BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

Supporting Information

for

Silanediol versus chlorosilanol: hydrolyses and hydrogen-bonding catalyses with fenchole-based silanes

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Copies of all NMR spectra, HPLC graphs, GC graphs of the kinetic study

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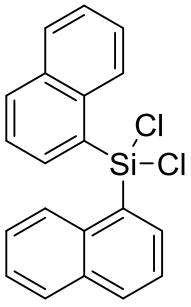
1. **General methods**

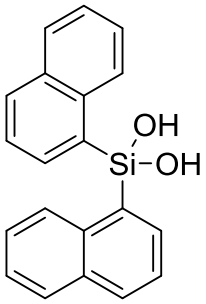
Diethyl ether, methyl *tert*-butyl ether, *n*-hexane and tetrahydrofuran were dried over sodium and fresh distilled before use. Methylene chloride was dried over phosphorus pentoxide and fresh distilled before use. Toluene, 1,2-DCE, dimethylformamide, acetonitrile, acetone, benzene, *m*-xylene, nitrobenzene and pyridine were purchased dry and used as received. Purification of reaction products was carried out by flash chromatography using silica gel (0.035–0.070 mm, 60 A). Analytical thin layer chromatography was performed on Merck silica gel 60 F_{254} plates. Visualization was accomplished with UV light (254 nm, 330 nm) and potassium permanganate stains followed by heating. Melting points (mp) were obtained on a Stuart Scientific SMP 3 and are uncorrected. Proton nuclear magnetic resonances (^{1}H NMR) were recorded in deuterated solvents on a Bruker Avance AV Avance II (300 MHz) spectrometer unless otherwise noted. Chemical shifts are reported in parts per million (ppm, δ) using the solvent as internal standard. ^{1}H NMR splitting patterns are designated as singlet (s), doublet (d), triplet (t), or quartet (q). Splitting patterns that could not be interpreted or easily visualized are designated as multiplet (m). Coupling constants are reported in Hertz (Hz). Proton-decoupled carbon (^{13}C NMR) spectra were recorded on a Bruker AV Avance II (300 MHz). Chemical shifts are reported in parts per million (ppm, δ) using the solvent as internal standard. Electrospray mass spectra (ESIMS) were obtained using a THERMO Scientific LTQ Orbitrap XL. HPLC analyses were obtained on a VWR Hitachi L-2130 (Pump) and VWR Hitachi L-2400 (UV Detector) equipped with a VWR Hitachi Chromaster 5310 (Column Oven). GC analyses were obtained on a Hewlett Packard 6890 GC-System. UV–vis spectra were obtained on a Perkin-Elmer UV–vis-Spectrometer Lambda 35, using quartz cuvettes with 1.00 cm width. Specific rotations were obtained on an Anton Paar MCP 200 polarimeter. X-ray structure analyses were obtained on a Bruker D8 Venture with KAPPA goniometer and a cupper microfocus source.

2. **Dichlorosilanes, chlorosilanol and silanediol preparation**

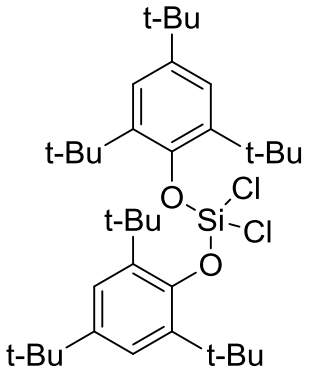


Synthesis of dichlorodi(naphthalen-1-yl)silane (13): In a dried round bottomed flask 1-bromonaphthalene (3.4 mL, 24.4 mmol, 1 equiv) was solved in 100 mL dried diethyl ether an cooled to -80 °C. Afterwards *n*-BuLi (2.5 *M* in hexane, 10.7 mL, 1.2 equiv) was added and stirred for 30 min at this temperature. In another flask, $SiCl_4$ (1.4 mL, 12.2 mmol, 0.5 equiv) was solved in 20 mL dried diethyl ether. That solution

was added drop wise to the 1-bromonaphthalen/*n*BuLi solution at -80 °C. The mixture was warmed to 20 °C and stirred for 2 d. The solvent was evaporated, the residue was solved in toluene and filtered through celite. After evaporation of the solvent, dichlorodi(naphthalen-1-yl)silane **13** was obtained as white solid (1.22 g, 3.45 mmol 14%). M.p.138.3°C; ^{1}H NMR (300 MHz, Chloroform-d): δ=8.29 (d, J = 6.9 Hz, 2H), 8.14 (d, J = 5.2 Hz, 2H), 8.06 (d, J = 8.2 Hz, 2H), 7.92 (d, J = 7.8 Hz, 2H), 7.59 – 7.40 (m, 6H); ^{13}C NMR (75 MHz, CDCl3): δ=136.11, 135.43, 133.59, 133.07, 129.61, 129.18, 127.91, 126.85, 126.22, 125.03, 109.99.

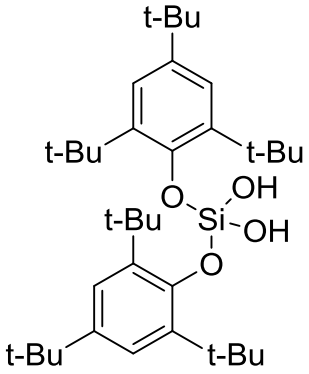


Synthesis of di(naphthalen-1-yl)silanediol (1): In a dried round bottomed flask dichlorodi(naphthalen-1-yl)silane **13** (0.5 g, 1.4 mmol, 1 equiv) was solved in 10 mL dried THF. To this solution, 5 mL water was added. This mixture was stirred for 2 h at 20 °C. The solvent was evaporated and the residue purified by silica gel flash column chromatography (*n*hexane/ethyl acetate: 4/1, R_f: 0.18). Di(naphthalen-1-yl)silanediol **1** was obtained as white solid (0.433 g, 1.3 mmol, 98%). M.p. 153.1°C; ^{1}H NMR (300 MHz, Chloroform-*d*): δ=8.28 (d, *J* = 8.2 Hz, 2H), 7.85 (dd, *J* = 18.7, 7.7 Hz, 6H), 7.46 – 7.27 (m, 6H), 3.74 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 135.61, 134.56, 132.25, 131.56, 130.21, 127.79, 127.35, 125.35, 124.63, 124.09.



Synthesis of dichlorobis(2,4,6-tri-*tert*-butylphenoxy)silane (14): In a dried round bottomed flask potassium (1.0 g, 25.6 mmol, 3 equiv) was added to 70 mL dried toluene and heated to reflux for 2 2,4,6-tri-*tert*-butylphenol (6 g, 25.6 mmol, 3 equiv) was solved in 70 mL dried diethyl ether and added to the potassium/toluene

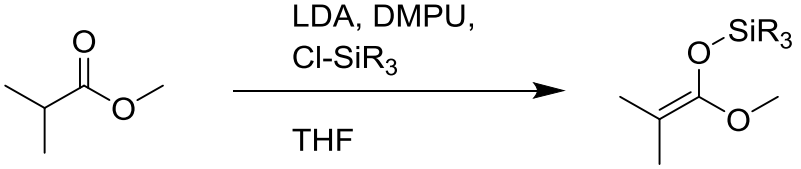
suspension. This mixture was heated to reflux for 24 h. After that, a solution of $SiCl_4$ (1.0 mL, 8.4 mmol, 1 equiv) and 16 mg 18-Crown-6 in 3 mL diethyl ether was added. This mixture was heated do reflux for 16 h. The diethyl ether was evaporated and the remaining mixture was heated to reflux for another 24 h. The solvent was evaporated, the residue solved in *n*-hexane and filtered through celite. After recrystallization with hexane, dichlorobis(2,4,6-tri-*tert*-butylphenoxy)silane (**14**) was obtained as white solid (0.97 g, 1.56 mmol, 19%). M.p. 205.6°C; ^{1}H NMR (300 MHz, chloroform-*d*): δ=7.29 (s, 4H), 1.50 (s, 36H), 1.31 (s, 18H).^{13}C NMR (75 MHz, $CDCl_3$): δ=148.17, 144.51, 140.37, 123.35, 35.75, 34.47, 32.17, 31.50.



Synthesis of bis(2,4,6-tri-*tert*-butylphenoxy)silandiol (15): In a dried round bottomed flask dichlorobis(2,4,6-tri-*tert*-butylphenoxy)silane (**14**, 310.9 mg, 0.5 mmol,1 equiv) and KOH (280 mg, 5 mmol, 10 equiv) were solved in 13 mL H_2O and 13 mL abs. THF. This mixture was heated to reflux for 16 h and extracted with diethyl ether thrice. The organic layer was dried over Na_2SO_4 and concentrated on a rotary evaporator. Bis(2,4,6-tri-*tert*-butylphenyl)silandiol **15** was obtained as white solid (289 mg, 0.49 mmol, 99%). M.p. 196.3°C; ^{1}H NMR (300 MHz, chloroform-*d*): δ=7.21 (s, 4H), 5.03 (s, 2H), 1.45 (s, 36H), 1.30 (s, 18H); ^{13}C NMR (75 MHz, $CDCl_3$):δ=151.33, 141.40, 134.93, 121.88, 31.73, 30.43.

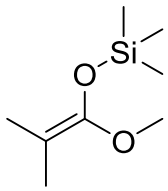
Di-*tert*-butoxydichlorosilane and di-*tert*-butoxysilandiol were obtained as reported in literature[1]. While concentrating on a rotary evaporator at 40 °C, the colorless oil turns to a white solid as well. With this behavior further kinetic experiments were discarded.

3. **General procedure for the preparation of silyl ketene acetals**

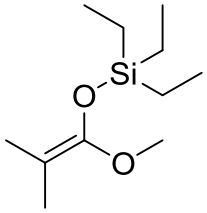


In a dried 250 mL round bottomed flask, di-*iso*propylamine (4.2 mL, 30 mmol, 1.2 equiv) was added to 50 mL anhydrous THF. The solution was cooled to 0 °C and *n*-

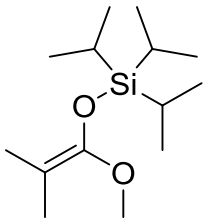
BuLi (11 mL, 27.5 mmol, 2.5 *M* in hexane, 1.1 equiv) was added dropwise. The mixture was stirred at 0 °C for 20 min. After that, the mixture was cooled to -78 °C and methyl isobutyrate (2.87 mL, 25 mmol, 1.0 equiv) was added slowly. The mixture was stirred at -78 °C for 30 min. Than DMPU (4.53 mL, 37.5 mmol, 1.2 equiv) and the respective chlorosilane (30 mmol, 1.2 equiv) were added. The mixture was stirred at −78 °C for 30 min and at 20 °C for 1 h. Afterwards, the solvent was removed under reduced pressure and the resulting mixture was taken up in 200 mL pentane, washed with water (1 × 100 mL), saturated $CuSO_4$ solution (1 × 100 mL), saturated $NaHCO_3$ solution (1 × 100 mL) and saturated NaCl solution (1 × 100 mL). The organic layer was dried over Na_2SO_4, concentrated on a rotary evaporator and purified via fractional distillation.



Synthesis of ((1-methoxy-2-methylprop-1-en-1-yl)oxy)trimethylsilane (11a): Chlorotrimethylsilane (3.77 mL, 30 mmol, 1.2 equiv) was added. After distillation, the product was obtained as clear colorless oil (2.25 g, 13.8 mmol, 55%). B.p: 47-49 °C (20 mbar), ^{1}H NMR (300 MHz, chloroform-*d*): δ=3.50 (s, 3H), 1.57 (s, 3H), 1.51 (s, 3H), 0.20 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 90.87, 56.51, 16.84, 16.10, 0.01.

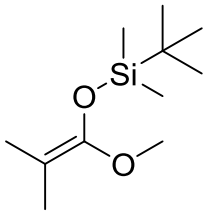


Synthesis of ((1-methoxy-2-methylprop-1-en-1-yl)oxy)triethylsilane (11b): Chlorotriethylsilane (5.08 mL, 30 mmol, 1.2 equiv) was added. After distillation, the product was obtained as clear colorless oil (3.09 g, 14.3 mmol, 57%). B.p: 57-59 °C (1.6 mbar). ^{1}H NMR (300 MHz, chloroform-*d*): δ=3.51 (s, 3H), 1.55 (s, 3H), 1.53 (s, 3H), 0.99 (t, *J* = 7.9 Hz, 9H), 0.69 (d, *J* = 8.6 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$): δ=90.93, 57.03, 16.79, 16.13, 6.54, 4.94.



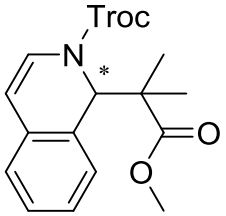
Synthesis of ((1-methoxy-2-methylprop-1-en-1-yl)oxy)tri*iso*propylsilane (11c): Chlorotri*iso*propylsilane (6.42 mL, 30 mmol, 1.2 equiv) was added. After distillation, the product was obtained as clear colorless oil (5.49 g, 14.3 mmol, 70%). B.p: 74 °C (0.4 mbar). ^{1}H NMR (300 MHz, chloroform-*d*): δ=3.56 (s, 3H), 1.57 (s, 6H), 1.14 –

1.07 (m, 21H); ^{13}C NMR (75 MHz, $CDCl_3$): δ=150.75, 90.97, 58.06, 17.76, 17.02, 16.27, 12.74.



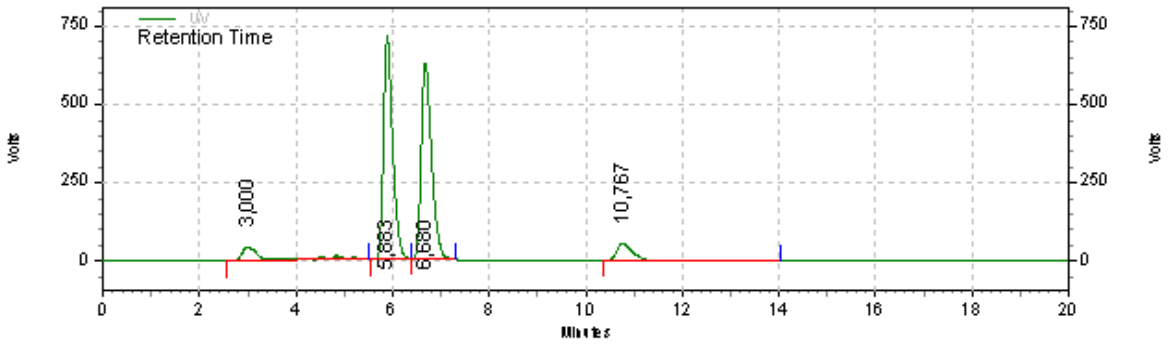
Synthesis of *tert*-butyl((1-methoxy-2-methylprop-1-en-1-yl)oxy)dimethylsilane (11d): *tert*-butylchlorodimethylsilane (4.52 g, 30 mmol, 1.2 equiv) was added. After distillation, the product was obtained as clear colorless oil (2.86 g, 13.0 mmol, 52%). B.p: 48-50 °C (1.8 mbar). ^{1}H NMR (300 MHz, chloroform-*d*): δ=3.51 (s, 3H), 1.57 (s, 3H), 1.53 (s, 3H), 0.96 (s, 9H), 0.14 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$): δ=91.51, 77.16, 57.19, 25.86, 17.03, 16.39, -4.47.

4. **General procedure for the catalytic reactions**



General procedure for the *N*-acyl Mannich reaction of isoquinolin 16 with silyl ketene acetals 11 to product 12: In a heat dried Schlenk tube isoquinolin **16** (11 µl, 0.1 mmol, 1 equiv) was solved in solvent (4 mL) and cooled to 0 °C under inert gas atmosphere. To this solution 2,2,2-trichlorethoxycarbonyl chloride (15 µL, 0.11 mmol, 1.1 equiv) was added. The cooling was removed. The solution warmed to 20 °C and stirred for 30 min. After this the solution was cooled to reaction temperature. The catalyst was added and stirred for 10 minutes. Then silyl ketene acetal **11** (0.15 mmol, 1.5 equiv) was added and the reaction mixture stirred for 6 h. The reaction was quenched by adding NaOMe (0.2 mL, 0.5 M in MeOH), filtered through silica gel with ethyl acetate as eluent and concentrated in vacuo. After further purification by silica gel flash column chromatography (*n*-hexane/ethyl acetate 95:5) product **12** was obtained. The enantiomeric excesses is determined by chiral HPLC analysis OD H, *n*-hexane/*i*PrOH 90/10, 1 mL/min, 220 nm, 25°C, t_r: 5.8 min (R) , t_r: 6.5 min (S), $[\alpha]^{20}_D$= -10.61 ° for 5% ee (c=1.1g/100 mL, (-)**12** correlates to **S-12**[2]); ^{1}H NMR (300 MHz, Chloroform-*d*): δ=7.33 – 7.17 (m, 2H), 7.10 (t, *J* = 6.3 Hz, 2H), 6.98 (s, 1H), 6.02 (d, *J* = 30.9, 7.7 Hz, 1H), 5.78 (s, 1H), 4.86 (d, 2H), 3.64 (s, 3H), 1.27 (s, 3H), 1.14 (s, 3H). NMR spectra contain the data set of two rotameres of **12**.

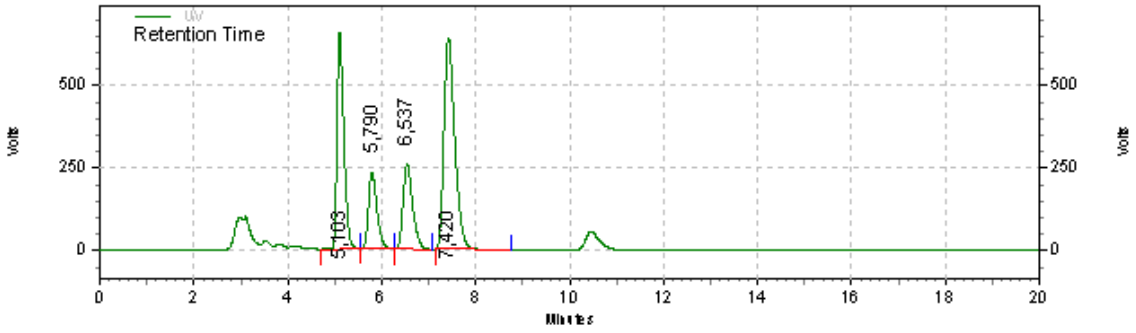
rac-12



UV Results

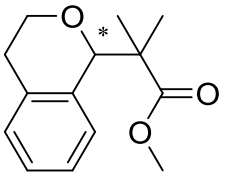
Retention Time	Area	Area %	Height	Height %
3,000	5540425	6,47	167367	2,91
5,883	37507028	43,78	2858708	49,66
6,680	37381215	43,64	2507394	43,56
10,767	5233162	6,11	223254	3,88
Totals	85661830	100,00	5756723	100,00

Table 7, entry 9

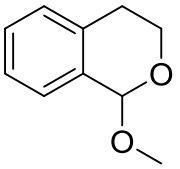


UV Results

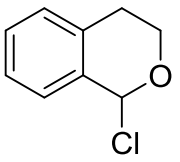
Retention Time	Area	Area %	Height	Height %
5,103	26654293	28,41	2622781	36,73
5,790	11576902	12,34	927275	12,99
6,537	14710908	15,68	1025196	14,36
7,420	40894509	43,58	2565081	35,92
Totals	93836612	100,00	7140333	100,00



General procedure for addition of silyl ketene acetals 11 to 1-chloroisochroman 18 to product 19: In a heat dried Schlenk tube 1-chloroisochroman (0.15 mmol, 0.3 mL of 0.5 M in toluene) was solved in solvent (1.2 mL) under inert gas atmosphere and cooled to −60 °C. After this catalyst (0.03 mmol, 0.2 equiv) was added and stirred for 10 min. Then silyl ketene acetal **11** (0.22 mmol, 1.5 equiv) was added and the resulting reaction mixture was stirred for 6 h. The reaction was quenched by adding NaOMe (0.2 mL, 0.5 M in MeOH), concentrated in vacuo and purified by silica gel flash column chromatography (*n*-hexane/Et_2O 9/1). The enantiomeric excesses is determined by chiral HPLC analysis OD H, n-hexane/*i*PrOH 100/0, 1.0 mL/min, 210 nm, 25°C, t_r: 23.9 min (S) , t_r: 29.1 min (R), $[\alpha]^{20}_D$= -0.63 ° for 1% ee (c=0.52g/100 mL (−)**19** correlates to ***S*-19**[3]). ^{1}H NMR (500 MHz, Chloroform-*d*): δ=7.20 – 7.08 (m, 3H), 6.97 (d, *J* = 7.1 Hz, 1H), 5.18 (s, 1H), 4.15 (dddd, *J* = 14.6, 10.7, 5.2, 1.6 Hz, 1H), 3.76 (s, 3H), 3.58 (tdd, *J* = 11.8, 10.8, 2.4, 1.0 Hz, 1H), 3.00 (ddt, *J* = 16.5, 11.2, 5.1, 4.7 Hz, 1H), 2.53 (d, *J* = 15.8 Hz, 1H), 1.13 (s, 3H), 1.11 (s, 3H).



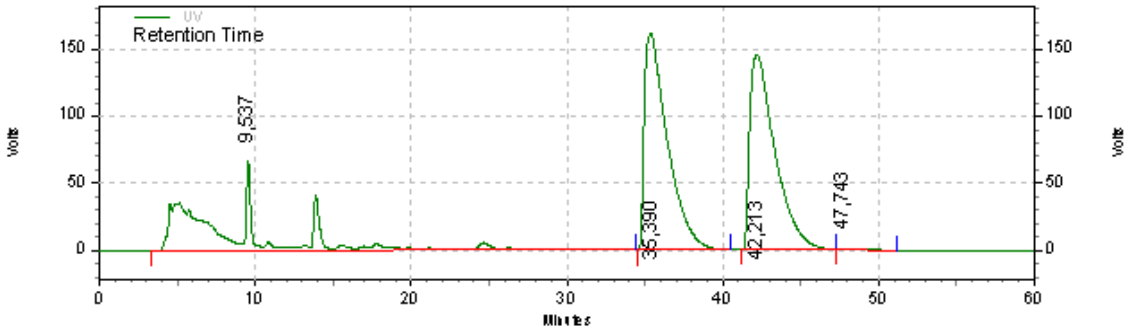
Synthesis of 1-methoxyisochroman: In a round bottomed flask isochromane (2.16 g, 16 mmol, 1 equiv) was solved in 100 mL DCM. methanol (0.44 mL, 10.8 mmol, 0.7 equiv) and 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (2.5 g, 11.0 mmol, 0.7 equiv) were added. This mixture was stirred at room temperature for 24 h, quenched with 200 mL $NaHCO_3$ (5%). The mixture was extracted with DCM (3 × 200 mL), dried over Na_2SO_4 and concentrated with a rotary evaporator. The residue was purified by flash chromatography (n-hexane/ethyl acetate 10/1). 1-Methoxyisochroman was obtained as colorless liquid (1.45 g, 8.8 mmol, 55%). ^{1}H NMR (300 MHz, Chloroform-*d*): δ=7.34 – 7.22 (m, 3H), 7.20 – 7.12 (m, 1H), 5.51 (s, 1H), 4.18 (td, *J* = 11.6, 3.4 Hz, 1H), 3.95 (ddd, *J* = 11.2, 6.0, 1.5 Hz, 1H), 3.60 (s, 3H), 3.07 (ddd, *J* = 17.3, 12.0, 6.0 Hz, 1H), 2.71 – 2.60 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ=134.19, 134.06, 128.48, 128.18, 127.47, 126.34, 97.84, 57.79, 55.36, 28.02.



Synthesis of 1-chloroisochroman: In a dried Schlenk tube 1- methoxyisochroman (1.0 g, 6.1 mmol, 1 equiv) was solved in 8 mL DCM. The mixture as cooled to 0 °C

and BCl_3 (1 *M*, 2.44 mL, 2.44 mmol, 0.4 equiv) was added dropwise. The mixture was warmed to 20 °C and stirred for 1.5 h. The solvent was evaporated and the residue distilled. 1-chloroisochroman was obtained as colorless liquid (0.69 g, 4.1 mmol, 67%). Bp: 75-77 °C (0.5 mbar), ^{1}H NMR (300 MHz, chloroform-*d*): δ=7.36 – 7.22 (m, 3H), 7.16 (d, *J* = 7.0 Hz, 2H), 4.48 – 4.29 (m, 1H), 4.19 (s, 1H), 3.29 – 3.01 (m, 1H), 2.77 (d, *J* = 15.9 Hz, 1H).

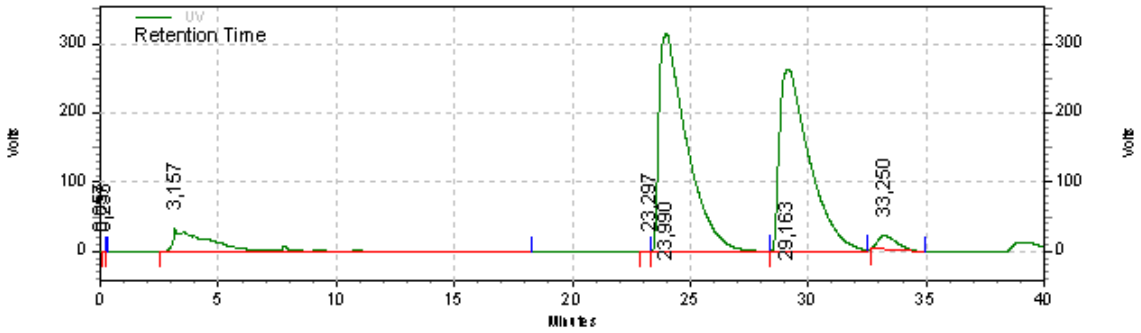
rac-18 with just 0.7 mL flow.



UV Results

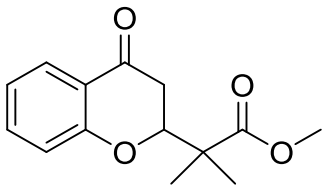
Retention Time	Area	Area %	Height	Height %
9,537	40758355	23,69	264537	17,77
35,390	66199736	38,47	644215	43,27
42,213	64833216	37,68	578814	38,88
47,743	277506	0,16	1203	0,08
Totals	172068813	100,00	1488769	100,00

Table 10, entry 7



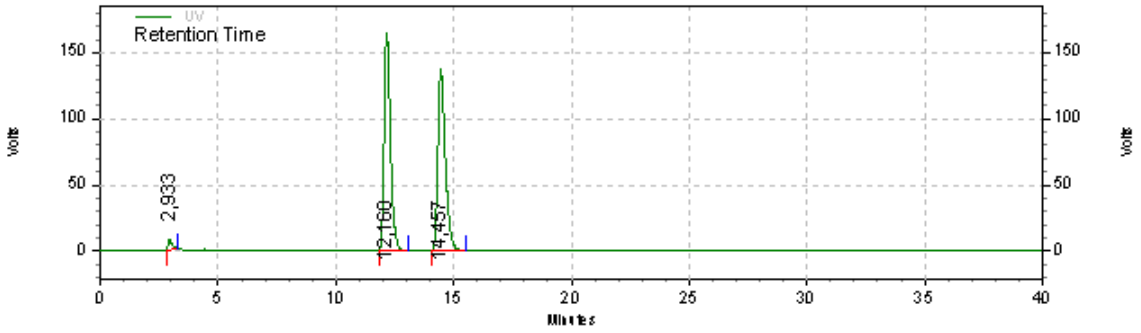
UV Results

Retention Time	Area	Area %	Height	Height %
0,057	520	0,00	94	0,00
0,233	322	0,00	85	0,00
3,157	15714805	7,24	130866	5,17
23,297	33222	0,02	1375	0,05
23,990	103230964	47,55	1261744	49,86
29,163	93668533	43,15	1057490	41,79
33,250	4452675	2,05	78696	3,11
Totals	217101041	100,00	2530350	100,00



General procedure for addition of silyl ketene acetals 11 to chromone 20 to product 22: In a heat dried Schlenk tube chromone (14.6 mg, 0.1 mmol, 1 equiv) was solved in 2 mL dried toluene under inert gas atmosphere. TIPSOTf (29.5 µL, 0.11 mmol, 1.1 equiv) was added and heated to 60 °C for 1 h. After this, the reaction mixture was cooled to -80 °C, catalyst (0.02 mmol, 0.2 equiv) and silyl ketene acetal **19** (0.14 mmol, 1.25 equiv), solved in 2 mL dried toluene, were added. The resulting reaction mixture was stirred for 4 h. The reaction was quenched by adding 3 M HCl (0.2 mL), concentrated in vacuo and purified by silica gel flash column chromatography (*n*hexane/ethyl acetate 9:1).The enantiomeric excesses is determined by chiral HPLC analysis AD H, *n*-hexane/*i*PrOH 98/2, 1 mL/min, 254 nm, 25 °C, t_r: 12.1 min (R), t_r: 14.5 min (S), $[\alpha]^{20}_D$=12.17 ° for 4% ee (c=0.05g/100 mL (+)**22** correlates to **S-22**[4]). ^{1}H NMR (300 MHz, chloroform-*d*): δ=7.87 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.46 (d, *J* = 8.2 Hz, 1H), 7.06 – 6.89 (m, 2H), 4.65 (dd, *J* = 14.1, 2.5 Hz, 1H), 3.73 (s, 3H), 2.88 – 2.52 (m, 2H), 1.38 (s, 3H), 1.28 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ=192.28, 175.51, 161.55, 136.00, 126.96, 121.48, 120.81, 117.88, 81.69, 52.25, 46.15, 38.36, 20.80, 20.62.

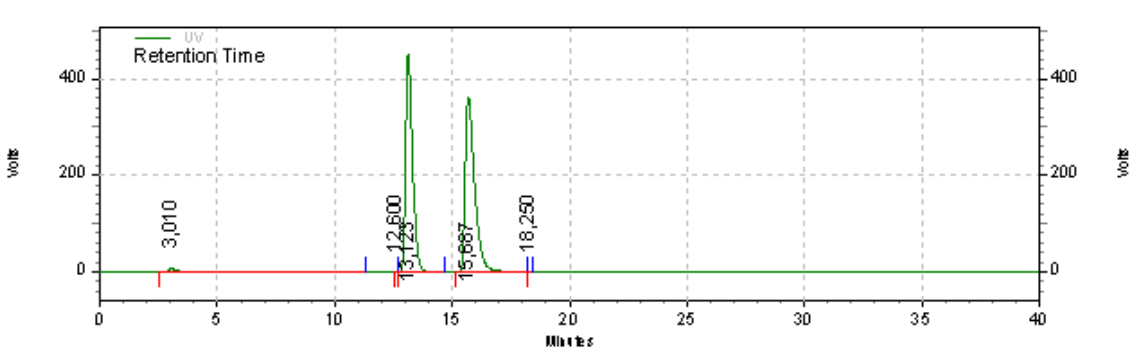
rac-22



UV Results

Retention Time	Area	Area %	Height	Height %
2,933	354942	1,44	28423	2,31
12,160	12167173	49,29	658212	53,41
14,457	12161171	49,27	545679	44,28
Totals	24683286	100,00	1232314	100,00

Table 10, entry 2



UV Results

Retention Time	Area	Area %	Height	Height %
3,010	905963	1,15	35793	1,09
12,600	3172	0,00	465	0,01
13,123	37468203	47,47	1806273	54,94
15,687	40546403	51,37	1445364	43,96
18,250	423	0,00	43	0,00
Totals	78924164	100,00	3287938	100,00

5. **General procedure for the kinetic hydrolysis**

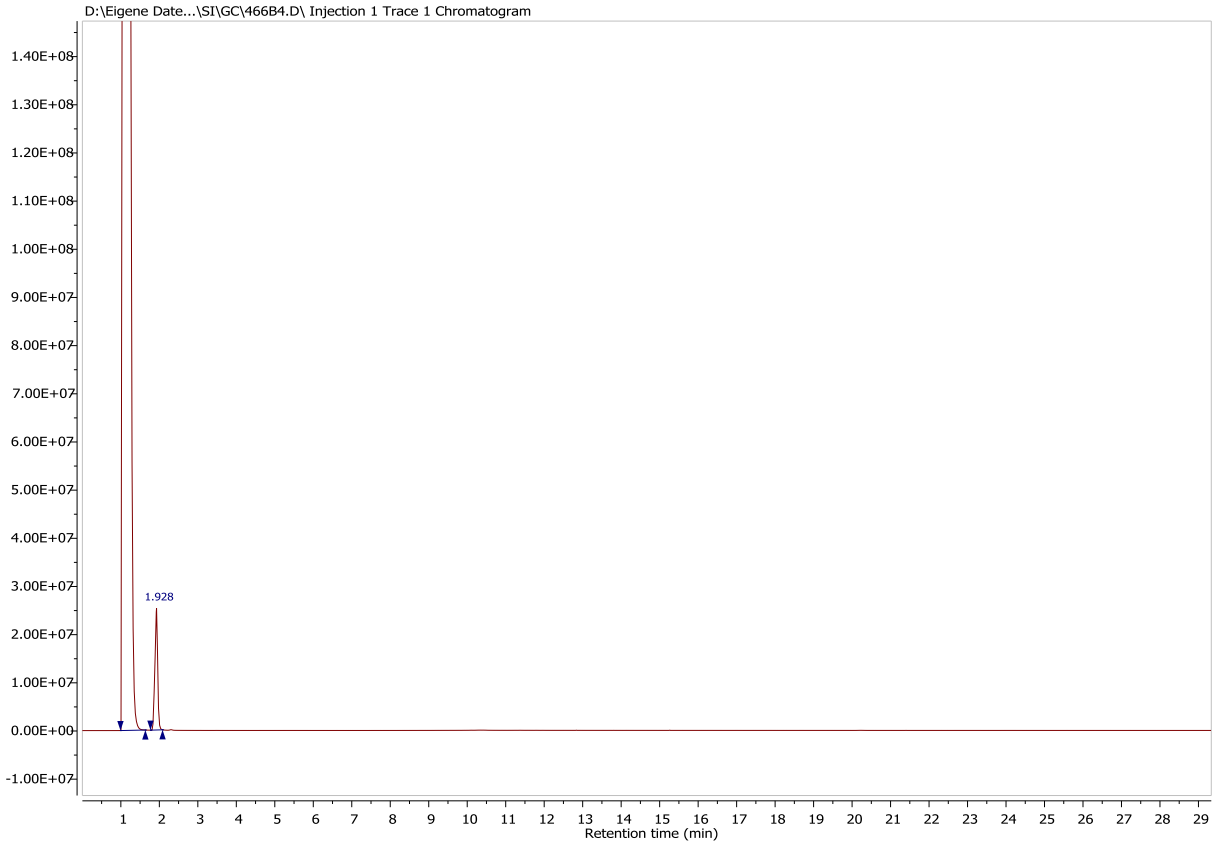
General procedure for the hydrolysis studies of dichlorosilanes 7, 13 and 14: Dichlorosilane (0.09 mmol) was solved in THF (2.5 mL) or THF/H_2O (1.25 mL/1.25 mL). For THF/H_2O/KOH conditions, KOH (0.9 mmol, 50.5 mg, 10 equiv) was added. The reaction mixture was heated and stirred as stated. After

reaction time the mixture was extracted two times with diethyl ether (2 mL) and concentrated in vacuo. The residue was solved in THF (5 mL). A sample (0.5 mL) was transferred to a GC vial and *n*-tetradecane solution (0.01 M in THF. 0.5 mL) was added as standard for GC analysis.

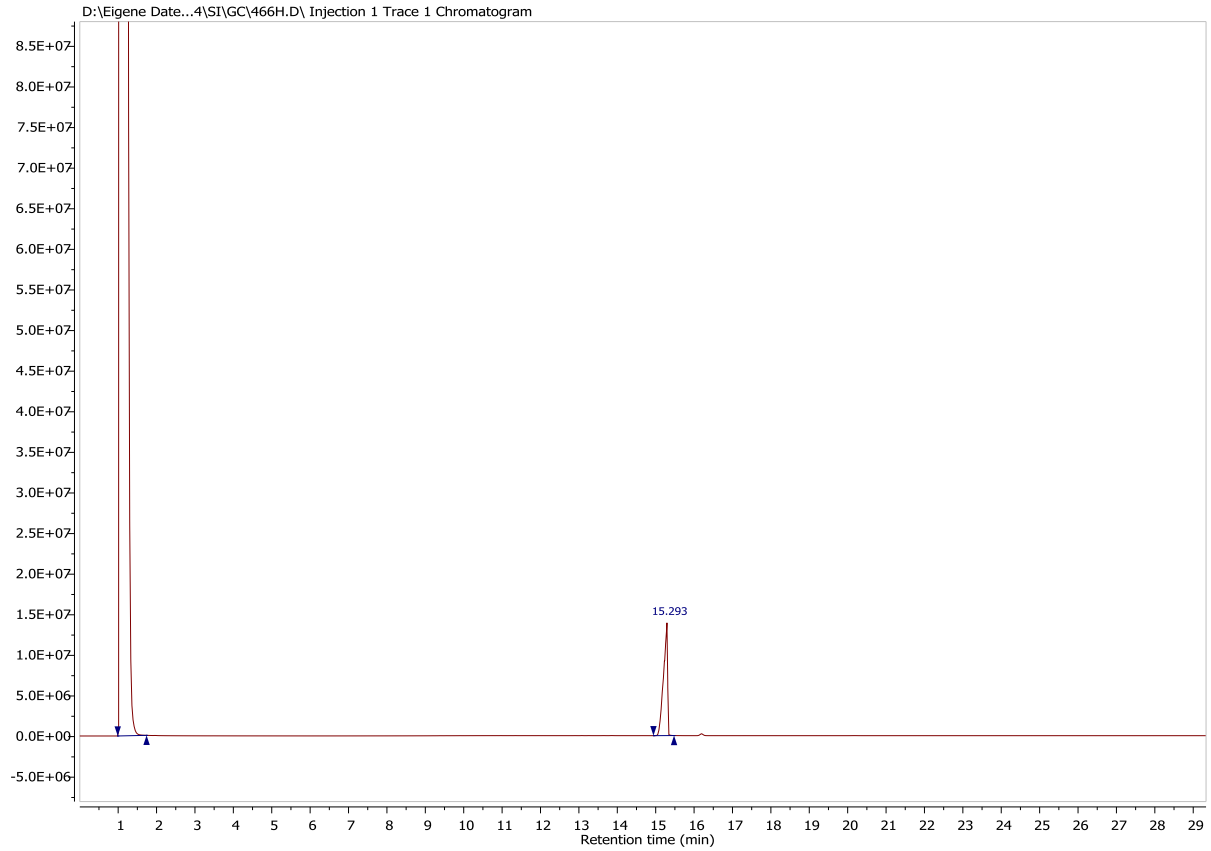
GC method: Inlet: 300 °C, carrier gas N_2, Split ratio 2.5/1, Flow: 4.5mL/min, column flow: 1.8 mL/min; oven: 150 °C (0m)-10 °C/min -> 200 °C (1min) – 30 °C/min -> 300 °C(20min) (Run Time 29.33 min)
column: HP-35, 30 m x 0.25 mm x 0.25 µm
For the dichlorosilanes, a calibration line was prepared according to the usual method of the internal standard. The internal standard used, was *n*-tetradecane.

substance	t_r [min]
ntetradecane	1.9
BIFOL **5**	15.3
BIFOXSiCl_2 **7**	23.2
BIFOXSiCl(OH) **8**	25.8
BIFOXSi$(OH)_2$ **9**	24.5
dichlorobis(2,4,6-tri-*tert*-butylphenoxy)silane **14**	11.4
bis(2,4,6-tri-*tert*-butylphenoxy)silandiol **15**	11.7

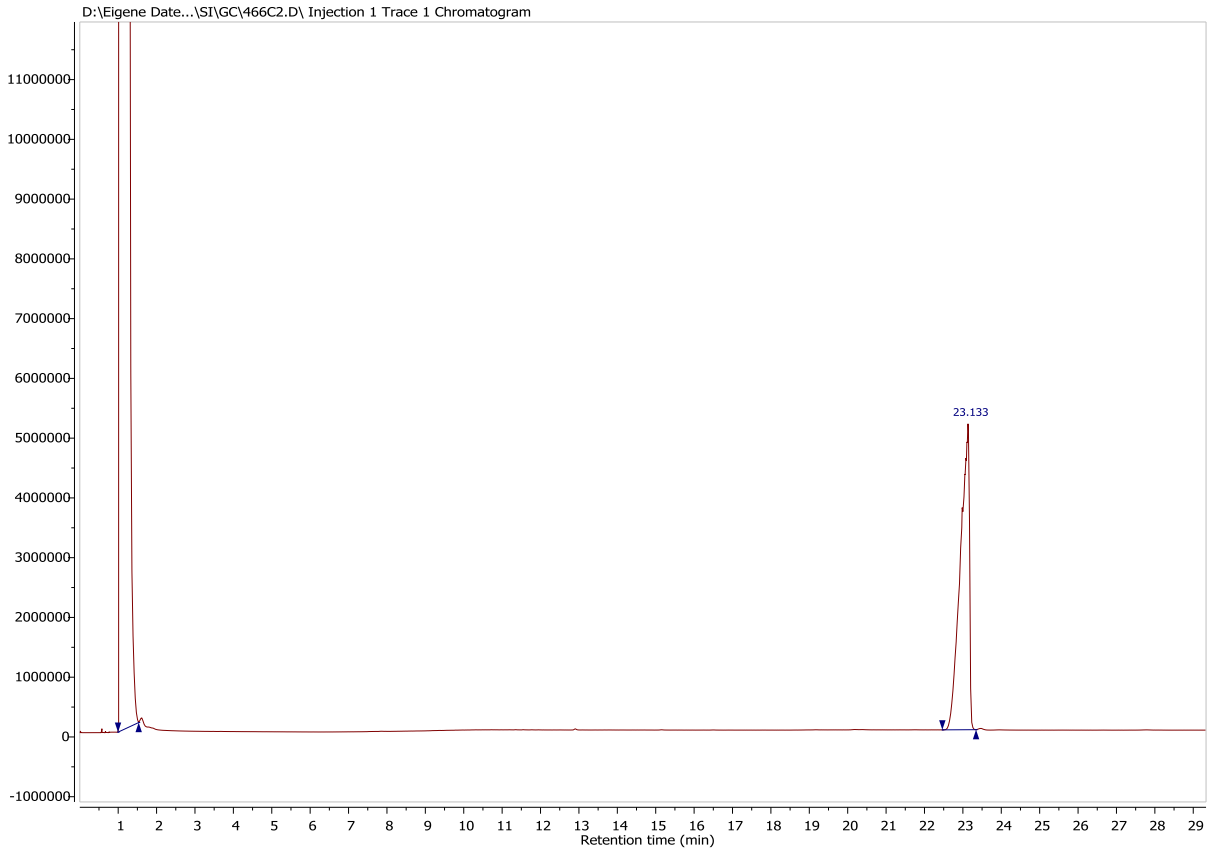
n-tetradecane



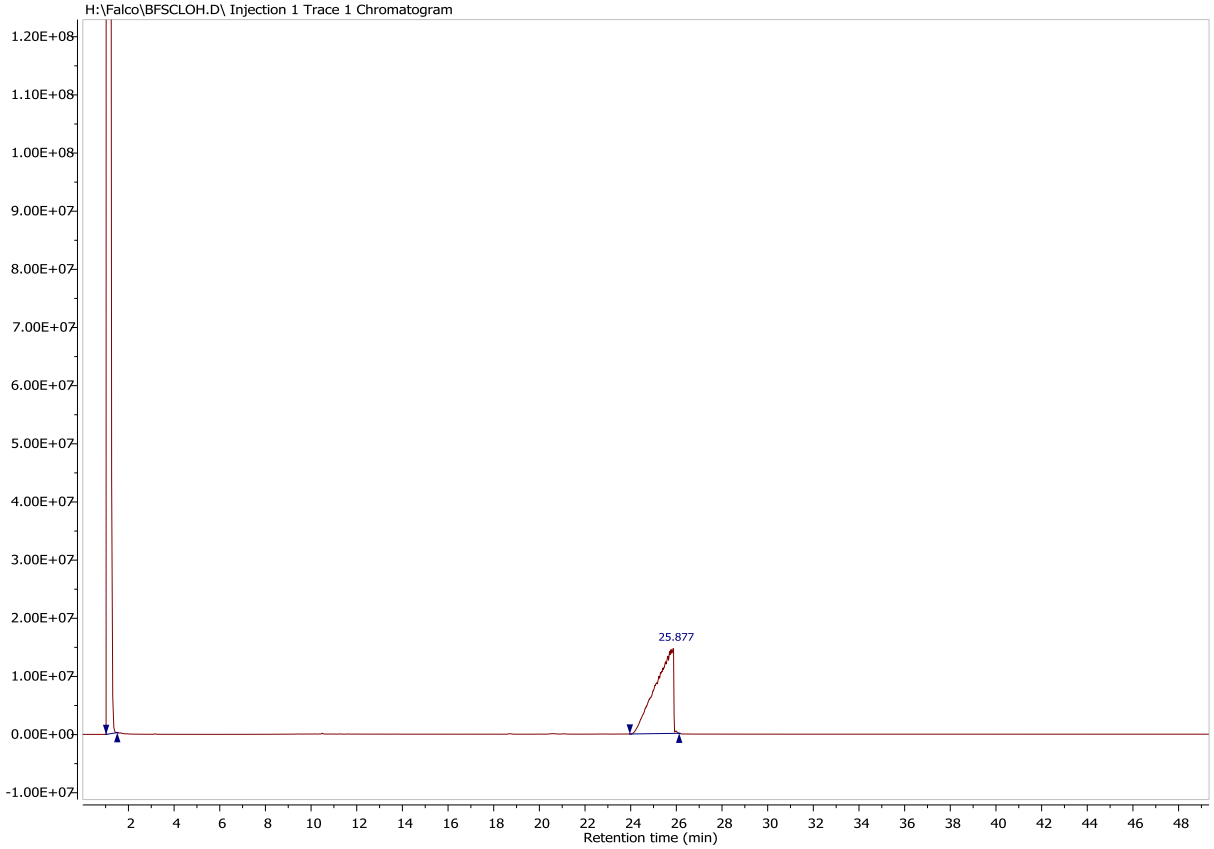
BIFOL **5**



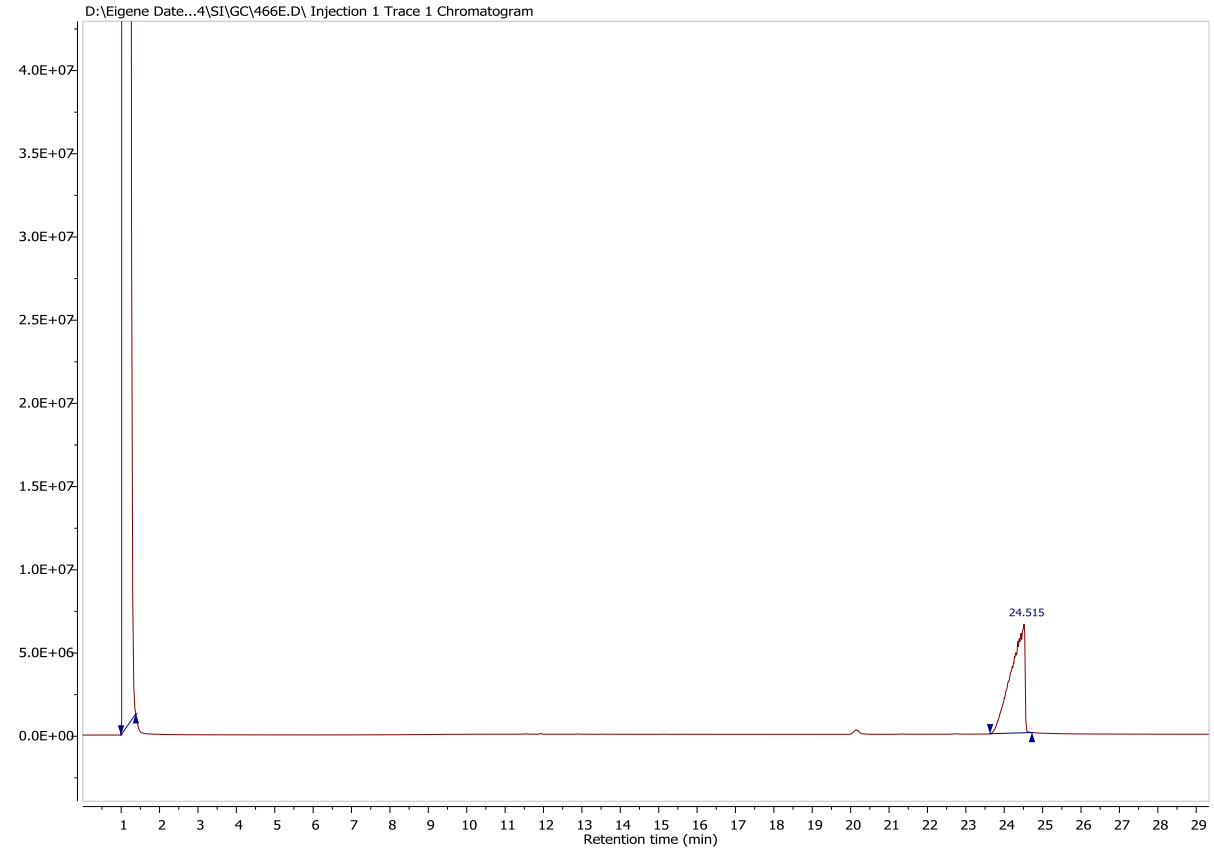
BIFOXSiCl$_2$ **7**



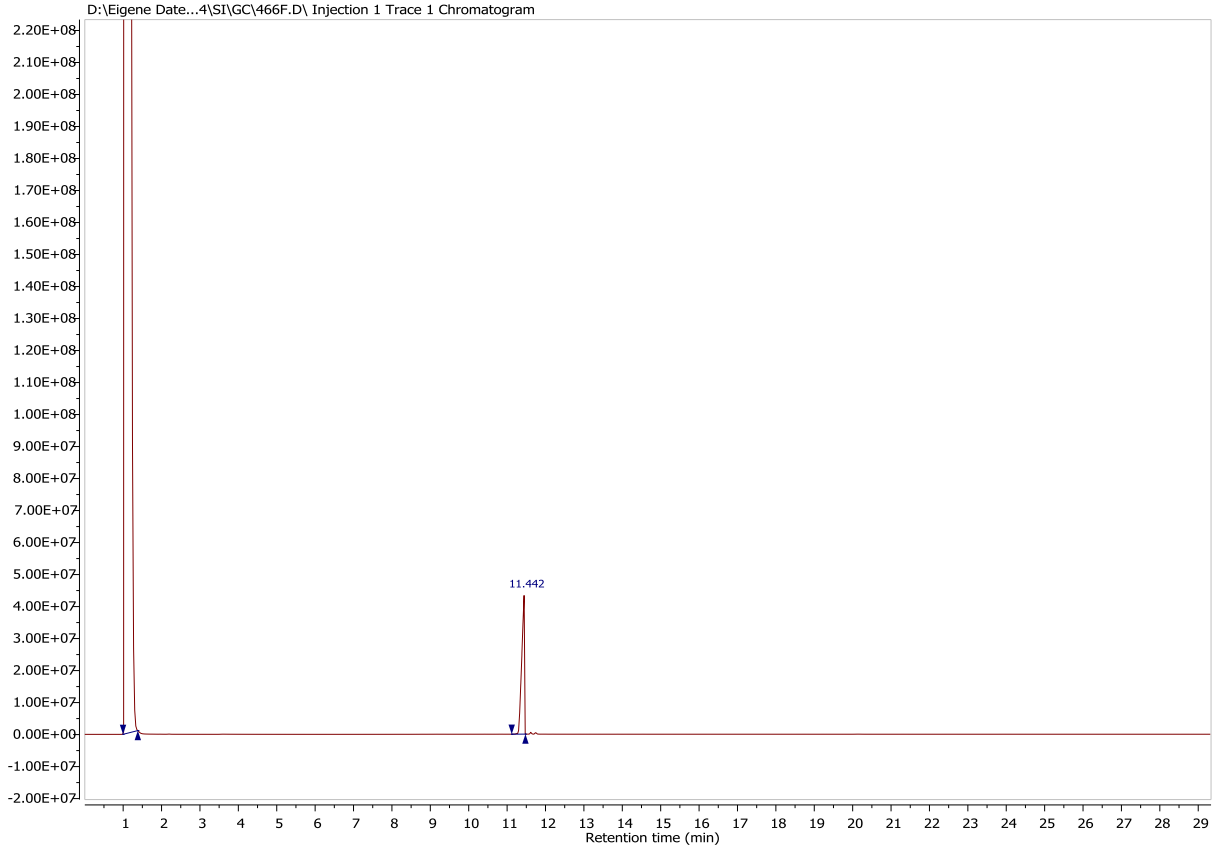
BIFOXSiCl(OH) **8**



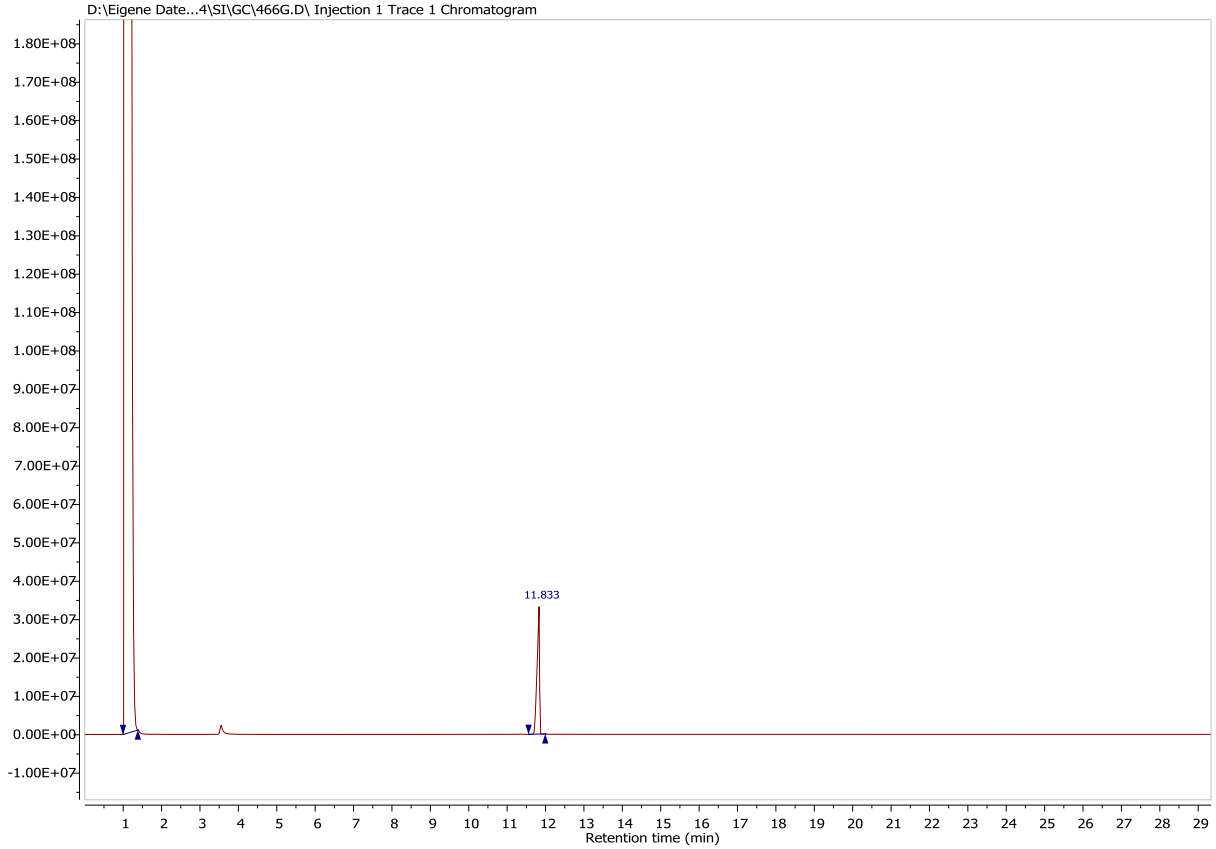
BIFOXSi(OH)$_2$ **9**



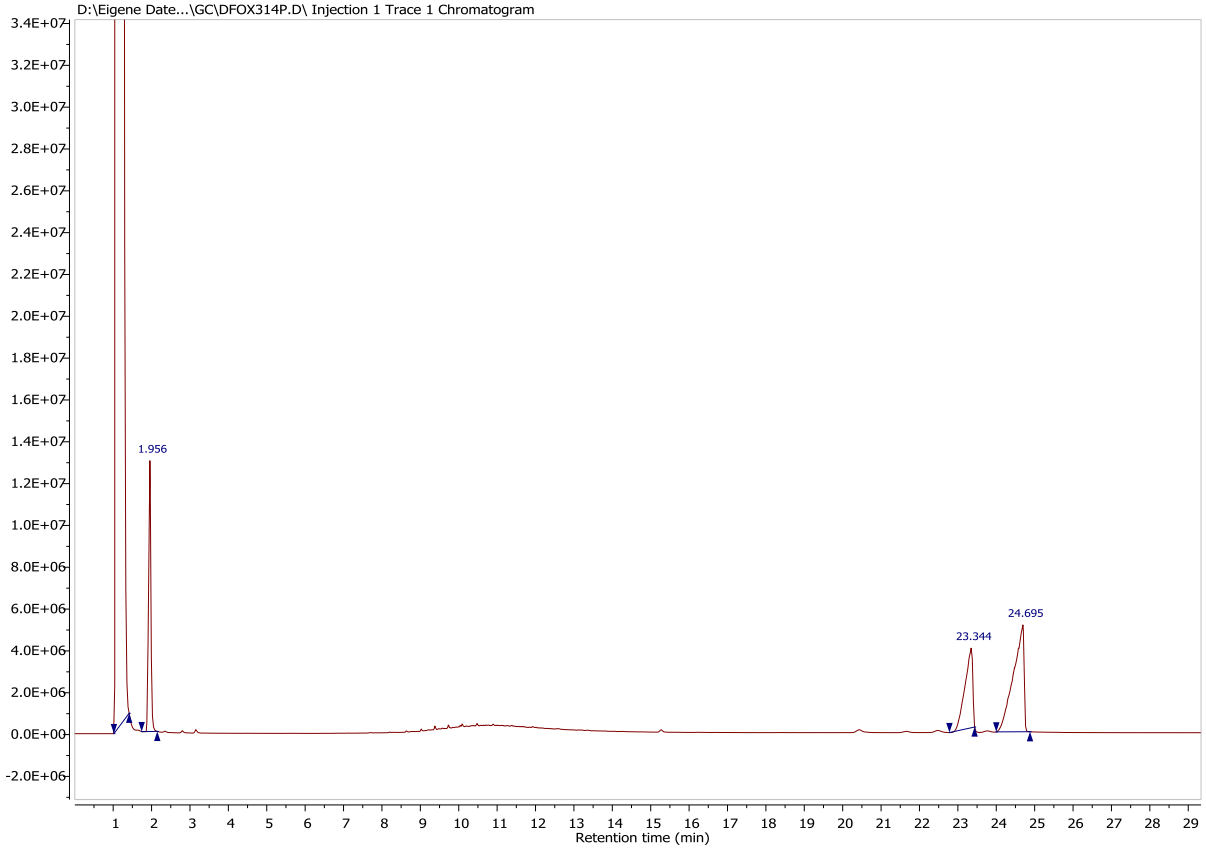
dichlorobis(2,4,6-tri-*tert*-butylphenoxy)silane (**14**)



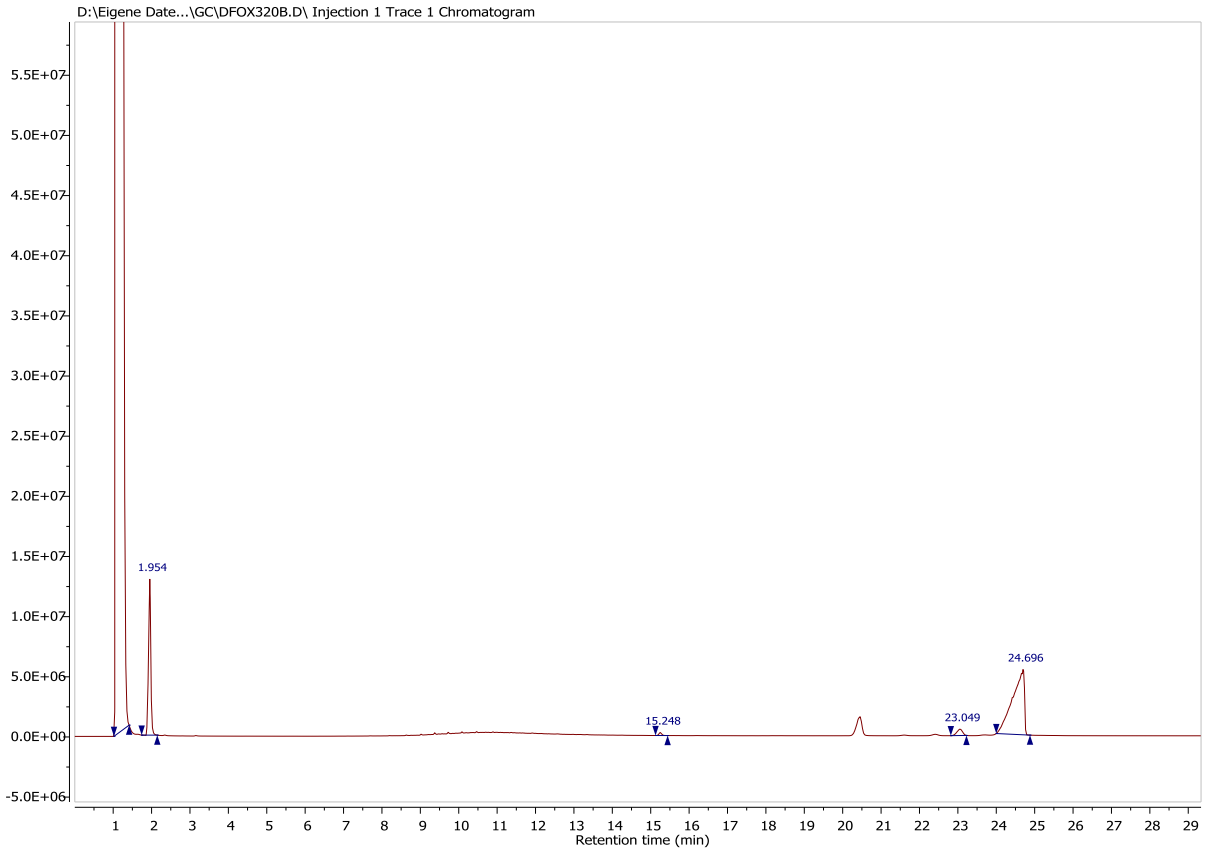
bis(2,4,6-tri-*tert*-butylphenoxy)silandiol (**15**)



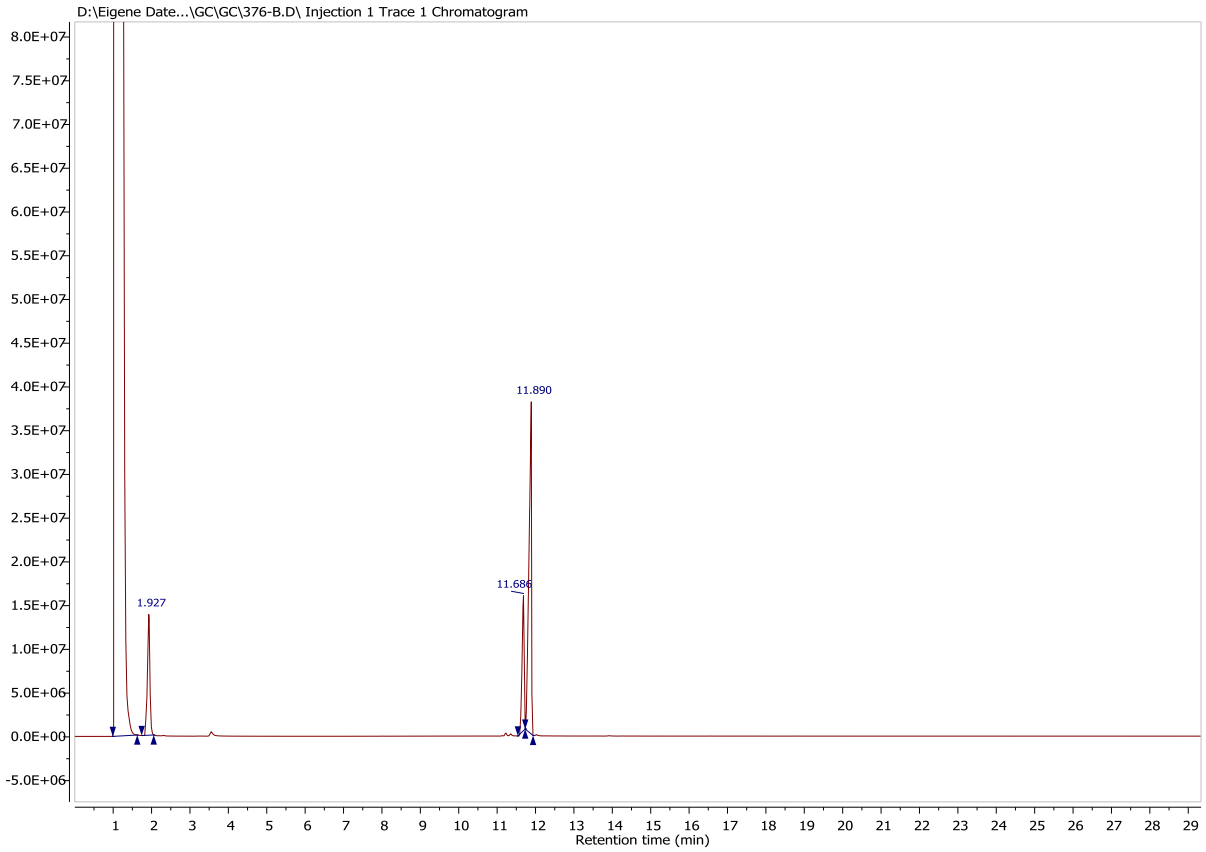
example for $BIFOXSiCl_2$ **7** to $BIFOXSi(OH)_2$ **9** in THF/H_2O reflux 10h



example for $BIFOXSiCl_2$ **7** to $BIFOXSi(OH)_2$ **9** in THF/H_2O/KOH reflux 10 h



example for dichlorobis(2,4,6-tri-*tert*-butylphenoxy)silane (**14**)
to bis(2,4,6-tri-*tert*-butylphenoxy)silandiol (**15**) in THF/H_2O reflux 30 min



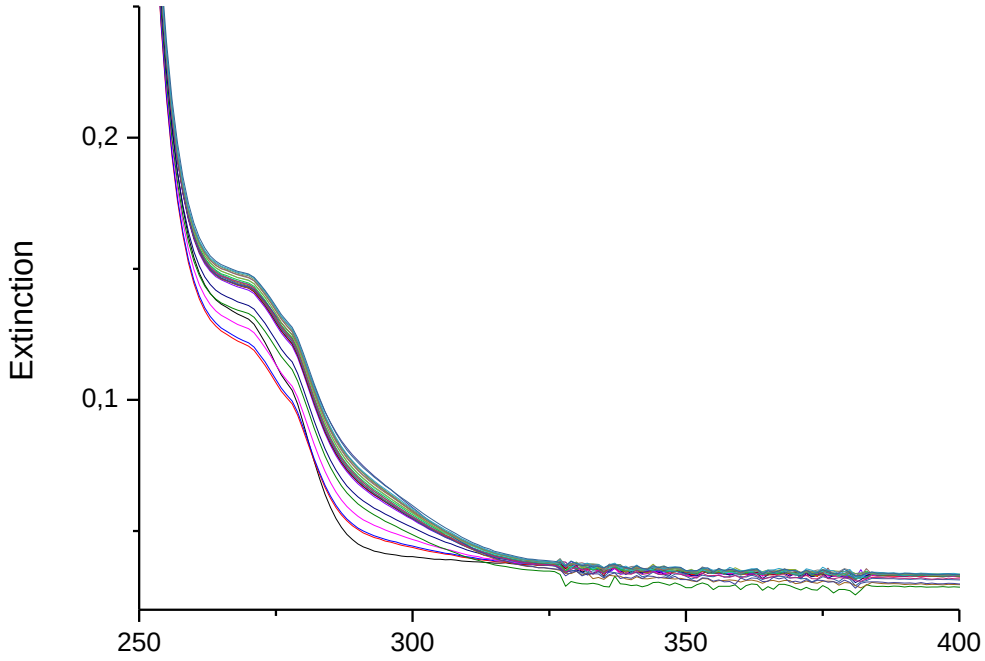
6. **General procedure for UV–vis titration**

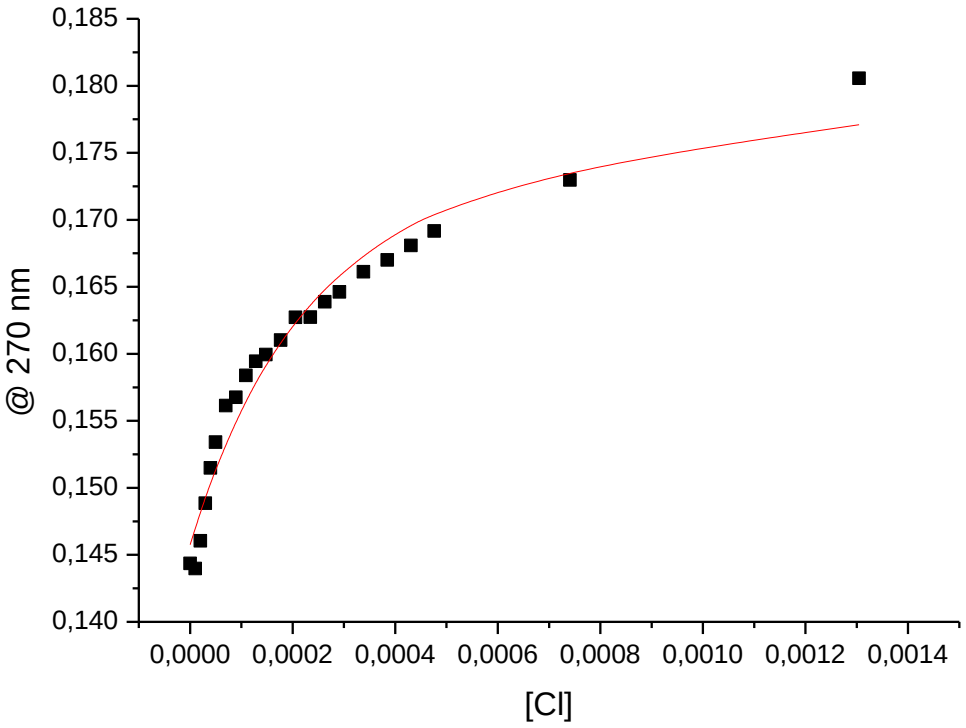
Stock solutions of the employed compounds with a concentration of 1×10^{-2} M in dry HPLC-grade chloroform were prepared. The examined anion Cl^- was employed as the *tert*-butylammonium salt and stock solution with a concentration of 1×10^{-2} M was prepared. The appropriate amount of anion stock solution was added between UV/Vis-measurements. The measurements were recorded on a Perkin Elmer Lambda35 spectrometer featuring a double-beam and all-reflecting system. A deuterium (UV) and a halogen (Vis) lamp, which automatically change at a wavelength of 326 nm, are used to cover the spectral range.

1) BIFOXSi(OH)$_2$ **9**

K	K error (%)	SSR	Data points fitted	Params fitted	H coeffs	HG coeffs	Raw coeffs 1	Raw coeffs 2
5274,85	13,93	6,4424E-05	22	3	1457,62	1819,75	1457,62	1819,75

RMS: 270.0	0,00171124
RMS: Total	0,00171124
Covariance: 270.0	0,03495925
Covariance: Total	0,03495925

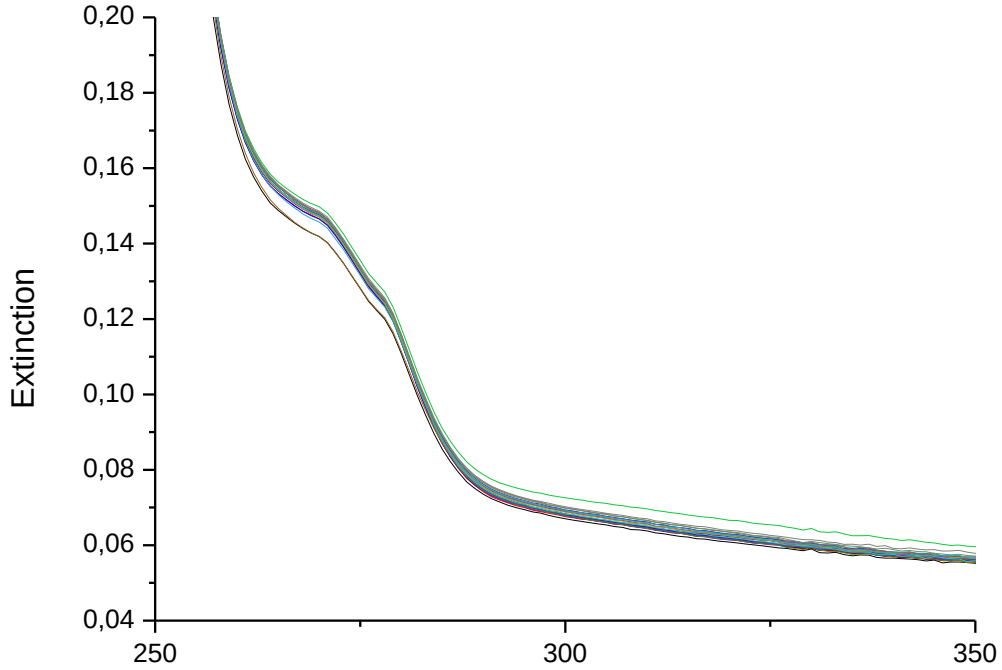


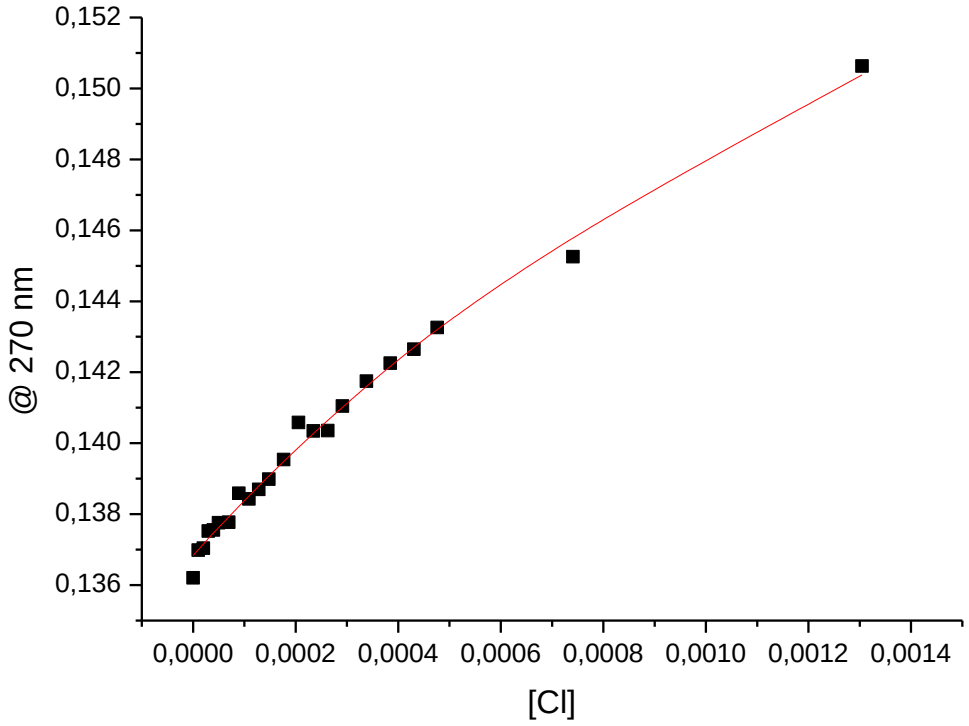


2) BIFOXSiCl(OH) **8**

K	K error (%)	SSR	Data points fitted	Params fitted	H coeffs	HG coeffs	Raw coeffs 1	Raw coeffs 2
451,10	4,10	1,7963E-06	22	3	1368,37	1740,62	1368,37	1740,62

RMS: 270.0	0,00028575
RMS: Total	0,00028575
Covariance: 270.0	0,00782941
Covariance: Total	0,00782941

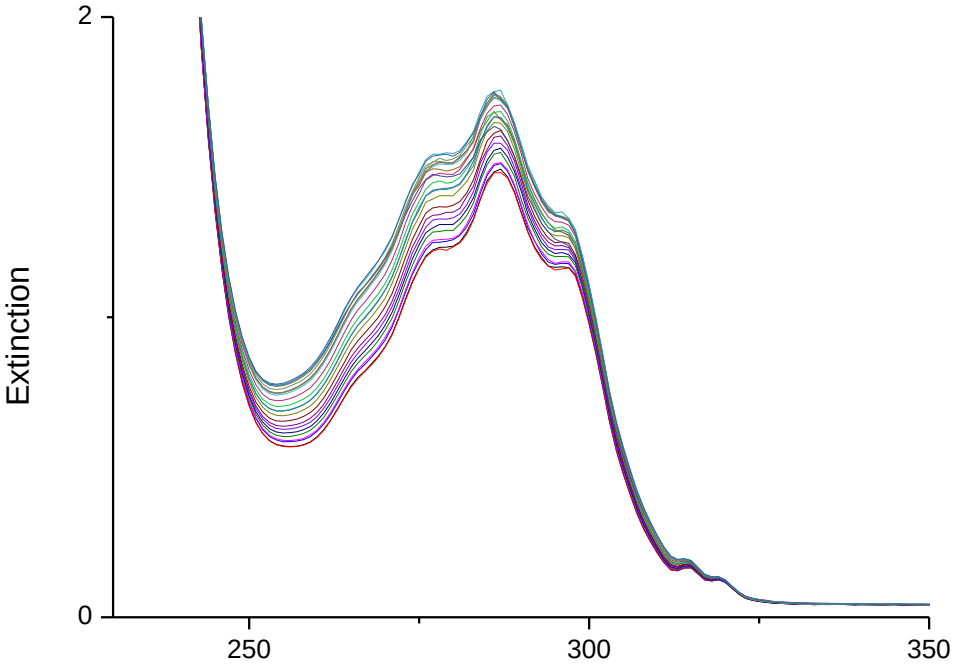


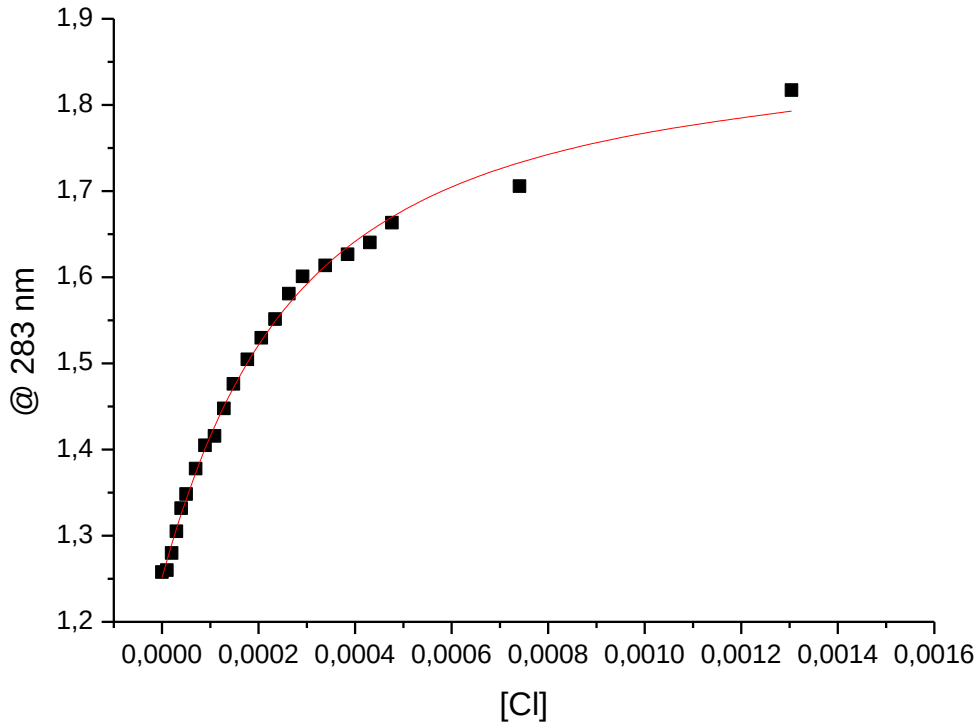


3) Kondo **1**

K	K error (%)	SSR	Data points fitted	Params fitted	H coeffs	HG coeffs	Raw coeffs 1	Raw coeffs 2
4688,04	4,96	0,00255167	22	3	12512,08	18875,09	12512,08	18875,09

RMS: 283.0	0,01076964
RMS: Total	0,01076964
Covariance: 283.0	0,00487214
Covariance: Total	0,00487214


Extinction
2
0
250
300
350


@ 283 nm
1,9
1,8
1,7
1,6
1,5
1,4
1,3
1,2
0,0000
0,0002
0,0004
0,0006
0,0008
0,0010
0,0012
0,0014
0,0016
[Cl]

7. **Computational details**

Computational details: In this work computations were performed using GAUSSIAN09[5]. Geometry optimizations were performed at the B3LYP-D3BJ/6-31G(d) level of theory. Zero-point energies were scaled by 0.96[6]. Frequency computations were performed at the M06-2X-D3/6-311++G(d,p) level of theory using the SCRF method with THF as solvent.

a. BIFOXSi derivatives

BIFOXSiCl_2 **7**

HF=-2603.7857186
Thermal correction to Gibbs Free Energy= 0.574622
NImag=0

1	17	0	0.516141	-2.107481	2.240961
2	14	0	0.033856	-1.590143	0.305178
3	1	0	2.940397	-2.745736	1.095431
4	17	0	-0.105566	-3.384988	-0.727559
5	8	0	-1.395317	-0.875870	0.508842
6	8	0	1.078348	-0.705556	-0.576413
7	6	0	3.609250	-1.885418	1.173689
8	1	0	-2.677805	-2.686673	-0.230420
9	6	0	-2.253639	0.016389	-0.195509
10	6	0	2.233556	0.055490	-0.151983
11	6	0	3.460861	-0.961795	-0.038686
12	1	0	3.422404	-1.420583	2.139770
13	1	0	4.632826	-2.278859	1.179029
14	6	0	-3.486864	-2.146637	-0.713262
15	6	0	-1.469470	1.266953	-0.632100
16	6	0	-3.028591	-0.781712	-1.321394
17	6	0	-3.457400	0.416064	0.819083
18	6	0	1.766283	0.798365	1.116305
19	6	0	2.737556	1.022597	-1.341862
20	6	0	4.662867	-0.056575	-0.381585
21	6	0	3.439236	-1.855120	-1.323442
22	6	0	-4.639509	-1.788329	0.260863
23	1	0	-3.844610	-2.775033	-1.535642
24	6	0	-0.408018	1.856520	0.104746
25	6	0	-1.980289	2.007746	-1.713486
26	6	0	-4.408355	-0.072274	-1.351420

27	6	0	-2.280229	-1.007032	-2.633444
28	6	0	-4.694576	-0.256763	0.148809
29	6	0	-3.188645	-0.079746	2.245954
30	6	0	-3.723420	1.930799	0.907867
31	6	0	0.450701	1.347494	1.250183
32	6	0	2.620381	0.888447	2.220801
33	6	0	4.110507	0.402236	-1.740873
34	6	0	1.746434	1.099432	-2.509232
35	6	0	3.039676	2.453770	-0.862473
36	1	0	4.842372	0.755224	0.326799
37	1	0	5.586481	-0.639912	-0.469855
38	6	0	3.930859	-0.936788	-2.467655
39	1	0	2.456522	-2.285779	-1.506488
40	1	0	4.132959	-2.686547	-1.160828
41	1	0	-5.589840	-2.219346	-0.072656
42	1	0	-4.466080	-2.145311	1.277791
43	6	0	-0.097060	3.206811	-0.160169
44	6	0	-1.576292	3.300427	-2.025329
45	1	0	-2.757810	1.577068	-2.321915
46	1	0	-4.406812	0.968800	-1.671764
47	1	0	-5.117892	-0.616211	-1.985673
48	1	0	-1.405574	-1.644669	-2.474419
49	1	0	-1.931006	-0.090061	-3.109257
50	1	0	-2.933313	-1.528412	-3.342618
51	1	0	-5.631606	0.178958	0.509362
52	1	0	-2.337833	0.445951	2.686322
53	1	0	-2.960491	-1.143418	2.292750
54	1	0	-4.070072	0.115119	2.868634
55	1	0	-4.552595	2.100518	1.603944
56	1	0	-3.997772	2.376740	-0.050513
57	1	0	-2.853660	2.477359	1.282037
58	6	0	0.044617	1.794346	2.516107
59	1	0	3.647387	0.567757	2.116352
60	6	0	2.200493	1.359529	3.462669
61	1	0	4.725125	1.122557	-2.289124
62	1	0	0.862645	1.680017	-2.241907
63	1	0	1.405800	0.114417	-2.830268
64	1	0	2.229341	1.593798	-3.361076
65	1	0	3.497460	3.010338	-1.688373
66	1	0	3.730819	2.484861	-0.016692
67	1	0	2.137682	2.982967	-0.573823
68	1	0	4.889395	-1.279876	-2.872530
69	1	0	3.230718	-0.878120	-3.303386
70	1	0	0.621587	3.690720	0.491870

71	6	0	-0.655910	3.934904	-1.202022
72	1	0	-2.015349	3.811401	-2.877174
73	6	0	0.883507	1.770335	3.626938
74	1	0	-0.948828	2.220849	2.611159
75	1	0	2.900062	1.387412	4.292923
76	1	0	-0.364113	4.967716	-1.366690
77	1	0	0.521956	2.116583	4.590628

BIFOXSiCl$_2$ **7** to BIFOXSiCl(OH) **8$_{ax}$** TS$_{front1}$ **7**

HF =-2680.1774268
Thermal correction to Gibbs Free Energy= 0.594561
NImag=1
Frequencies -- -221.4407 Hz

1	17	0	0.416731	-1.067098	2.744203
2	14	0	-0.013824	-1.557411	0.220395
3	1	0	2.823176	-2.200271	2.023649
4	17	0	-0.384123	-2.841157	-1.456155
5	8	0	-1.405572	-0.818768	0.544465
6	8	0	1.224974	-0.788050	-0.446024
7	6	0	3.547342	-1.398530	1.867665
8	1	0	-2.775585	-2.672825	0.196293
9	6	0	-2.338413	0.028661	-0.145596
10	6	0	2.337454	0.048295	-0.099013
11	6	0	3.515598	-0.905529	0.420517
12	1	0	3.336557	-0.641538	2.619417
13	1	0	4.543809	-1.814031	2.063030
14	6	0	-3.669867	-2.136500	-0.114169
15	6	0	-1.573477	1.115939	-0.922232
16	6	0	-3.356915	-0.882529	-0.984075
17	6	0	-3.310997	0.663986	0.982104
18	6	0	1.790742	1.128681	0.847582
19	6	0	2.976298	0.626467	-1.467279
20	6	0	4.777599	-0.176353	-0.094209
21	6	0	3.559273	-2.150969	-0.523622
22	6	0	-4.512064	-1.597869	1.072737
23	1	0	-4.258161	-2.824534	-0.729609
24	6	0	-0.396432	1.797005	-0.491668
25	6	0	-2.199456	1.591745	-2.089351
26	6	0	-4.706647	-0.145280	-0.794268
27	6	0	-3.005054	-1.256042	-2.438147
28	6	0	-4.644044	-0.099013	0.735869

29	6	0	-2.772073	0.490523	2.405981
30	6	0	-3.582804	2.167434	0.771697
31	6	0	0.477945	1.685325	0.756142
32	6	0	2.620163	1.582156	1.880239
33	6	0	4.331215	-0.132959	-1.564038
34	6	0	2.070323	0.411733	-2.686572
35	6	0	3.315497	2.126187	-1.383619
36	1	0	4.957034	0.805056	0.349414
37	1	0	5.674729	-0.785966	0.063369
38	6	0	4.122748	-1.624977	-1.866275
39	1	0	2.591506	-2.639073	-0.626589
40	1	0	4.240894	-2.879224	-0.071157
41	1	0	-5.502031	-2.066267	1.097953
42	1	0	-4.046311	-1.778551	2.043276
43	6	0	-0.016518	2.948040	-1.214982
44	6	0	-1.754894	2.683656	-2.822583
45	1	0	-3.097593	1.105206	-2.430718
46	1	0	-4.762942	0.833259	-1.273071
47	1	0	-5.536633	-0.752091	-1.174934
48	1	0	-2.003942	-0.941883	-2.733206
49	1	0	-3.712998	-0.804680	-3.142966
50	1	0	-3.052089	-2.338128	-2.580191
51	1	0	-5.484449	0.390313	1.237792
52	1	0	-1.853807	1.058897	2.557877
53	1	0	-2.532886	-0.542344	2.649557
54	1	0	-3.524323	0.853288	3.117513
55	1	0	-4.290921	2.505176	1.536722
56	1	0	-4.009822	2.401957	-0.205205
57	1	0	-2.674758	2.763716	0.870217
58	6	0	0.063437	2.547420	1.783480
59	1	0	3.642634	1.234664	1.919006
60	6	0	2.186466	2.447599	2.879024
61	1	0	5.015676	0.364586	-2.257964
62	1	0	1.190366	1.056456	-2.640075
63	1	0	1.718029	-0.616218	-2.773177
64	1	0	2.626368	0.666790	-3.597118
65	1	0	3.863842	2.412170	-2.288607
66	1	0	3.936574	2.381531	-0.522488
67	1	0	2.420356	2.739310	-1.336348
68	1	0	5.079860	-2.099231	-2.109766
69	1	0	3.452191	-1.801252	-2.709547
70	1	0	0.803666	3.533495	-0.819109
71	6	0	-0.651914	3.391676	-2.366394
72	1	0	-2.290395	2.987745	-3.717201

73	6	0	0.875781	2.903595	2.855219
74	1	0	-0.919588	2.996602	1.707296
75	1	0	2.869514	2.747571	3.668359
76	1	0	-0.296381	4.281211	-2.877939
77	1	0	0.497079	3.565659	3.628313
78	8	0	0.254825	-3.122875	1.163240
79	1	0	-0.300479	-3.882613	0.898929
80	1	0	0.229753	-2.799757	2.152212

BIFOXSiCl$_2$ **7** to BIFOXSiCl(OH) **8$_{eq}$** TS$_{front2}$ **7**

HF= -2680.172952
Thermal correction to Gibbs Free Energy= 0.594578
NImag=1
Frequencies -- -206.2297

1	8	0	1.399738	-0.753786	0.329382
2	8	0	-1.170442	-0.646519	-0.634608
3	6	0	2.257166	0.254004	-0.202464
4	6	0	-2.313276	0.076027	-0.152493
5	6	0	-1.855364	0.813108	1.121051
6	6	0	-2.724688	0.891242	2.214788
7	6	0	-2.321538	1.335065	3.471909
8	6	0	-1.003409	1.729228	3.662751
9	6	0	-0.155500	1.782712	2.559836
10	6	0	-0.548352	1.372737	1.276995
11	1	0	-3.752376	0.580202	2.090505
12	1	0	-3.033821	1.353222	4.291557
13	1	0	-0.650093	2.050050	4.638158
14	1	0	2.115507	0.367679	2.721030
15	6	0	-3.539755	-0.960427	-0.023685
16	6	0	-2.846743	1.046412	-1.333430
17	6	0	-3.515829	-1.877521	-1.285146
18	6	0	-4.750892	-0.078324	-0.403968
19	6	0	-4.184234	0.374883	-1.758126
20	6	0	-3.948086	-0.970607	-2.462502
21	1	0	-2.550459	-2.366984	-1.423814
22	1	0	-4.241520	-2.681039	-1.123818
23	1	0	-4.957053	0.737759	0.291106
24	1	0	-5.662341	-0.679620	-0.498379
25	1	0	-4.809811	1.062678	-2.334341
26	1	0	-3.206034	-0.906428	-3.261797
27	1	0	-4.876216	-1.331309	-2.918277

28	6	0	3.156419	-0.353508	-1.364016
29	6	0	3.363801	0.567819	0.945346
30	6	0	3.613404	-1.775397	-0.919013
31	6	0	4.505597	0.390042	-1.169762
32	6	0	4.669258	0.004926	0.308916
33	6	0	4.641861	-1.530492	0.215174
34	1	0	2.792240	-2.414982	-0.608707
35	1	0	4.088757	-2.255125	-1.781801
36	1	0	4.492199	1.466055	-1.343556
37	1	0	5.282684	-0.042862	-1.810140
38	1	0	5.559311	0.401830	0.807333
39	1	0	4.362247	-2.018956	1.149836
40	1	0	5.634106	-1.904801	-0.059156
41	6	0	-3.716765	-1.861809	1.204858
42	1	0	-3.490486	-1.393504	2.159673
43	1	0	-4.759945	-2.200160	1.230781
44	1	0	-3.090498	-2.753323	1.133176
45	6	0	-3.206653	2.459891	-0.837302
46	1	0	-3.783670	2.971405	-1.616287
47	1	0	-3.804897	2.459615	0.075940
48	1	0	-2.316804	3.053197	-0.650810
49	6	0	-1.847020	1.196928	-2.486516
50	1	0	-0.900019	3.693391	0.589488
51	1	0	-1.515889	0.238344	-2.888353
52	1	0	-2.316030	1.762939	-3.300496
53	6	0	3.569118	2.071581	1.211858
54	1	0	4.334628	2.187952	1.987166
55	1	0	3.902303	2.625376	0.331337
56	1	0	2.655870	2.554444	1.568303
57	6	0	3.008279	-0.087846	2.286152
58	1	0	0.831790	2.216539	2.676035
59	1	0	2.809085	-1.154769	2.201039
60	1	0	3.839826	0.056354	2.986486
61	6	0	1.437690	1.511099	-0.545150
62	6	0	1.977185	2.378857	-1.514612
63	6	0	0.297341	1.973457	0.164499
64	6	0	1.496312	3.656741	-1.768561
65	1	0	2.840182	2.062172	-2.075380
66	6	0	-0.109130	3.309806	-0.044730
67	6	0	0.454324	4.149590	-0.994518
68	1	0	1.965392	4.266105	-2.535520
69	1	0	-0.955772	1.739212	-2.167803
70	1	0	0.086646	5.164090	-1.116074
71	6	0	2.568241	-0.415989	-2.774491

72	1	0	3.358319	-0.702889	-3.478353
73	1	0	1.789369	-1.178654	-2.829898
74	1	0	2.132639	0.519818	-3.125989
75	8	0	0.183465	-2.287374	-1.632235
76	1	0	0.460237	-3.262652	-1.434132
77	1	0	-0.656751	-2.190215	-2.119243
78	17	0	0.954802	-4.081949	0.144539
79	14	0	0.025023	-1.532485	0.085809
80	17	0	-0.615262	-2.024011	1.987794

BIFOXSiCl$_2$ **7** to BIFOXSiCl(OH) **8$_{eq}$** TS$_{side}$ **7**

HF=-2680.1727746
Thermal correction to Gibbs Free Energy= 0.596455
NImag=1
Frequencies -- -189.6553

1	17	0	0.642859	-2.133150	1.937293
2	14	0	-0.038703	-1.568625	0.075775
3	1	0	3.008919	-2.878636	0.908728
4	8	0	-1.409755	-0.773095	0.354003
5	8	0	1.093959	-0.609169	-0.640155
6	6	0	3.670902	-2.017038	1.012233
7	1	0	-2.863777	-2.361690	-0.646065
8	6	0	-2.204340	0.280383	-0.180579
9	6	0	2.279519	0.048408	-0.161017
10	6	0	3.478628	-1.024280	-0.140766
11	1	0	3.511185	-1.610266	2.008535
12	1	0	4.699636	-2.394442	0.961836
13	6	0	-3.631364	-1.672288	-0.985398
14	6	0	-1.341422	1.515952	-0.492555
15	6	0	-3.079270	-0.270738	-1.382307
16	6	0	-3.336844	0.626002	0.928246
17	6	0	1.875439	0.722591	1.165251
18	6	0	2.812648	1.078395	-1.291551
19	6	0	4.705850	-0.149423	-0.477515
20	6	0	3.384214	-1.842354	-1.468426
21	6	0	-4.690649	-1.391571	0.109661
22	1	0	-4.097732	-2.107857	-1.876450
23	6	0	-0.247370	1.969681	0.290334
24	6	0	-1.799288	2.380709	-1.504591
25	6	0	-4.396509	0.538166	-1.238457
26	6	0	-2.385484	-0.311607	-2.759602

27	6	0	-4.641921	0.141687	0.226359
28	6	0	-3.061431	-0.075303	2.264359
29	6	0	-3.481477	2.131735	1.221199
30	6	0	0.588545	1.312310	1.373906
31	6	0	2.761262	0.710040	2.246947
32	6	0	4.130642	0.414160	-1.784120
33	6	0	1.803695	1.314694	-2.420630
34	6	0	3.212033	2.448315	-0.712235
35	1	0	4.948602	0.606135	0.272890
36	1	0	5.597221	-0.767694	-0.633477
37	6	0	3.858359	-0.872257	-2.578257
38	1	0	2.385055	-2.240103	-1.638291
39	1	0	4.062895	-2.696898	-1.379796
40	1	0	-5.687820	-1.711027	-0.211533
41	1	0	-4.473085	-1.907470	1.045760
42	6	0	0.146251	3.317158	0.145802
43	6	0	-1.319044	3.670422	-1.698276
44	1	0	-2.590894	2.054124	-2.158582
45	1	0	-4.313778	1.613651	-1.393561
46	1	0	-5.167925	0.156187	-1.917110
47	1	0	-1.363774	0.086853	-2.729953
48	1	0	-2.915518	0.286141	-3.508325
49	1	0	-2.365239	-1.333912	-3.159434
50	1	0	-5.531258	0.577597	0.691627
51	1	0	-2.161460	0.327989	2.735372
52	1	0	-2.910037	-1.148412	2.159875
53	1	0	-3.906695	0.095281	2.941874
54	1	0	-4.286889	2.270026	1.951111
55	1	0	-3.728519	2.722878	0.336471
56	1	0	-2.568545	2.555162	1.646745
57	6	0	0.226357	1.671469	2.679590
58	1	0	3.774303	0.366935	2.090519
59	6	0	2.389279	1.100838	3.531722
60	1	0	4.761264	1.132862	-2.316265
61	1	0	0.947741	1.894539	-2.074939
62	1	0	1.425446	0.381270	-2.840390
63	1	0	2.288836	1.878219	-3.227017
64	1	0	3.709274	3.030859	-1.496567
65	1	0	3.899843	2.371018	0.132279
66	1	0	2.347120	3.015570	-0.384016
67	1	0	4.781878	-1.227187	-3.048833
68	1	0	3.125454	-0.737519	-3.377191
69	1	0	0.895910	3.692640	0.833347
70	6	0	-0.365392	4.170709	-0.822181

71	1	0	-1.721862	4.280686	-2.501300
72	6	0	1.089681	1.532879	3.763788
73	1	0	-0.746708	2.126380	2.833747
74	1	0	3.111351	1.048041	4.341300
75	1	0	-0.010148	5.194260	-0.893360
76	1	0	0.762716	1.813527	4.760573
77	17	0	-1.184505	-4.018216	0.159299
78	8	0	-0.201100	-2.348866	-1.631310
79	1	0	-0.534304	-1.728864	-2.309885
80	1	0	-0.802679	-3.162915	-1.459060

BIFOXSiCl(OH) **8_{ax}**

HF=-2219.4193095
Thermal correction to Gibbs Free Energy= 0.587261
NImag=0

1	1	0	-5.530435	-2.302116	0.280819
2	6	0	-4.597425	-1.796562	0.552854
3	1	0	-4.444923	-1.958600	1.621558
4	6	0	-3.410765	-2.298644	-0.310725
5	6	0	-4.675145	-0.310942	0.164994
6	1	0	-3.734540	-3.066107	-1.021709
7	1	0	-2.611412	-2.731584	0.282681
8	6	0	-2.949452	-1.052097	-1.132298
9	6	0	-4.337812	-0.389169	-1.333479
10	1	0	-5.631625	0.160364	0.412384
11	6	0	-3.474009	0.497774	0.744298
12	17	0	-0.049955	-3.500260	0.083796
13	6	0	-2.224826	-0.057450	-0.136064
14	6	0	-2.148592	-1.482404	-2.359049
15	1	0	-4.342960	0.579147	-1.832805
16	1	0	-5.014721	-1.052452	-1.884349
17	6	0	-3.762228	1.998074	0.549521
18	6	0	-3.259849	0.273244	2.247046
19	14	0	0.061456	-1.519559	0.675865
20	1	0	-1.257523	-2.045199	-2.064381
21	8	0	-1.385899	-0.790856	0.745063
22	6	0	-1.441626	1.110389	-0.764845
23	1	0	-2.758828	-2.147587	-2.980656
24	1	0	-1.813854	-0.652325	-2.982899
25	1	0	-4.609630	2.278032	1.185705
26	1	0	-4.020165	2.256999	-0.479551

27	1	0	-2.907891	2.618400	0.834861
28	1	0	-2.465995	0.922515	2.626844
29	1	0	-2.978491	-0.750734	2.487776
30	1	0	-4.182878	0.519048	2.785687
31	8	0	1.032129	-0.789861	-0.430353
32	8	0	0.578593	-1.617209	2.230884
33	6	0	-0.393718	1.817001	-0.119691
34	6	0	-1.931212	1.661738	-1.962194
35	6	0	2.209204	-0.026566	-0.088327
36	1	0	0.507567	-0.778743	2.712945
37	6	0	0.446380	1.488084	1.098606
38	6	0	-0.071112	3.104553	-0.594317
39	1	0	-2.695026	1.134141	-2.509007
40	6	0	-1.520243	2.887767	-2.472915
41	6	0	3.400513	-1.051503	0.206059
42	6	0	2.775950	0.752253	-1.381405
43	6	0	1.753332	0.903179	1.059410
44	6	0	0.030734	2.114899	2.283714
45	6	0	-0.612777	3.650978	-1.750506
46	1	0	0.643123	3.685882	-0.021386
47	1	0	-1.943426	3.251436	-3.404728
48	6	0	3.382791	-2.108619	-0.948277
49	6	0	3.482356	-1.803877	1.537310
50	6	0	4.639307	-0.231404	-0.215063
51	6	0	4.143507	0.050991	-1.642472
52	6	0	3.100197	2.231257	-1.101895
53	6	0	1.820550	0.684857	-2.578044
54	6	0	2.593179	1.128017	2.157284
55	6	0	0.853461	2.226474	3.402974
56	1	0	-0.956179	2.565637	2.301307
57	1	0	-0.316168	4.642301	-2.079481
58	1	0	4.027008	-2.942581	-0.651139
59	1	0	2.385891	-2.512894	-1.112329
60	6	0	3.954444	-1.372023	-2.183559
61	1	0	4.469886	-2.277425	1.595661
62	1	0	2.736094	-2.598505	1.590415
63	1	0	3.352551	-1.191482	2.428242
64	1	0	4.819867	0.666272	0.380741
65	1	0	5.549423	-0.841687	-0.190990
66	1	0	4.795997	0.674797	-2.261043
67	1	0	3.598687	2.653269	-1.982238
68	1	0	3.765927	2.369684	-0.246249
69	1	0	2.203208	2.816816	-0.924865
70	1	0	0.947097	1.319248	-2.421584

71	1	0	1.458626	-0.326446	-2.764237
72	1	0	2.339804	1.040765	-3.476401
73	1	0	3.612838	0.773341	2.116139
74	6	0	2.164240	1.769332	3.318317
75	1	0	0.486173	2.707833	4.304469
76	1	0	4.921326	-1.790072	-2.485618
77	1	0	3.298234	-1.419505	-3.055473
78	1	0	2.851470	1.894182	4.149913

BIFOXSiCl(OH) **8**$_{eq}$

HF=- 2219.4141309
Thermal correction to Gibbs Free Energy= 0.586319
NImag=0

1	1	0	-5.550817	-2.304345	-0.470583
2	6	0	-4.609119	-1.917196	-0.066347
3	1	0	-4.433396	-2.425724	0.883251
4	6	0	-3.447550	-2.101240	-1.077137
5	6	0	-4.684399	-0.387107	0.062769
6	1	0	-3.786281	-2.604005	-1.989238
7	1	0	-2.630009	-2.689452	-0.666643
8	6	0	-3.002554	-0.653532	-1.459095
9	6	0	-4.390821	0.035423	-1.386528
10	1	0	-5.630529	-0.028299	0.479854
11	6	0	-3.461201	0.187271	0.840734
12	6	0	-2.243555	-0.037123	-0.210236
13	6	0	-2.248355	-0.661971	-2.788028
14	1	0	-4.396229	1.114220	-1.535773
15	1	0	-5.089795	-0.406263	-2.106540
16	6	0	-3.746878	1.666241	1.162166
17	6	0	-3.197803	-0.521763	2.175589
18	14	0	0.010598	-1.711757	-0.106720
19	1	0	-1.401759	-1.353375	-2.743742
20	8	0	-1.376517	-1.007401	0.359558
21	6	0	-1.471218	1.272156	-0.440515
22	1	0	-2.916022	-1.011306	-3.584609
23	1	0	-1.859345	0.314092	-3.081063
24	1	0	-4.582047	1.717219	1.869953
25	1	0	-4.019773	2.253722	0.282783
26	1	0	-2.885279	2.156238	1.623352
27	1	0	-2.362982	-0.054890	2.703700

28	1	0	-2.942670	-1.573891	2.057819
29	1	0	-4.089839	-0.445829	2.809238
30	8	0	1.082873	-0.666295	-0.739248
31	6	0	-0.411927	1.727780	0.387698
32	6	0	-1.975757	2.180839	-1.387759
33	6	0	2.224322	-0.012368	-0.159068
34	6	0	0.434834	1.027320	1.435416
35	6	0	-0.095359	3.101574	0.351350
36	1	0	-2.749836	1.858663	-2.065158
37	6	0	-1.566218	3.506052	-1.479728
38	6	0	3.453528	-1.039186	-0.205518
39	6	0	2.751812	1.148622	-1.149746
40	6	0	1.744669	0.493300	1.217463
41	6	0	0.025865	1.265959	2.755629
42	6	0	-0.647717	3.992918	-0.558981
43	1	0	0.621320	3.468008	1.077848
44	1	0	-1.999162	4.152370	-2.237695
45	6	0	3.442025	-1.702059	-1.622096
46	6	0	3.601107	-2.153873	0.835180
47	6	0	4.660803	-0.091960	-0.378886
48	6	0	4.121696	0.594616	-1.642977
49	6	0	3.061527	2.469067	-0.420292
50	6	0	1.775621	1.444543	-2.294322
51	6	0	2.591181	0.389489	2.327263
52	6	0	0.856704	1.050616	3.851716
53	1	0	-0.962027	1.686450	2.913699
54	1	0	-0.352504	5.037839	-0.550742
55	1	0	4.135628	-2.549460	-1.598234
56	1	0	2.459178	-2.093286	-1.881946
57	6	0	3.943571	-0.601728	-2.588069
58	1	0	4.637524	-2.511538	0.804908
59	1	0	2.962319	-3.004651	0.589997
60	1	0	3.372897	-1.870293	1.860736
61	1	0	4.836875	0.585540	0.459666
62	1	0	5.583957	-0.655483	-0.557412
63	1	0	4.744997	1.393103	-2.057193
64	1	0	3.553633	3.151106	-1.123386
65	1	0	3.725776	2.339625	0.437553
66	1	0	2.159200	2.959557	-0.069492
67	1	0	0.885585	1.961861	-1.934537
68	1	0	1.443041	0.537826	-2.800315
69	1	0	2.267682	2.092372	-3.030429
70	1	0	3.616784	0.084552	2.175679
71	6	0	2.169422	0.654424	3.628181

72	1	0	0.493120	1.240816	4.857298
73	1	0	4.905972	-0.872990	-3.036432
74	1	0	3.252018	-0.402433	-3.409481
75	1	0	2.864692	0.537936	4.454431
76	17	0	0.481582	-2.713779	1.647025
77	8	0	-0.133606	-2.837204	-1.305744
78	1	0	-0.748706	-3.562168	-1.127955

BIFOXSiCl(OH) **8_{ax}** to BIFOXSi(OH)$_2$ **9** TS_{front1} **8ax**

HF=-2295.8124297
Thermal correction to Gibbs Free Energy= 0.608924
NImag=1
Frequencies -- -208.0116

1	1	0	5.483668	-2.027748	-1.089875
2	6	0	4.510804	-1.524373	-1.111990
3	1	0	4.160240	-1.552927	-2.145510
4	6	0	3.516820	-2.179467	-0.115744
5	6	0	4.648923	-0.092729	-0.556348
6	1	0	4.006936	-2.973136	0.456811
7	1	0	2.649379	-2.622697	-0.596100
8	6	0	3.149572	-1.044133	0.885803
9	6	0	4.536183	-0.353460	0.951937
10	1	0	5.556457	0.421872	-0.888433
11	6	0	3.375335	0.757945	-0.836655
12	6	0	2.266526	0.019319	0.090699
13	6	0	2.576030	-1.592461	2.204474
14	1	0	4.578331	0.548914	1.563602
15	1	0	5.299969	-1.045500	1.325236
16	6	0	3.659522	2.214470	-0.422363
17	6	0	2.978229	0.782851	-2.318632
18	14	0	-0.052693	-1.336168	-0.919091
19	1	0	1.517042	-1.359691	2.324693
20	8	0	1.399606	-0.665288	-0.799384
21	6	0	1.487735	1.034910	0.944784
22	1	0	2.656187	-2.680808	2.234315
23	1	0	3.110172	-1.198188	3.076314
24	1	0	4.454028	2.614605	-1.062660
25	1	0	3.983884	2.316826	0.614737
26	1	0	2.778617	2.849824	-0.545234

27	1	0	2.100371	1.413121	-2.480124
28	1	0	2.737175	-0.203572	-2.710550
29	1	0	3.806377	1.198030	-2.905941
30	8	0	-1.107810	-0.802248	0.215927
31	6	0	0.383746	1.817560	0.512605
32	6	0	2.040956	1.359023	2.196501
33	6	0	-2.261430	0.032197	0.026384
34	6	0	-0.474620	1.785559	-0.741481
35	6	0	0.033539	2.947521	1.281707
36	1	0	2.863580	0.772613	2.568416
37	6	0	1.615469	2.422265	2.982658
38	6	0	-3.468544	-0.871724	-0.522453
39	6	0	-2.830028	0.472708	1.472955
40	6	0	-1.785682	1.215840	-0.844401
41	6	0	-0.073844	2.705405	-1.723453
42	6	0	0.617775	3.259018	2.501620
43	1	0	-0.730723	3.606522	0.885699
44	1	0	2.090451	2.606557	3.941816
45	6	0	-3.450645	-2.198919	0.303097
46	6	0	-3.591076	-1.236695	-2.005670
47	6	0	-4.700857	-0.194787	0.116812
48	6	0	-4.183358	-0.292322	1.560358
49	6	0	-3.168755	1.972273	1.558350
50	6	0	-1.864631	0.129755	2.614623
51	6	0	-2.634774	1.729298	-1.836285
52	6	0	-0.906634	3.118868	-2.760606
53	1	0	0.912646	3.146746	-1.632606
54	1	0	0.293673	4.134758	3.055802
55	1	0	-4.134547	-2.903371	-0.183227
56	1	0	-2.465334	-2.660521	0.336581
57	6	0	-3.967236	-1.805406	1.708252
58	1	0	-4.582145	-1.678319	-2.162942
59	1	0	-2.850373	-1.984608	-2.294560
60	1	0	-3.490707	-0.405962	-2.704353
61	1	0	-4.894963	0.825700	-0.221930
62	1	0	-5.608546	-0.785106	-0.053879
63	1	0	-4.831431	0.138001	2.329936
64	1	0	-3.678510	2.161945	2.509956
65	1	0	-3.827517	2.313897	0.755865
66	1	0	-2.274982	2.588760	1.540744
67	1	0	-0.993051	0.786960	2.604725
68	1	0	-1.499226	-0.895256	2.556724
69	1	0	-2.379619	0.267728	3.573532
70	1	0	-3.658955	1.387106	-1.871468

71	6	0	-2.217637	2.659987	-2.787725
72	1	0	-0.545228	3.825879	-3.501291
73	1	0	-4.916619	-2.301433	1.938858
74	1	0	-3.264901	-2.063300	2.502666
75	1	0	-2.916111	3.008988	-3.542565
76	1	0	0.240507	-3.662075	-0.978937
77	8	0	0.348216	-2.978460	-1.732967
78	1	0	-0.224681	-3.115140	-2.511324
79	8	0	-0.653472	-0.985310	-2.435844
80	1	0	-1.061923	-0.111218	-2.521833
81	17	0	0.087724	-3.344104	0.871462

BIFOXSiCl(OH) **8_{eq}** to BIFOXSi(OH)$_2$ **9** TS_{front2} **8eq**

HF=-2295.796119
Thermal correction to Gibbs Free Energy= 0.607763
NImag=1
Frequencies -- -242.4084

1	1	0	-5.566429	-2.243600	-0.515697
2	6	0	-4.587712	-1.897179	-0.164768
3	1	0	-4.294411	-2.546055	0.662368
4	6	0	-3.550467	-1.878087	-1.317128
5	6	0	-4.668731	-0.412804	0.224221
6	1	0	-3.994087	-2.229211	-2.255244
7	1	0	-2.682951	-2.501651	-1.123437
8	6	0	-3.174020	-0.373349	-1.503988
9	6	0	-4.548955	0.254041	-1.152370
10	1	0	-5.562101	-0.157373	0.803030
11	6	0	-3.372317	0.067937	0.941504
12	6	0	-2.275670	0.055404	-0.261217
13	6	0	-2.647536	-0.126172	-2.920309
14	1	0	-4.578161	1.343096	-1.118213
15	1	0	-5.319857	-0.079894	-1.857011
16	6	0	-3.650056	1.473397	1.509782
17	6	0	-2.965825	-0.835599	2.110574
18	14	0	0.002126	-1.575576	-0.650951
19	1	0	-1.832994	-0.811228	-3.153128
20	8	0	-1.310938	-0.958019	0.061778
21	6	0	-1.548146	1.406967	-0.355921
22	1	0	-3.459582	-0.315193	-3.633134
23	1	0	-2.286900	0.888286	-3.093633
24	1	0	-4.403360	1.387642	2.300997

25	1	0	-4.030538	2.173729	0.762397
26	1	0	-2.757775	1.926247	1.945665
27	1	0	-2.096116	-0.438790	2.635995
28	1	0	-2.695522	-1.841636	1.797381
29	1	0	-3.800317	-0.897010	2.820454
30	8	0	1.180620	-0.481953	-0.897579
31	6	0	-0.445509	1.781267	0.458237
32	6	0	-2.127947	2.415409	-1.147329
33	6	0	2.257566	0.118102	-0.160000
34	6	0	0.391190	0.995654	1.452615
35	6	0	-0.116646	3.150983	0.529914
36	1	0	-2.967062	2.170357	-1.776634
37	6	0	-1.715558	3.742568	-1.134307
38	6	0	3.499704	-0.897977	-0.206904
39	6	0	2.840540	1.365199	-1.002003
40	6	0	1.701457	0.475841	1.230642
41	6	0	-0.047750	1.128552	2.778346
42	6	0	-0.714631	4.129132	-0.253220
43	1	0	0.632246	3.446610	1.255450
44	1	0	-2.209048	4.465752	-1.777228
45	6	0	3.589412	-1.455544	-1.669600
46	6	0	3.575683	-2.030181	0.840807
47	6	0	4.712218	0.056365	-0.252418
48	6	0	4.231497	0.847504	-1.476172
49	6	0	3.114803	2.603038	-0.128229
50	6	0	1.923470	1.788753	-2.155819
51	6	0	2.508820	0.256198	2.353778
52	6	0	0.744095	0.809730	3.876332
53	1	0	-1.033296	1.545328	2.949496
54	1	0	-0.407029	5.166786	-0.163649
55	1	0	4.313518	-2.277040	-1.674356
56	1	0	2.644778	-1.840132	-2.056704
57	6	0	4.100036	-0.267546	-2.523293
58	1	0	3.830714	-2.988977	0.367069
59	1	0	2.657831	-2.157739	1.419340
60	1	0	4.374373	-1.851634	1.566454
61	1	0	4.838736	0.655029	0.651335
62	1	0	5.645005	-0.491834	-0.430125
63	1	0	4.875058	1.671345	-1.797764
64	1	0	3.679606	3.332983	-0.719724
65	1	0	3.693835	2.378829	0.770394
66	1	0	2.192171	3.080969	0.184099
67	1	0	1.006456	2.247698	-1.781808
68	1	0	1.630916	0.951405	-2.790161

69	1	0	2.443460	2.529108	-2.776116
70	1	0	3.532251	-0.056236	2.211988
71	6	0	2.054898	0.409198	3.659694
72	1	0	0.349428	0.918686	4.882110
73	1	0	5.077006	-0.492714	-2.964046
74	1	0	3.426298	-0.011599	-3.342879
75	1	0	2.722657	0.203769	4.491074
76	17	0	0.085328	-2.682170	1.911158
77	8	0	-0.521233	-2.160683	-2.105938
78	1	0	0.031020	-2.865928	-2.468557
79	1	0	0.886970	-3.423160	0.492375
80	8	0	1.083206	-3.185501	-0.509369
81	1	0	2.032135	-2.961616	-0.556432

BIFOXSiCl(OH) **8_{ax}** to BIFOXSi(OH)$_2$ **9** TS_{side} **8ax**

HF=-2295.8158455
Thermal correction to Gibbs Free Energy= 0.609060
NImag=1
Frequencies -- -162.8018

1	1	0	5.623777	1.925985	0.119717
2	6	0	4.633092	1.535025	0.376545
3	1	0	4.380669	1.927291	1.363186
4	6	0	3.584927	1.905979	-0.704598
5	6	0	4.644602	-0.003344	0.311163
6	1	0	4.053515	2.459304	-1.525911
7	1	0	2.780335	2.522809	-0.314950
8	6	0	3.096312	0.542406	-1.277121
9	6	0	4.439402	-0.230648	-1.192833
10	1	0	5.542345	-0.456486	0.743557
11	6	0	3.348027	-0.615771	0.919183
12	6	0	2.220042	-0.170173	-0.159892
13	6	0	2.449989	0.703868	-2.667546
14	1	0	4.397384	-1.282215	-1.478157
15	1	0	5.208394	0.254031	-1.805701
16	6	0	3.538462	-2.141404	1.021429
17	6	0	3.039026	-0.098901	2.330376
18	14	0	0.001210	1.568675	0.270019
19	1	0	1.427104	0.321492	-2.699663
20	8	0	1.385842	0.778678	0.492921
21	6	0	1.389913	-1.377807	-0.629851

22	1	0	2.412854	1.757011	-2.958658
23	1	0	3.019086	0.174556	-3.440110
24	1	0	4.335420	-2.349641	1.744390
25	1	0	3.818615	-2.605254	0.073293
26	1	0	2.631873	-2.643061	1.367997
27	1	0	2.154785	-0.589875	2.743686
28	1	0	2.849907	0.973236	2.356474
29	1	0	3.889486	-0.319057	2.987283
30	8	0	-1.120289	0.682239	-0.588585
31	6	0	0.286927	-1.929130	0.072114
32	6	0	1.873060	-2.106514	-1.732377
33	6	0	-2.277562	0.001974	-0.080338
34	6	0	-0.531026	-1.422429	1.246293
35	6	0	-0.110562	-3.242224	-0.256759
36	1	0	2.678862	-1.696136	-2.318051
37	6	0	1.394974	-3.358347	-2.100654
38	6	0	-3.460873	1.075575	0.140814
39	6	0	-2.898240	-0.910962	-1.262913
40	6	0	-1.813514	-0.800028	1.153037
41	6	0	-0.140260	-1.958393	2.482933
42	6	0	0.416951	-3.961665	-1.320845
43	1	0	-0.867736	-3.704799	0.366199
44	1	0	1.816091	-3.863411	-2.965156
45	6	0	-3.459008	2.033907	-1.088768
46	6	0	-3.556652	1.933359	1.410273
47	6	0	-4.718741	0.249590	-0.216810
48	6	0	-4.226936	-0.178609	-1.606850
49	6	0	-3.283874	-2.327777	-0.796775
50	6	0	-1.961609	-1.058382	-2.468501
51	6	0	-2.661258	-0.905291	2.262244
52	6	0	-0.966265	-1.951696	3.602974
53	1	0	0.826697	-2.446543	2.543754
54	1	0	0.060002	-4.964817	-1.534356
55	1	0	-4.149071	2.855680	-0.871475
56	1	0	-2.482643	2.492689	-1.253817
57	6	0	-3.969464	1.181659	-2.276092
58	1	0	-4.595200	2.272049	1.516662
59	1	0	-2.925191	2.819048	1.327695
60	1	0	-3.262700	1.429811	2.327365
61	1	0	-4.926513	-0.582328	0.458060
62	1	0	-5.611264	0.885121	-0.252570
63	1	0	-4.901684	-0.823373	-2.177974
64	1	0	-3.871666	-2.811879	-1.585477
65	1	0	-3.880655	-2.335272	0.117417

66	1	0	-2.405179	-2.941688	-0.621769
67	1	0	-1.083616	-1.655041	-2.218757
68	1	0	-1.604616	-0.099708	-2.847077
69	1	0	-2.496686	-1.565450	-3.280875
70	1	0	-3.673247	-0.533946	2.186698
71	6	0	-2.260264	-1.463295	3.473340
72	1	0	-0.616994	-2.372523	4.541341
73	1	0	-4.901016	1.589003	-2.683549
74	1	0	-3.261077	1.118985	-3.105295
75	1	0	-2.957099	-1.502290	4.305705
76	8	0	-0.748907	1.836093	1.705771
77	1	0	-0.361039	2.581658	2.188721
78	17	0	0.869805	3.937923	0.653608
79	8	0	0.226725	2.400836	-1.462626
80	1	0	-0.575125	2.228003	-1.991125
81	1	0	0.394636	3.364798	-1.299359

BIFOXSi(OH)$_2$ **9**

HF=-1835.0468439
Thermal correction to Gibbs Free Energy= 0.599402
NImag=0

1	14	0	0.043969	-1.618470	0.703806
2	8	0	1.001473	-0.882301	-0.410549
3	8	0	-1.375464	-0.814914	0.826736
4	8	0	-0.059922	-3.173646	0.159032
5	8	0	0.556555	-1.709574	2.268252
6	6	0	2.183843	-0.134170	-0.085365
7	6	0	-2.204574	-0.154176	-0.112614
8	1	0	-0.475486	-3.788171	0.779699
9	6	0	3.366546	-1.169355	0.221118
10	6	0	2.754095	0.615881	-1.393751
11	6	0	1.748999	0.820644	1.050559
12	6	0	-2.869517	-1.206580	-1.094415
13	6	0	-3.495699	0.403509	0.702407
14	6	0	-1.432255	1.005359	-0.768542
15	6	0	3.315887	-2.252959	-0.906050
16	6	0	4.613116	-0.380975	-0.233275
17	6	0	3.455458	-1.891238	1.568664
18	6	0	4.102624	-0.118526	-1.658983
19	6	0	3.106629	2.092611	-1.137666
20	6	0	1.787448	0.550129	-2.581615
21	6	0	0.449273	1.419971	1.087952

22	6	0	2.599419	1.058904	2.137187
23	6	0	-3.317114	-2.436301	-0.244418
24	6	0	-2.018963	-1.656244	-2.280511
25	6	0	-4.271995	-0.596818	-1.357087
26	6	0	-3.317403	0.258397	2.219421
27	6	0	-3.822105	1.883909	0.431941
28	6	0	-4.651873	-0.470558	0.128531
29	6	0	-0.392674	1.730374	-0.132725
30	6	0	-1.911860	1.521339	-1.985319
31	6	0	3.873697	-1.549297	-2.167464
32	1	0	3.960831	-3.084373	-0.601890
33	1	0	2.311217	-2.651554	-1.038013
34	1	0	4.817424	0.525476	0.341808
35	1	0	5.512893	-1.006780	-0.208646
36	1	0	4.439938	-2.371402	1.629153
37	1	0	2.701844	-2.676802	1.645165
38	1	0	3.337597	-1.257549	2.446288
39	1	0	4.759028	0.477421	-2.300836
40	1	0	3.599667	2.496691	-2.029626
41	1	0	3.785455	2.231052	-0.292349
42	1	0	2.220718	2.694147	-0.954670
43	1	0	2.309199	0.870955	-3.491851
44	1	0	0.934232	1.212708	-2.433057
45	1	0	1.394485	-0.453985	-2.741199
46	6	0	0.046712	2.071859	2.263621
47	6	0	2.185458	1.727118	3.288520
48	1	0	3.616283	0.695707	2.093772
49	1	0	-3.607289	-3.234012	-0.936761
50	1	0	-2.512372	-2.825060	0.372942
51	6	0	-4.532528	-1.936837	0.579405
52	1	0	-2.614264	-2.305086	-2.933886
53	1	0	-1.159721	-2.240703	-1.937784
54	1	0	-1.635279	-0.831329	-2.882812
55	1	0	-4.293241	0.350773	-1.893712
56	1	0	-4.913658	-1.301320	-1.899322
57	1	0	-2.547221	0.943981	2.584352
58	1	0	-3.018155	-0.745156	2.517993
59	1	0	-4.259389	0.509188	2.722078
60	1	0	-4.697400	2.166595	1.028244
61	1	0	-4.052638	2.090659	-0.614978
62	1	0	-2.994100	2.539681	0.716472
63	1	0	-5.631516	-0.026647	0.332422
64	6	0	-0.071731	3.008058	-0.634072
65	6	0	-1.504358	2.738501	-2.519796

66	1	0	-2.660763	0.970116	-2.530864
67	1	0	4.825144	-1.991988	-2.483594
68	1	0	3.196884	-1.598833	-3.023277
69	1	0	-0.937269	2.529895	2.280037
70	6	0	0.879284	2.197336	3.374178
71	1	0	2.880441	1.863057	4.112043
72	1	0	-4.393474	-2.048497	1.656602
73	1	0	-5.443955	-2.484114	0.314696
74	1	0	0.640385	3.603374	-0.072632
75	6	0	-0.609120	3.524772	-1.806149
76	1	0	-1.918765	3.077145	-3.464970
77	1	0	0.523499	2.699354	4.269165
78	1	0	-0.315060	4.509551	-2.156565
79	1	0	0.448851	-0.879932	2.757183

b. Kondo-silanes

dichlorodi(naphthalen-1-yl)silane **13**

HF=-1980.4604433
Thermal correction to Gibbs Free Energy= 0.220359
NImag=0

1	14	0	0.039826	-1.091581	0.137046
2	6	0	-1.745247	-0.809108	-0.331616
3	6	0	-2.503205	0.295948	0.193226
4	6	0	-2.359088	-1.687271	-1.211268
5	6	0	-1.962261	1.253476	1.094002
6	6	0	-3.870419	0.456449	-0.210336
7	6	0	-3.706516	-1.524524	-1.605108
8	1	0	-1.801936	-2.527333	-1.611733
9	6	0	-2.721430	2.300113	1.566615
10	1	0	-0.931940	1.164979	1.418446
11	6	0	-4.627647	1.545129	0.295828
12	6	0	-4.443982	-0.475592	-1.113721
13	1	0	-4.150835	-2.234973	-2.295748
14	6	0	-4.068794	2.450659	1.166564
15	1	0	-2.280698	3.015540	2.254644
16	1	0	-5.662089	1.648400	-0.021835
17	1	0	-5.481550	-0.341749	-1.409509

18	1	0	-4.657113	3.280027	1.547988
19	6	0	1.175782	0.279032	-0.406476
20	6	0	2.584715	0.323337	-0.126422
21	6	0	0.603922	1.294958	-1.159737
22	6	0	3.262785	-0.680748	0.614948
23	6	0	3.355750	1.427124	-0.621460
24	6	0	1.368702	2.378672	-1.646886
25	1	0	-0.457531	1.271918	-1.383100
26	6	0	4.615652	-0.596940	0.857521
27	1	0	2.711005	-1.530376	0.998555
28	6	0	4.747863	1.486131	-0.352099
29	6	0	2.714150	2.441934	-1.378717
30	1	0	0.884557	3.156290	-2.230012
31	6	0	5.368878	0.496371	0.372880
32	1	0	5.108475	-1.379638	1.426733
33	1	0	5.314698	2.331322	-0.734378
34	1	0	3.312590	3.271847	-1.746464
35	1	0	6.435047	0.549959	0.572815
36	17	0	0.158237	-1.372180	2.204740
37	17	0	0.686591	-2.882231	-0.716004

dichlorodi(naphthalen-1-yl)silane **13** to **13$_{ClOH}$** TS$_{front}$ 13

HF=-2056.8616445
Thermal correction to Gibbs Free Energy= 0.241033
NImag=1
Frequencies -- -167.5153

1	6	0	-1.848525	-0.791494	-0.169168
2	6	0	-2.494839	0.464303	0.108600
3	6	0	-2.623217	-1.881569	-0.542198
4	6	0	-1.805508	1.636171	0.522349
5	6	0	-3.919693	0.552206	-0.048261
6	6	0	-4.026481	-1.794876	-0.659730
7	1	0	-2.148562	-2.830822	-0.767031
8	6	0	-2.474240	2.819088	0.742094
9	1	0	-0.739013	1.597823	0.690884
10	6	0	-4.578934	1.788012	0.184490
11	6	0	-4.657672	-0.597679	-0.427438
12	1	0	-4.594873	-2.674110	-0.947543
13	6	0	-3.873976	2.903740	0.567183
14	1	0	-1.917608	3.694672	1.063180
15	1	0	-5.657454	1.830463	0.055153
16	1	0	-5.736517	-0.511475	-0.530881

17	1	0	-4.387431	3.844412	0.743741
18	6	0	1.250065	0.203664	-0.505613
19	6	0	2.615709	0.253736	-0.080763
20	6	0	0.792907	1.121633	-1.438676
21	6	0	3.176692	-0.653284	0.855470
22	6	0	3.474832	1.262162	-0.630759
23	6	0	1.639023	2.123747	-1.964861
24	1	0	-0.236898	1.085948	-1.783425
25	6	0	4.501138	-0.584151	1.220685
26	1	0	2.539122	-1.394125	1.319826
27	6	0	4.836159	1.312580	-0.231456
28	6	0	2.952022	2.190071	-1.568429
29	1	0	1.242321	2.832422	-2.685522
30	6	0	5.344462	0.408283	0.670794
31	1	0	4.899588	-1.288668	1.944911
32	1	0	5.472043	2.084072	-0.658135
33	1	0	3.614450	2.951645	-1.971844
34	1	0	6.387903	0.456467	0.967774
35	14	0	-0.014501	-1.092863	-0.063676
36	17	0	0.378180	-2.456652	-1.706689
37	8	0	0.304610	-2.552224	1.051122
38	1	0	1.007853	-3.170318	0.773903
39	1	0	0.414959	-2.096808	1.973885
40	17	0	0.088096	-0.314629	2.451850

dichlorodi(naphthalen-1-yl)silane **13** to **13$_{\mathbf{ClOH}}$** TS$_{side}$ 13

HF=-2056.8492045
Thermal correction to Gibbs Free Energy= 0.240761
NImag=1
Frequencies -- -176.0179

1	6	0	-1.720998	0.478477	0.478878
2	6	0	-2.332555	-0.680779	-0.110886
3	6	0	-2.486636	1.311712	1.277966
4	6	0	-1.629571	-1.641970	-0.894579
5	6	0	-3.737520	-0.898668	0.089754
6	6	0	-3.853873	1.060239	1.518726
7	1	0	-2.039567	2.205234	1.701662
8	6	0	-2.274828	-2.705438	-1.486872
9	1	0	-0.545940	-1.604824	-0.946132
10	6	0	-4.373375	-2.003049	-0.536594
11	6	0	-4.470174	-0.011004	0.918251
12	1	0	-4.418370	1.735925	2.153839

13	6	0	-3.666765	-2.882591	-1.322541
14	1	0	-1.704062	-3.425291	-2.066466
15	1	0	-5.439689	-2.141489	-0.377026
16	1	0	-5.531117	-0.194970	1.066757
17	1	0	-4.167253	-3.721089	-1.797083
18	6	0	1.260009	-0.357577	0.488459
19	6	0	2.626152	-0.347813	0.046423
20	6	0	0.831612	-1.388160	1.310851
21	6	0	3.172890	0.694439	-0.750724
22	6	0	3.495719	-1.421612	0.432675
23	6	0	1.692615	-2.440776	1.699437
24	1	0	-0.194948	-1.404629	1.665235
25	6	0	4.487644	0.669642	-1.157429
26	1	0	2.549097	1.532652	-1.041091
27	6	0	4.844719	-1.423011	-0.009155
28	6	0	2.993760	-2.459689	1.260732
29	1	0	1.315499	-3.231604	2.341306
30	6	0	5.333712	-0.401910	-0.789562
31	1	0	4.879895	1.482182	-1.761943
32	1	0	5.487362	-2.247585	0.289146
33	1	0	3.663756	-3.266459	1.547513
34	1	0	6.368641	-0.411060	-1.118923
35	14	0	0.025043	1.011039	0.093817
36	17	0	0.782276	2.502853	1.345295
37	17	0	-0.982848	3.041489	-1.297120
38	8	0	0.260718	0.744255	-1.792018
39	1	0	-0.288656	1.538115	-2.151265
40	1	0	-0.116499	-0.110280	-2.084670

chlorodi(naphthalen-1-yl)silanol **13_{ClOH}**

HF=-1596.0871036
Thermal correction to Gibbs Free Energy= 0.231269
NImag=0

1	14	0	-0.037083	1.140379	0.377626
2	6	0	1.747597	0.887859	-0.121529
3	6	0	2.464182	-0.286869	0.302165
4	6	0	2.400060	1.818090	-0.915271
5	6	0	1.878513	-1.300151	1.111188
6	6	0	3.827275	-0.462495	-0.109149
7	6	0	3.744355	1.643623	-1.315952
8	1	0	1.872329	2.707678	-1.243315
9	6	0	2.594450	-2.413910	1.488634

10	1	0	0.850872	-1.196460	1.441083
11	6	0	4.538540	-1.621416	0.298726
12	6	0	4.440390	0.527190	-0.920731
13	1	0	4.219722	2.396557	-1.937790
14	6	0	3.938123	-2.579821	1.080773
15	1	0	2.122136	-3.172846	2.105634
16	1	0	5.570856	-1.735979	-0.022415
17	1	0	5.474267	0.382943	-1.224914
18	1	0	4.491050	-3.463320	1.386384
19	6	0	-1.176286	-0.125078	-0.366335
20	6	0	-2.565940	-0.246079	-0.025374
21	6	0	-0.644374	-0.964231	-1.334121
22	6	0	-3.194515	0.571787	0.952083
23	6	0	-3.365249	-1.229543	-0.697097
24	6	0	-1.433106	-1.936863	-1.989478
25	1	0	0.405101	-0.884263	-1.600687
26	6	0	-4.532893	0.430019	1.242860
27	1	0	-2.605459	1.307388	1.487928
28	6	0	-4.741466	-1.352030	-0.372259
29	6	0	-2.764590	-2.063404	-1.676236
30	1	0	-0.979940	-2.578402	-2.739550
31	6	0	-5.317272	-0.538974	0.575560
32	1	0	-4.991015	1.067072	1.993998
33	1	0	-5.332592	-2.103050	-0.890539
34	1	0	-3.382349	-2.805788	-2.175823
35	1	0	-6.371887	-0.639540	0.815621
36	17	0	-0.618533	3.048464	-0.277053
37	8	0	-0.219996	1.095528	2.030795
38	1	0	0.424331	1.618349	2.530411

chlorodi(naphthalen-1-yl)silanol **13**$_{\mathbf{ClOH}}$ to di(naphthalen-1-yl)silanediol **1** TS_{front} **13**$_{\mathbf{ClOH}}$

HF=-1672.4874734
Thermal correction to Gibbs Free Energy= 0.253637
NImag=1
Frequencies -- -137.2984

1	6	0	1.846112	-0.747651	-0.078352
2	6	0	2.457123	0.543675	-0.262620
3	6	0	2.654820	-1.823622	0.249298
4	6	0	1.723345	1.721337	-0.577678
5	6	0	3.877210	0.674388	-0.094567
6	6	0	4.054556	-1.696210	0.386548

7	1	0	2.205651	-2.791444	0.441399
8	6	0	2.345392	2.941326	-0.712991
9	1	0	0.651896	1.660865	-0.715615
10	6	0	4.489961	1.946728	-0.244211
11	6	0	4.651725	-0.470980	0.220503
12	1	0	4.648692	-2.569968	0.637993
13	6	0	3.744124	3.060862	-0.545695
14	1	0	1.754858	3.821571	-0.950840
15	1	0	5.566513	2.020500	-0.111322
16	1	0	5.726901	-0.357015	0.335639
17	1	0	4.222844	4.029690	-0.655330
18	6	0	-1.290233	0.041170	0.459956
19	6	0	-2.621578	0.216986	-0.038967
20	6	0	-0.886879	0.753479	1.577056
21	6	0	-3.138446	-0.512198	-1.147094
22	6	0	-3.492454	1.154251	0.611462
23	6	0	-1.746850	1.672766	2.217456
24	1	0	0.112700	0.607321	1.976390
25	6	0	-4.422829	-0.310204	-1.601374
26	1	0	-2.520776	-1.265073	-1.626109
27	6	0	-4.810242	1.339235	0.117249
28	6	0	-3.020197	1.873088	1.739645
29	1	0	-1.393578	2.219263	3.086880
30	6	0	-5.267954	0.630130	-0.968856
31	1	0	-4.793963	-0.885481	-2.444783
32	1	0	-5.456260	2.054090	0.620908
33	1	0	-3.688228	2.581904	2.222441
34	1	0	-6.279121	0.780874	-1.335327
35	8	0	-0.078687	-0.430183	-2.005504
36	1	0	-0.882539	0.065606	-2.215073
37	14	0	0.014511	-0.978100	-0.403007
38	8	0	-0.355987	-2.707962	-1.132756
39	1	0	0.139124	-2.886145	-1.954296
40	1	0	-0.210189	-3.360535	-0.386791
41	17	0	-0.200619	-2.645812	1.528318

chlorodi(naphthalen-1-yl)silanol **13$_{ClOH}$** to di(naphthalen-1-yl)silanediol **1** TS$_{side}$ **13$_{ClOH}$**

HF=-1672.4883422
Thermal correction to Gibbs Free Energy= 0.255458
NImag=1
Frequencies -- -119.7494

1	6	0	1.651865	0.660487	-0.360388
2	6	0	2.490314	-0.327957	0.258758
3	6	0	2.100578	1.300831	-1.503142
4	6	0	2.115405	-1.037166	1.435158
5	6	0	3.764512	-0.629791	-0.330337
6	6	0	3.354481	1.002160	-2.079600
7	1	0	1.485843	2.063843	-1.969211
8	6	0	2.944523	-1.986233	1.988644
9	1	0	1.165592	-0.817202	1.909973
10	6	0	4.596591	-1.611676	0.269645
11	6	0	4.167875	0.055304	-1.504602
12	1	0	3.670490	1.527385	-2.976251
13	6	0	4.198255	-2.279629	1.403143
14	1	0	2.634456	-2.512737	2.886772
15	1	0	5.558911	-1.825062	-0.189187
16	1	0	5.135049	-0.183066	-1.940351
17	1	0	4.843006	-3.029563	1.852375
18	6	0	-1.162075	-0.478278	-0.145862
19	6	0	-2.589920	-0.448938	0.029123
20	6	0	-0.599780	-1.590340	-0.747628
21	6	0	-3.265654	0.647841	0.640937
22	6	0	-3.389465	-1.542093	-0.447056
23	6	0	-1.382734	-2.687753	-1.180216
24	1	0	0.472683	-1.632388	-0.904036
25	6	0	-4.639808	0.676251	0.746352
26	1	0	-2.681577	1.443738	1.093004
27	6	0	-4.801228	-1.484419	-0.316334
28	6	0	-2.748383	-2.659878	-1.042512
29	1	0	-0.894723	-3.544154	-1.636880
30	6	0	-5.418798	-0.396414	0.256955
31	1	0	-5.126570	1.520398	1.226486
32	1	0	-5.389711	-2.322116	-0.682559
33	1	0	-3.360185	-3.488179	-1.391270
34	1	0	-6.500680	-0.364907	0.346922
35	8	0	-0.373853	1.039194	1.926849
36	1	0	-0.008894	1.828015	2.360465
37	14	0	-0.064639	1.016292	0.289568
38	8	0	-1.038015	1.886240	-1.240616
39	1	0	-1.025932	2.856507	-1.060219
40	17	0	0.344569	3.423736	0.506304
41	1	0	-1.954872	1.550568	-1.303228

di(naphthalen-1-yl)silanediol **1**

HF=-1211.7094702
Thermal correction to Gibbs Free Energy= 0.243783
NImag=0

1	14	0	0.095655	-1.234555	0.378628
2	6	0	-1.678756	-1.001736	-0.154514
3	6	0	-2.521035	0.071583	0.295109
4	6	0	-2.175857	-1.884228	-1.102158
5	6	0	-2.097078	1.028520	1.258048
6	6	0	-3.840594	0.207362	-0.251271
7	6	0	-3.482359	-1.760849	-1.628264
8	1	0	-1.542555	-2.689939	-1.462966
9	6	0	-2.920490	2.061140	1.646638
10	1	0	-1.116228	0.923585	1.707011
11	6	0	-4.666861	1.280876	0.173603
12	6	0	-4.294363	-0.733737	-1.211996
13	1	0	-3.834854	-2.475717	-2.366416
14	6	0	-4.217991	2.193133	1.099482
15	1	0	-2.573421	2.779098	2.384388
16	1	0	-5.664065	1.368241	-0.250888
17	1	0	-5.297831	-0.622360	-1.615900
18	1	0	-4.857543	3.012342	1.415661
19	6	0	1.241525	0.045561	-0.353404
20	6	0	2.657063	0.046878	-0.110324
21	6	0	0.688258	1.094016	-1.071046
22	6	0	3.315358	-0.998996	0.594575
23	6	0	3.453371	1.141417	-0.583998
24	6	0	1.477184	2.161576	-1.559672
25	1	0	-0.380825	1.110685	-1.260105
26	6	0	4.669826	-0.953352	0.840327
27	1	0	2.746209	-1.871577	0.900292
28	6	0	4.847263	1.158089	-0.316556
29	6	0	2.828421	2.187106	-1.313186
30	1	0	1.005966	2.963584	-2.120635
31	6	0	5.445392	0.138604	0.387171
32	1	0	5.149702	-1.767914	1.375594
33	1	0	5.435708	1.996418	-0.681478
34	1	0	3.441787	3.010060	-1.672247
35	1	0	6.512803	0.163516	0.586816
36	8	0	0.129161	-1.151131	2.048169
37	1	0	1.011792	-1.002966	2.419016
38	8	0	0.633344	-2.728422	-0.140640
39	1	0	0.154486	-3.474633	0.249460

c. glycol-silanes

$[CH_2O]_2SiCl_2$

HF=-1439.0996514
Thermal correction to Gibbs Free Energy= 0.034383
NImag=0

1	14	0	-0.204228	-0.000020	-0.000004
2	8	0	0.861880	0.001303	-1.261716
3	8	0	0.861874	-0.001408	1.261714
4	17	0	-1.403498	-1.656669	0.059959
5	17	0	-1.403343	1.656768	-0.059961
6	6	0	2.182184	-0.242475	-0.731840
7	1	0	2.394862	-1.316143	-0.792918
8	1	0	2.904816	0.301695	-1.344740
9	6	0	2.182173	0.242403	0.731853
10	1	0	2.394828	1.316076	0.792930
11	1	0	2.904815	-0.301753	1.344754

$[CH_2O]_2SiCl_2$ to $[CH_2O]_2SiCl(OH)$ TS

HF=-1515.5045843
Thermal correction to Gibbs Free Energy= 0.052212
NImag=1
Frequencies -- -542.4420

1	14	0	-0.089418	0.161017	0.113565
2	8	0	-0.695409	-0.996653	-0.890077
3	8	0	-1.546680	0.696434	0.735825
4	17	0	0.803082	1.895403	-0.515565
5	17	0	2.225039	-1.112919	-0.239748
6	6	0	-2.136916	-0.899452	-0.925884
7	1	0	-2.422226	-0.292293	-1.792029
8	1	0	-2.539280	-1.908272	-1.043705
9	6	0	-2.575778	-0.238131	0.390323
10	1	0	-2.677406	-0.985325	1.188833
11	1	0	-3.523099	0.297736	0.285721
12	8	0	0.615658	-0.372059	1.675814
13	1	0	0.623224	0.291817	2.391378
14	1	0	1.600183	-0.756424	1.261105

$[CH_2O]_2SiCl(OH)$

HF=-1054.7318979
Thermal correction to Gibbs Free Energy= 0.046244
NImag=0

1	14	0	-0.294771	0.357477	-0.031878
2	8	0	0.744011	-0.013241	-1.262059
3	8	0	0.728754	0.132912	1.247174
4	17	0	-1.885840	-0.956245	0.103768
5	8	0	-0.902811	1.866336	-0.186878
6	1	0	-1.861805	1.968040	-0.122308
7	6	0	2.055590	-0.106555	0.743224
8	1	0	2.614326	0.837039	0.756552
9	1	0	2.555898	-0.825549	1.397515
10	6	0	1.907632	-0.641892	-0.696419
11	1	0	1.765215	-1.729701	-0.699508
12	1	0	2.773492	-0.395709	-1.316734

$[CH_2O]_2SiCl(OH)$ to $[CH_2O]_2Si(OH)_2$ TS

HF=-1131.1452959
Thermal correction to Gibbs Free Energy= 0.068673
NImag=1
Frequencies -- -189.6398

1	14	0	-0.062709	-0.322960	-0.147171
2	8	0	-0.575751	1.233491	-0.291797
3	8	0	-1.526402	-1.018715	0.239196
4	17	0	2.463509	0.640670	-0.026017
5	8	0	0.558961	-1.234357	-1.348273
6	1	0	1.452464	-0.937503	-1.597267
7	6	0	-2.572926	-0.082538	-0.042853
8	1	0	-2.943210	-0.248772	-1.062652
9	1	0	-3.396451	-0.241838	0.659225
10	6	0	-1.961043	1.324405	0.100024
11	1	0	-2.004138	1.674275	1.137886
12	1	0	-2.451424	2.058349	-0.544308
13	8	0	0.700172	-0.735226	1.467320
14	1	0	1.681515	-0.417461	1.300094
15	1	0	0.607489	-1.669740	1.735120

$[CH_2O]_2Si(OH)_2$

HF=-670.3596105
Thermal correction to Gibbs Free Energy= 0.058973
NImag=0

1	14	0	0.610310	-0.000008	-0.000021
2	8	0	-0.462803	-0.878679	0.906572
3	8	0	-0.462820	0.878548	-0.906702
4	8	0	1.546123	-1.037266	-0.874116
5	1	0	2.213829	-0.625291	-1.440173
6	8	0	1.545925	1.037381	0.874157
7	1	0	2.212948	0.625452	1.441054
8	6	0	-1.775247	0.684234	-0.357147
9	1	0	-1.990626	1.494283	0.351471
10	1	0	-2.509033	0.720411	-1.167788
11	6	0	-1.775271	-0.684235	0.357151
12	1	0	-1.990784	-1.494265	-0.351446
13	1	0	-2.508981	-0.720350	1.167864

d. tetrachlorosilane

$SiCl_4$

HF=-2130.4665922
Thermal correction to Gibbs Free Energy= -0.025732
NImag=0

1	14	0	-0.000005	0.000075	-0.000001
2	17	0	-0.003935	-1.186855	-1.664245
3	17	0	1.683258	1.159942	0.005767
4	17	0	-1.654683	1.200265	-0.015092
5	17	0	-0.024635	-1.173414	1.673571

$SiCl_4$ to $SiCl_3(OH)$ TS

HF=-2206.8642365
Thermal correction to Gibbs Free Energy= -0.007501
NImag=1
Frequencies -- -415.7825

1	17	0	0.036314	-1.717792	-1.039395
2	17	0	0.059213	1.797232	-0.943552

3	17	0	2.272203	-0.045248	0.531969
4	14	0	0.231330	0.015789	0.030062
5	8	0	-0.228225	0.025069	1.768232
6	1	0	0.317882	-0.474693	2.407351
7	1	0	-1.318640	-0.110597	1.685383
8	17	0	-2.391969	-0.024563	0.353362

$SiCl_3(OH)$

HF=-1746.1009766
Thermal correction to Gibbs Free Energy= -0.013842
NImag=0

1	14	0	-0.016938	-0.000048	0.269229
2	17	0	0.977207	1.661665	-0.415182
3	17	0	-1.931228	-0.003039	-0.427155
4	17	0	0.982712	-1.658338	-0.415533
5	8	0	-0.119992	-0.000470	1.901467
6	1	0	0.709324	-0.000474	2.402835

$SiCl_3(OH)$ to $SiCl_2(OH)_2$TS

HF=-1822.5078623
Thermal correction to Gibbs Free Energy= 0.008208
NImag=1
Frequencies -- -209.8226

1	17	0	2.281689	-0.460400	-0.095700
2	17	0	-2.389483	-0.302319	-0.046539
3	8	0	0.010191	-0.847455	1.629410
4	1	0	-0.935396	-0.899892	1.859562
5	14	0	0.249836	-0.114610	0.196651
6	8	0	-0.179507	-1.048579	-1.320623
7	1	0	0.335600	-0.884533	-2.135098
8	1	0	-1.209998	-0.937564	-1.373835
9	17	0	0.088184	1.909472	-0.067999

$SiCl_2(OH)_2$

HF=-1361.733971
Thermal correction to Gibbs Free Energy= -0.001124
NImag=0

1	14	0	0.000042	0.357332	-0.008058
2	17	0	1.652812	-0.865062	-0.020343
3	17	0	-1.652545	-0.865464	-0.021007
4	8	0	-0.000701	1.340131	1.306135
5	1	0	-0.002900	0.931518	2.183220
6	8	0	0.000666	1.312476	-1.333097
7	1	0	-0.001929	2.263923	-1.151761

$SiCl_2(OH)_2$ to $SiCl(OH)_3$TS

HF=-1438.1494687
Thermal correction to Gibbs Free Energy= 0.023028
NImag=1
Frequencies -- -145.4944

1	17	0	2.272156	0.115499	-0.018123
2	17	0	-2.318430	0.085900	-0.010331
3	8	0	0.045957	-1.242430	-1.238496
4	1	0	-0.885893	-1.429864	-1.442102
5	14	0	0.214314	-0.230493	0.030431
6	8	0	-0.078294	1.568739	-0.399751
7	1	0	0.534654	2.211620	0.007465
8	1	0	-1.048187	1.744348	-0.232793
9	8	0	0.041876	-0.578505	1.620626
10	1	0	-0.890615	-0.705422	1.866086

$SiCl(OH)_3$

HF=-977.366064
Thermal correction to Gibbs Free Energy= 0.011647
NImag=0

1	14	0	-0.350156	0.012021	-0.024510
2	17	0	1.708722	0.014335	0.123412
3	8	0	-0.798804	-1.302260	-0.910594
4	1	0	-0.253752	-1.503311	-1.684438
5	8	0	-1.105015	-0.120713	1.425913
6	1	0	-1.224469	-1.025863	1.747104
7	8	0	-0.724534	1.469093	-0.675796
8	1	0	-1.641058	1.748224	-0.533719

$SiCl(OH)_3$ to $Si(OH)_4$TS

HF=-1053.7820771

Thermal correction to Gibbs Free Energy= 0.036029
NImag=1
Frequencies -- -128.5474

1	8	0	0.345356	-0.192231	1.711552
2	1	0	-0.581877	-0.292466	1.979430
3	8	0	0.429053	-1.453277	-0.941957
4	1	0	-0.482285	-1.740200	-1.109941
5	8	0	2.133633	0.219860	-0.060213
6	1	0	2.619043	-0.404083	-0.616402
7	14	0	0.520104	-0.169121	0.080549
8	8	0	0.178309	1.543306	-0.642744
9	1	0	0.871005	2.186941	-0.399674
10	1	0	-0.745338	1.830094	-0.450415
11	17	0	-1.979578	-0.009051	-0.062575

$Si(OH)_4$

HF=-592.9959338
Thermal correction to Gibbs Free Energy= 0.025173
NImag=0

1	14	0	-0.000025	0.000003	-0.000019
2	8	0	1.155739	-0.795337	-0.866630
3	1	0	1.896571	-0.236966	-1.141150
4	8	0	-0.795328	-1.155965	0.866414
5	1	0	-0.236761	-1.896560	1.141198
6	8	0	-1.156043	0.795546	-0.866115
7	1	0	-1.896507	0.237098	-1.141453
8	8	0	0.795600	1.155755	0.866344
9	1	0	0.237308	1.896380	1.141572

Water

HF=-76.4273616
Thermal correction to Gibbs Free Energy= 0.002654
NImag=0

1	8	0	0.000000	0.000000	0.119721
2	1	0	0.000000	0.761555	-0.478885
3	1	0	0.000000	-0.761555	-0.478885

Hydrogen chloride

HF=-460.7992656
Thermal correction to Gibbs Free Energy= -0.011484
NImag=0

1	17	0	0.000000	0.000000	0.071638
2	1	0	0.000000	0.000000	-1.217838

e. NBO geometries

CH_3OH H_2O

C	1.63812900	-0.33878900	-0.01116500
H	2.50727300	0.07150500	0.51205400
H	1.94620800	-0.58470000	-1.03985200
H	1.34978600	-1.27629400	0.49104700
O	0.61811400	0.64154400	0.03194700
H	-0.17968800	0.25926400	-0.37862900
O	-2.01803800	-0.25629500	-0.04061400
H	-1.71386500	-0.03756500	0.85549100
H	-2.53909300	0.51853200	-0.30378900

SiH_3OH H_2O

Si	1.16559500	-0.33062100	-0.00006600
H	2.60169000	0.03811100	0.00514200
H	0.89548000	-1.18854400	-1.19669500
H	0.88789200	-1.19275800	1.19189000
O	0.28859300	1.07014300	-0.00003100
H	-0.67534800	0.89817900	-0.00134400
O	-2.23386400	-0.13036300	0.00005800
H	-2.22963600	-0.72123900	0.76911800
H	-2.23624100	-0.72329800	-0.76740100

$Si(OH)_4$ H_2O

Si	-0.55228900	-0.02310400	-0.00964900
O	0.35927500	-1.20388000	-0.66792000
H	1.32761500	-1.01800000	-0.61479300
O	0.39426300	0.69659700	1.16607900
H	0.06518700	1.56065200	1.45324100
O	-0.98955000	1.23947800	-0.97982700
H	-1.75718100	1.06558600	-1.54226600

O	-1.95287500	-0.69736800	0.54038200
H	-1.85493900	-1.62663000	0.79266800
O	2.78355500	-0.10731100	-0.04564800
H	2.21759100	0.32584900	0.62641300
H	2.97642000	0.59587900	-0.68470300

$SiCl(OH)_3$ H_2O double bonding

Si	0.51626500	-0.39184200	0.00016600
O	-0.17522200	-0.96827000	-1.36817100
H	-1.14693600	-0.92331400	-1.31966900
O	-0.17649100	-0.96489600	1.36943700
H	-1.14801300	-0.91507200	1.32180000
O	2.11708300	-0.70793300	-0.00070700
H	2.70044500	0.06180600	0.01344000
Cl	0.27029500	1.70706600	-0.00131000
O	-2.55597300	-0.14916900	0.00026900
H	-3.52054500	-0.24330200	-0.00014600
H	-2.38284100	0.80770700	-0.00210800

$SiCl(OH)_3$ H_2O single bonding

Si	0.36978900	-0.38261000	-0.02481900
O	-0.55531200	-0.66605900	-1.33631900
H	-1.48168300	-0.35524700	-1.19039200
O	-0.47344800	-0.56322900	1.39788700
H	-0.27219100	-1.39458800	1.85349500
O	1.63830600	-1.42495200	-0.00007300
H	1.83309700	-1.83853500	-0.85353900
Cl	1.01552100	1.58002100	-0.00638700
O	-2.78545900	0.26501300	-0.07213600
H	-2.77688400	1.23295600	-0.01039000
H	-2.33594300	-0.03459200	0.74198500

$(CH_2)_2O_2SiClOH$ H_2O

Si	0.09892300	-0.22073700	0.00742600
O	1.17072600	-0.16711700	1.26681400
O	1.18010000	-0.20895800	-1.24619400
Cl	-1.02949500	1.54150200	-0.09064700
O	-0.91826400	-1.47065000	0.08759400
H	-1.89059500	-1.30849400	-0.00591300

C	2.50981300	-0.33270400	-0.71358700
H	2.81173600	-1.38633500	-0.75598300
H	3.19352800	0.25801500	-1.32952700
C	2.46664700	0.17009000	0.74455900
H	2.60117300	1.25831900	0.78968900
H	3.22938900	-0.30692300	1.36600900
O	-3.50521800	-0.68652200	-0.03450900
H	-3.31948500	0.23229500	-0.29442500
H	-3.78675500	-0.62044500	0.89170500

$(CH_2)_2O_2Si(OH)_2$ H_2O

Si	0.09892300	-0.22073700	0.00742600
O	1.17072600	-0.16711700	1.26681400
O	1.18010000	-0.20895800	-1.24619400
Cl	-1.02949500	1.54150200	-0.09064700
O	-0.91826400	-1.47065000	0.08759400
H	-1.89059500	-1.30849400	-0.00591300
C	2.50981300	-0.33270400	-0.71358700
H	2.81173600	-1.38633500	-0.75598300
H	3.19352800	0.25801500	-1.32952700
C	2.46664700	0.17009000	0.74455900
H	2.60117300	1.25831900	0.78968900
H	3.22938900	-0.30692300	1.36600900
O	-3.50521800	-0.68652200	-0.03450900
H	-3.31948500	0.23229500	-0.29442500
H	-3.78675500	-0.62044500	0.89170500

$(CH_2)_2O_{2C}(OH)_2$ H_2O

O	0.02556300	0.85369200	0.39615000
O	1.29685200	-0.98196100	-0.01937600
O	-0.48998400	-0.61313700	-1.32699900
H	-1.42162000	-0.32466200	-1.30848100
O	-0.75363900	-1.24373500	0.88716800
H	-1.66822600	-0.90404700	0.81957100
C	2.18120800	0.12914000	0.14163500
H	2.60146700	0.11313500	1.15454800
H	2.99001500	0.05172700	-0.59004600
C	1.27719500	1.34510400	-0.07632200
H	1.21019300	1.61562200	-1.13760000
H	1.55678000	2.21870000	0.51659500
O	-2.65558100	0.64500900	0.02204100
H	-3.44581900	1.09606600	0.35146600
H	-1.88753300	1.20417200	0.25612100
C	-0.01189300	-0.53251900	-0.02098600

BIFOXSiCl(OH) H_2O

H	5.48397600	2.39343400	-0.21359400
C	4.55104600	1.94275900	0.14292900
H	4.33409300	2.38485100	1.11726500
C	3.40349600	2.13899300	-0.88192900
C	4.69241500	0.41312100	0.18409900
H	3.74625500	2.69963700	-1.75803900
H	2.55531700	2.67697100	-0.46982300
C	3.02855000	0.69763900	-1.35332600
C	4.44398000	0.06412200	-1.29365300
H	5.64574300	0.07009200	0.59857500
C	3.48219200	-0.25931300	0.90156000
Cl	-0.01272900	3.18169600	-1.10125900
C	2.27377400	-0.02072900	-0.15867500
C	2.29389000	0.74674400	-2.69165800
H	4.50098000	-1.00297500	-1.50423000
H	5.13618800	0.57720700	-1.97155200
C	3.82767500	-1.74165800	1.13881600
C	3.16327800	0.35265300	2.27198200
Si	-0.10893100	1.48588500	0.17238500
H	1.35481800	1.29998200	-2.59892000
O	1.36841800	0.89213700	0.44359800
C	1.56626900	-1.34994100	-0.48274000
H	2.90955100	1.27573100	-3.42840300
H	2.04938000	-0.23377800	-3.10151000
H	4.65142200	-1.79817200	1.85952900
H	4.14339900	-2.26261700	0.23228800
H	2.98169200	-2.29685200	1.55229500
H	2.33482800	-0.17703200	2.74885200
H	2.87199100	1.40024400	2.21341100
H	4.04367000	0.26889300	2.92090800
O	-1.03953700	0.44628000	-0.68514500
O	-0.62893400	2.02190800	1.61205400
C	0.52694800	-1.91991900	0.29763800
C	2.12859600	-2.16477800	-1.48180400
C	-2.17205900	-0.27456000	-0.14958900
H	-1.02313800	2.92437900	1.65745200
C	-0.35634400	-1.34305700	1.38786900
C	0.27642900	-3.30041500	0.15509500
H	2.89734100	-1.75926900	-2.11776200
C	1.78780300	-3.49842100	-1.67555200
C	-3.42398000	0.71785100	-0.12003100
C	-2.67222100	-1.38262000	-1.20920500
C	-1.68549400	-0.85320200	1.19573400
C	0.05552000	-1.66221800	2.69077200
C	0.88122200	-4.09509300	-0.80974900
H	-0.42959300	-3.75334400	0.84222700
H	2.26428300	-4.06592700	-2.46969500

C	-3.45499900	1.46453400	-1.49301500
C	-3.56996500	1.75646800	0.99947600
C	-4.60789800	-0.25070800	-0.33652300
C	-4.06773300	-0.84375500	-1.64729100
C	-2.92469800	-2.76037800	-0.56973700
C	-1.69713500	-1.56641900	-2.37827200
C	-2.54135000	-0.85931000	2.30369800
C	-0.79048200	-1.56359500	3.79125400
H	1.05997200	-2.05019700	2.82619700
H	0.63639600	-5.15049800	-0.88292100
H	-4.16987600	2.29006500	-1.40663800
H	-2.48692400	1.89578900	-1.74272500
C	-3.93928400	0.41274800	-2.51956100
H	-4.62975100	2.02275500	1.09312400
H	-3.04010300	2.67865800	0.75037200
H	-3.21027900	1.43702500	1.97510900
H	-4.75543600	-0.98354500	0.45999700
H	-5.54836800	0.29648100	-0.47007100
H	-4.67385000	-1.63423700	-2.10037100
H	-3.39240400	-3.41321900	-1.31596700
H	-3.58910000	-2.71500800	0.29632500
H	-2.00054000	-3.23551600	-0.25550300
H	-0.78220300	-2.06441600	-2.05389900
H	-1.40772500	-0.61826900	-2.83188700
H	-2.16780400	-2.19138400	-3.14739000
H	-3.57678600	-0.57919500	2.16987700
C	-2.11630800	-1.20221300	3.58472500
H	-0.42666400	-1.81370800	4.78358200
H	-4.91510300	0.68265200	-2.93868700
H	-3.25336500	0.28314800	-3.35903400
H	-2.82022800	-1.17232300	4.41147000
O	-1.42916200	4.63294600	1.46866500
H	-1.17889300	4.69098700	0.52935600
H	-0.72681400	5.11311600	1.93502300

BIFOXSi(OH)$_2$ H_2O

Si	-0.08542700	1.62324700	0.26443800
O	-1.06787000	0.59379300	-0.57164200
O	1.31921200	0.88929000	0.62173100
O	0.11054300	2.93530700	-0.72631000
O	-0.65396100	2.12187400	1.72931600
C	-2.13872800	-0.22045600	-0.09869000
C	2.27758700	0.15081700	-0.11547200
H	-0.45900500	3.68547200	-0.48066600
C	-3.41587900	0.72249200	0.19110400
C	-2.67868500	-1.11674300	-1.32651100
C	-1.59669000	-1.01846200	1.10366900
C	3.01454500	1.09303000	-1.16181500

C	3.48760100	-0.21930200	0.90377700
C	1.63160400	-1.12670900	-0.68330400
C	-3.45654400	1.76582700	-0.96939800
C	-4.59973100	-0.16703500	-0.24573700
C	-3.57383900	1.38753500	1.57358600
C	-4.05553700	-0.46506000	-1.64658900
C	-2.95254000	-2.57985400	-0.93121400
C	-1.72919300	-1.11952200	-2.53077800
C	-0.26030900	-1.51286000	1.16476700
C	-2.41907900	-1.24664100	2.21442700
C	3.32165800	2.44809200	-0.45056000
C	2.30267500	1.34765000	-2.49076500
C	4.45411400	0.51507700	-1.18431900
C	3.13573700	0.13125900	2.35491000
C	3.89789200	-1.70400100	0.87946100
C	4.67223100	0.61898300	0.33463500
C	0.59936000	-1.85045700	-0.03507700
C	2.21695800	-1.73028200	-1.81089400
C	-3.89489200	0.95602200	-2.21761600
H	-4.21454800	2.52081000	-0.71812300
H	-2.49720200	2.25981300	-1.12597200
H	-4.74313200	-1.05035300	0.37961800
H	-5.54082900	0.39676100	-0.25468700
H	-4.42383400	0.96671800	2.12124000
H	-3.77597000	2.46014100	1.46886800
H	-2.68765900	1.28587400	2.19597100
H	-4.67097300	-1.11666200	-2.27447900
H	-3.48728600	-3.07599500	-1.74997400
H	-3.55759100	-2.68032000	-0.02716700
H	-2.02655900	-3.12542900	-0.76796300
H	-2.23634600	-1.58096400	-3.38775900
H	-0.82807400	-1.69739900	-2.32250800
H	-1.41056400	-0.11637200	-2.81176400
C	0.19055700	-2.07439700	2.36899900
C	-1.95737000	-1.82504800	3.39412000
H	-3.45911100	-0.95765900	2.16577900
H	3.66243200	3.15402600	-1.21615300
H	2.43939300	2.88263100	0.01065600
C	4.45752000	2.12612900	0.55481600
H	2.96809100	1.91452500	-3.15337600
H	1.40712100	1.95400000	-2.33243400
H	2.00235300	0.44040600	-3.01658300
H	4.55862700	-0.49814000	-1.57128400
H	5.12993700	1.16335000	-1.75481100
H	2.34521400	-0.52230000	2.73135500
H	2.77627900	1.15277300	2.46732000
H	4.02277400	-0.00370700	2.98641300
H	4.72079700	-1.85350300	1.58814900
H	4.23941900	-2.04021200	-0.10220300
H	3.07598500	-2.36071400	1.17618700
H	5.63630200	0.25291900	0.70279700

C	0.35094700	-3.17405600	-0.45250400
C	1.88930300	-3.00321300	-2.26384300
H	2.98852500	-1.20342900	-2.34786700
H	-4.85360600	1.31663600	-2.60649800
H	-3.17216000	1.01257400	-3.03326200
H	1.20225100	-2.46540200	2.40122700
C	-0.62437600	-2.20507600	3.48960800
H	-2.63819500	-1.96407800	4.22912500
H	4.20082400	2.37865400	1.58545700
H	5.37492600	2.67279200	0.30838100
H	-0.35819300	-3.75637900	0.12532100
C	0.96848800	-3.75905000	-1.55002100
H	2.38296800	-3.40429000	-3.14446500
H	-0.22997400	-2.64009700	4.40344600
H	0.72755400	-4.77855900	-1.83644400
H	-1.17635800	2.94034900	1.66546300
O	-1.99470300	4.36540300	0.52235100
H	-2.25299400	5.26734600	0.76548700
H	-2.76371100	3.97448000	0.07585000

BIFOXSiCl(OH) Cl^-

1 1

H	5.31260800	2.56961700	-0.74039100
C	4.43185900	2.11936800	-0.27340700
H	4.24629300	2.66698400	0.65170200
C	3.21813600	2.13044800	-1.23782300
C	4.66764600	0.61590100	-0.06070600
H	3.47809200	2.58882600	-2.19723200
H	2.36903000	2.68250800	-0.84679800
C	2.90485000	0.62947000	-1.51441100
C	4.34655700	0.06477500	-1.45756800
H	5.66485600	0.37355900	0.31860500
C	3.57206500	-0.02864800	0.83260500
Cl	-0.26191000	2.98950300	-1.27790000
C	2.23745400	0.02564100	-0.17209900
C	2.07431300	0.45475600	-2.77949400
H	4.45386900	-1.01616500	-1.54135700
H	4.96089900	0.51708000	-2.24357500
C	4.02036600	-1.44926300	1.21638500
C	3.28135100	0.73057200	2.13032900
Si	-0.18216400	1.40939700	0.02922800
H	1.11956900	0.98485300	-2.70521800
O	1.34310400	0.94949300	0.37060100
C	1.61496800	-1.34797900	-0.27075200
H	2.61418500	0.89640700	-3.62399400
H	1.85275600	-0.58375200	-3.03132300
H	4.88015400	-1.36229500	1.88836200
H	4.33681700	-2.05291500	0.36401400
H	3.24110800	-2.00092900	1.75072600

H	2.55160800	0.19558000	2.74548200
H	2.89496400	1.73430000	1.96639000
H	4.21171700	0.80472400	2.70483300
O	-0.87227800	0.11376400	-0.77078300
O	-0.88162300	1.79437400	1.43414200
C	0.67730900	-1.85054200	0.71220700
C	2.21094800	-2.29860000	-1.12652600
C	-2.00907900	-0.54858500	-0.23651700
H	-1.23746400	2.72306800	1.51877800
C	-0.29454900	-1.16435600	1.60485500
C	0.68026900	-3.24522900	0.96052200
H	2.85107700	-1.95521300	-1.92163400
C	2.06827200	-3.66245600	-0.95451100
C	-3.34325400	0.33949300	-0.55904200
C	-2.36586000	-1.92035900	-1.08648200
C	-1.66129900	-0.81342600	1.20309500
C	-0.01120400	-1.26228600	2.98259300
C	1.33945100	-4.14647300	0.14209800
H	0.06338700	-3.62181000	1.76848500
H	2.55853700	-4.34852300	-1.63739200
C	-3.24325700	0.75075400	-2.05881700
C	-3.64420300	1.56506100	0.29672700
C	-4.42692100	-0.75821600	-0.64505000
C	-3.73083100	-1.57393700	-1.73862400
C	-2.57688000	-3.13994900	-0.17296900
C	-1.26819200	-2.24292600	-2.09841600
C	-2.63779500	-0.74820400	2.21390700
C	-0.97550200	-1.04204100	3.94683500
H	0.99835800	-1.52324300	3.27974900
H	1.25345800	-5.21205800	0.32745400
H	-3.98671500	1.53418400	-2.23398300
H	-2.27182900	1.17465800	-2.30657400
C	-3.57959900	-0.53292000	-2.85681700
H	-4.67894400	1.86170500	0.08795300
H	-3.02625800	2.42408900	0.02662800
H	-3.55037200	1.41883600	1.37151300
H	-4.61318300	-1.31133100	0.27762100
H	-5.37831800	-0.32452100	-0.97062100
H	-4.24872100	-2.48618500	-2.04931900
H	-2.85897000	-3.99317400	-0.79868900
H	-3.37336900	-2.99442600	0.56022600
H	-1.66953800	-3.41707000	0.36235800
H	-0.39102200	-2.67415100	-1.61820600
H	-0.94509800	-1.37221700	-2.66875900
H	-1.65621000	-2.99007300	-2.80157500
H	-3.66479700	-0.56780800	1.93571300
C	-2.31522900	-0.83387900	3.55322300
H	-0.71331200	-1.06853100	4.99938700
H	-4.52462100	-0.42839500	-3.39775200
H	-2.81799900	-0.79512600	-3.59315200
H	-3.09040900	-0.72394000	4.30453700

Cl	-1.67647300	4.66840800	1.16402100

BIFOXSi(OH)$_2$ Cl$^-$

1 1

Si	-0.11476200	1.51431600	-0.08363700
O	-0.84288200	0.16904200	-0.80570900
O	1.35376700	0.95037600	0.38284500
O	-0.10121400	2.67695700	-1.21397700
O	-0.84843100	1.89775500	1.32702700
C	-2.01309100	-0.36443000	-0.24823300
C	2.18868100	-0.00178600	-0.19027000
H	-0.31941000	3.57858000	-0.87509200
C	-3.29531500	0.59402200	-0.66390900
C	-2.47164100	-1.77453000	-0.99968000
C	-1.70885700	-0.54841200	1.20377400
C	2.80376100	0.54288300	-1.58994000
C	3.56736700	-0.09017100	0.73807800
C	1.50210400	-1.34621500	-0.23144500
C	-3.12042300	0.89873900	-2.17900200
C	-4.44659800	-0.43009000	-0.71039800
C	-3.53089000	1.88503900	0.10941400
C	-3.78021500	-1.36660700	-1.72167900
C	-2.79550500	-2.89703400	0.00126400
C	-1.38043800	-2.26242000	-1.95030000
C	-0.36574600	-0.96946700	1.64577700
C	-2.70401000	-0.39554400	2.19507100
C	3.16814000	2.04083000	-1.37348300
C	1.90773100	0.35700300	-2.80878100
C	4.22794800	-0.06041800	-1.58447300
C	3.36776600	0.68837800	2.04236200
C	3.99501200	-1.51819800	1.11781400
C	4.63070700	0.51538700	-0.21782900
C	0.56707100	-1.74883100	0.80159700
C	2.02949300	-2.36397700	-1.05319800
C	-3.50762600	-0.41681100	-2.89952500
H	-3.81857500	1.70387000	-2.42864900
H	-2.12022500	1.25998400	-2.41277800
H	-4.70122100	-0.90090200	0.24112700
H	-5.35450200	0.04515700	-1.09732600
H	-4.52931600	2.24433100	-0.16811400
H	-2.83317100	2.67399100	-0.17771600
H	-3.50512400	1.79274400	1.19454400
H	-4.35668400	-2.25555900	-1.99521400
H	-3.12513800	-3.77522300	-0.56380800
H	-3.59508200	-2.63782200	0.69811700
H	-1.92208200	-3.19480800	0.58282800
H	-1.82601800	-2.99921000	-2.63002500
H	-0.57648500	-2.76199400	-1.41394700
H	-0.94570800	-1.46241600	-2.54877700

C	-0.11824500	-1.03278000	3.03520800
C	-2.41116800	-0.45457700	3.53764700
H	-3.71103500	-0.15962000	1.88595900
H	3.41701500	2.45044400	-2.35809300
H	2.34143100	2.63172400	-0.98987900
C	4.41135600	2.02088900	-0.44768800
H	2.45110800	0.69420900	-3.69843100
H	1.00788000	0.97435200	-2.73506200
H	1.59509600	-0.67462000	-2.98318200
H	4.29908400	-1.14632800	-1.64372800
H	4.81634800	0.35190000	-2.41140500
H	2.66897600	0.17013900	2.70696900
H	2.98639700	1.69551500	1.88942800
H	4.33207700	0.75330400	2.55894300
H	4.88723800	-1.44786300	1.74811000
H	4.25549300	-2.14140700	0.26075100
H	3.22620100	-2.04005100	1.69650400
H	5.64094800	0.26295900	0.11790700
C	0.52765900	-3.12696900	1.13984900
C	1.84232100	-3.70704600	-0.78965300
H	2.65753500	-2.08865100	-1.88508300
H	-4.41862200	-0.29074500	-3.49172300
H	-2.73435400	-0.77956000	-3.57859400
H	0.87103000	-1.33063200	3.36374000
C	-1.08827500	-0.72608000	3.96539600
H	-3.18983600	-0.27444600	4.27155800
H	4.26392100	2.58346300	0.47548600
H	5.28430600	2.45041400	-0.94768600
H	-0.08711100	-3.43311500	1.97864300
C	1.12932900	-4.09594000	0.35733600
H	2.28619000	-4.45389100	-1.43979800
H	-0.84978100	-0.72761900	5.02400100
H	1.00788300	-5.14521000	0.60538200
H	-1.17677300	2.83991600	1.38833000
Cl	-1.07373800	4.77307100	0.82638900

Dimer

0 1

Si	1.98349600	-0.26048100	0.01108200
O	2.21893000	1.34660600	0.14007800
O	3.37177000	-1.06096100	0.37132400
O	1.41412600	-0.41295000	-1.55146200
O	0.85531800	-0.91575200	1.00139500
C	2.98907300	2.17168300	0.99313800
C	4.18378300	-1.76084400	-0.58386700
H	1.88350300	0.16234700	-2.17628600
H	-0.01310000	-0.47756100	0.92574300
C	4.48429000	1.83411900	0.83757600
C	2.68195900	3.70403500	0.55500300

C	2.41666700	2.13370900	2.47295200
C	4.35085300	-0.77256100	-1.76126700
C	5.57270000	-2.22753600	0.08664800
C	3.48940200	-3.17117200	-0.88387700
C	5.07194100	1.29381500	-0.33445800
C	5.36545300	2.25467400	1.84994700
C	1.90825800	4.25215900	1.79254500
C	1.87209900	3.76703000	-0.74720900
C	3.94143100	4.56318800	0.34044000
C	0.86114600	2.17178500	2.39170600
C	2.64328700	3.58673200	2.96997800
C	2.86883000	0.95747400	3.33491500
C	4.46682900	0.64054800	-1.56085700
C	4.28008900	-1.23161500	-3.08203200
C	5.44023000	-3.78016800	0.11747600
C	5.79434800	-1.61237600	1.47290700
C	6.80112000	-1.90993600	-0.78537000
C	3.07506300	-3.77041400	0.50040800
C	4.70318100	-4.06920500	-1.20117800
C	2.28060700	-3.26472200	-1.81772200
C	6.46863900	1.40949100	-0.49107600
C	6.74863700	2.26657000	1.71458800
H	4.95854300	2.61743800	2.77965900
H	1.88914800	5.34671600	1.80271900
C	0.51600900	3.60754700	1.92047000
H	1.56558700	4.80303700	-0.93618300
H	0.98493900	3.13664900	-0.72760800
H	2.48147600	3.43621300	-1.59396100
H	3.63428600	5.57157900	0.03957900
H	4.57684900	4.15449900	-0.45109400
H	4.56059600	4.65854700	1.23498700
H	0.46830000	1.40318600	1.73902300
H	0.46730800	1.97875100	3.39557100
H	2.14319500	3.75653300	3.93089700
H	3.67796100	3.91042500	3.07462500
H	2.47284000	1.07068200	4.35095600
H	3.95264600	0.85163800	3.40324700
H	2.47114700	0.01935100	2.93358100
C	4.32972600	1.48720600	-2.67157800
C	4.17104500	-0.37310300	-4.17504500
H	4.28304000	-2.29685400	-3.26517400
H	6.41696600	-4.26003000	0.23447000
C	4.40059100	-4.23399100	1.15224800
H	6.63135600	-2.12192300	1.96632700
H	4.91249600	-1.69711700	2.10806200
H	6.04305300	-0.55279600	1.39918200
H	7.68593700	-2.36754500	-0.32751000
H	6.98422700	-0.84078000	-0.84995300
H	6.71664500	-2.29770600	-1.80375600
H	2.52146800	-3.05141100	1.10215000
H	2.40947300	-4.61963600	0.31348600

H	4.40803000	-5.11988200	-1.30468300
H	5.26305700	-3.78659900	-2.09604000
H	2.10197100	-4.32415000	-2.03826300
H	2.37826400	-2.73554400	-2.76408400
H	1.38269400	-2.88365200	-1.33021300
H	6.89462600	1.09806300	-1.43886400
C	7.31228800	1.88656000	0.50339900
H	7.36756300	2.60635800	2.53996100
H	-0.05320100	3.62268100	0.98938600
H	-0.07820300	4.14121300	2.67033100
H	4.41800900	2.55681700	-2.50877900
C	4.14162700	1.00173700	-3.96502800
H	4.09049200	-0.78375900	-5.17722500
H	4.56634000	-3.80582700	2.14316500
H	4.43132800	-5.32388300	1.26293900
H	8.38363000	1.93962500	0.33465200
H	4.02618400	1.69178000	-4.79568500
O	-1.26939700	-0.57503100	-2.14086300
H	-0.29267300	-0.61210300	-2.02304900
Si	-2.07718900	-0.12207600	-0.79816300
O	-2.25268000	-1.26340200	0.36631200
O	-3.55173700	0.41020000	-1.29025500
O	-1.09060000	0.95748000	-0.00047100
C	-3.14774800	-2.35430800	0.51144200
C	-4.09708800	1.69204700	-0.94285200
H	-1.51692000	1.43935700	0.72512300
C	-4.58626300	-1.81622000	0.61867100
C	-2.73395300	-3.15219800	1.86408000
C	-2.87068600	-3.44154300	-0.60868900
C	-3.91968000	1.79613300	0.59102600
C	-5.62841300	1.80177200	-1.43276700
C	-3.39552000	2.80499500	-1.86259600
C	-4.92308100	-0.55090700	1.16534500
C	-5.64947700	-2.69592500	0.35364800
C	-2.19624400	-4.50085300	1.29690900
C	-1.69970600	-2.38601800	2.69748800
C	-3.91908200	-3.45494100	2.80158000
C	-1.32456800	-3.59238900	-0.75338400
C	-3.15751000	-4.77630100	0.12713600
C	-3.51395800	-3.19044900	-1.97098900
C	-4.07269200	0.66802500	1.46034000
C	-3.50399600	3.00371500	1.16923000
C	-5.56108700	2.87469900	-2.56004700
C	-6.19183400	0.45937000	-1.91321200
C	-6.56857600	2.36424400	-0.35065600
C	-3.38010600	2.23150000	-3.31803600
C	-4.51459300	3.85728100	-2.00887700
C	-1.99071100	3.33158200	-1.55356300
C	-6.24669400	-0.34870800	1.60395000
C	-6.97073800	-2.43208900	0.69760800
H	-5.43848700	-3.64726100	-0.10840300

H	-2.15686600	-5.27445900	2.07046700
C	-0.86756900	-4.30977900	0.54195000
H	-1.40843600	-2.99820200	3.55983900
H	-0.79849500	-2.13285300	2.14565200
H	-2.12301500	-1.45217200	3.07813300
H	-3.54272700	-3.99335400	3.67880400
H	-4.40345300	-2.53839500	3.15134800
H	-4.69221800	-4.07299200	2.34066600
H	-0.82589900	-2.64234500	-0.91318200
H	-1.13111500	-4.20725300	-1.63913700
H	-2.84888700	-5.63491000	-0.48092800
H	-4.18909500	-4.94355500	0.43681100
H	-3.33342300	-4.05176100	-2.62506900
H	-4.59115600	-3.02138600	-1.92512000
H	-3.06135800	-2.31956300	-2.45521100
C	-3.67582700	0.79875000	2.79955200
C	-3.11927200	3.11080100	2.50584100
H	-3.46543100	3.89036200	0.55312200
H	-6.55020700	3.29516200	-2.76702200
C	-4.84519500	2.33655700	-3.80717100
H	-7.14909700	0.63019400	-2.42134700
H	-5.51828000	-0.04898500	-2.60313300
H	-6.37045400	-0.21641300	-1.07660900
H	-7.55782300	2.52752700	-0.79395600
H	-6.69352400	1.67191200	0.47715100
H	-6.22762100	3.31806300	0.06013700
H	-2.97980000	1.21943800	-3.34893300
H	-2.71940400	2.86388000	-3.92062600
H	-4.23824300	4.63674200	-2.72842300
H	-4.80871600	4.34689400	-1.07731400
H	-1.80219000	4.19079700	-2.20837400
H	-1.82913300	3.66375000	-0.52872700
H	-1.22864200	2.58178700	-1.77084900
H	-6.46739700	0.57302900	2.13151900
C	-7.27043300	-1.26216900	1.38368400
H	-7.74346000	-3.15881600	0.46402300
H	-0.12612300	-3.73545200	1.09874900
H	-0.42106600	-5.28570300	0.32015300
H	-3.80692300	-0.05760500	3.45271100
C	-3.16522400	1.98534400	3.32133800
H	-2.77914200	4.06642400	2.89306800
H	-5.25075400	1.38554500	-4.15848200
H	-4.94003500	3.05154400	-4.63234600
H	-8.27806000	-1.04930300	1.72787300
H	-2.85113300	2.03463700	4.35965700

8. **X-ray details**

BIFOXSiCl$_2$ **7**

Empirical formula	C41 H50.50 Cl2 O2 Si	
Moiety formula	C32 H40 Cl2 O2 Si, 3/4(C6 H14)	
Formula weight	674.30	
Temperature	0(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 10.4216(14) Å	α= 90°.
	b = 16.463(2) Å	β= 90°.
	c = 18.727(2) Å	γ = 90°.
Volume	3213.0(7) Å^3	
Z	4	
Density (calculated)	1.394 Mg/m^3	
Absorption coefficient	2.462 mm^{-1}	
F(000)	1442	
Crystal size	0.200 x 0.200 x 0.200 mm^3	
Theta range for data collection	3.575 to 72.283°.	
Index ranges	-6<=h<=12, -20<=k<=20, -23<=l<=19	
Reflections collected	13374	
Independent reflections	5946 [R(int) = 0.0239]	
Completeness to theta = 67.679°	97.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7536 and 0.5292	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5946 / 0 / 340	
Goodness-of-fit on F^2	0.558	
Final R indices [I>2sigma(I)]	R1 = 0.0286, wR2 = 0.0862	
R indices (all data)	R1 = 0.0295, wR2 = 0.0892	
Absolute structure parameter	0.041(5)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.234 and -0.478 e.Å^{-3}	

BIFOXSiCl(OH) **8**

Empirical formula	C36.50 H51.50 Cl O3 Si
Moiety formula	C32 H41 Cl O3 Si, 3/4(C6 H14)
Formula weight	601.81

Temperature	100(2) K
Wavelength	1.54178 Å
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
Unit cell dimensions	a = 10.4969(12) Å α= 90°.
	b = 15.9441(16) Å β= 90°.
	c = 18.801(3) Å γ = 90°.
Volume	3146.6(7) $Å^3$
Z	4
Density (calculated)	1.270 Mg/m^3
Absorption coefficient	1.708 mm^{-1}
F(000)	1302
Crystal size	0.300 x 0.250 x 0.200 mm^3
Theta range for data collection	3.635 to 72.173°.
Index ranges	-12<=h<=9, -15<=k<=19, -22<=l<=21
Reflections collected	12083
Independent reflections	5493 [R(int) = 0.0408]
Completeness to theta = 67.679°	98.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7535 and 0.5042
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5493 / 0 / 340
Goodness-of-fit on F^2	1.046
Final R indices [I>2sigma(I)]	R1 = 0.0335, wR2 = 0.0846
R indices (all data)	R1 = 0.0348, wR2 = 0.0855
Absolute structure parameter	0.091(8)
Extinction coefficient	n/a
Largest diff. peak and hole	0.283 and -0.409 $e.Å^{-3}$

BIFOXSi$(OH)_2$ **9** in toluene

Empirical formula	C32 H42 O4 Si
Moiety formula	C32 H42 O4 Si
Formula weight	518.74
Temperature	100(2) K
Wavelength	1.54178 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 15.3371(5) Å α= 90°.

	b = 12.8277(5) Å	β= 107.4350(10)°.
	c = 14.6917(5) Å	γ = 90°.
Volume	2757.65(17) Å^3	
Z	4	
Density (calculated)	1.249 Mg/m^3	
Absorption coefficient	1.028 mm^{-1}	
F(000)	1120	
Crystal size	0.200 x 0.200 x 0.100 mm^3	
Theta range for data collection	4.584 to 72.350°.	
Index ranges	-18<=h<=18, -15<=k<=15, -18<=l<=17	
Reflections collected	36980	
Independent reflections	5435 [R(int) = 0.0233]	
Completeness to theta = 67.679°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7536 and 0.6518	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5435 / 0 / 348	
Goodness-of-fit on F^2	1.047	
Final R indices [I>2sigma(I)]	R1 = 0.0337, wR2 = 0.0841	
R indices (all data)	R1 = 0.0344, wR2 = 0.0847	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.318 and -0.401 e.Å^{-3}	

BIFOXSi(OH)$_2$ **9** in hexane

Empirical formula	C131 H175 O16 Si4	
Moiety formula	4(C32 H42 O4 Si), 0.5(C6 H14)	
Formula weight	2118.06	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	C2	
Unit cell dimensions	a = 29.2834(10) Å	α= 90°.
	b = 12.5929(4) Å	β= 113.8850(10)°.
	c = 34.1671(11) Å	γ = 90°.
Volume	11520.5(7) Å^3	
Z	4	
Density (calculated)	1.221 Mg/m^3	
Absorption coefficient	0.994 mm^{-1}	

F(000)	4580
Crystal size	0.200 x 0.150 x 0.100 mm^3
Theta range for data collection	3.301 to 72.230°.
Index ranges	-36<=h<=36, -15<=k<=14, -39<=l<=42
Reflections collected	69567
Independent reflections	22299 [R(int) = 0.0325]
Completeness to theta = 67.679°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7536 and 0.6262
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	22299 / 1 / 1417
Goodness-of-fit on F^2	1.031
Final R indices [I>2sigma(I)]	R1 = 0.0327, wR2 = 0.0841
R indices (all data)	R1 = 0.0339, wR2 = 0.0851
Absolute structure parameter	0.028(4)
Extinction coefficient	n/a
Largest diff. peak and hole	0.391 and -0.353 e.$Å^{-3}$

$BIFOXSi(OH)_2$ **9** in acetone

Empirical formula	C35 H48 O5 Si	
Moiety formula	C32 H42 O4 Si, C3 H6 O	
Formula weight	576.82	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Tetragonal	
Space group	$P4_12_12$	
Unit cell dimensions	a = 12.8327(4) Å	α= 90°.
	b = 12.8327(4) Å	β= 90°.
	c = 37.7649(11) Å	γ = 90°.
Volume	6219.1(4) $Å^3$	
Z	8	
Density (calculated)	1.232 Mg/m^3	
Absorption coefficient	0.986 mm^{-1}	
F(000)	2496	
Crystal size	0.200 x 0.200 x 0.100 mm^3	
Theta range for data collection	3.638 to 74.528°.	
Index ranges	-13<=h<=15, -16<=k<=13, -47<=l<=46	
Reflections collected	51773	

Independent reflections	6351 [R(int) = 0.0298]
Completeness to theta = 67.679°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7538 and 0.6308
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6351 / 0 / 410
Goodness-of-fit on F^2	1.086
Final R indices [I>2sigma(I)]	R1 = 0.0306, wR2 = 0.0799
R indices (all data)	R1 = 0.0318, wR2 = 0.0801
Absolute structure parameter	0.032(4)
Extinction coefficient	n/a
Largest diff. peak and hole	0.222 and -0.324 e.$Å^{-3}$

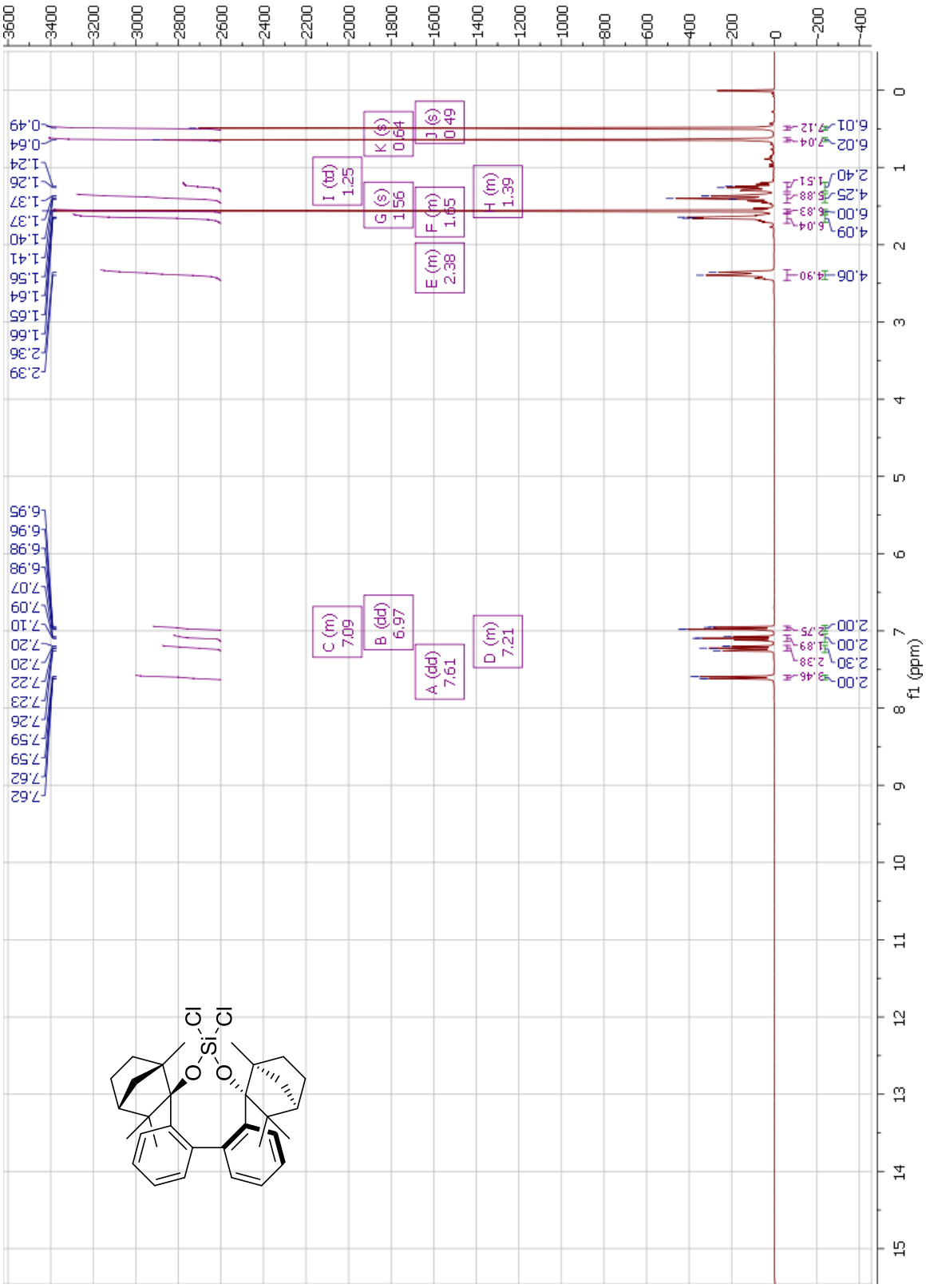
BIFOXSiCl(OH) **8** in acetone

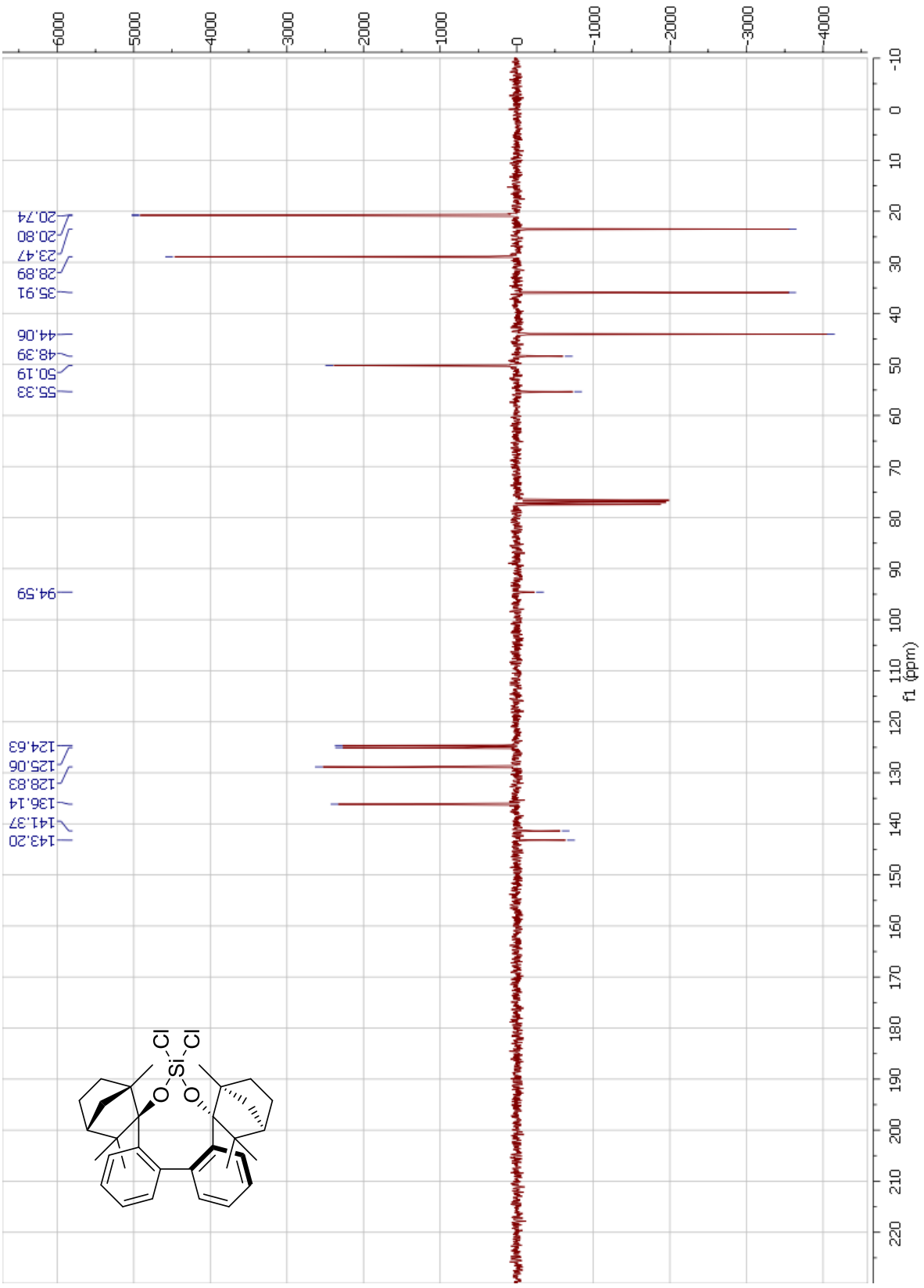
Empirical formula	C35 H47 Cl O4 Si
Moiety formula	C32 H41 Cl O3 Si, C3 H6 O
Formula weight	595.26
Temperature	100(2) K
Wavelength	1.54178 Å
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
Unit cell dimensions	a = 10.5180(16) Å α= 90°. b = 16.3280(13) Å β= 90°. c = 18.1007(18) Å γ = 90°.
Volume	3108.6(6) $Å^3$
Z	4
Density (calculated)	1.272 Mg/m^3
Absorption coefficient	1.750 mm^{-1}
F(000)	1280
Crystal size	0.300 x 0.200 x 0.100 mm^3
Theta range for data collection	3.646 to 72.159°.
Index ranges	-12<=h<=12, -18<=k<=20, -21<=l<=22
Reflections collected	23558
Independent reflections	6088 [R(int) = 0.0407]
Completeness to theta = 67.679°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7536 and 0.5440
Refinement method	Full-matrix least-squares on F^2

Data / restraints / parameters	6088 / 1 / 382
Goodness-of-fit on F^2	1.020
Final R indices [I>2sigma(I)]	R1 = 0.0303, wR2 = 0.0733
R indices (all data)	R1 = 0.0316, wR2 = 0.0742
Absolute structure parameter	0.051(6)
Extinction coefficient	n/a
Largest diff. peak and hole	0.237 and -0.356 e.$Å^{-3}$

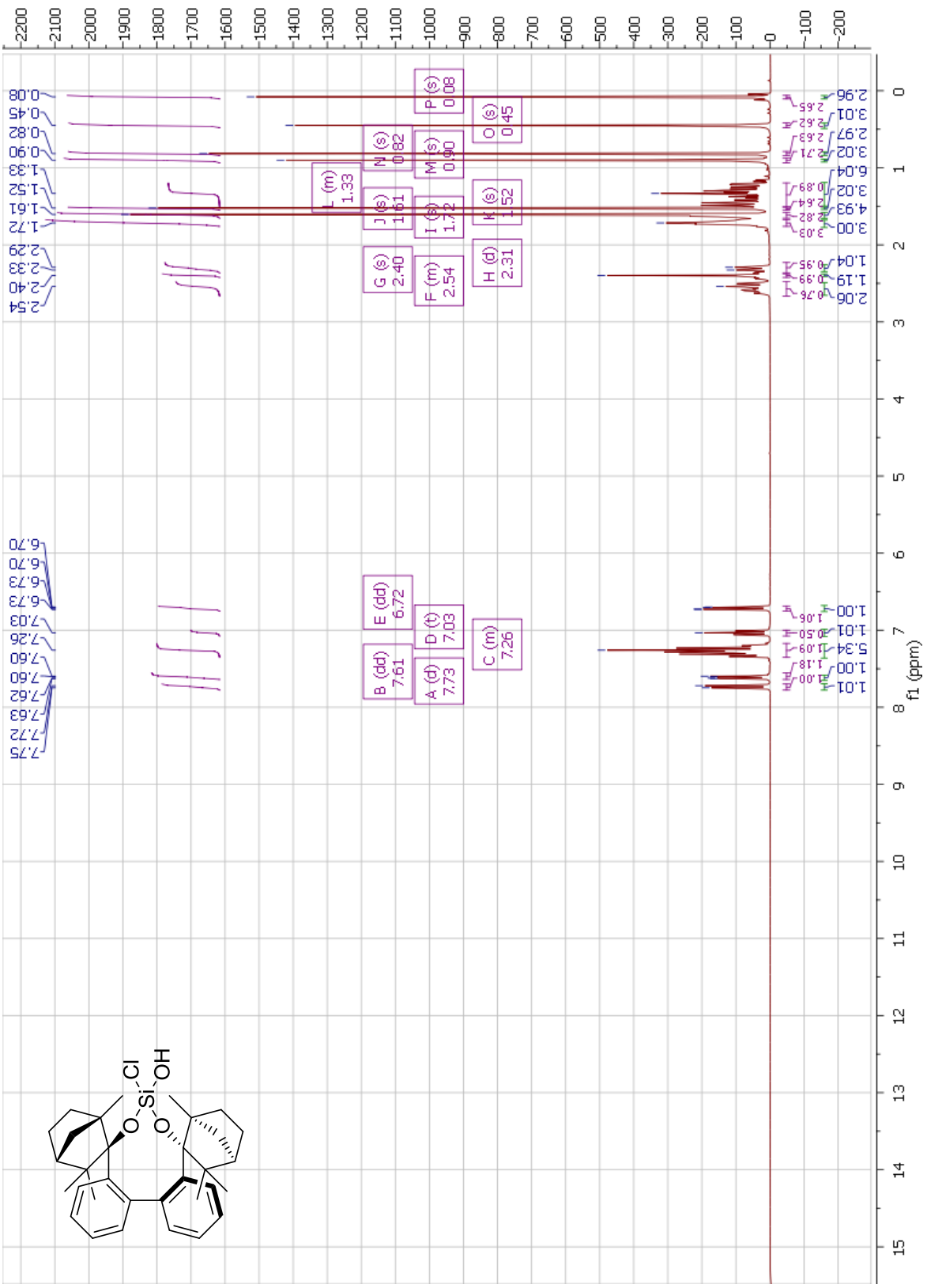
9. **Selected NMR spectra**

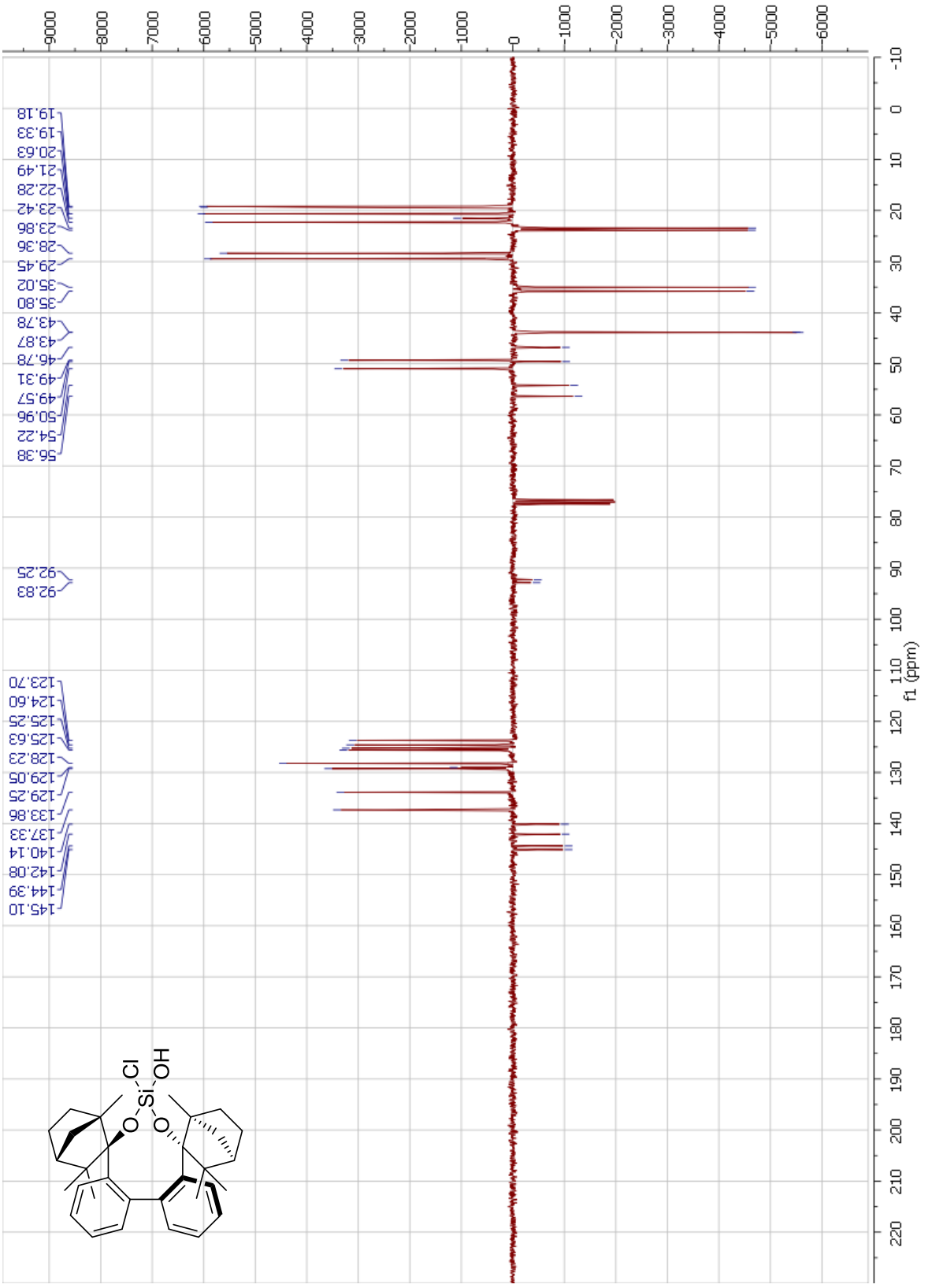
a. BIFOXSiCl$_2$



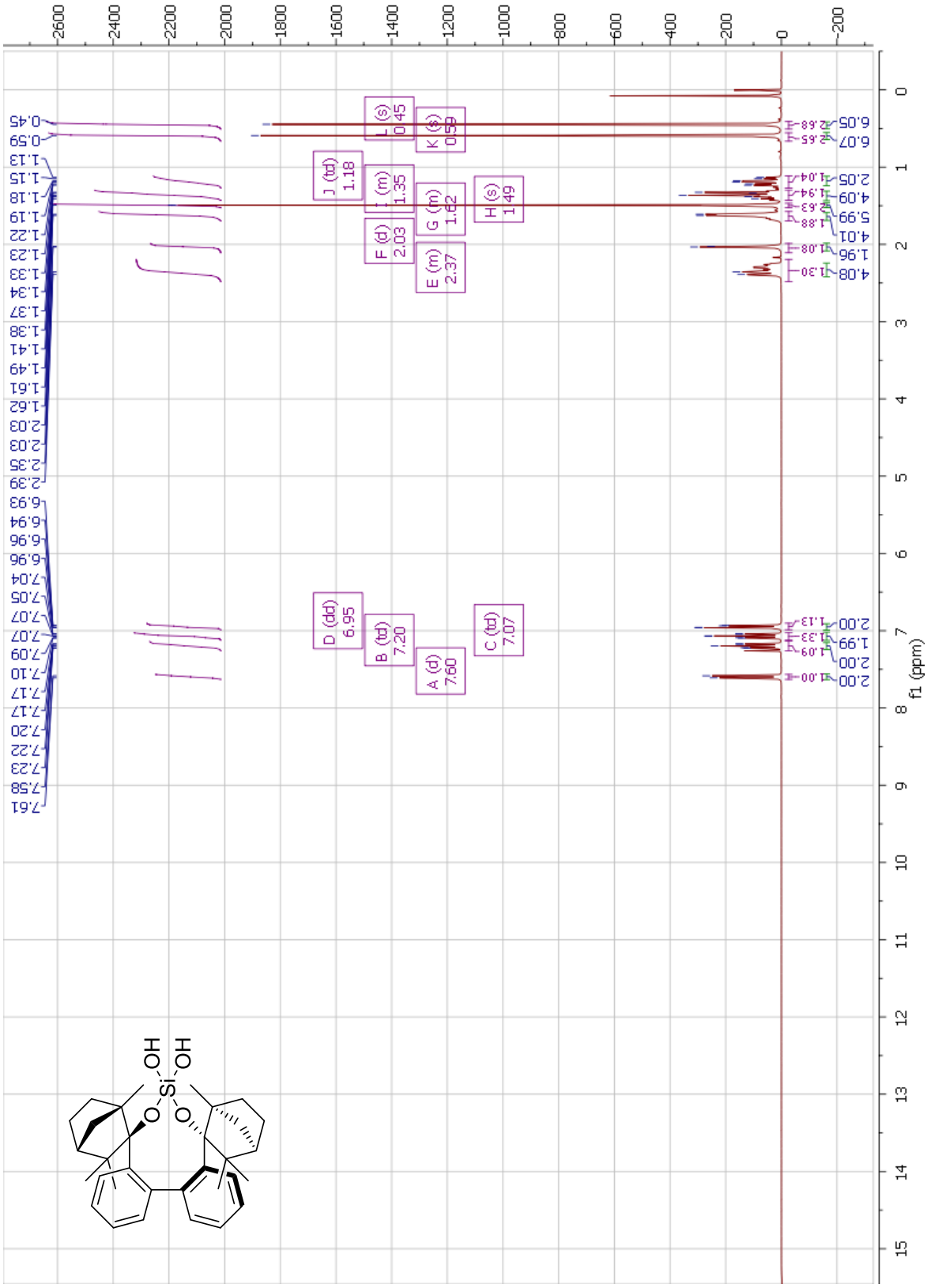

20.74
20.80
23.47
28.89
35.91
44.06
48.39
50.19
55.33
94.59
124.63
125.06
128.83
136.14
141.37
143.20
f1 (ppm)
Cl
Si
Cl
O
O

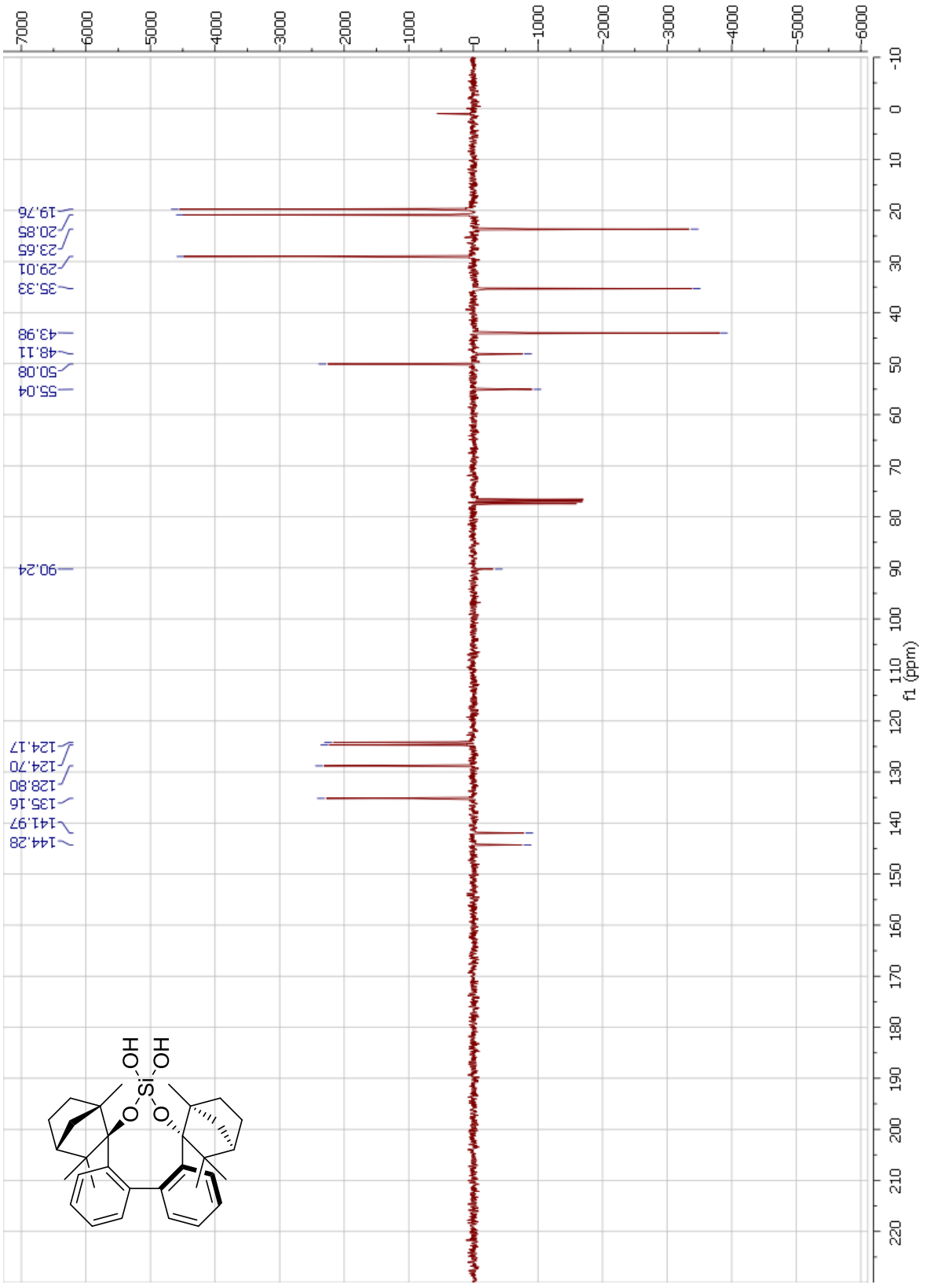
b. BIFOXSiCl(OH) 8



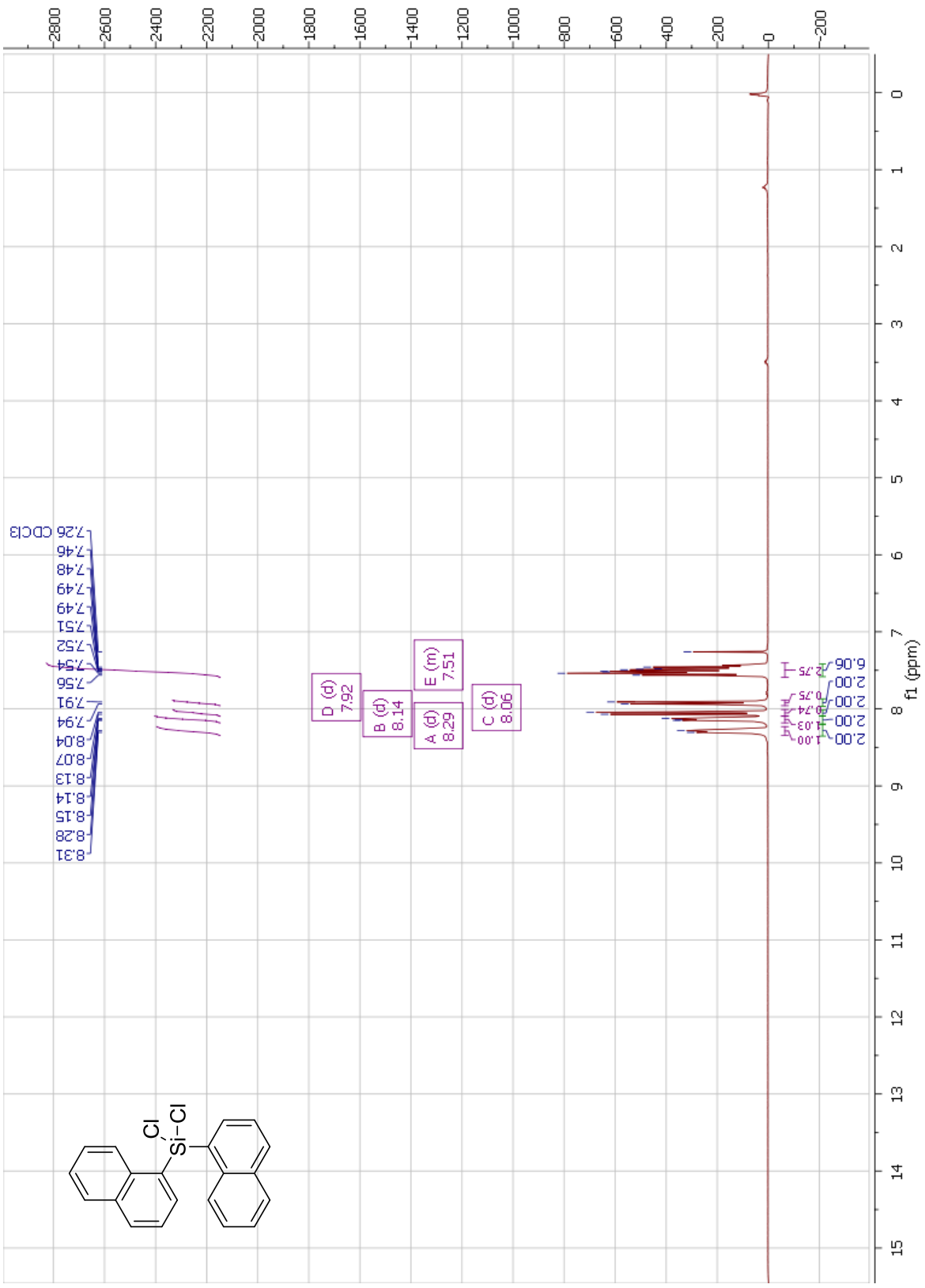

19.18
19.33
20.63
21.49
22.28
23.42
23.86
28.36
29.45
35.02
35.80
43.78
43.87
46.78
49.31
49.57
50.96
54.22
56.38
92.83
92.25
123.70
124.60
125.25
125.63
128.23
129.05
129.25
133.86
137.33
140.14
142.08
144.39
145.10
Cl
Si
OH
O
O
f1 (ppm)

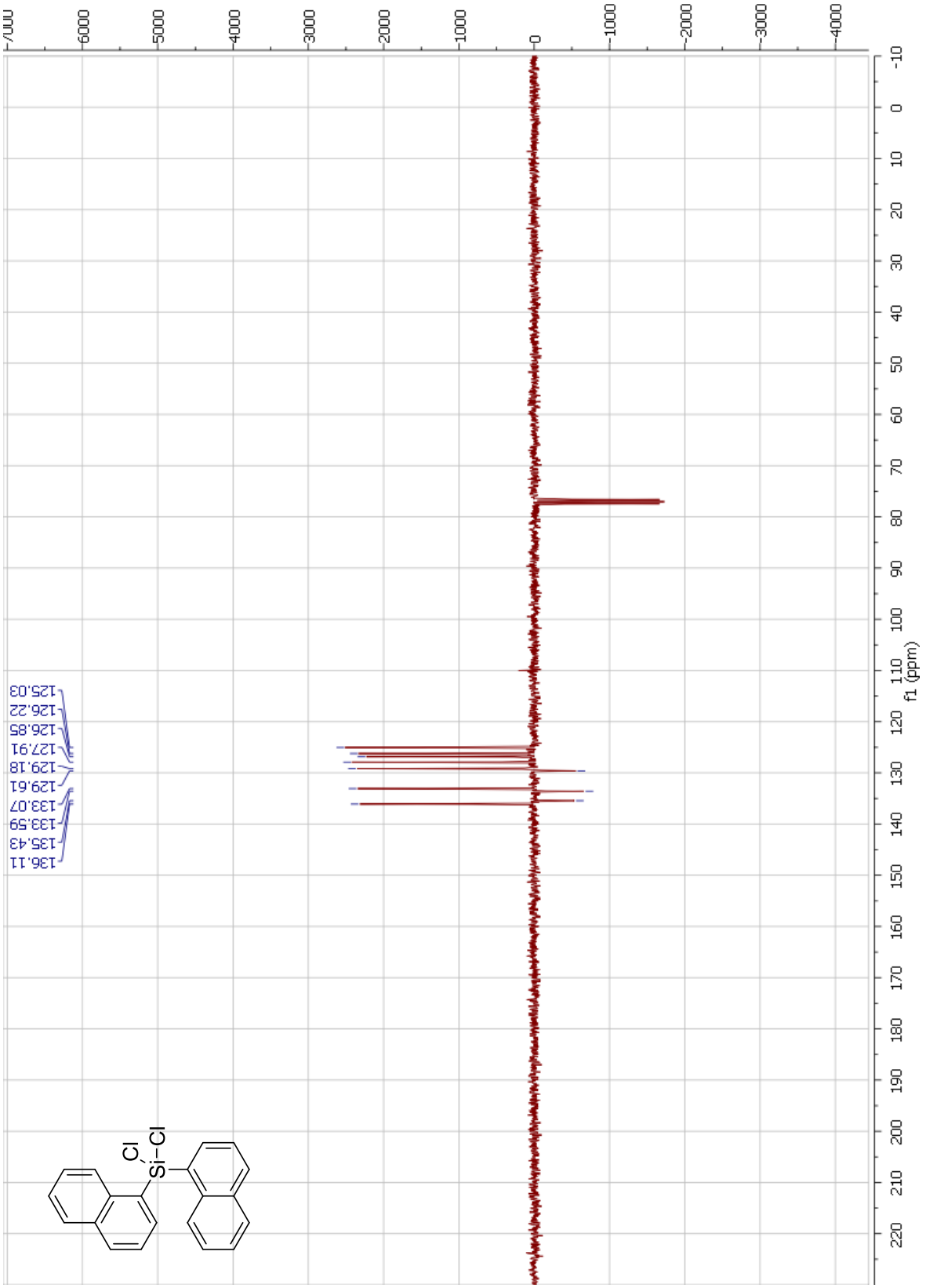
c. BIFOXSi(OH)$_2$ 9



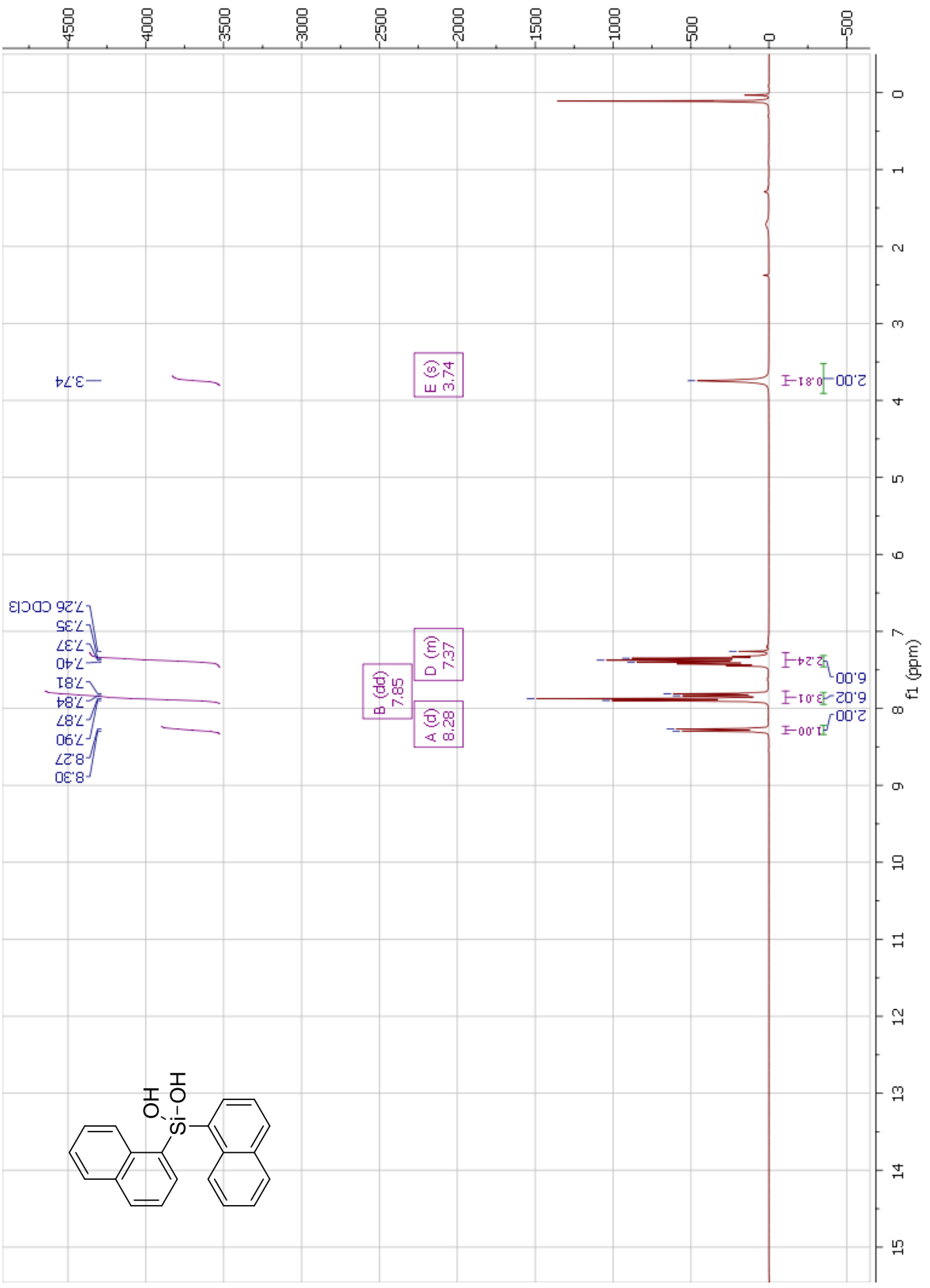

144.28
141.97
135.16
128.80
124.70
124.17
90.24
55.04
50.08
48.11
43.98
35.33
29.01
23.65
20.85
19.76
f1 (ppm)
OH
OH
Si
O
O

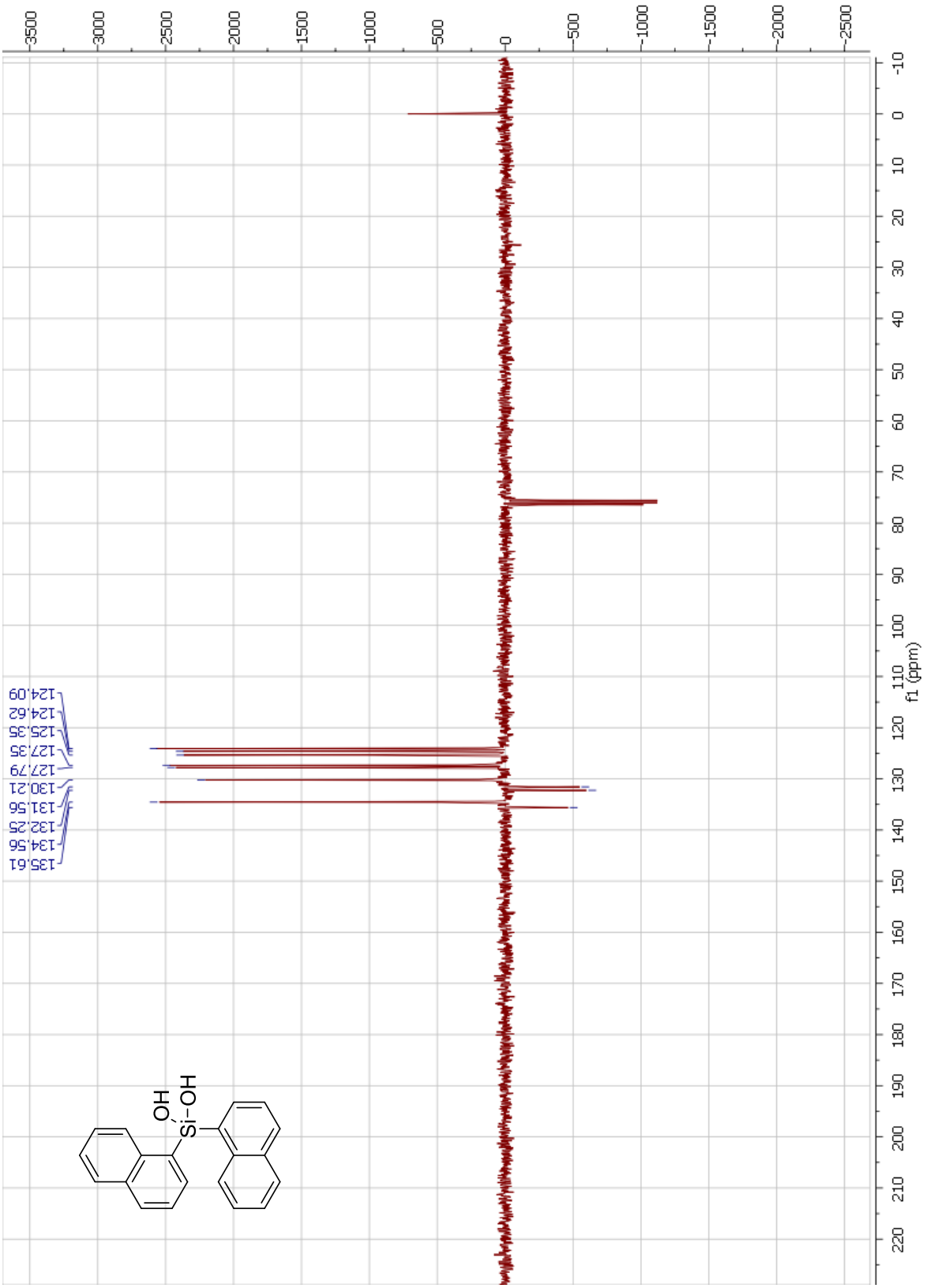
d. Kondo-$SiCl_2$ 13



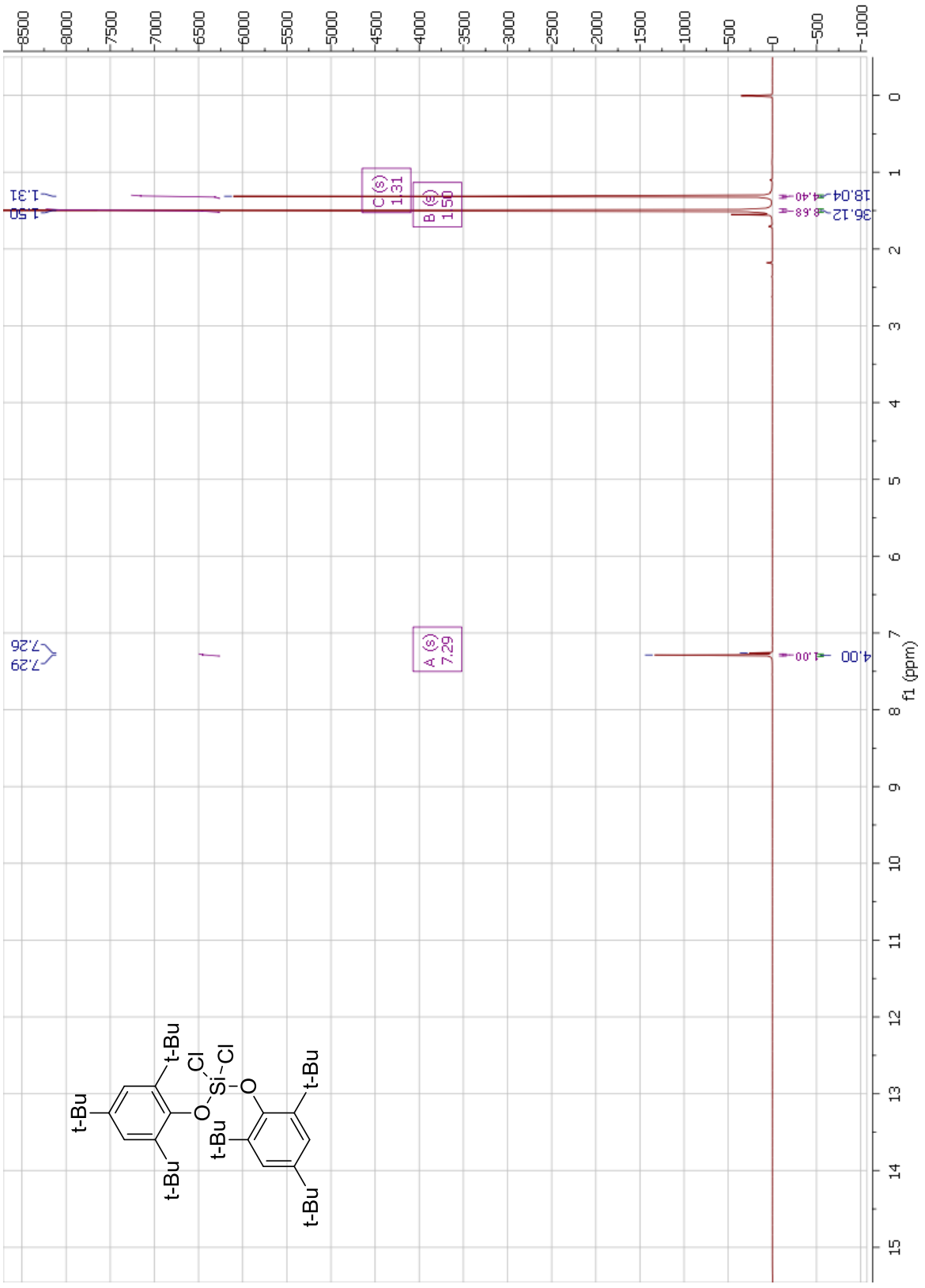

136.11
135.43
133.59
133.07
129.61
129.18
127.91
126.85
126.22
125.03
Cl
Si
Cl
f1 (ppm)

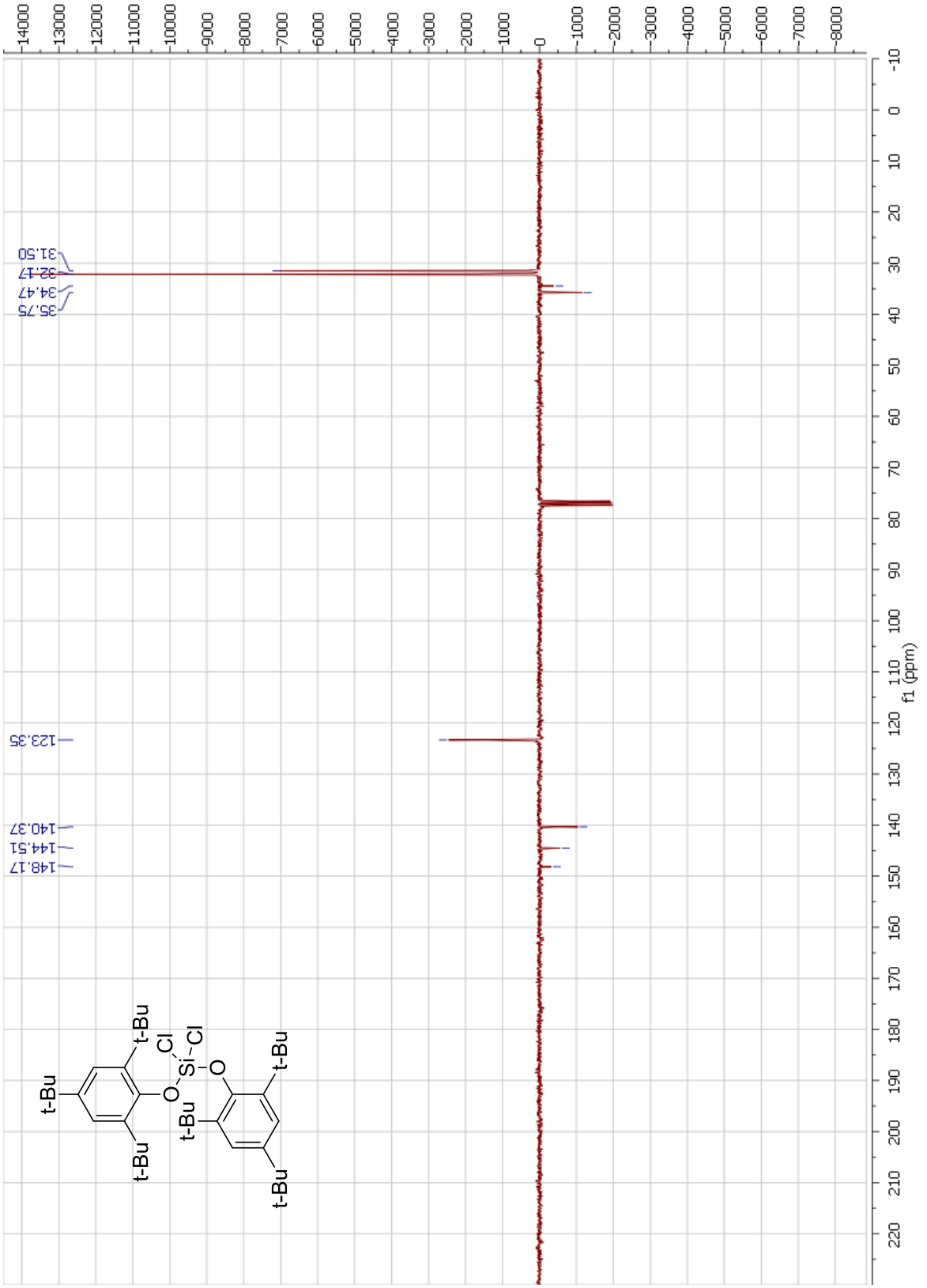
e. KondoSi(OH)$_2$ 1



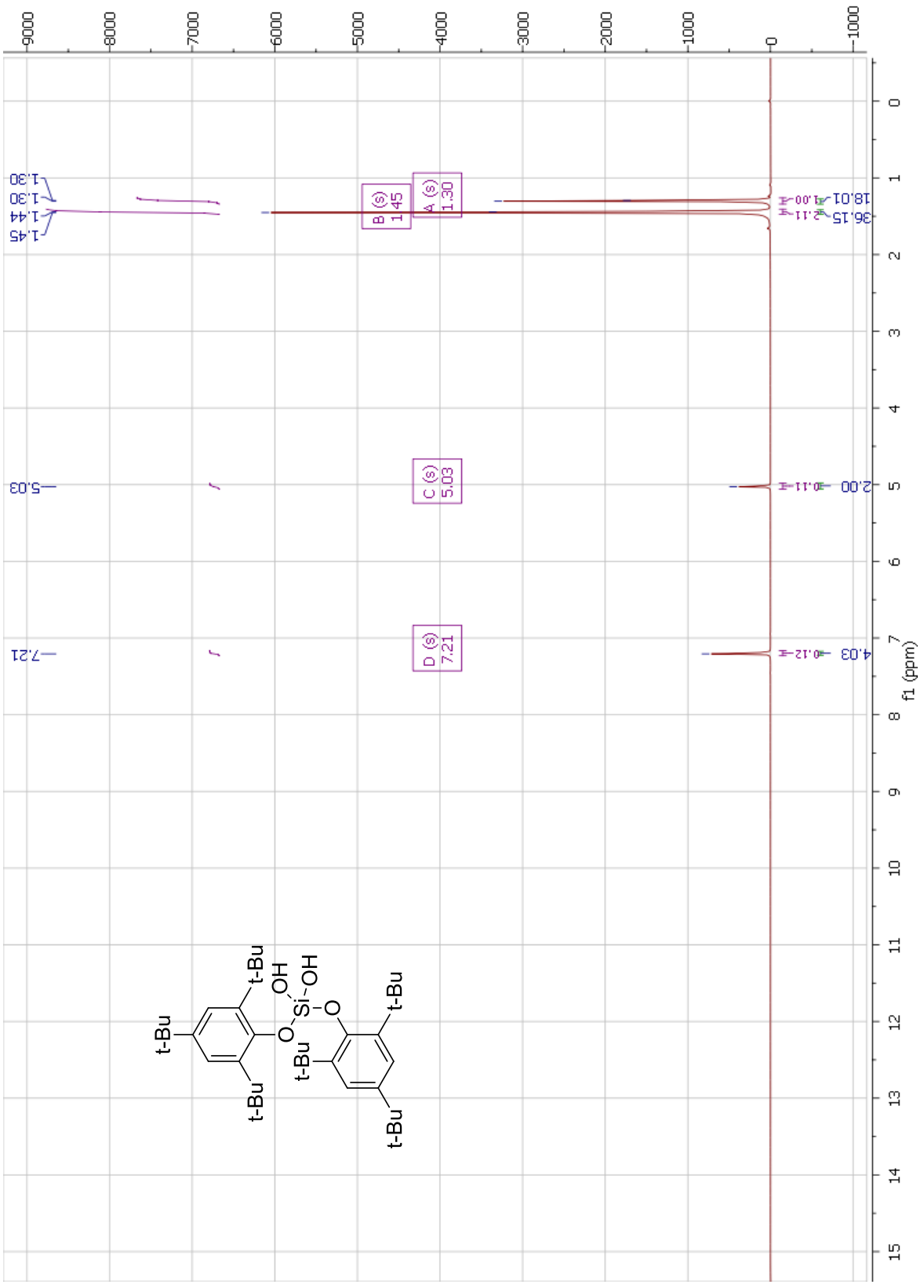

135,61
134,56
132,25
131,56
130,21
127,79
127,35
125,35
124,62
124,09
OH
Si
OH
f1 (ppm)

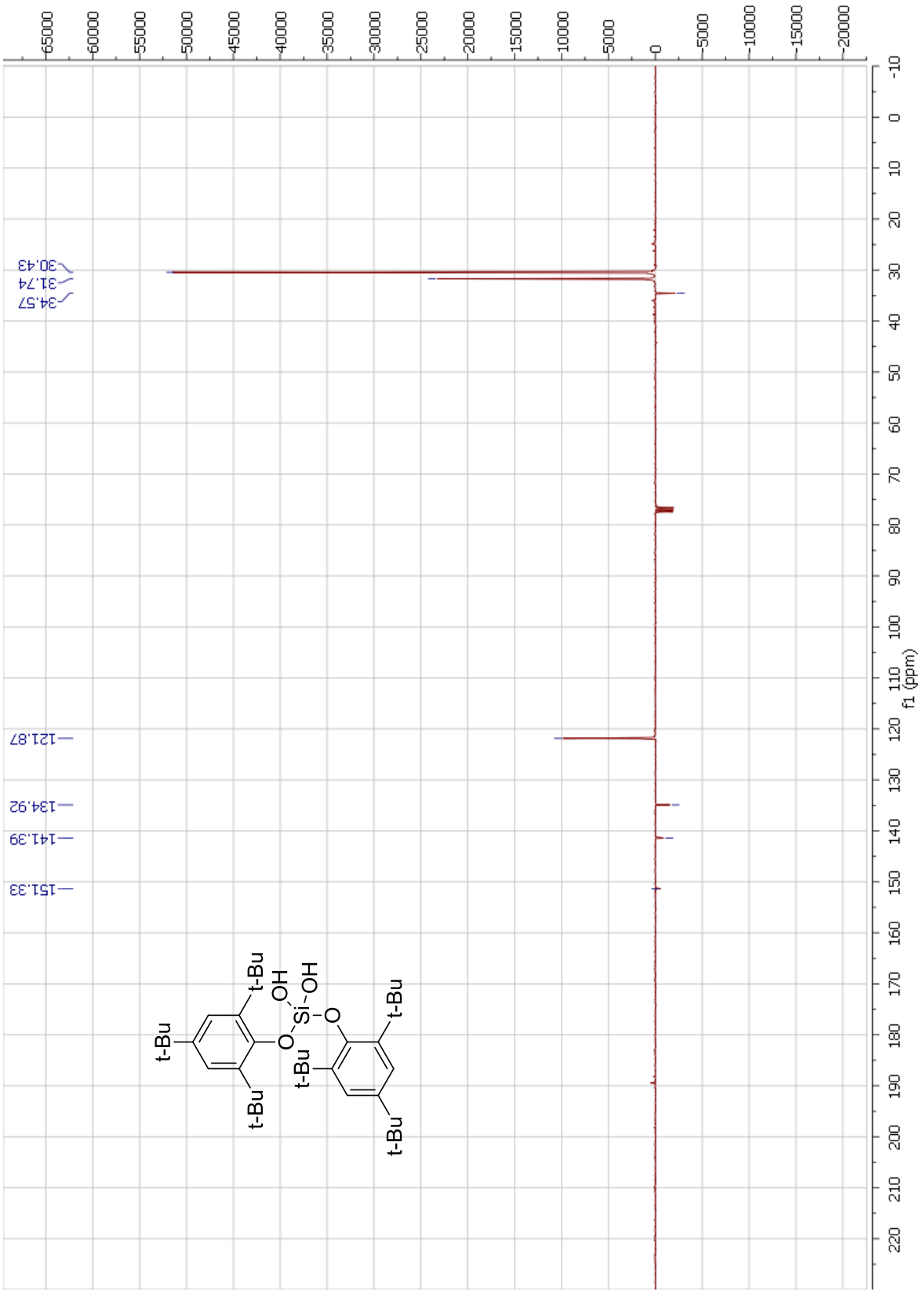
f. dichlorobis(2,4,6-tri-*tert*-butylphenoxy)silane 14




31.50
32.17
34.47
35.75
123.35
140.37
144.51
148.17
f1 (ppm)
t-Bu
t-Bu
t-Bu
t-Bu
t-Bu
Cl
Si
Cl
O
O

g. bis(2,4,6-tri-*tert*-butylphenoxy)silandiol 15




34.57
31.74
30.43
121.87
134.92
141.39
151.33
f1 (ppm)
t-Bu
t-Bu
t-Bu
t-Bu
t-Bu
OH
HO
Si
O
O

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[6] NIST Computational Chemistry Comparison and Benchmark Database, "NIST Standard Reference Database Number 101", to be found under http://cccbdb.nist.gov/, **Release 18, 2016**.