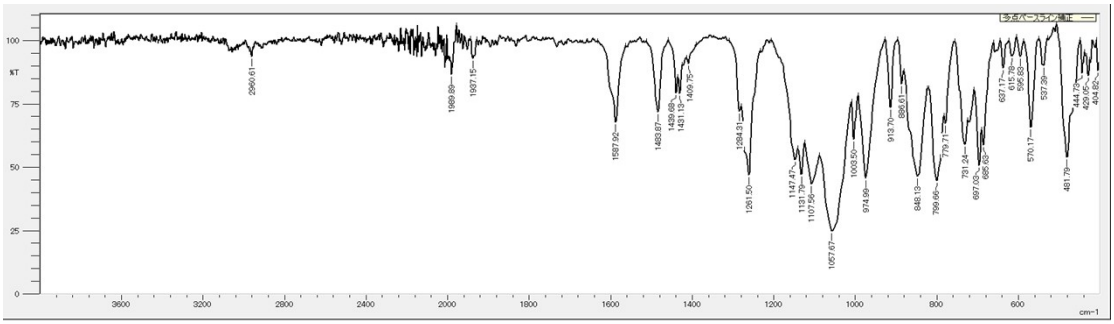


Figure S16: Infrared spectrum for **7**.

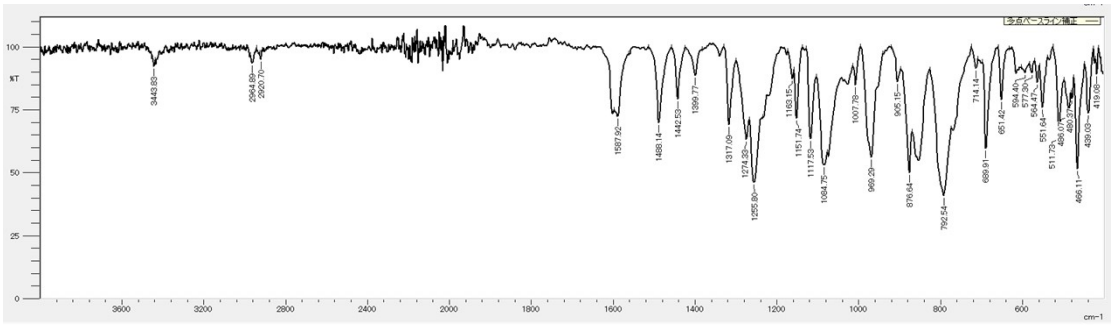


Figure S17: Infrared spectrum for **8**.

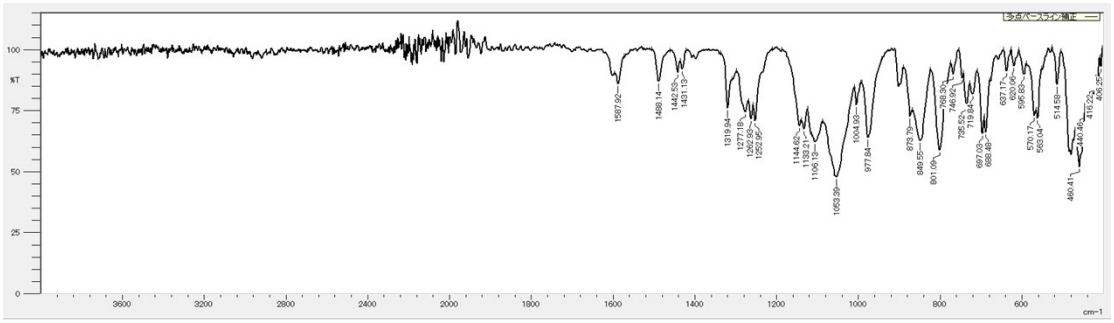


Figure S18: Infrared spectrum for **9**.

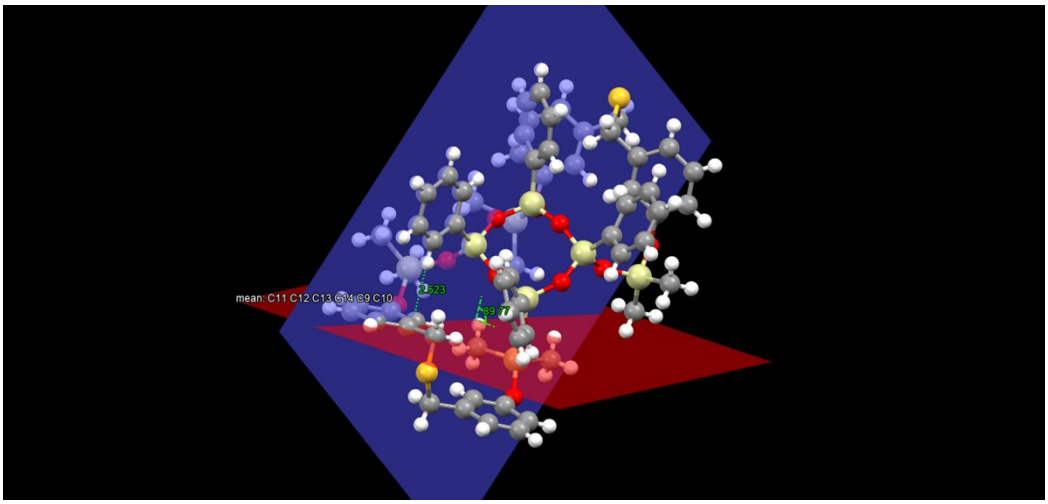


Figure S19: X-ray structure for compound **7**.

4. MALDI-TOF spectrum for compounds 5, 7, 8 and 9

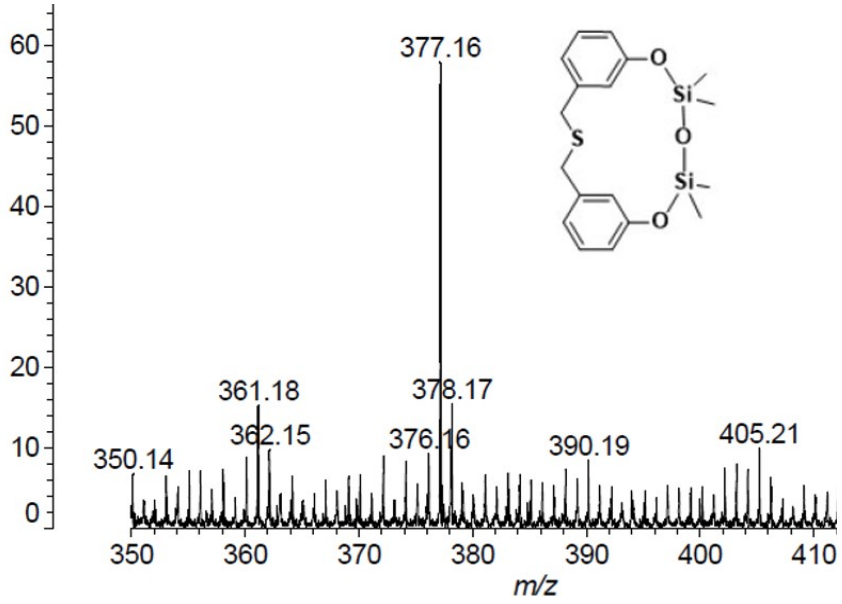


Figure S20: MALDI-TOF spectrum of compound **5**

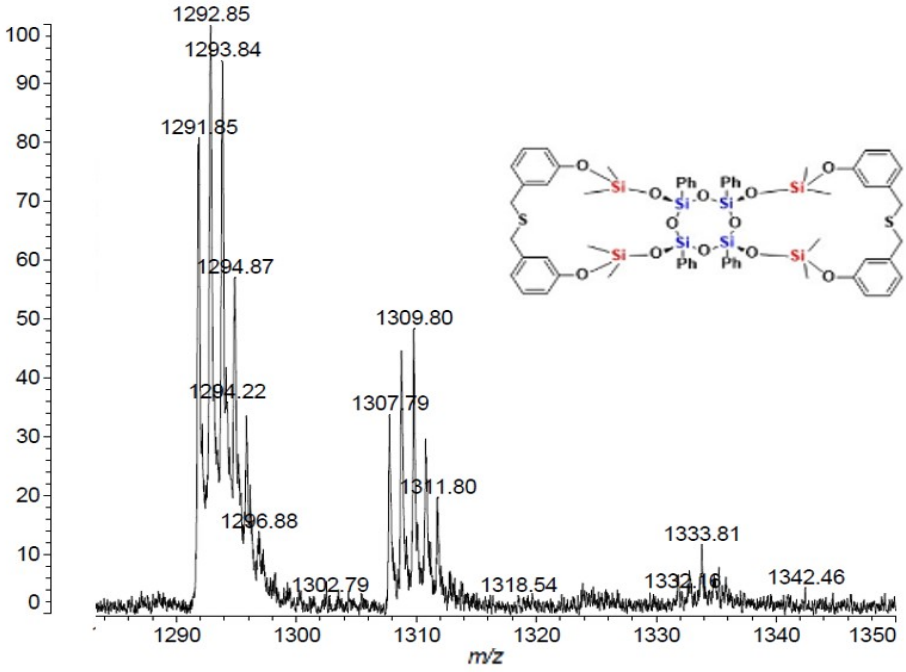


Figure S21: MALDI-TOF spectrum of compound **7**

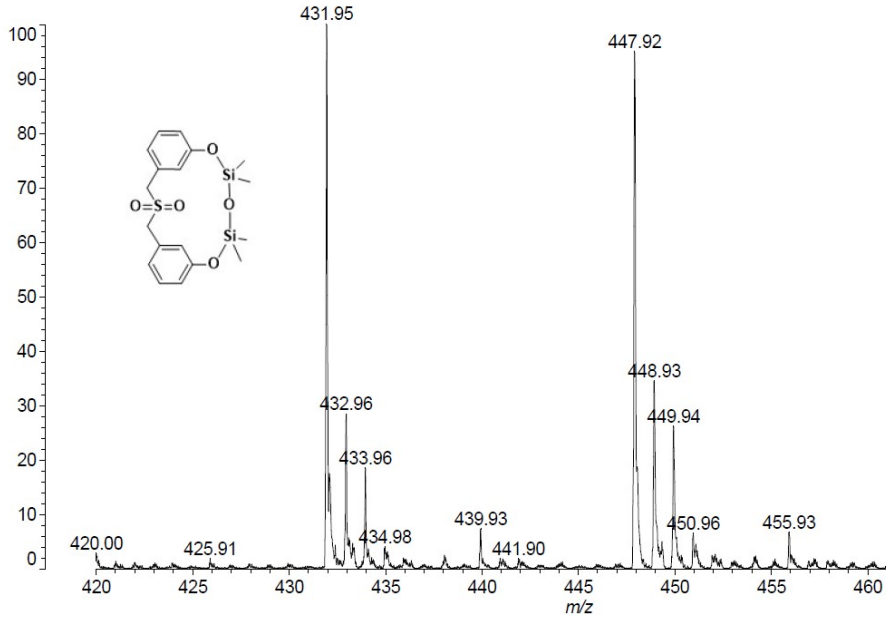


Figure S22: MALDI-TOF spectrum of compound **8**

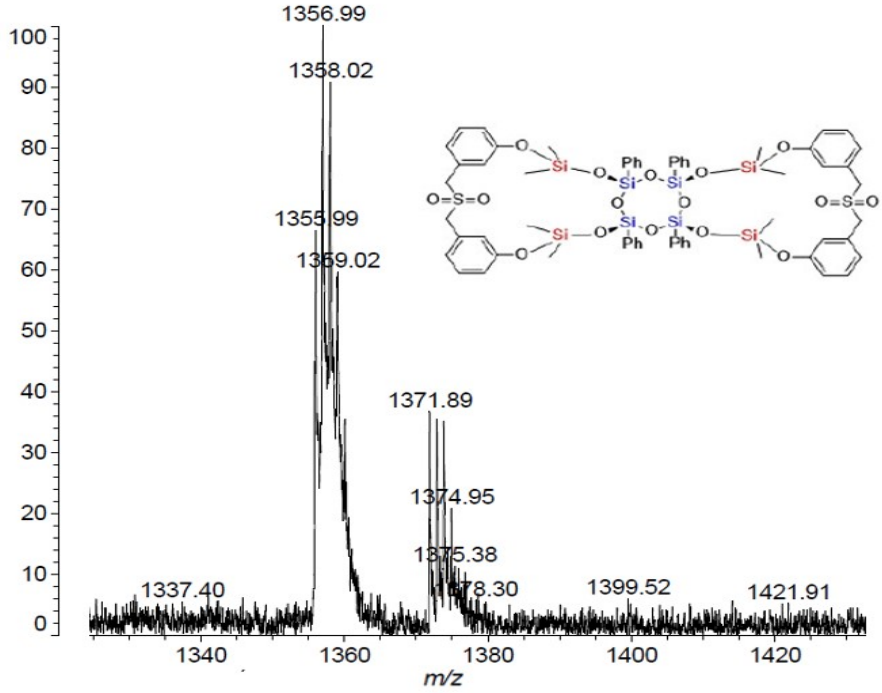


Figure S23: MALDI-TOF spectrum of compound **9**

5. X-ray diffraction and crystallography for compound 7

Table S1. Crystal data and structure refinement for **7**.

Identification code	22z03	
Empirical formula	C60 H68 O12 S2 Si8	
Formula weight	1269.98	
Temperature	120 K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 20.8502(18) Å	α= 90°.
	b = 10.6548(7) Å	β= 95.342(2)°.
	c = 29.707(3) Å	γ = 90°.
Volume	6570.9(10) $Å^3$	
Z	4	
Density (calculated)	1.284 Mg/m^3	
Absorption coefficient	0.284 mm^{-1}	
F(000)	2672	
Crystal size	0.38 x 0.23 x 0.09 mm^3	
Theta range for data collection	2.502 to 27.498°.	
Index ranges	-27<=h<=27, -13<=k<=13, -38<=l<=38	
Reflections collected	103916	
Independent reflections	14962 [R(int) = 0.0254]	
Completeness to theta = 25.242°	99.5 %	
Absorption correction	Numerical	
Max. and min. transmission	1.000 and 0.950	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14962 / 0 / 739	
Goodness-of-fit on F^2	1.056	
Final R indices [I>2sigma(I)][a]	R1 = 0.0296, wR2 = 0.0775	
R indices (all data)	R1 = 0.0361, wR2 = 0.0819	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.381 and -0.322 $e.Å^{-3}$	

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, $wR_2 = [(\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$.

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **7**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Si(1)	1813(1)	4538(1)	1870(1)	16(1)
O(1)	2584(1)	4656(1)	1968(1)	23(1)
Si(2)	3313(1)	5019(1)	2151(1)	16(1)
O(2)	3388(1)	5013(1)	2699(1)	21(1)
Si(3)	3056(1)	5044(1)	3172(1)	16(1)
O(3)	2290(1)	5155(1)	3065(1)	24(1)
Si(4)	1553(1)	4862(1)	2883(1)	16(1)
O(4)	1487(1)	4679(1)	2340(1)	23(1)
O(5)	1630(1)	3183(1)	1656(1)	27(1)
Si(5)	1752(1)	1690(1)	1582(1)	20(1)
O(6)	1318(1)	1278(1)	1113(1)	27(1)
C(1)	1128(1)	2034(1)	748(1)	23(1)
C(2)	478(1)	2250(2)	644(1)	28(1)
C(3)	278(1)	3024(2)	280(1)	32(1)
C(4)	722(1)	3552(2)	17(1)	30(1)
C(5)	1378(1)	3302(1)	112(1)	24(1)
C(6)	1577(1)	2546(1)	479(1)	23(1)
C(7)	1859(1)	3830(2)	-188(1)	27(1)
S(1)	1946(1)	5523(1)	-154(1)	27(1)
C(8)	2359(1)	5642(2)	409(1)	25(1)
C(9)	3039(1)	5136(1)	451(1)	21(1)
C(10)	3493(1)	5610(2)	178(1)	26(1)
C(11)	4128(1)	5213(2)	241(1)	30(1)
C(12)	4323(1)	4347(2)	575(1)	26(1)
C(13)	3874(1)	3874(1)	848(1)	20(1)
C(14)	3233(1)	4250(1)	782(1)	21(1)
O(7)	4068(1)	3016(1)	1185(1)	23(1)
Si(6)	4358(1)	3411(1)	1704(1)	17(1)

O(8)	3770(1)	3940(1)	1976(1)	22(1)
O(9)	3248(1)	3764(1)	3443(1)	23(1)
Si(7)	3703(1)	2530(1)	3384(1)	25(1)
O(10)	3781(1)	1806(1)	3878(1)	28(1)
C(15)	4001(1)	2427(1)	4272(1)	25(1)
C(16)	4657(1)	2569(2)	4391(1)	32(1)
C(17)	4861(1)	3211(2)	4787(1)	35(1)
C(18)	4418(1)	3701(2)	5059(1)	31(1)
C(19)	3758(1)	3542(1)	4944(1)	26(1)
C(20)	3555(1)	2897(1)	4550(1)	25(1)
C(21)	3272(1)	4079(2)	5236(1)	31(1)
S(2)	3162(1)	5767(1)	5177(1)	31(1)
C(22)	2756(1)	5866(2)	4610(1)	29(1)
C(23)	2080(1)	5346(1)	4564(1)	24(1)
C(24)	1602(1)	5866(2)	4805(1)	30(1)
C(25)	980(1)	5393(2)	4751(1)	34(1)
C(26)	822(1)	4398(2)	4460(1)	29(1)
C(27)	1295(1)	3883(1)	4220(1)	23(1)
C(28)	1922(1)	4352(1)	4269(1)	23(1)
O(11)	1161(1)	2852(1)	3948(1)	28(1)
Si(8)	848(1)	2854(1)	3416(1)	22(1)
C(29)	1512(1)	5768(1)	1466(1)	20(1)
C(30)	1030(1)	5520(2)	1117(1)	27(1)
C(31)	820(1)	6448(2)	812(1)	39(1)
C(32)	1085(1)	7635(2)	845(1)	40(1)
C(33)	1567(1)	7902(2)	1182(1)	37(1)
C(34)	1777(1)	6979(1)	1493(1)	29(1)
C(35)	3532(1)	6594(1)	1952(1)	20(1)
C(36)	3559(1)	6832(2)	1491(1)	34(1)
C(37)	3710(1)	8008(2)	1331(1)	34(1)
C(38)	3838(1)	8976(2)	1630(1)	32(1)
C(39)	3825(1)	8766(2)	2090(1)	43(1)
C(40)	3674(1)	7585(2)	2249(1)	32(1)

C(41)	3340(1)	6414(1)	3516(1)	20(1)
C(42)	3905(1)	6361(2)	3809(1)	27(1)
C(43)	4117(1)	7396(2)	4066(1)	36(1)
C(44)	3770(1)	8494(2)	4037(1)	36(1)
C(45)	3204(1)	8570(2)	3755(1)	35(1)
C(46)	2992(1)	7536(1)	3495(1)	28(1)
C(47)	1047(1)	6189(1)	3037(1)	20(1)
C(48)	1159(1)	6752(1)	3463(1)	25(1)
C(49)	756(1)	7690(2)	3598(1)	33(1)
C(50)	229(1)	8068(2)	3311(1)	36(1)
C(51)	114(1)	7535(2)	2888(1)	36(1)
C(52)	523(1)	6606(2)	2750(1)	29(1)
C(53)	1452(1)	759(2)	2042(1)	35(1)
C(54)	2613(1)	1389(2)	1531(1)	35(1)
C(55)	4664(1)	1953(1)	1979(1)	28(1)
C(56)	4979(1)	4642(2)	1696(1)	32(1)
C(57)	3291(1)	1418(2)	2982(1)	44(1)
C(58)	4490(1)	3076(2)	3220(1)	38(1)
C(59)	62(1)	3665(2)	3360(1)	38(1)
C(60)	813(1)	1178(2)	3270(1)	44(1)
O(12)	1342(1)	3566(1)	3107(1)	24(1)

Table S3. Bond lengths [Å] and angles [°] for **7**.

Si(1)-O(5)	1.6090(10)	C(6)-H(4)	0.9500
Si(1)-O(1)	1.6120(10)	C(7)-S(1)	1.8153(16)
Si(1)-O(4)	1.6182(10)	C(7)-H(5)	0.9900
Si(1)-C(29)	1.8460(14)	C(7)-H(6)	0.9900
O(1)-Si(2)	1.6130(10)	S(1)-C(8)	1.8135(14)
Si(2)-O(8)	1.6099(10)	C(8)-C(9)	1.5110(19)
Si(2)-O(2)	1.6189(10)	C(8)-H(7)	0.9900
Si(2)-C(35)	1.8511(14)	C(8)-H(8)	0.9900
O(2)-Si(3)	1.6232(10)	C(9)-C(14)	1.395(2)
Si(3)-O(3)	1.6039(10)	C(9)-C(10)	1.3967(19)
Si(3)-O(9)	1.6150(10)	C(10)-C(11)	1.385(2)
Si(3)-C(41)	1.8479(14)	C(10)-H(9)	0.9500
O(3)-Si(4)	1.6117(10)	C(11)-C(12)	1.389(2)
Si(4)-O(12)	1.6116(10)	C(11)-H(10)	0.9500
Si(4)-O(4)	1.6167(10)	C(12)-C(13)	1.3889(19)
Si(4)-C(47)	1.8466(14)	C(12)-H(11)	0.9500
O(5)-Si(5)	1.6287(11)	C(13)-O(7)	1.3865(17)
Si(5)-O(6)	1.6506(11)	C(13)-C(14)	1.3914(19)
Si(5)-C(53)	1.8438(16)	C(14)-H(12)	0.9500
Si(5)-C(54)	1.8445(16)	O(7)-Si(6)	1.6575(10)
O(6)-C(1)	1.3786(17)	Si(6)-O(8)	1.6297(10)
C(1)-C(2)	1.382(2)	Si(6)-C(55)	1.8417(15)
C(1)-C(6)	1.396(2)	Si(6)-C(56)	1.8452(15)
C(2)-C(3)	1.393(2)	O(9)-Si(7)	1.6405(11)
C(2)-H(1)	0.9500	Si(7)-O(10)	1.6533(11)
C(3)-C(4)	1.385(2)	Si(7)-C(57)	1.8380(18)
C(3)-H(2)	0.9500	Si(7)-C(58)	1.8489(18)
C(4)-C(5)	1.396(2)	O(10)-C(15)	1.3838(18)
C(4)-H(3)	0.9500	C(15)-C(16)	1.389(2)
C(5)-C(6)	1.390(2)	C(15)-C(20)	1.393(2)
C(5)-C(7)	1.510(2)	C(16)-C(17)	1.391(2)

C(16)-H(13)	0.9500	C(30)-H(25)	0.9500
C(17)-C(18)	1.386(2)	C(31)-C(32)	1.381(3)
C(17)-H(14)	0.9500	C(31)-H(26)	0.9500
C(18)-C(19)	1.397(2)	C(32)-C(33)	1.381(3)
C(18)-H(15)	0.9500	C(32)-H(27)	0.9500
C(19)-C(20)	1.390(2)	C(33)-C(34)	1.390(2)
C(19)-C(21)	1.509(2)	C(33)-H(28)	0.9500
C(20)-H(16)	0.9500	C(34)-H(29)	0.9500
C(21)-S(2)	1.8193(18)	C(35)-C(40)	1.390(2)
C(21)-H(17)	0.9900	C(35)-C(36)	1.3984(19)
C(21)-H(18)	0.9900	C(36)-C(37)	1.388(2)
S(2)-C(22)	1.8164(15)	C(36)-H(30)	0.9500
C(22)-C(23)	1.509(2)	C(37)-C(38)	1.371(2)
C(22)-H(19)	0.9900	C(37)-H(31)	0.9500
C(22)-H(20)	0.9900	C(38)-C(39)	1.385(2)
C(23)-C(28)	1.394(2)	C(38)-H(32)	0.9500
C(23)-C(24)	1.396(2)	C(39)-C(40)	1.390(2)
C(24)-C(25)	1.387(2)	C(39)-H(33)	0.9500
C(24)-H(21)	0.9500	C(40)-H(34)	0.9500
C(25)-C(26)	1.387(2)	C(41)-C(46)	1.396(2)
C(25)-H(22)	0.9500	C(41)-C(42)	1.399(2)
C(26)-C(27)	1.383(2)	C(42)-C(43)	1.390(2)
C(26)-H(23)	0.9500	C(42)-H(35)	0.9500
C(27)-O(11)	1.3777(17)	C(43)-C(44)	1.375(3)
C(27)-C(28)	1.392(2)	C(43)-H(36)	0.9500
C(28)-H(24)	0.9500	C(44)-C(45)	1.384(3)
O(11)-Si(8)	1.6521(11)	C(44)-H(37)	0.9500
Si(8)-O(12)	1.6299(10)	C(45)-C(46)	1.394(2)
Si(8)-C(60)	1.8383(18)	C(45)-H(38)	0.9500
Si(8)-C(59)	1.8452(18)	C(46)-H(39)	0.9500
C(29)-C(30)	1.3993(19)	C(47)-C(52)	1.395(2)
C(29)-C(34)	1.404(2)	C(47)-C(48)	1.402(2)
C(30)-C(31)	1.385(2)	C(48)-C(49)	1.390(2)

C(48)-H(40)	0.9500	O(5)-Si(1)-O(1)	109.81(6)
C(49)-C(50)	1.386(3)	O(5)-Si(1)-O(4)	108.73(6)
C(49)-H(41)	0.9500	O(1)-Si(1)-O(4)	109.11(5)
C(50)-C(51)	1.380(3)	O(5)-Si(1)-C(29)	109.08(6)
C(50)-H(42)	0.9500	O(1)-Si(1)-C(29)	109.62(6)
C(51)-C(52)	1.394(2)	O(4)-Si(1)-C(29)	110.47(6)
C(51)-H(43)	0.9500	Si(1)-O(1)-Si(2)	166.60(7)
C(52)-H(44)	0.9500	O(8)-Si(2)-O(1)	106.70(6)
C(53)-H(45)	0.9800	O(8)-Si(2)-O(2)	108.52(5)
C(53)-H(46)	0.9800	O(1)-Si(2)-O(2)	109.73(5)
C(53)-H(47)	0.9800	O(8)-Si(2)-C(35)	111.94(6)
C(54)-H(48)	0.9800	O(1)-Si(2)-C(35)	111.18(6)
C(54)-H(49)	0.9800	O(2)-Si(2)-C(35)	108.73(6)
C(54)-H(50)	0.9800	Si(2)-O(2)-Si(3)	149.34(7)
C(55)-H(51)	0.9800	O(3)-Si(3)-O(9)	110.84(6)
C(55)-H(52)	0.9800	O(3)-Si(3)-O(2)	109.14(5)
C(55)-H(53)	0.9800	O(9)-Si(3)-O(2)	108.03(5)
C(56)-H(54)	0.9800	O(3)-Si(3)-C(41)	108.18(6)
C(56)-H(55)	0.9800	O(9)-Si(3)-C(41)	109.85(6)
C(56)-H(56)	0.9800	O(2)-Si(3)-C(41)	110.82(6)
C(57)-H(57)	0.9800	Si(3)-O(3)-Si(4)	162.39(7)
C(57)-H(58)	0.9800	O(12)-Si(4)-O(3)	108.41(6)
C(57)-H(59)	0.9800	O(12)-Si(4)-O(4)	107.90(6)
C(58)-H(60)	0.9800	O(3)-Si(4)-O(4)	110.40(5)
C(58)-H(61)	0.9800	O(12)-Si(4)-C(47)	111.65(6)
C(58)-H(62)	0.9800	O(3)-Si(4)-C(47)	108.50(6)
C(59)-H(63)	0.9800	O(4)-Si(4)-C(47)	109.97(6)
C(59)-H(64)	0.9800	Si(4)-O(4)-Si(1)	150.38(7)
C(59)-H(65)	0.9800	Si(1)-O(5)-Si(5)	153.45(7)
C(60)-H(66)	0.9800	O(5)-Si(5)-O(6)	107.00(6)
C(60)-H(67)	0.9800	O(5)-Si(5)-C(53)	111.02(7)
C(60)-H(68)	0.9800	O(6)-Si(5)-C(53)	106.65(7)
		O(5)-Si(5)-C(54)	110.25(7)

O(6)-Si(5)-C(54)	110.21(7)	H(7)-C(8)-H(8)	107.6
C(53)-Si(5)-C(54)	111.55(8)	C(14)-C(9)-C(10)	119.08(13)
C(1)-O(6)-Si(5)	127.14(9)	C(14)-C(9)-C(8)	120.54(12)
O(6)-C(1)-C(2)	118.40(13)	C(10)-C(9)-C(8)	120.26(13)
O(6)-C(1)-C(6)	121.30(13)	C(11)-C(10)-C(9)	120.11(14)
C(2)-C(1)-C(6)	120.28(14)	C(11)-C(10)-H(9)	119.9
C(1)-C(2)-C(3)	119.19(14)	C(9)-C(10)-H(9)	119.9
C(1)-C(2)-H(1)	120.4	C(10)-C(11)-C(12)	120.81(13)
C(3)-C(2)-H(1)	120.4	C(10)-C(11)-H(10)	119.6
C(4)-C(3)-C(2)	120.75(14)	C(12)-C(11)-H(10)	119.6
C(4)-C(3)-H(2)	119.6	C(11)-C(12)-C(13)	119.34(13)
C(2)-C(3)-H(2)	119.6	C(11)-C(12)-H(11)	120.3
C(3)-C(4)-C(5)	120.20(15)	C(13)-C(12)-H(11)	120.3
C(3)-C(4)-H(3)	119.9	O(7)-C(13)-C(12)	119.57(13)
C(5)-C(4)-H(3)	119.9	O(7)-C(13)-C(14)	120.20(12)
C(6)-C(5)-C(4)	118.96(13)	C(12)-C(13)-C(14)	120.22(13)
C(6)-C(5)-C(7)	120.87(13)	C(13)-C(14)-C(9)	120.40(12)
C(4)-C(5)-C(7)	120.16(14)	C(13)-C(14)-H(12)	119.8
C(5)-C(6)-C(1)	120.57(13)	C(9)-C(14)-H(12)	119.8
C(5)-C(6)-H(4)	119.7	C(13)-O(7)-Si(6)	124.07(9)
C(1)-C(6)-H(4)	119.7	O(8)-Si(6)-O(7)	108.86(5)
C(5)-C(7)-S(1)	113.91(10)	O(8)-Si(6)-C(55)	108.51(6)
C(5)-C(7)-H(5)	108.8	O(7)-Si(6)-C(55)	106.23(6)
S(1)-C(7)-H(5)	108.8	O(8)-Si(6)-C(56)	108.84(7)
C(5)-C(7)-H(6)	108.8	O(7)-Si(6)-C(56)	111.33(6)
S(1)-C(7)-H(6)	108.8	C(55)-Si(6)-C(56)	112.94(8)
H(5)-C(7)-H(6)	107.7	Si(2)-O(8)-Si(6)	154.38(7)
C(8)-S(1)-C(7)	99.08(7)	Si(3)-O(9)-Si(7)	137.88(6)
C(9)-C(8)-S(1)	114.43(9)	O(9)-Si(7)-O(10)	106.80(5)
C(9)-C(8)-H(7)	108.7	O(9)-Si(7)-C(57)	110.21(8)
S(1)-C(8)-H(7)	108.7	O(10)-Si(7)-C(57)	106.11(7)
C(9)-C(8)-H(8)	108.7	O(9)-Si(7)-C(58)	108.25(7)
S(1)-C(8)-H(8)	108.7	O(10)-Si(7)-C(58)	111.38(7)

C(57)-Si(7)-C(58)	113.87(9)	C(28)-C(23)-C(24)	118.99(14)
C(15)-O(10)-Si(7)	121.64(9)	C(28)-C(23)-C(22)	120.13(13)
O(10)-C(15)-C(16)	120.63(14)	C(24)-C(23)-C(22)	120.86(14)
O(10)-C(15)-C(20)	119.04(13)	C(25)-C(24)-C(23)	120.12(14)
C(16)-C(15)-C(20)	120.33(14)	C(25)-C(24)-H(21)	119.9
C(15)-C(16)-C(17)	119.03(15)	C(23)-C(24)-H(21)	119.9
C(15)-C(16)-H(13)	120.5	C(26)-C(25)-C(24)	120.93(14)
C(17)-C(16)-H(13)	120.5	C(26)-C(25)-H(22)	119.5
C(18)-C(17)-C(16)	120.76(15)	C(24)-C(25)-H(22)	119.5
C(18)-C(17)-H(14)	119.6	C(27)-C(26)-C(25)	119.03(14)
C(16)-C(17)-H(14)	119.6	C(27)-C(26)-H(23)	120.5
C(17)-C(18)-C(19)	120.36(15)	C(25)-C(26)-H(23)	120.5
C(17)-C(18)-H(15)	119.8	O(11)-C(27)-C(26)	120.20(13)
C(19)-C(18)-H(15)	119.8	O(11)-C(27)-C(28)	118.98(13)
C(20)-C(19)-C(18)	118.81(14)	C(26)-C(27)-C(28)	120.73(14)
C(20)-C(19)-C(21)	120.35(14)	C(27)-C(28)-C(23)	120.20(13)
C(18)-C(19)-C(21)	120.83(14)	C(27)-C(28)-H(24)	119.9
C(19)-C(20)-C(15)	120.67(14)	C(23)-C(28)-H(24)	119.9
C(19)-C(20)-H(16)	119.7	C(27)-O(11)-Si(8)	126.94(9)
C(15)-C(20)-H(16)	119.7	O(12)-Si(8)-O(11)	109.01(6)
C(19)-C(21)-S(2)	113.81(11)	O(12)-Si(8)-C(60)	109.35(7)
C(19)-C(21)-H(17)	108.8	O(11)-Si(8)-C(60)	103.21(7)
S(2)-C(21)-H(17)	108.8	O(12)-Si(8)-C(59)	109.47(7)
C(19)-C(21)-H(18)	108.8	O(11)-Si(8)-C(59)	110.81(7)
S(2)-C(21)-H(18)	108.8	C(60)-Si(8)-C(59)	114.74(10)
H(17)-C(21)-H(18)	107.7	C(30)-C(29)-C(34)	117.84(13)
C(22)-S(2)-C(21)	100.99(8)	C(30)-C(29)-Si(1)	121.58(11)
C(23)-C(22)-S(2)	114.47(10)	C(34)-C(29)-Si(1)	120.55(11)
C(23)-C(22)-H(19)	108.6	C(31)-C(30)-C(29)	120.77(16)
S(2)-C(22)-H(19)	108.6	C(31)-C(30)-H(25)	119.6
C(23)-C(22)-H(20)	108.6	C(29)-C(30)-H(25)	119.6
S(2)-C(22)-H(20)	108.6	C(32)-C(31)-C(30)	120.49(16)
H(19)-C(22)-H(20)	107.6	C(32)-C(31)-H(26)	119.8

C(30)-C(31)-H(26)	119.8	C(41)-C(42)-H(35)	119.4
C(31)-C(32)-C(33)	119.98(15)	C(44)-C(43)-C(42)	120.13(15)
C(31)-C(32)-H(27)	120.0	C(44)-C(43)-H(36)	119.9
C(33)-C(32)-H(27)	120.0	C(42)-C(43)-H(36)	119.9
C(32)-C(33)-C(34)	119.89(17)	C(43)-C(44)-C(45)	120.13(15)
C(32)-C(33)-H(28)	120.1	C(43)-C(44)-H(37)	119.9
C(34)-C(33)-H(28)	120.1	C(45)-C(44)-H(37)	119.9
C(33)-C(34)-C(29)	121.01(15)	C(44)-C(45)-C(46)	119.80(16)
C(33)-C(34)-H(29)	119.5	C(44)-C(45)-H(38)	120.1
C(29)-C(34)-H(29)	119.5	C(46)-C(45)-H(38)	120.1
C(40)-C(35)-C(36)	117.22(13)	C(45)-C(46)-C(41)	121.10(15)
C(40)-C(35)-Si(2)	122.04(11)	C(45)-C(46)-H(39)	119.5
C(36)-C(35)-Si(2)	120.74(11)	C(41)-C(46)-H(39)	119.5
C(37)-C(36)-C(35)	122.00(14)	C(52)-C(47)-C(48)	118.12(13)
C(37)-C(36)-H(30)	119.0	C(52)-C(47)-Si(4)	121.70(11)
C(35)-C(36)-H(30)	119.0	C(48)-C(47)-Si(4)	120.05(11)
C(38)-C(37)-C(36)	119.60(14)	C(49)-C(48)-C(47)	120.99(14)
C(38)-C(37)-H(31)	120.2	C(49)-C(48)-H(40)	119.5
C(36)-C(37)-H(31)	120.2	C(47)-C(48)-H(40)	119.5
C(37)-C(38)-C(39)	119.80(15)	C(50)-C(49)-C(48)	119.80(15)
C(37)-C(38)-H(32)	120.1	C(50)-C(49)-H(41)	120.1
C(39)-C(38)-H(32)	120.1	C(48)-C(49)-H(41)	120.1
C(38)-C(39)-C(40)	120.44(15)	C(51)-C(50)-C(49)	120.18(15)
C(38)-C(39)-H(33)	119.8	C(51)-C(50)-H(42)	119.9
C(40)-C(39)-H(33)	119.8	C(49)-C(50)-H(42)	119.9
C(39)-C(40)-C(35)	120.91(14)	C(50)-C(51)-C(52)	120.06(15)
C(39)-C(40)-H(34)	119.5	C(50)-C(51)-H(43)	120.0
C(35)-C(40)-H(34)	119.5	C(52)-C(51)-H(43)	120.0
C(46)-C(41)-C(42)	117.73(13)	C(51)-C(52)-C(47)	120.83(15)
C(46)-C(41)-Si(3)	120.96(11)	C(51)-C(52)-H(44)	119.6
C(42)-C(41)-Si(3)	121.31(11)	C(47)-C(52)-H(44)	119.6
C(43)-C(42)-C(41)	121.10(15)	Si(5)-C(53)-H(45)	109.5
C(43)-C(42)-H(35)	119.4	Si(5)-C(53)-H(46)	109.5

H(45)-C(53)-H(46)	109.5	H(61)-C(58)-H(62)	109.5
Si(5)-C(53)-H(47)	109.5	Si(8)-C(59)-H(63)	109.5
H(45)-C(53)-H(47)	109.5	Si(8)-C(59)-H(64)	109.5
H(46)-C(53)-H(47)	109.5	H(63)-C(59)-H(64)	109.5
Si(5)-C(54)-H(48)	109.5	Si(8)-C(59)-H(65)	109.5
Si(5)-C(54)-H(49)	109.5	H(63)-C(59)-H(65)	109.5
H(48)-C(54)-H(49)	109.5	H(64)-C(59)-H(65)	109.5
Si(5)-C(54)-H(50)	109.5	Si(8)-C(60)-H(66)	109.5
H(48)-C(54)-H(50)	109.5	Si(8)-C(60)-H(67)	109.5
H(49)-C(54)-H(50)	109.5	H(66)-C(60)-H(67)	109.5
Si(6)-C(55)-H(51)	109.5	Si(8)-C(60)-H(68)	109.5
Si(6)-C(55)-H(52)	109.5	H(66)-C(60)-H(68)	109.5
H(51)-C(55)-H(52)	109.5	H(67)-C(60)-H(68)	109.5
Si(6)-C(55)-H(53)	109.5	Si(4)-O(12)-Si(8)	147.45(7)
H(51)-C(55)-H(53)	109.5		
H(52)-C(55)-H(53)	109.5		
Si(6)-C(56)-H(54)	109.5		
Si(6)-C(56)-H(55)	109.5		
H(54)-C(56)-H(55)	109.5		
Si(6)-C(56)-H(56)	109.5		
H(54)-C(56)-H(56)	109.5		
H(55)-C(56)-H(56)	109.5		
Si(7)-C(57)-H(57)	109.5		
Si(7)-C(57)-H(58)	109.5		
H(57)-C(57)-H(58)	109.5		
Si(7)-C(57)-H(59)	109.5		
H(57)-C(57)-H(59)	109.5		
H(58)-C(57)-H(59)	109.5		
Si(7)-C(58)-H(60)	109.5		
Si(7)-C(58)-H(61)	109.5		
H(60)-C(58)-H(61)	109.5		
Si(7)-C(58)-H(62)	109.5		
H(60)-C(58)-H(62)	109.5		

6. X-ray diffraction and crystallography for compound 9

Table S4. Crystal data and structure refinement for **9**.

Identification code	22z02m	
Empirical formula	C60 H68 O16 S2 Si8	
Formula weight	1333.98	
Temperature	120 K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 21.122(3) Å	α= 90°.
	b = 10.6780(18) Å	β= 94.396(4)°.
	c = 29.541(5) Å	γ = 90°.
Volume	6643.1(18) $Å^3$	
Z	4	
Density (calculated)	1.334 Mg/m^3	
Absorption coefficient	0.289 mm^{-1}	
F(000)	2800	
Crystal size	0.25 x 0.23 x 0.13 mm^3	
Theta range for data collection	2.766 to 27.499°.	
Index ranges	-27<=h<=27, -13<=k<=13, -38<=l<=38	
Reflections collected	51908	
Independent reflections	7612 [R(int) = 0.0239]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Numerical	
Max. and min. transmission	1.000 and 0.949	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7612 / 0 / 388	
Goodness-of-fit on F^2	1.096	
Final R indices [I>2sigma(I)][a]	R1 = 0.0296, wR2 = 0.0786	
R indices (all data)	R1 = 0.0346, wR2 = 0.0833	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.398 and -0.318 $e.Å^{-3}$	

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, $wR_2 = [(\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$.

Table S5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **9**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	4057(1)	6999(1)	7330(1)	24(1)
Si(1)	4383(1)	6994(1)	6852(1)	16(1)
O(2)	5130(1)	7268(1)	6949(1)	26(1)
Si(2)	5868(1)	7191(1)	7126(1)	16(1)
O(3)	6171(1)	5976(1)	6900(1)	22(1)
Si(3)	6715(1)	5425(1)	6592(1)	17(1)
O(4)	6404(1)	5297(1)	6062(1)	20(1)
C(1)	6264(1)	6291(1)	5774(1)	18(1)
C(2)	6735(1)	6800(1)	5528(1)	22(1)
C(3)	6586(1)	7787(2)	5234(1)	25(1)
C(4)	5975(1)	8259(1)	5180(1)	23(1)
C(5)	5499(1)	7740(1)	5424(1)	18(1)
C(6)	5646(1)	6750(1)	5721(1)	18(1)
C(7)	4836(1)	8282(1)	5380(1)	19(1)
S(1)	4416(1)	8020(1)	4839(1)	19(1)
O(5)	4819(1)	8352(1)	4486(1)	28(1)
O(6)	3809(1)	8636(1)	4843(1)	26(1)
C(8)	4293(1)	6364(1)	4809(1)	21(1)
C(9)	3829(1)	5845(1)	5123(1)	19(1)
C(10)	3180(1)	6080(1)	5038(1)	24(1)
C(11)	2750(1)	5539(2)	5311(1)	28(1)
C(12)	2958(1)	4765(2)	5670(1)	26(1)
C(13)	3602(1)	4553(1)	5761(1)	21(1)
C(14)	4036(1)	5084(1)	5487(1)	19(1)
O(7)	3799(1)	3783(1)	6117(1)	28(1)
Si(4)	4255(1)	4135(1)	6577(1)	20(1)
O(8)	4266(1)	5654(1)	6615(1)	33(1)
C(15)	4041(1)	8219(1)	6467(1)	17(1)

C(16)	3522(1)	7966(2)	6158(1)	24(1)
C(17)	3276(1)	8888(2)	5863(1)	32(1)
C(18)	3542(1)	10064(2)	5869(1)	34(1)
C(19)	4057(1)	10338(2)	6169(1)	32(1)
C(20)	4304(1)	9423(1)	6467(1)	25(1)
C(21)	6283(1)	8624(1)	6964(1)	22(1)
C(22)	6158(1)	9138(2)	6530(1)	28(1)
C(23)	6530(1)	10098(2)	6375(1)	39(1)
C(24)	7034(1)	10555(2)	6653(1)	43(1)
C(25)	7158(1)	10086(2)	7087(1)	43(1)
C(26)	6786(1)	9128(2)	7241(1)	32(1)
C(27)	7410(1)	6478(2)	6629(1)	28(1)
C(28)	6901(1)	3801(2)	6763(1)	29(1)
C(29)	5069(1)	3566(2)	6524(1)	40(1)
C(30)	3885(1)	3426(2)	7057(1)	44(1)

Table S6. Bond lengths [Å] and angles [°] for **9**.

O(1)-Si(1)	1.6161(11)	C(8)-C(9)	1.5064(19)
O(1)-Si(2)#1	1.6165(11)	C(8)-H(33)	0.9900
Si(1)-O(8)	1.6040(12)	C(8)-H(34)	0.9900
Si(1)-O(2)	1.6083(11)	C(9)-C(14)	1.391(2)
Si(1)-C(15)	1.8439(14)	C(9)-C(10)	1.3955(19)
O(2)-Si(2)	1.6083(11)	C(10)-C(11)	1.387(2)
Si(2)-O(3)	1.6133(10)	C(10)-H(5)	0.9500
Si(2)-O(1)#1	1.6164(11)	C(11)-C(12)	1.390(2)
Si(2)-C(21)	1.8454(16)	C(11)-H(6)	0.9500
O(3)-Si(3)	1.6301(10)	C(12)-C(13)	1.384(2)
Si(3)-O(4)	1.6579(11)	C(12)-H(7)	0.9500
Si(3)-C(28)	1.8400(16)	C(13)-O(7)	1.3752(18)
Si(3)-C(27)	1.8460(16)	C(13)-C(14)	1.390(2)
O(4)-C(1)	1.3786(17)	C(14)-H(8)	0.9500
C(1)-C(2)	1.385(2)	O(7)-Si(4)	1.6474(11)
C(1)-C(6)	1.3922(19)	Si(4)-O(8)	1.6258(12)
C(2)-C(3)	1.387(2)	Si(4)-C(30)	1.8338(18)
C(2)-H(1)	0.9500	Si(4)-C(29)	1.8421(18)
C(3)-C(4)	1.385(2)	C(15)-C(16)	1.3988(19)
C(3)-H(2)	0.9500	C(15)-C(20)	1.400(2)
C(4)-C(5)	1.395(2)	C(16)-C(17)	1.389(2)
C(4)-H(3)	0.9500	C(16)-H(9)	0.9500
C(5)-C(6)	1.395(2)	C(17)-C(18)	1.376(3)
C(5)-C(7)	1.5111(19)	C(17)-H(10)	0.9500
C(6)-H(4)	0.9500	C(18)-C(19)	1.380(3)
C(7)-S(1)	1.7892(14)	C(18)-H(11)	0.9500
C(7)-H(31)	0.9900	C(19)-C(20)	1.390(2)
C(7)-H(32)	0.9900	C(19)-H(12)	0.9500
S(1)-O(6)	1.4404(11)	C(20)-H(13)	0.9500
S(1)-O(5)	1.4414(11)	C(21)-C(26)	1.398(2)
S(1)-C(8)	1.7885(15)	C(21)-C(22)	1.401(2)

C(22)-C(23)	1.390(2)	O(2)-Si(2)-C(21)	109.92(7)
C(22)-H(14)	0.9500	O(3)-Si(2)-C(21)	110.34(6)
C(23)-C(24)	1.382(3)	O(1)#1-Si(2)-C(21)	110.60(6)
C(23)-H(15)	0.9500	Si(2)-O(3)-Si(3)	147.20(7)
C(24)-C(25)	1.381(3)	O(3)-Si(3)-O(4)	108.16(6)
C(24)-H(16)	0.9500	O(3)-Si(3)-C(28)	109.39(7)
C(25)-C(26)	1.389(3)	O(4)-Si(3)-C(28)	104.08(7)
C(25)-H(17)	0.9500	O(3)-Si(3)-C(27)	109.82(6)
C(26)-H(18)	0.9500	O(4)-Si(3)-C(27)	111.18(6)
C(27)-H(19)	0.9800	C(28)-Si(3)-C(27)	113.95(8)
C(27)-H(20)	0.9800	C(1)-O(4)-Si(3)	124.82(9)
C(27)-H(21)	0.9800	O(4)-C(1)-C(2)	119.71(12)
C(28)-H(22)	0.9800	O(4)-C(1)-C(6)	119.66(12)
C(28)-H(23)	0.9800	C(2)-C(1)-C(6)	120.60(13)
C(28)-H(24)	0.9800	C(1)-C(2)-C(3)	119.30(13)
C(29)-H(25)	0.9800	C(1)-C(2)-H(1)	120.3
C(29)-H(26)	0.9800	C(3)-C(2)-H(1)	120.3
C(29)-H(27)	0.9800	C(4)-C(3)-C(2)	120.80(13)
C(30)-H(28)	0.9800	C(4)-C(3)-H(2)	119.6
C(30)-H(29)	0.9800	C(2)-C(3)-H(2)	119.6
C(30)-H(30)	0.9800	C(3)-C(4)-C(5)	119.96(14)
		C(3)-C(4)-H(3)	120.0
Si(1)-O(1)-Si(2)#1	148.52(7)	C(5)-C(4)-H(3)	120.0
O(8)-Si(1)-O(2)	110.86(7)	C(4)-C(5)-C(6)	119.49(13)
O(8)-Si(1)-O(1)	108.83(6)	C(4)-C(5)-C(7)	120.24(13)
O(2)-Si(1)-O(1)	108.79(6)	C(6)-C(5)-C(7)	120.23(12)
O(8)-Si(1)-C(15)	108.90(6)	C(1)-C(6)-C(5)	119.84(12)
O(2)-Si(1)-C(15)	108.21(6)	C(1)-C(6)-H(4)	120.1
O(1)-Si(1)-C(15)	111.25(6)	C(5)-C(6)-H(4)	120.1
Si(2)-O(2)-Si(1)	164.06(8)	C(5)-C(7)-S(1)	114.17(9)
O(2)-Si(2)-O(3)	108.13(6)	C(5)-C(7)-H(31)	108.7
O(2)-Si(2)-O(1)#1	110.41(6)	S(1)-C(7)-H(31)	108.7
O(3)-Si(2)-O(1)#1	107.39(6)	C(5)-C(7)-H(32)	108.7

S(1)-C(7)-H(32)	108.7	O(8)-Si(4)-O(7)	106.80(6)
H(31)-C(7)-H(32)	107.6	O(8)-Si(4)-C(30)	111.31(9)
O(6)-S(1)-O(5)	117.91(7)	O(7)-Si(4)-C(30)	106.71(8)
O(6)-S(1)-C(8)	109.06(7)	O(8)-Si(4)-C(29)	108.99(8)
O(5)-S(1)-C(8)	107.31(7)	O(7)-Si(4)-C(29)	110.14(8)
O(6)-S(1)-C(7)	107.65(7)	C(30)-Si(4)-C(29)	112.71(10)
O(5)-S(1)-C(7)	109.15(7)	Si(1)-O(8)-Si(4)	157.08(8)
C(8)-S(1)-C(7)	105.03(7)	C(16)-C(15)-C(20)	117.89(13)
C(9)-C(8)-S(1)	115.56(10)	C(16)-C(15)-Si(1)	121.06(11)
C(9)-C(8)-H(33)	108.4	C(20)-C(15)-Si(1)	121.03(11)
S(1)-C(8)-H(33)	108.4	C(17)-C(16)-C(15)	120.70(15)
C(9)-C(8)-H(34)	108.4	C(17)-C(16)-H(9)	119.7
S(1)-C(8)-H(34)	108.4	C(15)-C(16)-H(9)	119.7
H(33)-C(8)-H(34)	107.5	C(18)-C(17)-C(16)	120.32(15)
C(14)-C(9)-C(10)	119.28(13)	C(18)-C(17)-H(10)	119.8
C(14)-C(9)-C(8)	120.61(12)	C(16)-C(17)-H(10)	119.8
C(10)-C(9)-C(8)	120.05(13)	C(17)-C(18)-C(19)	120.24(15)
C(11)-C(10)-C(9)	120.00(14)	C(17)-C(18)-H(11)	119.9
C(11)-C(10)-H(5)	120.0	C(19)-C(18)-H(11)	119.9
C(9)-C(10)-H(5)	120.0	C(18)-C(19)-C(20)	119.78(16)
C(10)-C(11)-C(12)	120.53(14)	C(18)-C(19)-H(12)	120.1
C(10)-C(11)-H(6)	119.7	C(20)-C(19)-H(12)	120.1
C(12)-C(11)-H(6)	119.7	C(19)-C(20)-C(15)	121.07(15)
C(13)-C(12)-C(11)	119.55(14)	C(19)-C(20)-H(13)	119.5
C(13)-C(12)-H(7)	120.2	C(15)-C(20)-H(13)	119.5
C(11)-C(12)-H(7)	120.2	C(26)-C(21)-C(22)	117.86(15)
O(7)-C(13)-C(12)	118.69(13)	C(26)-C(21)-Si(2)	121.37(12)
O(7)-C(13)-C(14)	121.06(13)	C(22)-C(21)-Si(2)	120.22(12)
C(12)-C(13)-C(14)	120.22(14)	C(23)-C(22)-C(21)	121.20(16)
C(13)-C(14)-C(9)	120.40(13)	C(23)-C(22)-H(14)	119.4
C(13)-C(14)-H(8)	119.8	C(21)-C(22)-H(14)	119.4
C(9)-C(14)-H(8)	119.8	C(24)-C(23)-C(22)	119.59(17)
C(13)-O(7)-Si(4)	128.19(9)	C(24)-C(23)-H(15)	120.2

C(22)-C(23)-H(15)	120.2	Si(3)-C(28)-H(23)	109.5
C(25)-C(24)-C(23)	120.39(17)	H(22)-C(28)-H(23)	109.5
C(25)-C(24)-H(16)	119.8	Si(3)-C(28)-H(24)	109.5
C(23)-C(24)-H(16)	119.8	H(22)-C(28)-H(24)	109.5
C(24)-C(25)-C(26)	119.98(18)	H(23)-C(28)-H(24)	109.5
C(24)-C(25)-H(17)	120.0	Si(4)-C(29)-H(25)	109.5
C(26)-C(25)-H(17)	120.0	Si(4)-C(29)-H(26)	109.5
C(25)-C(26)-C(21)	120.94(17)	H(25)-C(29)-H(26)	109.5
C(25)-C(26)-H(18)	119.5	Si(4)-C(29)-H(27)	109.5
C(21)-C(26)-H(18)	119.5	H(25)-C(29)-H(27)	109.5
Si(3)-C(27)-H(19)	109.5	H(26)-C(29)-H(27)	109.5
Si(3)-C(27)-H(20)	109.5	Si(4)-C(30)-H(28)	109.5
H(19)-C(27)-H(20)	109.5	Si(4)-C(30)-H(29)	109.5
Si(3)-C(27)-H(21)	109.5	H(28)-C(30)-H(29)	109.5
H(19)-C(27)-H(21)	109.5	Si(4)-C(30)-H(30)	109.5
H(20)-C(27)-H(21)	109.5	H(28)-C(30)-H(30)	109.5
Si(3)-C(28)-H(22)	109.5	H(29)-C(30)-H(30)	109.5