

Supporting Information

Synthesis and Reactivity of Martin's Spirosilane-Derived Chloromethylsilicate

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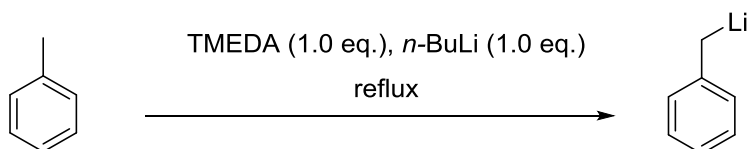
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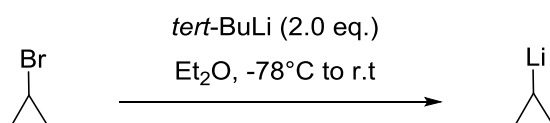
I. Synthesis of organolithium reagents

Synthesis of benzyllithium:



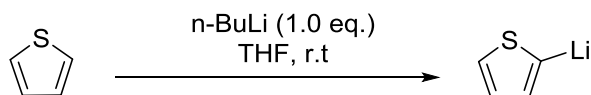
In a dry Schlenk flask was added TMEDA (45 μ L, 0.30 mmol, 1.0 eq.) and toluene (0.24 mL, 0.30 mmol, 1.0 eq.). *n*-BuLi 2.5M in hexane (0.12 mL, 0.30 mmol, 1.0 eq.) was added dropwise at room temperature, and the reaction was refluxed for 1h. The resulting deep orange mixture was allowed to reach room temperature and was used immediately for the synthesis of phenylethylsilicate **3c**.

Synthesis of cyclopropyllithium:



In a dry Schlenk flask was added cyclopropyl bromide (16 μ L, 0.20 mmol, 1.0 eq.) and Et₂O (0.5 mL). The resulting solution was cooled down to -78°C and *tert*-BuLi 1.7 M in pentane (0.24 mL, 0.40 mmol, 2.0 eq.) was added dropwise and the reaction mixture was stirred at -78°C for 1h. The solution of cyclopropyllithium was used immediately for the synthesis of the mixture of cyclopropylmethylsilicate **3e** and cyclopropyllithium.

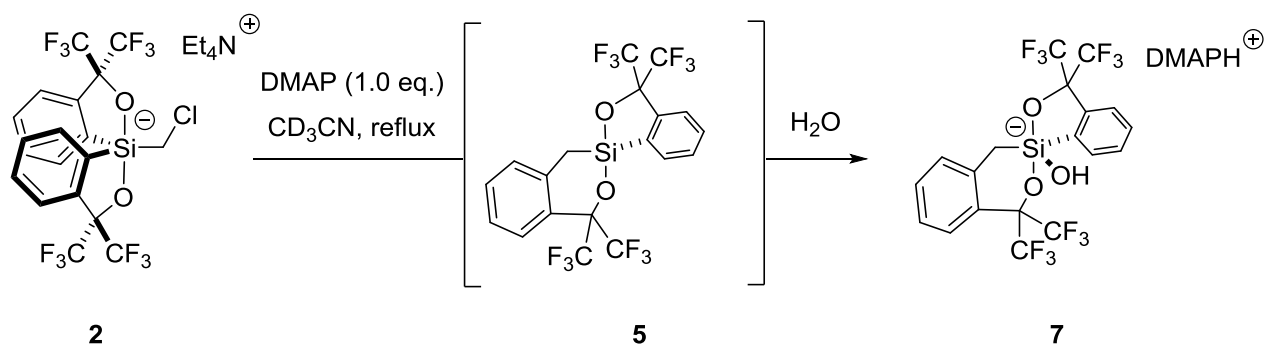
Synthesis of 2-thienyllithium:



In a dry Schlenk flask was diluted thiophene (25 μ L, 0.31 mmol, 1.0 eq.) in THF (0.5 mL), and *n*-BuLi 2.5 M in hexane (0.12 mL, 0.30 mmol, 1.0 eq.) was added dropwise at room temperature. The reaction mixture was stirred for 1h at room temperature. until the solution turns yellow. was used immediately for the synthesis of thienylmethylsilicate **3g**

II. NMR monitoring following the method B

Synthesis of hydroxysilicate **7**:



Synthesis of hydroxysilicate **7** according to the method B was NMR-monitored by means of a J. Young's tube starting from chloromethylsilicate **2** (20 mg, 0.029 mmol, 1.0 eq.) and DMAP (3.5 mg, 0.029 mmol, 1.0 eq.) in anhydrous acetonitrile- d_3 (0.4 mL). The reaction was heated at 80°C overnight, and then water was added to afford silicate **7**.

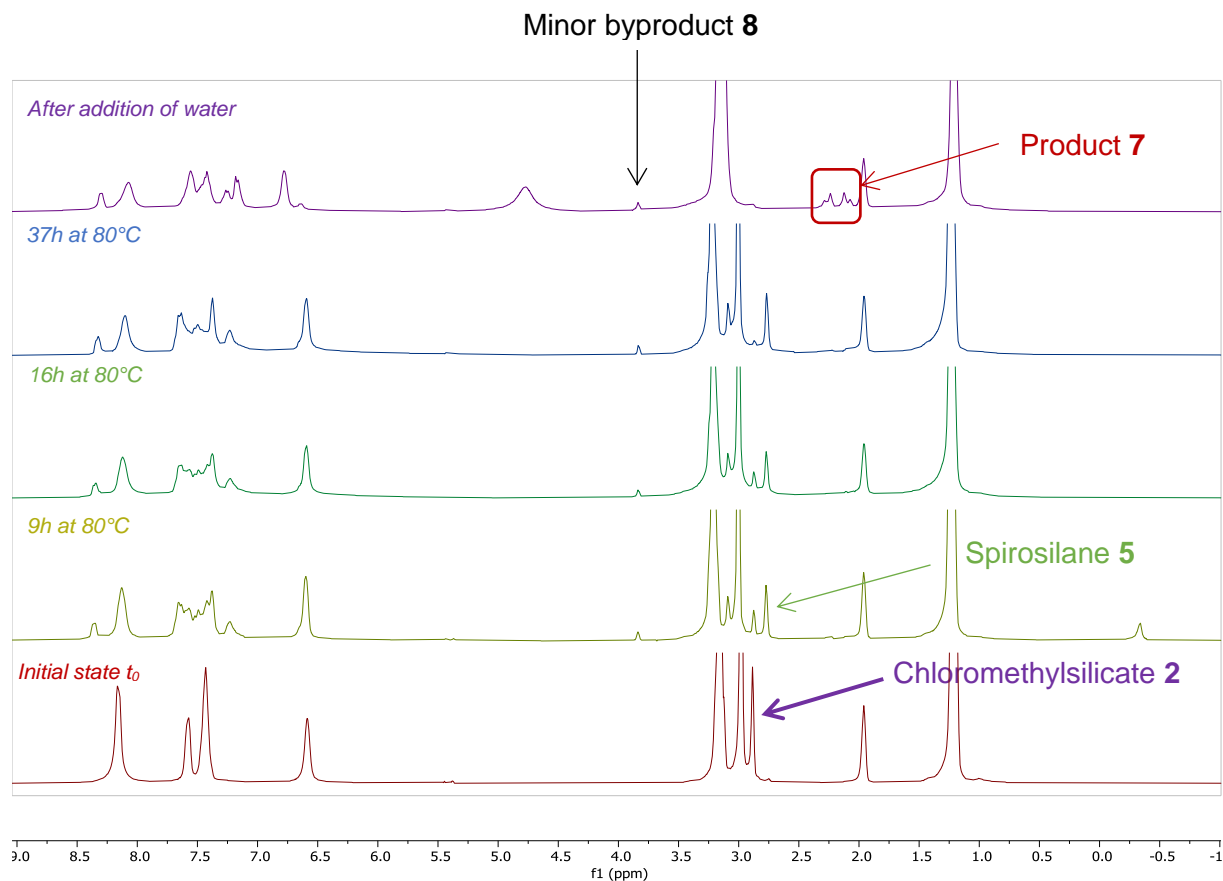


Figure S1 | ^1H NMR monitoring in CD_3CN for the reaction of chloromethylsilicate **2** with DMAP as Lewis base (method B).

Formation of spirosilane **5** results in appearance of a singlet (2.76 ppm) in CD_3CN associated to the benzylic protons. Air bubbling into the mixture affords hydroxysilicate **7**, which is highlighted by the AB system at 2.20 & 2.10 ppm. The singlet observed at 3.82 ppm indicated the presence of a minor byproduct, which was identified as the silicate **8** as a consequence of the direct substitution of chlorine atom of **2** by DMAP.

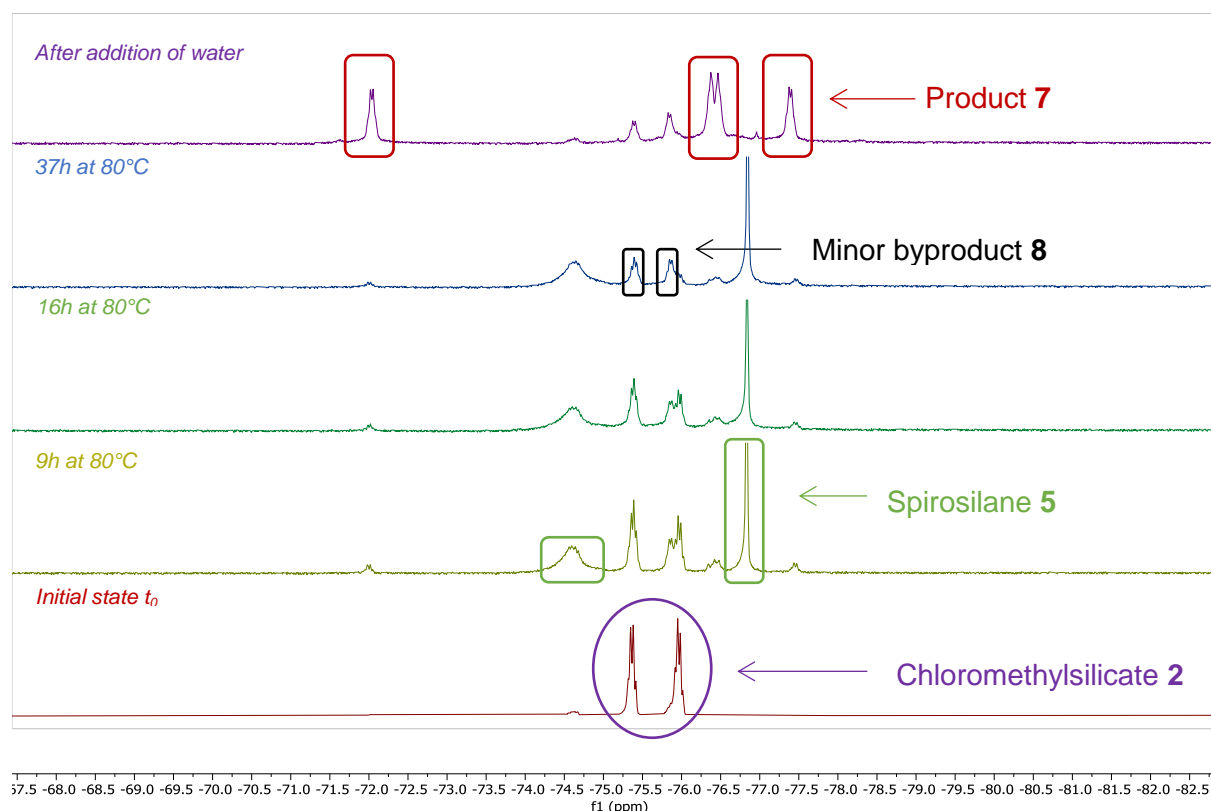
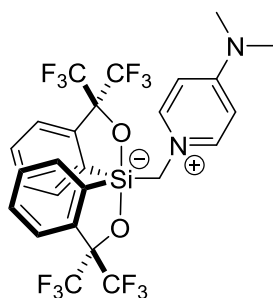


Figure S2 | ^{19}F NMR monitoring in CD_3CN for the reaction of chloromethylsilicate **2** with DMAP as Lewis base (method B).

Due to the loss of symmetry caused by the ring expansion, the transformation of chloromethylsilicate **2** (purple ellipse) to spirosilane **5** (green box) could be monitored by ^{19}F NMR with the apparition of the 1 broad signal at -74.6 and the singlet at -76.9 ppm. Air bubbling into the mixture triggers the transformation of **5** to hydroxysilicate **7** (red box), as highlighted by the appearance of the four quadruplets (-72.1, -76.4, -76.5, -77.4 ppm).

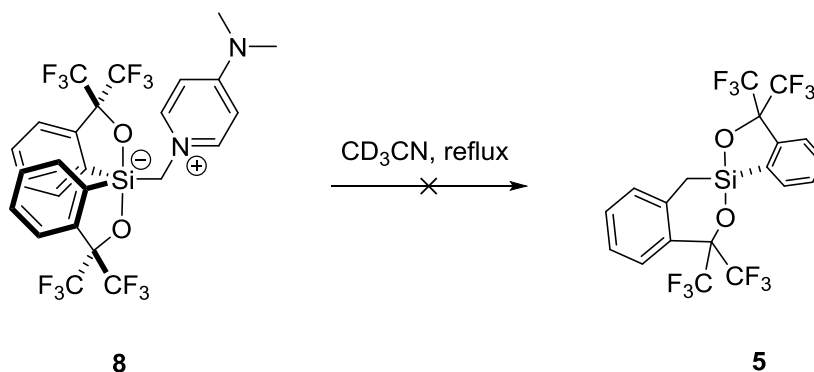
Isolation and Stability's assessment of the zwitterionic silicate byproduct **8** upon heating



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Zwitterionic nature of byproduct **8** allowed its isolation by chromatography over SiO₂ (DCM 100%) as a colorless solid (1.9 mg, 9%).

¹H NMR: (400 MHz, CDCl₃) δ 8.11 (d, *J* = 6.9 Hz, 2H), 7.62 (m, 4H), 6.51 (d, *J* = 7.3 Hz, 2H), 3.98 (d, *J* = 14.8 Hz, 1H), 3.88 (d, *J* = 14.8 Hz, 1H), 3.19 (s, 6H). **¹³C NMR:** (101 MHz, CDCl₃) δ 155.1, 143.3, 141.0, 140.4, 137.5, 129.4, 128.9, 123.8, 106.3, 56.4, 39.9, 29.7, 1.1. **¹⁹F NMR:** (376 MHz, CDCl₃) δ -74.77 (q, *J* = 9.2 Hz), -75.33 (q, *J* = 9.4 Hz). **¹H/²⁹Si HMQC:** (400 MHz/79 MHz, CD₃CN) 3.85/-74.7. **HRMS (ESI⁺):** *m/z* calcd for C₂₆H₂₀F₁₂N₂O₂SiH [M+H] 649.1175, found 649.1171.

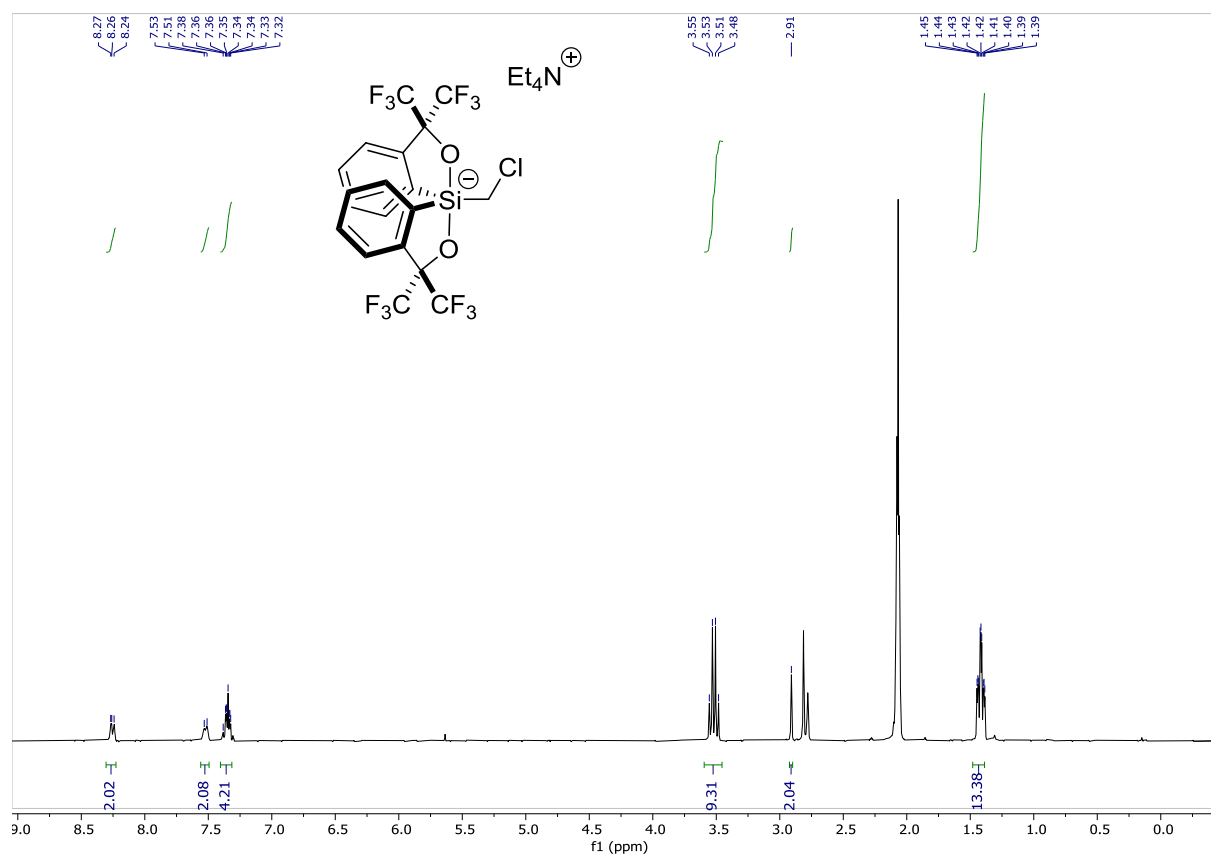


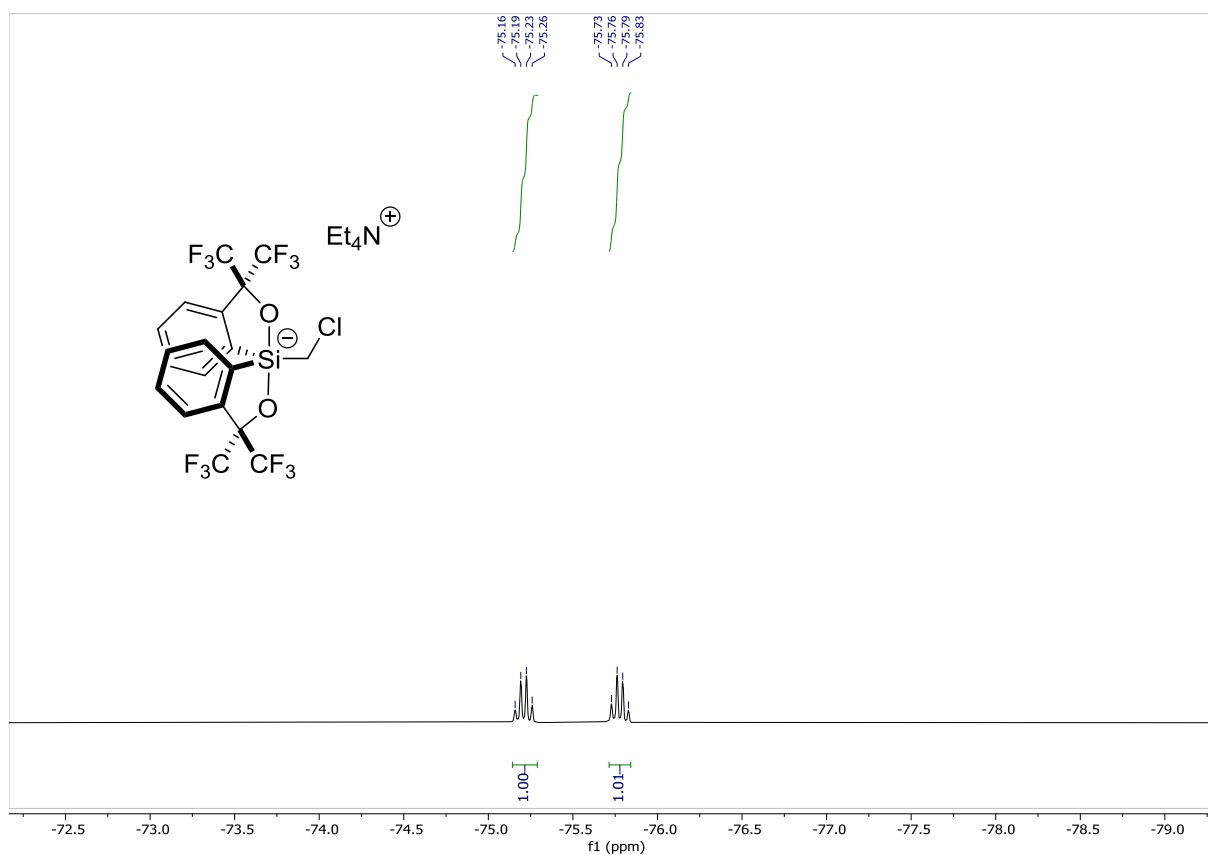
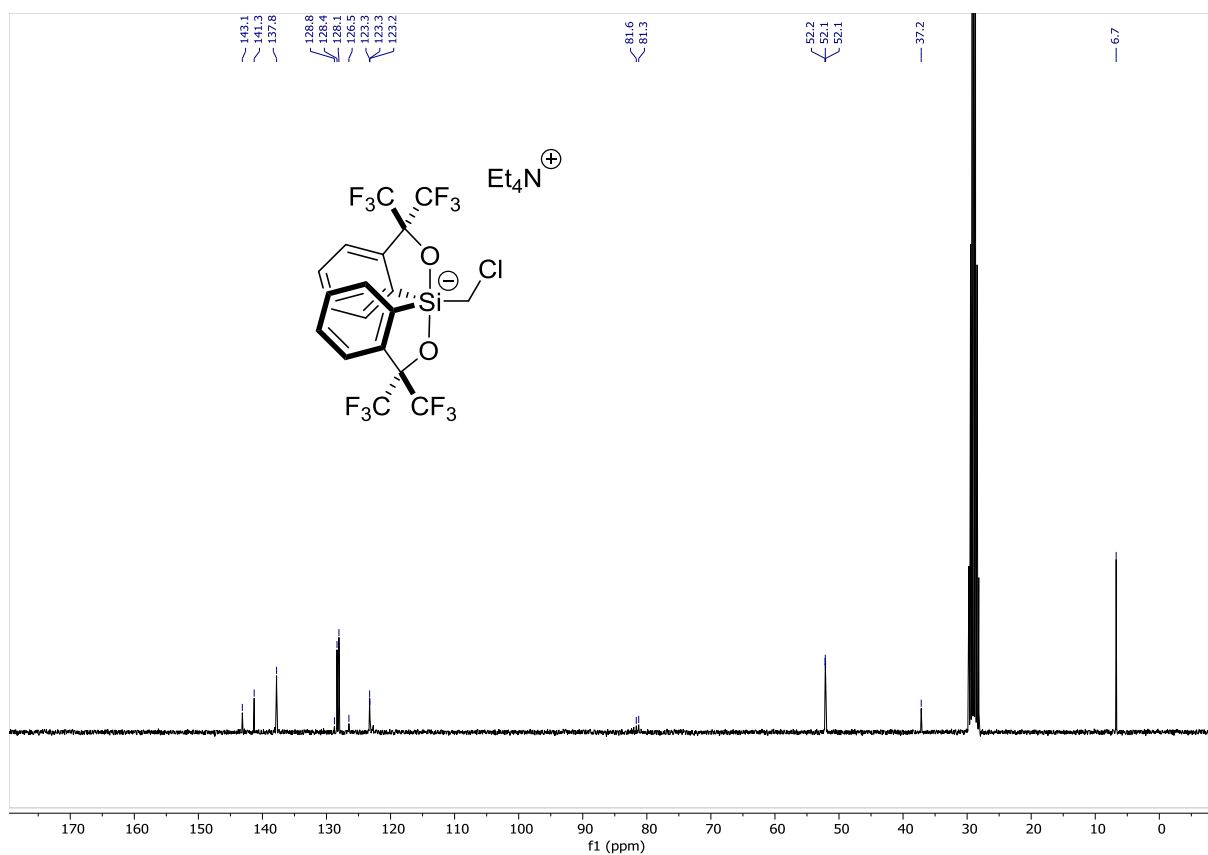
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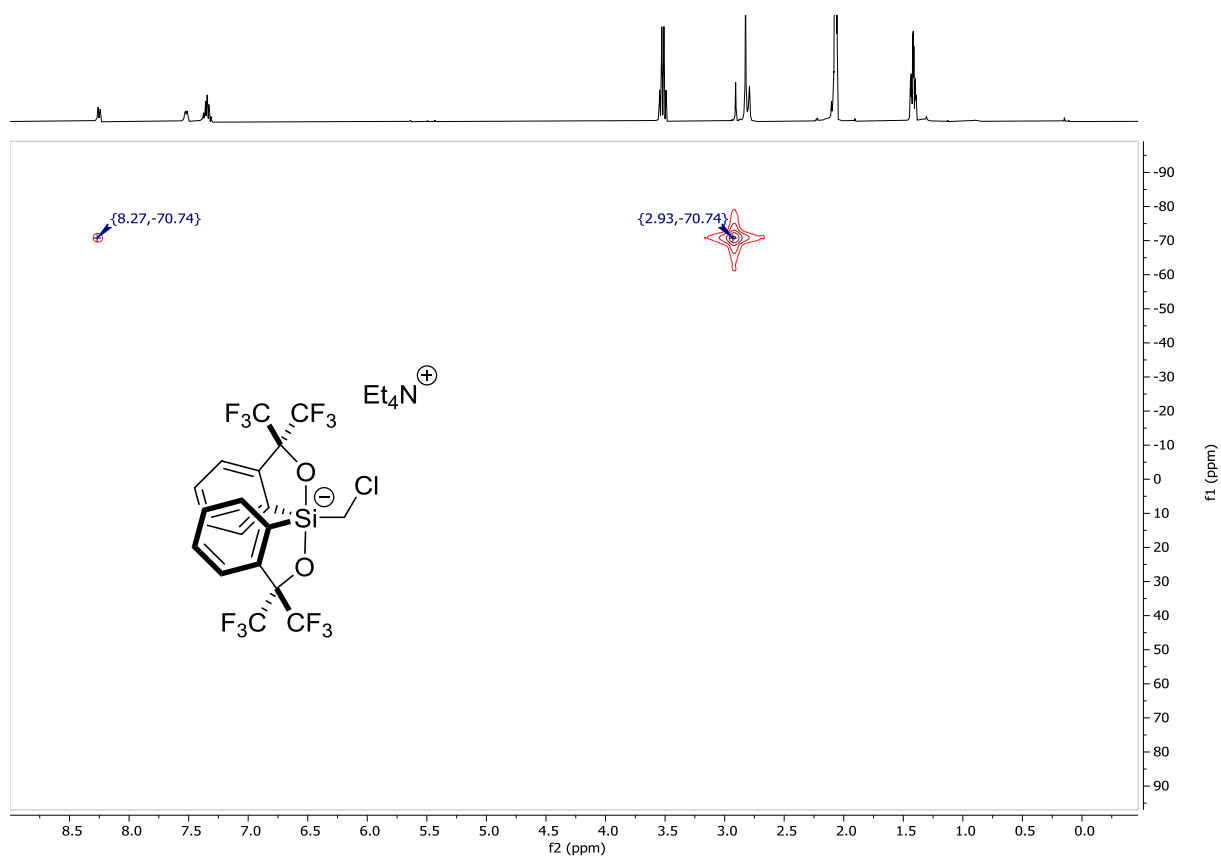
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Thermal stability of silicate **8** was assessed by means of ¹H and ¹⁹F NMR: Silicate **8** was added to a dried J. Young's tube with anhydrous acetonitrile-d₃, and the mixture was refluxed overnight. No reaction occurred.

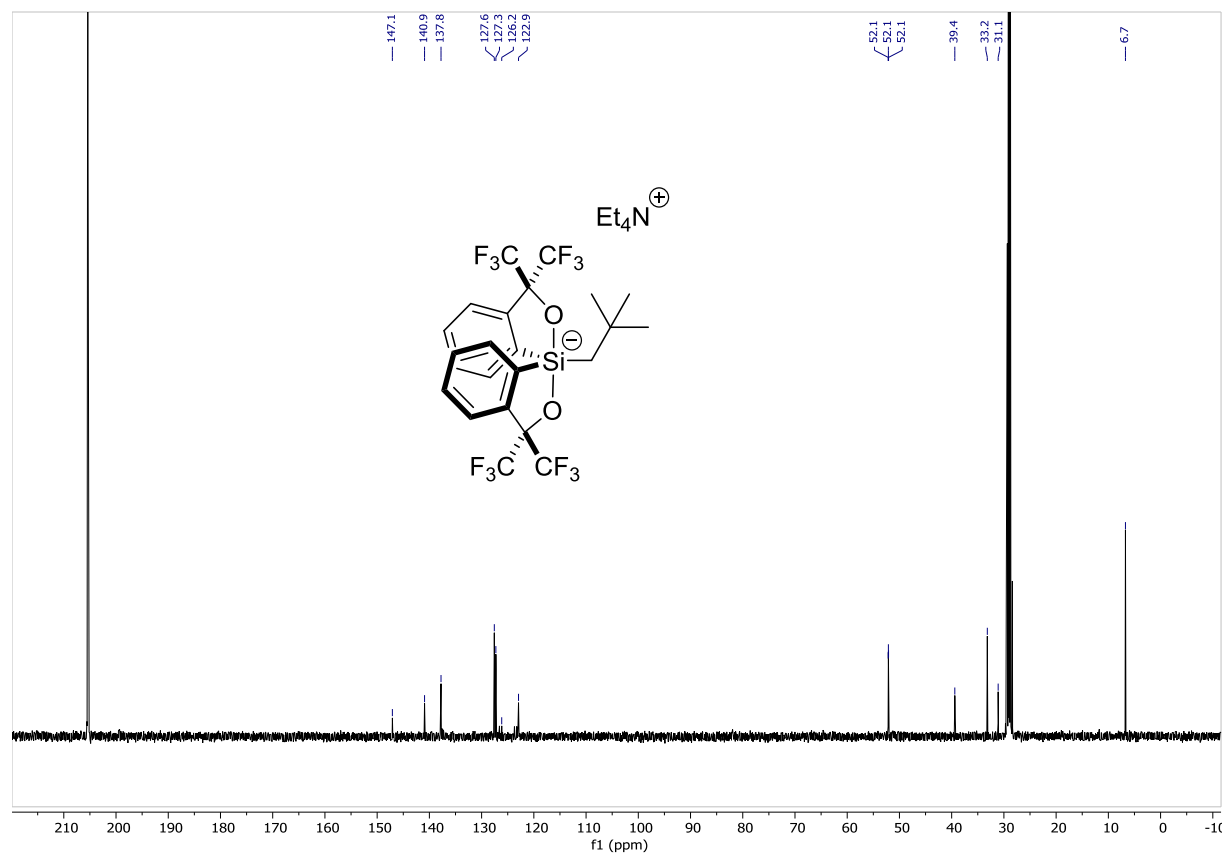
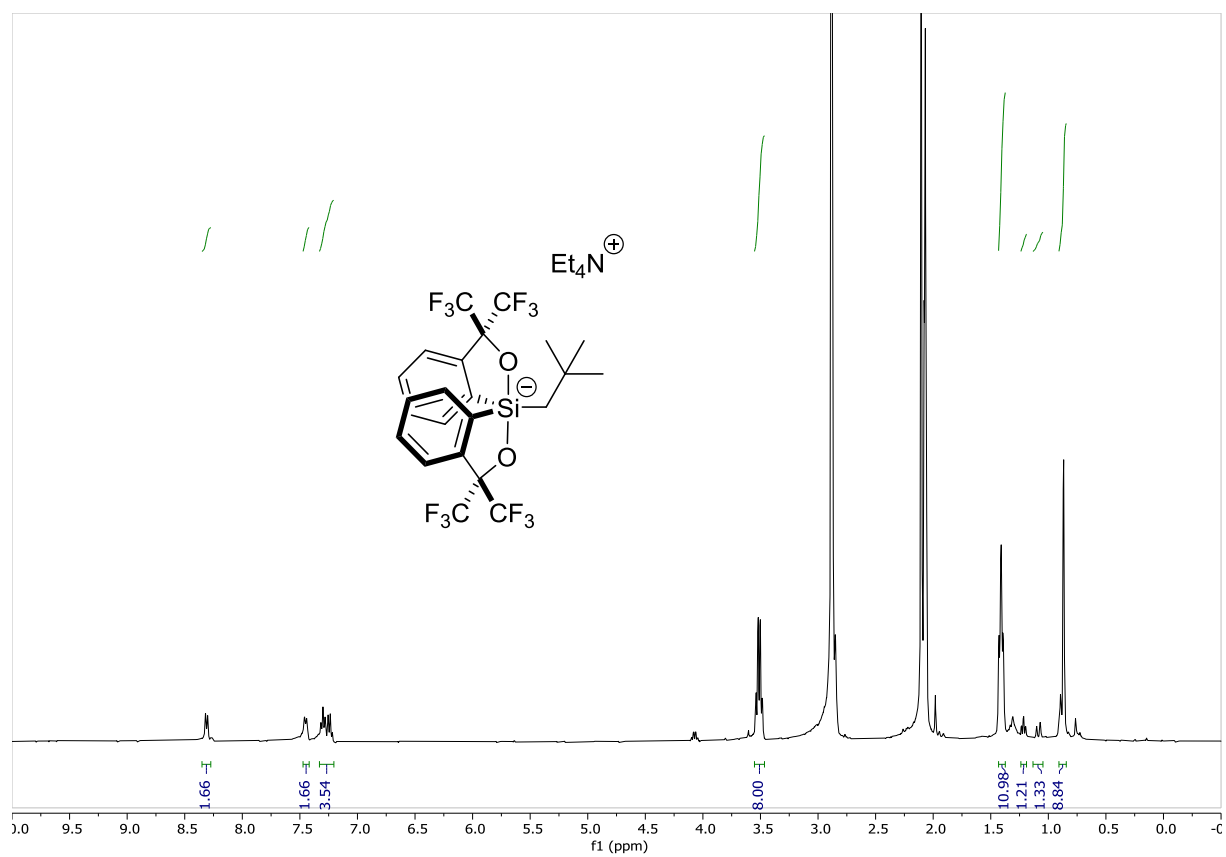
III. NMR Spectra

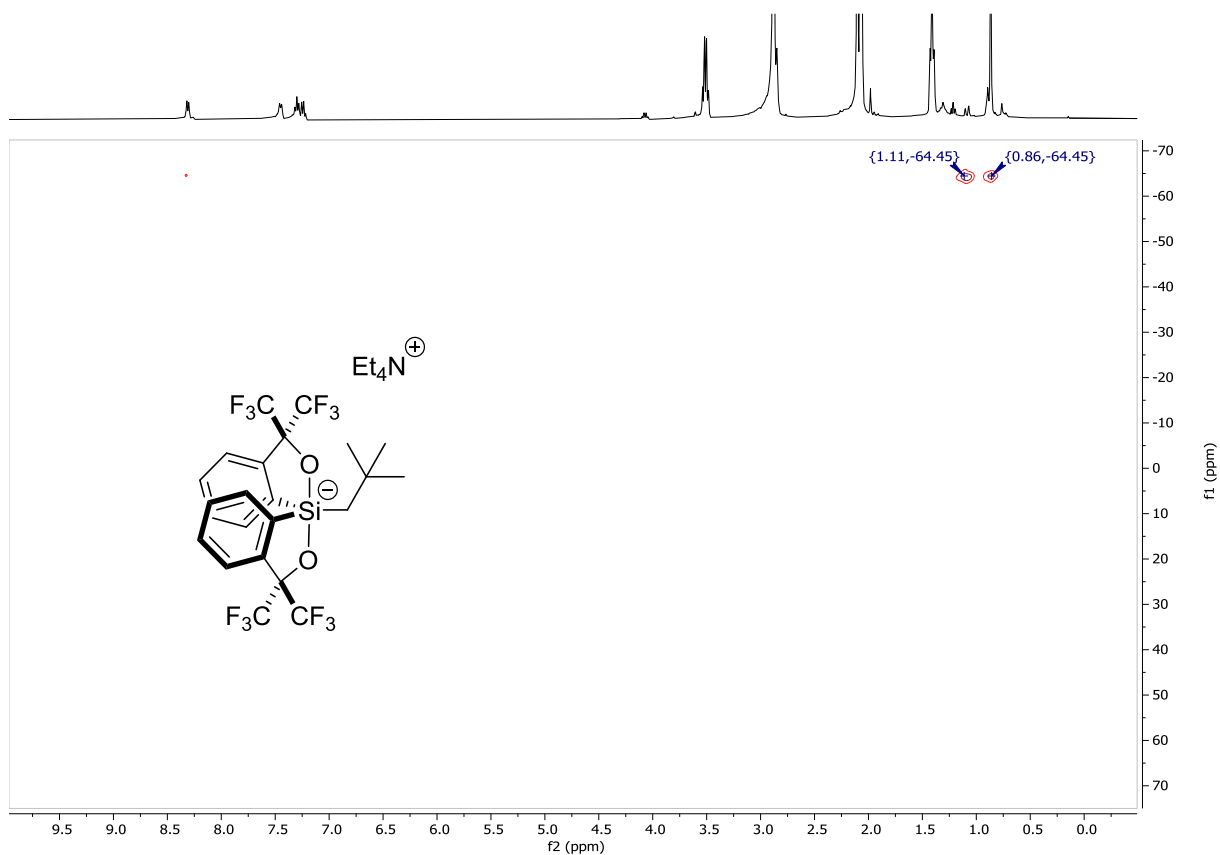
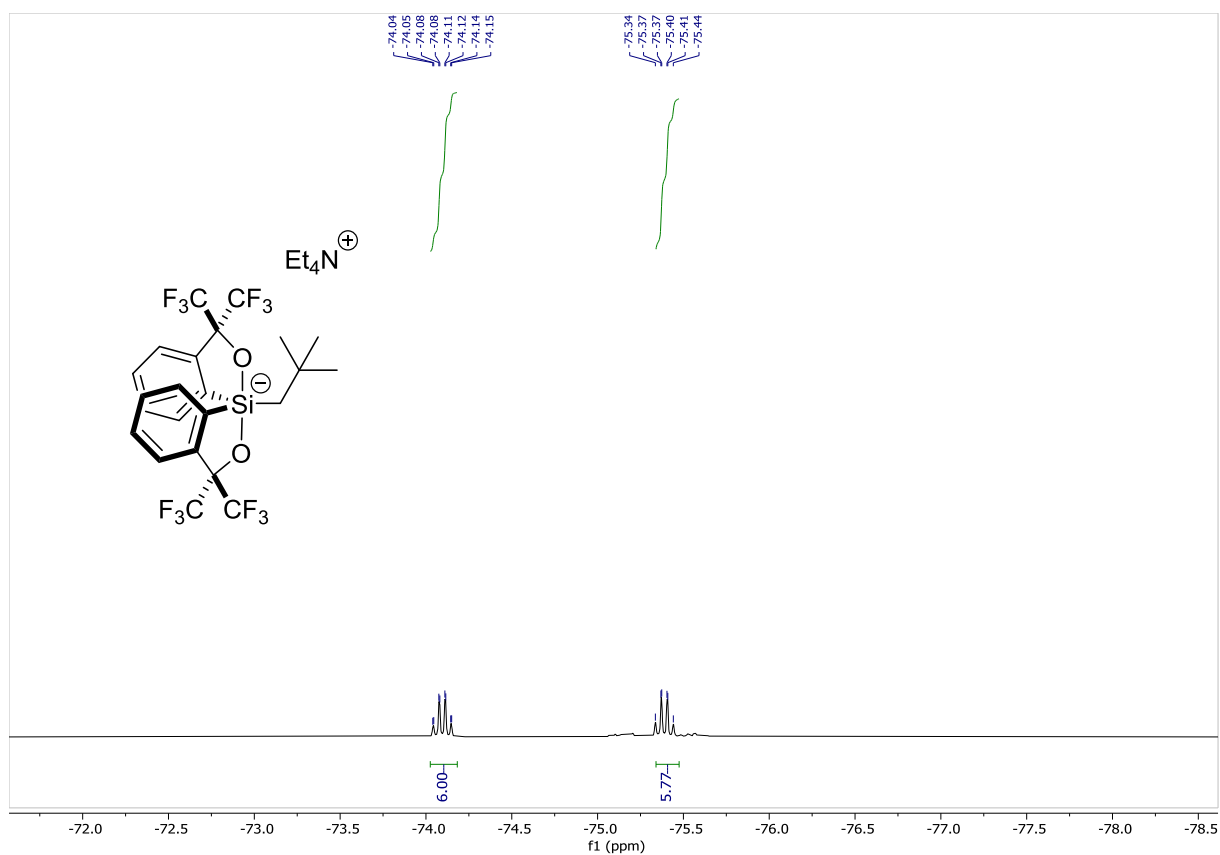
¹H, ¹³C, ¹⁹F, and ¹H/²⁹Si HMQC NMR spectra of 2 in (CD₃)₂CO



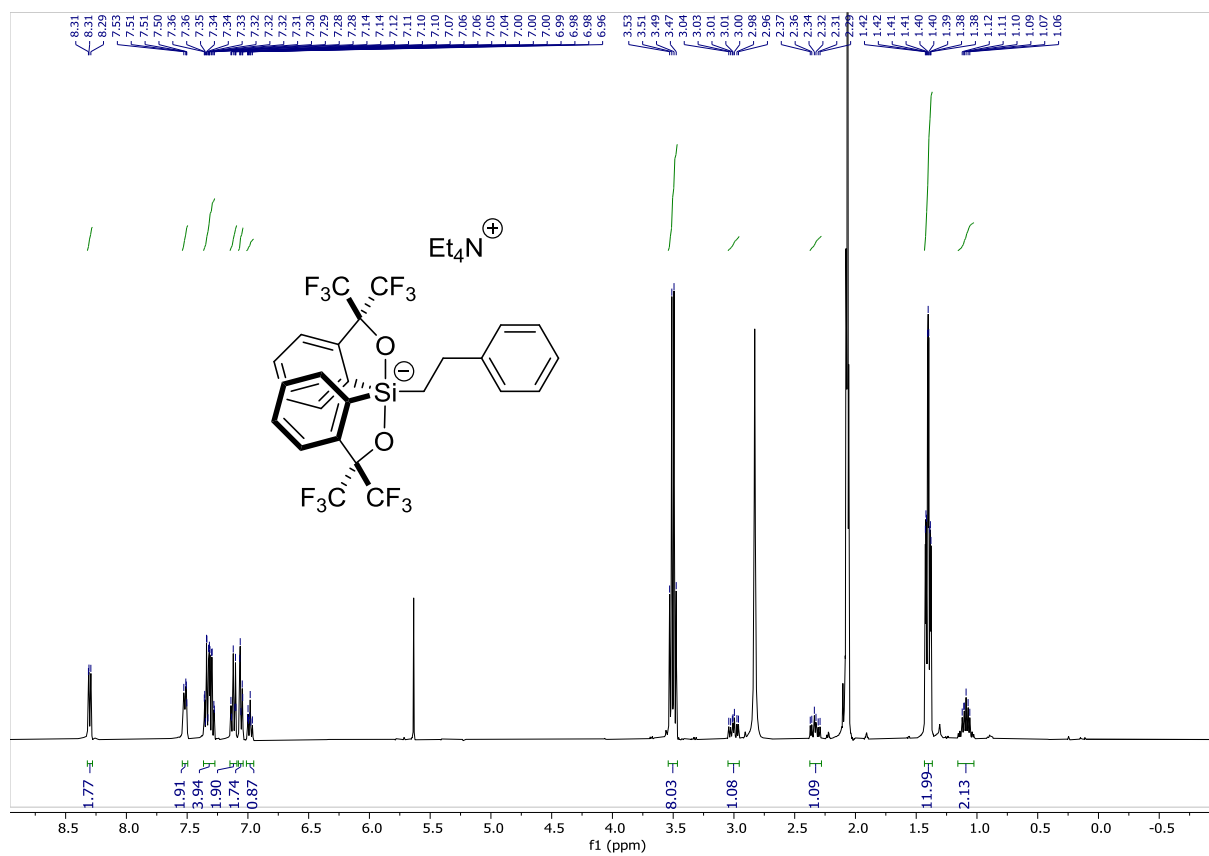


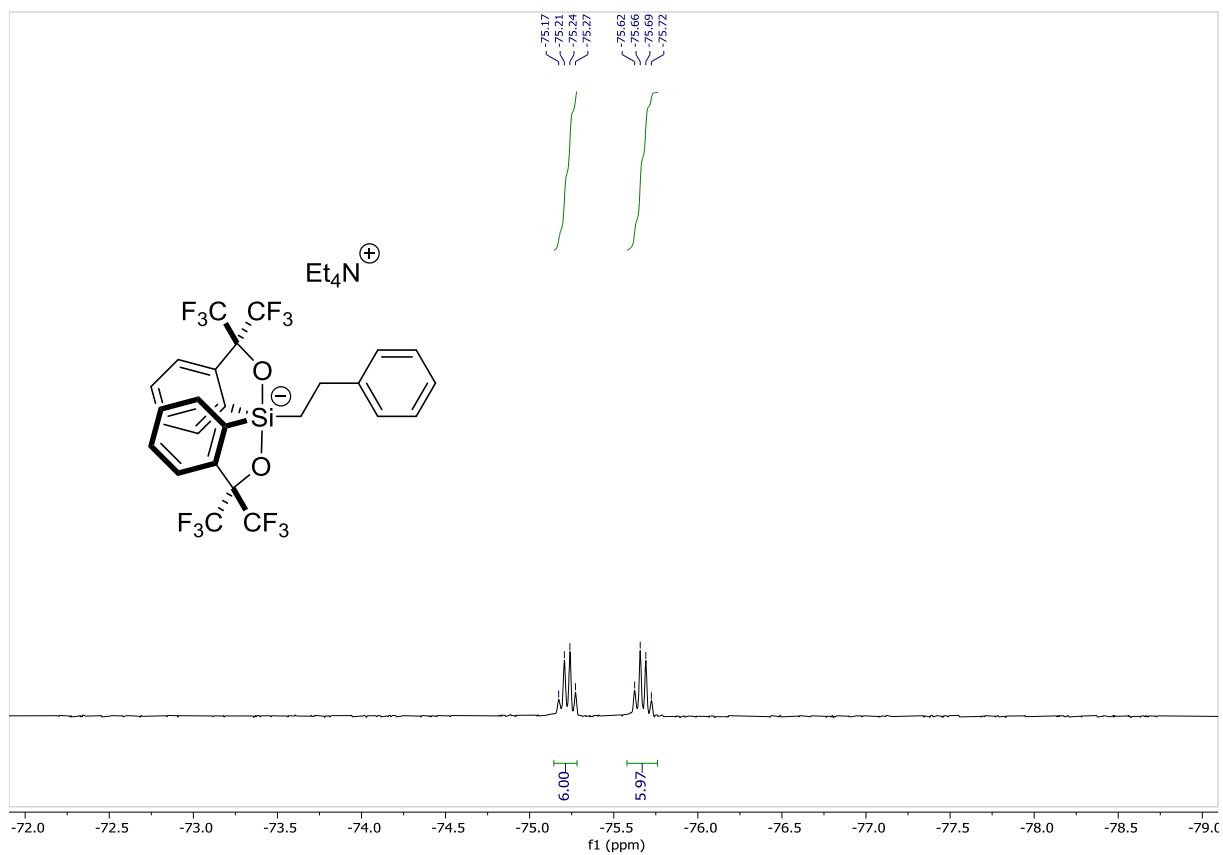
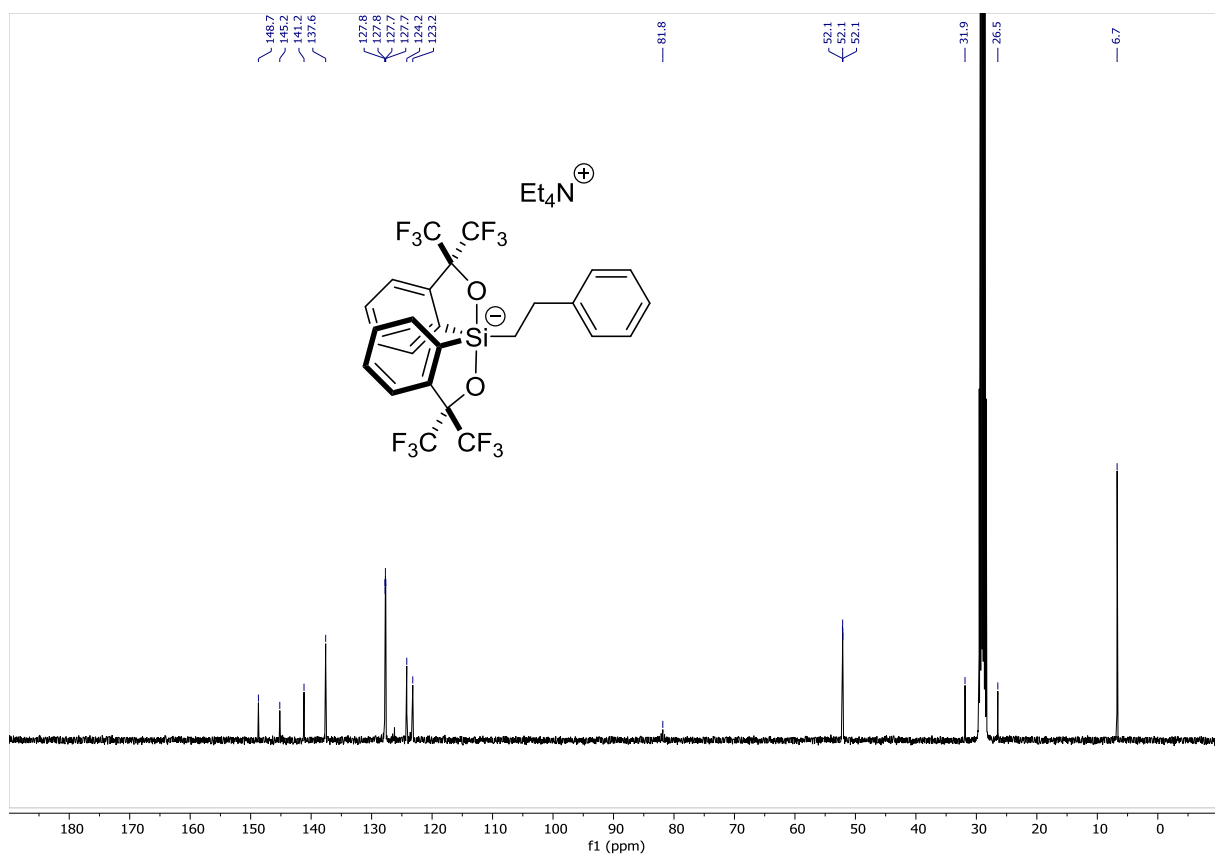
^1H , ^{13}C , ^{19}F , and $^1\text{H}/^{29}\text{Si}$ HMQC NMR spectra of 3b in $(\text{CD}_3)_2\text{CO}$

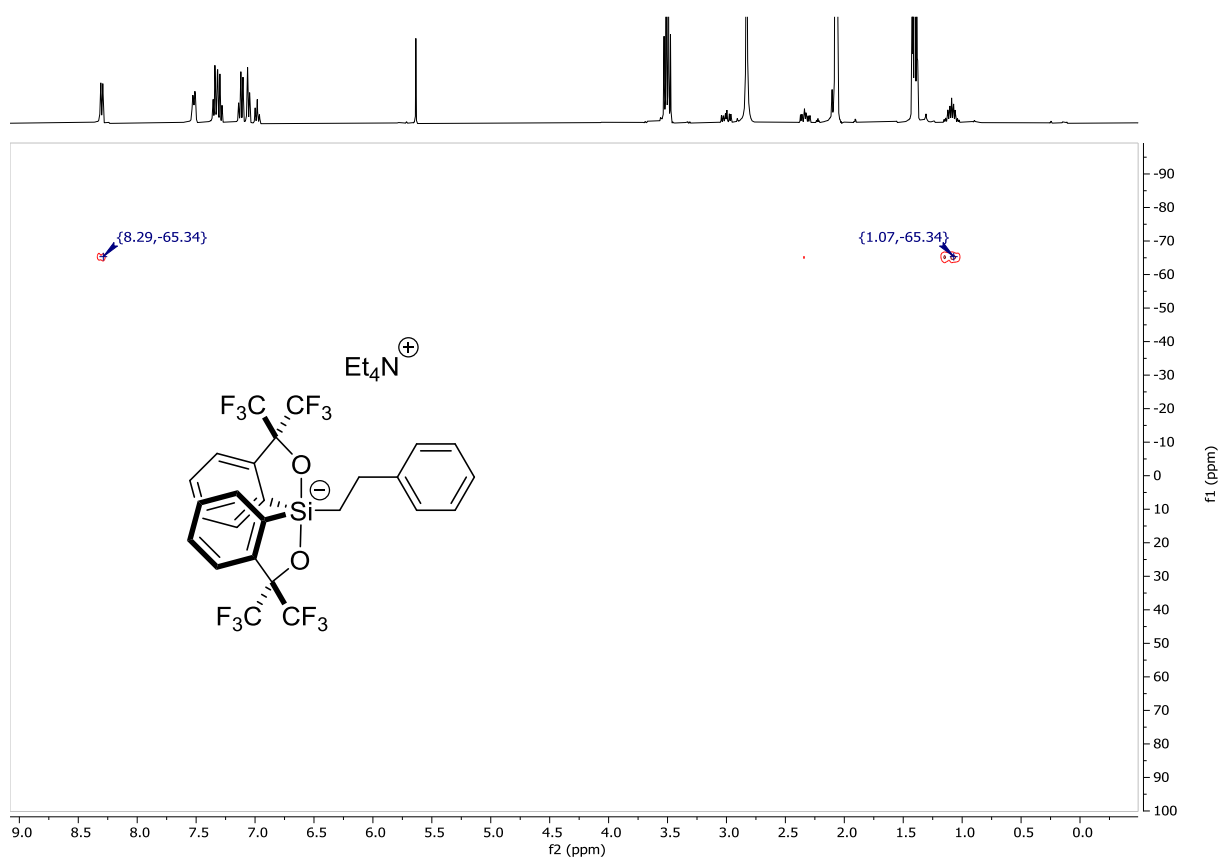




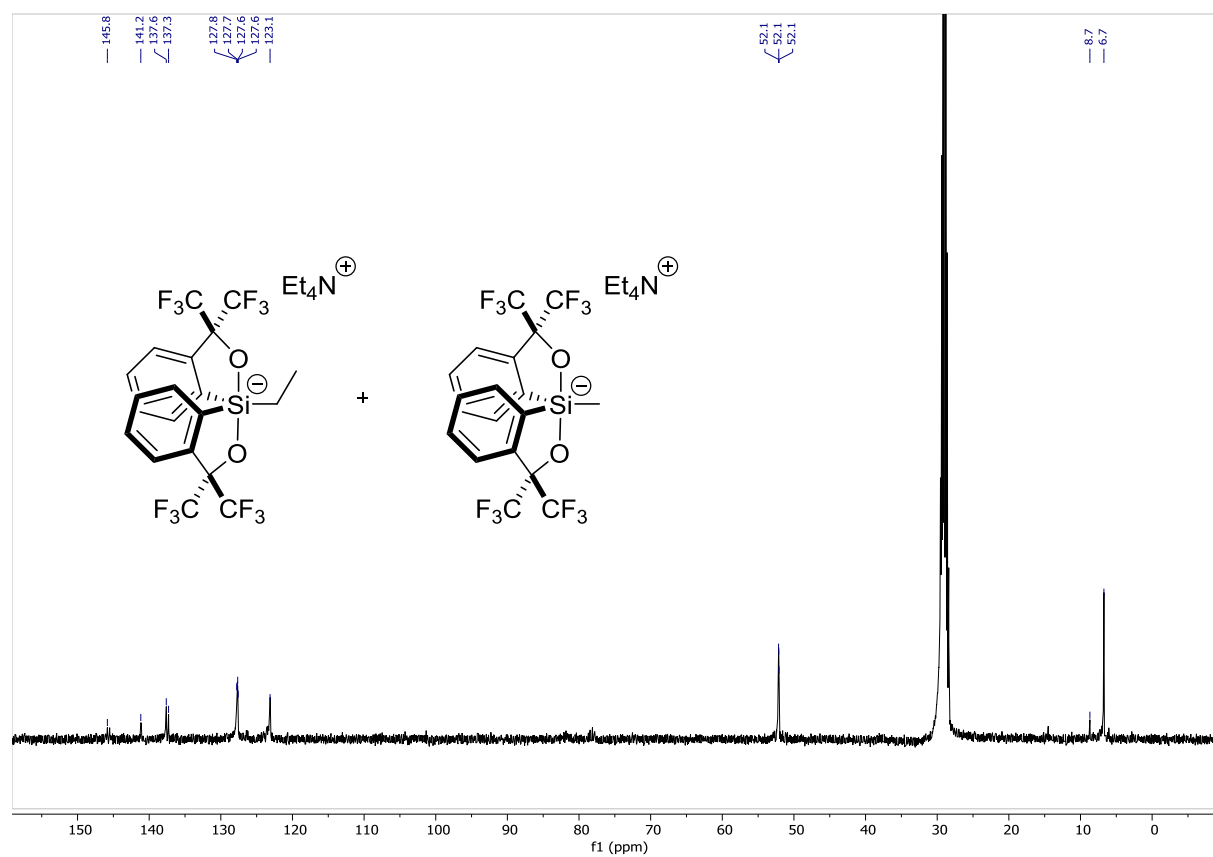
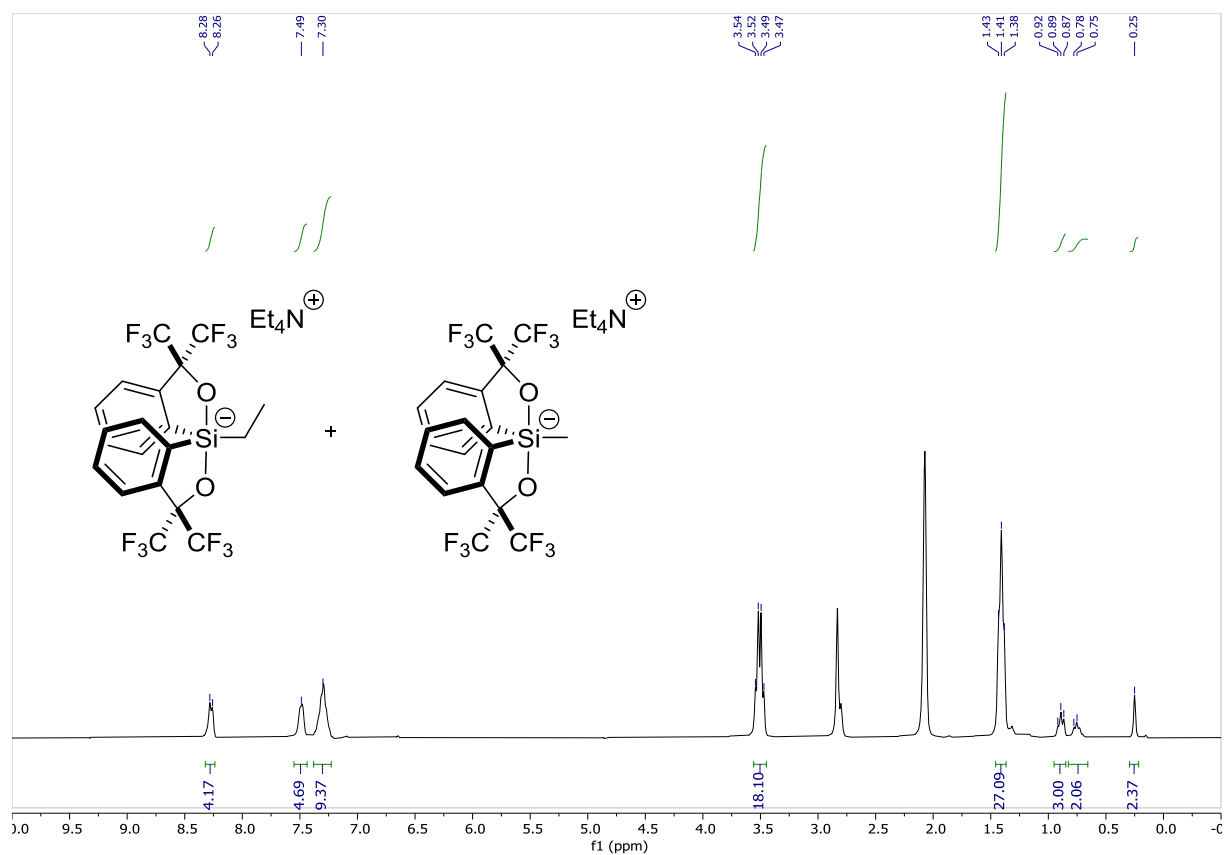
^1H , ^{13}C , ^{19}F , and $^1\text{H}/^{29}\text{Si}$ HMQC NMR spectra of 3c in $(\text{CD}_3)_2\text{CO}$

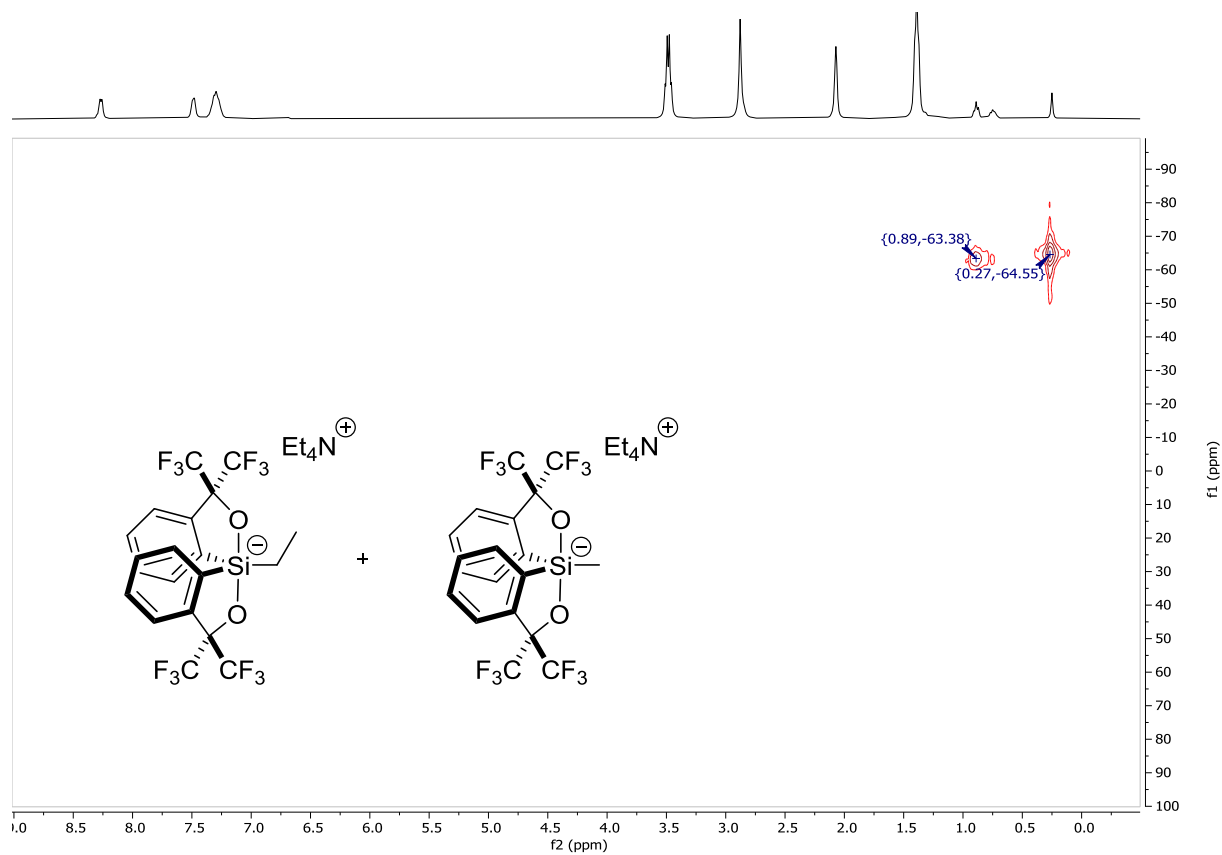
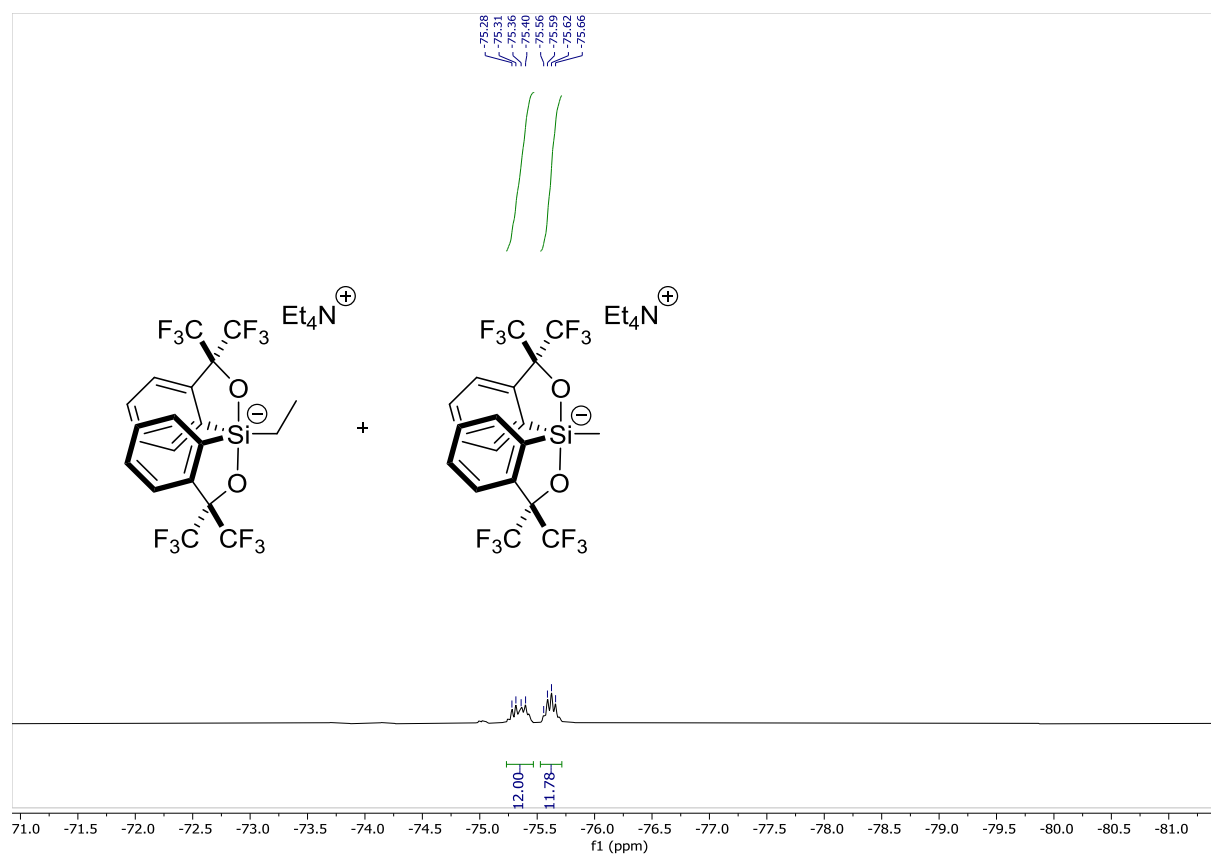




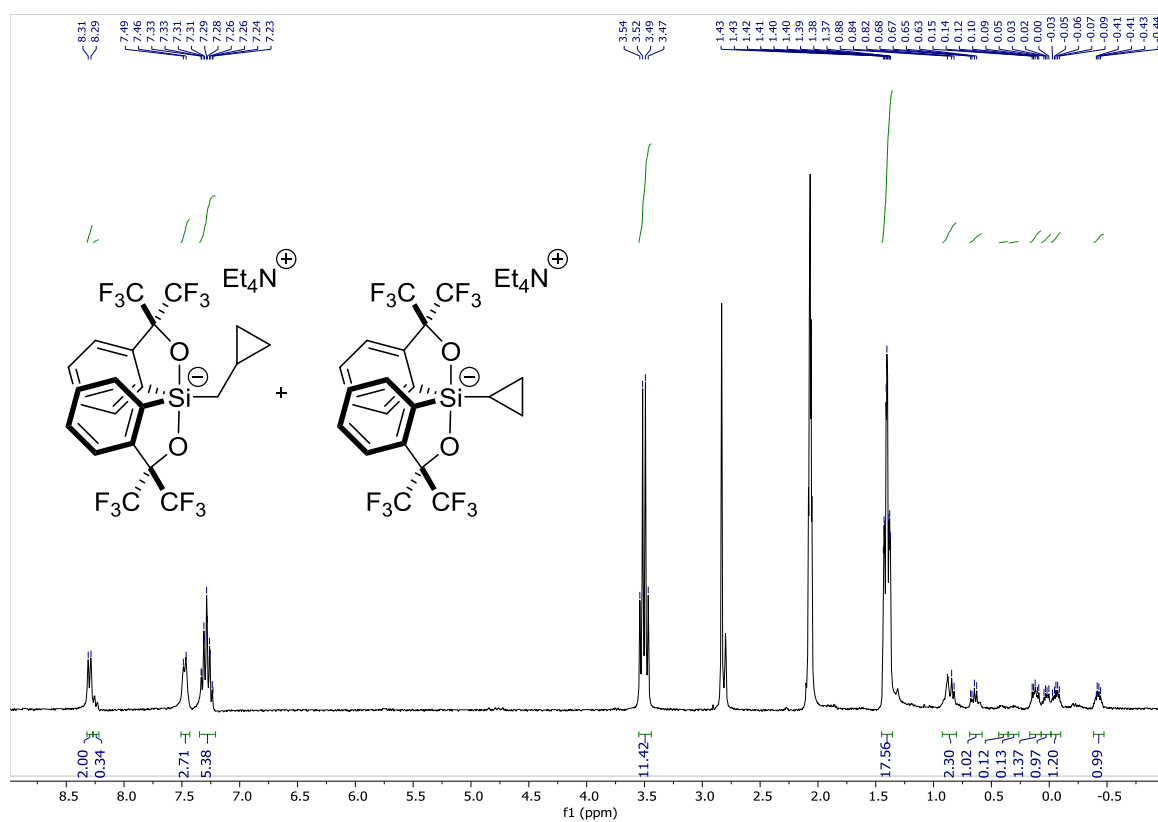


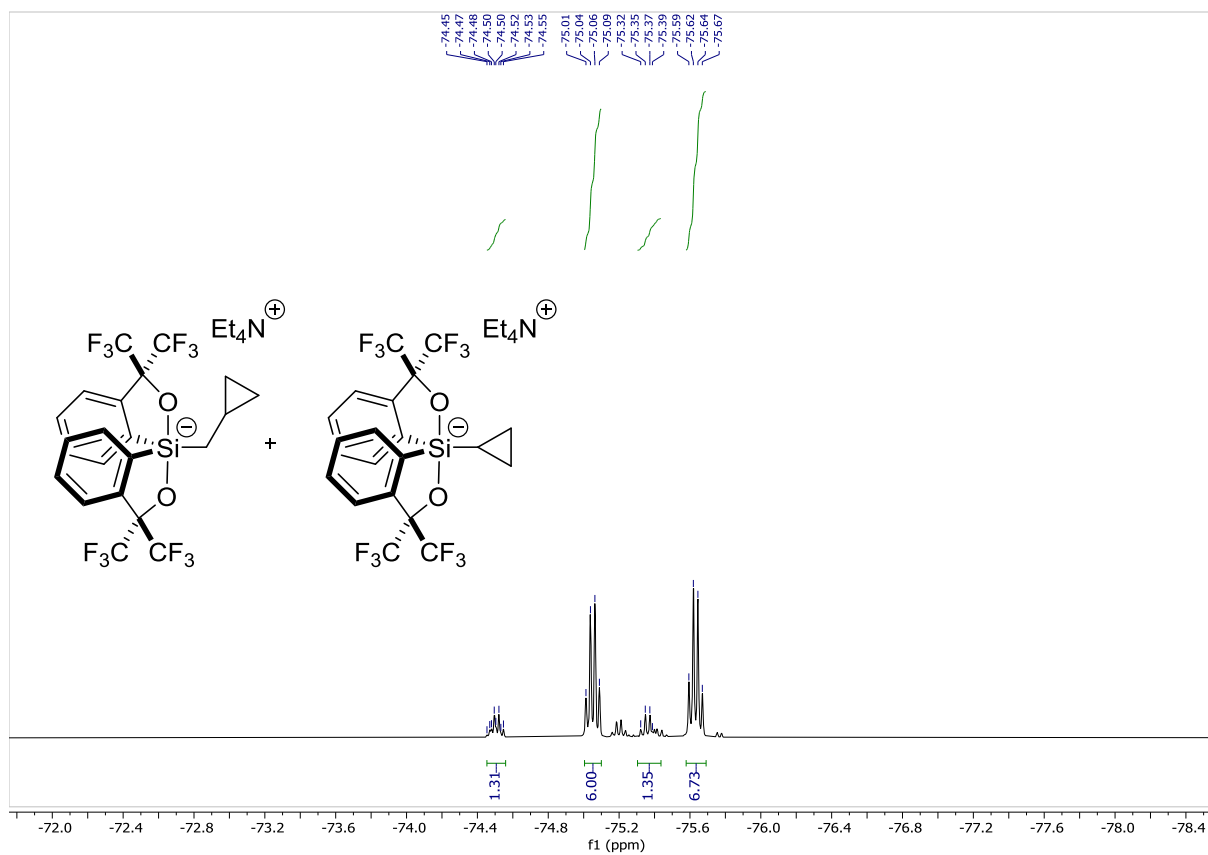
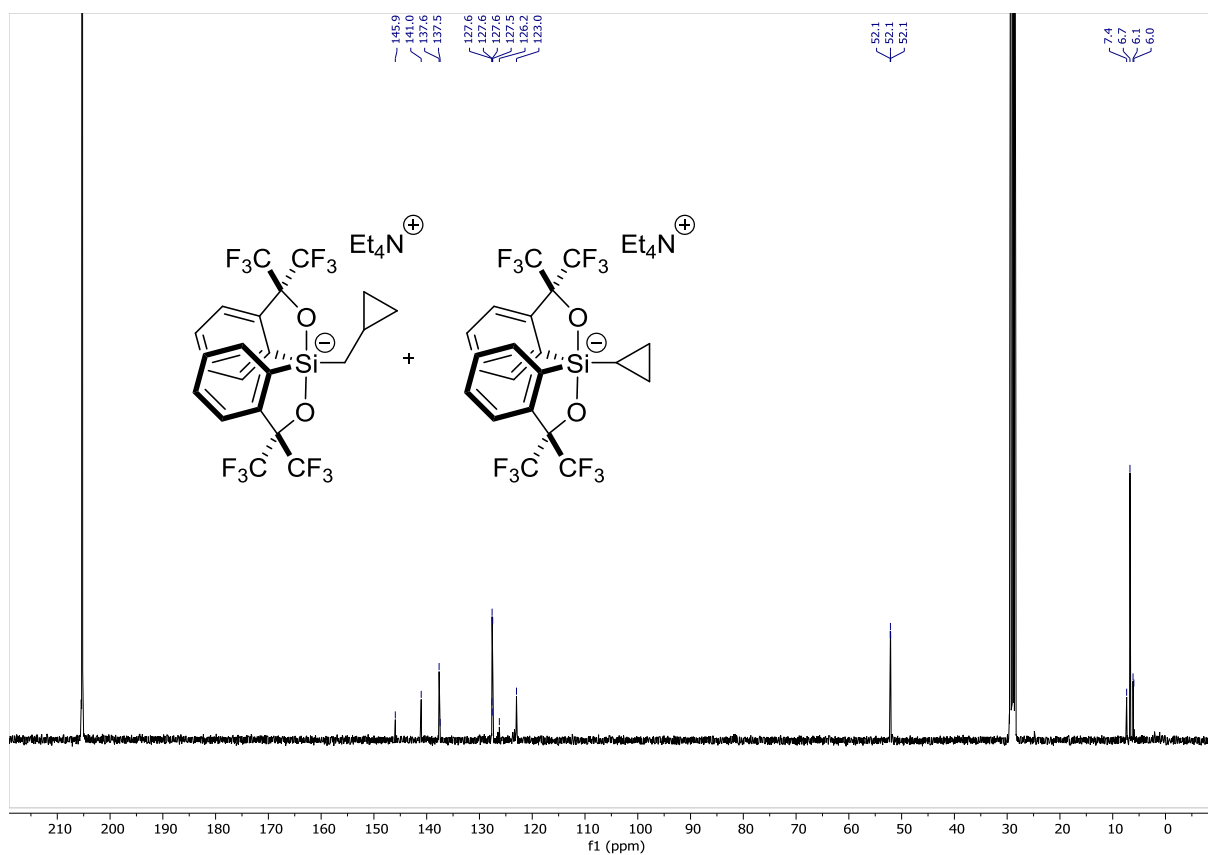
^1H , ^{13}C , ^{19}F , and $^1\text{H}/^{29}\text{Si}$ HMQC NMR spectra of mixture 3d/4d in $(\text{CD}_3)_2\text{CO}$

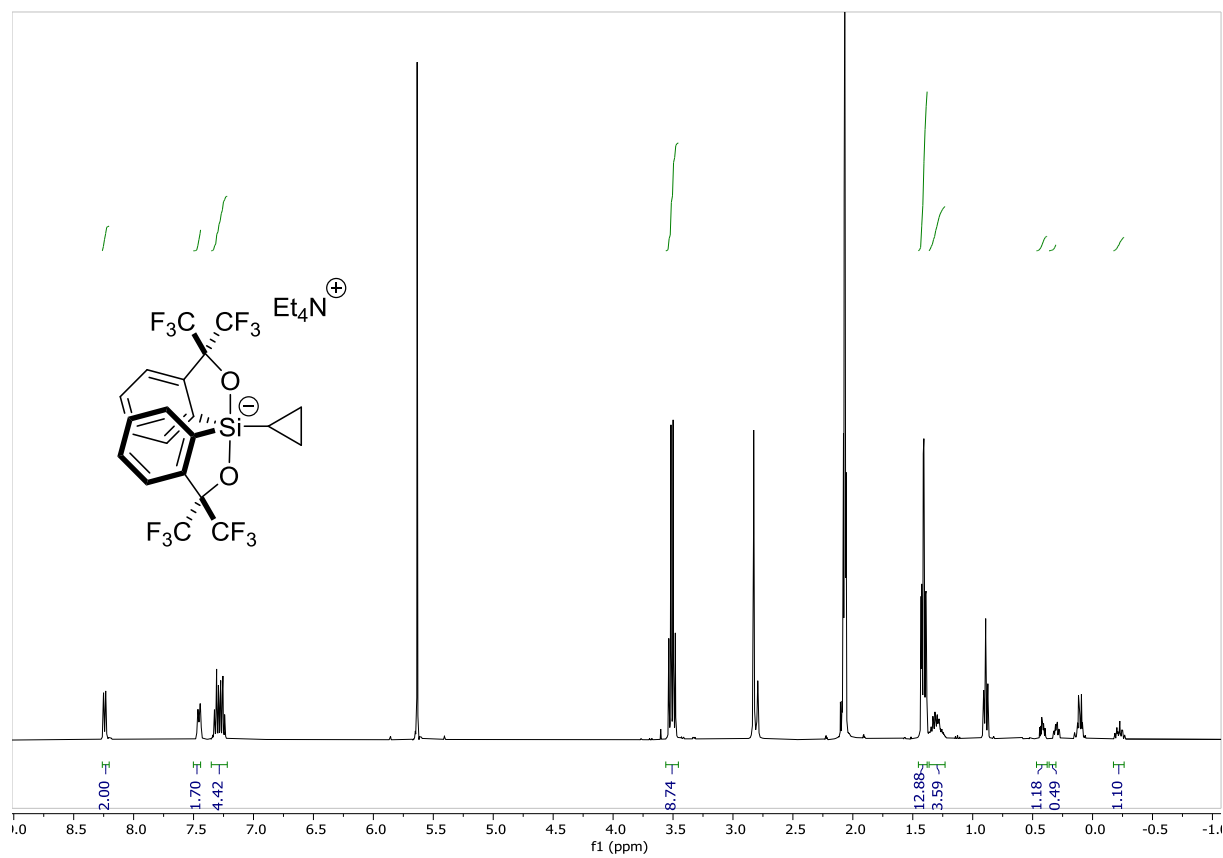
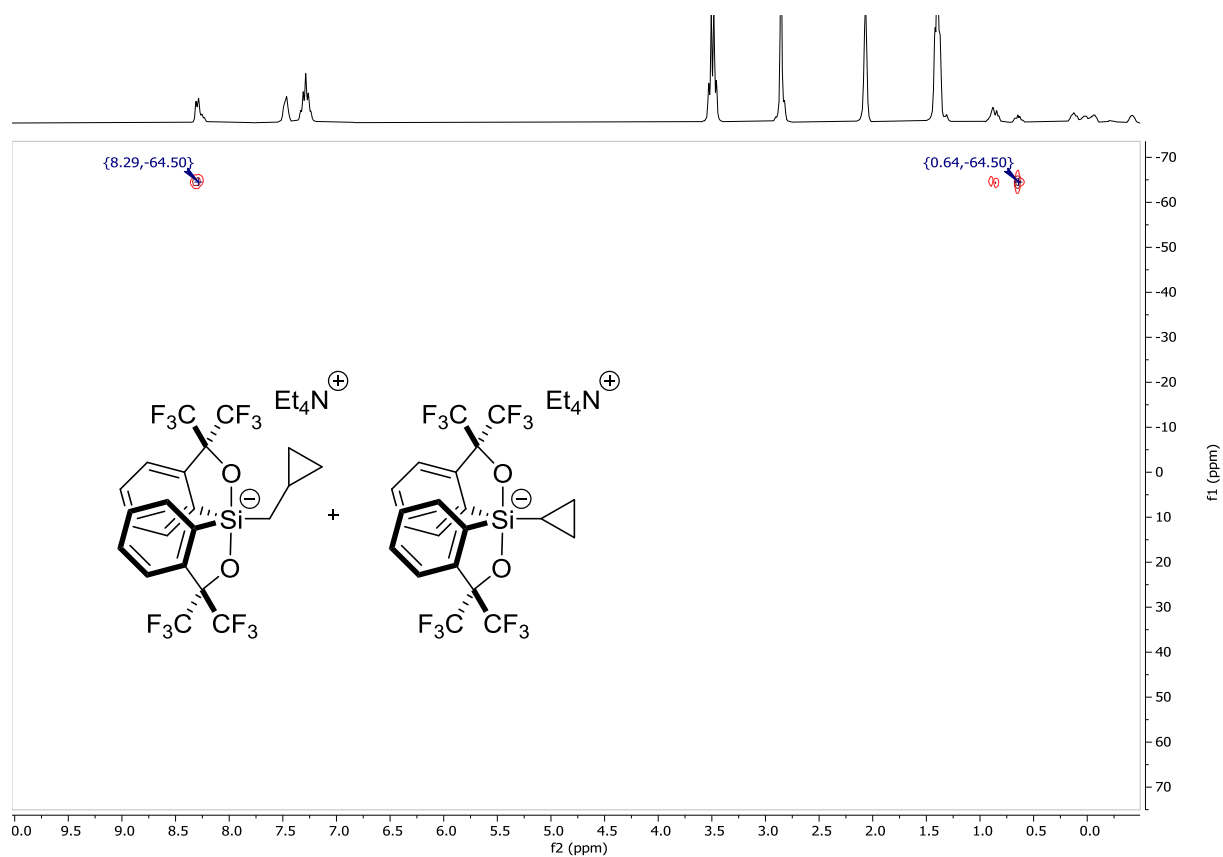


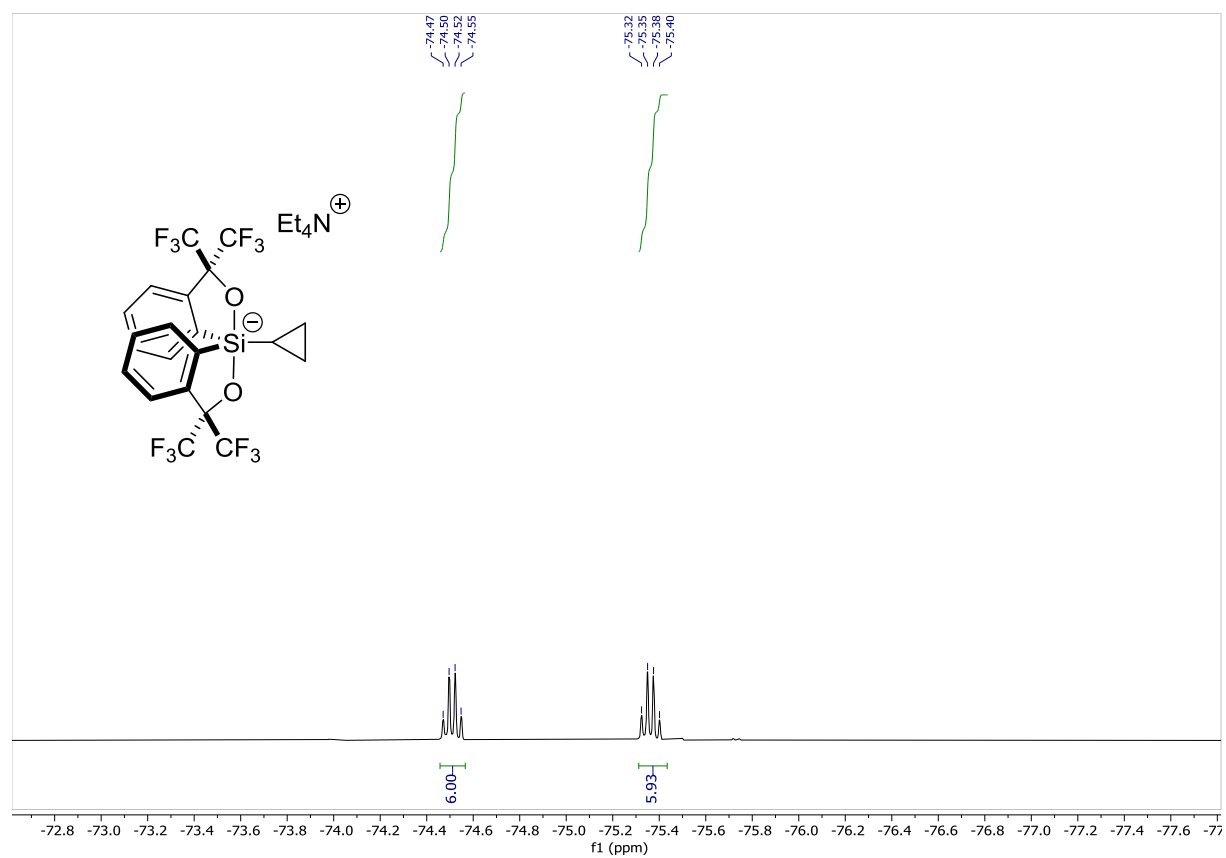
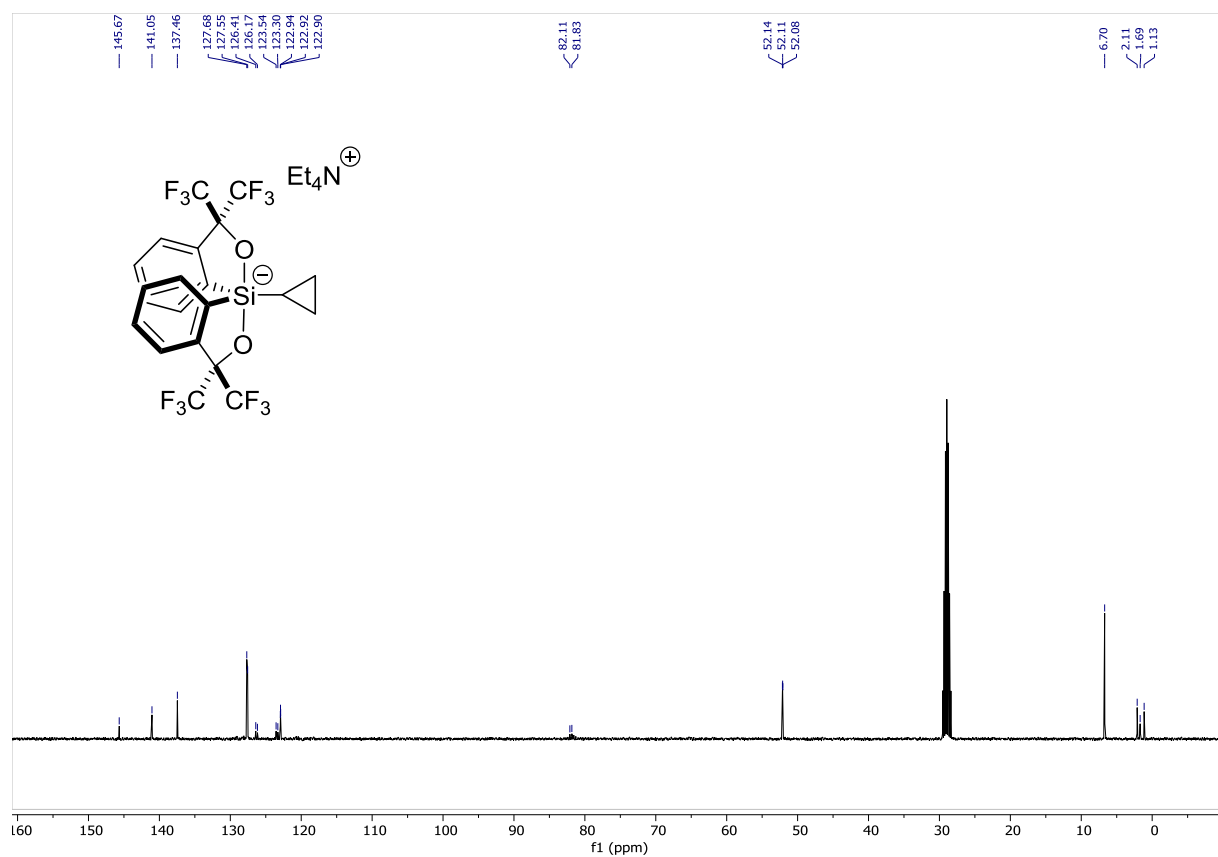


^1H , ^{13}C , ^{19}F , and $^1\text{H}/^{29}\text{Si}$ HMQC NMR spectra of mixture 3e/4e in $(\text{CD}_3)_2\text{CO}$ and 4e in $(\text{CD}_3)_2\text{CO}$

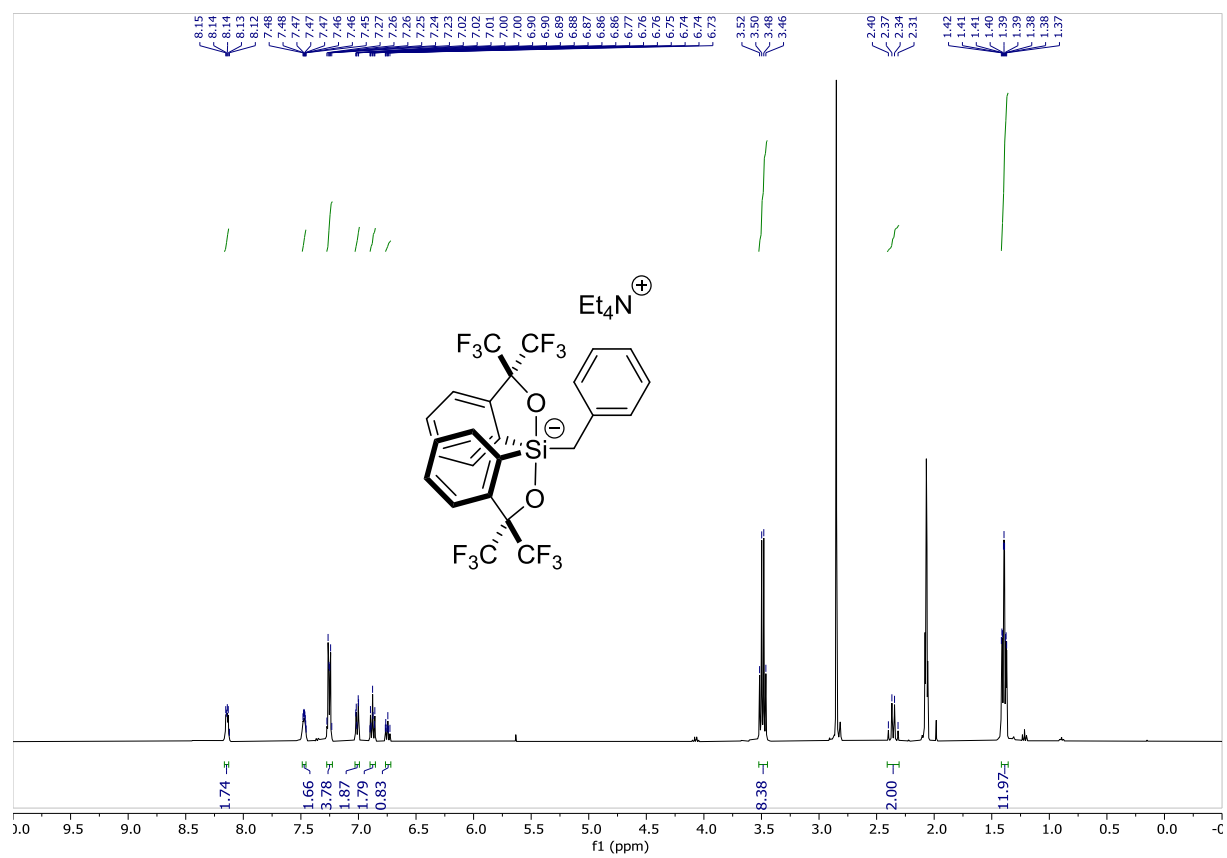


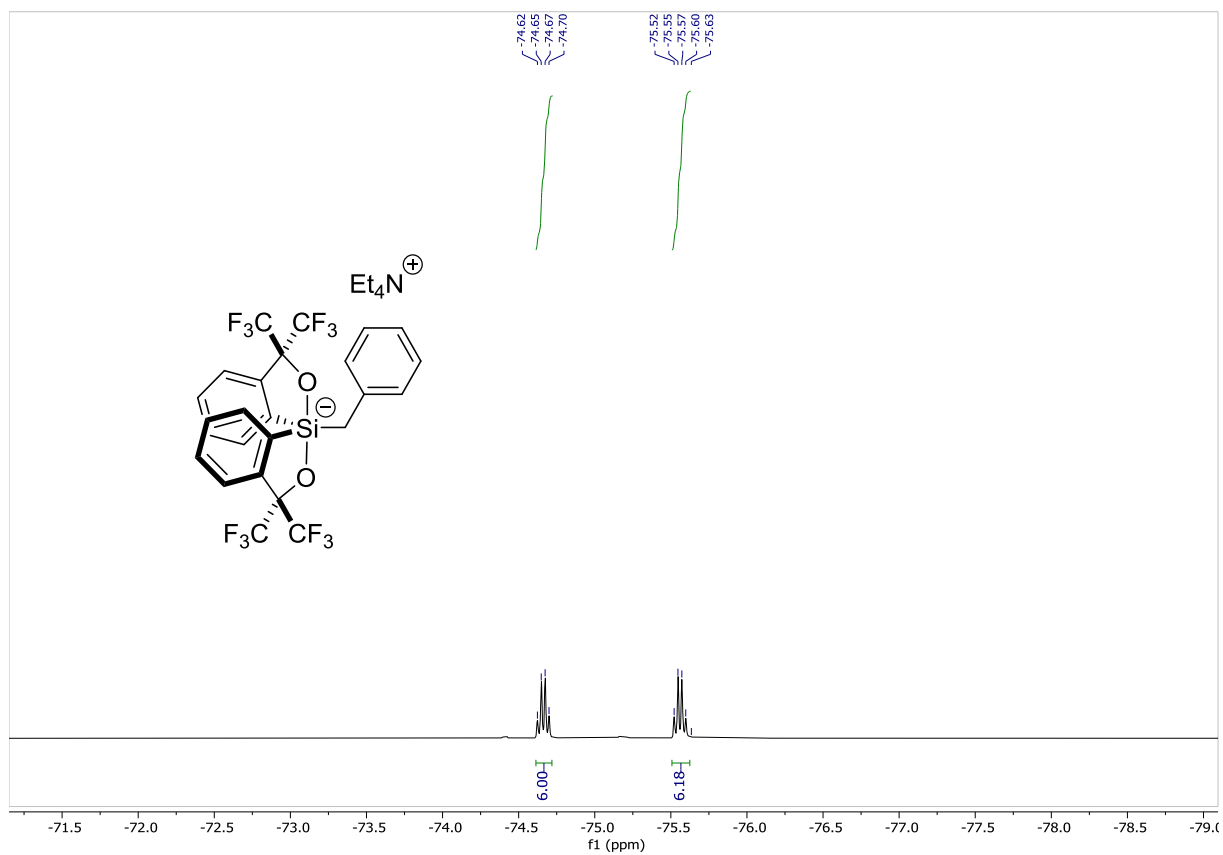
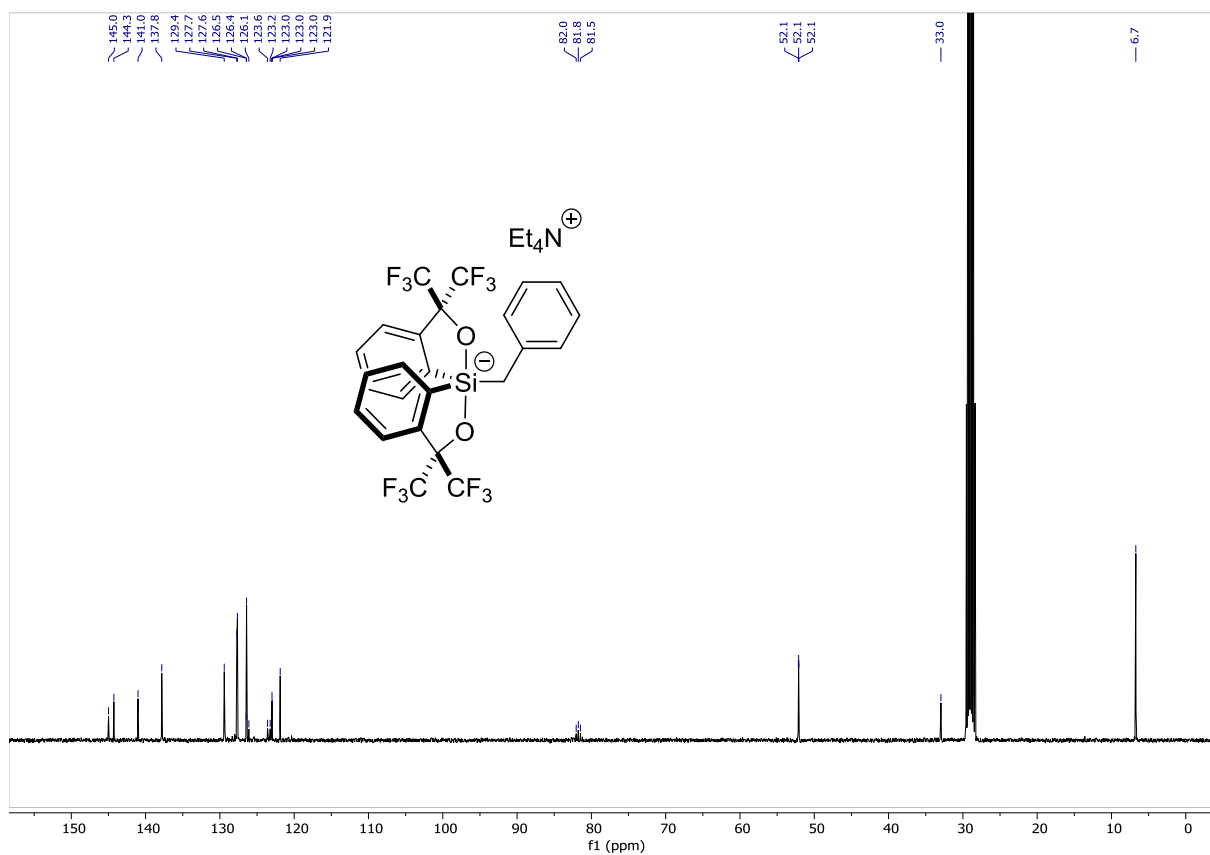


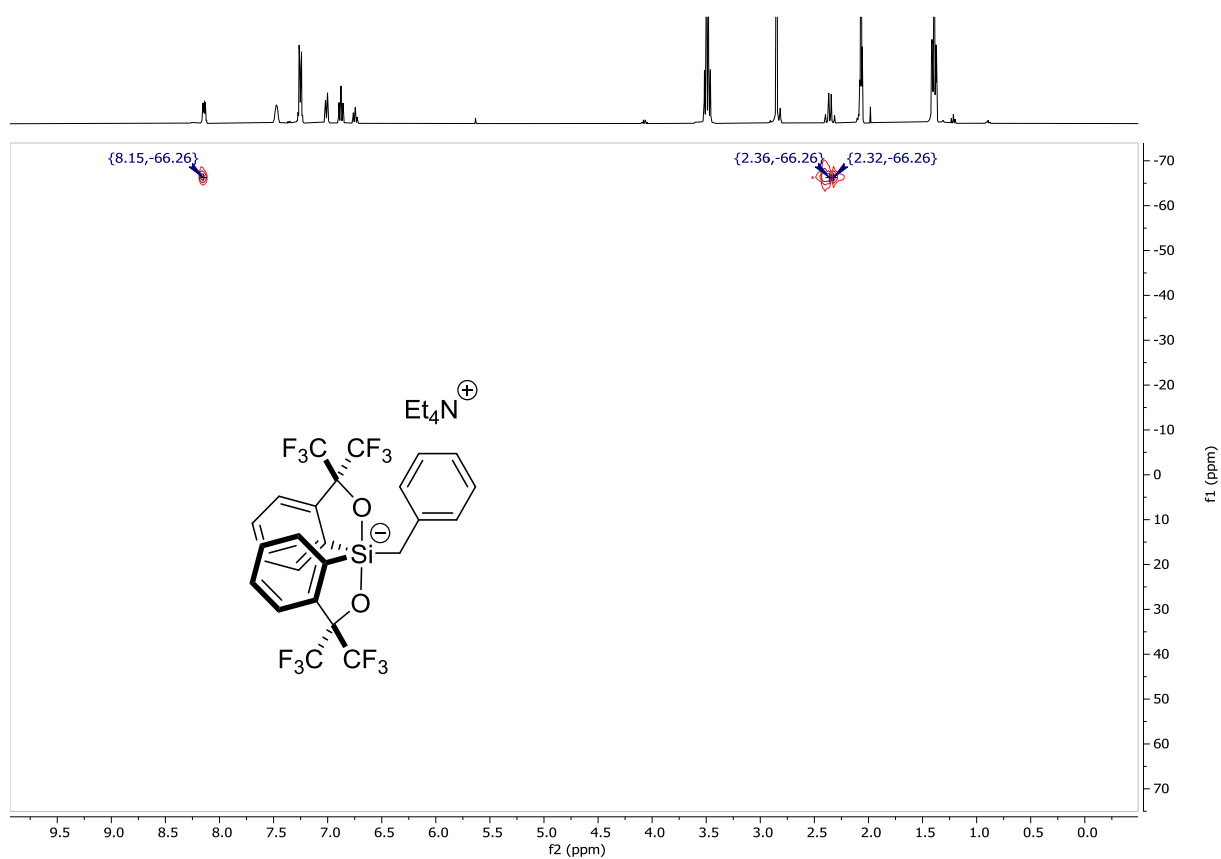




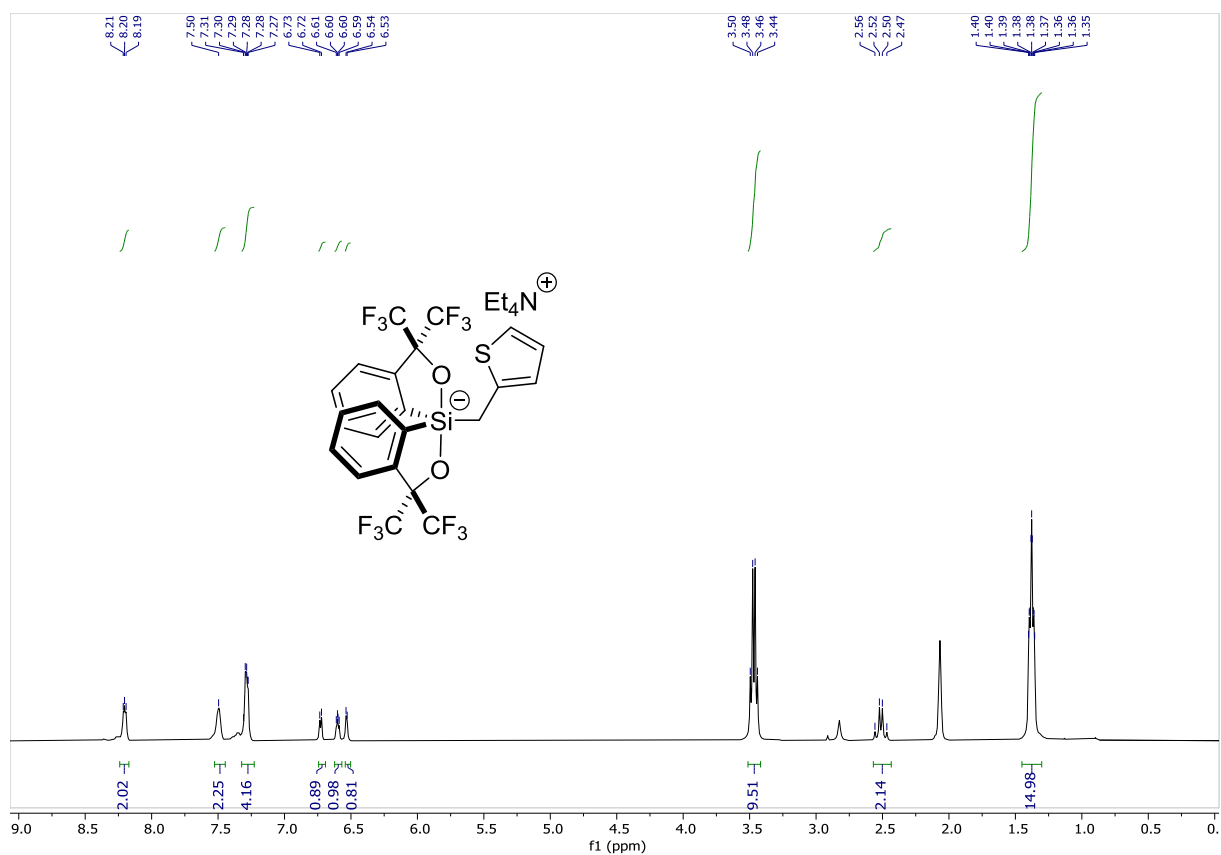
^1H , ^{13}C , ^{19}F , and $^1\text{H}/^{29}\text{Si}$ HMQC NMR spectra of 3f in $(\text{CD}_3)_2\text{CO}$

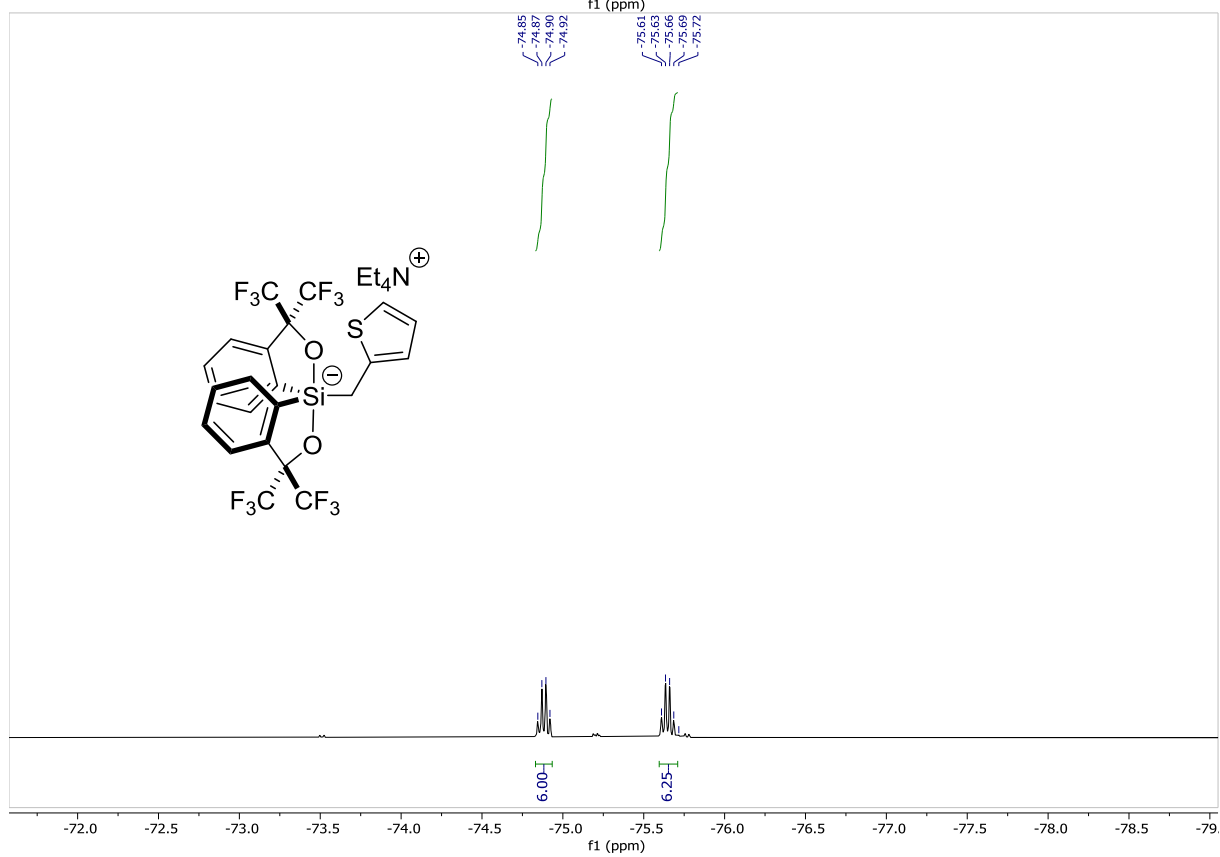
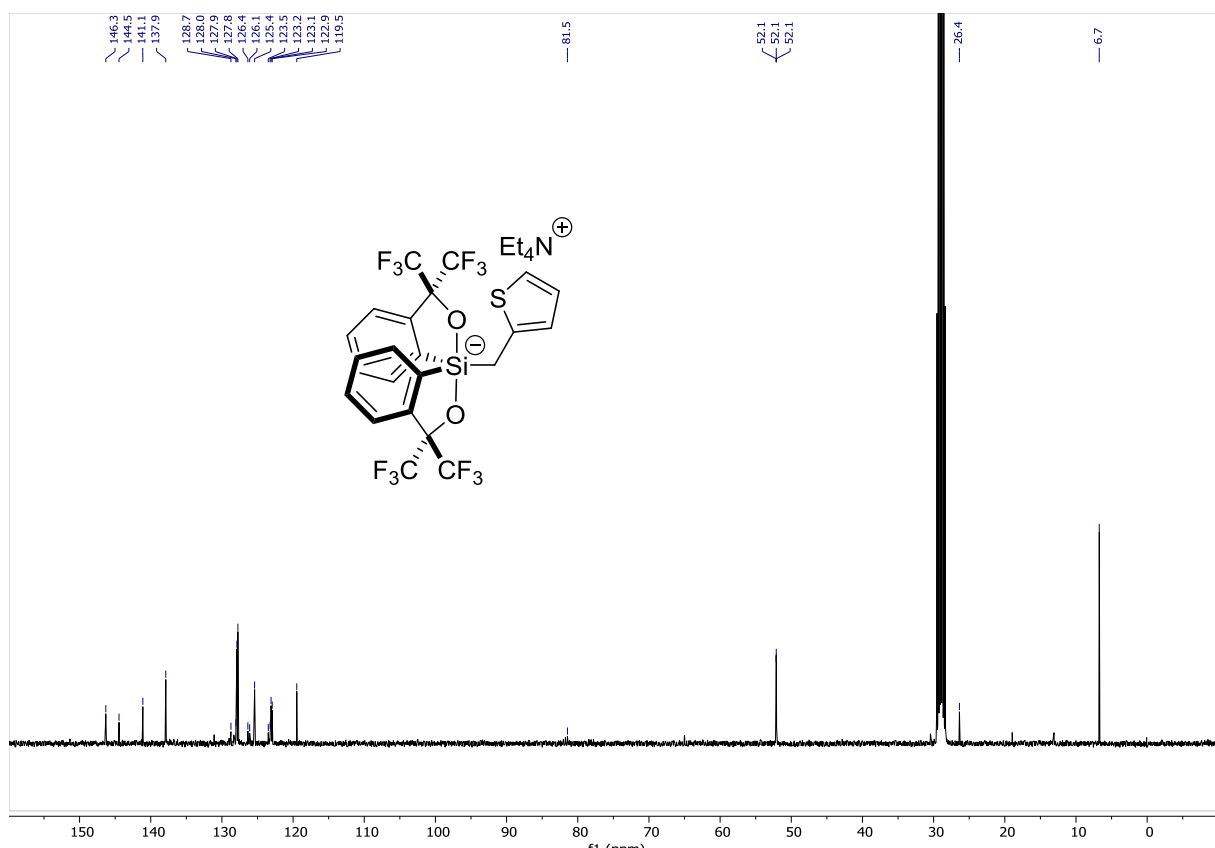


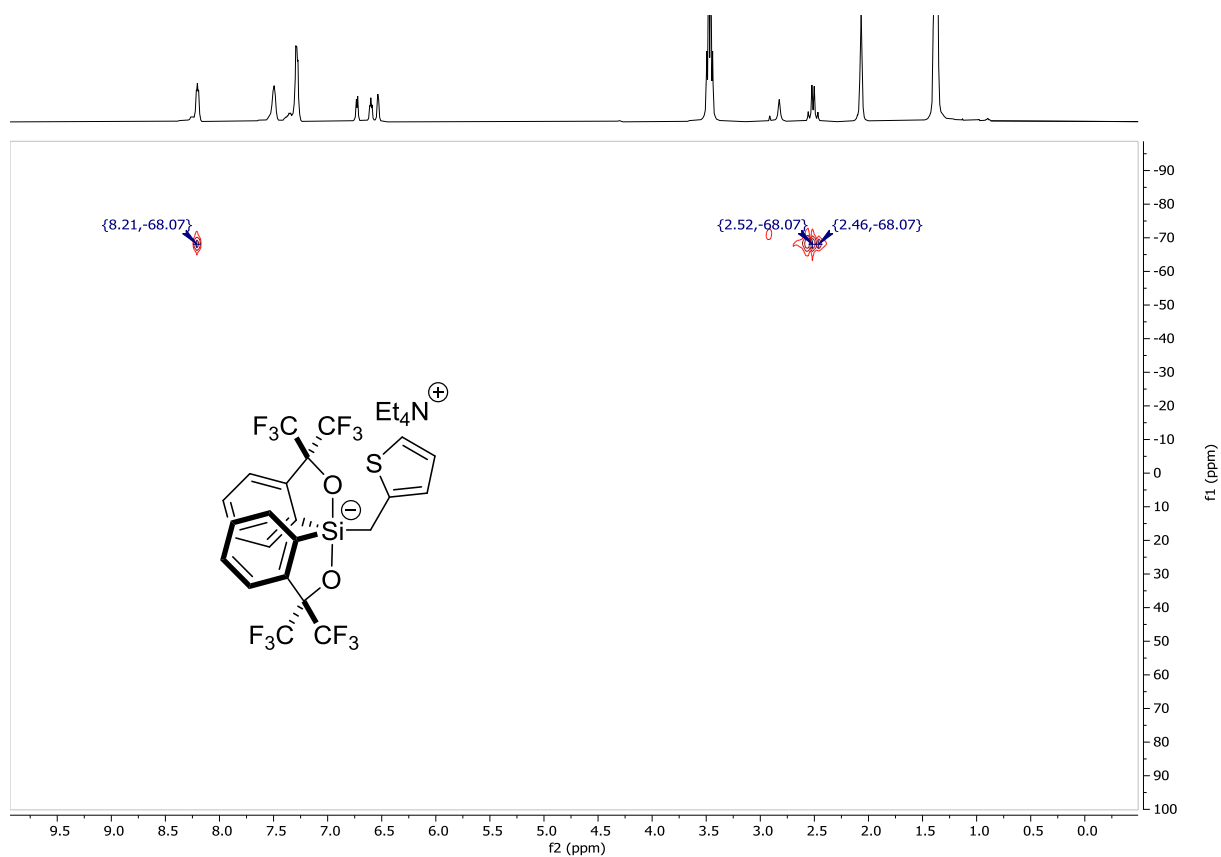




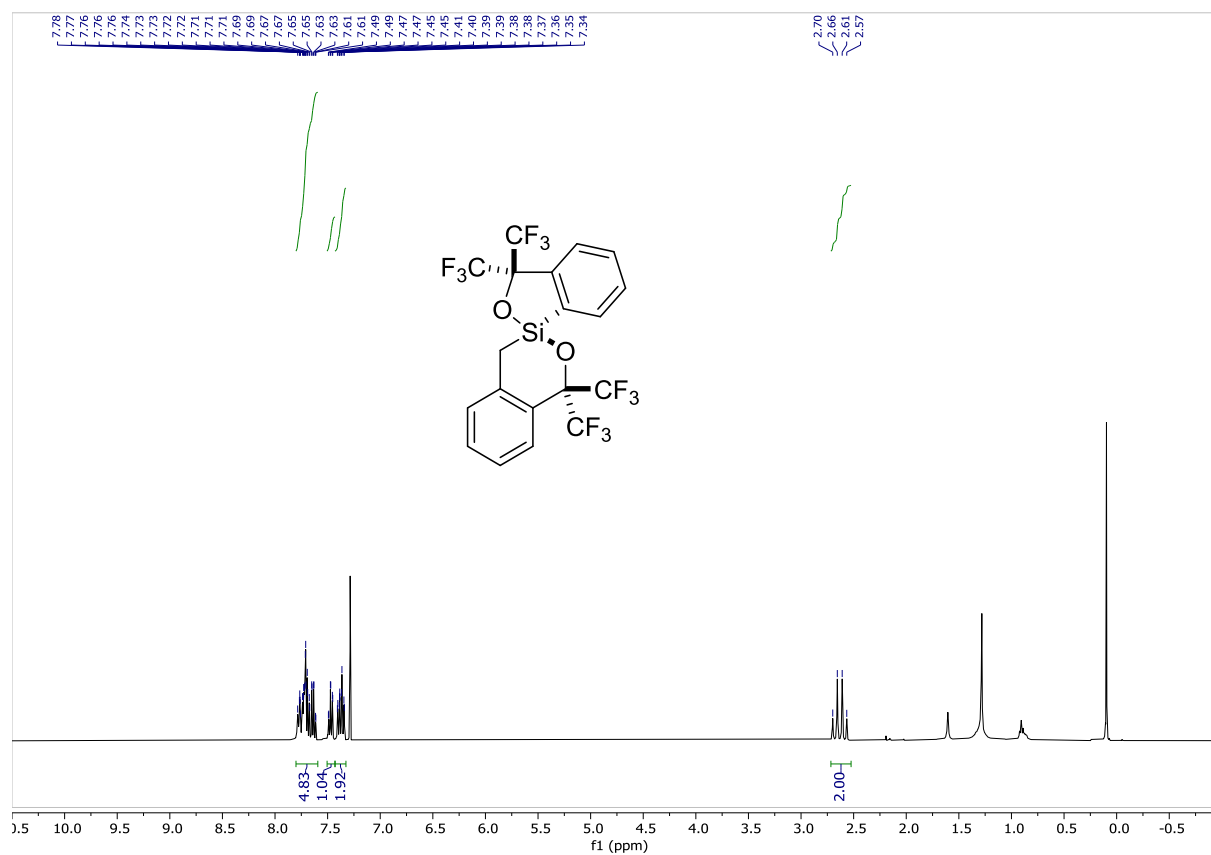
^1H , ^{13}C , ^{19}F , and $^1\text{H}/^{29}\text{Si}$ HMQC NMR spectra of 3g in $(\text{CD}_3)_2\text{CO}$

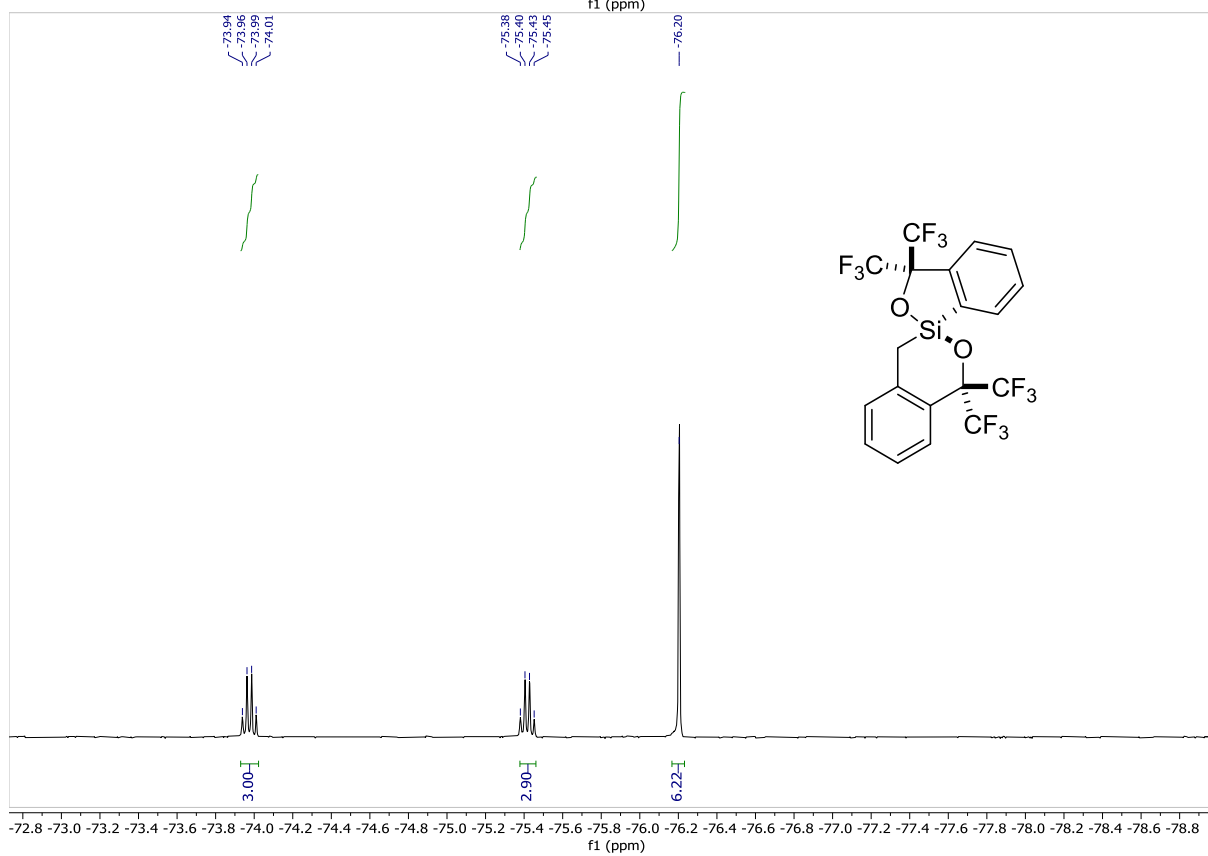
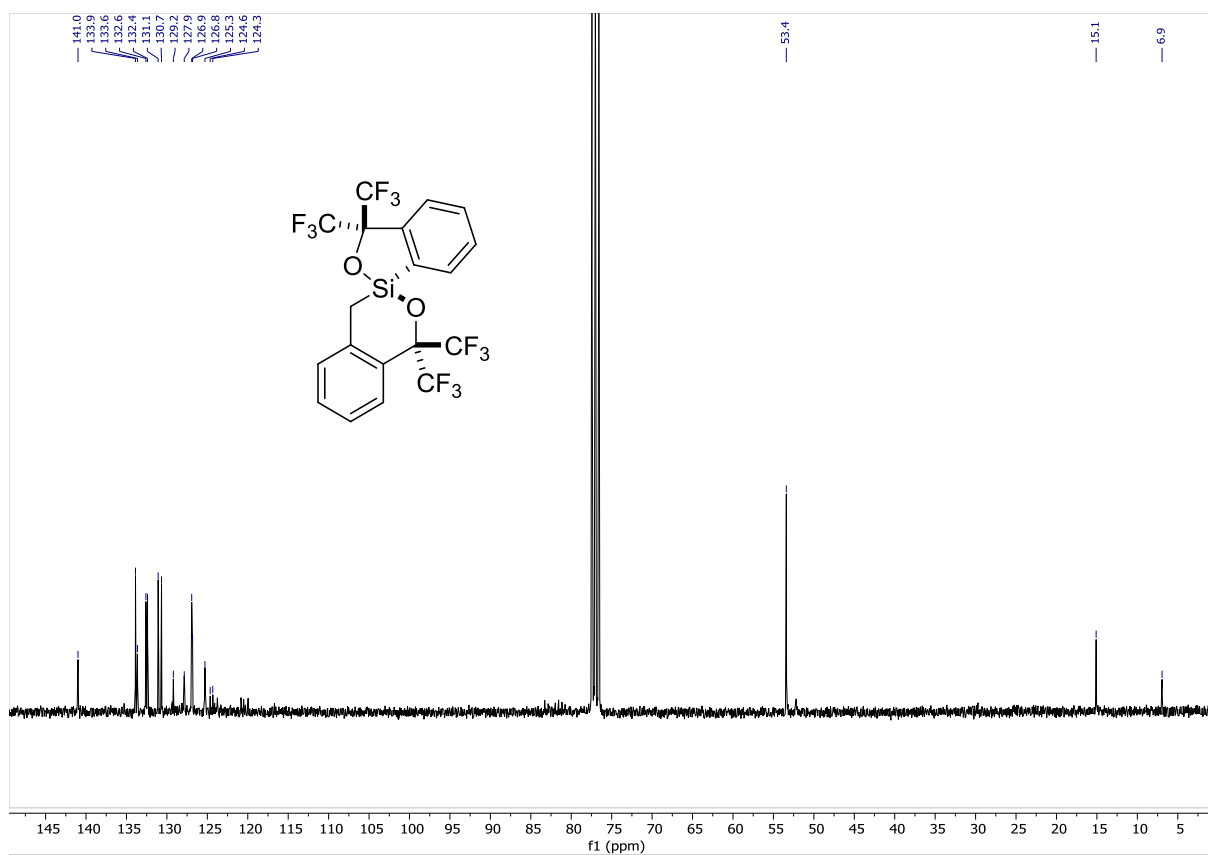


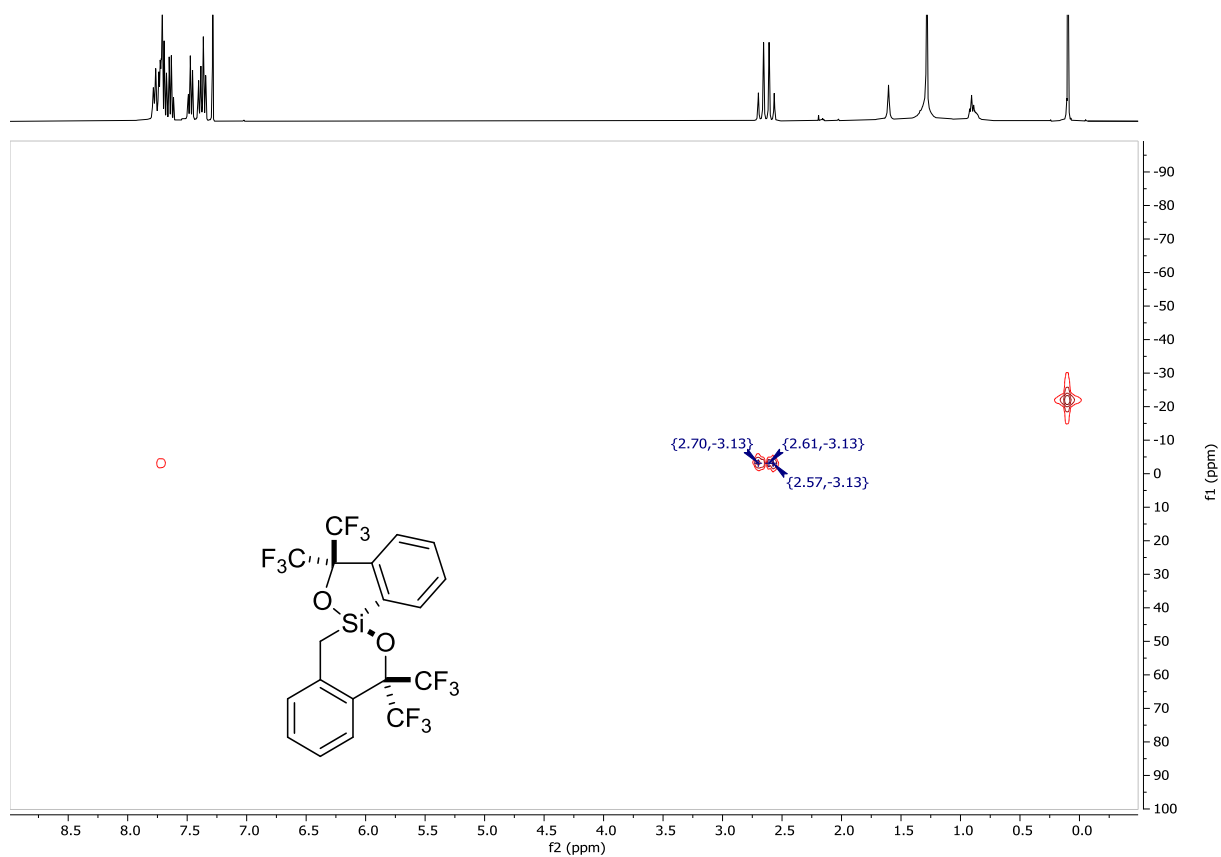




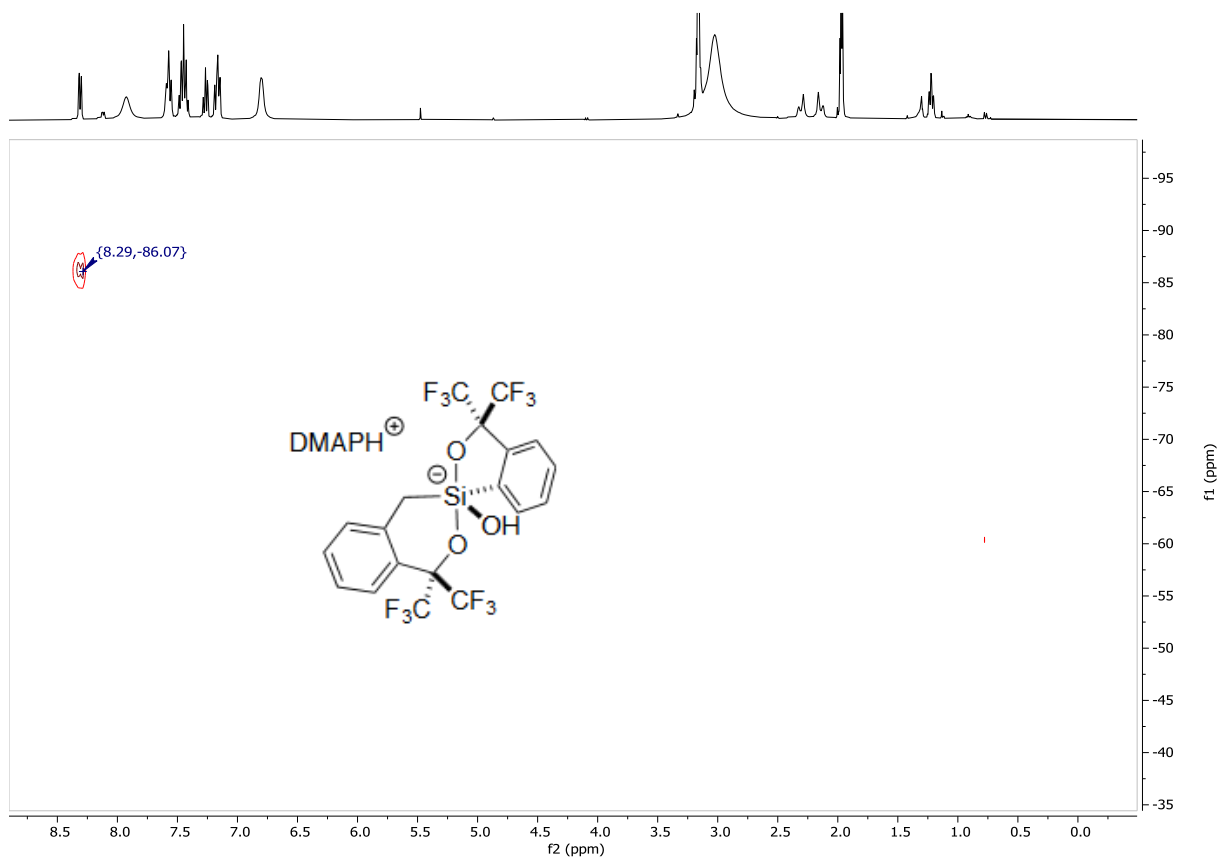
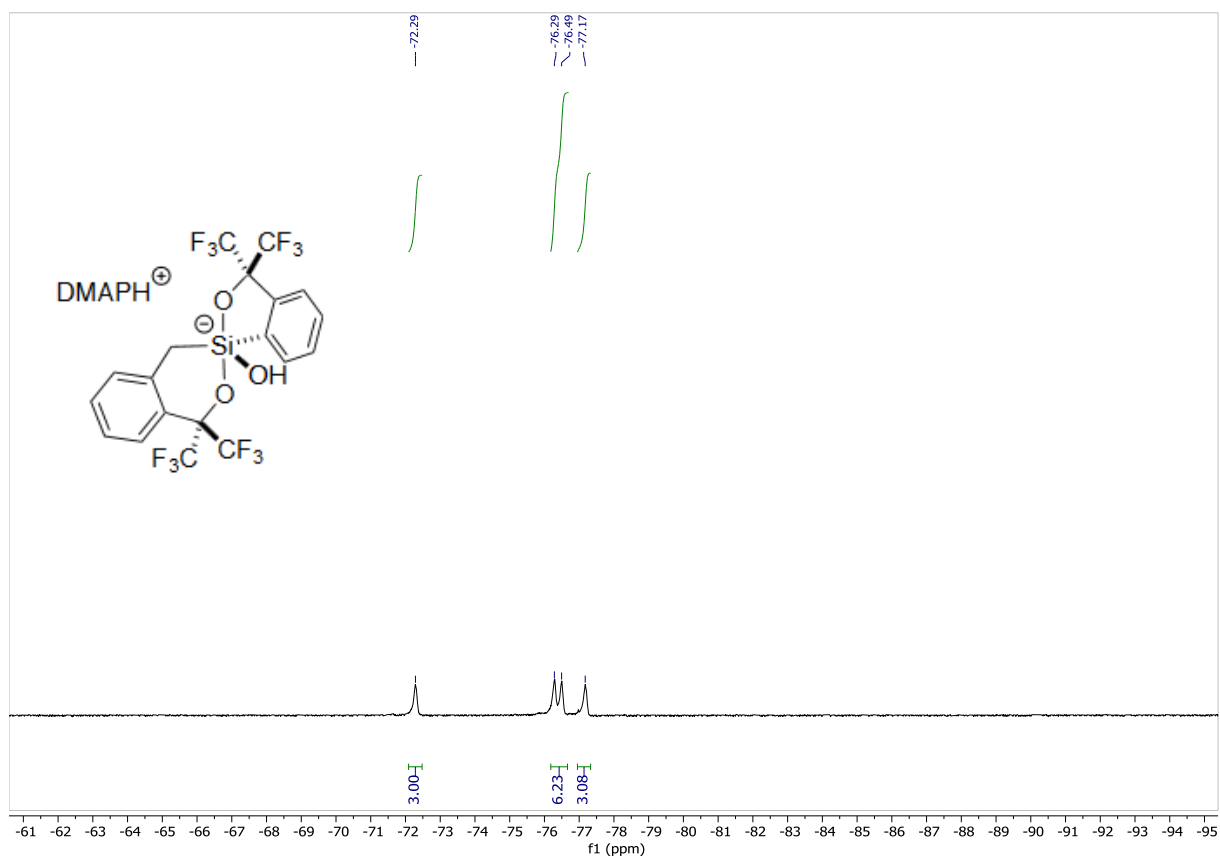
^1H , ^{13}C , ^{19}F , and $^1\text{H}/^{29}\text{Si}$ HMQC NMR spectra of 5 in CDCl_3





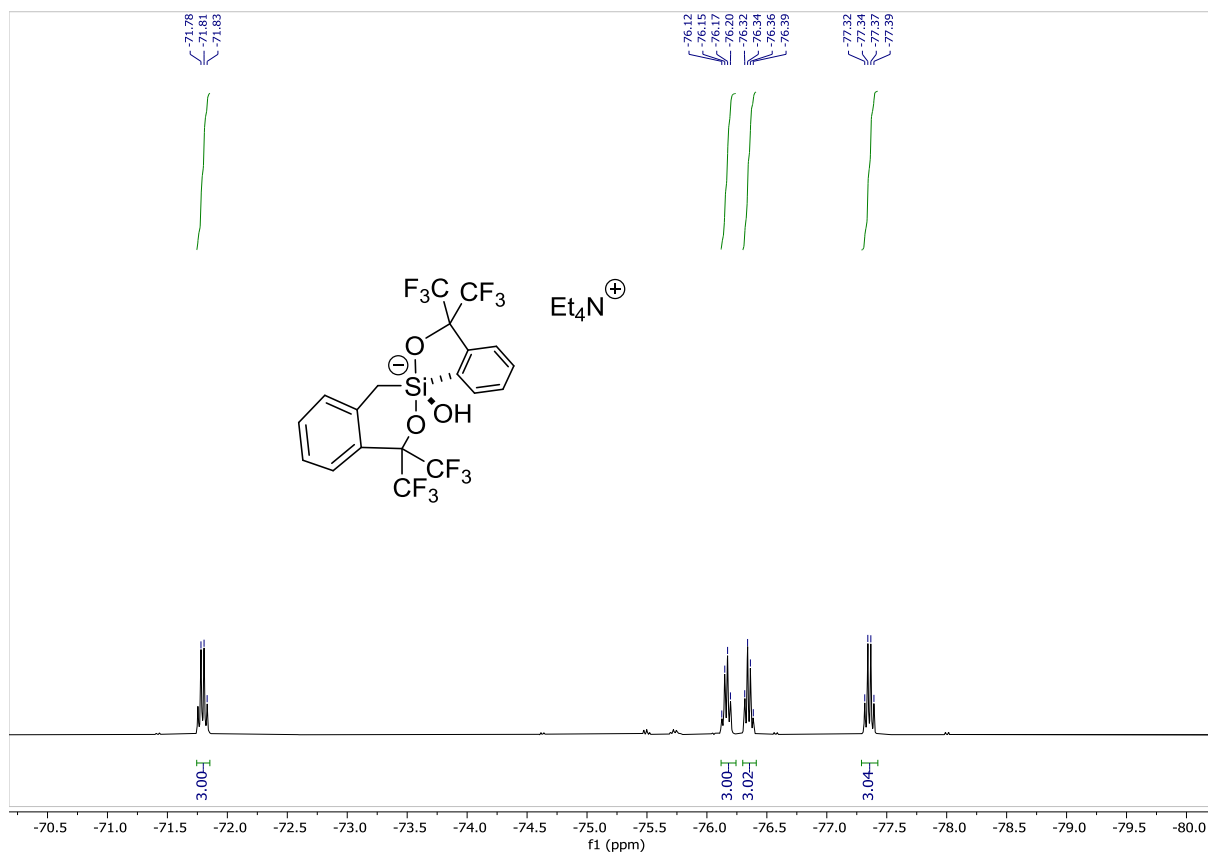
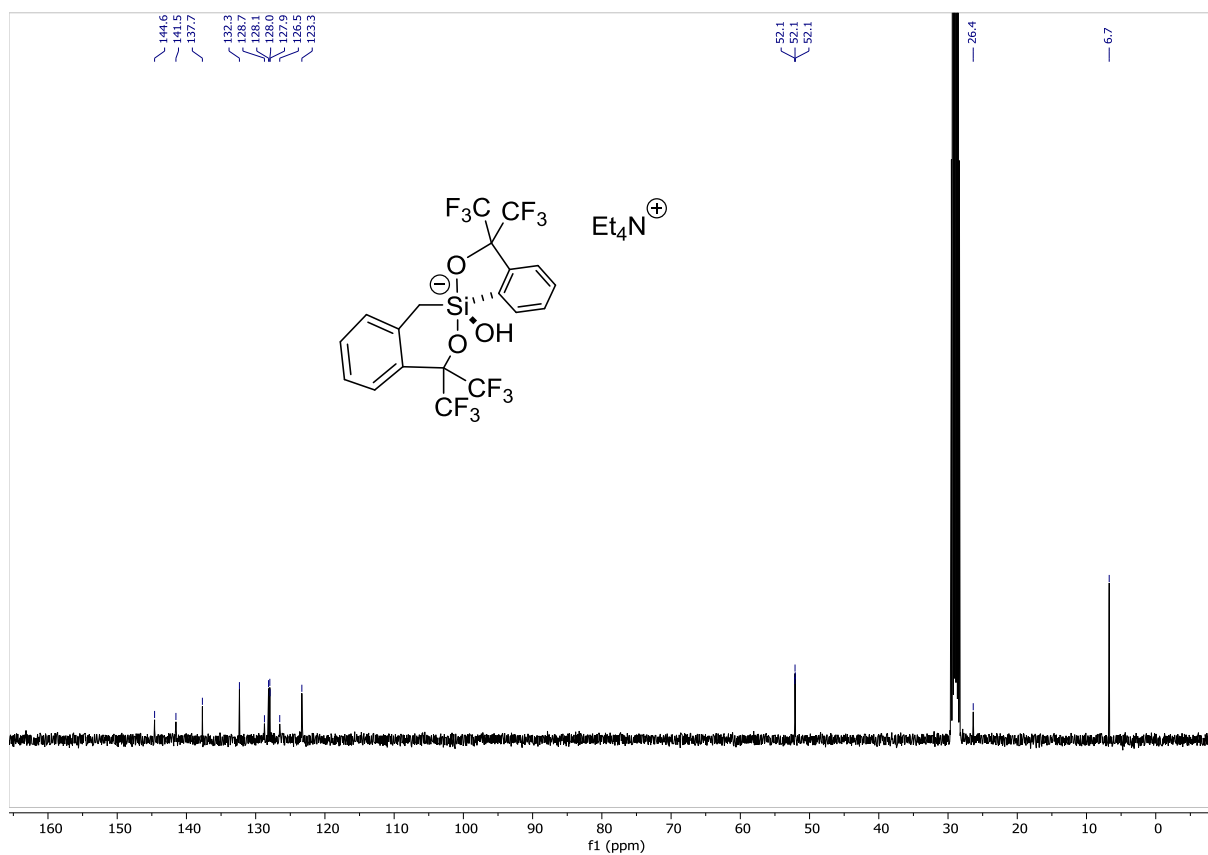


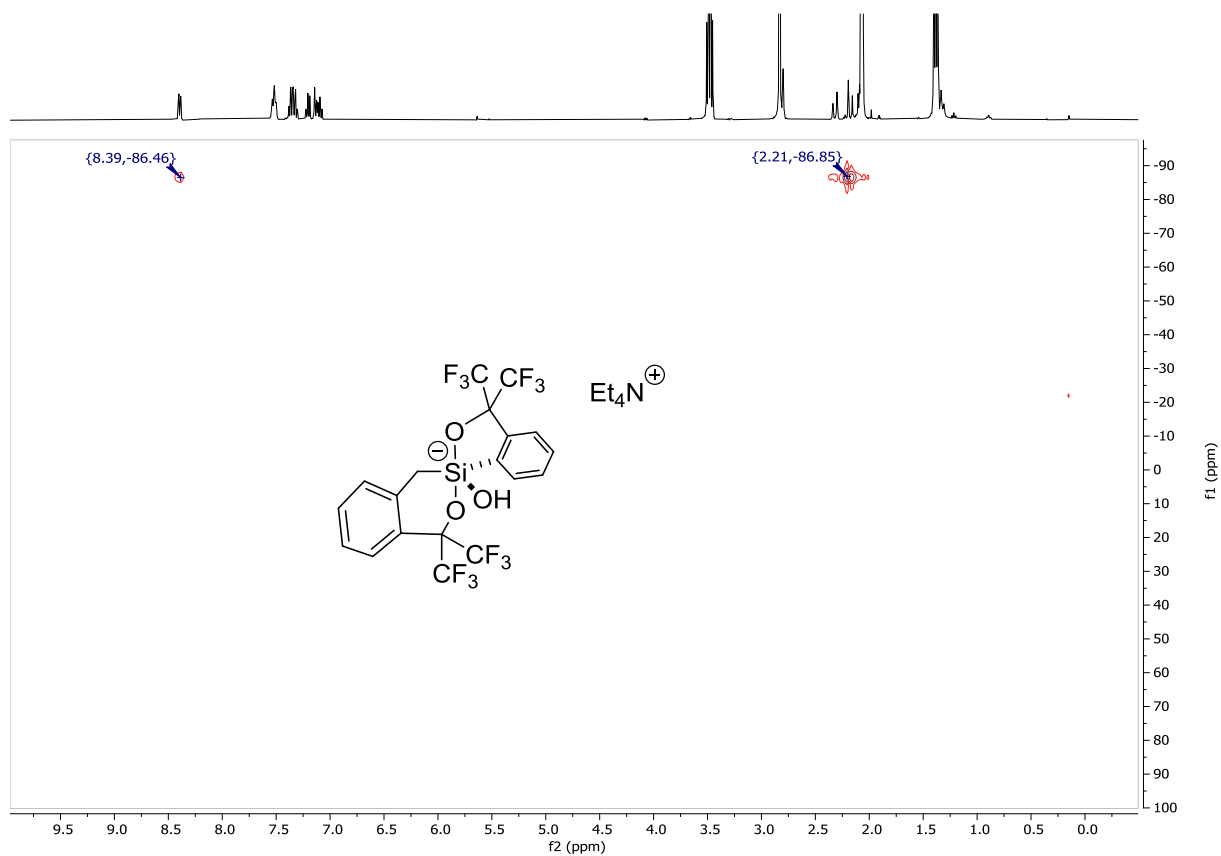
^1H , ^{13}C , ^{19}F , and $^1\text{H}/^{29}\text{Si}$ HMQC NMR spectra of 7 in CD_3CN



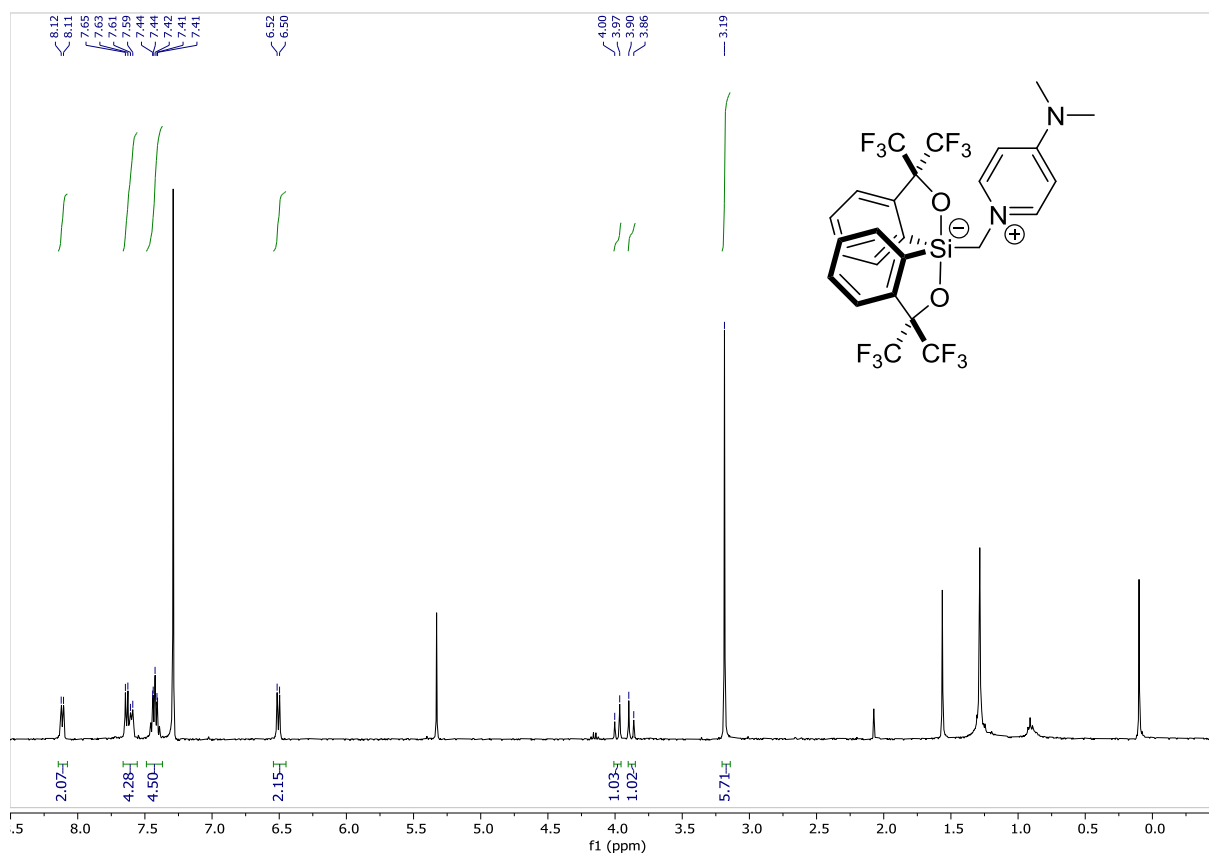
Chemical structure of the silanone ynone salt is shown above the spectrum. The structure consists of a central silicon atom double-bonded to an oxygen atom (silanone) and single-bonded to a phenyl ring, a hydroxyl group, and a ynone group. The ynone group is a 1,1,1-trifluoro-2-phenylethan-2-ylidene group. The counterion is Et_4N^+ .

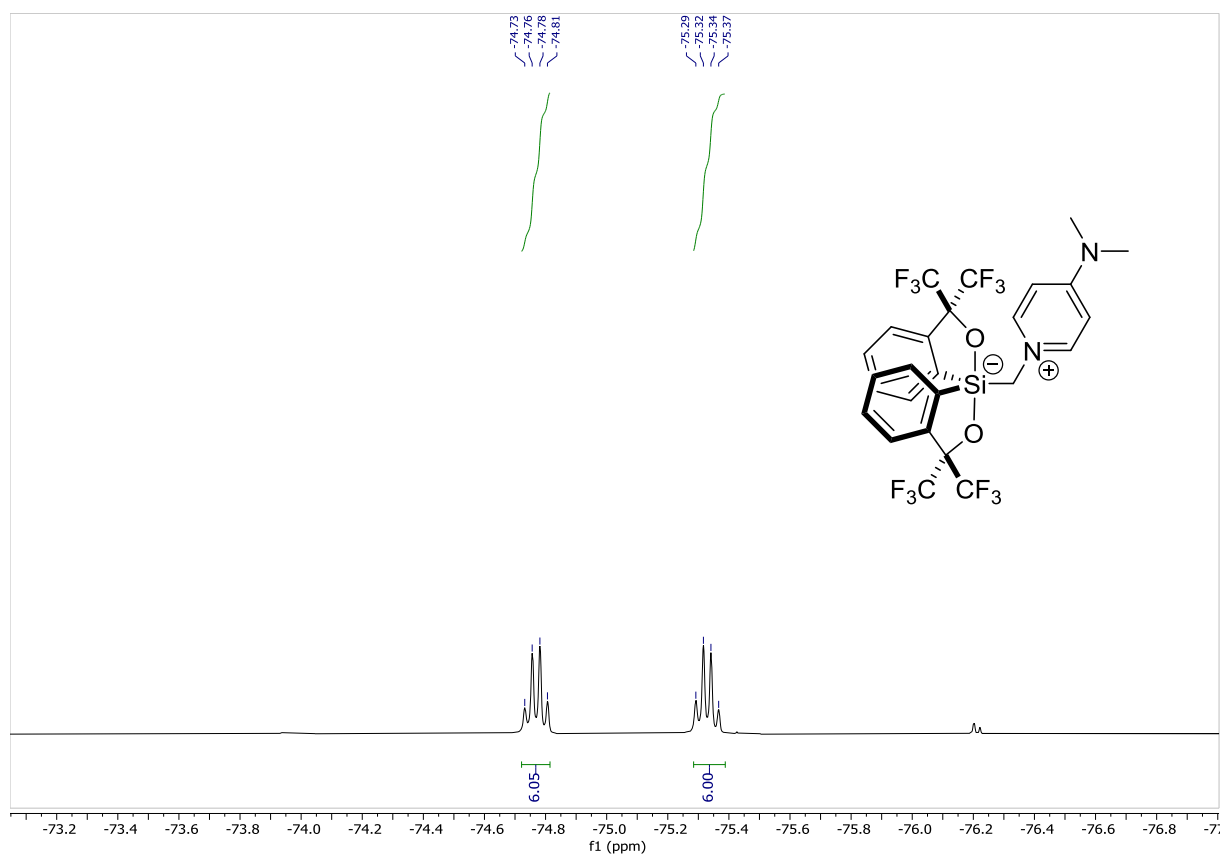
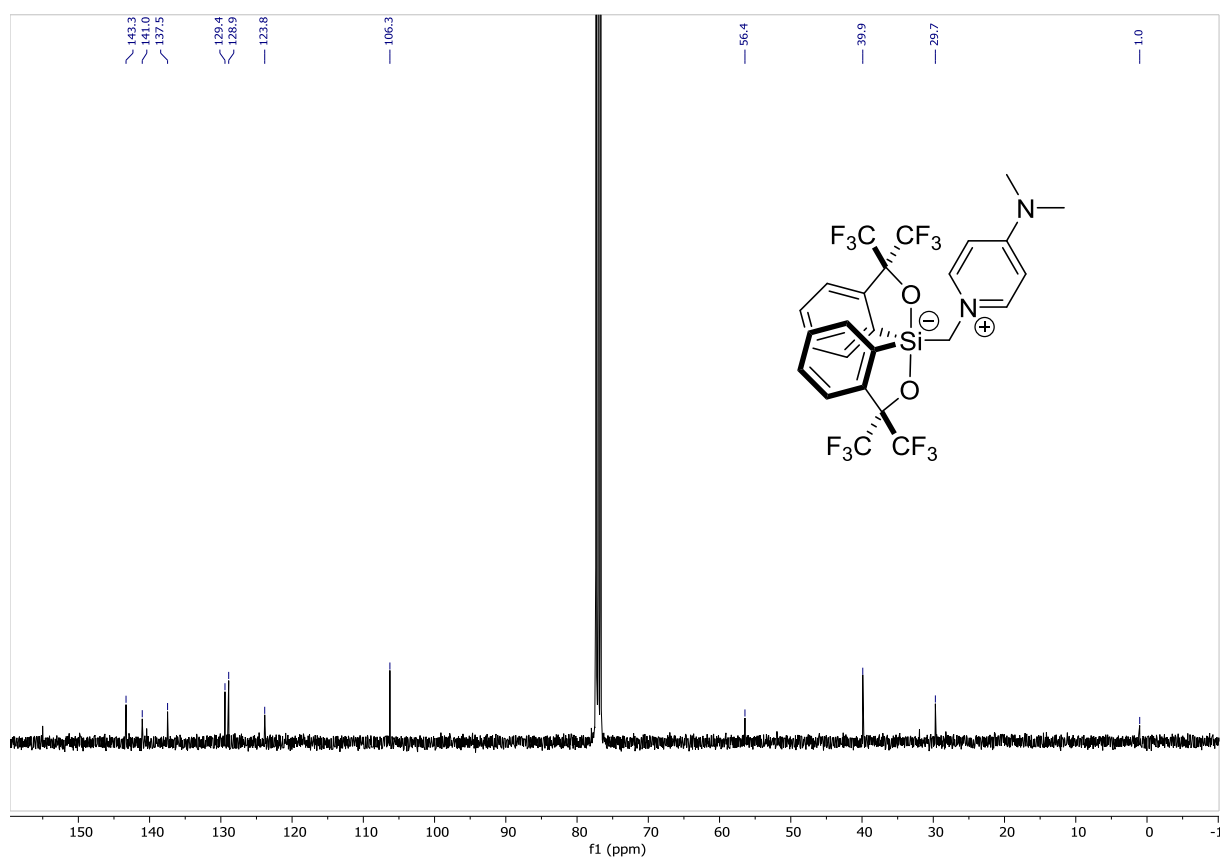
^1H NMR spectrum (CDCl₃) showing peaks from 0 to 10 ppm. The spectrum is characterized by several multiplets in the aromatic region (7.0-7.5 ppm), a sharp singlet at 3.5 ppm, a sharp singlet at 2.3 ppm, and a large multiplet in the aliphatic region (1.3-1.4 ppm). Integration values are provided below the peaks: 0.53, 1.69, 1.94, 2.49, 6.75, 0.80, 0.93, and 11.17. A list of chemical shifts (ppm) is provided at the top of the spectrum: 8.41, 8.40, 8.39, 8.38, 7.54, 7.53, 7.52, 7.50, 7.38, 7.37, 7.36, 7.35, 7.34, 7.33, 7.32, 7.31, 7.30, 7.23, 7.22, 7.11, 7.10, 7.09, 7.08, 7.07, 7.06, 7.05, 7.04, 7.03, 7.02, 7.01, 7.00, 6.99, 6.98, 6.97, 6.96, 6.95, 6.94, 6.93, 6.92, 6.91, 6.90, 6.89, 6.88, 6.87, 6.86, 6.85, 6.84, 6.83, 6.82, 6.81, 6.80, 6.79, 6.78, 6.77, 6.76, 6.75, 6.74, 6.73, 6.72, 6.71, 6.70, 6.69, 6.68, 6.67, 6.66, 6.65, 6.64, 6.63, 6.62, 6.61, 6.60, 6.59, 6.58, 6.57, 6.56, 6.55, 6.54, 6.53, 6.52, 6.51, 6.50, 6.49, 6.48, 6.47, 6.46, 6.45, 6.44, 6.43, 6.42, 6.41, 6.40, 6.39, 6.38, 6.37, 6.36, 6.35, 6.34, 6.33, 6.32, 6.31, 6.30, 6.29, 6.28, 6.27, 6.26, 6.25, 6.24, 6.23, 6.22, 6.21, 6.20, 6.19, 6.18, 6.17, 6.16, 6.15, 6.14, 6.13, 6.12, 6.11, 6.10, 6.09, 6.08, 6.07, 6.06, 6.05, 6.04, 6.03, 6.02, 6.01, 6.00, 5.99, 5.98, 5.97, 5.96, 5.95, 5.94, 5.93, 5.92, 5.91, 5.90, 5.89, 5.88, 5.87, 5.86, 5.85, 5.84, 5.83, 5.82, 5.81, 5.80, 5.79, 5.78, 5.77, 5.76, 5.75, 5.74, 5.73, 5.72, 5.71, 5.70, 5.69, 5.68, 5.67, 5.66, 5.65, 5.64, 5.63, 5.62, 5.61, 5.60, 5.59, 5.58, 5.57, 5.56, 5.55, 5.54, 5.53, 5.52, 5.51, 5.50, 5.49, 5.48, 5.47, 5.46, 5.45, 5.44, 5.43, 5.42, 5.41, 5.40, 5.39, 5.38, 5.37, 5.36, 5.35, 5.34, 5.33, 5.32, 5.31, 5.30, 5.29, 5.28, 5.27, 5.26, 5.25, 5.24, 5.23, 5.22, 5.21, 5.20, 5.19, 5.18, 5.17, 5.16, 5.15, 5.14, 5.13, 5.12, 5.11, 5.10, 5.09, 5.08, 5.07, 5.06, 5.05, 5.04, 5.03, 5.02, 5.01, 5.00, 4.99, 4.98, 4.97, 4.96, 4.95, 4.94, 4.93, 4.92, 4.91, 4.90, 4.89, 4.88, 4.87, 4.86, 4.85, 4.84, 4.83, 4.82, 4.81, 4.80, 4.79, 4.78, 4.77, 4.76, 4.75, 4.74, 4.73, 4.72, 4.71, 4.70, 4.69, 4.68, 4.67, 4.66, 4.65, 4.64, 4.63, 4.62, 4.61, 4.60, 4.59, 4.58, 4.57, 4.56, 4.55, 4.54, 4.53, 4.52, 4.51, 4.50, 4.49, 4.48, 4.47, 4.46, 4.45, 4.44, 4.43, 4.42, 4.41, 4.40, 4.39, 4.38, 4.37, 4.36, 4.35, 4.34, 4.33, 4.32, 4.31, 4.30, 4.29, 4.28, 4.27, 4.26, 4.25, 4.24, 4.23, 4.22, 4.21, 4.20, 4.19, 4.18, 4.17, 4.16, 4.15, 4.14, 4.13, 4.12, 4.11, 4.10, 4.09, 4.08, 4.07, 4.06, 4.05, 4.04, 4.03, 4.02, 4.01, 4.00, 3.99, 3.98, 3.97, 3.96, 3.95, 3.94, 3.93, 3.92, 3.91, 3.90, 3.89, 3.88, 3.87, 3.86, 3.85, 3.84, 3.83, 3.82, 3.81, 3.80, 3.79, 3.78, 3.77, 3.76, 3.75, 3.74, 3.73, 3.72, 3.71, 3.70, 3.69, 3.68, 3.67, 3.66, 3.65, 3.64, 3.63, 3.62, 3.61, 3.60, 3.59, 3.58, 3.57, 3.56, 3.55, 3.54, 3.53, 3.52, 3.51, 3.50, 3.49, 3.48, 3.47, 3.46, 3.45, 3.44, 3.43, 3.42, 3.41, 3.40, 3.39, 3.38, 3.37, 3.36, 3.35, 3.34, 3.33, 3.32, 3.31, 3.30, 3.29, 3.28, 3.27, 3.26, 3.25, 3.24, 3.23, 3.22, 3.21, 3.20, 3.19, 3.18, 3.17, 3.16, 3.15, 3.14, 3.13, 3.12, 3.11, 3.10, 3.09, 3.08, 3.07, 3.06, 3.05, 3.04, 3.03, 3.02, 3.01, 3.00, 2.99, 2.98, 2.97, 2.96, 2.95, 2.94, 2.93, 2.92, 2.91, 2.90, 2.89, 2.88, 2.87, 2.86, 2.85, 2.84, 2.83, 2.82, 2.81, 2.80, 2.79, 2.78, 2.77, 2.76, 2.75, 2.74, 2.73, 2.72, 2.71, 2.70, 2.69, 2.68, 2.67, 2.66, 2.65, 2.64, 2.63, 2.62, 2.61, 2.60, 2.59, 2.58, 2.57, 2.56, 2.55, 2.54, 2.53, 2.52, 2.51, 2.50, 2.49, 2.48, 2.47, 2.46, 2.45, 2.44, 2.43, 2.42, 2.41, 2.40, 2.39, 2.38, 2.37, 2.36, 2.35, 2.34, 2.33, 2.32, 2.31, 2.30, 2.29, 2.28, 2.27, 2.26, 2.25, 2.24, 2.23, 2.22, 2.21, 2.20, 2.19, 2.18, 2.17, 2.16, 2.15, 2.14, 2.13, 2.12, 2.11, 2.10, 2.09, 2.08, 2.07, 2.06, 2.05, 2.04, 2.03, 2.02, 2.01, 2.00, 1.99, 1.98, 1.97, 1.96, 1.95, 1.94, 1.93, 1.92, 1.91, 1.90, 1.89, 1.88, 1.87, 1.86, 1.85, 1.84, 1.83, 1.82, 1.81, 1.80, 1.79, 1.78, 1.77, 1.76, 1.75, 1.74, 1.73, 1.72, 1.71, 1.70, 1.69, 1.68, 1.67, 1.66, 1.65, 1.64, 1.63, 1.62, 1.61, 1.60, 1.59, 1.58, 1.57, 1.56, 1.55, 1.54, 1.53, 1.52, 1.51, 1.50, 1.49, 1.48, 1.47, 1.46, 1.45, 1.44, 1.43, 1.42, 1.41, 1.40, 1.39, 1.38, 1.37, 1.36, 1.35, 1.34, 1.33, 1.32, 1.31, 1.30, 1.29, 1.28, 1.27, 1.26, 1.25, 1.24

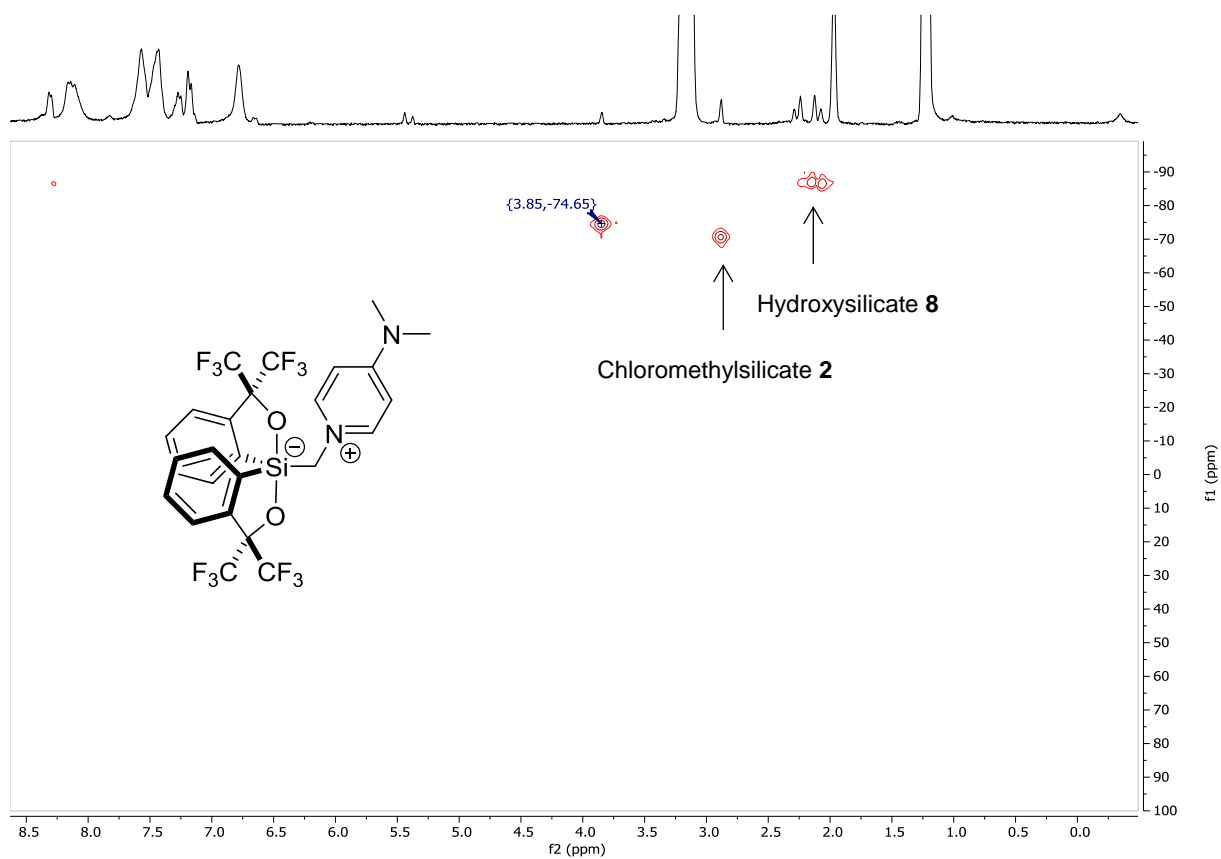




^1H , ^{13}C , ^{19}F , NMR spectra of 8 in CDCl_3 and $^1\text{H}/^{29}\text{Si}$ HMQC spectrum of 8 in CD_3CN







IV. Computational details

All DFT computations were carried out using the Gaussian 09^[2] software package.

Optimization of geometries and frequencies were performed using the B3LYP-D3 functional and the 6-311G(2d,p) basis set for all elements. The nature of all stationary points was confirmed by analyzing the harmonic vibrational frequencies.

In the following table is reported the energy (in Hartree) and the cartesian coordinates (x,y,z) of the computed species.

A				TS _A ‡			
E(B3LYP-D3) = -2829.28571261				E(RB3LYP-D3) = -2829.23036311			
N _{imag} = 0				N _{imag} = 1 (- 480.07 cm ⁻¹)			
Si	0.00392400	-0.15835100	-0.53838497	Si	-0.09187700	0.66518199	0.33781800
F	-2.25630593	2.06888199	1.46054304	F	-1.58827901	-2.47315907	-0.28454700
F	-4.31937981	1.40451503	1.34532106	F	-3.72134495	-2.29238200	-0.63906401
F	-3.46464109	2.58647895	-0.25899601	F	-2.95735502	-2.34927106	1.38887596
F	-4.91092014	-0.62417102	-0.35780901	F	-4.89466476	0.07042000	-0.07125700
F	-4.14080191	0.58106798	-1.98627806	F	-4.06961918	0.07789000	1.93416905
F	-3.31528711	-1.38634801	-1.61569798	F	-3.63379312	1.71224105	0.58025002
F	3.46918011	-1.63350904	1.77978802	F	2.67069411	-2.07649708	2.23759890
F	4.31524515	0.36123100	1.85441005	F	4.39877415	-1.07936001	1.39019895
F	2.25064611	0.03117100	2.43559289	F	2.89582992	0.06637400	2.45915103
F	3.34271789	-0.22693200	-2.17909408	F	1.77664900	-1.62037206	-1.82754695
F	4.13100100	-1.75804901	-0.86611003	F	1.82427895	-3.01099300	-0.16959800
F	4.92788696	0.25593501	-0.77783602	F	3.67634511	-2.23155499	-0.96894902
O	-1.61510396	0.66206700	-0.86781901	O	-1.49192095	-0.03663200	1.01272702
O	1.62007201	-0.92075598	-0.10940800	O	0.94085598	-0.63255900	0.64770001
C	-0.90520298	-1.06346798	0.85626298	C	-0.90324903	0.71778703	-1.35568798
C	-0.38710701	-1.99289095	1.76201499	C	-0.45701900	1.17342806	-2.59634089
H	0.65942299	-2.26101208	1.70488095	H	0.52970803	1.60867703	-2.68756509
C	-1.20204604	-2.56747603	2.73266792	C	-1.26888001	1.06215405	-3.71948099

H	-0.79062200	-3.28896689	3.42939091	H	-0.91506201	1.41929901	-4.68033695
C	-2.54883194	-2.21533394	2.81418705	C	-2.53391504	0.48688501	-3.61580396
H	-3.18284988	-2.66096306	3.57160211	H	-3.16452289	0.40005001	-4.49344778
C	-3.08297491	-1.28793001	1.92531395	C	-2.99253011	0.01787500	-2.39026403
H	-4.12631989	-1.01193202	1.99263597	H	-3.97145796	-0.43258700	-2.30670404
C	-2.25349402	-0.72540700	0.95813799	C	-2.17154002	0.13926800	-1.27349496
C	-2.68065596	0.31180200	-0.08378900	C	-2.52214909	-0.33518299	0.14094301
C	-3.19677305	1.60000205	0.61837298	C	-2.70697403	-1.87919700	0.15947001
C	-3.78045702	-0.27689701	-1.01156700	C	-3.79449797	0.38879201	0.66454703
C	0.91128701	1.50169098	-0.39488900	C	1.87176502	1.66472602	-0.34261501
C	0.39350599	2.78802299	-0.56742698	C	2.24128294	2.83765888	-1.00401497
H	-0.65388000	2.90820789	-0.81050903	H	1.56327796	3.68593693	-1.01041496
C	1.20940495	3.90613389	-0.42181301	C	3.46694493	2.95165610	-1.65010798
H	0.79814500	4.89986086	-0.55820698	H	3.73187900	3.87305307	-2.15834093
C	2.55641603	3.75240993	-0.09610000	C	4.36008406	1.88290501	-1.63139403
H	3.19049311	4.62327719	0.02103300	H	5.32391691	1.96556997	-2.12043095
C	3.09096909	2.48034096	0.08349000	C	4.01238680	0.70271301	-0.98741603
H	4.13467884	2.36252689	0.34069300	H	4.70338821	-0.12858599	-0.98320299
C	2.26105499	1.37259805	-0.06985600	C	2.76919293	0.59779298	-0.35957301
C	2.68550801	-0.08809800	0.10186700	C	2.27888894	-0.69413298	0.30015799
C	3.19719601	-0.33431000	1.55048704	C	3.06955409	-0.95949203	1.61185503
C	3.79017591	-0.45693901	-0.92829698	C	2.39570093	-1.90889096	-0.66962600
C	0.03146700	-0.95159698	-2.28536391	C	0.48256001	2.14557791	1.18496597
H	0.96577799	-0.73979700	-2.80015993	H	0.30694300	3.12300301	0.77124500
H	-0.81179601	-0.65355802	-2.90131497	H	1.23938203	2.07330203	1.94865894
Cl	-0.06167800	-2.79539108	-2.20849609	Cl	-0.99293298	2.91360092	2.95841599
B				C			
E(B3LYP-D3) = -2829.32130998				E(B3LYP-D3) = -8177.91061921			
N _{imag} = 0				N _{imag} = 0			
Si	0.17184500	0.51182997	0.49798000	Si	-0.83663702	0.24887000	-0.57611603
F	2.16070199	-0.82968497	-2.26371098	F	-3.84964204	1.63904798	0.96819699

F	4.29034424	-0.70401597	-1.86011195	F	-5.47745705	0.20154400	0.94044799
F	3.21918201	1.02674699	-2.60561991	F	-5.03522301	1.38430095	-0.82324600
F	5.08162785	0.74986500	0.29660800	F	-5.11330986	-2.10448003	-0.46335000
F	3.98757505	2.46694708	-0.44815800	F	-4.72816896	-0.91310602	-2.23206902
F	3.54266000	1.67595005	1.51619101	F	-3.24486995	-2.33337808	-1.54639804
F	-1.98506498	-2.07203007	-2.17789602	F	2.28286004	0.67971998	2.58458209
F	-3.73411298	-0.79756200	-2.31234908	F	1.92160904	2.81943393	2.54068995
F	-1.75274706	0.04564700	-2.55954099	F	0.25624499	1.44057405	2.48170304
F	-3.14507890	-1.40495396	1.76127994	F	2.98156595	2.02267098	-1.35300100
F	-2.29708195	-2.85232496	0.39956000	F	3.77221203	0.78181398	0.24919200
F	-4.26563311	-2.06329489	0.01685200	F	3.57567596	2.92264104	0.52027702
O	1.58916295	1.10112798	-0.37727600	O	-2.53550100	0.28589699	-1.08401406
O	-1.02641201	-0.65645999	0.02449800	O	1.15432894	0.31690100	0.06177900
C	1.29680002	-0.94303399	1.05012703	C	-1.35835099	-0.75831598	0.92422301
C	0.97363001	-2.03277206	1.86026704	C	-0.58978200	-1.33734703	1.93341506
H	-0.03332300	-2.12879300	2.24893689	H	0.48287001	-1.21133494	1.94750702
C	1.93217599	-2.98966098	2.16625404	C	-1.19164300	-2.10454702	2.92243195
H	1.67420006	-3.83486390	2.79606295	H	-0.57784802	-2.56176591	3.68951988
C	3.23077893	-2.87226605	1.66420400	C	-2.57202697	-2.29252100	2.92237091
H	3.97655106	-3.62201500	1.90471697	H	-3.04001307	-2.88671088	3.69917703
C	3.56917500	-1.79680705	0.85357302	C	-3.35525799	-1.73182201	1.92008698
H	4.57121277	-1.70178604	0.45730299	H	-4.42522621	-1.88634706	1.91131794
C	2.58971596	-0.84838998	0.56053001	C	-2.73675799	-0.98068899	0.92472100
C	2.77067900	0.38699901	-0.32051700	C	-3.45029998	-0.34616199	-0.26960400
C	3.11979389	-0.02741200	-1.77515602	C	-4.47099304	0.72461200	0.20498800
C	3.85626507	1.32979000	0.26010701	C	-4.15165520	-1.43174505	-1.13317502
C	-2.25369501	1.96201301	0.00732400	C	-0.59554201	2.11547589	-0.61644101
C	-2.88431001	3.16275096	0.35583299	C	-1.54318702	3.01095700	-1.12318397
H	-2.27651000	4.05805302	0.42144200	H	-2.46540594	2.62562490	-1.53665805
C	-4.24423790	3.23285389	0.61183202	C	-1.31482100	4.38114882	-1.08707297
H	-4.69881487	4.18069983	0.87897700	H	-2.05433297	5.06368780	-1.49050105
C	-5.01824522	2.08177900	0.51916897	C	-0.14359000	4.87768221	-0.52171701

H	-6.08586788	2.11590195	0.70285797	H	0.03367000	5.94640923	-0.48317200
C	-4.41150379	0.87506199	0.20097201	C	0.80211198	4.00471020	0.00169000
H	-5.02716208	-0.00917200	0.14269701	H	1.70409203	4.39314890	0.45320001
C	-3.03655791	0.79475200	-0.03510300	C	0.57282400	2.63263106	-0.06263100
C	-2.35778308	-0.55439597	-0.33137101	C	1.53792298	1.58570302	0.48343599
C	-2.46213794	-0.85640502	-1.85910201	C	1.51060200	1.63103294	2.04444599
C	-3.02635598	-1.73093104	0.46417001	C	2.97976494	1.84999704	-0.03189800
C	-0.79300600	1.95380497	-0.30727100	C	-0.20978600	-0.77837199	-2.05628395
H	-0.33536300	2.90469193	-0.03509800	H	0.65761203	-0.37387300	-2.57576990
H	-0.64706397	1.82154298	-1.38292003	H	-1.00690901	-1.00574696	-2.75780797
Cl	-0.15741500	1.22555900	2.56338692	Cl	0.34997499	-2.42057705	-1.41382694
				Mg	2.43017197	-1.24285698	-0.36106101
				Br	3.00629997	-2.66822290	1.52285099
				Br	3.60527992	-1.12789798	-2.51664090
T₀₀₀ E(B3LYP-D3) = -8177.86039854 N _{imag} = 1 (- 407.47 cm ⁻¹)				D E(B3LYP-D3) = -8177.93989166 N _{imag} = 0			
Si	0.61682600	0.39350700	0.76983601	Si	0.88539600	1.08174300	0.36461499
F	-0.60569602	1.07691300	-2.53246808	F	-1.65131903	1.09405005	-2.35750890
F	-2.21992612	2.52735209	-2.52512693	F	-3.36859488	2.21134901	-1.63648403
F	-2.62762904	0.44408500	-2.07433510	F	-3.10314202	0.14157800	-1.05607796
F	-3.19385600	3.31309295	-0.14822100	F	-3.36601901	2.98279190	0.97540897
F	-3.68399405	1.26273406	0.34654200	F	-3.14754605	0.90420598	1.55354702
F	-2.38320303	2.40214396	1.64729202	F	-1.67736399	2.36124706	2.19397902
F	2.13306689	-2.71144605	-1.86673796	F	2.65298510	-1.21065998	-2.60306311
F	4.13212013	-2.58503890	-1.03825700	F	4.48534489	-1.87440705	-1.67656803
F	2.44453096	-2.96658802	0.26661399	F	2.57555199	-2.62705302	-0.96719098
F	3.01458001	1.38133705	-1.53245294	F	3.87469697	1.84534097	-0.01349900
F	2.49931002	-0.21564700	-2.90175104	F	3.97957897	1.15225196	-2.06436110
F	4.48204994	-0.13239600	-2.03633308	F	5.37594700	0.39389199	-0.59100002
O	-1.05101204	0.44118199	0.14397199	O	-0.74116403	0.66692603	0.24835500

O	1.28601205	-0.49249899	-0.49019301	O	1.80442500	0.16968299	-0.64842999
C	0.74993700	2.24159503	0.52861398	C	0.58470702	2.80796504	-0.25799799
C	1.79376996	3.12103009	0.81706297	C	1.44105899	3.87604308	-0.52883798
H	2.65770197	2.77171111	1.36729503	H	2.51084399	3.76067996	-0.41256300
C	1.74113297	4.43875122	0.38091001	C	0.92101002	5.09077406	-0.95817101
H	2.55453897	5.11778688	0.60988599	H	1.58645594	5.91872692	-1.17411995
C	0.65371001	4.88454103	-0.36759999	C	-0.45552099	5.24837399	-1.11499703
H	0.62053603	5.90873814	-0.72061002	H	-0.85640597	6.19791985	-1.44989502
C	-0.39327499	4.02197218	-0.66701198	C	-1.32223105	4.19592905	-0.84739500
H	-1.23889399	4.36819601	-1.24320495	H	-2.38846707	4.31973410	-0.96874303
C	-0.33642000	2.70968390	-0.20606700	C	-0.78906399	2.98183203	-0.42383400
C	-1.44183505	1.67520499	-0.40322599	C	-1.60244298	1.73313200	-0.08426100
C	-1.73717999	1.42599702	-1.90573800	C	-2.44997406	1.27350998	-1.30048895
C	-2.70345592	2.16371393	0.36591700	C	-2.47842908	1.98567104	1.17352104
C	2.51470208	0.11053700	1.74380100	C	2.70548606	-0.18576799	2.13305402
C	3.09841704	0.57750702	2.92298293	C	3.01433301	-0.62933302	3.42241311
H	2.47447395	0.95811802	3.72489190	H	2.48079491	-0.18953300	4.25659609
C	4.47849607	0.57179302	3.09300494	C	3.94825101	-1.62261105	3.65308809
H	4.91416693	0.93792099	4.01616383	H	4.15202093	-1.95191598	4.66525412
C	5.29847479	0.08902300	2.07696009	C	4.60581589	-2.20226598	2.57481694
H	6.37459803	0.07527000	2.20446897	H	5.33804083	-2.98552608	2.72936296
C	4.74009085	-0.36790201	0.88958597	C	4.30835819	-1.78621495	1.28840005
H	5.37924385	-0.72524297	0.09490400	H	4.82688999	-2.25353408	0.46631899
C	3.35514903	-0.35088399	0.72872901	C	3.35542488	-0.79001701	1.04572105
C	2.64695811	-0.75560600	-0.56413001	C	3.07667208	-0.35856199	-0.40313599
C	2.82529092	-2.28120589	-0.81467599	C	3.18707800	-1.54343295	-1.42877698
C	3.17001390	0.06724700	-1.78092098	C	4.10110378	0.75460899	-0.79093701
C	0.45587200	-0.52257299	2.32156110	C	1.69232702	0.93597102	2.02115202
H	0.55714399	-0.02379300	3.27168012	H	2.18908811	1.89298606	2.22143602
H	0.65662098	-1.58720696	2.31592202	H	0.92196602	0.80441397	2.78212404
Cl	-1.85665298	-0.89545703	2.95967603	Cl	-0.07364000	-1.90419698	2.26703811
Mg	-2.36795592	-1.43615401	0.68897098	Mg	-1.59519100	-2.09191108	0.56842101

Br	-4.73013496	-1.73557699	0.14958400	Br	-3.92907310	-2.47486591	1.17945600
Br	-0.84726202	-3.21346307	0.01139300	Br	-0.80622900	-2.51796699	-1.69474804
E E(B3LYP-D3) = -2751.371693 $N_{\text{imag}} = 0$				T_{SE} E(B3LYP-D3) = -2751.29882958 $N_{\text{imag}} = 1$ (- 533.0 cm ⁻¹)			
F	-1.64788306	-2.18193507	-2.61845899	F	-1.41407394	-2.08959603	-2.81126308
F	-3.74023104	-1.66302800	-2.35488391	F	-3.40464091	-2.54165792	-2.07536006
F	-2.23095393	-0.11779600	-2.35384297	F	-2.66212392	-0.51197100	-2.02083611
F	-2.67874193	-3.08262610	1.37007594	F	-0.97654802	-3.81010604	0.99933100
F	-2.16286802	-3.90998006	-0.56176800	F	-0.88635498	-4.17571306	-1.13065100
F	-4.14446783	-3.10347795	-0.21565400	F	-2.79811597	-4.17466307	-0.10395900
O	-0.96333802	-1.47587800	-0.09445800	O	-0.42399099	-1.52126396	-0.38568300
C	-2.18823695	0.45491600	1.05213296	C	-1.89545798	-0.40691301	1.41529703
C	-2.76353097	1.50070000	1.77725601	C	-2.60979605	0.29198501	2.39093304
H	-2.12616897	2.17098904	2.34536195	H	-2.09631205	1.01983202	3.00975490
C	-4.13998413	1.71330595	1.77008200	C	-3.97251797	0.07937300	2.56611705
H	-4.56846094	2.53183508	2.33884096	H	-4.51888990	0.63403898	3.32054305
C	-4.97228193	0.87880099	1.02408600	C	-4.63888407	-0.85151601	1.76918697
H	-6.04285192	1.04746699	1.00817597	H	-5.70137310	-1.01824903	1.90096402
C	-4.42514181	-0.17676499	0.29970199	C	-3.94305801	-1.56885195	0.79996598
H	-5.07025099	-0.82530397	-0.27877101	H	-4.46527576	-2.28288889	0.17710800
C	-3.04649210	-0.38062999	0.33803999	C	-2.57719803	-1.34859002	0.64383799
C	-2.30070901	-1.50473201	-0.39141899	C	-1.69966197	-2.01956797	-0.41432500
C	-2.48236609	-1.36517000	-1.93974698	C	-2.30011010	-1.78782403	-1.84363306
C	-2.83331609	-2.90628505	0.04372400	C	-1.60009801	-3.55813503	-0.16614500
C	-0.52861702	-1.01101696	2.60287094	C	0.03226100	-1.08766305	2.24511194
H	-1.32233703	-1.74177694	2.50827098	H	-0.24404500	-2.13129210	2.27350092
H	-0.82376200	-0.30307701	3.37592506	H	-0.16971000	-0.58602500	3.18125391
Cl	0.82440501	-2.00736189	3.44535398	Cl	2.20883203	-1.69732404	3.22843790
C	1.74049699	-1.64665902	-0.65516502	C	2.30648494	-1.62925506	-0.30445200
C	2.61815596	-0.66846901	1.21706200	C	2.81387210	0.56006902	0.14938000

C	2.96510196	-2.14482808	-1.03080702	C	3.61300111	-1.92047906	-0.60352802
H	0.86485797	-1.82198596	-1.25995696	H	1.55079401	-2.39562988	-0.35538900
C	3.88464093	-1.11682296	0.92477202	C	4.14438581	0.36172199	-0.12090400
H	2.45541191	-0.06785200	2.09787798	H	2.47295094	1.53412497	0.45818999
C	4.11019802	-1.89161003	-0.23695800	C	4.60745192	-0.91516900	-0.52088201
H	3.02470994	-2.71811199	-1.94327497	H	3.85385203	-2.93337297	-0.88742697
H	4.68653488	-0.85786003	1.59897995	H	4.81349277	1.20181596	-0.01789800
N	1.53700197	-0.91692901	0.45913199	N	1.87313795	-0.40160599	0.06044000
N	5.33937502	-2.35582995	-0.57055700	N	5.90777779	-1.15814996	-0.79799497
C	6.49158907	-2.05070400	0.26953799	C	6.89657116	-0.09071200	-0.68319499
H	6.66610622	-0.97243702	0.33219099	H	6.66427422	0.73870599	-1.35657299
H	6.35821295	-2.43933797	1.28305197	H	6.94921112	0.29428300	0.33904099
H	7.37663794	-2.51392388	-0.15721200	H	7.87405109	-0.48135501	-0.95057899
C	5.52651215	-3.13251996	-1.79064202	C	6.33997583	-2.49605489	-1.19027197
H	6.57207012	-3.41477799	-1.87603903	H	7.41063404	-2.48448110	-1.37240100
H	4.92722082	-4.04718685	-1.77579904	H	6.13399410	-3.22695494	-0.40340900
H	5.25460911	-2.55406189	-2.67848611	H	5.84076691	-2.82036901	-2.10717106
O	-0.08446800	0.78635597	-0.76256001	O	-0.46463200	0.88559401	-0.81630802
C	0.51966703	1.56005096	1.59458196	C	0.31110600	1.64221203	1.46996403
C	0.81796700	1.89469695	2.91989994	C	0.81304902	1.93961298	2.74142694
C	0.80149299	2.51837397	0.62196398	C	-0.05250000	2.71328092	0.65717101
C	1.37146199	3.12904906	3.25317001	C	0.93009102	3.25658393	3.17783809
H	0.63102502	1.18192303	3.71508503	H	1.13988101	1.13757002	3.39328289
C	1.35869205	3.75858307	0.92931098	C	0.05264300	4.03920078	1.07362199
C	1.64371896	4.06408119	2.25647998	C	0.54575598	4.30776787	2.34599090
H	1.59521198	3.36262608	4.28850079	H	1.32512999	3.46809793	4.16539001
H	1.57170105	4.48016310	0.15197501	H	-0.23777300	4.85300016	0.42313200
H	2.07710600	5.02448606	2.51029301	H	0.63629198	5.33313513	2.68469596
C	0.44346100	2.04534698	-0.79096699	C	-0.54040098	2.25316000	-0.71824402
C	-0.61379802	2.99375200	-1.43680406	C	-2.02060199	2.68505311	-0.94846803
C	1.71883500	2.01985002	-1.68894196	C	0.34565899	2.85122490	-1.85030401
F	2.70154595	1.31927800	-1.09596002	F	1.64257300	2.56133199	-1.63297403

F	2.22322202	3.25171304	-1.94728601	F	0.25541601	4.19655800	-1.94566500
F	1.49027395	1.43812096	-2.88397694	F	0.03444000	2.35107899	-3.06132197
F	-0.19532700	4.27776194	-1.55791903	F	-2.19473004	4.02680492	-0.88072503
F	-0.97257501	2.59116006	-2.67349410	F	-2.49272203	2.29641390	-2.14835596
F	-1.73098397	3.02276802	-0.69169402	F	-2.81436610	2.14162588	-0.01362600
Si	-0.31277600	-0.05432400	0.86746699	Si	-0.01074500	-0.08784700	0.63993299
F E(B3LYP-D3) = -3211.72472818 $N_{\text{imag}} = 0$				TS_{FG} E(B3LYP-D3) = -3211.70507892 $N_{\text{imag}} = 1$ (- 362.57 cm ⁻¹)			
Si	-0.55892599	0.35692400	-0.46548399	Si	0.58620697	0.00677000	0.47071099
F	-3.92801905	0.72584701	1.04016495	F	0.33209899	2.31428003	-2.25129104
F	-5.01607895	-1.15183604	1.03542197	F	-1.33989596	3.67236710	-1.98527801
F	-4.96934605	0.08389000	-0.74625701	F	-1.66991401	1.68465900	-2.78579092
F	-3.96424603	-3.22595811	-0.36395901	F	-3.09633994	3.13450909	0.00960300
F	-3.91196203	-2.00219893	-2.15104604	F	-3.40906596	1.13425803	-0.76491898
F	-2.08827305	-2.90164804	-1.40653706	F	-2.70813990	1.40840805	1.26617706
F	2.55808711	1.84879303	2.23731089	F	2.48173499	-2.25154901	-2.70134997
F	1.85781097	3.88440490	1.97124398	F	4.03288603	-2.94888210	-1.35518301
F	0.45197901	2.30346894	2.45509791	F	1.94101596	-3.15835190	-0.81108499
F	2.28442788	2.39809608	-1.92081201	F	3.82321596	1.19002903	-0.73733300
F	3.61938906	1.93517995	-0.27930701	F	3.35807705	0.31265700	-2.66047812
F	2.87823296	3.95608211	-0.53185701	F	5.04960299	-0.42038700	-1.52697802
O	-2.24179912	-0.15675101	-0.98427403	O	-0.76737303	0.47845101	-0.49242100
O	1.09086502	0.93098700	0.11067100	O	1.55977702	-0.43615401	-0.83978701
C	-0.82501900	-0.75419801	1.04223502	C	0.72843599	1.74496901	1.14644301
C	0.05589000	-1.00489104	2.09694290	C	1.61898303	2.31170702	2.05926609
H	1.01208496	-0.49934700	2.12101293	H	2.37274694	1.69757104	2.53464103
C	-0.28832400	-1.89622700	3.10811305	C	1.54595006	3.66772699	2.36014891
H	0.40194201	-2.08821011	3.92149806	H	2.23898506	4.10234880	3.07052398
C	-1.52207804	-2.54537201	3.07857895	C	0.58588099	4.47127819	1.74744403
H	-1.79004395	-3.23872304	3.86691499	H	0.53261298	5.52720594	1.98309398

C	-2.41529608	-2.30570889	2.03890300	C	-0.30652201	3.92626691	0.82983601
H	-3.37257195	-2.80806303	2.02063489	H	-1.04760504	4.55464792	0.35598901
C	-2.05296397	-1.41430700	1.03214002	C	-0.22430700	2.56785297	0.53952301
C	-2.91261792	-1.04070401	-0.17885900	C	-1.12276804	1.81733894	-0.44706500
C	-4.22571278	-0.35028401	0.28891900	C	-0.95943499	2.38381410	-1.88382804
C	-3.23900604	-2.30187201	-1.02635002	C	-2.60514498	1.87830198	0.01154300
C	-0.97512400	2.19511294	-0.65148699	C	2.17515492	-0.90613103	1.68811500
C	-2.16640806	2.76862597	-1.10428500	C	2.46987510	-0.94643801	3.05160093
H	-2.98379588	2.12628508	-1.40348804	H	1.68594694	-0.77008998	3.78045893
C	-2.30797791	4.15179777	-1.16348803	C	3.75931811	-1.21391499	3.49935889
H	-3.23460388	4.58758116	-1.51904297	H	3.97160006	-1.23977804	4.56176376
C	-1.26202404	4.98115396	-0.76085502	C	4.77544117	-1.45774996	2.57843804
H	-1.37506294	6.05797100	-0.80223799	H	5.77984715	-1.67644298	2.91956401
C	-0.07086600	4.42989111	-0.29955801	C	4.50694084	-1.41052103	1.21533597
H	0.73705298	5.07378912	0.01941100	H	5.30556488	-1.58200300	0.50743699
C	0.05687700	3.04418206	-0.25500101	C	3.21202707	-1.12860596	0.77993798
C	1.28984499	2.28158307	0.23296700	C	2.83659506	-0.96613598	-0.69252998
C	1.55230904	2.59042311	1.73481905	C	2.83259106	-2.34467292	-1.40796900
C	2.53396702	2.65524912	-0.61889899	C	3.78567791	0.03158700	-1.41950500
C	0.26188299	-0.56953698	-1.95499599	C	0.13914800	-1.46646297	1.41408801
H	0.59506398	0.15155999	-2.70048904	H	-0.06306300	-1.41154397	2.47287989
H	-0.44903401	-1.24057305	-2.43059492	H	0.42541400	-2.43939805	1.04408896
C	1.25959098	-2.55962801	-0.92624801	C	-2.87773108	-1.64144194	1.93544900
C	2.69228005	-0.89087802	-1.68928301	C	-2.26767802	-2.44260502	-0.11757300
C	2.30470800	-3.29262209	-0.44401601	C	-4.21839905	-1.68920803	1.62001097
H	0.23920099	-2.89636707	-0.82531101	H	-2.56206799	-1.27802098	2.90778303
C	3.78646588	-1.56672001	-1.22968304	C	-3.57689404	-2.52990699	-0.53690302
H	2.78463697	0.06238200	-2.18390298	H	-1.46173298	-2.72031498	-0.78857797
C	3.63803911	-2.81569099	-0.56956398	C	-4.62108803	-2.13905501	0.33855200
H	2.08016706	-4.23206615	0.03499600	H	-4.93585014	-1.36588097	2.35885692
H	4.75424290	-1.11689401	-1.38241994	H	-3.77831602	-2.88397694	-1.53652000
N	1.43580401	-1.36948597	-1.54963195	N	-1.90490305	-2.01340389	1.09674501

N	4.69065189	-3.50395107	-0.09450900	N	-5.92573690	-2.18572497	-0.03100000
C	6.04665422	-2.97771311	-0.24495600	C	-6.29591799	-2.64014912	-1.36609101
H	6.15815115	-2.02225089	0.27373099	H	-5.88037682	-1.98917305	-2.14139390
H	6.74977589	-3.68449998	0.18451101	H	-5.94873810	-3.66093493	-1.54787302
H	6.29950285	-2.83968306	-1.29883802	H	-7.37831402	-2.63079596	-1.45771801
C	4.49206877	-4.78103924	0.58982098	C	-6.96463680	-1.72717404	0.88340902
H	4.03303289	-5.51667118	-0.07511300	H	-6.82291317	-0.67653000	1.15382802
H	5.45606899	-5.16420603	0.90963697	H	-7.93272495	-1.82587504	0.40056399
H	3.86045790	-4.65963602	1.47302997	H	-6.97911882	-2.32226396	1.80104101
<p style="text-align: center;">G</p> <p style="text-align: center;">E(B3LYP-D3) = -2751.38585347</p> <p style="text-align: center;">$N_{\text{imag}} = 0$</p>				<p style="text-align: center;">DMAP</p> <p style="text-align: center;">E(B3LYP-D3) = -382.391238753</p> <p style="text-align: center;">$N_{\text{imag}} = 0$</p>			
F	-2.53487897	1.67243302	2.50695109	N	2.66828704	0.00000000	0.00011300
F	-4.50376177	1.28760302	1.71836603	C	1.95030999	-1.13352501	0.00005700
F	-3.18167806	-0.36710000	2.18209696	C	1.95030999	1.13352501	0.00004200
F	-2.40117002	2.33930993	-1.66868305	H	2.51832795	2.05939507	0.00012500
F	-2.58853102	3.31040692	0.25994399	C	0.56881601	-1.19673204	-0.00008800
F	-4.31310797	2.36834908	-0.66106802	H	0.09239200	-2.16586995	-0.00007900
O	-1.22504997	0.91387600	0.42065799	C	0.56881601	1.19673204	-0.00010500
C	-2.28837991	-0.85995901	-1.58365202	N	-1.54713905	0.00000000	-0.00051700
C	-2.78701401	-1.93515801	-2.32846808	C	-2.27978492	-1.25865901	0.00018600
H	-2.13272095	-2.41416311	-3.04721904	H	-2.05037999	-1.85628998	0.88786697
C	-4.08798981	-2.39005399	-2.17405891	H	-3.34634995	-1.05113006	-0.00044400
H	-4.44519615	-3.22305608	-2.76782489	H	-2.04965091	-1.85757399	-0.88641500
C	-4.92872477	-1.76508296	-1.25941098	C	-2.27978611	1.25865805	0.00021600
H	-5.95179081	-2.09705591	-1.13313901	H	-3.34635091	1.05113006	-0.00033800
C	-4.44765806	-0.70943999	-0.49774900	H	-2.05032301	1.85629904	0.88787597
H	-5.11767721	-0.23986700	0.20644499	H	-2.04971004	1.85756505	-0.88640702
C	-3.13037801	-0.25991800	-0.63389403	C	-0.18576799	0.00000000	-0.00023800
C	-2.58984590	0.89379102	0.22583200	H	0.09239200	2.16586995	-0.00011400
C	-3.21805406	0.87547803	1.66836596	H	2.51832795	-2.05939507	0.00015500

C	-2.98972297	2.24388003	-0.45656899
C	-0.87974501	-0.39520600	-1.83384001
C	0.77175802	2.57787395	-0.87409300
C	2.38015389	1.42773402	0.33192399
C	1.53888404	3.70784497	-0.90448600
H	-0.20013399	2.56703591	-1.33753800
C	3.20104909	2.51843095	0.36497101
C	2.81303096	3.72736001	-0.27430901
H	1.14494705	4.57385588	-1.41232598
H	4.14275122	2.42771506	0.88264900
N	1.16987205	1.42844796	-0.27768299
N	3.59829998	4.81703520	-0.28107399
C	4.89854908	4.79635096	0.38862801
H	4.78752804	4.59108877	1.45582902
H	5.55472183	4.04125977	-0.05068400
H	5.37020302	5.76749182	0.27533501
C	3.16568089	6.03784323	-0.96076000
H	3.94475007	6.78833580	-0.86980498
H	2.98882198	5.85290813	-2.02277207
H	2.25115895	6.43470287	-0.51344103
O	1.53627503	-1.06311500	-0.90797299
C	0.36614600	-1.11953700	1.32447600
C	-0.18928599	-0.91358501	2.58835411
C	1.26277101	-2.17750812	1.16288400
C	0.12665799	-1.75949502	3.64708400
H	-0.85672498	-0.08196600	2.75094509
C	1.56650805	-3.05000806	2.20221591
C	0.99088597	-2.83462501	3.45063090
H	-0.30142999	-1.58314204	4.62687922
H	2.24833488	-3.87612796	2.05472302
H	1.22738898	-3.49954391	4.27262402
C	1.85764098	-2.22252297	-0.24387400

C	3.40775108	-2.33476806	-0.20877200
C	1.26012397	-3.43163610	-1.02676797
F	-0.07981600	-3.30671406	-1.09225702
F	1.51833403	-4.62031794	-0.44517699
F	1.71322703	-3.49849200	-2.29237390
F	3.84624100	-3.51570511	0.27493700
F	3.94871402	-2.18133998	-1.42886198
Si	0.10534700	-0.10553300	-0.24852900
H	-0.90334702	0.56852901	-2.35298800
H	-0.36754200	-1.09463406	-2.48811889
H	2.67267203	0.50537997	0.80492002
F	3.92939305	-1.37112606	0.57799000

V. Experimental references

- [1] Frisch, M.J.; Trucks, G.W.; Schlegel, H.B.; Scuseria, G.E.; Robb, M.A.; Cheeseman, J.R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G.A.; et al. *Gaussian 09, Revision D.01*; Gaussian, Inc.: Wallingford, CT, USA, 2009.