

Tuning the Si-N Interaction in Metallated Oligosilanylsilatrane

Mohammad Aghazadeh Meshgi,[†] Rainer Zitz,[†] Malgorzata Walewska,[†]
Judith Baumgartner,^{*,‡} and Christoph Marschner^{*,†}

[†]Institut für Anorganische Chemie, Technische Universität Graz, Stremayrgasse 9, 8010 Graz,
Austria

[‡]Institut für Chemie, Karl Franzens Universität Graz, Stremayrgasse 9, 8010 Graz, Austria

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Table S1. Crystallographic data for compounds **3**, **5**, **6**, and **7**

	3	5	6	7
Empirical formula	C ₂₄ H ₆₀ N ₂ O ₆ Si ₈ Zn	C ₂₂ H ₄₀ ClHfNO ₃ Si ₄	C ₁₂ H ₃₁ NO ₃ Si ₄	C ₃₂ H ₇₆ N ₂ O ₈ Si ₈ Yb
M _w	762.83	692.85	349.74	1014.71
Temperature [K]	100(2)	100(2)	100(2)	100(2)
Size [mm]	0.18×0.12×0.05	0.24×0.14×0.09	0.20×0.11×0.08	0.12×0.08×0.06
Crystal system	monoclinic	monoclinic	triclinic	triclinic
Space group	C2/c	P2(1)/c	P-1	P-1
a [Å]	22.934(7)	11.397(3)	7.679(3)	9.969(2)
b [Å]	11.727(3)	11.523(3)	11.337(4)	15.459(2)
c [Å]	15.772(4)	21.702(5)	12.014(5)	16.395(2)
α [°]	90	90	88.725(6)	81.587(3)
β [°]	103.32(2)	98.649(4)	87.958(6)	87.487(2)
γ [°]	90	90	70.280(6)	86.698(3)
V [Å ³]	4128(2)	2818(2)	984(2)	2494(2)
Z	4	4	2	2
ρ _{calc} [gcm ⁻³]	1.227	1.633	1.181	1.351
Absorption coefficient [mm ⁻¹]	0.861	3.991	0.308	2.109
F(000)	1632	1392	380	1056
θ range	1.82<θ<26.38	1.81<θ<26.34	1.70<θ<25.50	1.70<θ<26.36
Reflections collected/unique	16118/4215	21898/5719	7218/3571	20142/10041
Completeness to θ [%]	99.7	99.5	97.6	98.3
Data/restraints/parameters	4215/28/221	5719/0/295	3571/0/210	10041/0/472
Goodness of fit on F ²	1.08	1.13	1.08	0.95
Final R indices [I>2σ(I)]	R1=0.064 wR2=0.139	R1=0.043 wR2=0.096	R1=0.070 wR2=0.192	R1=0.081 wR2=0.173
R indices (all data)	R1=0.072 wR2=0.144	R1=0.047 wR2=0.098	R1=0.0752 wR2=0.197	R1=0.113 wR2=0.191
Largest diff. Peak/hole [e ⁻ / Å ³]	0.83/−0.68	2.82/−1.72	1.01/−0.42	2.27/−2.67

3. NMR spectra

Compound **3**: ^1H , ^{13}C , and ^{29}Si NMR spectra:

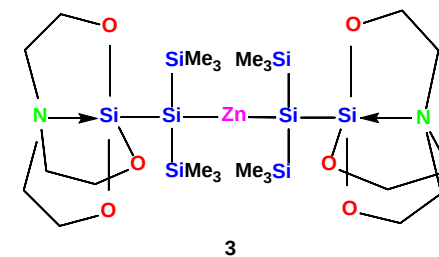
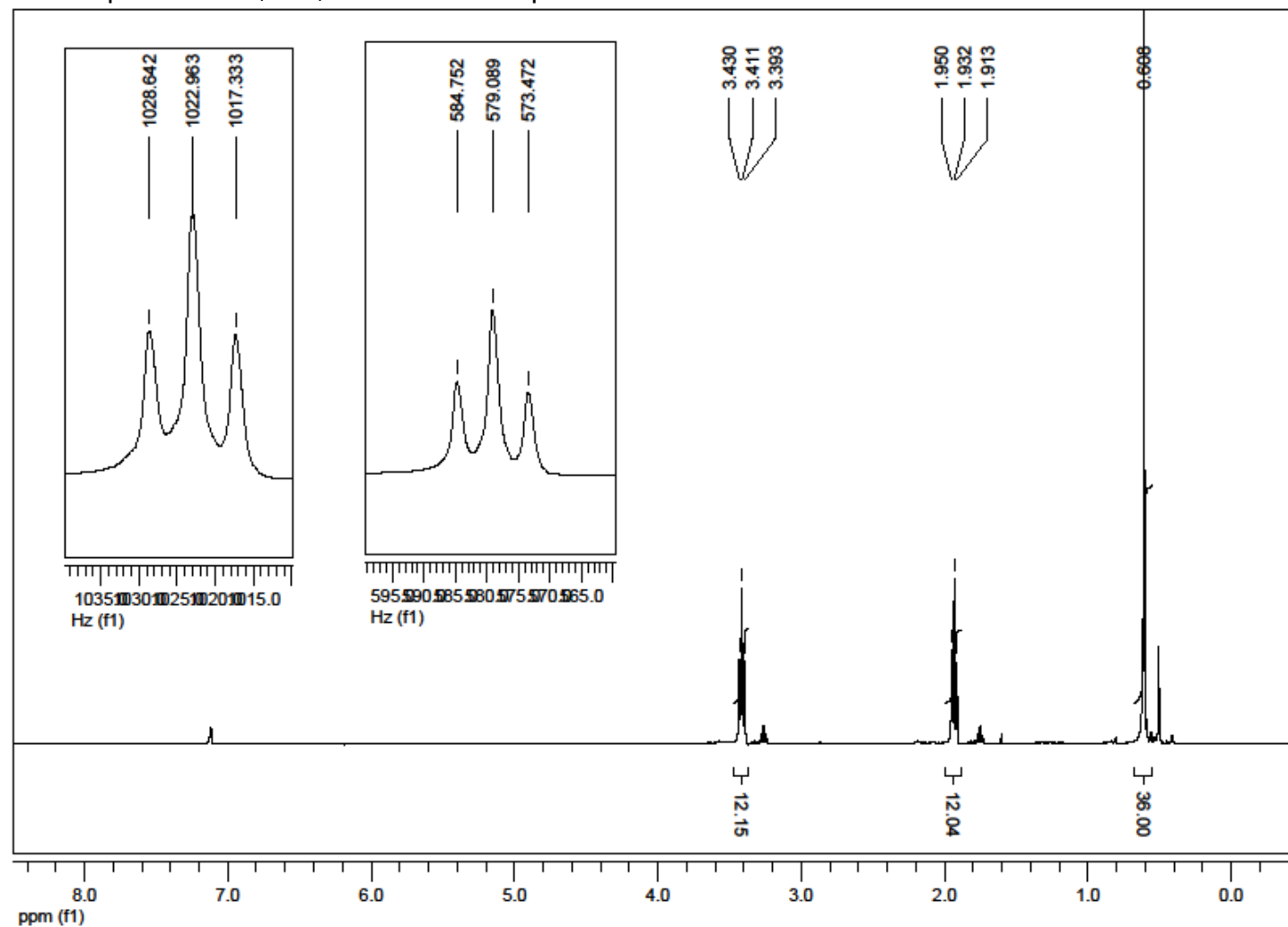


Figure S1. ^1H NMR spectrum of **3** in C_6D_6

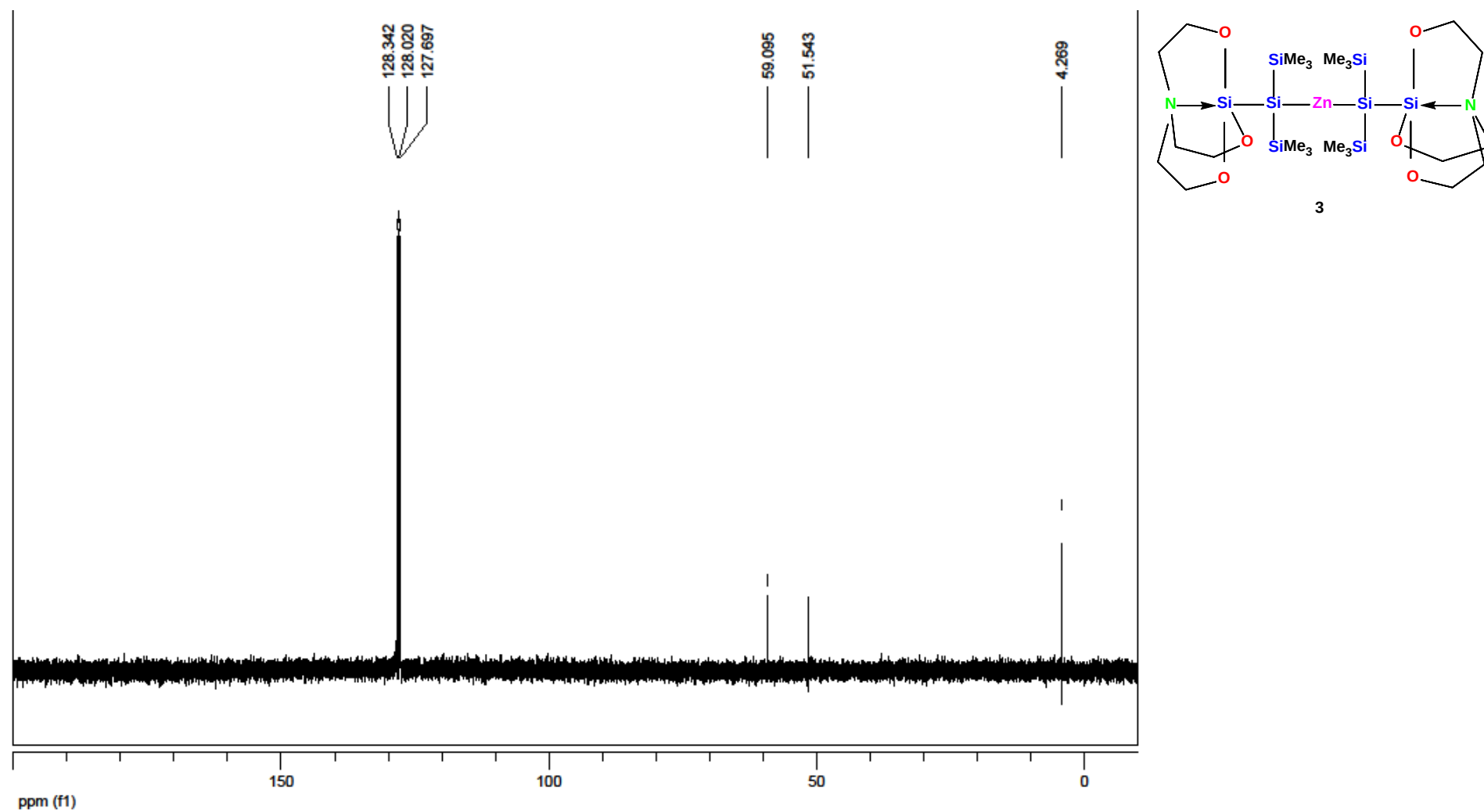


Figure S2. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3** in C_6D_6

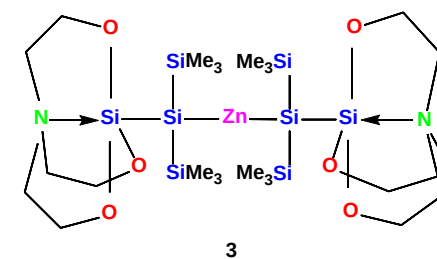
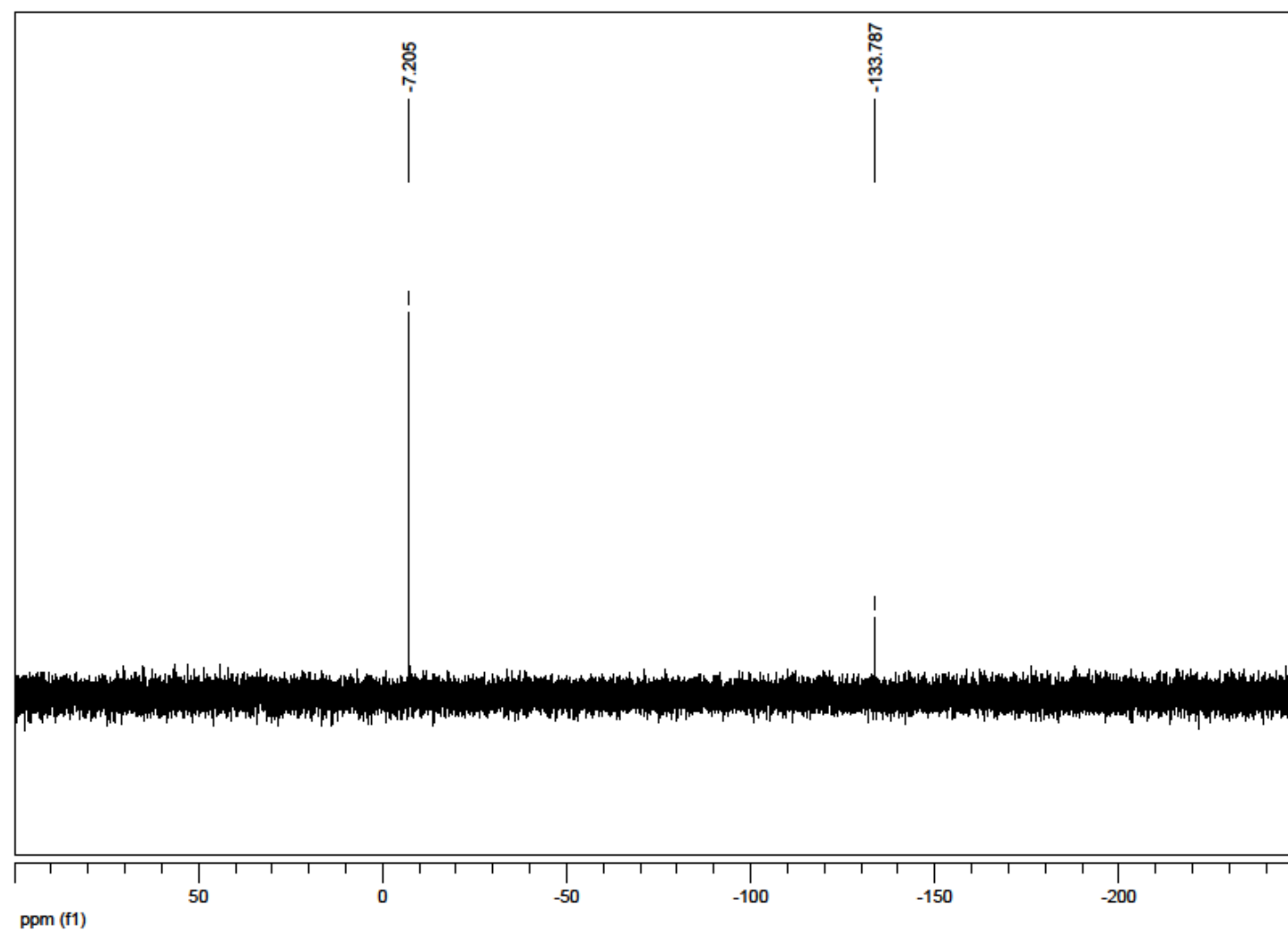


Figure S3. $^{29}\text{Si}\{^1\text{H}\}$ INEPT NMR spectrum of **3** in C_6D_6

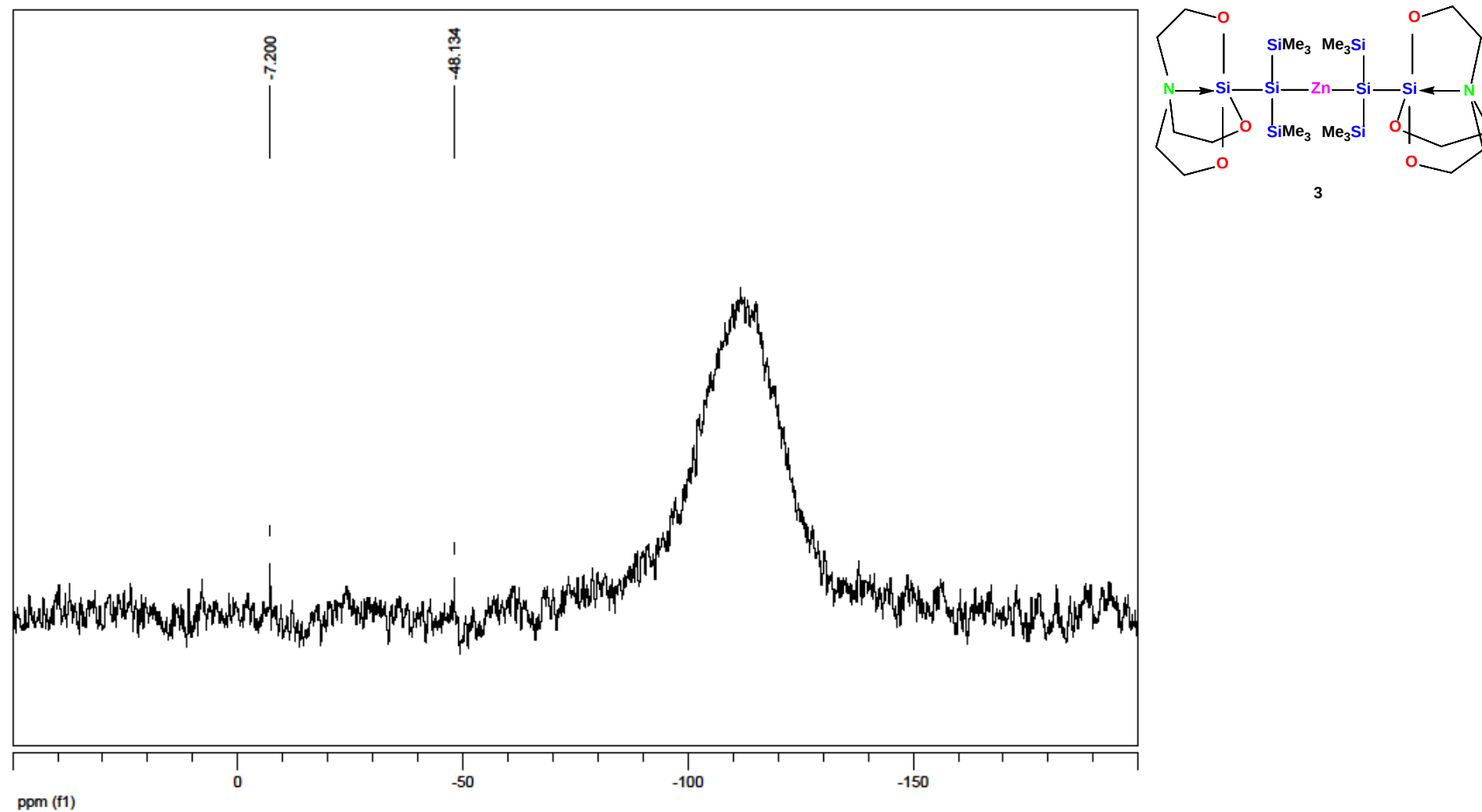


Figure S4. $^{29}\text{Si}\{^1\text{H}\}$ NMR spectrum of **3** in C_6D_6

Compound **5**: ^1H , ^{13}C , and ^{29}Si spectra:

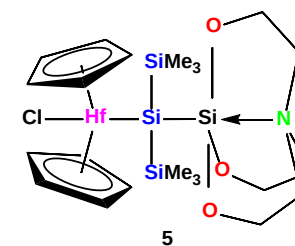
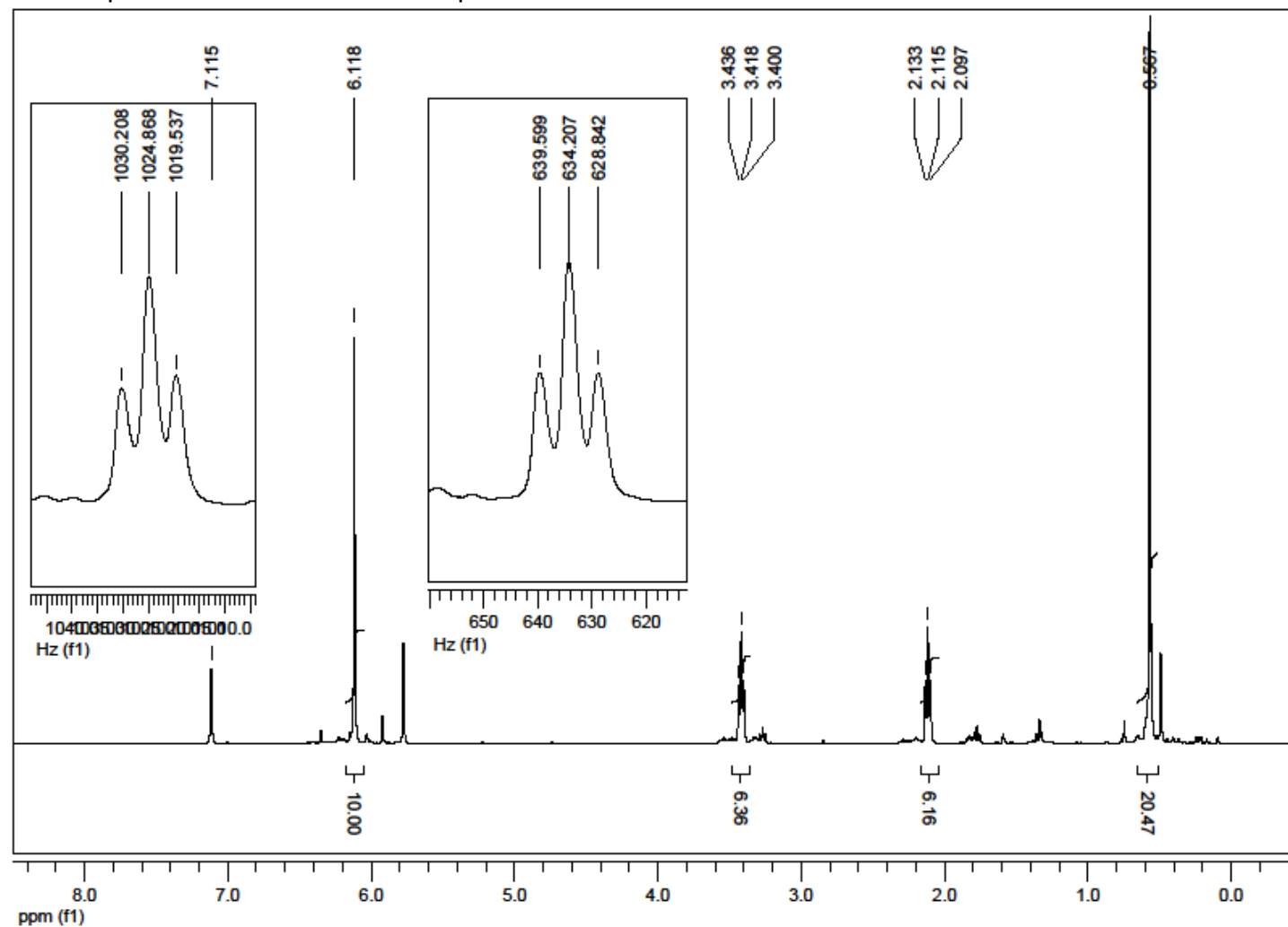


Figure S5. ^1H NMR spectrum of **5** in C_6D_6

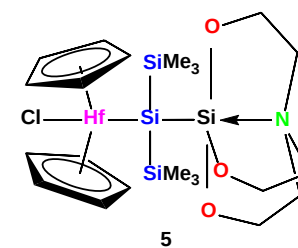
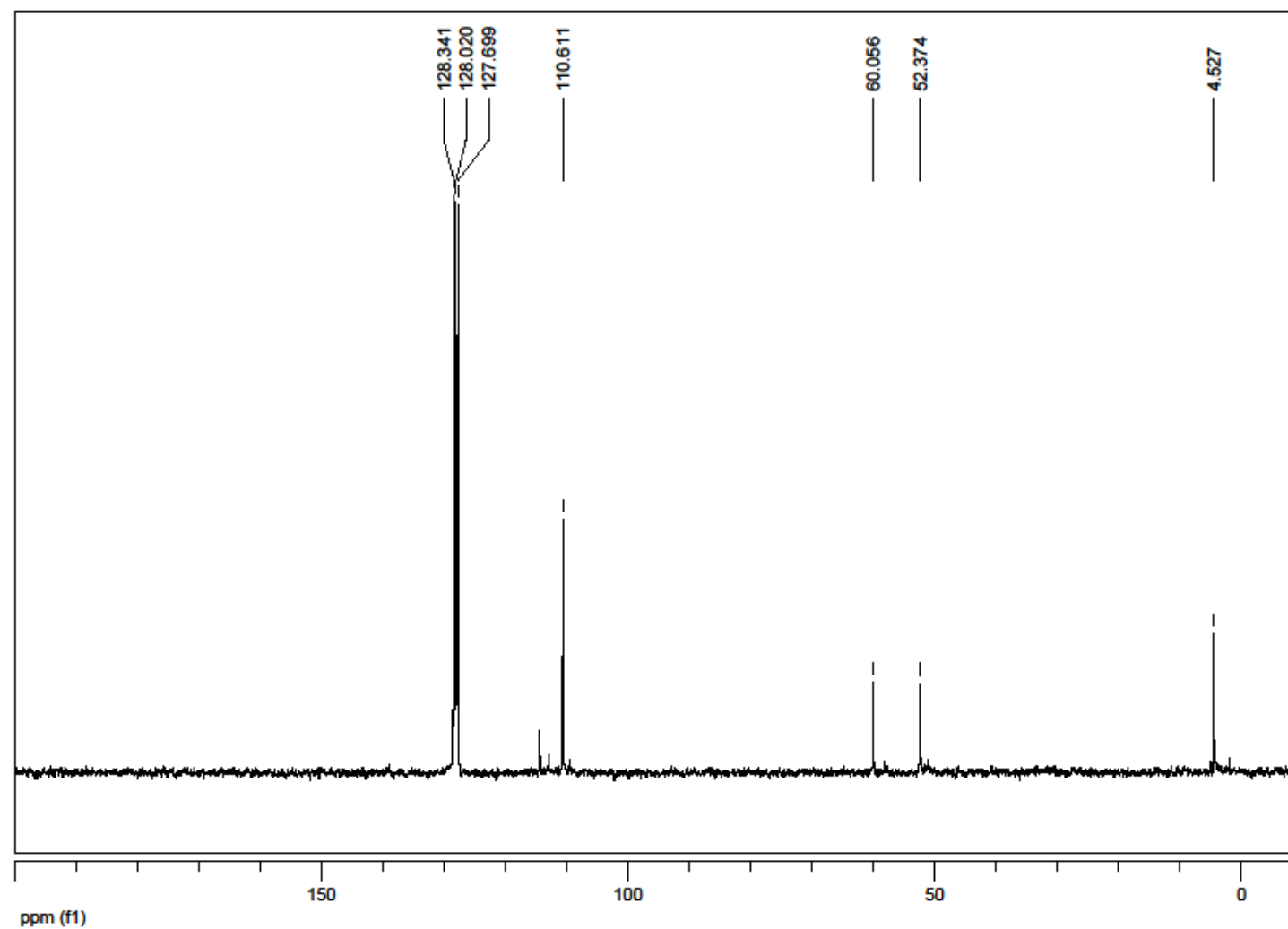


Figure S6. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **5** in C_6D_6

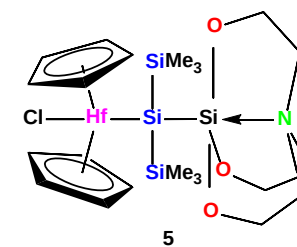
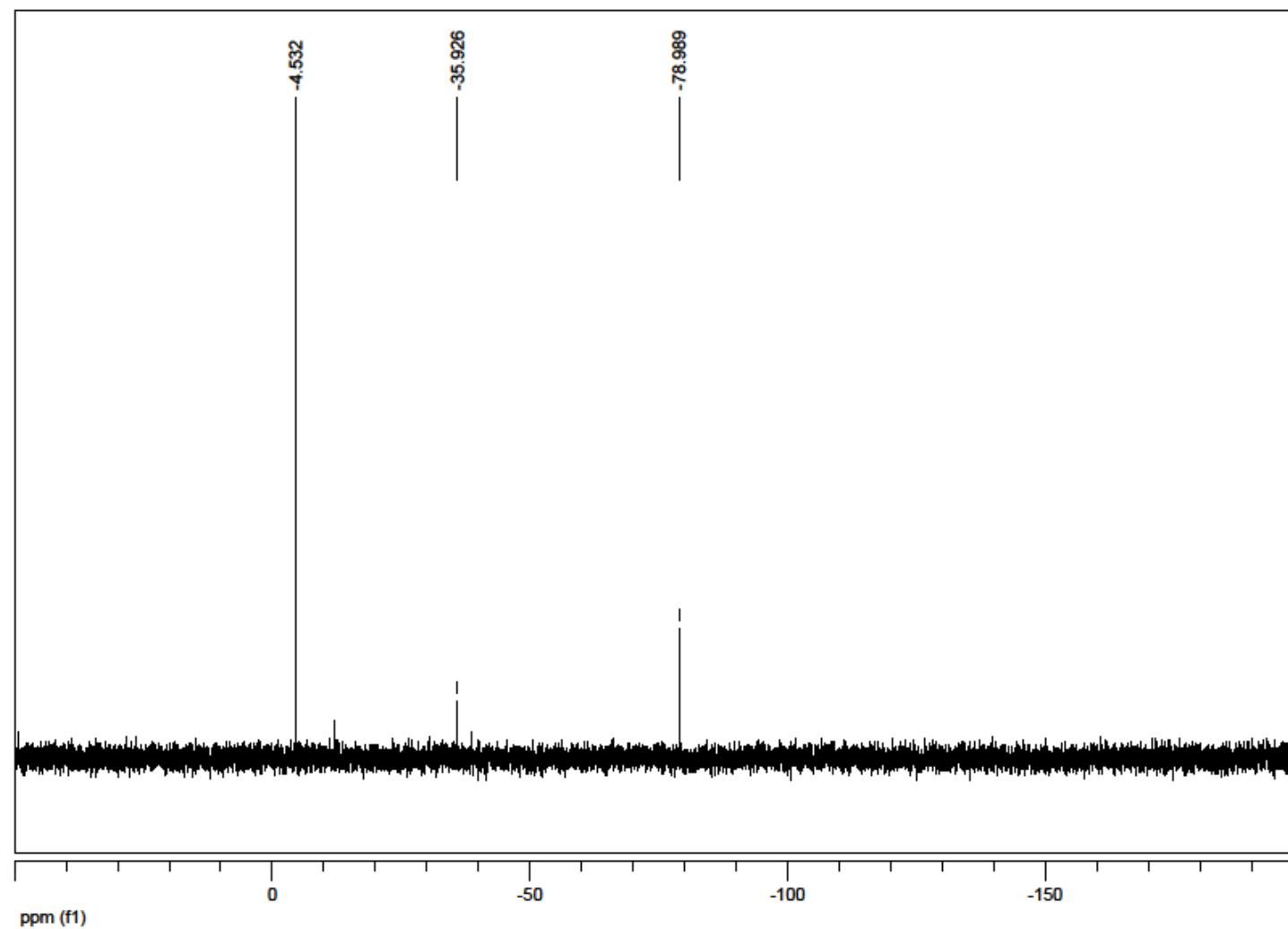


Figure S7. $^{29}\text{Si}\{^1\text{H}\}$ NMR spectrum of **5** in C_6D_6

Compound **6**: ^1H , ^{13}C , and ^{29}Si NMR spectra:

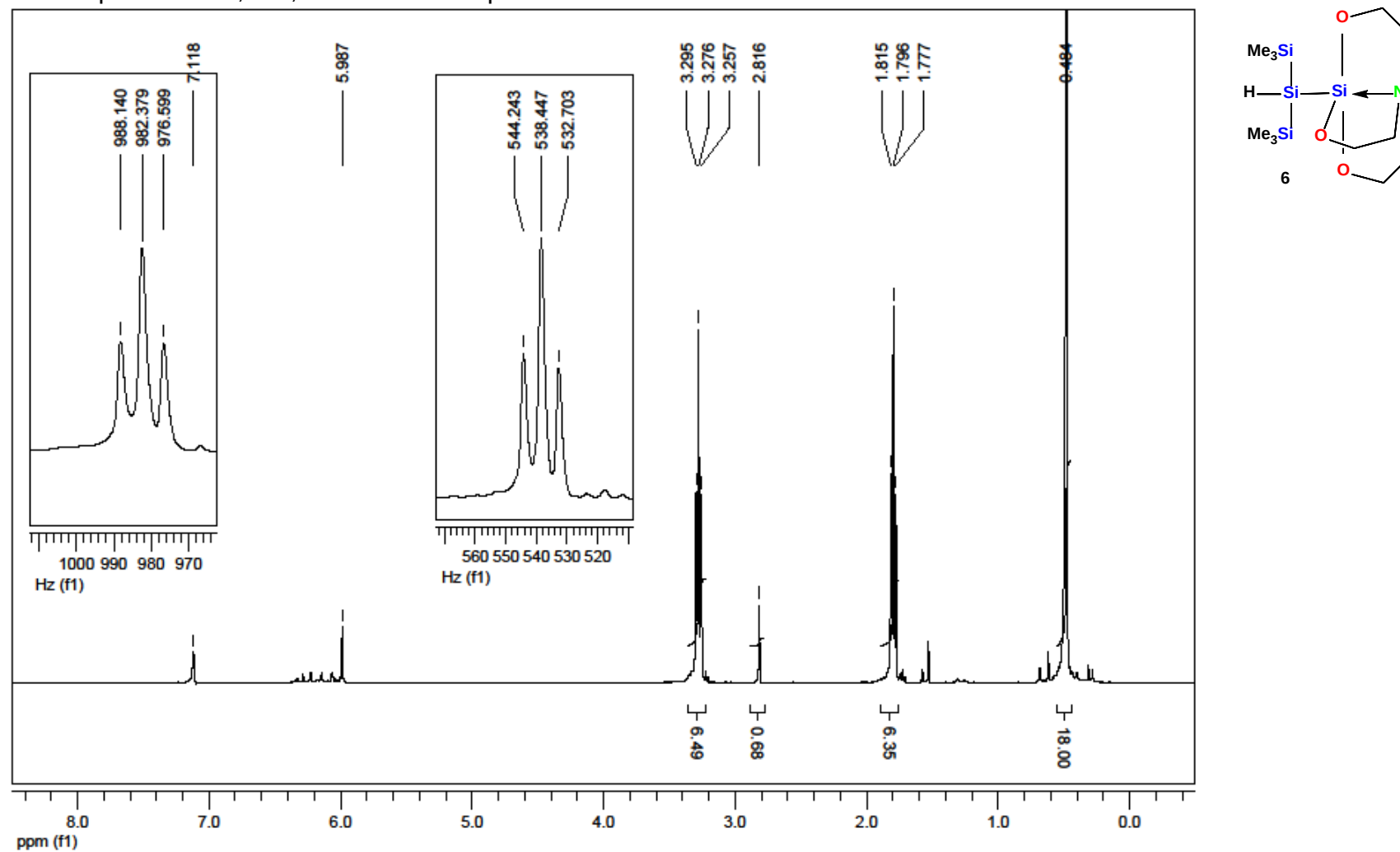


Figure S8. ^1H NMR spectrum of **6** in C_6D_6

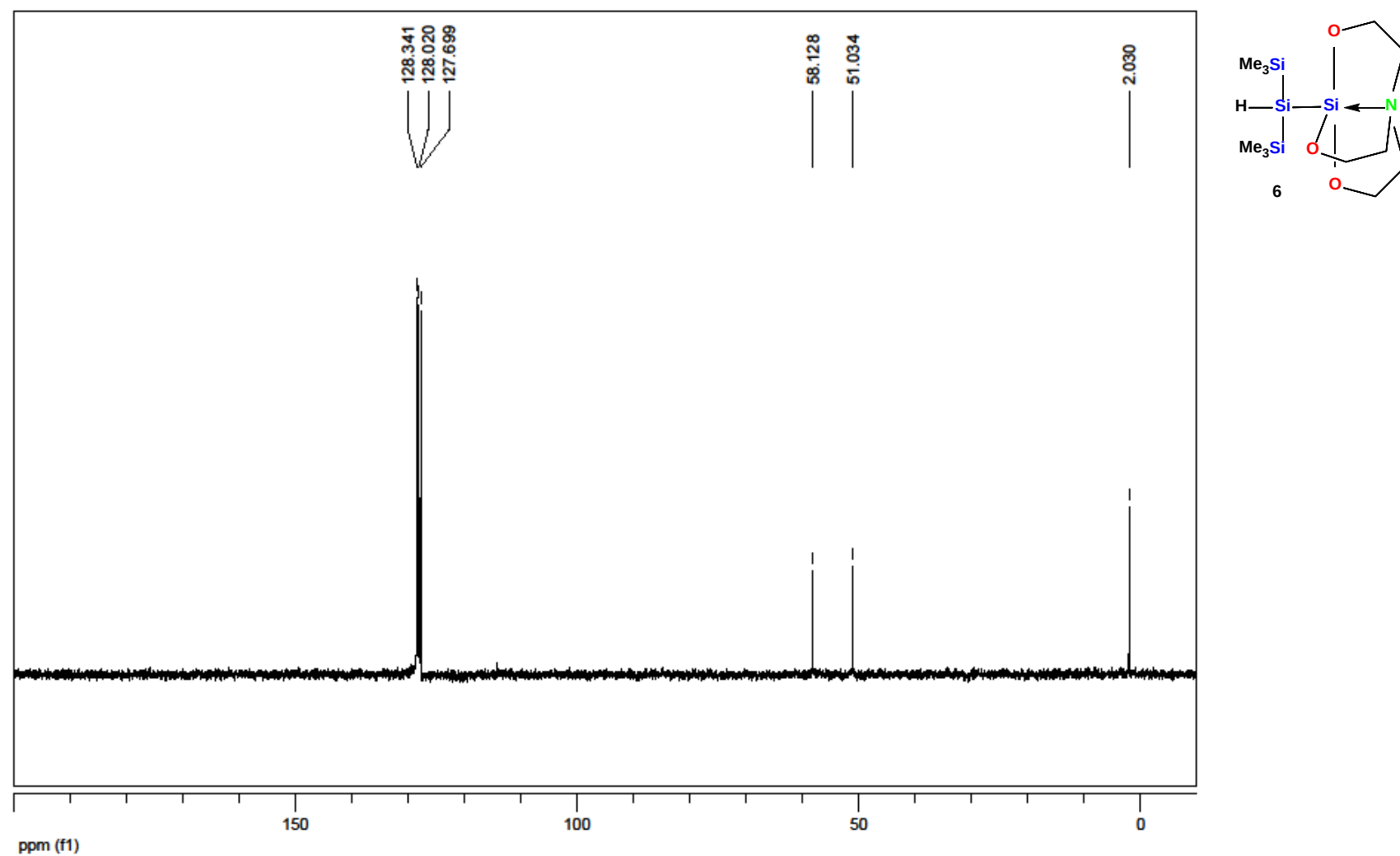


Figure S9. ¹³C{¹H} NMR spectrum of **6** in C₆D₆

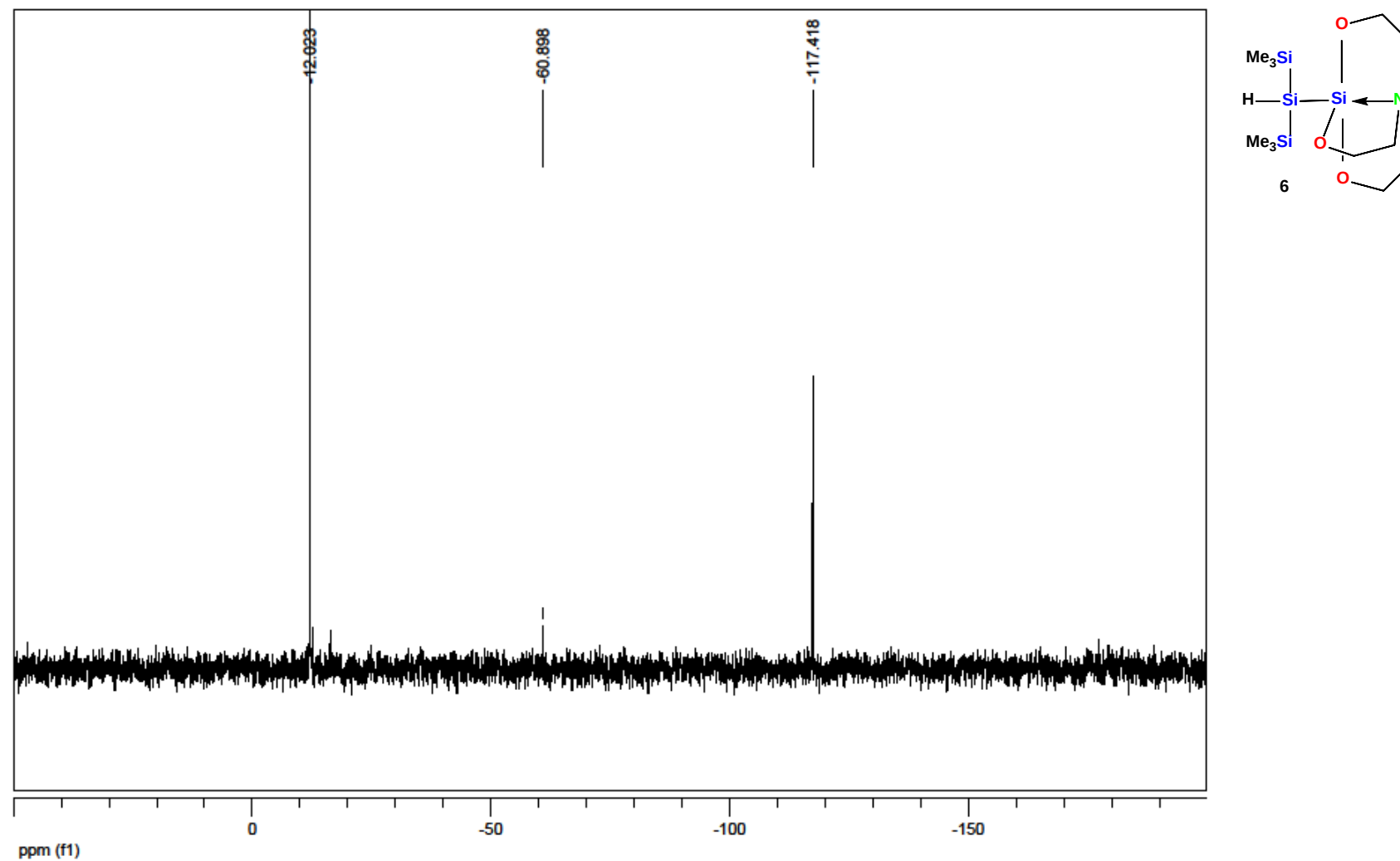


Figure S10. $^{29}\text{Si}\{^1\text{H}\}$ INEPT NMR spectrum of **6** in C_6D_6

Compound **7**: ^1H , ^{13}C , and ^{29}Si NMR spectra:

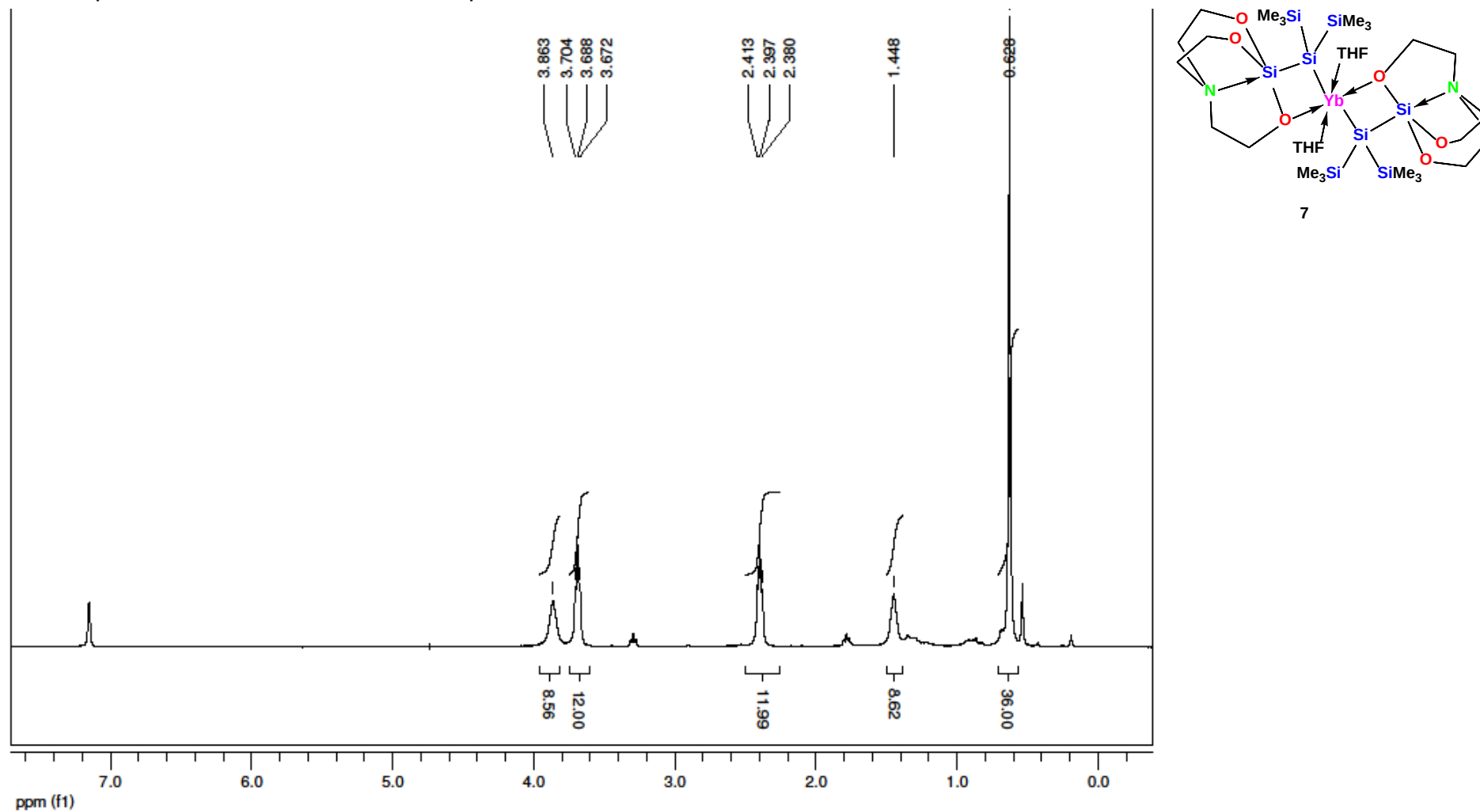


Figure S11. ^1H NMR spectrum of **7** in C_6D_6

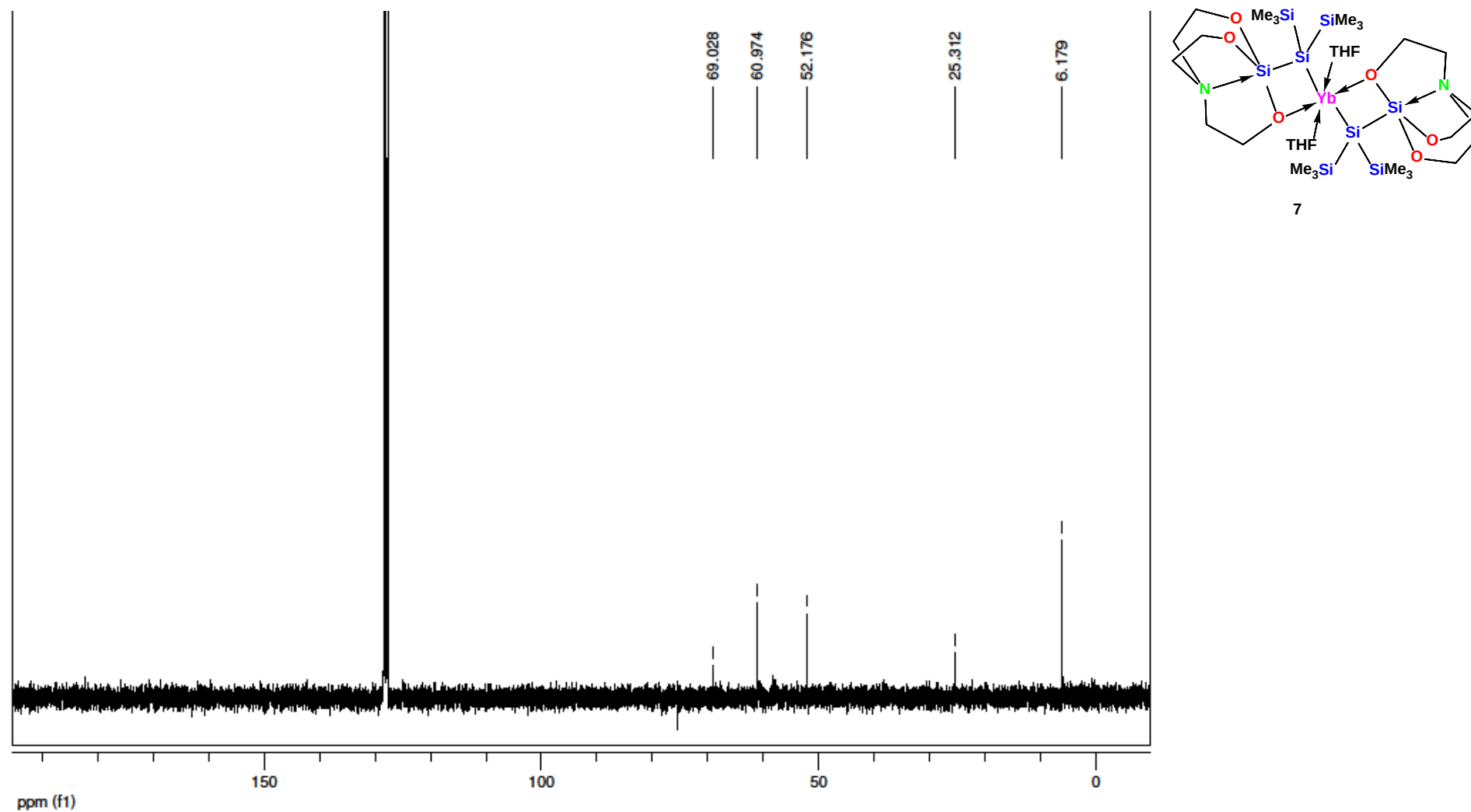


Figure S12. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **7** in C_6D_6

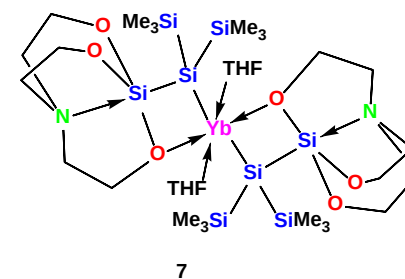
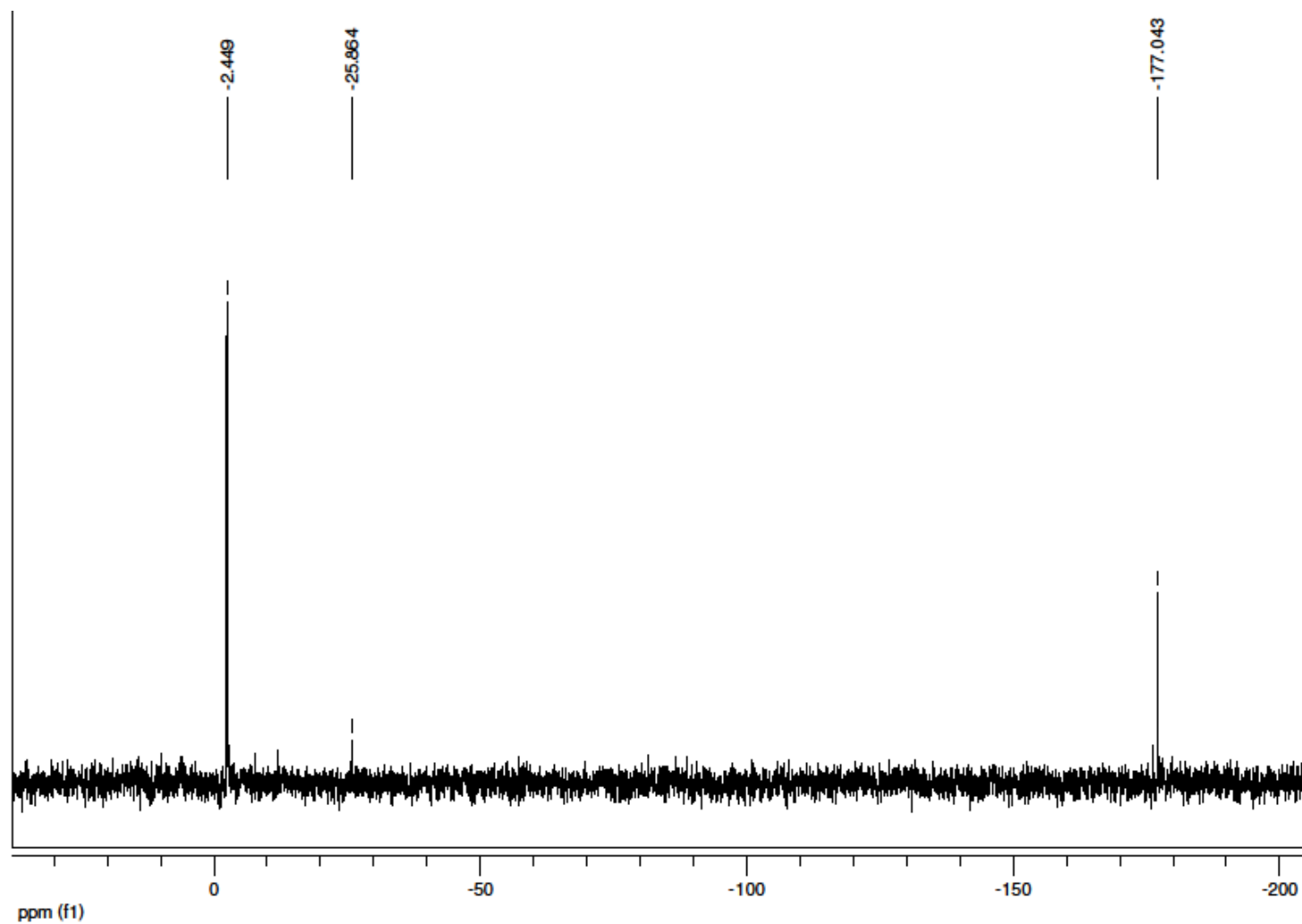


Figure S13. $^{29}\text{Si}\{^1\text{H}\}$ INEPT NMR spectrum of **7** in C_6D_6

Compound **8**: ^1H , ^{13}C , ^{29}Si , and ^{31}P NMR spectra:

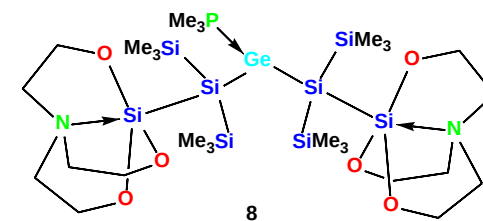
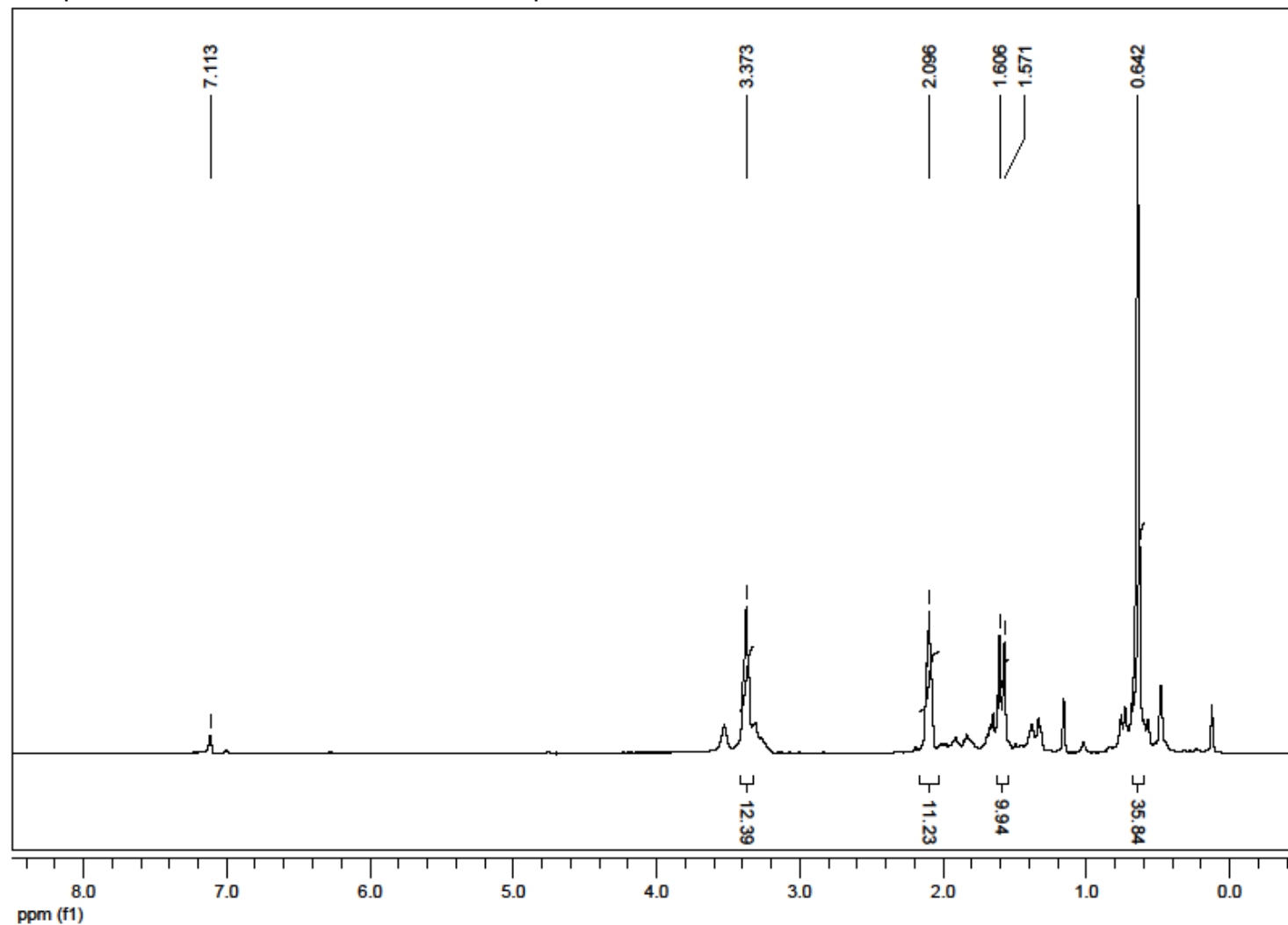


Figure S14. ^1H NMR spectrum of **8** in C_6D_6

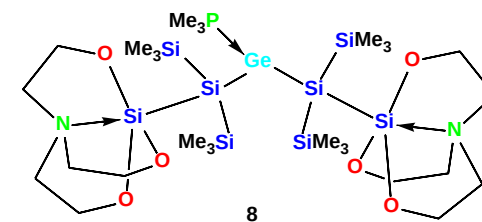
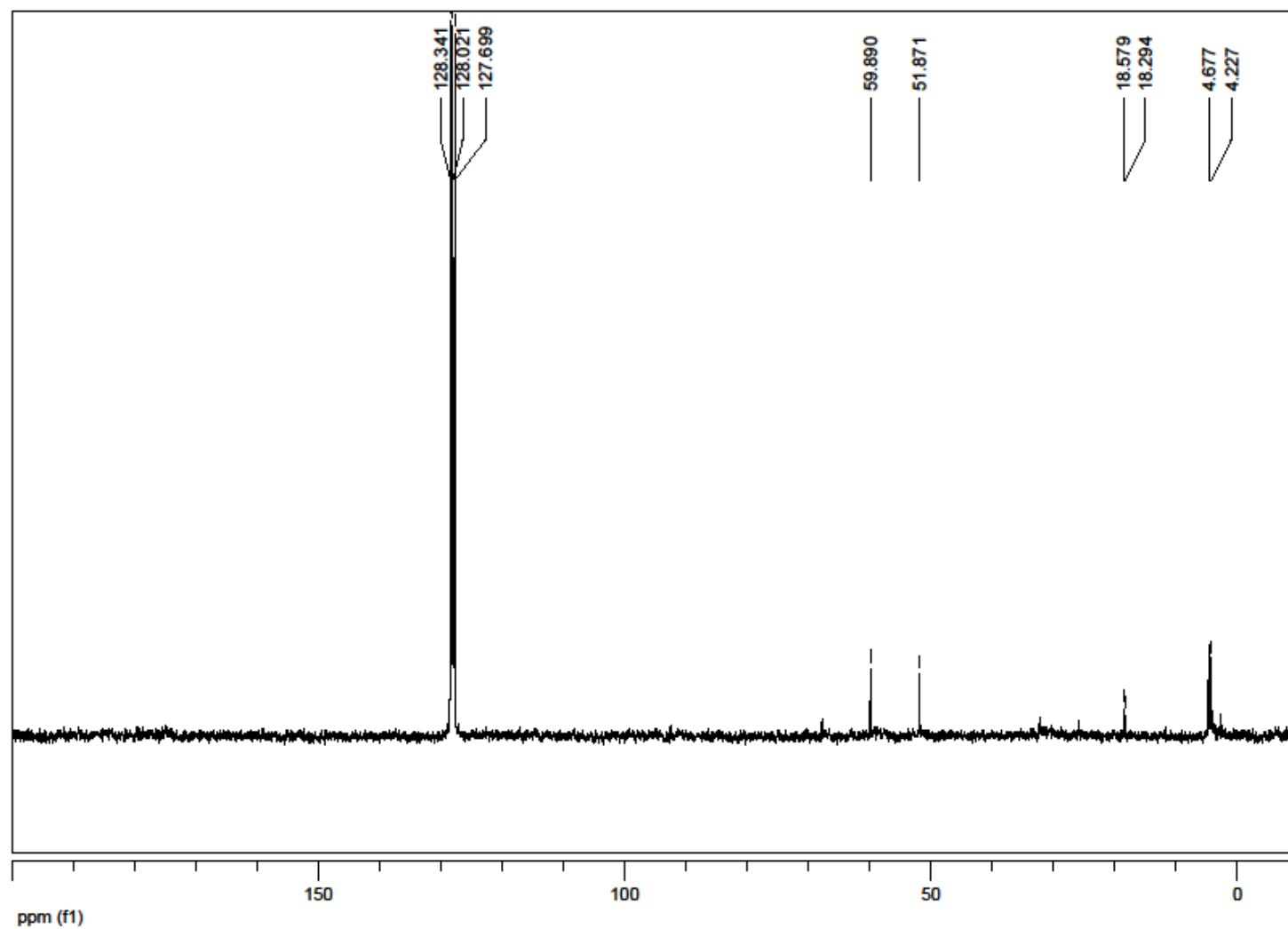


Figure S15. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **8** in C_6D_6

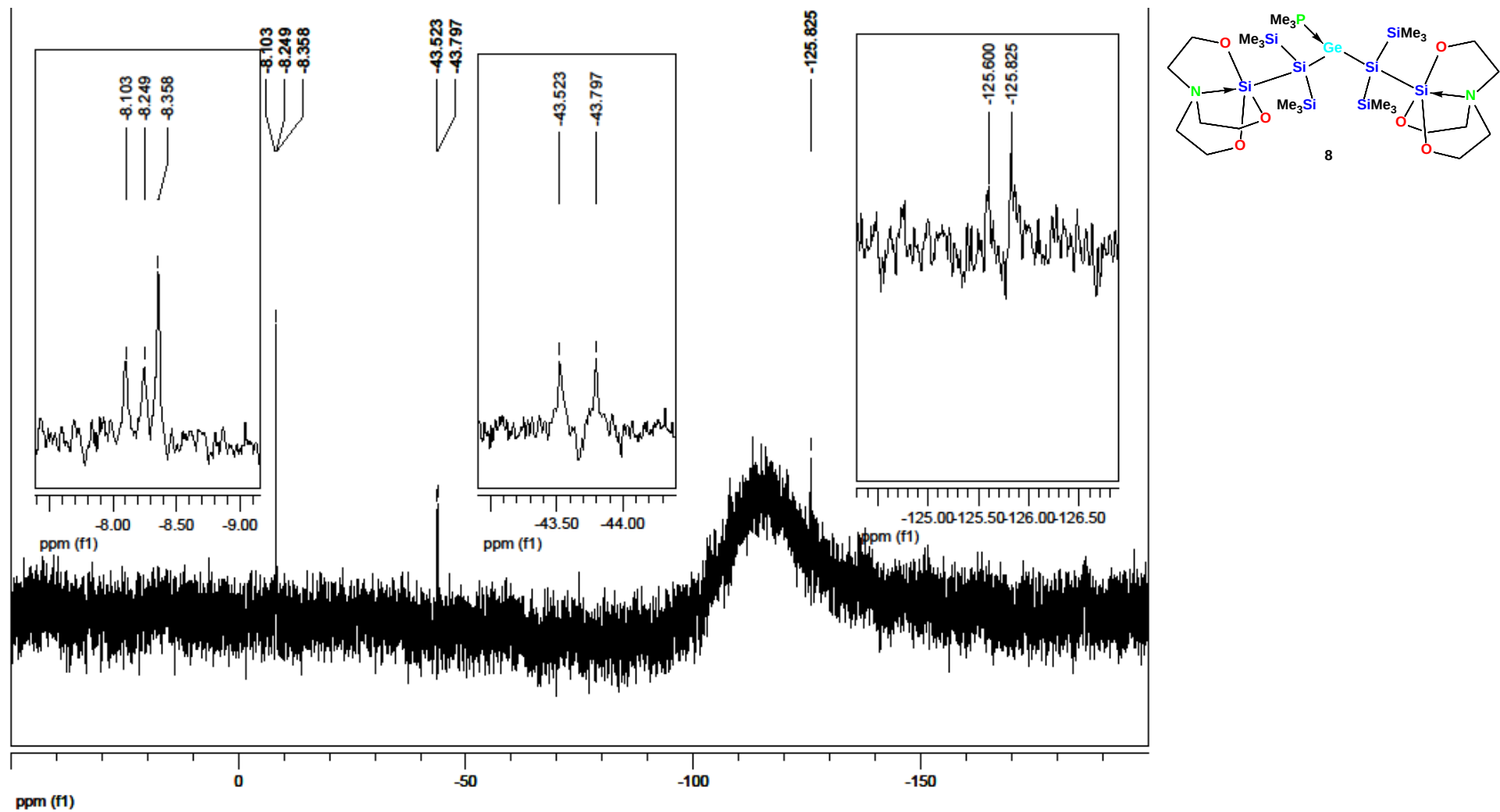


Figure S16. $^{29}\text{Si}\{^1\text{H}\}$ NMR spectrum of **8** in C_6D_6

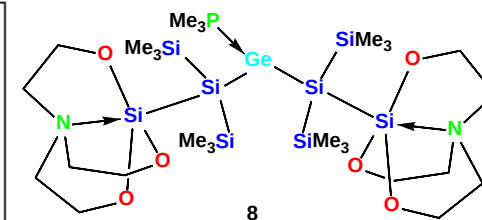
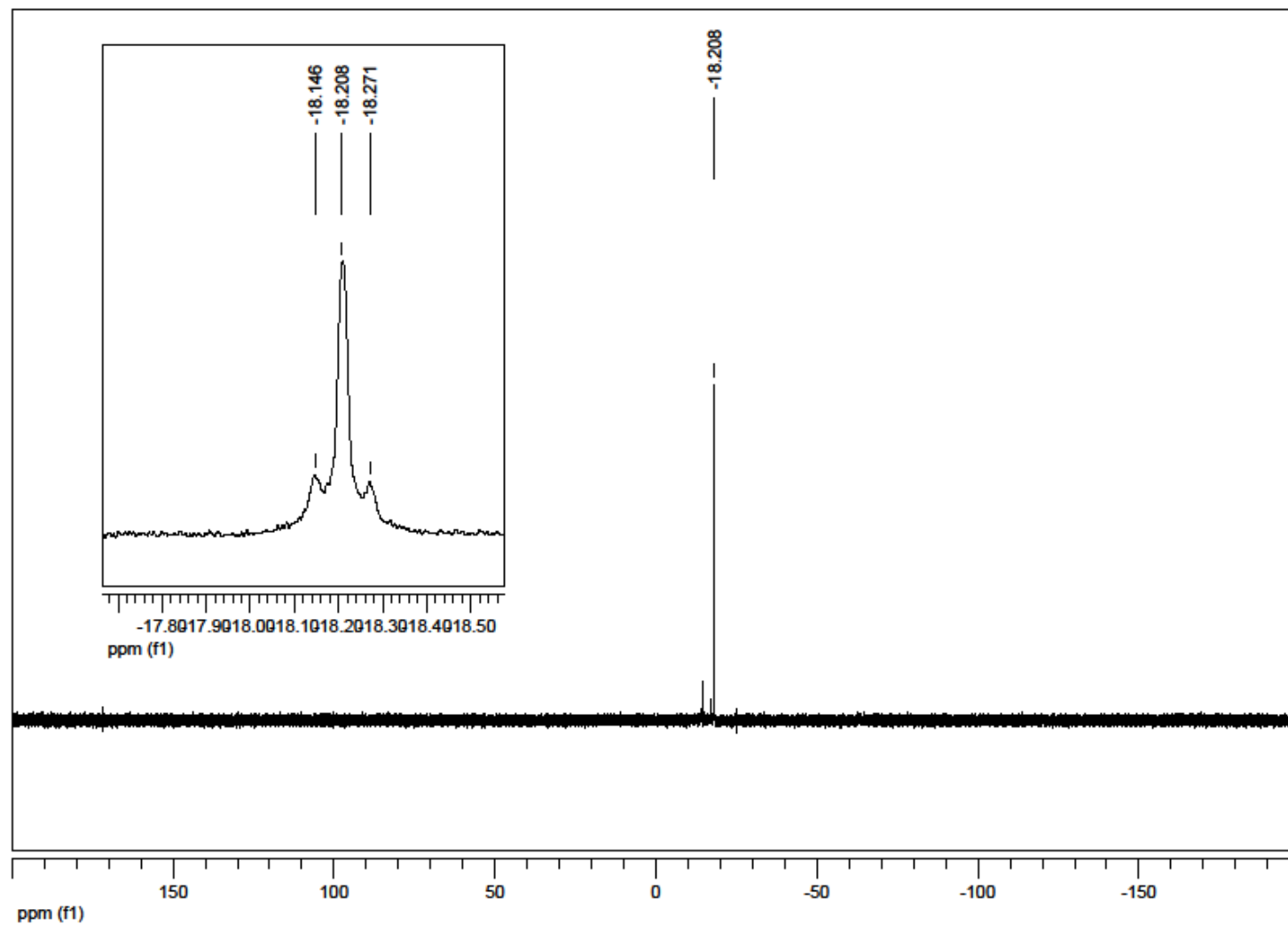


Figure S17. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **8** in C_6D_6

Compound **9**: ^1H and ^{29}Si NMR spectra:

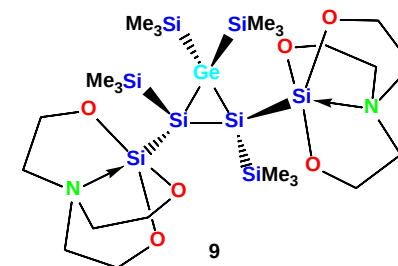
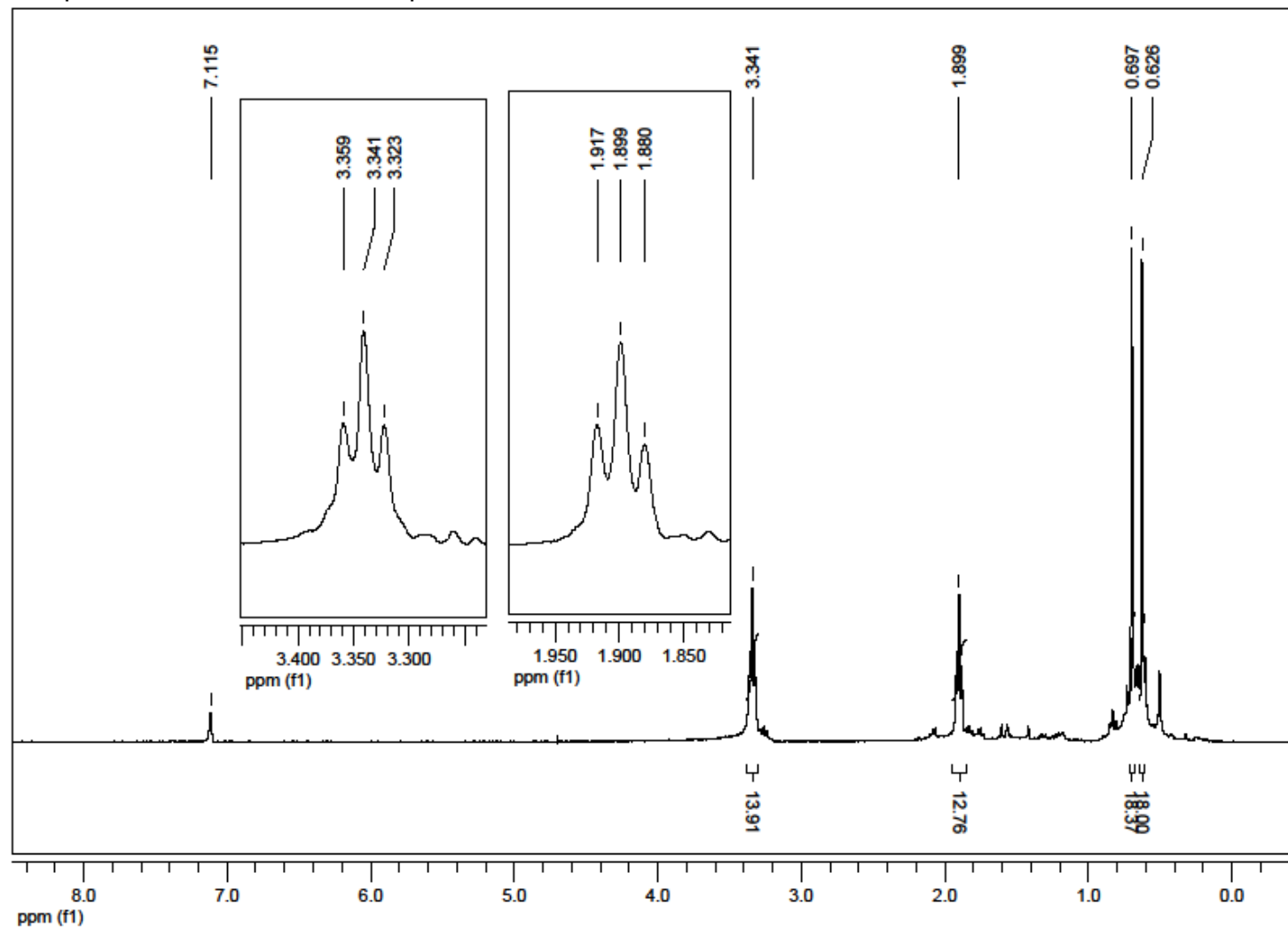


Figure S18. ^1H NMR spectrum of **9** in C_6D_6

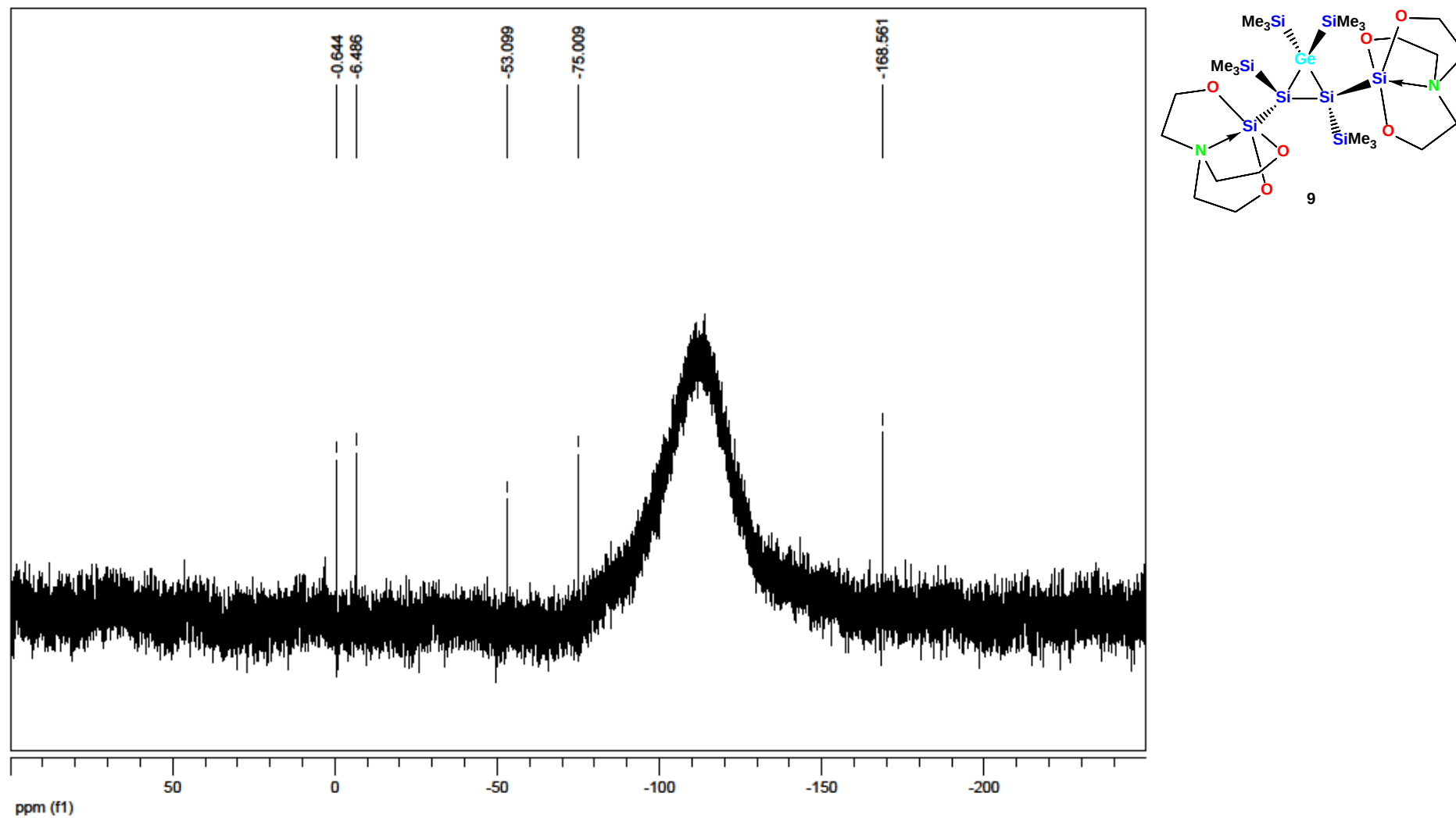


Figure S19. $^{29}\text{Si}\{^1\text{H}\}$ NMR spectrum of **9** in C_6D_6

Compound **10**: ^1H , ^{13}C , and ^{29}Si NMR spectra:

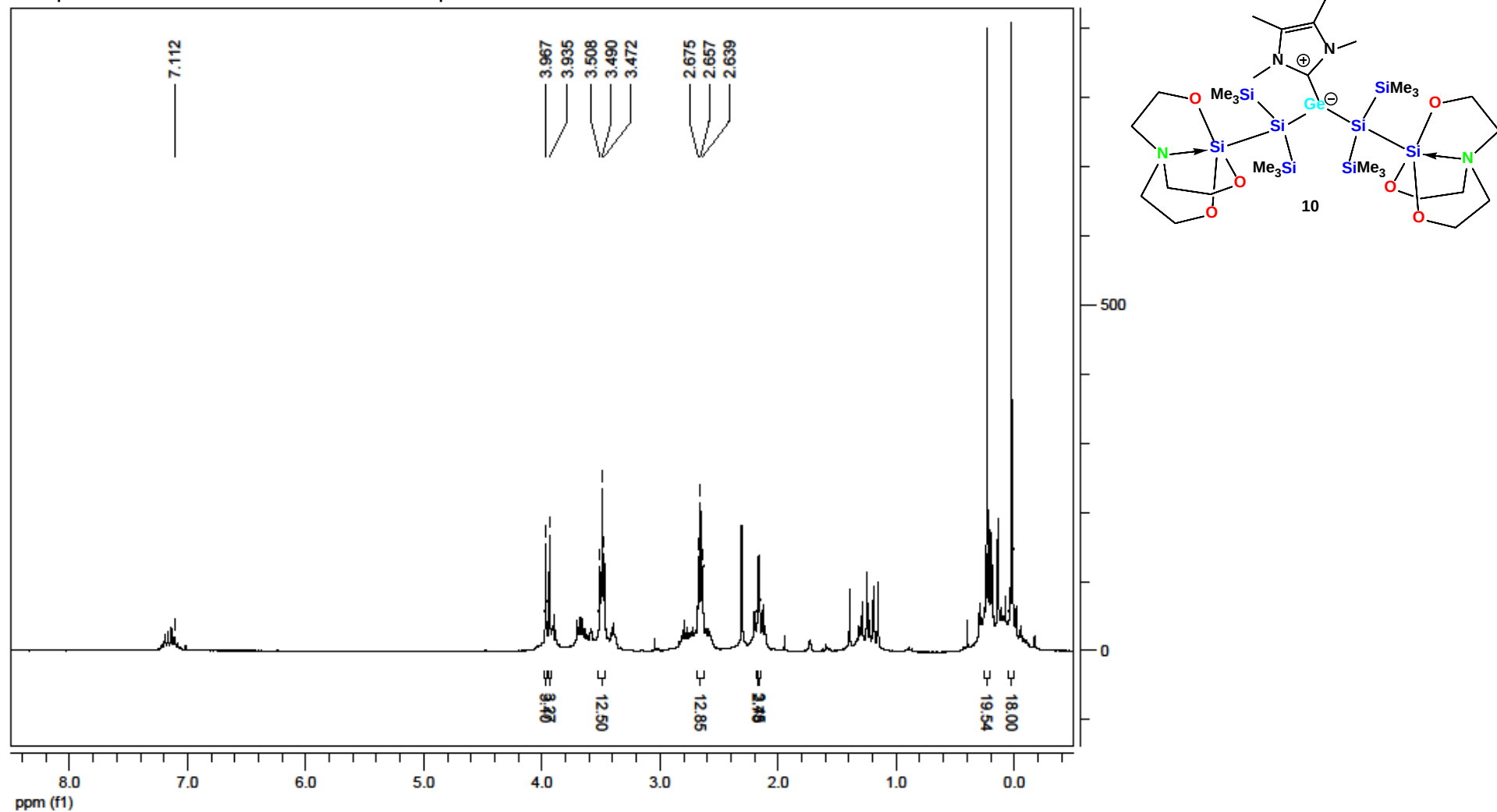


Figure S20. ^1H NMR spectrum of **10** in THF-d_8 (contaminated with toluene)

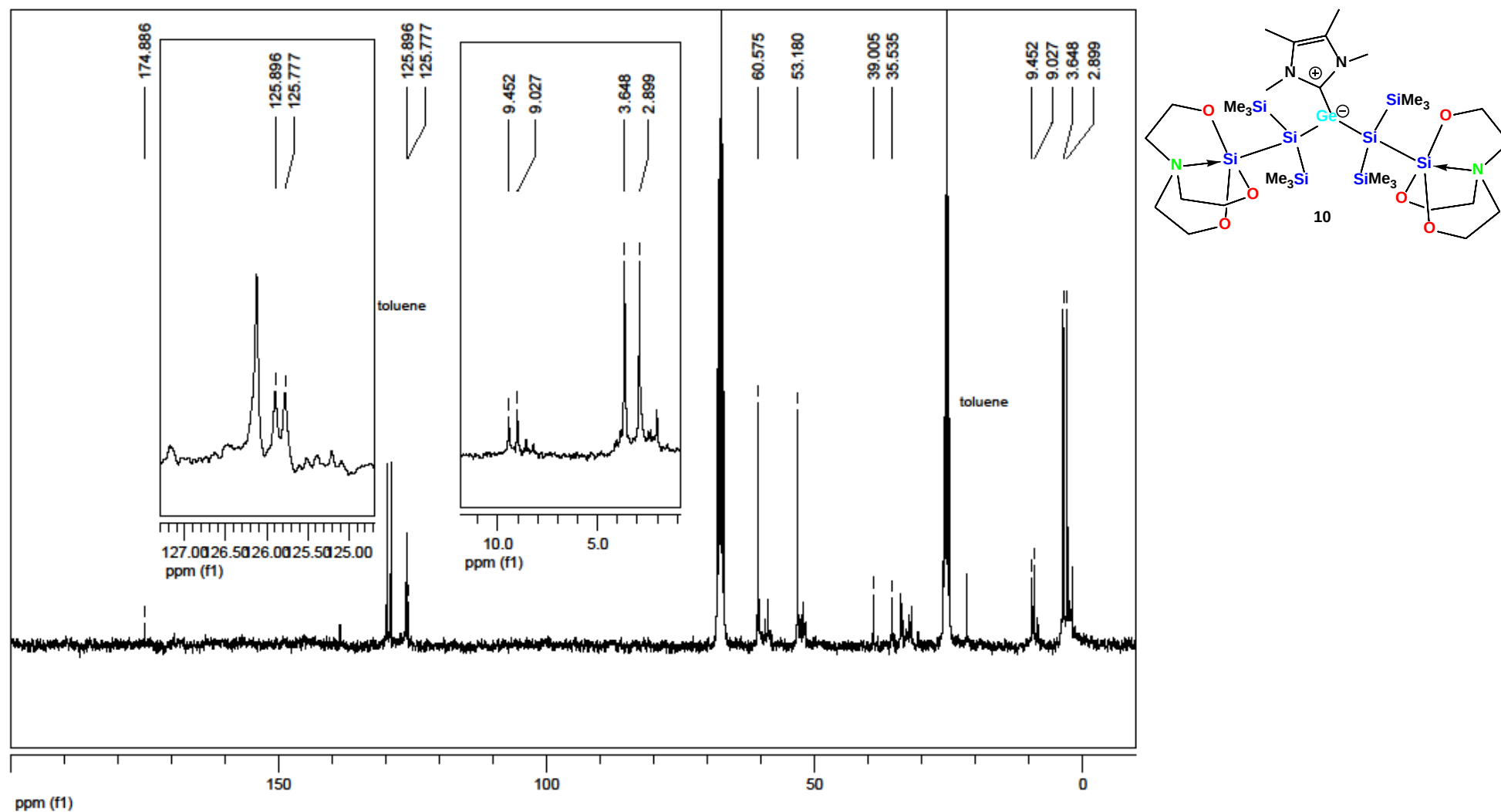


Figure S21. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **10** in THF-d_8 (contaminated with toluene)

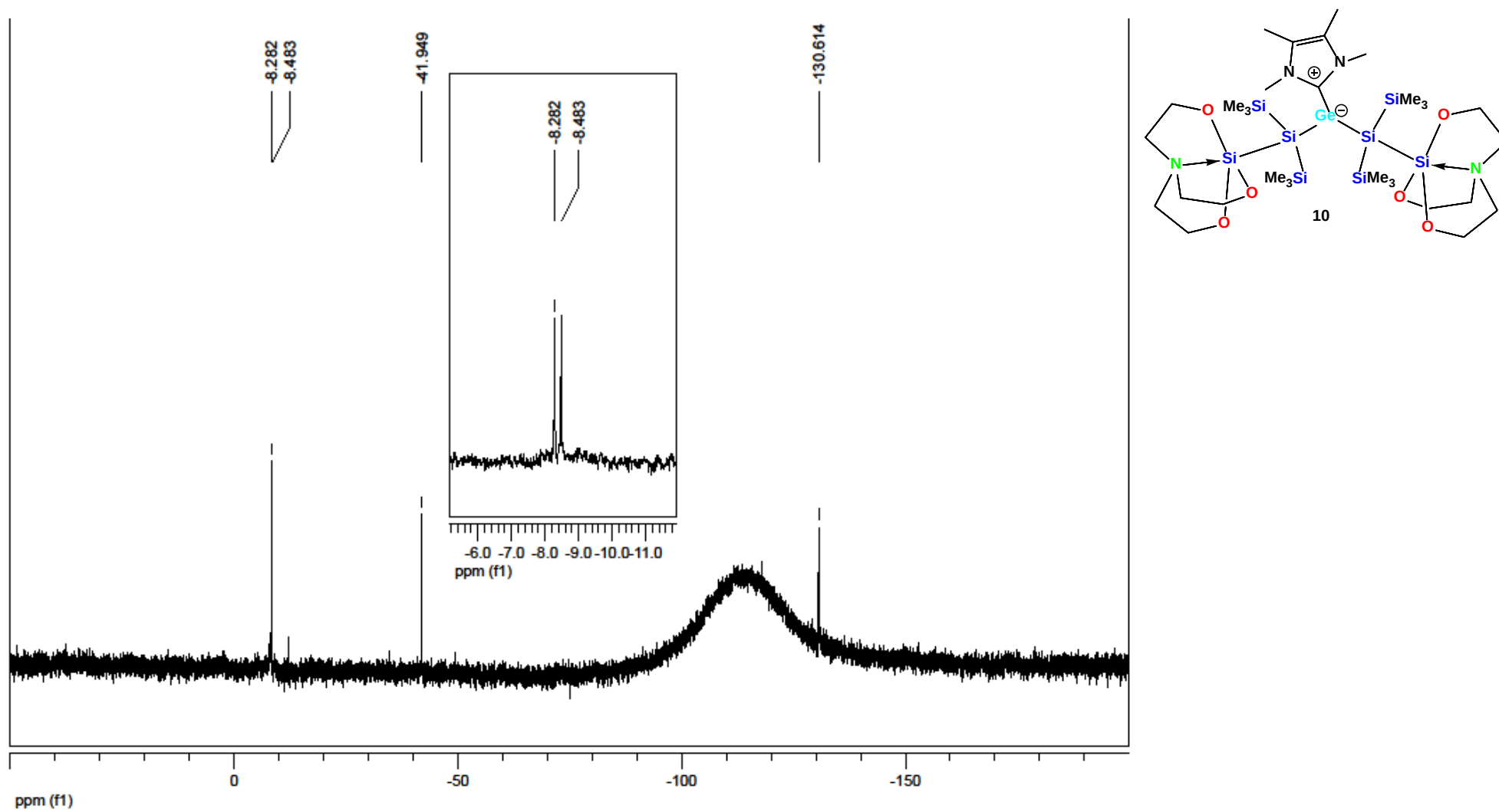


Figure S22. $^{29}\text{Si}\{^1\text{H}\}$ NMR spectrum of **10** in THF-d_8