

Supporting Information

Yb/Si frustrated Lewis pairs with a labile naphthalenyl ridge

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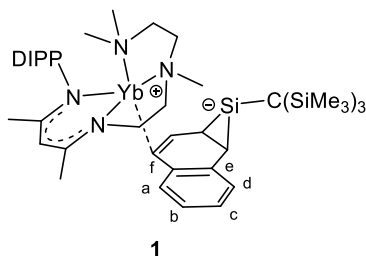
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General

All operations were carried out under an atmosphere of argon using Schlenk techniques or in an argon filled glovebox. Toluene, tetrahydrofuran, hexane, C₆D₆ and THF-*d*₈ were dried over Na/K alloy, transferred under vacuum, and stored in the glovebox. [L1YbI]₂ (L1 = [MeC(NDIPP)CHC(Me)(NCH₂CH₂N(Me)CH₂CH₂NMe₂)]⁺), [L2K]₂ (L2 = [MeC(NDIPP)CHC(^tBu)(NCH₂CH₂N(Me)CH₂CH₂NMe₂)]⁺), [L3YbI]₂ (L3 = [^tBuC(NDIPP)CHC(^tBu)(NCH₂CH₂N(Me)CH₂CH₂NMe₂)]⁺) and **K-Si** were synthesized as we previously reported.¹⁻⁴ [L2YbI]₂ was synthesized from the reaction of [L2K]₂ with YbI₂(THF)₂ using the same procedure reported for [L1YbI]₂.¹ Phenylacetylene and 3-hexyne were dried over CaH₂, distilled under vacuum, degassed by three freeze-pump-thaw cycles, and stored in the glovebox under -35 °C. Triphenylphosphine sulfide and 2,6-dimethylphenyl isocyanide were dried under vacuum for 12 h before use. ¹H, ¹³C{¹H} and ²⁹Si{¹H} NMR spectra were recorded on a Bruker AV III 400 spectrometer or an Agilent MR400 spectrometer. Chemical shifts were reported in δ units with references to the residual solvent resonance of the deuterated solvents for proton and carbon chemical shifts, and to the external PhSiH₃ (δ = -59.7 ppm) for silicon chemical shifts. The assignment of ¹H and ¹³C{¹H} resonances was assisted with gCOSY, gHSQC and gHMBC spectra. Elemental analysis was performed by the Analytical Laboratory of Shanghai Institute of Organic Chemistry.

Synthesis

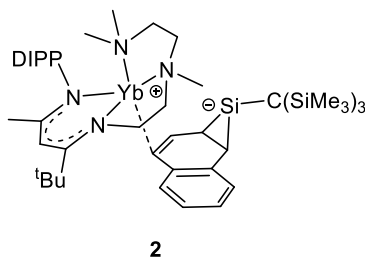
1: [L1YbI]₂ (1.0 g, 0.729 mmol) and **K-Si** (653 mg, 0.765 mmol) were mixed in 10 mL of toluene at room temperature. After stirring for 0.5 h, the precipitate was separated by centrifugation. The volatiles of the solution were removed under vacuum, the residue was washed with cold hexane (3 mL × 2) and dried under vacuum to give **1** as a dark-red solid (1.26 g, 91% yield).



The NMR spectra of **1** in C₆D₆ revealed there are two isomers. These two isomers are in a 1.6:1 ratio according to the integration of CH=CH–Ar in the major isomer at δ = 5.66(d, $^3J_{\text{H-H}}$ = 9.0 Hz) ppm and in the minor isomer at δ = 5.24(d, $^3J_{\text{H-H}}$ = 9.2 Hz) ppm. The ^1H – ^1H NOESY spectrum of **1** revealed that in the major isomer the MeC(N)CH (4.81 ppm) is close to the CH=CH–Ar (5.66 ppm) and the CHMe₂ of DIPP (1.21, 1.52 ppm) is close to the SiCH–CH=C (6.77 ppm), which has been subjected to single crystal XRD. In the minor isomer, the CH=CH–Ar (5.24 ppm) is away from the MeC(N)CH (4.80 ppm). The ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR data of the major isomer are given as the following. ^1H NMR (400 MHz, C₆D₆, 25 °C): δ 7.27–7.13 (m, overlapped with the residue solvent resonance of the deuterated solvent, *m*-ArH of DIPP), 7.12 (m, 1H, *p*-ArH of DIPP), 7.05 (m, 1H, ArH_a), 6.88 (t, $^3J_{\text{H-H}}$ = 7.0 Hz, 1H, ArH_b), 6.77 (m, 1H, SiCH–CH=), 6.68 (t, $^3J_{\text{H-H}}$ = 7.0 Hz, 1H, ArH_c), 6.49 (d, $^3J_{\text{H-H}}$ = 7.0 Hz, 1H, ArH_d), 5.66 (d, $^3J_{\text{H-H}}$ = 9.0 Hz, 1H, CH=CH–Ar), 4.81 (s, 1H, MeC(N)CH), 3.28, 3.16, 3.03, 2.69, 2.21, 2.05 (m, overlapped with the signals of the minor isomer, SiCH–Ar, NCH₂ and CHMe₂), 2.92 (d, $^3J_{\text{H-H}}$ = 9.0 Hz, 1H, SiCH–Ar), 2.77 (dd, $^3J_{\text{H-H}}$ = 9.0 Hz, $^3J_{\text{H-H}}$ = 5.4 Hz, 1H, SiCH–CH=), 1.80 (s, 3H, NMe), 1.74 (s, 3H, CMe), 1.65 (s, 3H, CMe), 1.53 (m, 9H, CHMe₂ and NMe₂), 1.22 (d, $^3J_{\text{H-H}}$ = 6.8 Hz, 3H, CHMe₂), 1.13 (d, $^3J_{\text{H-H}}$ = 7.0 Hz, 3H, CHMe₂), 1.08 (d, $^3J_{\text{H-H}}$ = 6.8 Hz, 3H, CHMe₂), 0.51 (s, 27H, SiMe₃). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C₆D₆, 25 °C): δ 165.9, 164.9 (MeC(N)CH), 149.6 (*i*-ArC of DIPP), 146.6 (SiCH–CH=C), 142.3 (C_e), 129.8 (*o*-ArC of DIPP), 131.0 (C_f), 128.5 (C_d, overlapped with the resonance of the deuterated solvent), 128.1 (C_b), 126.6, 126.5 (*m*-ArC of DIPP), 126.5 (*p*-ArC of DIPP), 124.7(C_a), 122.3 (C_c), 111.3 (CH=CH–Ar), 97.0 (MeC(N)CH), 60.3, 57.3, 55.9, 48.4 (NCH₂), 45.9 (NMe₂), 41.0 (NMe), 32.1 (SiCH–CH=C), 30.0 (SiCH–Ar), 28.5, 27.7, 25.9, 25.5, 25.3, 24.8, 23.3 (CHMe₂, CHMe₂, CMe), 7.3 (SiMe₃). $^{29}\text{Si}\{^1\text{H}\}$ NMR (80 MHz, C₆D₆, 25 °C): for the major isomer, δ -95.7 (Si(Np)C), -2.8 (SiMe₃); for the minor isomer, δ -94.5 (Si(Np)C), -2.6 (SiMe₃). Anal. Calcd for C₄₄H₇₆N₄Si₄Yb: C, 55.83; H, 8.09; N, 5.92. Found: C: 55.88; H: 8.44; N: 5.54.

2: [L2YbI]₂ (200 mg, 0.137 mmol) and **K-Si** (128 mg, 0.150 mmol) were mixed in 5 mL of toluene at room temperature. After stirring for 0.5 h, the precipitate was separated by centrifugation. The volatiles

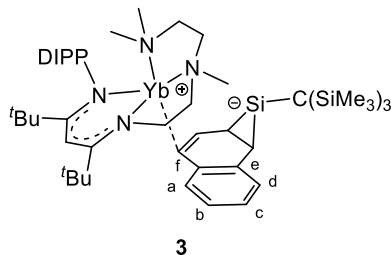
of the solution were removed under vacuum, the residue was washed with cold hexane (1 mL $\times$ 2) and dried under vacuum to give **2** as a dark-red solid (235 mg, 87% yield).



The NMR spectra of **2** in C₆D₆ revealed there are two isomers. These two isomers are in a 1.2:1 ratio according to the integration of CH=CH–Ar in the major isomer at δ = 5.33 (d, $^3J_{\text{H-H}}$ = 9.03 Hz) ppm and in the minor isomer at δ = 5.52 (d, $^3J_{\text{H-H}}$ = 9.0 Hz) ppm. ^1H NMR (400 MHz, C₆D₆, 25 °C): δ 7.18–7.09 (m, overlapped with the residue solvent resonance of the deuterated solvent, *m*-ArH of DIPP), 7.06, 6.85, 6.63, 6.43 (m, 6H in total, *p*-ArH of DIPP, SiCH–CH=C and ArH of Np), 5.52 (d, $^3J_{\text{H-H}}$ = 9.0 Hz, 0.45H, CH=CH–Ar in minor isomer), 5.33 (d, $^3J_{\text{H-H}}$ = 9.0 Hz, 0.55H, CH=CH–Ar in major isomer), 5.08, 5.06 (s, 1H in total, MeC(N)CH), 3.71 (m, 1H, N(CH₂)), 3.30, 3.14 (m, 2H, CHMe₂), 2.91, 2.67, 2.42, 2.10 (m, 7H in total, NCH₂, SiCH–Ar and SiCH–CH=), 2.10, 1.86 (s, 3H in total, NMe), 1.71–0.94 (m, ~20H in total, NMe₂, C^{*t*}Bu, CMe, NCH₂ and CHMe₂), 0.53, 0.52 (s, 27H in total, SiMe₃). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C₆D₆, 25 °C) δ 172.8, 171.7 (^{*t*}BuC(N)CH), 164.5, 164.4 (MeC(N)CH), 151.2, 150.1, 147.3, 146.7, 146.1, 143.4, 142.8, 142.6, 142.1, 141.8, 132.1, 127.4, 126.4, 126.3, 125.1, 125.1, 124.4, 124.3, 124.1, 124.0, 122.5, 122.2 (SiCH–CH=C, ArC of DIPP and ArC of Np), 113.3, 109.7 (CH=CH–Ar), 94.7, 92.9 (MeC(N)CH), 60.9, 60.3, 58.0, 57.0, 53.2, 52.5, 48.7, 48.3 (NCH₂), 46.0, 45.2, 42.8, 39.2, 39.1 (NMe and NMe₂), 33.0, 32.5, 31.8, 31.4, 31.3, 30.0, 30.7, 29.8, 29.1, 28.1, 28.1, 27.9, 27.6, 26.9, 26.1, 26.1, 25.7, 24.7, 24.7, 24.2, 23.6 (SiCH–CH=C, SiCH–Ar, CMe₃, CMe, CMe, CHMe₂ and CHMe₂), 7.3, 7.1 (SiMe₃). $^{29}\text{Si}\{^1\text{H}\}$ NMR (80 MHz, C₆D₆, 25 °C): for the major isomer, δ -91.2 (Si(Np)C), -2.7 (SiMe₃); for the minor isomer, δ -89.6 (Si(Np)C), -2.8 (SiMe₃). Anal. Calcd for C₄₇H₈₂N₄Si₄Yb: C, 57.10; H, 8.36; N, 5.67. Found: C: 57.10; H: 8.77; N: 5.46.

3: [L3YbI]₂ (200 mg, 0.130 mmol) and **K-Si** (122 mg, 0.143 mmol) were mixed in 5 mL of toluene at room temperature. After stirring for 0.5 h, the precipitate was separated by centrifugation. The volatiles

of the solution were removed under vacuum, the residue was washed with cold hexane (1 mL $\times$ 2) and dried under vacuum to give **3** as a dark-red solid (242 mg, 90% yield).



¹H NMR (400 MHz, C₆D₆, 25 °C): δ 7.22-7.13 (m, overlapped with the residue solvent resonance of the deuterated solvent, *m* and *p*-ArH of DIPP), 6.99 (m, 1H, ArH_a), 6.93, 6.88 (m, 2H, *m*-ArH of DIPP and ArH_b), 6.78 (m, 1H, SiCH-CH=), 6.64 (t, ³J_{H-H} = 7.0 Hz, 1H, ArH_c), 6.59 (d, ³J_{H-H} = 8.0 Hz, 1H, ArH_d), 5.53 (d, ³J_{H-H} = 8.9 Hz, 1H, CH=CH-Ar), 5.48 (s, 1H, ^tBuC(N)CH), 3.64 (m, 2H, NCH₂), 3.57 (m, 1H, CHMe₂), 2.89 (d, ³J_{H-H} = 8.6 Hz, 1H, SiCH-Ar), 3.87 (m, 1H, CHMe₂), 2.70 (dd, ³J_{H-H} = 8.6 Hz, ³J_{H-H} = 5.6 Hz, 1H, CH=CH-Ar), 2.57 (m, 1H, NCH₂), 2.00 (m, 2H, NCH₂), 1.83 (s, 3H, NMe), 1.73 (d, ³J_{H-H} = 6.8 Hz, 3H, CHMe₂), 1.55 (br, 6H, NMe₂), 1.32, 1.22 (m, 24H, C^tBu and CHMe₂), 0.91 (d, ³J_{H-H} = 6.8 Hz, 3H, CHMe₂), 0.53 (s, 27H, SiMe₃). ¹³C{¹H} NMR (100 MHz, C₆D₆, 25 °C): δ 172.9, 172.4 (MeC(N)CH), 150.7 (*i*-ArC of DIPP), 148.4 (SiCH-CH=C) 146.4 (C_e), 141.9 (*o*-ArC of DIPP), 139.9 (C_f), 129.5 (C_d), 128.7 (C_b), 126.5, 126.1 (*m*-ArC of DIPP), 125.1 (*p*-ArC of DIPP), 124.3(C_a) 122.5 (C_c), 108.9 (CH=CH-Ar), 94.1 (^tBuC(N)CH), 60.4, 57.6, 53.6, 48.9 (NCH₂), 46.6 (NMe₂), 46.2 (NMe), 45.7, 40.4 (C of ^tBu), 34.0 (SiCH-CH=C), 33.6 (CMe₃), 32.6 (SiCH-Ar), 31.8 (CMe₃), 30.0, 27.2, 25.7, 25.6, 25.1 (CHMe₂ and CHMe₂), 7.3 (SiMe₃). ²⁹Si{¹H} NMR (80 MHz, C₆D₆, 25 °C): δ -84.3 (Si(Np)C), -2.8 (SiMe₃). Anal. Calcd for C₅₀H₈₈N₄Si₄Yb: C, 58.27; H, 8.61; N, 5.44. Found: C; 58.04; H; 9.31; N; 5.27.

4: Complex **1** (100 mg, 0.106 mmol) and triphenylphosphine sulfide (62 mg, 0.211 mmol) were mixed in 5 mL of toluene at room temperature. After stirring for 4 h, the volatiles of the solution were removed under vacuum, and the residue was extracted by cold pentane (3 mL). Pentane was removed under vacuum to give **4** as a dark-green solid (68 mg, 73% yield). ¹H NMR (400 MHz, C₆D₆, 25 °C): δ 7.24-7.18 (m, 2H, *m*- and *p*-ArH of DIPP), 7.17-7.14 (m, overlapped with the residue solvent resonance of the deuterated solvent, *m*-ArH of DIPP), 4.70 (s, 1H, MeC(N)CH), 3.50 (hept, ³J_{H-H} = 6.8 Hz, 1H, CHMe₂), 3.17-3.00

(m, 4H, NCH_2 and CHMe_2), 2.50 (s, 3H, NMe), 2.31 (m, 1H, NCH_2), 2.19 (m, 1H, NCH_2), 2.12 (br, 3H, NMe_2), 1.95 (br, 3H, NMe_2), 1.92 (m, 1H, NCH_2), 1.71 (s, 3H, CMe), 1.70 (s, 3H, CMe), 1.58 (m, 1H, NCH_2), 1.56 (d, $^3J_{\text{H-H}} = 6.8$ Hz, 3H, CHMe_2), 1.54 (d, $^3J_{\text{H-H}} = 6.8$ Hz, 3H, CHMe_2), 1.46 (m, 1H, NCH_2), 1.27 (d, $^3J_{\text{H-H}} = 6.8$ Hz, 3H, CHMe_2), 1.23 (d, $^3J_{\text{H-H}} = 6.8$ Hz, 3H, CHMe_2), 0.51 (s, 27H, SiMe_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C_6D_6 , 25 °C): δ 165.3, 163.9 (MeC(N)CH) 147.7 (*i*-ArC of DIPP), 142.9, 140.7 (*o*-ArC of DIPP), 124.7, 124.1 (*m*-ArC of DIPP), 123.1 (*p*-ArC of DIPP), 95.5 (MeC(N)CH), 57.9, 57.8, 50.7, 47.9 (NCH_2), 47.8, 44.1 (NMe_2), 45.4 (NMe), 29.7, 28.1 (CHMe_2), 25.6, 25.13, 25.06, 25.0, 24.1, 23.4 (CHMe_2 , CMe), 6.2 (SiMe_3). $^{29}\text{Si}\{^1\text{H}\}$ NMR (80 MHz, C_6D_6 , 25 °C): δ 170.1 (S–Si), -2.7 (SiMe_3). Anal. Calcd for $\text{C}_{34}\text{H}_{68}\text{N}_4\text{S}_2\text{Si}_4\text{Yb}$: C 46.28; H 7.77; N 6.35. Found: C 46.03; H 7.78; N 6.36.

5: Complex **2** (200 mg, 0.202 mmol) and 2,6-dimethylphenyl isocyanide (29 mg, 0.221 mol) were mixed in 5 mL of toluene at room temperature, and then the solution was heated at 50 °C for 1 h. The volatiles of the solution were removed under vacuum at room temperature, the black residue was washed with 1 mL of cold hexane and dried under vacuum to give **5** as a dark-red solid (110 mg, 55% yield). ^1H NMR (400 MHz, C_6D_6 , 25 °C): δ 7.20-7.11 (m, overlapped with the residue solvent resonance of the deuterated solvent, 1H, *p*-ArH of DIPP), 7.06-6.98 (m, 4H, *m*-ArH of DIPP and *m*-ArH of Me_2Ar), 6.93 (m, 1H, *p*-ArH of Me_2Ar), 4.97 (s, 1H, MeC(N)CH), 4.02 (m, 1H, $\text{N(CH}_2\text{)}$), 3.25-3.16 (m, 2H, CHMe_2 and $\text{N(CH}_2\text{)}$), 3.04 (hept, $^3J_{\text{H-H}} = 6.8$ Hz, 1H, CHMe_2), 2.60 (s, 6H, Me_2Ar), 2.56 (s, 3H, NMe), 2.50-1.66 (br, 6H, NCH_2), 1.69 (s, 3H, CMe), 1.56 (br, 3H, NMe_2), 1.49 (br, 3H, NMe_2), 1.25-1.21 (br, 12H, C^tBu and CHMe_2), 1.09-1.01 (m, 9H, CHMe_2), 0.45 (s, 27H, SiMe_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C_6D_6 , 25 °C): δ 266.2 (Si=C=N), 172.8 (C^tBu), 164.7 (CMe), 149.8 (*i*-ArC of DIPP), 146.5 (*i*-ArC of Me_2Ar), 142.3, 141.6 (*o*-ArC of DIPP), 130.6 (*o*-ArC of Me_2Ar), 129.0 (*m*-ArC of Me_2Ar) 128.3 (*p*-ArC of DIPP), 124.3 (*p*-ArC of Me_2Ar), 123.9 (*m*-ArC of Me_2Ar), 123.8, 123.4 (*m*-ArC of DIPP), 91.9 (MeC(N)CH), 61.2, 58.0, 56.7, 47.9 (NCH_2), 43.6 (NMe), 40.7 (CMe_3), 30.8 (CMe_3), 26.4 (CMe), 28.4, 27.3 (CHMe_2), 25.0, 24.7, 24.7, 24.3 (CHMe_2), 19.2 (Me_2Ar), 5.3 (SiMe_3). $^{29}\text{Si}\{^1\text{H}\}$ NMR (80 MHz, C_6D_6 , 25 °C): δ -67.1 (Si=C=N), -2.7 (SiMe_3). The satisfied elemental analysis result of **7** was not obtained. In the interest of transparency, the elemental

analysis result is listed below. Anal. Calcd for $C_{46}H_{83}N_5Si_4Yb$: C 55.72; H 8.44; N 7.06. Found: C 56.98; H: 9.33; N 6.97.

X-ray crystallography

Single crystals of **1-3** suitable for single-crystal X-ray diffraction were grown from the hexane solutions, those of **4** were grown from the hexane/benzene mixture, and those of **5** were grown from the hexane/hexamethyldisiloxane mixture. The single crystals of **1-5** were mounted under nitrogen atmosphere on a glass fiber at low temperature. Data collections of **1-3** and **5** were performed on a Bruker D8 Venture with Ga $K\alpha$ radiation ($\lambda = 1.34139 \text{ \AA}$). The absorption correction was applied using SADABS program.⁴ Data collections of **4** were performed on a XtaLAB Synergy R with Mo $K\alpha$ radiation ($\lambda = 0.71073 \text{ \AA}$). For **1-3** and **5**, the absorption correction was applied using SADABS program.⁵ The absorption correction for **4** was applied using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm. The structure was solved with the ShelXT structure solution program using Intrinsic Phasing and refined with the ShelXL refinement package using Least Squares minimisation. Hydrogen atoms were placed at calculated positions and were included in the structure calculation. Calculations were carried out using the SHELXL-2016/2018 and Olex2 program.⁶ Crystallographic data and refinement parameters are listed in Table S1.

Table S1. Crystallographic Data and Refinement for **1-5**

	1	2	3
formula	C ₄₄ H ₇₆ N ₄ Si ₄ Yb	C ₄₇ H ₈₂ N ₄ Si ₄ Yb	C ₅₀ H ₈₈ N ₄ Si ₄ Yb
fw	946.48	988.56	1031.65
color	red	red	red
cryst syst.	orthorhombic	orthorhombic	monoclinic
space group	<i>Pbca</i>	<i>Pbca</i>	<i>P2₁/c</i>
a (Å)	17.7955(10)	17.9657(8)	14.1534(9)
b (Å)	22.5894(13)	22.4892(10)	17.7808(11)
c (Å)	27.3617(16)	28.4392(14)	22.4677(14)
α (deg)	90	90	90
β (deg)	90	90	100.898(4)
γ (deg)	90	90	90
V (Å ³)	10999.1(11)	11490.4(9)	5552.2(6)
Z	8	8	4
<i>D</i> _{calcd} (g/cm ³)	1.143	1.143	1.233
<i>F</i> (000)	3952	4144	2168
<i>T</i> (K)	170	170	193
θ range (deg)	3.088 to 55.062	2.703 to 55.217	2.777 to 55.020
no. of refns collected	111621	107233	57766
no. of unique refns	10419	10961	10555
no. of obsd refns (<i>I</i> > 2 σ (<i>I</i>))	8167	6275	8320
No. of params	496	525	554
Final R, R _w (<i>I</i> > 2 σ (<i>I</i>))	0.0961, 0.2800	0.0672, 0.1726	0.0399, 0.0913
Goodness-of-fit on <i>F</i> ²	1.100	1.121	1.039
$\Delta\rho_{\text{max, min}}$, eÅ ⁻³	2.004, -4.094	1.647, -1.215	0.458, -1.202

	4	5
formula	[C ₃₄ H ₆₈ N ₄ S ₂ Si ₄ Yb] ₂	C ₄₆ H ₈₃ N ₅ Si ₄ Yb
fw	1763.87	991.57
color	green	red
cryst syst.	triclinic	monoclinic
space group	<i>P</i> -1	<i>P</i> 2 ₁ /n
a (Å)	15.4962(3)	13.2397(4)
b (Å)	17.7037(3)	22.4875(8)
c (Å)	19.3080(3)	18.0354(5)
α (deg)	78.3820(10)	90
β (deg)	69.4360(10)	105.208(2)
γ (deg)	69.691(2)	90
V (Å ³)	4632.04(15)	5181.6(3)
Z	2	4
D _{calcd} (g/cm ³)	1.268	1.271
<i>F</i> (000)	1836	2080
<i>T</i> (K)	173	182
θ range (deg)	2.113 to 31.139	2.793 to 55.022
no. of refns collected	103679	45017
no. of unique refns	24544	9759
no. of obsd refns (<i>I</i> > 2σ(<i>I</i>))	18946	6756
No. of params	812	527
Final R, R _w (<i>I</i> > 2σ(<i>I</i>))	0.0337, 0.0793	0.0674, 0.1511
Goodness-of-fit on <i>F</i> ²	1.053	1.048
Δρ _{max, min} , eÅ ⁻³	1.014, -0.854	0.979, -2.591

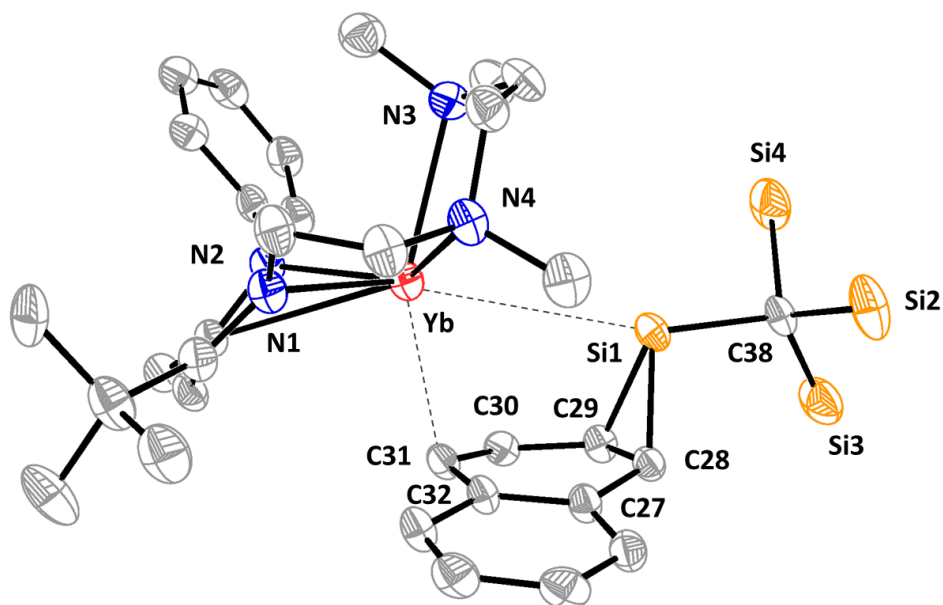


Figure S1. Molecular structure of **2** with thermal ellipsoids set at 30% probability level. For the clarity, SiMe₃ group is represented by one Si atom, isopropyl groups of DIPP and hydrogen atoms are omitted. Selected bond distances [Å] and angles [°]: Yb–Si1 3.718(3), Yb–N1 2.429(6), Yb–N2 2.376(5), Yb–C30 3.428(10), Yb–C31 2.765(7), Yb–C32 3.126(6), C28–C29 1.541(9), C31–C32 1.475(9), C30–C31 1.368(9), C29–C30 1.441(9), C28–C37 1.497(8), Si1–C38 1.999(7), C38–Si2 1.900(7), C38–Si3 1.907(7), C38–Si4 1.857(7); Yb–Si1–C38 162.1(3), C28–Si1–C29 46.7(3).

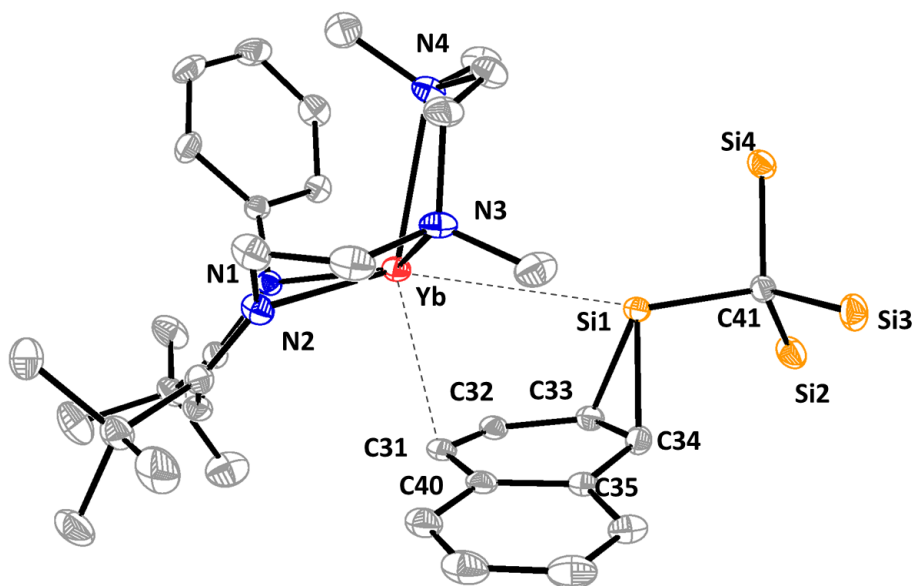


Figure S2. Molecular structure of **3** with thermal ellipsoids set at 30% probability level. For the clarity, SiMe₃ group is represented by one Si atom, isopropyl groups of DIPP and hydrogen atoms are omitted. Selected bond distances [Å] and angles [°]: Yb–Si1 3.6149(12), Yb–N1 2.432(3), Yb–N2 2.404(3), Yb–C31 2.758(4), Yb–C32 3.222(4), Yb–C40 3.293(4), C32–C33 1.454(6), C33–C34 1.535(6), C31–C32 1.348(6), C31–C40 1.457(6), Si1–C41 2.009(4), C41–Si2 1.886(4), C41–Si3 1.903(4), C41–Si4 1.903(4); Yb–Si1–C41 161.73(14), C33–Si1–C34 46.2(2).

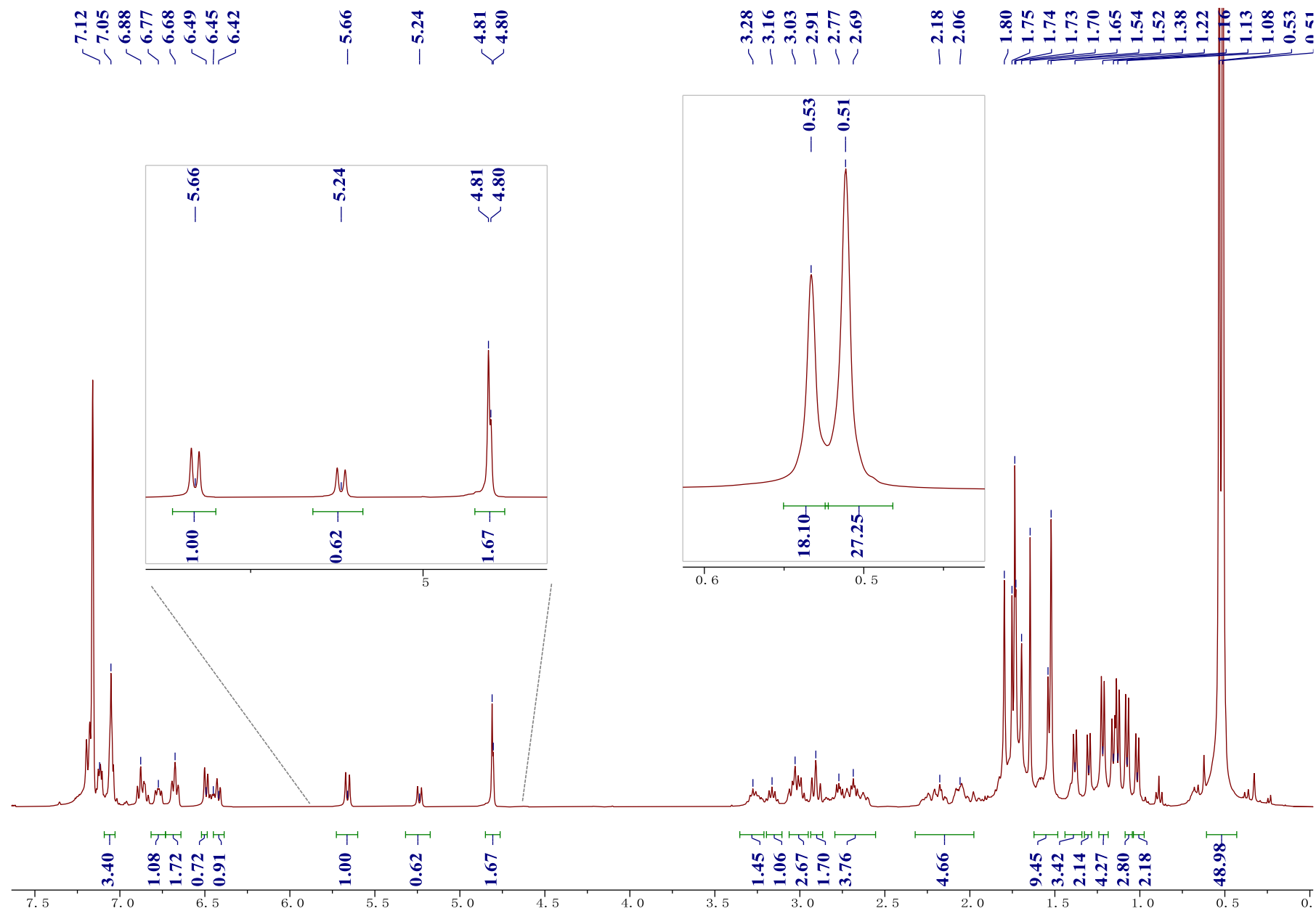


Figure S3. ^1H NMR of complex **1** (400 MHz, C_6D_6 , 25 $^\circ\text{C}$).

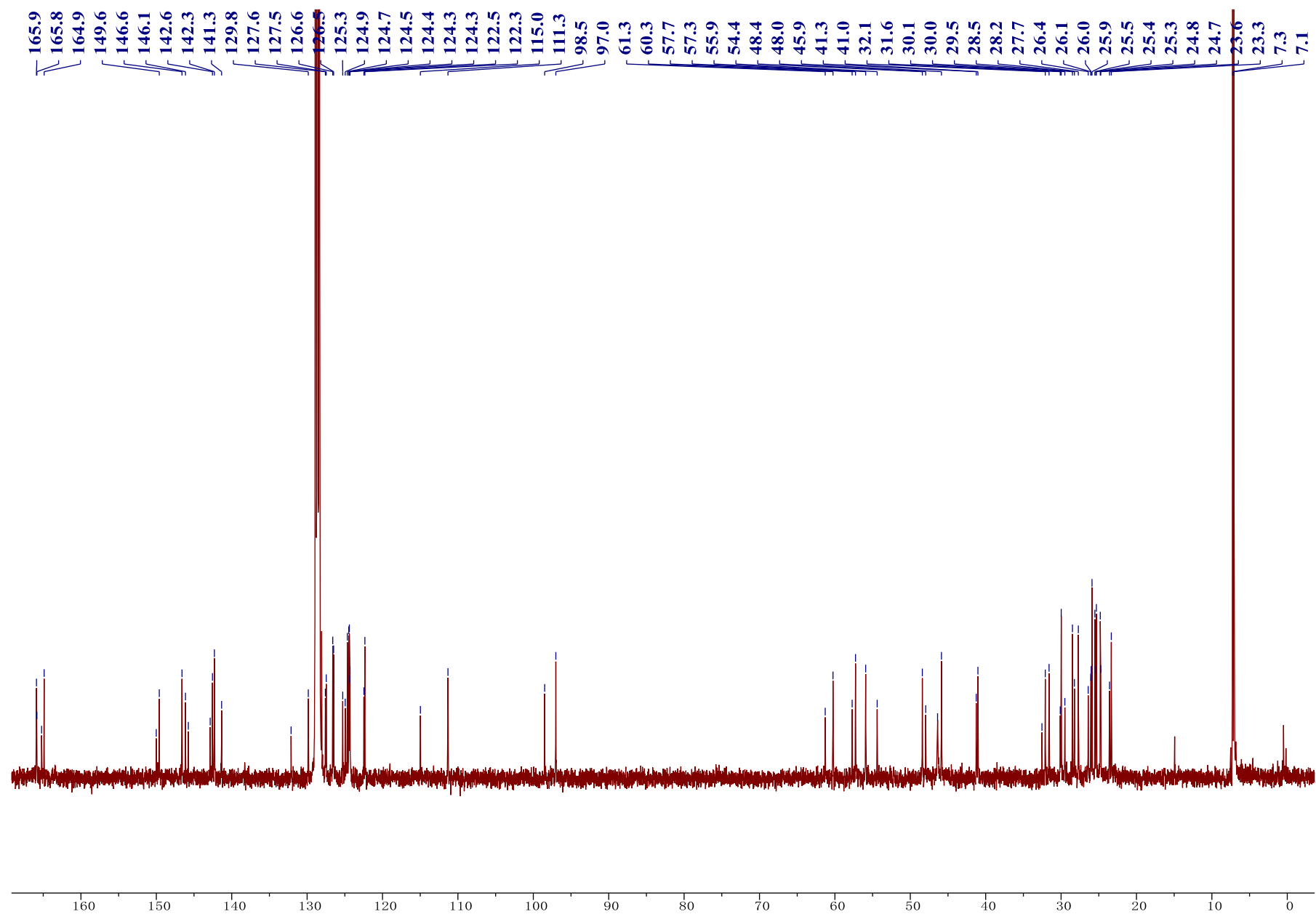


Figure S4. $^{13}\text{C}\{^1\text{H}\}$ NMR of complex **1** (100 MHz, C_6D_6 , 25 °C).

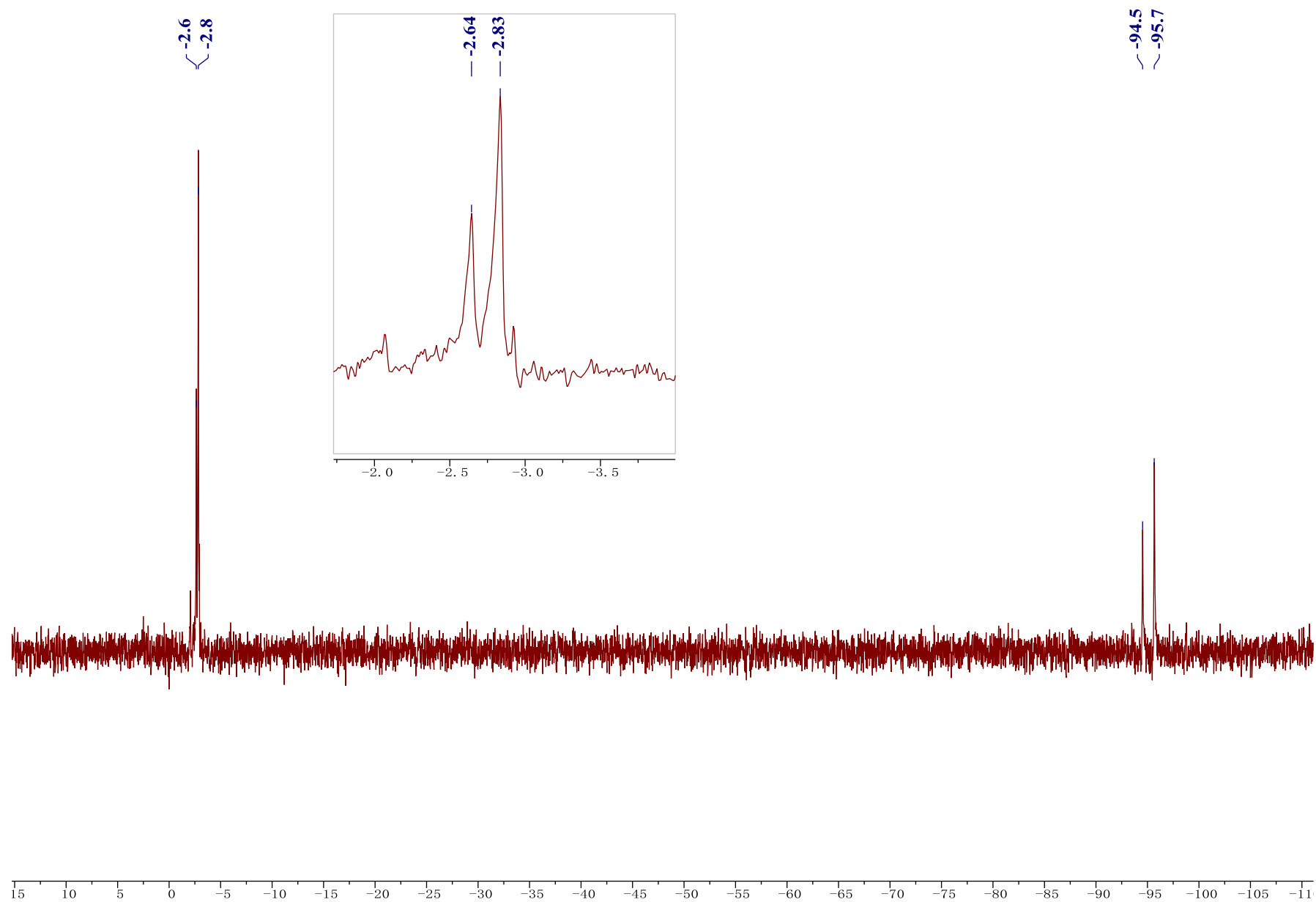


Figure S5. $^{29}\text{Si}\{^1\text{H}\}$ NMR of complex **1** (80 MHz, C_6D_6 , 25 °C).

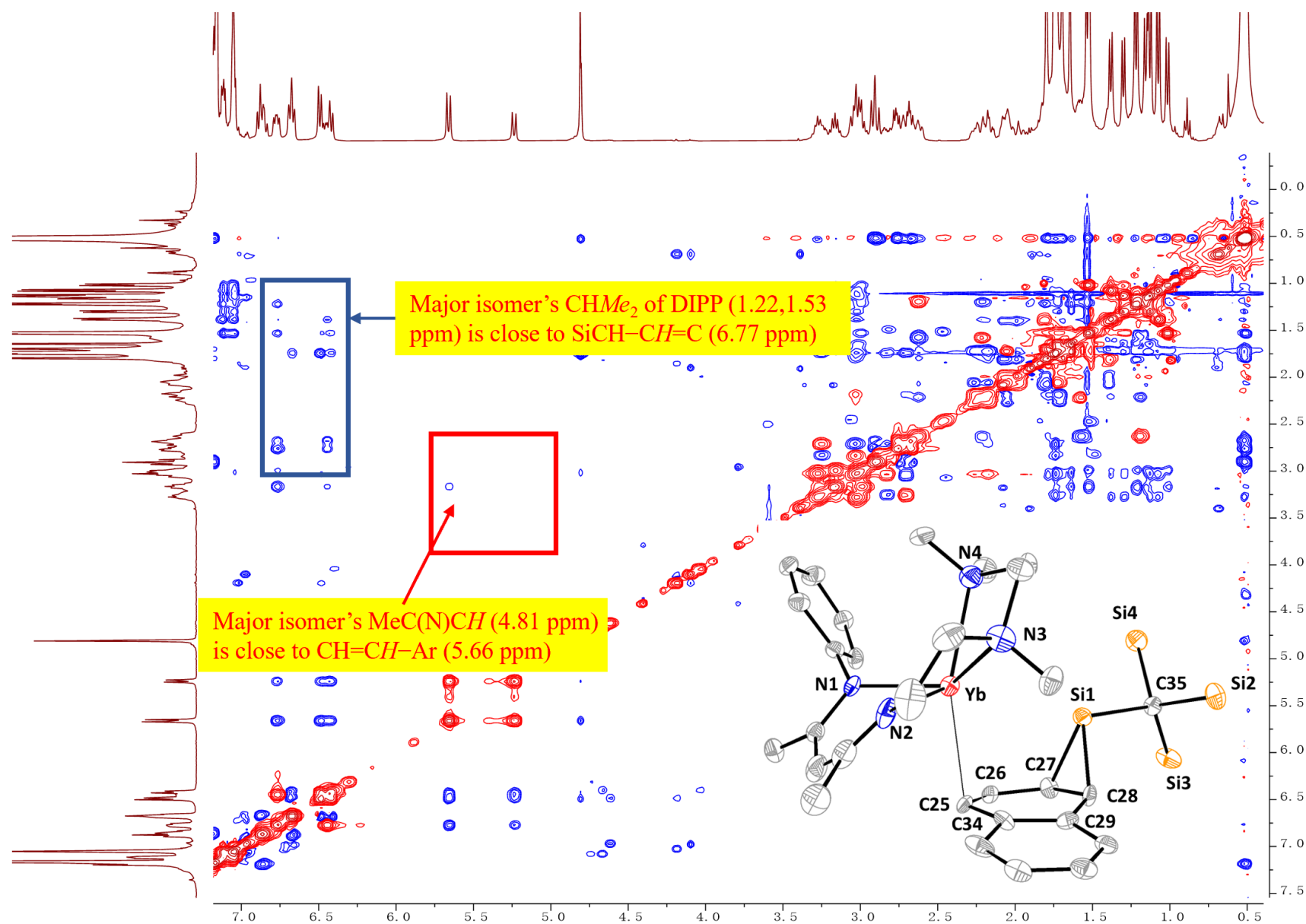


Figure S6. ^1H - ^1H NOESY spectrum of complex **1** (400 MHz, C_6D_6 , 25 $^\circ\text{C}$).

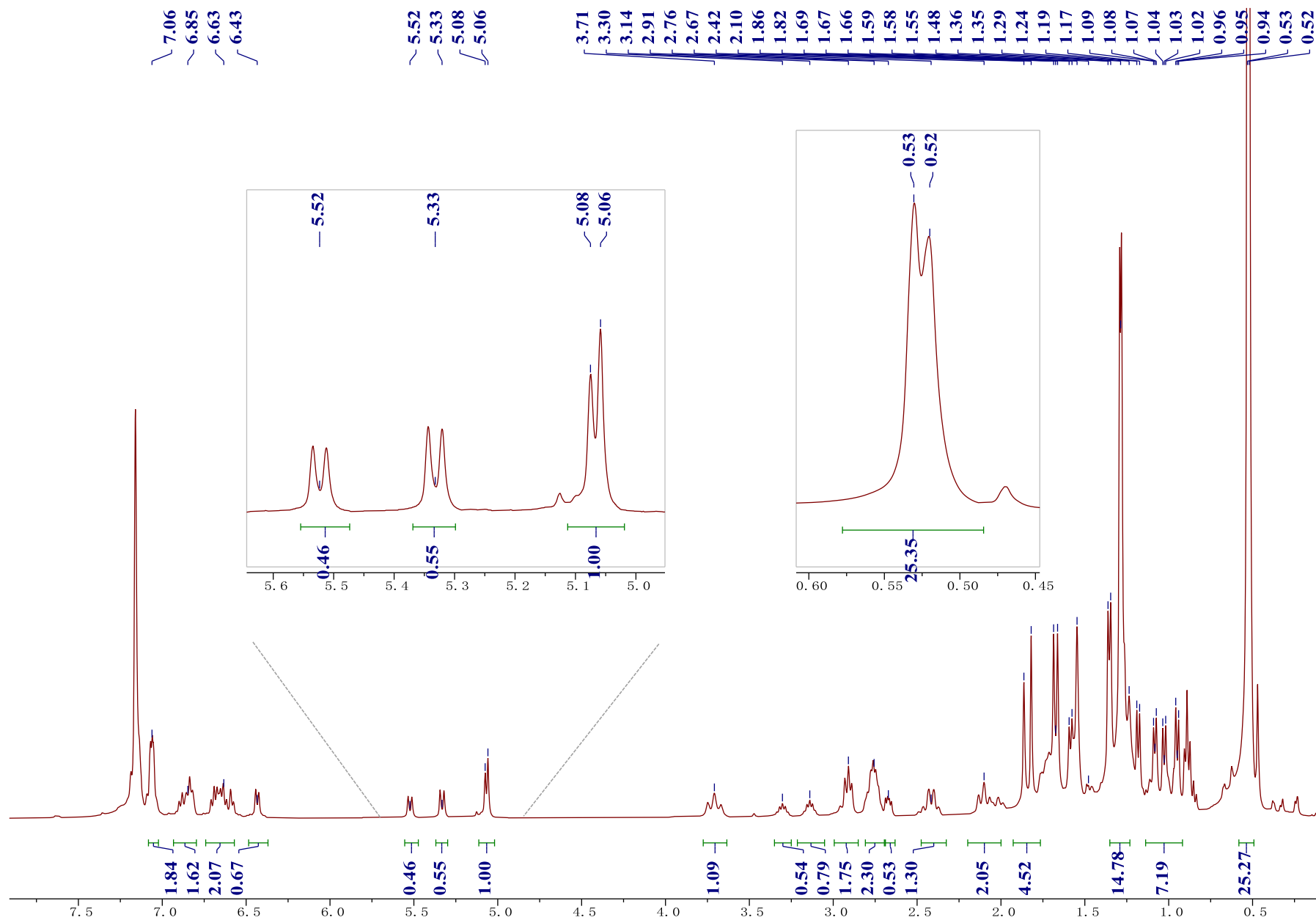


Figure S7. ^1H NMR of complex **2** (400 MHz, C_6D_6 , 25 °C).

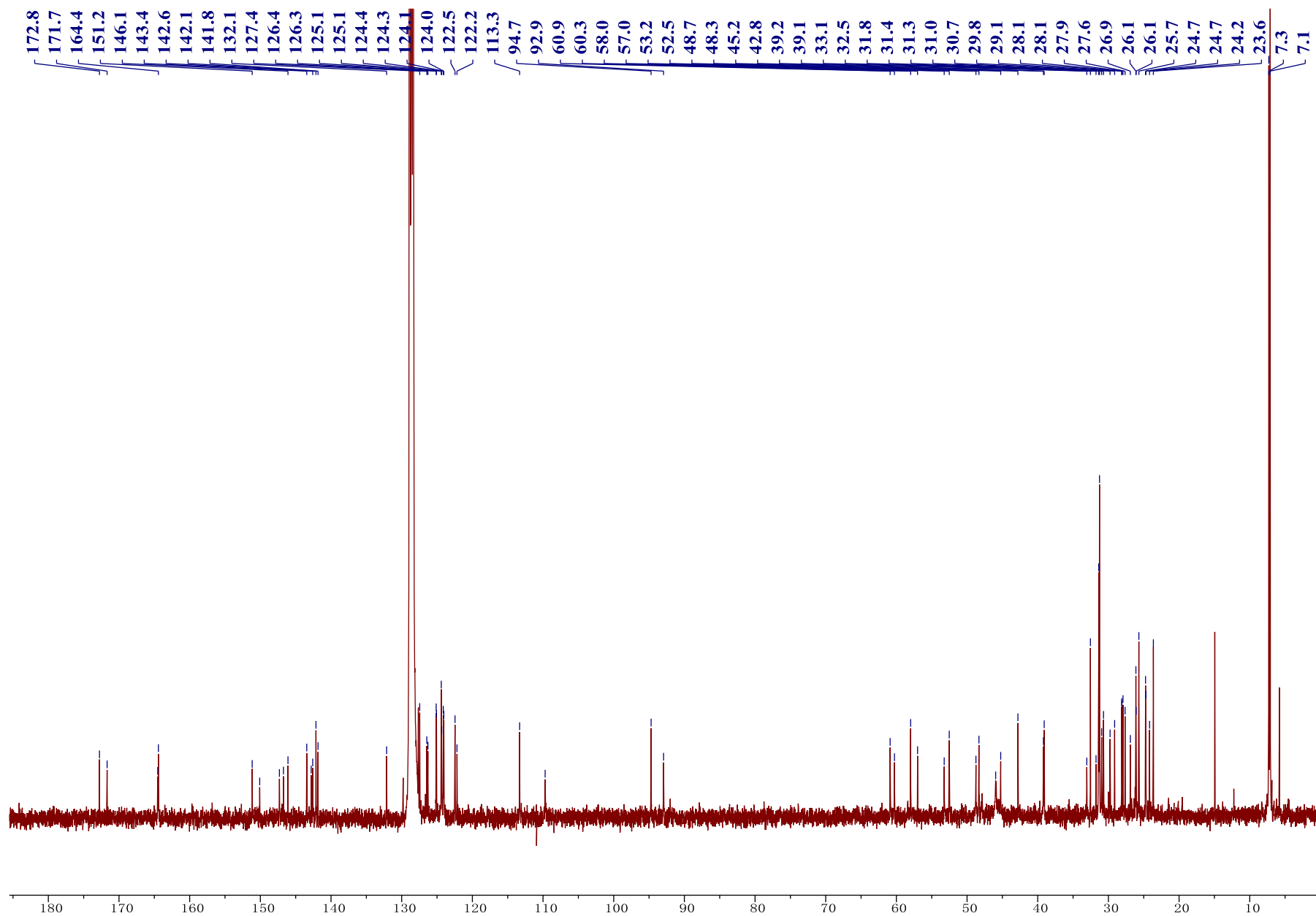


Figure S8. $^{13}\text{C}\{^1\text{H}\}$ NMR of complex **2** (100 MHz, C_6D_6 , 25 °C).

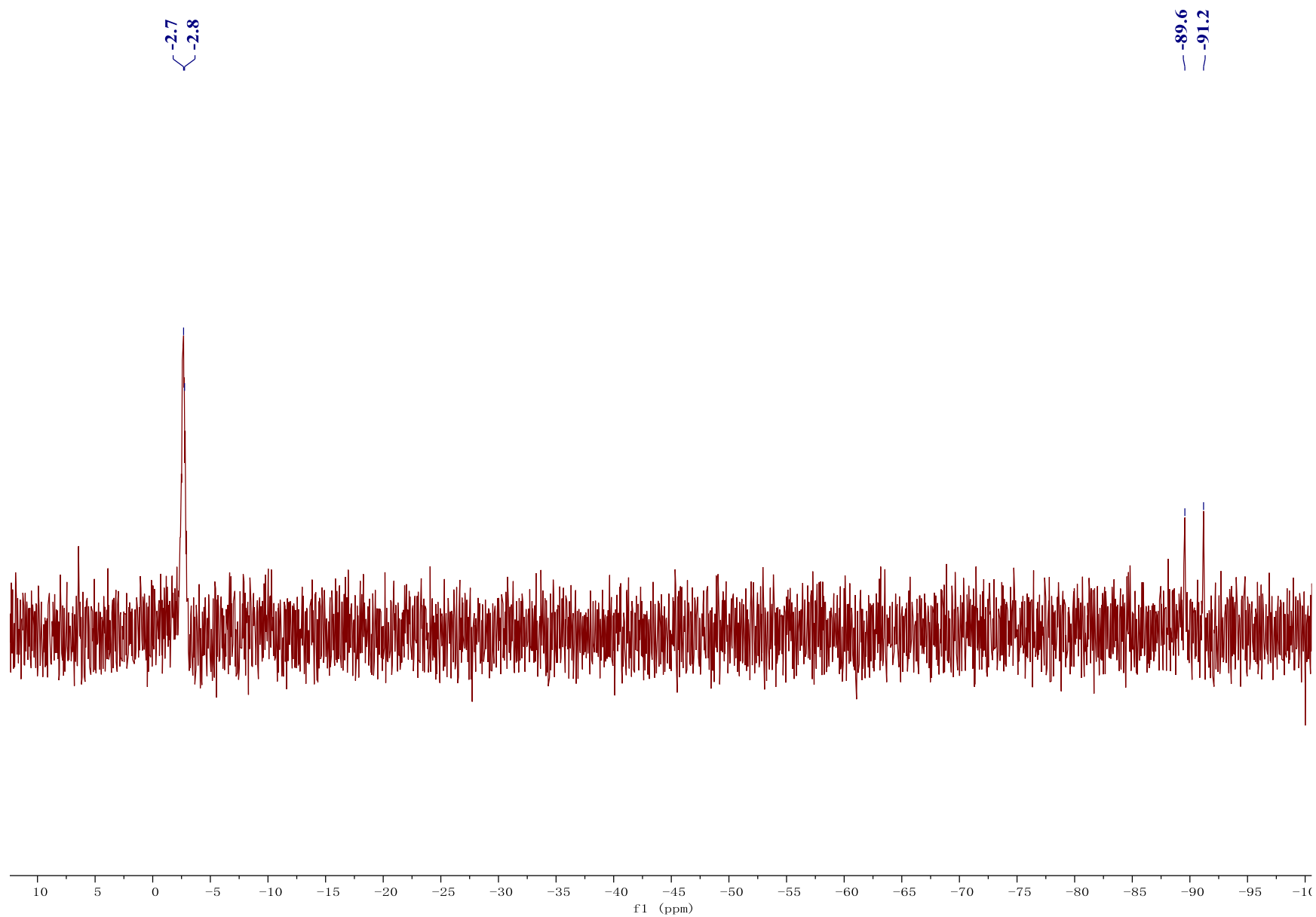


Figure S9. $^{29}\text{Si}\{^1\text{H}\}$ NMR of complex **2** (80 MHz, C_6D_6 , 25 °C).

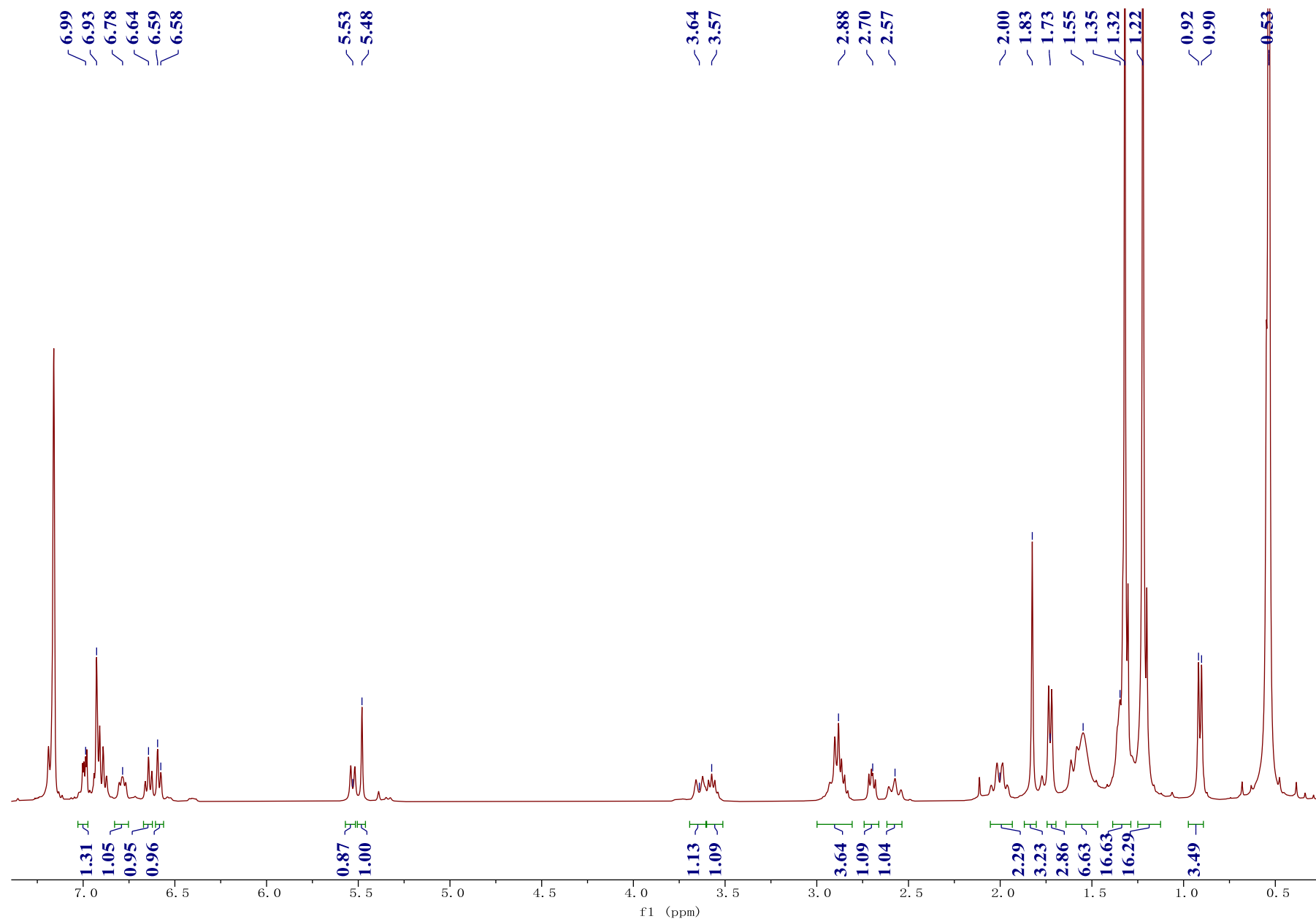


Figure S10. ^1H NMR of complex **3** (400 MHz, C_6D_6 , 25°C)

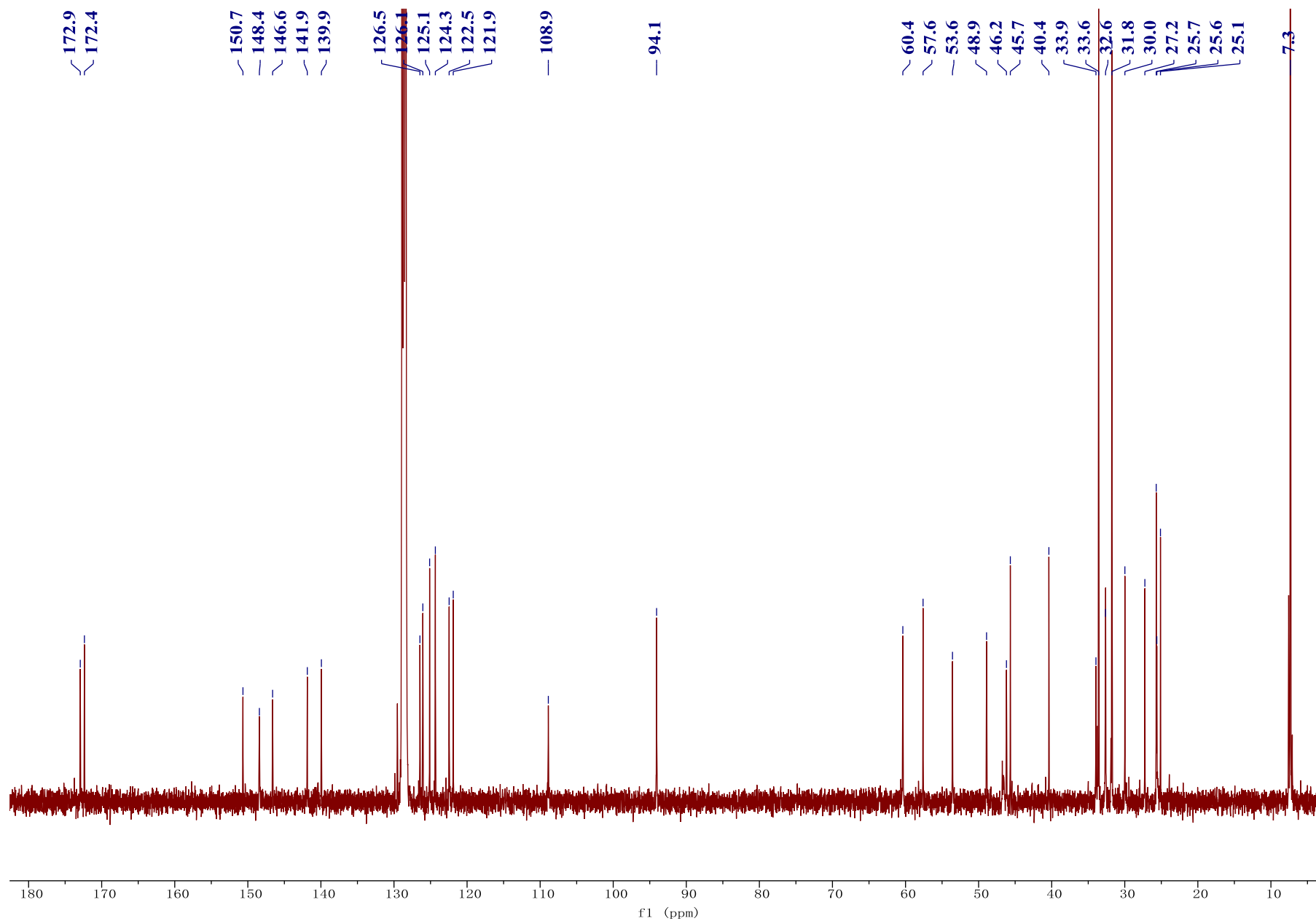


Figure S11. $^{13}\text{C}\{^1\text{H}\}$ NMR of complex **3** (100 MHz, C_6D_6 , 25 $^\circ\text{C}$).

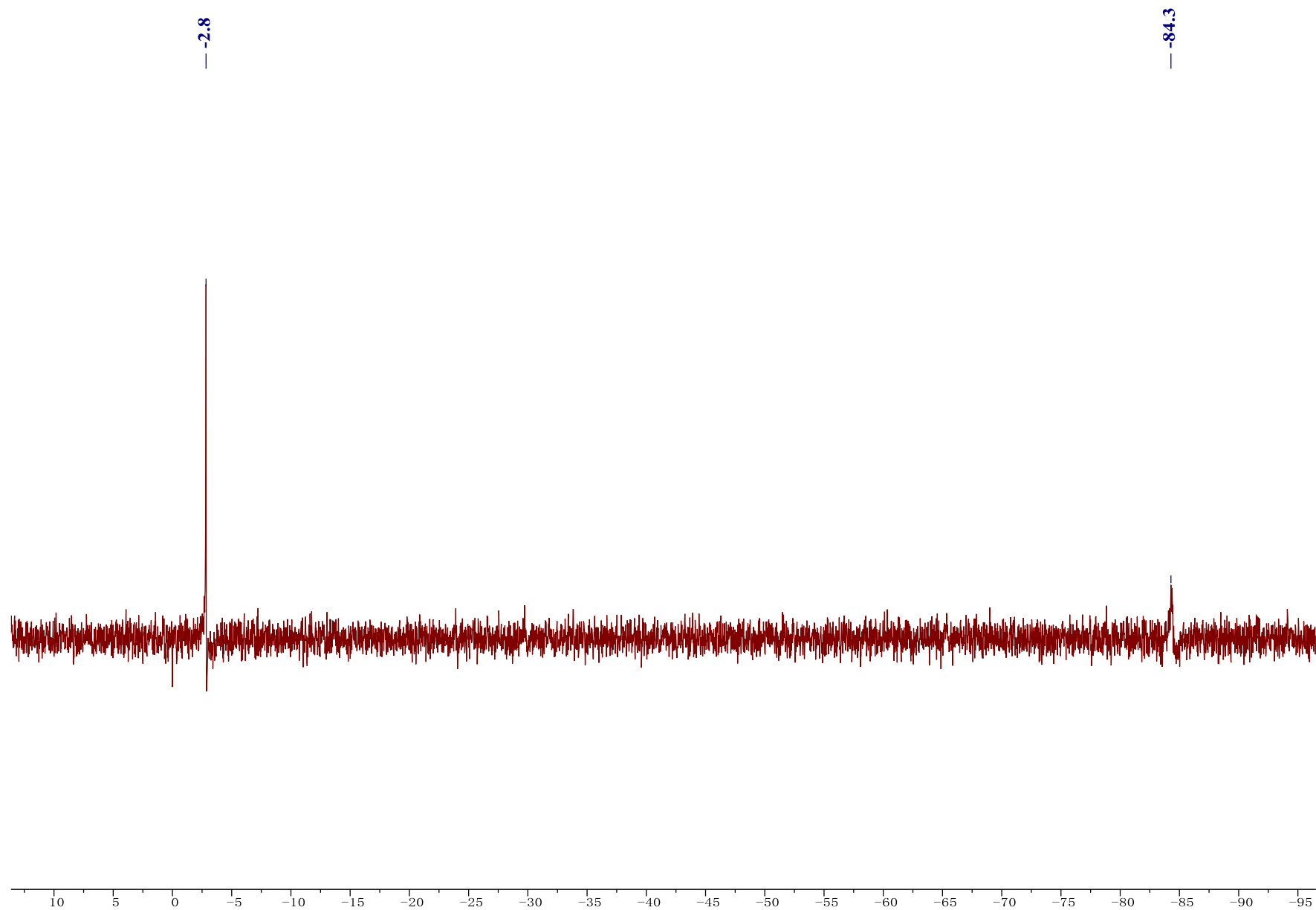


Figure S12. $^{29}\text{Si}\{^1\text{H}\}$ NMR of complex **3** (80 MHz, C_6D_6 , 25 °C).

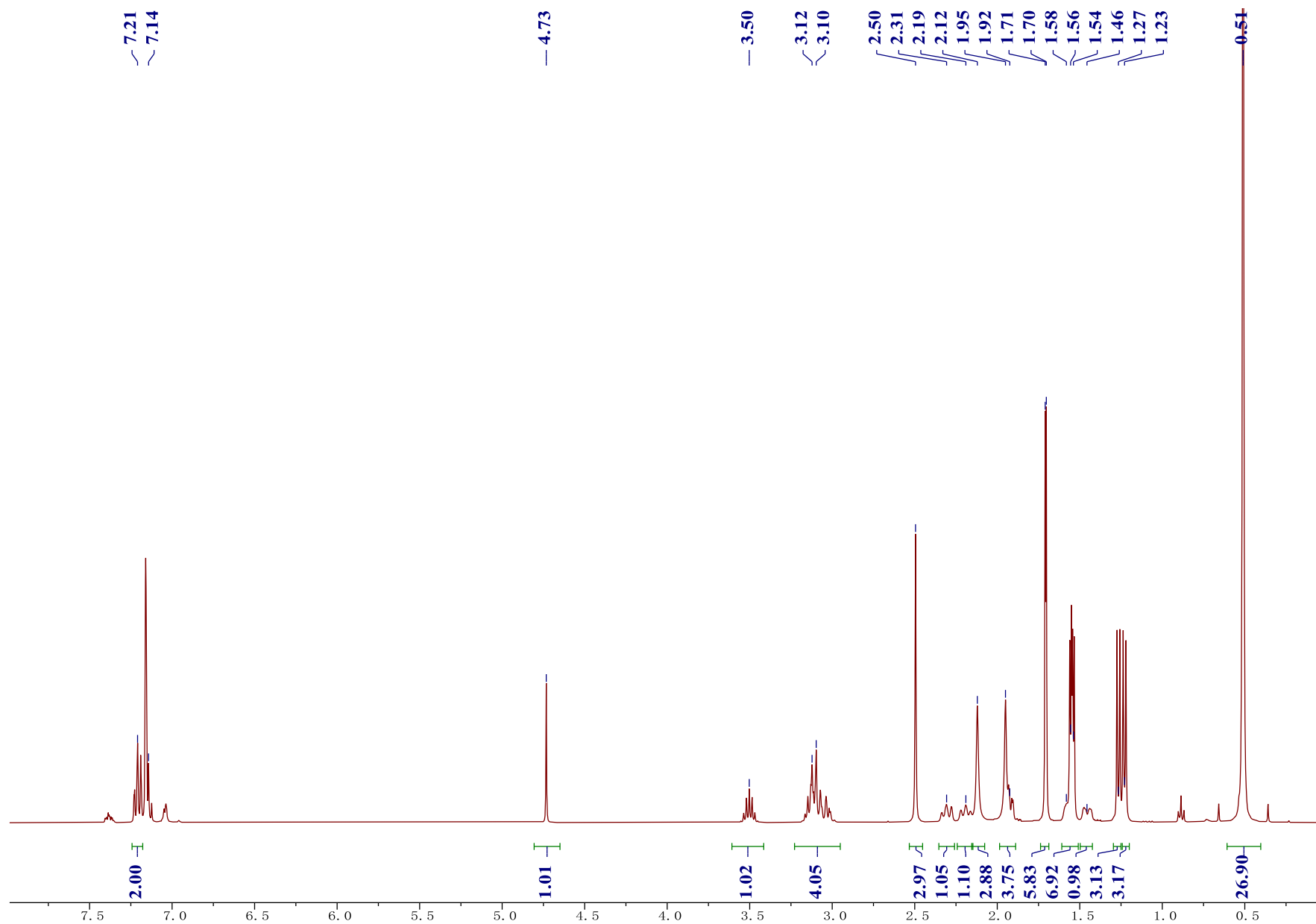


Figure S13. ¹H NMR of complex 4 (400 MHz, CDCl₃, 25 °C)

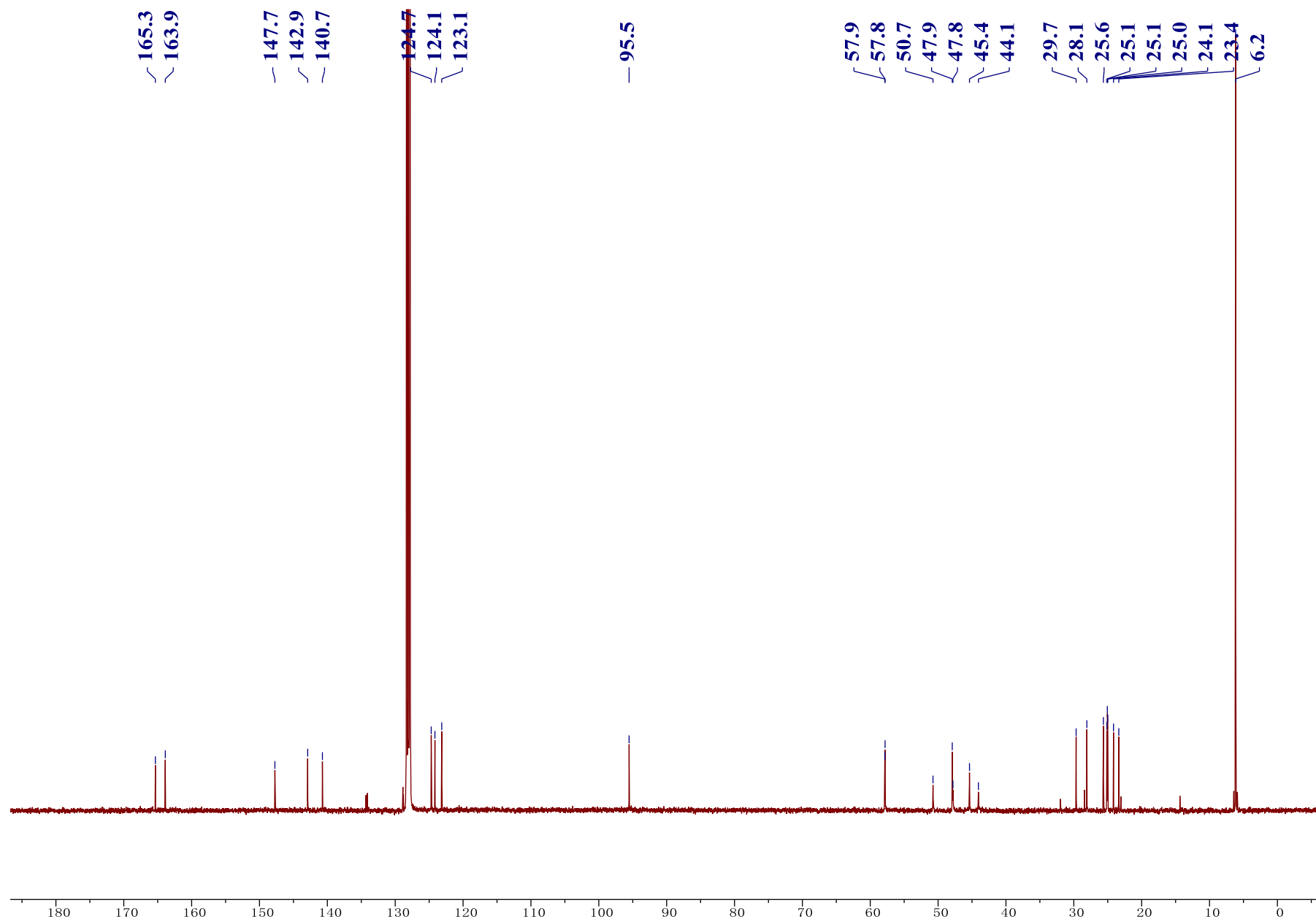


Figure S14. $^{13}\text{C}\{^1\text{H}\}$ NMR of complex **4** (100 MHz, C_6D_6 , 25 °C).

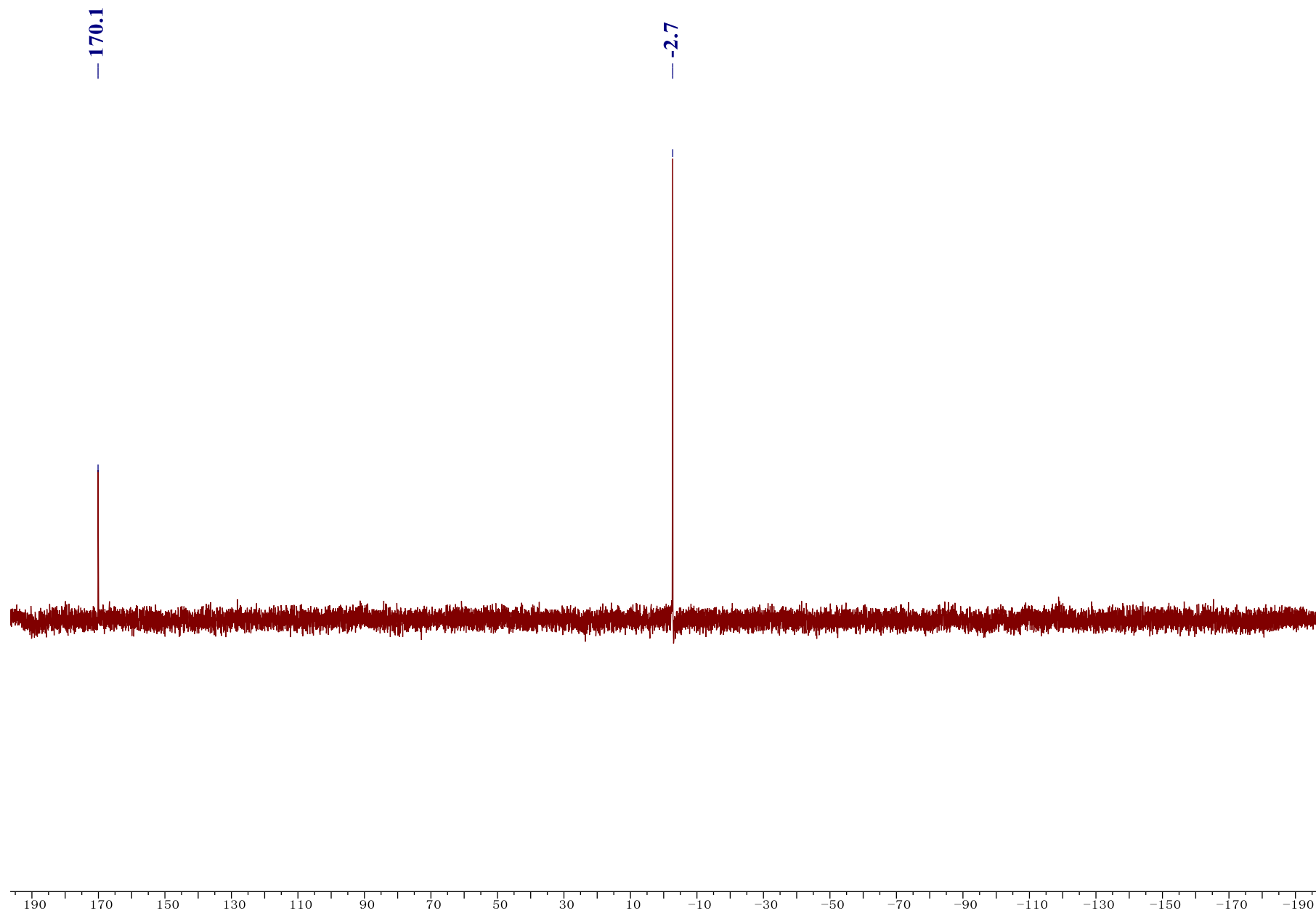


Figure S15. $^{29}\text{Si}\{^1\text{H}\}$ NMR of complex **4** (80 MHz, C_6D_6 , 25 °C).

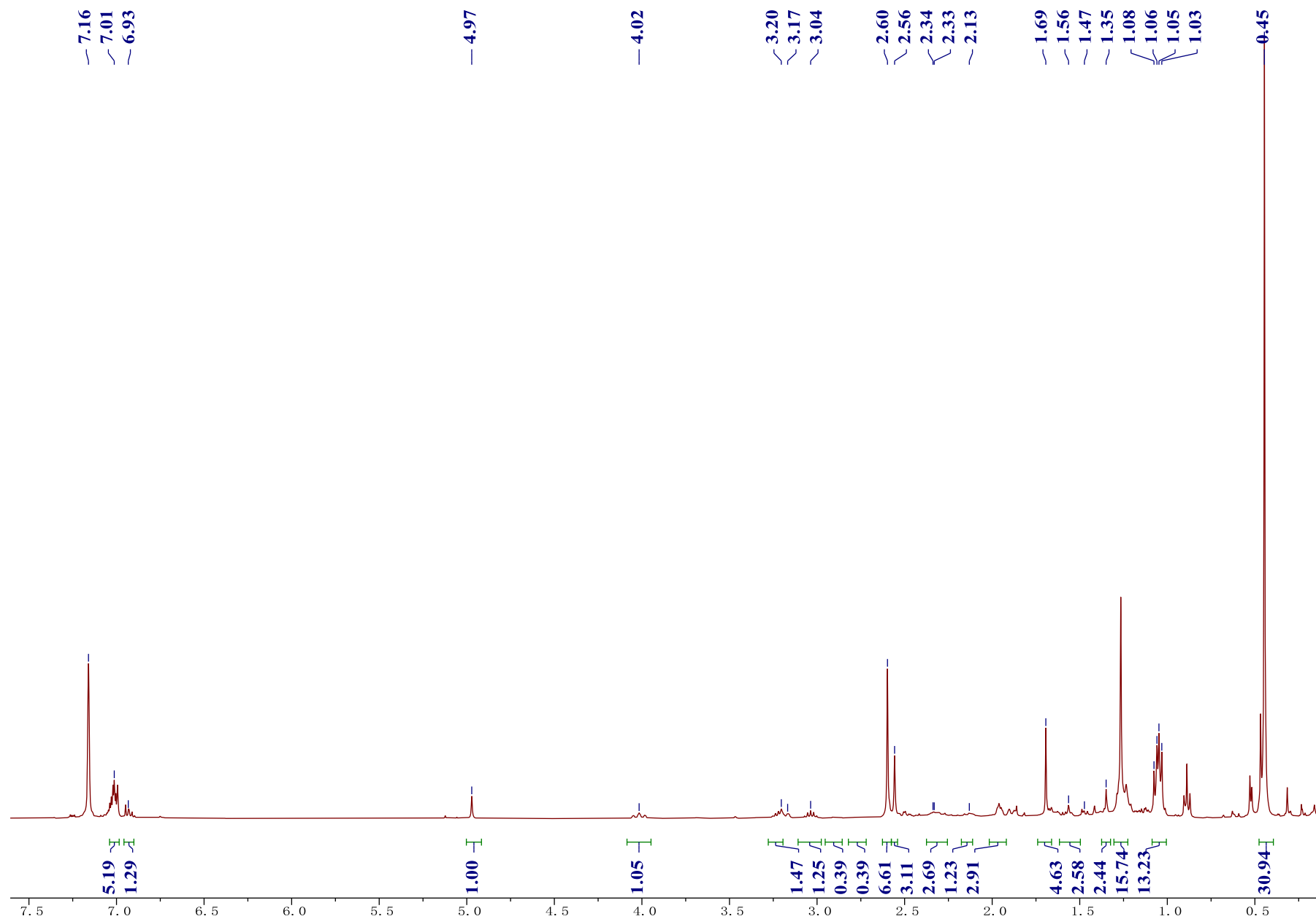


Figure S16. ^1H NMR of complex **5** (400 MHz, C_6D_6 , 25 $^\circ\text{C}$)

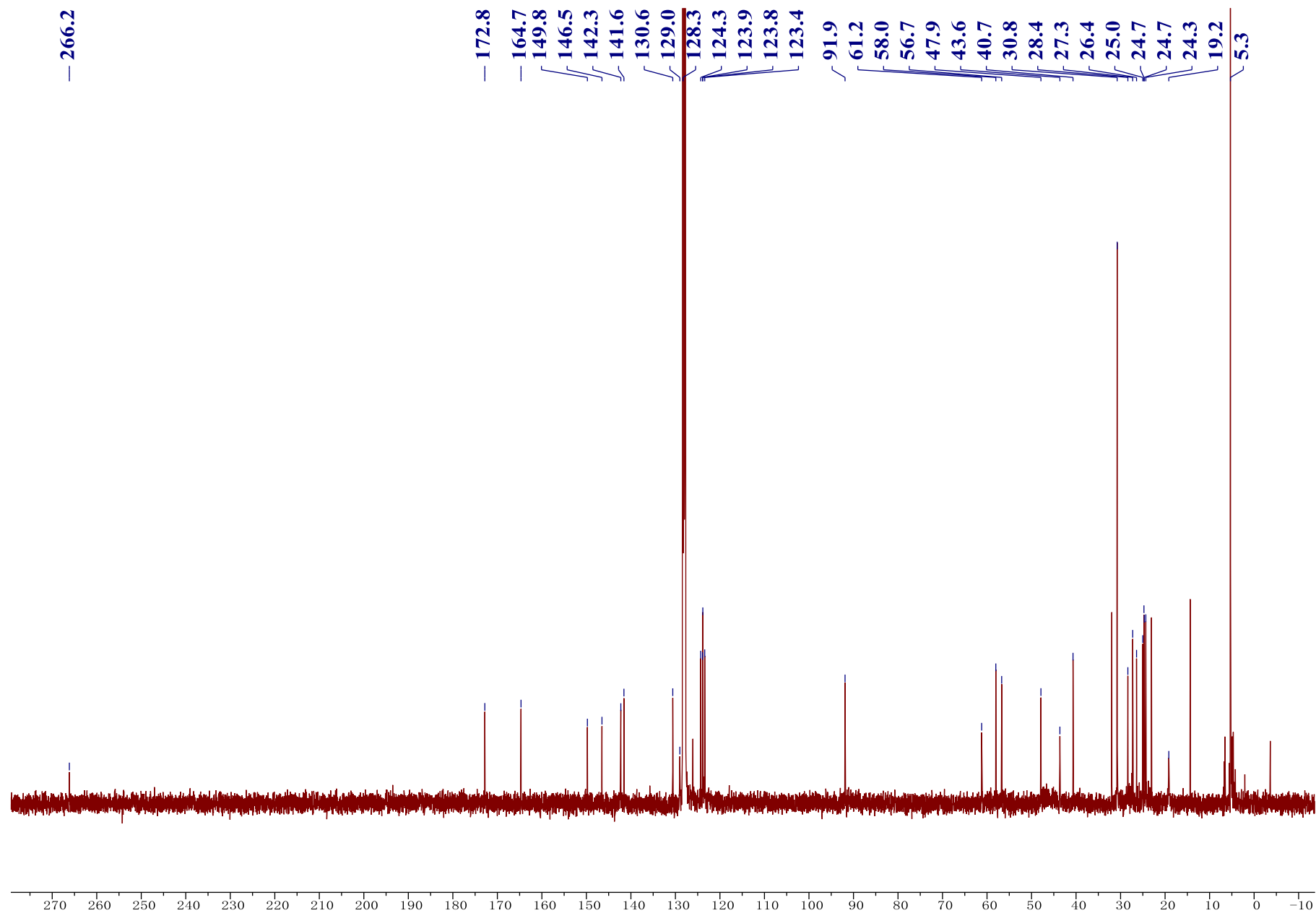


Figure S17. $^{13}\text{C}\{^1\text{H}\}$ NMR of complex **5** (100 MHz, C_6D_6 , 25 °C).

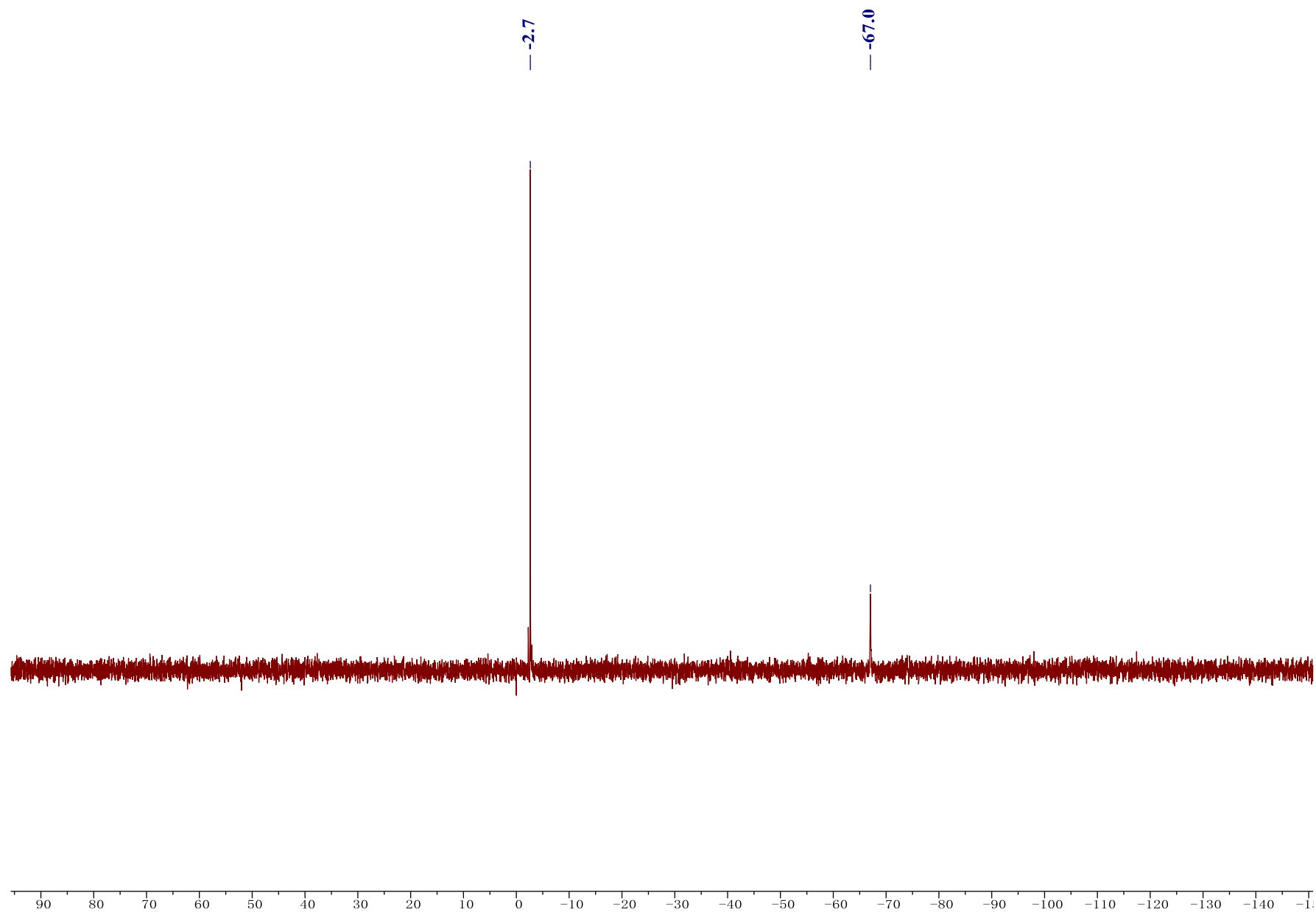


Figure S18. $^{29}\text{Si}\{^1\text{H}\}$ NMR of complex **5** (80 MHz, C_6D_6 , 25 °C).

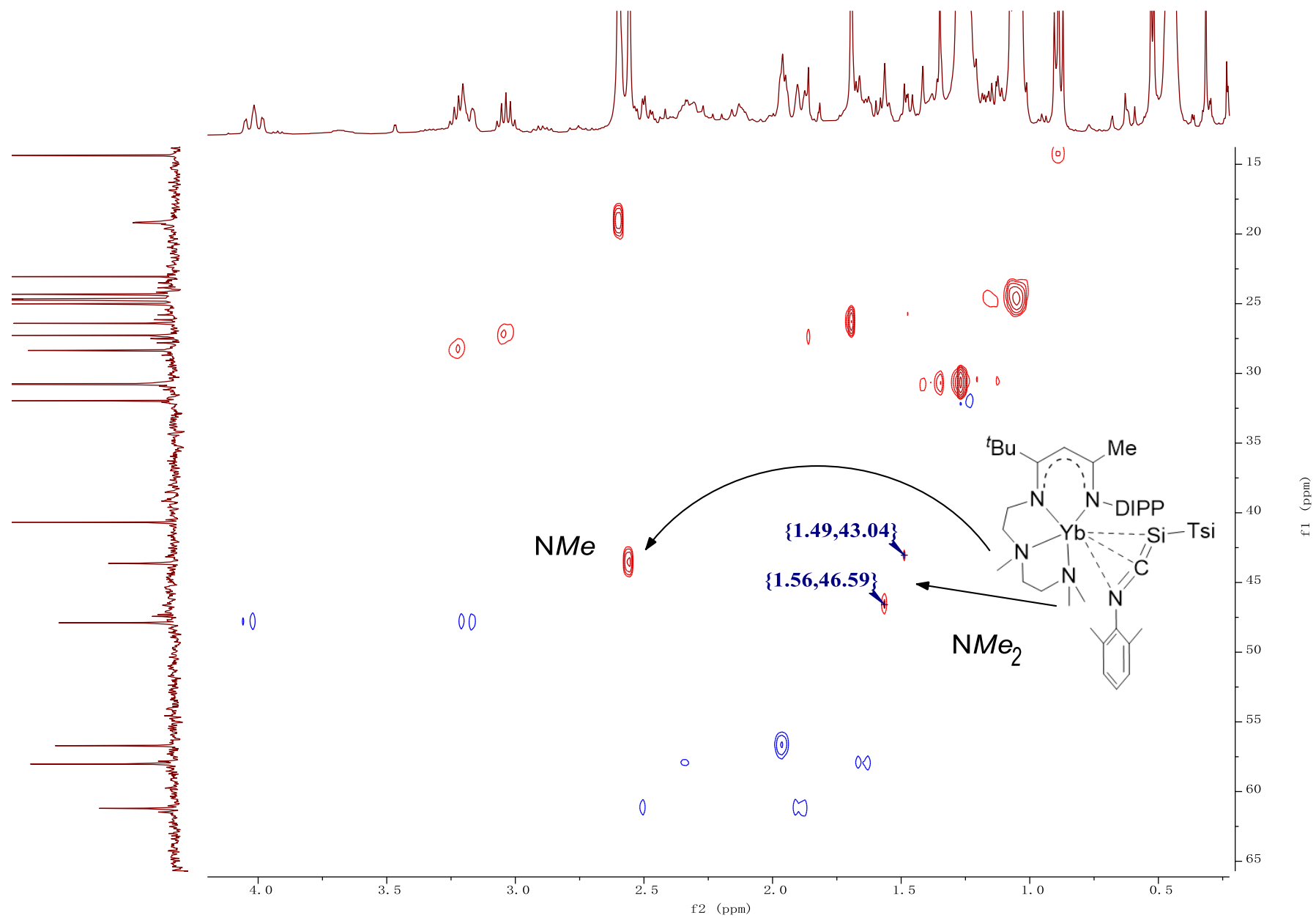


Figure S19. gHSQC NMR of complex **5** (400 MHz, C₆D₆, 25 °C).

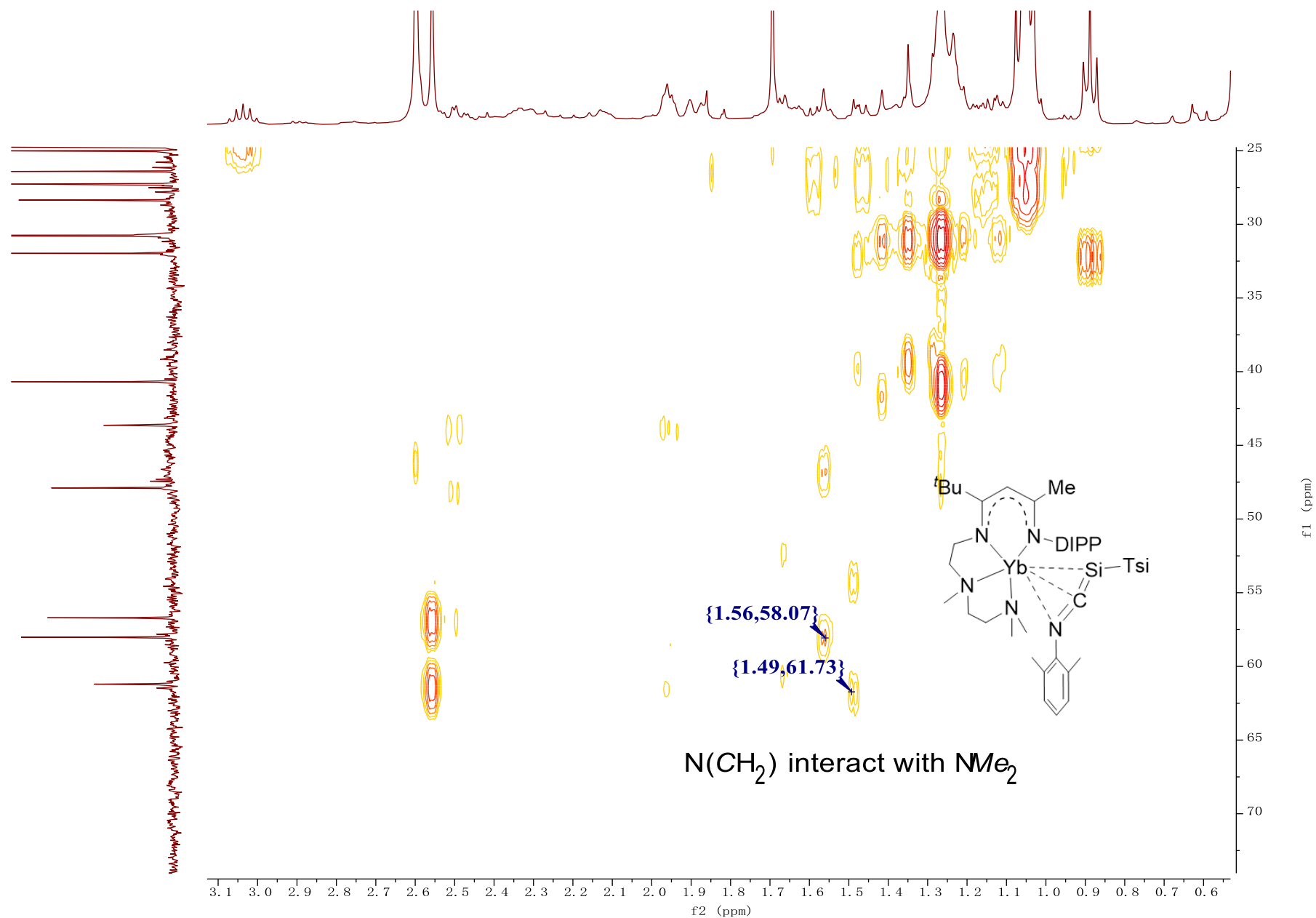
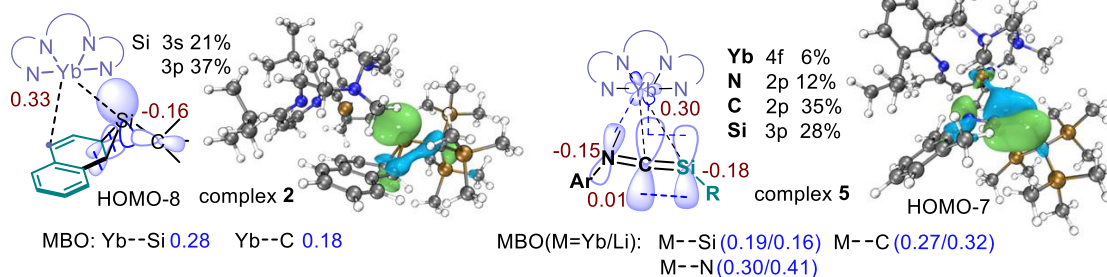


Figure S20. HMBC NMR of complex **5** (400 MHz, C₆D₆, 25 °C).

Computational Details

All DFT calculations were carried out with Gaussian 09 program⁷ and structures were displayed by CYLview software.⁸ B3LYP level of density functional theory,⁹ which has been successfully applied to propose the reaction mechanism,⁴ was used to locate all the intermediates and transition states, as well as calculating the corresponding single point energy. The relativistic effective core potential SDD was used on ytterbium atom.¹⁰ For other atoms, 6-31G(d) basis set was used to perform geometry optimizations.¹¹ Grimme's DFT-D3 dispersion correction was also considered in all of the calculations.¹² Frequency analysis at the same level of geometry optimizations has been performed to confirm each stationary point to be either a minimum (no imaginary frequency) or a transition structure (only one imaginary frequency). Single point energies were further calculated with the SMD solvation model (toluene solvent) on optimized geometries,¹³ using a mixed basis set of SDD for ytterbium and larger 6-311+G(d,p) for rest atoms.^{10,11} Cube files of orbital wavefunctions were generated by using Multiwfn 3.8(dev),¹⁴ then the frontier molecular orbital isosurfaces were displayed by VMD software. (isovalue = ± 0.05).¹⁵ Mayer bond orders and the charge distributions of atomic dipole corrected Hirshfield population(ADCH) calculated by Multiwfn 3.8(dev) were used to analyze structures.^{16,17}

a. Molecular orbitals of complex **2** and **5**



b. The generative mechanism from **2** to **5**

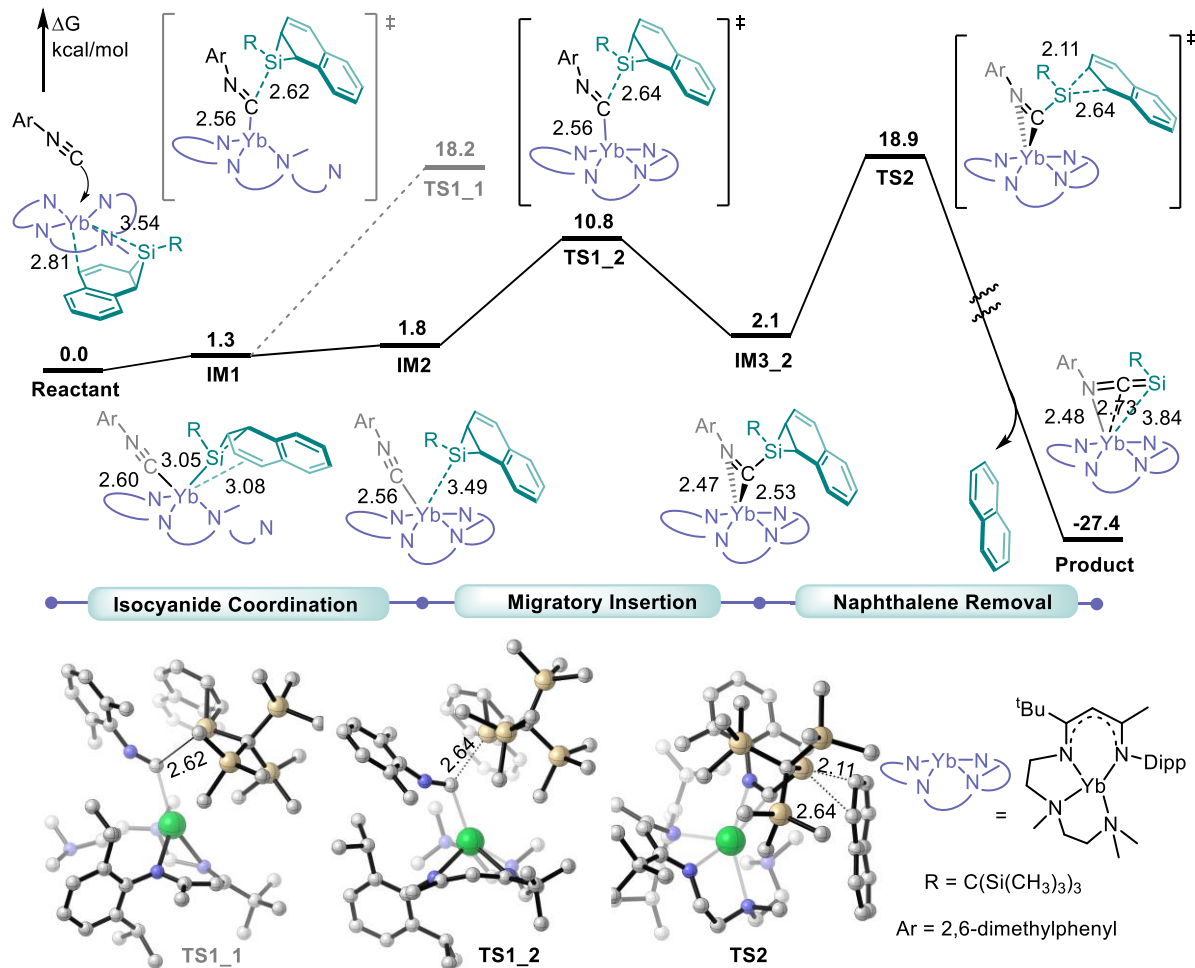


Figure S21. Electronic structures of **2** and **5**, free energy profile of mechanism from complex **2** with isocyanide reactant at SMD-B3LYP-D3/SDD(Yb)/6-311+G(d,p) level of theory. Energy and bond distances were shown in kcal/mol and Å, respectively. The charge distributions of atomic dipole corrected Hirshfeld population (ADCH) shown in dark red, and Mayer bond order shown in blue.

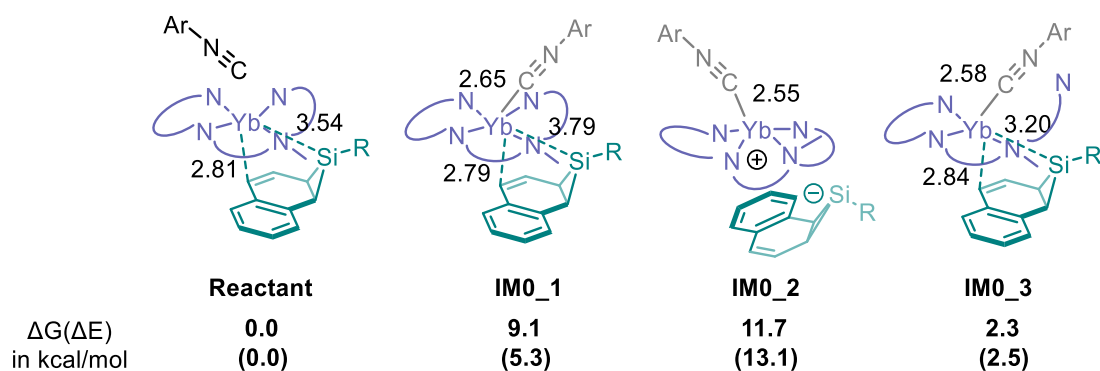


Figure S22. Other unstable intermediates with isocyanide coordination. Two intermediates **IM0_1** and **IM0_2** can be located for the isocyanide directly attacking to Yb centre without the amide dissociation. Note that the silyl substrate had been dissociated in **IM0_2**. The **IM0_3** is the different conformation with the stable **IM1**.

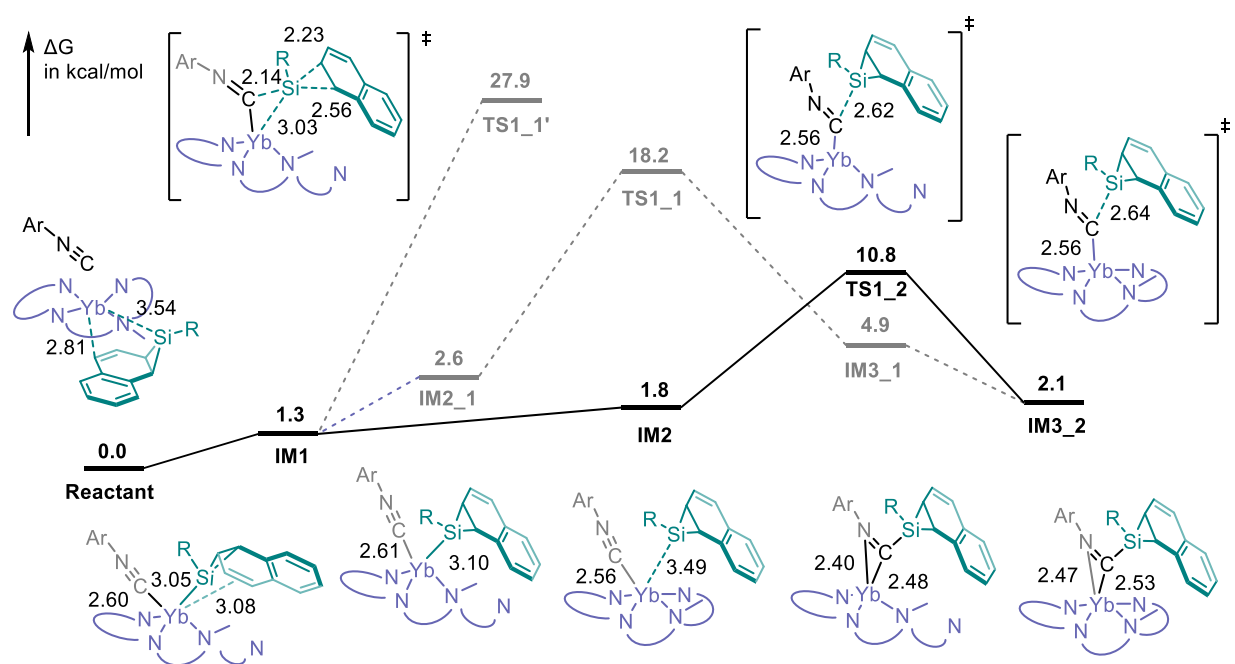


Figure S23. Calculated energy profiles for isocyanide insertion reaction. The **TS1-1'** is the concerted mechanism of migratory insertion and naphthalene removal, which is not available for the highest energy barrier. We can not locate the pathway with naphthalene removal before the migratory insertion.

Table S2. Molecular orbitals, orbital compositions, ADCH charges, MBOs of **2** and **5**.

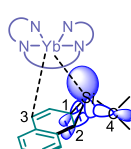
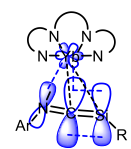
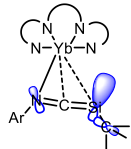
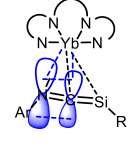
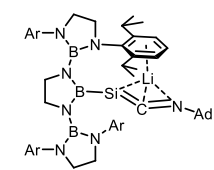
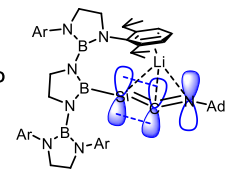
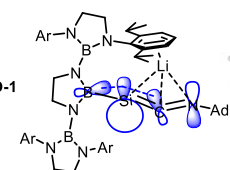
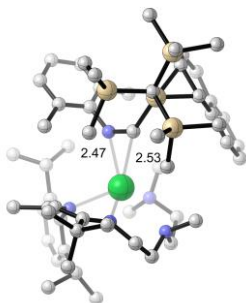
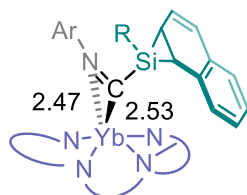
complex 2					
Molecular orbitals		Orbital composition	ADCH charge		MBO
HOMO-8		Si 3s 21.3%	Yb 0.33	Yb-Si 0.28	
		3p 37.1%	Si -0.16	Yb-C3 0.18	
		C1 2p 6.7%	C1 -0.13	Si-C2 0.67	
		C2 2p 5.3%	C2 -0.09	Si-C1 0.73	
		C4 2p 10.0%	C3 -0.23		
complex 5					
Molecular orbitals		Orbital composition	ADCH charge		MBO
HOMO-7		Yb 4f 5.8%			
		N 2p 11.6%			
		C 2p 34.6%			
		Si 3p 27.7%			
HOMO-9		N 2p 8.5%	Yb 0.30	Yb-Si 0.19	
		Si 3s 20.7%	Si -0.18	Yb-C 0.27	
		3p 32.1%	C 0.01	Yb-N 0.30	
		C 2p 13.1%	N -0.15	N-C 1.47	
HOMO-28		N 2p 19.6%		Si-C 1.53	
		C 2p 12.9%			
complex 					
Molecular orbitals		Orbital composition	ADCH charge		MBO
HOMO		Si 3p 35.2%	Li 0.12	Li-Si 0.16	
		N 2p 15.6%	Si -0.18	Li-C 0.32	
		C 2p 28.3%	C 0.04	Li-N 0.41	
HOMO-1		Si 3s 14.9%	N -0.16	Si-C 1.53	
		3p 38.1%		C-N 1.36	
		N 2p 11.6%			
		C 2p 8.2%			

Table S3. Structures, electron energies and imaginary vibrational frequencies of calculated stationary points.

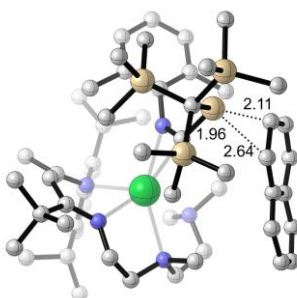
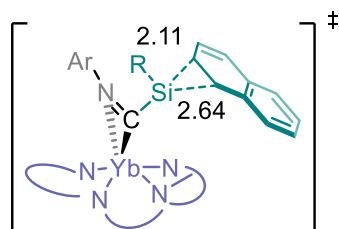
		E = -4780.235932 au E_{SMD} = -4781.079756 au
Reactant		
		E = -4780.240496 au E_{SMD} = -4781.078232 au
IM1		
		E = -4780.241603 au E_{SMD} = -4781.083111 au
IM2		
		E = -4780.225436 au E_{SMD} = -4781.067838 au Frequency = -92.13 cm⁻¹
TS1_2		



E = -4780.250719 au

E_{SMD} = -4781.088241 au

IM3_2

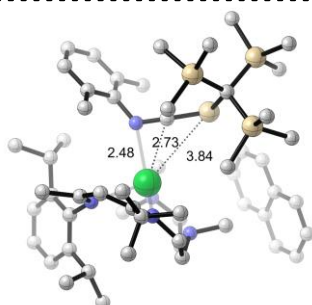
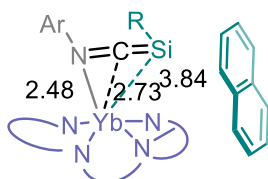


E = -4780.221542 au

E_{SMD} = -4781.059766 au

Frequency = -142.52 cm⁻¹

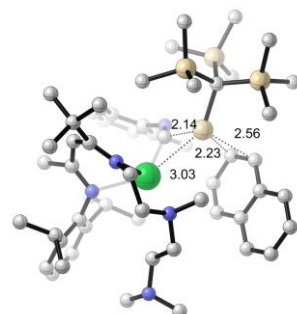
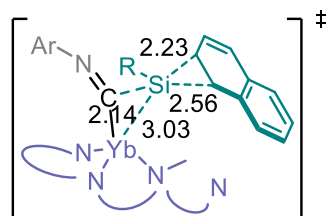
TS2



E = -4780.281536 au

E_{SMD} = -4781.124132 au

Product

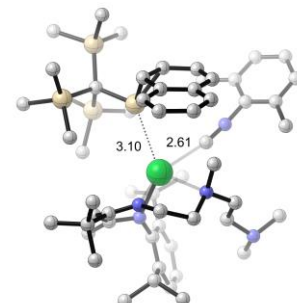
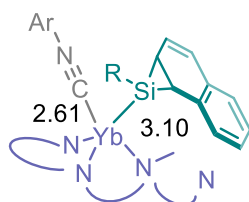


E = -4780.200799 au

E_{SMD} = -4781.040009 au

Frequency = -184.34 cm⁻¹

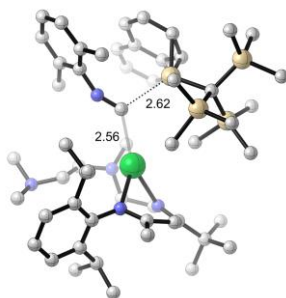
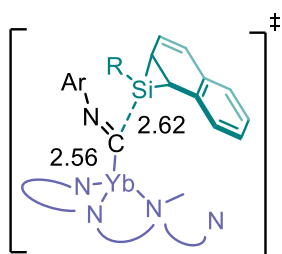
TS1_1'



E = -4780.234229 au

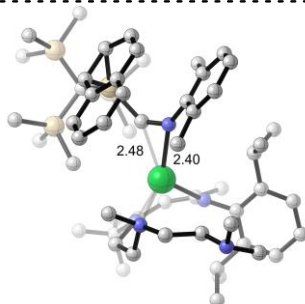
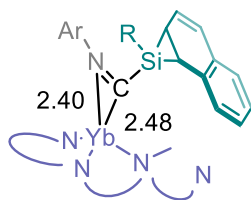
E_{SMD} = -4781.077555 au

IM2_1 S35



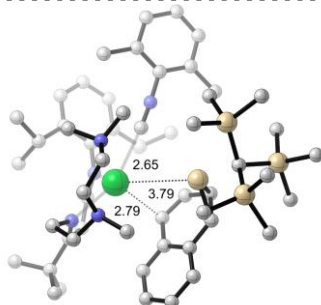
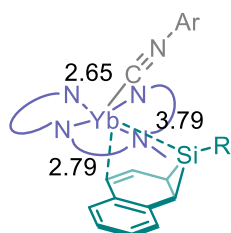
E = -4780.20056 au
 E_{SMD} = -4781.047293 au
 Frequency = -104.44 cm^{-1}

TS1_1



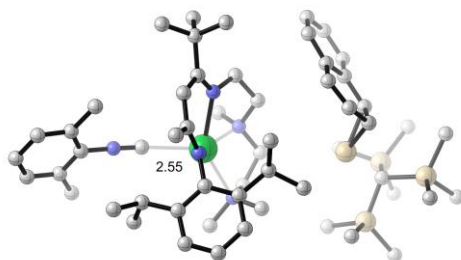
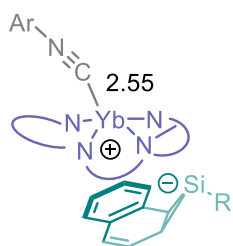
E = -4780.236008 au
 E_{SMD} = -4781.076604 au

IM3_1



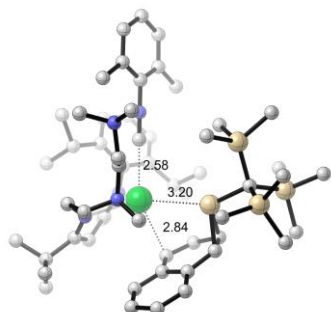
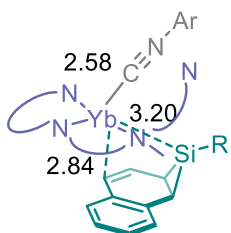
E = -4780.230109 au
 E_{SMD} = -4781.071283 au

IM0_1



E = -4780.205401 au
 E_{SMD} = -4781.058838 au

IM0_2



E = -4780.237008 au
 E_{SMD} = -4781.075829 au

IM0_3

E: Optimized electronic energy under B3LYP-D3/SDD(Yb)/6-31G(d) level of theory.

E_{SMD}: Single point energy at SMD-B3LYP-D3/SDD(Yb)/6-311+G(d,p) level of theory.

Cartesian Coordinates of Optimized Structures

Reactant

Charge=0, Multiplicity=1

Yb	0.10374600	0.46888700	-0.24443300
Si	-3.38400000	0.00719600	0.14507400
Si	-4.69577800	-2.63689900	1.08738200
Si	-6.51599300	-0.80795300	-0.68713700
Si	-5.77475200	0.07409400	2.23618000
N	1.57942100	-0.07569500	-2.10068000
N	2.04091900	1.95508300	-0.03390500
N	0.35003000	1.17555700	2.25382100
N	0.56249400	-1.66482200	1.14777200
C	2.11227900	0.75767200	-4.36791100
H	2.68255400	-0.15170500	-4.57897100
H	2.61668300	1.60337400	-4.84173100
H	1.13195000	0.63347600	-4.84323900
C	1.94299800	0.96366500	-2.86649800
C	2.20117200	2.26346700	-2.39090300
H	2.40418700	2.97663900	-3.17284900
C	2.49769500	2.66720200	-1.05269700
C	3.43096700	3.91842500	-0.89846900
C	2.51258500	2.05369700	1.34314000
H	3.23930300	2.84284800	1.54011700
H	3.02800200	1.11738100	1.59694000
C	1.34268400	2.27010000	2.30539800
H	1.71836600	2.40593300	3.33371100
H	0.82403300	3.18770800	2.01170900
C	0.79842300	-0.00750700	3.02410800
H	0.54932600	0.11869600	4.09085000
H	1.88552100	-0.08205500	2.97316600
C	0.15295200	-1.29935500	2.52268500
H	0.38999100	-2.11990300	3.22212700
H	-0.93369300	-1.18413000	2.51165800
C	1.97882700	-2.06033200	1.09296200
H	2.20463800	-2.41396100	0.08725400
H	2.20124000	-2.86559200	1.81414700
H	2.63054300	-1.21346400	1.31165700
C	-0.27255300	-2.77652900	0.65371100
H	-1.31929100	-2.47065500	0.65890300
H	-0.15821400	-3.67962100	1.27620200
H	0.01902700	-3.01787900	-0.37292600
C	-0.95152600	1.64930600	2.75627000
H	-1.68552000	0.84854400	2.68501400

H	-1.30696600	2.47614100	2.14014800
H	-0.88318300	1.98457900	3.80506400
C	2.83461700	4.96616700	0.07528800
H	1.94049500	5.42301100	-0.36257300
H	3.56353200	5.76758900	0.24708200
H	2.54830200	4.56736700	1.04760700
C	4.83609100	3.44131100	-0.44857400
H	4.84843000	2.99039200	0.54468100
H	5.53315500	4.28869500	-0.43505500
H	5.22017800	2.69706200	-1.15597600
C	3.65399700	4.67953700	-2.22735700
H	4.18167000	4.07245600	-2.96885000
H	4.26839800	5.56572900	-2.02861100
H	2.71174800	5.02528800	-2.66545700
C	1.84609500	-1.40155400	-2.54536100
C	0.87479100	-2.16310900	-3.23451000
C	1.14076800	-3.50945700	-3.51892700
H	0.38926700	-4.10142500	-4.03548400
C	2.35204600	-4.09494100	-3.16672100
H	2.54486400	-5.13896400	-3.39916600
C	3.32322700	-3.32902500	-2.52150500
H	4.26947900	-3.79175500	-2.25896200
C	3.09571400	-1.98757400	-2.19567400
C	4.16242400	-1.16330100	-1.47564000
H	3.63123800	-0.43654700	-0.84854400
C	5.02990500	-0.35750400	-2.46558600
H	5.53093100	-1.02710300	-3.17558300
H	5.80456000	0.20159400	-1.92398700
H	4.43744600	0.36496500	-3.02965600
C	5.08491200	-2.00029100	-0.57468600
H	4.52743800	-2.62911900	0.12775100
H	5.73505800	-1.34060600	0.00500800
H	5.74235200	-2.65502100	-1.15902900
C	-0.43867800	-1.54213700	-3.69009700
H	-0.37590700	-0.46960400	-3.48689400
C	-0.67060000	-1.71989300	-5.20153500
H	0.18366200	-1.35618800	-5.78245300
H	-1.56325500	-1.16621800	-5.51714200
H	-0.82755700	-2.77263100	-5.46348300
C	-1.62759300	-2.08815700	-2.88671400
H	-1.68146600	-3.18122900	-2.94527800
H	-2.57780100	-1.68158400	-3.25056700
H	-1.54804900	-1.81067100	-1.83076400
C	-3.85175300	1.83959100	-0.35090600
H	-4.89802200	2.09040100	-0.19797100
C	-3.58308800	0.97648900	-1.59601300
H	-4.42219000	0.70073000	-2.22715000

C	-2.36518400	1.27227300	-2.32027000
H	-2.20084000	0.75480900	-3.26288900
C	-1.42233900	2.16015100	-1.88669200
H	-0.53805600	2.36071900	-2.49055700
C	-1.68427700	3.05463300	-0.74737500
C	-0.76833900	4.05237600	-0.38245300
H	0.17616500	4.10230800	-0.91528300
C	-1.06248500	4.97172000	0.62834900
H	-0.33528500	5.73152800	0.90256000
C	-2.30609700	4.91356600	1.26101600
H	-2.55780200	5.62825100	2.04066800
C	-3.23067500	3.92596100	0.90230200
H	-4.19325300	3.87977700	1.40744500
C	-2.93150200	2.95994600	-0.06757300
C	-5.15777200	-0.82463500	0.65828100
C	-3.72015600	-3.51674500	-0.29189400
H	-4.39804500	-3.99046700	-1.00881600
H	-3.09857700	-4.30833000	0.14643400
H	-3.06637500	-2.84906600	-0.85291700
C	-6.13359000	-3.84309700	1.40693900
H	-6.85955200	-3.50141900	2.14863900
H	-5.69866700	-4.78274600	1.77387600
H	-6.67330800	-4.07788600	0.48306000
C	-3.61638800	-2.72579700	2.65618400
H	-2.76662800	-2.04014600	2.60578400
H	-3.22203000	-3.74389200	2.76738600
H	-4.17922100	-2.48766900	3.56466800
C	-6.02215900	-1.88902500	-2.17375800
H	-4.96768100	-1.75625000	-2.43879700
H	-6.62951000	-1.61628900	-3.04591300
H	-6.18617700	-2.95493900	-1.98058200
C	-8.20198100	-1.44660300	-0.06334400
H	-8.16100500	-2.42480100	0.42025500
H	-8.88211500	-1.52568900	-0.92196900
H	-8.65789600	-0.74405800	0.64419100
C	-7.01172800	0.88045000	-1.42455400
H	-7.39324200	1.57586000	-0.67347000
H	-7.83650300	0.67443000	-2.12055900
H	-6.23349100	1.39706100	-1.99000800
C	-6.85388600	1.61413100	1.94041100
H	-6.37262400	2.37417400	1.31807800
H	-7.04513800	2.06730600	2.92221800
H	-7.82751600	1.37834900	1.49831800
C	-6.87033300	-1.00942100	3.35765900
H	-7.74014600	-1.40406900	2.82252200
H	-7.24309100	-0.38639600	4.18135300
H	-6.33866900	-1.85633000	3.80295100

C	-4.37023100	0.72032400	3.34179500
H	-3.62661200	-0.04206900	3.59179700
H	-4.80512100	1.08142100	4.28326900
H	-3.85386900	1.56203500	2.86814600
C	7.59438800	-0.27371900	1.71564000
C	8.85891000	-0.71477400	1.31822800
C	9.29591100	-2.00436300	1.62263300
C	8.47130200	-2.88151700	2.32801800
C	7.19834300	-2.48864500	2.74830600
C	6.79048900	-1.17839000	2.43541100
H	9.50164300	-0.03984500	0.75990800
H	10.28208000	-2.32957800	1.30367500
H	8.81482400	-3.88709900	2.55457600
C	6.27432800	-3.41873100	3.49042300
H	5.99229900	-3.00654400	4.46664000
H	5.34248400	-3.57307800	2.93237300
H	6.74349500	-4.39329800	3.65055800
C	7.07306600	1.09430800	1.36208500
H	6.21353900	1.02039100	0.68471300
H	6.72842600	1.63690000	2.24996100
H	7.84153500	1.69408900	0.86699700
N	5.52503200	-0.76939800	2.82888500
C	4.44883200	-0.42828900	3.16435200

IM1

Charge=0, Multiplicity=1

Yb	-0.75130600	-0.36073700	0.11652700
N	-2.72503700	1.07963700	0.08745200
N	-1.17175300	0.14520900	2.41884800
N	-1.46056100	-2.61586500	1.33339100
N	-4.62761900	-3.28517100	-0.61296800
C	-3.16795300	3.51446500	0.24389400
H	-3.12296000	3.61405800	-0.84373300
H	-2.72541800	4.40338200	0.70107600
H	-4.23010900	3.49689700	0.50735600
C	-2.46708900	2.24165600	0.71281500
C	-1.61852900	2.40053500	1.82750300
H	-1.46002600	3.42909400	2.10688800
C	-1.24613400	1.41252700	2.79199400
C	-1.05297200	1.91594500	4.25842400
C	-1.20682000	-1.01833000	3.29130100
H	-1.67520400	-0.83649900	4.26385300
H	-0.19101000	-1.38071200	3.49919100
C	-2.02263400	-2.13069700	2.61846500
H	-2.12986900	-2.97833900	3.31864700
H	-3.02397100	-1.73895400	2.41590200
C	-2.47178200	-3.45391400	0.63902500
H	-3.08918200	-3.99567400	1.37243700

H	-1.93480100	-4.19535700	0.04498100
C	-3.37276200	-2.61850800	-0.27571400
H	-3.62527400	-1.67324300	0.21716700
H	-2.79255100	-2.35200300	-1.18558500
C	-4.44863600	-4.60308700	-1.21273900
H	-3.88410000	-5.26444800	-0.55004700
H	-3.92914100	-4.56814500	-2.19058500
H	-5.43234300	-5.05663300	-1.37569000
C	-5.44295600	-2.44320100	-1.48224900
H	-6.42115300	-2.91241500	-1.63560700
H	-4.98006000	-2.28379000	-2.47630400
H	-5.59815100	-1.46631500	-1.02473300
C	-0.23337200	-3.40648500	1.56302600
H	0.17281700	-3.73181000	0.60340600
H	-0.43247500	-4.28940600	2.19313200
H	0.52729700	-2.78999700	2.04368600
C	0.14628300	1.23204100	4.94889100
H	0.05196900	0.15091100	5.03929600
H	0.26550700	1.63293600	5.96249300
H	1.06447500	1.43984500	4.39291200
C	-2.36816100	1.67222400	5.03892900
H	-3.20291700	2.17695900	4.54080100
H	-2.28045000	2.07352900	6.05642300
H	-2.62421300	0.61265500	5.12308900
C	-0.76177000	3.43525700	4.33053200
H	0.10367500	3.70881300	3.71628900
H	-0.53394200	3.70489300	5.36804000
H	-1.61700500	4.04184500	4.01936500
C	-3.97749200	1.00685800	-0.58264700
C	-5.14945800	0.85480800	0.20865100
C	-6.39956100	0.93264700	-0.41338400
H	-7.30102900	0.85102900	0.18896900
C	-6.50832100	1.09370600	-1.79396900
H	-7.48606300	1.16002100	-2.26361700
C	-5.35339900	1.12787500	-2.57144700
H	-5.44449400	1.21091300	-3.65107200
C	-4.07829000	1.07081100	-1.99265800
C	-2.84333600	1.07811600	-2.88877900
H	-1.99193800	0.75596500	-2.28031000
C	-2.97793100	0.08745600	-4.06005400
H	-3.30022600	-0.89974200	-3.71135300
H	-2.01820700	-0.02504100	-4.57793500
H	-3.70989300	0.43132500	-4.79964600
C	-2.49716500	2.48091500	-3.42140700
H	-3.34606400	2.91148900	-3.96580600
H	-1.64521000	2.43095600	-4.11156300
H	-2.22807200	3.16452900	-2.61157300

C	-5.05851500	0.56760400	1.70752300
H	-4.00387200	0.39445500	1.94011800
C	-5.53298500	1.75361900	2.56748000
H	-4.90388300	2.63529700	2.41301300
H	-5.49016600	1.49633400	3.63297000
H	-6.56883000	2.02529500	2.32900700
C	-5.83424500	-0.71086300	2.08627600
H	-6.91504700	-0.58439900	1.95095600
H	-5.66410200	-0.95337200	3.14292800
H	-5.52672000	-1.57384700	1.48538400
C	1.88630100	3.91869500	-3.13492600
C	2.52243100	5.08543900	-3.56402700
C	2.56999700	6.21738300	-2.74933800
C	1.97484700	6.20520700	-1.48722900
C	1.32619300	5.06438100	-1.00902300
C	1.30416800	3.93581700	-1.85243300
H	2.98454600	5.10258800	-4.54719000
H	3.07146000	7.11460700	-3.10099000
H	2.01186300	7.09160200	-0.85998400
C	0.66927800	5.01905500	0.34570200
H	-0.39224300	4.76143200	0.26033100
H	1.12042900	4.24987700	0.98207700
H	0.75275800	5.98402500	0.85354300
C	1.81518500	2.68282300	-3.99299000
H	2.30493300	1.83205400	-3.50595600
H	0.77474700	2.38905200	-4.17802600
H	2.29980500	2.84774500	-4.95909400
N	0.68943600	2.78575400	-1.39111600
C	0.21273100	1.81031900	-0.94565400
Si	2.21350400	-1.01731200	-0.18423400
Si	3.69867200	0.49696500	1.98954700
Si	5.16772000	0.28524800	-0.79860400
Si	4.82829300	-2.26172500	1.02958200
C	2.41718400	-2.29471800	-1.63772400
H	3.45614000	-2.56019600	-1.81509000
C	2.02314800	-0.92097400	-2.19315600
H	2.75785100	-0.35060200	-2.75505800
C	0.65745800	-0.80502000	-2.66776900
H	0.34944000	0.13898000	-3.11287100
C	-0.26237500	-1.80929300	-2.55501200
H	-1.27096200	-1.66159800	-2.93021500
C	0.13517700	-3.17695400	-2.20207300
C	-0.75753800	-4.25019100	-2.32018400
H	-1.77814300	-4.05015600	-2.63644000
C	-0.35467700	-5.56183000	-2.05592700
H	-1.06741600	-6.37802000	-2.13940200
C	0.97318600	-5.81001100	-1.70458500

H	1.30612900	-6.82480100	-1.50229300
C	1.88288100	-4.75076600	-1.61652300
H	2.91993900	-4.95135100	-1.35639500
C	1.48348000	-3.42547600	-1.83117000
C	4.04562000	-0.60767800	0.45715300
C	2.44200400	1.89467700	1.68426300
H	2.61919300	2.42937200	0.74835700
H	2.52879700	2.61913000	2.50640300
H	1.40999000	1.53312800	1.67265600
C	5.22060600	1.40113600	2.68810900
H	6.08082800	0.75033700	2.86522000
H	4.93723700	1.85029200	3.64914000
H	5.54149400	2.21703100	2.03038100
C	2.95333100	-0.49854000	3.42922900
H	1.95860900	-0.86887500	3.15748900
H	2.83680000	0.16172600	4.29582100
H	3.56067400	-1.34963700	3.74651000
C	4.46670100	2.00183100	-1.22413200
H	3.39858500	1.94330700	-1.45416300
H	4.97916000	2.41549600	-2.10137800
H	4.58937000	2.71825000	-0.40396900
C	6.95517700	0.54101100	-0.19182000
H	7.03775000	1.10975900	0.73674600
H	7.50985200	1.08510700	-0.96796900
H	7.46577700	-0.41790900	-0.04460100
C	5.46624400	-0.59588100	-2.46532800
H	6.19996500	-1.40034800	-2.36105700
H	5.90267900	0.14896700	-3.14480700
H	4.59039900	-1.01623400	-2.96253700
C	5.79688600	-3.21185500	-0.30761300
H	5.23614300	-3.40478900	-1.22659600
H	6.06752400	-4.18562200	0.12230500
H	6.73145000	-2.71059900	-0.58205600
C	6.13053600	-2.03623200	2.40321600
H	6.94137800	-1.37452600	2.07983500
H	6.57325500	-3.01601700	2.62583600
H	5.72998700	-1.63679200	3.33989100
C	3.54530100	-3.50851400	1.67685800
H	2.90021900	-3.09829600	2.45888600
H	4.07754900	-4.36991500	2.10228200
H	2.90110200	-3.87764300	0.87215200

IM2

Charge=0, Multiplicity=1

Yb	0.91872400	-0.65190500	0.27968100
N	3.06379400	0.12723100	-0.71506500
N	1.19842400	-2.01509000	-1.69996400
N	0.96155000	-3.16677600	0.98068100

N	1.86613000	-0.89412100	2.77417500
N	0.42529100	3.03126700	0.56689700
C	3.88593100	1.46860000	-2.63568000
H	3.53755200	2.48438100	-2.41618100
H	3.93917300	1.35956600	-3.72145800
H	4.89598400	1.37938000	-2.22723600
C	2.94449000	0.44191000	-2.01068300
C	2.01402500	-0.12618300	-2.90772600
H	1.98588600	0.38021800	-3.85813000
C	1.40780500	-1.41746300	-2.86795100
C	1.16037200	-2.08169700	-4.26771700
C	0.97720900	-3.44656800	-1.51721200
H	1.46257300	-4.06776500	-2.27724400
H	-0.09185600	-3.68659100	-1.55329000
C	1.54906700	-3.89299200	-0.16531300
H	1.40669200	-4.98207100	-0.04822200
H	2.62270900	-3.69776100	-0.16530800
C	1.78021200	-3.32051800	2.19997600
H	2.83315200	-3.25415000	1.91135100
H	1.63104200	-4.31571900	2.65227500
C	1.45963700	-2.24255700	3.23378200
H	0.38662900	-2.22822800	3.43588600
H	1.95577300	-2.48840000	4.18820800
C	3.31842100	-0.71480200	2.95341200
H	3.87633700	-1.43082800	2.34849400
H	3.60459500	-0.83989100	4.01154000
H	3.61486700	0.27888100	2.62170700
C	1.14669900	0.13675000	3.54303400
H	1.46854400	1.12542900	3.20917100
H	1.33946600	0.05172700	4.62608300
H	0.07109800	0.05140600	3.37208000
C	-0.41534000	-3.62565700	1.23980300
H	-0.87830000	-3.02632600	2.01989700
H	-0.43643700	-4.68238600	1.55113400
H	-1.02214500	-3.50820600	0.34524600
C	2.38144800	-2.97841000	-4.59270900
H	2.28322600	-3.39383400	-5.60356100
H	2.49028500	-3.81854000	-3.90097200
H	3.30421400	-2.39011900	-4.54928400
C	1.05241300	-1.04021700	-5.41079800
H	0.28735000	-0.28600600	-5.19685800
H	0.76553000	-1.55553900	-6.33433200
H	1.99977300	-0.53144500	-5.60915300
C	-0.15212500	-2.89345800	-4.33851900
H	-0.20706200	-3.71770600	-3.62989800
H	-0.25566300	-3.32389200	-5.34160700
H	-1.01616100	-2.24555700	-4.16461900

C	4.32522000	0.30173000	-0.06648700
C	5.19493800	-0.82531500	-0.03590300
C	6.38637000	-0.75179600	0.69120200
H	7.05175400	-1.60970400	0.71946900
C	6.74296800	0.40554900	1.38141800
H	7.66950800	0.44413300	1.94810000
C	5.91028100	1.51614800	1.31735000
H	6.20045200	2.42774500	1.83365100
C	4.70722800	1.49388200	0.59622900
C	3.87444900	2.76859900	0.53959400
H	2.99657400	2.55542800	-0.07279700
C	3.38261200	3.20445800	1.93209700
H	2.77311100	2.42604500	2.39731000
H	2.77272200	4.11210000	1.86102500
H	4.22343400	3.41709600	2.60205800
C	4.65220100	3.92795000	-0.11486000
H	5.51655600	4.21752200	0.49388800
H	4.01060500	4.81238300	-0.21362000
H	5.02414300	3.65778200	-1.10758100
C	4.85568900	-2.07975200	-0.83259900
H	3.76756800	-2.10420900	-0.94029700
C	5.44195400	-1.99441000	-2.25678700
H	5.05387700	-1.12340300	-2.79199700
H	5.17901100	-2.88781900	-2.83656900
H	6.53585700	-1.91715400	-2.22264000
C	5.30709600	-3.38403700	-0.15569300
H	6.39836800	-3.48764100	-0.14499000
H	4.91007000	-4.24899500	-0.70034900
H	4.95918400	-3.44600200	0.88253300
C	0.55667400	1.86618900	0.54045600
C	0.27318600	4.40163100	0.62622700
C	0.64252900	5.17338200	-0.49295200
C	0.47924200	6.55686200	-0.39182500
H	0.74988100	7.18214700	-1.23814900
C	-0.02910500	7.13817100	0.77078200
H	-0.14865400	8.21639700	0.82652400
C	-0.39344900	6.34318800	1.85860500
H	-0.79790900	6.80136100	2.75684600
C	-0.25409400	4.95495200	1.80924000
C	-0.64881100	4.05779400	2.95320000
H	0.21682700	3.50544500	3.34011400
H	-1.38158200	3.30790000	2.63250600
H	-1.08102600	4.63539800	3.77482000
C	1.18468400	4.52073500	-1.73874200
H	2.19619700	4.13579300	-1.57146000
H	1.22933800	5.23596700	-2.56467500
H	0.57007000	3.66926800	-2.05120200

Si	-2.51244000	-0.11063400	0.57860300
Si	-2.91369200	1.64708700	-1.93337000
Si	-5.58232600	0.95622800	-0.51748000
Si	-3.98831200	-1.32003500	-1.91526200
C	-3.64365600	-1.10305600	1.84000000
H	-4.60465600	-1.35020400	1.40161500
C	-3.46656200	0.37280600	2.23478800
H	-4.32719300	1.02874900	2.11358900
C	-2.72839500	0.60716100	3.47388800
H	-2.63517700	1.63871900	3.81346100
C	-2.17490600	-0.38002600	4.21687300
H	-1.62920500	-0.14221100	5.12836900
C	-2.37974800	-1.79427600	3.90462800
C	-1.88044000	-2.81017300	4.73452300
H	-1.27499300	-2.53225000	5.59617900
C	-2.16437900	-4.15634600	4.48897900
H	-1.76233300	-4.92754700	5.14080500
C	-2.98985600	-4.49416800	3.41432400
H	-3.23657300	-5.53502000	3.21907700
C	-3.49528000	-3.49240100	2.58061600
H	-4.12869200	-3.76156700	1.73726500
C	-3.17456800	-2.14172300	2.77718200
C	-3.82526500	0.30456100	-0.92744200
C	-2.47054800	3.16512900	-0.87698100
H	-3.28963500	3.88829900	-0.84829600
H	-1.60720700	3.67679100	-1.31477600
H	-2.22113700	2.90015900	0.15422000
C	-3.85088900	2.40277600	-3.41208900
H	-4.19841700	1.66923200	-4.14473200
H	-3.15980900	3.08417500	-3.92683800
H	-4.71265700	2.99915100	-3.09356900
C	-1.27814400	1.01332500	-2.67314100
H	-0.50696400	0.86952300	-1.91169300
H	-0.88792400	1.75438000	-3.38323400
H	-1.37761000	0.06537900	-3.21058500
C	-5.59643400	2.75486300	0.11235400
H	-4.82095700	2.94978200	0.85999300
H	-6.57074200	2.95090000	0.57807500
H	-5.47099900	3.48066600	-0.69821100
C	-6.72810000	0.94078800	-2.04469500
H	-6.30249100	1.43752600	-2.91942400
H	-7.65777600	1.46346800	-1.78295800
H	-7.00330300	-0.07675100	-2.34287600
C	-6.61975300	0.01966700	0.78026700
H	-6.74630900	-1.04455900	0.56679400
H	-7.61896200	0.47561100	0.75059400
H	-6.24734700	0.11863900	1.80356900

C	-5.39805300	-2.46624600	-1.34489400
H	-5.30861800	-2.72165200	-0.28360100
H	-5.31474200	-3.40154300	-1.91447000
H	-6.40286800	-2.06883400	-1.51509600
C	-4.25746100	-1.09322500	-3.78788000
H	-5.16555300	-0.52444600	-4.01295700
H	-4.36387100	-2.08471300	-4.24760200
H	-3.41669200	-0.59225700	-4.28074900
C	-2.46735100	-2.43919600	-1.73701600
H	-2.49909000	-2.92107100	-0.75563900
H	-1.51261400	-1.91392000	-1.82686400
H	-2.50392500	-3.22618300	-2.50050700

IM3_2

Charge=0, Multiplicity=1

Yb	-1.26005300	-0.06053300	0.60032100
N	-3.14613200	0.56779700	-0.82348800
N	-1.61211000	2.34203300	1.00484500
N	-1.69399200	0.40299100	3.22981000
N	-2.18695900	-2.25930900	1.84873300
N	0.22317200	-1.01415800	-1.12384200
C	-3.82290500	1.78980700	-2.86144100
H	-3.42017900	1.11454100	-3.62364500
H	-3.79858100	2.80773500	-3.25731000
H	-4.86624000	1.50212700	-2.70248800
C	-3.01661800	1.66358400	-1.57450000
C	-2.17118400	2.75715400	-1.27946300
H	-2.08944300	3.45919500	-2.09291500
C	-1.68669700	3.19392000	-0.01520700
C	-1.38024000	4.73092200	0.09091900
C	-1.58786400	2.76777000	2.39941400
H	-2.09246500	3.72405500	2.57489100
H	-0.56074800	2.88790600	2.76480900
C	-2.31886100	1.74219300	3.26966200
H	-2.37967700	2.10964200	4.31010200
H	-3.34012200	1.64597700	2.89443200
C	-2.63979200	-0.63510600	3.67951800
H	-3.60293400	-0.44069800	3.19961300
H	-2.80508500	-0.57448700	4.77029700
C	-2.16577400	-2.03684200	3.31128500
H	-1.14365200	-2.19749400	3.66322800
H	-2.79379800	-2.78584800	3.82265300
C	-3.54457600	-2.63155600	1.40837500
H	-4.25759000	-1.84079800	1.64830400
H	-3.87640200	-3.56907400	1.88607800
H	-3.56515900	-2.75929500	0.32595700
C	-1.23580200	-3.32841600	1.49946500
H	-1.30288000	-3.53190200	0.43162200

H	-1.44192600	-4.26092500	2.04972200
H	-0.21638600	-3.00935500	1.72838800
C	-0.48055500	0.38055000	4.06393600
H	0.09302000	-0.52787000	3.87965700
H	-0.73063100	0.43830500	5.13803800
H	0.15802900	1.22428300	3.81108300
C	-2.66751800	5.45356200	0.55821900
H	-2.50425300	6.53855800	0.58689800
H	-2.99033900	5.14041700	1.55583500
H	-3.48883200	5.24581100	-0.13625200
C	-0.98924700	5.34588000	-1.27844300
H	-0.15933000	4.80331400	-1.74112300
H	-0.67319900	6.38402800	-1.12631200
H	-1.82387700	5.37070400	-1.98414100
C	-0.19975700	5.05400100	1.04045200
H	-0.43448900	4.91997400	2.09570900
H	0.09136200	6.10285400	0.91513300
H	0.67352400	4.43683500	0.80995900
C	-4.30727100	-0.24588000	-0.96481600
C	-5.40587500	0.02558500	-0.10325800
C	-6.53106100	-0.80249500	-0.15494500
H	-7.37758700	-0.60178000	0.49561900
C	-6.58704300	-1.88937200	-1.02730500
H	-7.46835300	-2.52491400	-1.05463600
C	-5.50657600	-2.15066900	-1.86340700
H	-5.55217000	-2.99729300	-2.54406700
C	-4.35849400	-1.34581300	-1.85246800
C	-3.20168200	-1.68767100	-2.78203800
H	-2.42134900	-0.93909900	-2.62994800
C	-2.59015300	-3.05649500	-2.43845100
H	-2.14081800	-3.03731400	-1.44143400
H	-1.80132900	-3.31574300	-3.15012300
H	-3.34744100	-3.84940600	-2.45697600
C	-3.61161400	-1.65982200	-4.26639400
H	-4.30848000	-2.47351100	-4.50153300
H	-2.72450300	-1.78514300	-4.89833200
H	-4.10165800	-0.71904600	-4.53674200
C	-5.34972200	1.21237100	0.85237400
H	-4.28953100	1.39721700	1.05404400
C	-5.90180700	2.49485500	0.19776400
H	-5.32993500	2.76428600	-0.69376500
H	-5.84555600	3.33887800	0.89697300
H	-6.95123900	2.36125000	-0.09316700
C	-6.06278800	0.95743700	2.19038200
H	-7.15282300	0.93021700	2.07618200
H	-5.83479100	1.76182100	2.90016200
H	-5.75609100	0.00639300	2.64163100

C	1.06871700	-0.64142500	-0.21088400
C	0.45249200	-1.61155900	-2.40383200
C	0.16931000	-0.86369400	-3.56986200
C	0.35945700	-1.45593300	-4.82325000
H	0.15944000	-0.86318200	-5.71340200
C	0.79705100	-2.77153800	-4.94649900
H	0.95324100	-3.21213700	-5.92737800
C	0.99615600	-3.52398400	-3.79277100
H	1.27982500	-4.57139700	-3.86962100
C	0.79835100	-2.97711100	-2.51912200
C	0.78703900	-3.91628800	-1.34261500
H	-0.19632900	-4.40232200	-1.28078900
H	0.97599800	-3.42131000	-0.39416600
H	1.53110900	-4.70601000	-1.45962600
C	-0.32674300	0.55848600	-3.52393000
H	-0.71989500	0.83669200	-2.54751400
H	-1.12111400	0.70655700	-4.26423500
H	0.47344700	1.26426100	-3.76436800
Si	3.00083300	-0.71293500	-0.12414400
Si	3.35337200	1.79191000	-1.92541600
Si	5.90487900	0.69664700	-0.43677500
Si	3.62571300	2.07057400	1.21238200
C	3.64130100	-1.65650600	1.37833900
H	4.41569800	-1.15033400	1.95441600
C	4.13627100	-2.26303300	0.01994500
H	5.16108200	-2.01641100	-0.24940500
C	3.88280200	-3.69592300	-0.17738700
H	4.32025700	-4.16052800	-1.05949800
C	3.18976700	-4.45234500	0.69581200
H	3.04571700	-5.51406400	0.50743500
C	2.57796100	-3.89739900	1.90214100
C	1.80796500	-4.70054300	2.75890800
H	1.64286400	-5.74241600	2.49175800
C	1.27094000	-4.19398400	3.94311400
H	0.68082900	-4.83467000	4.59304700
C	1.50931500	-2.86202100	4.28832800
H	1.11517700	-2.45612100	5.21711800
C	2.26802200	-2.04904200	3.43873000
H	2.46466200	-1.01410000	3.71097200
C	2.79965100	-2.53670700	2.23935300
C	3.99227100	0.94910600	-0.31067100
C	3.26485900	0.56934900	-3.37174000
H	4.26440400	0.30129100	-3.72449000
H	2.74074200	1.04391000	-4.21073900
H	2.73441800	-0.35856500	-3.14389300
C	4.41162200	3.22631700	-2.58562100
H	4.57598500	4.02278400	-1.85456600

H	3.86539700	3.66274300	-3.43245400
H	5.38536200	2.89806800	-2.96382700
C	1.64141700	2.55309600	-1.63535700
H	0.90910200	1.84373000	-1.24425200
H	1.25019300	2.94699100	-2.57989500
H	1.69283300	3.39185500	-0.93680200
C	6.39467600	-0.13378700	-2.07364700
H	5.75477800	-0.98903900	-2.31366200
H	7.42817400	-0.49404300	-1.99834800
H	6.35139700	0.56400000	-2.91662000
C	6.86484000	2.33718900	-0.33086400
H	6.53073500	3.11260300	-1.02142300
H	7.91552100	2.11633400	-0.56062500
H	6.84041100	2.75200700	0.68289400
C	6.78024600	-0.30798300	0.93052300
H	6.69444400	0.15153100	1.91763700
H	7.84560200	-0.29067100	0.66226100
H	6.49007500	-1.35622900	1.02423700
C	4.68038900	1.70632500	2.75379500
H	4.64249200	0.65871500	3.06635500
H	4.26819000	2.30956900	3.57346000
H	5.73060800	1.99166300	2.64014100
C	3.91244800	3.92600800	0.89429500
H	4.93857500	4.14560200	0.58574800
H	3.73286300	4.45556300	1.83925800
H	3.23928400	4.35830700	0.14853700
C	1.85561800	1.89705700	1.84581400
H	1.66020600	0.87053700	2.16774000
H	1.08817400	2.15244400	1.11315300
H	1.74627000	2.56605300	2.70970600

Product

Charge=0, Multiplicity=1

Yb	0.93728800	0.26227500	0.12069900
N	3.23188600	-0.48016200	0.42468900
N	1.27618900	0.33607500	2.51941600
N	0.51638600	2.77543700	1.06549300
N	1.27142400	2.07174600	-1.82262400
N	0.10778100	-1.62699200	-1.26214000
C	4.54968200	-2.43064900	1.19493500
H	4.29437100	-3.21811600	0.47635000
H	4.78459000	-2.90665600	2.15014200
H	5.44643600	-1.92985000	0.82145500
C	3.38345400	-1.45785500	1.32195400
C	2.51791300	-1.69785000	2.41418100
H	2.71499600	-2.63611500	2.90685500
C	1.69434500	-0.77437900	3.12062500
C	1.45662700	-1.11576400	4.63367900

C	0.86402300	1.54539900	3.22301100
H	1.37084800	1.68117400	4.18571100
H	-0.21190200	1.54060200	3.43195900
C	1.20575200	2.77589400	2.37495900
H	0.97076700	3.69657400	2.93766300
H	2.28083800	2.77124700	2.18605100
C	1.20371200	3.65077900	0.09588700
H	2.27953600	3.47281700	0.18097500
H	1.03027500	4.71463900	0.33399400
C	0.75119900	3.36820200	-1.33301600
H	-0.33870500	3.34211800	-1.38440500
H	1.07130800	4.18650100	-1.99813900
C	2.66902500	2.22352000	-2.27108900
H	3.30948200	2.53727500	-1.44528900
H	2.74509200	2.96372800	-3.08547100
H	3.05396600	1.26813800	-2.62472400
C	0.44587200	1.59325500	-2.94559900
H	0.84648700	0.64566900	-3.30524900
H	0.43064000	2.31308600	-3.78030600
H	-0.58107500	1.42972700	-2.60767100
C	-0.88353600	3.22128400	1.21907600
H	-1.48443400	2.91185700	0.36338000
H	-0.94966300	4.31597500	1.31547300
H	-1.32164400	2.77322500	2.10830500
C	2.59260300	-0.46030300	5.45603900
H	2.50007200	-0.73352700	6.51490000
H	2.57826500	0.63235300	5.39237600
H	3.56849400	-0.80217100	5.09435300
C	1.50859600	-2.64322700	4.89820000
H	0.82789700	-3.18626300	4.23330500
H	1.19973000	-2.83794800	5.93129600
H	2.51314000	-3.05945600	4.78445100
C	0.07672600	-0.66252600	5.16340700
H	-0.06360900	0.41696800	5.17444600
H	-0.04130000	-1.00789600	6.19711900
H	-0.73169100	-1.10299700	4.57291500
C	4.34449100	-0.04143300	-0.35270400
C	5.09388500	1.05977200	0.14517700
C	6.12222700	1.59216000	-0.63813200
H	6.69972700	2.43298800	-0.26525500
C	6.42115000	1.06167400	-1.89287700
H	7.22201800	1.48809800	-2.49126900
C	5.69447300	-0.02616400	-2.36489200
H	5.93865200	-0.44972200	-3.33581700
C	4.65533700	-0.59651500	-1.61590500
C	3.90977500	-1.79969800	-2.17876800
H	3.14103600	-2.08275500	-1.45665100

C	3.19775900	-1.47800900	-3.50429800
H	2.41237200	-0.73039400	-3.35972200
H	2.72228000	-2.37498900	-3.91009000
H	3.90037400	-1.09258900	-4.25276400
C	4.84583700	-3.00766900	-2.37911900
H	5.57262300	-2.81525300	-3.17772200
H	4.26026400	-3.88976000	-2.66263700
H	5.40892500	-3.24070200	-1.47035700
C	4.79376100	1.62179000	1.52984800
H	3.74279700	1.39665400	1.73699700
C	5.62006600	0.90060500	2.61401900
H	5.41584100	-0.17344500	2.61911300
H	5.37565700	1.29259500	3.60940800
H	6.69433100	1.04387900	2.44341600
C	4.99579700	3.14192400	1.63564300
H	6.05493800	3.42103400	1.58569200
H	4.61295600	3.50874800	2.59560100
H	4.47559900	3.67882400	0.83341400
C	-1.06774800	-1.23020100	-0.96674600
C	0.35610600	-2.68608000	-2.20297300
C	1.06811400	-3.80686500	-1.71857000
C	1.38720800	-4.84297500	-2.59907000
H	1.93280900	-5.70439300	-2.22071900
C	1.00139100	-4.79361000	-3.93822100
H	1.25301300	-5.60686300	-4.61353200
C	0.28313100	-3.69512100	-4.39685400
H	-0.02533400	-3.64732000	-5.43922100
C	-0.05022700	-2.62555300	-3.55239300
C	-0.76756400	-1.44700300	-4.17340200
H	-0.08106900	-0.87743400	-4.81482400
H	-1.19882700	-0.76993400	-3.44005200
H	-1.58585800	-1.79622300	-4.81353800
C	1.42074500	-3.93216400	-0.25898600
H	1.71173700	-2.97855200	0.18231500
H	2.23541000	-4.64905000	-0.11159600
H	0.55867100	-4.28370000	0.31890800
Si	-2.66782300	-0.51706700	-0.93747800
Si	-2.97964000	-3.28298800	0.76468100
Si	-5.43817300	-1.78879100	-0.53891400
Si	-3.95094500	-0.51154200	1.91414400
C	-3.44136500	3.27497300	-1.89740900
H	-4.06060200	2.47917300	-1.49436700
C	-2.86541100	3.13223400	-3.14077900
H	-3.03887700	2.22408200	-3.71047800
C	-2.04032600	4.15595400	-3.66918300
H	-1.60176100	4.03626200	-4.65628400
C	-1.78172600	5.29126900	-2.93232500

H	-1.13635900	6.07178600	-3.32914000
C	-2.34437300	5.46152000	-1.63818000
C	-2.07179600	6.60274000	-0.83497200
H	-1.40953200	7.37166400	-1.22662100
C	-2.63865800	6.74015600	0.41295100
H	-2.42306500	7.61838400	1.01557400
C	-3.51200800	5.74210700	0.91562400
H	-3.95926400	5.86501700	1.89827500
C	-3.79137800	4.62142800	0.16585400
H	-4.45338300	3.85142800	0.55272400
C	-3.21107300	4.44206200	-1.12010100
C	-3.75274900	-1.58214300	0.35272100
C	-2.41605900	-4.27592600	-0.75665600
H	-3.22385200	-4.91550200	-1.12686700
H	-1.58306700	-4.93275400	-0.47800700
H	-2.07373400	-3.65277400	-1.58504300
C	-4.18938900	-4.45653500	1.65589300
H	-4.60794900	-4.04261300	2.57756200
H	-3.65130600	-5.37746500	1.91760500
H	-5.02395100	-4.74423100	1.00645700
C	-1.48360600	-3.13198700	1.93525500
H	-0.70433100	-2.46499100	1.55383600
H	-1.03655600	-4.12705300	2.05559000
H	-1.77189500	-2.78566000	2.93383300
C	-5.40859400	-3.17667600	-1.83399300
H	-4.54670500	-3.08786400	-2.50469000
H	-6.31865900	-3.11005000	-2.44387900
H	-5.38292700	-4.17546900	-1.38621900
C	-6.85758300	-2.19179000	0.66261300
H	-6.65044900	-3.07269600	1.27812100
H	-7.76590800	-2.39718300	0.08131800
H	-7.08411600	-1.35851300	1.33711000
C	-5.99205700	-0.24498300	-1.50536900
H	-5.94511800	0.67895900	-0.92280100
H	-7.03575900	-0.39257800	-1.81429100
H	-5.39351200	-0.09864400	-2.41061400
C	-5.03046100	1.03153500	1.63302300
H	-4.66144500	1.60963700	0.77872500
H	-4.96651100	1.67093500	2.52309900
H	-6.08755900	0.80713500	1.45916100
C	-4.67335500	-1.41486700	3.42243400
H	-5.62279500	-1.91284000	3.20582900
H	-4.85291300	-0.68190900	4.21990400
H	-3.98128400	-2.16618100	3.81875800
C	-2.28801500	0.19822400	2.46122800
H	-1.91986100	0.87120200	1.68482800
H	-1.51520200	-0.55384000	2.61998900

H	-2.40791900	0.77251500	3.38889200
IM2_1			
Charge=0, Multiplicity=1			
Yb	0.74047500	-0.09050500	0.28633000
N	2.43803500	-1.15480300	-1.02635000
N	1.68435800	-1.74922300	1.74175800
N	1.97951800	1.10435300	2.24155800
N	4.56109300	3.13964300	0.36017600
C	2.55310800	-3.20108700	-2.40773200
H	2.01973200	-2.73096800	-3.23992200
H	2.27730700	-4.25758700	-2.36935600
H	3.62117200	-3.13038400	-2.63449200
C	2.21891700	-2.48397800	-1.10611500
C	1.70238300	-3.28263400	-0.07041700
H	1.48282800	-4.29550300	-0.36753800
C	1.69618200	-3.00748400	1.33468900
C	1.78331700	-4.23615800	2.29415000
C	2.09388500	-1.27612400	3.05639100
H	2.78911400	-1.94242200	3.57576000
H	1.22696200	-1.15376300	3.71859300
C	2.81683500	0.06586700	2.88792700
H	3.16432400	0.42641600	3.87234300
H	3.69725300	-0.09506600	2.26044800
C	2.79552600	2.29205000	1.89653800
H	3.53878600	2.49482000	2.68442300
H	2.11603100	3.14594300	1.86307500
C	3.50334000	2.15090400	0.54589500
H	3.94499100	1.15485200	0.45887400
H	2.74441300	2.22068200	-0.26048000
C	4.05992500	4.50766600	0.41553500
H	3.66123900	4.73773400	1.40860200
H	3.26646900	4.70772900	-0.33445300
H	4.88377300	5.20319200	0.22500300
C	5.26498800	2.90411900	-0.89810800
H	6.09899400	3.60879200	-0.98914900
H	4.61302100	3.01886900	-1.78477000
H	5.66535800	1.88948500	-0.91736900
C	0.87892500	1.49837800	3.13767600
H	0.23089800	2.21481200	2.62947300
H	1.24566900	1.94683800	4.07514000
H	0.26267900	0.63775100	3.39799000
C	0.87238000	-4.05021200	3.53108800
H	1.20640200	-3.26426500	4.20801300
H	0.84495200	-4.98025900	4.11061600
H	-0.15122300	-3.81461900	3.22029900
C	3.26164400	-4.44585000	2.70656800
H	3.88391100	-4.59363300	1.81717500

H	3.35040000	-5.33748200	3.33977600
H	3.67691600	-3.60274000	3.26498700
C	1.32359400	-5.54985500	1.61627200
H	0.30939300	-5.46369800	1.21530100
H	1.32382800	-6.35281600	2.36206000
H	1.99423200	-5.86028300	0.80974600
C	3.48990400	-0.62926100	-1.82909800
C	4.82958100	-0.83957700	-1.39695000
C	5.87776500	-0.38518700	-2.20334300
H	6.90444000	-0.57007600	-1.89771000
C	5.63202600	0.32119500	-3.38031700
H	6.45884300	0.67555900	-3.99013900
C	4.31851500	0.58279600	-3.75764100
H	4.12762900	1.14782400	-4.66672100
C	3.23408700	0.10868700	-3.00698300
C	1.81547000	0.38017200	-3.49189500
H	1.12685200	-0.14320700	-2.81925900
C	1.48503900	1.88314800	-3.43859500
H	1.60859800	2.27925400	-2.42517400
H	0.45007000	2.06255700	-3.75178400
H	2.14530100	2.45436700	-4.10198200
C	1.57270800	-0.17866000	-4.90606100
H	2.19584300	0.33139100	-5.64998000
H	0.52597900	-0.04166700	-5.19916100
H	1.80464700	-1.24769400	-4.95640900
C	5.13248100	-1.54318400	-0.07389000
H	4.19695500	-1.58028200	0.49258300
C	5.60429300	-2.99518500	-0.28441500
H	4.83561900	-3.59919100	-0.77367700
H	5.83615700	-3.46643900	0.67875700
H	6.51046800	-3.02678100	-0.90225400
C	6.16399000	-0.77809700	0.77860600
H	7.15798400	-0.77793700	0.31625300
H	6.26390500	-1.25471500	1.76159000
H	5.87514700	0.26658700	0.93746800
C	-2.07330500	4.79343900	-1.28315400
C	-2.75638100	6.01006000	-1.34374100
C	-2.44597100	7.05249900	-0.46954800
C	-1.44667800	6.89464400	0.49144900
C	-0.73230300	5.69902300	0.59345400
C	-1.06004400	4.67104400	-0.31090000
H	-3.54531400	6.13366700	-2.08022300
H	-2.99175000	7.98965000	-0.53153700
H	-1.21823300	7.70547600	1.17747400
C	0.33223700	5.49012300	1.63797900
H	0.08033700	4.64189600	2.28589700
H	1.30228400	5.27035900	1.17778700

H	0.44651800	6.37792400	2.26590200
C	-2.40709600	3.63301400	-2.17950600
H	-3.24729700	3.87025200	-2.83762500
H	-1.55209000	3.34856900	-2.80371000
H	-2.66762400	2.74734600	-1.58885700
N	-0.38095300	3.46836800	-0.22562000
C	0.11651200	2.40798300	-0.15994800
Si	-2.35159900	-0.24547000	0.10735500
Si	-2.51031800	-1.39503200	-2.72759800
Si	-5.28739700	-0.88684600	-1.38515300
Si	-3.42675300	-3.16398500	-0.29730200
C	-3.37926900	-0.04257200	1.74080400
H	-4.25088800	-0.69240200	1.78290300
C	-3.52143900	1.17653000	0.82082600
H	-4.46036200	1.27031300	0.28226500
C	-3.07434300	2.45924400	1.36841500
H	-3.24289900	3.34824600	0.76418400
C	-2.51931100	2.59614100	2.59264600
H	-2.22584600	3.58002500	2.95635800
C	-2.35453200	1.45879900	3.49888800
C	-1.81323500	1.62402900	4.78262400
H	-1.52562700	2.62368800	5.10509200
C	-1.61662700	0.53629700	5.63573900
H	-1.17986200	0.68504200	6.61989500
C	-1.98518600	-0.74173900	5.20876400
H	-1.83289900	-1.60226500	5.85562600
C	-2.56489600	-0.91339500	3.94780500
H	-2.86551200	-1.90741900	3.62219000
C	-2.75835500	0.16499400	3.07452400
C	-3.47368300	-1.41374500	-1.07415800
C	-1.98165300	0.35375100	-3.25560400
H	-2.82359600	1.04521800	-3.33142900
H	-1.50814000	0.29430400	-4.24346000
H	-1.25657100	0.78724600	-2.55964200
C	-3.42419300	-2.10043600	-4.24051300
H	-3.77216000	-3.12633200	-4.08588000
H	-2.71813300	-2.11332600	-5.08142800
H	-4.28286800	-1.49253500	-4.54423200
C	-0.88899800	-2.37998500	-2.66137600
H	-1.04071100	-3.45798000	-2.55223700
H	-0.23431500	-2.06989700	-1.84397900
H	-0.34423400	-2.21337900	-3.59895700
C	-5.40159600	0.70256500	-2.42929200
H	-4.80771200	1.52027400	-2.00684400
H	-6.44788300	1.03152100	-2.46449100
H	-5.07114200	0.54806300	-3.46233600
C	-6.30702000	-2.20686100	-2.31049500

H	-5.85167400	-2.57083400	-3.23357300
H	-7.27913100	-1.76629200	-2.56906800
H	-6.50819500	-3.07409000	-1.67129000
C	-6.39633600	-0.56796400	0.13460100
H	-6.51876100	-1.45589200	0.75980200
H	-7.38953500	-0.31632100	-0.26224200
H	-6.08662500	0.25474700	0.78207100
C	-4.77156500	-3.50404100	1.00631200
H	-4.77849800	-2.77052300	1.81833200
H	-4.55324400	-4.48416100	1.45085700
H	-5.78073000	-3.55761100	0.58530000
C	-3.65836200	-4.56740000	-1.56720600
H	-4.60614800	-4.47655000	-2.10750900
H	-3.67449200	-5.52518300	-1.03048800
H	-2.85676100	-4.62305900	-2.31043900
C	-1.80785600	-3.53016100	0.62053800
H	-0.91258400	-3.40823700	0.00595600
H	-1.84012700	-4.57341700	0.96297500
H	-1.69188300	-2.89238500	1.50385500

IM3_1

Charge=0, Multiplicity=1

Yb	1.01955700	0.13934200	-0.34752000
N	2.81663000	0.91450600	1.00976800
N	1.56367700	2.30124000	-1.25690900
N	1.79067400	-0.22380000	-2.79413400
N	4.66702200	-2.55027300	-1.93488700
C	2.98929100	2.36765400	2.99853400
H	2.60593800	1.59111000	3.67026300
H	2.65654500	3.34306400	3.36239600
H	4.08095900	2.32785500	3.06681300
C	2.51658300	2.10076800	1.57424600
C	1.80621100	3.14331100	0.94865600
H	1.57232200	3.96458100	1.60647000
C	1.56400600	3.34780600	-0.44606000
C	1.38316200	4.82451900	-0.92233200
C	1.70278500	2.31428400	-2.70299900
H	2.26759600	3.16865600	-3.09359800
H	0.71963300	2.34148500	-3.19235500
C	2.46402500	1.05474200	-3.14699000
H	2.63852500	1.09160700	-4.23654500
H	3.43874600	1.06447400	-2.65289000
C	2.73146300	-1.36304000	-2.93815000
H	3.34214800	-1.25597900	-3.84808900
H	2.12572100	-2.26369600	-3.06002000
C	3.65647500	-1.52298300	-1.72534700
H	4.16280400	-0.57734600	-1.51645900

H	3.04940600	-1.73957800	-0.81855700
C	4.10400000	-3.89822900	-1.94839200
H	3.35879200	-4.00478100	-2.74209400
H	3.62469800	-4.17302400	-0.98881600
H	4.90297700	-4.62002500	-2.14746100
C	5.73340100	-2.45683500	-0.93740700
H	6.50572500	-3.20015500	-1.16384500
H	5.37835600	-2.62483200	0.09394600
H	6.19204400	-1.46591100	-0.96865600
C	0.61246900	-0.44771100	-3.65623400
H	0.07535800	-1.34210400	-3.32810600
H	0.90020900	-0.57385400	-4.71305900
H	-0.07330700	0.39727300	-3.58163700
C	0.28481500	4.94876200	-2.00497200
H	0.54643600	4.47030100	-2.94843500
H	0.10460200	6.00761400	-2.22362700
H	-0.65843500	4.51455200	-1.65713400
C	2.74253600	5.33892900	-1.45555800
H	3.50747500	5.26618700	-0.67506400
H	2.65622600	6.39054100	-1.75690800
H	3.09698500	4.77424500	-2.32258200
C	0.95597800	5.76895000	0.22694300
H	0.03760300	5.42242500	0.71356100
H	0.76246000	6.76666700	-0.18295400
H	1.73274600	5.87763300	0.98895200
C	4.02067100	0.27927900	1.42171200
C	5.24562300	0.79433500	0.90920700
C	6.44973200	0.23417500	1.34534600
H	7.39040100	0.64105600	0.98261700
C	6.46674700	-0.84193900	2.23170400
H	7.41144700	-1.26234700	2.56640900
C	5.26217900	-1.38844100	2.66453100
H	5.27667700	-2.24609200	3.33226700
C	4.02823700	-0.85425700	2.26767200
C	2.74399700	-1.52139800	2.74716000
H	1.89599300	-0.96979200	2.32650000
C	2.65657300	-2.97277200	2.23754500
H	2.68053200	-3.00843200	1.14302600
H	1.72892500	-3.44825600	2.56666300
H	3.49779100	-3.57152400	2.60658900
C	2.59172600	-1.48011200	4.27845200
H	3.38614900	-2.05154500	4.77334400
H	1.63056800	-1.91709500	4.57462400
H	2.63505300	-0.45362200	4.65837500
C	5.25567400	1.94017300	-0.10399300
H	4.23540200	2.04170400	-0.48626900
C	5.64498000	3.28144500	0.54724000

H	4.93082400	3.56997600	1.32283300
H	5.66546800	4.08244400	-0.20236700
H	6.64120000	3.21939000	1.00273300
C	6.17384600	1.65974000	-1.30878400
H	7.23095300	1.61564400	-1.02170300
H	6.07233600	2.46056000	-2.05169500
H	5.92633500	0.71217000	-1.79968300
C	-1.01608200	-3.08769100	2.42057600
C	-1.00222800	-4.40909900	2.88722200
C	-0.58084600	-5.46231300	2.07968300
C	-0.14168100	-5.19644700	0.78142900
C	-0.12108400	-3.89281600	0.28722900
C	-0.58636800	-2.83696200	1.10240800
H	-1.32602600	-4.60605500	3.90711800
H	-0.57983700	-6.47957800	2.46172300
H	0.20258600	-6.00860300	0.14514300
C	0.40965000	-3.59144300	-1.08851300
H	-0.31395300	-3.02894100	-1.68580300
H	1.32185400	-2.98808600	-1.01375900
H	0.65671400	-4.50750700	-1.63270900
C	-1.46009800	-1.97808500	3.33756100
H	-1.30063100	-2.24890100	4.38703100
H	-0.91874400	-1.04928800	3.13491700
H	-2.52552200	-1.76062800	3.20976600
N	-0.42290600	-1.52699700	0.59178800
C	-1.25718300	-0.54886700	0.37205700
Si	-3.14604200	-0.50553300	0.37810500
Si	-3.16013800	2.16231600	1.98124700
Si	-5.85624400	1.22053000	0.72615800
Si	-3.55863000	2.17392200	-1.18561700
C	-3.97055500	-1.57439800	-0.96212800
H	-4.75136200	-1.03144200	-1.49185800
C	-4.35458400	-2.00416400	0.47616400
H	-5.35856800	-1.73934700	0.80318700
C	-3.98096400	-3.37508000	0.85952900
H	-4.22589100	-3.69609400	1.86981800
C	-3.37785500	-4.23629800	0.01821400
H	-3.11380200	-5.23335500	0.35837700
C	-3.02330200	-3.87763500	-1.35526200
C	-2.42680300	-4.81016700	-2.21715200
H	-2.22902100	-5.81281500	-1.84455900
C	-2.06765200	-4.46755100	-3.52069800
H	-1.59771100	-5.20344200	-4.16790700
C	-2.30915600	-3.17154200	-3.98322000
H	-2.03046300	-2.88798800	-4.99520500
C	-2.92156400	-2.23842900	-3.14110600
H	-3.12265400	-1.23135800	-3.50237800

C	-3.28596200	-2.56985400	-1.83055800
C	-3.94018100	1.25214400	0.46377400
C	-3.16195800	1.07482800	3.54775000
H	-3.61144800	1.62635000	4.38245700
H	-2.13754800	0.81689200	3.83529600
H	-3.71809500	0.14128300	3.43691100
C	-4.03210400	3.77226300	2.49844600
H	-4.11274400	4.51055900	1.69609300
H	-3.41922800	4.21648000	3.29415600
H	-5.03079400	3.60676200	2.91526900
C	-1.35877600	2.64132500	1.67623800
H	-1.19569800	3.22514700	0.76664800
H	-0.73649700	1.74640100	1.59555800
H	-0.98751700	3.23499100	2.52100600
C	-6.32562100	0.65608800	2.47785400
H	-5.93192400	-0.33981800	2.70945600
H	-7.41983700	0.60283300	2.54128600
H	-5.98200300	1.33944000	3.26071900
C	-6.65669600	2.92716300	0.45596900
H	-6.19279000	3.74686000	1.00581400
H	-7.70021700	2.85268700	0.78911900
H	-6.67884400	3.20251100	-0.60387800
C	-6.90124600	0.12708800	-0.43400300
H	-6.75924400	0.35451200	-1.49283400
H	-7.94784000	0.35829200	-0.19349800
H	-6.77306000	-0.94951200	-0.30173700
C	-4.76842100	1.78604400	-2.60208300
H	-4.80749800	0.71908900	-2.84450900
H	-4.39725500	2.30930700	-3.49301800
H	-5.79056900	2.13290000	-2.42639600
C	-3.59178000	4.06822300	-1.01288900
H	-4.56800400	4.44404400	-0.69210400
H	-3.37704400	4.50417200	-1.99734100
H	-2.83850100	4.45004600	-0.31626800
C	-1.87419400	1.76580600	-1.94966300
H	-1.03914100	2.09469600	-1.32783200
H	-1.80713100	2.28768600	-2.91385800
H	-1.76508900	0.69188900	-2.12802100

IM0_2

Charge=0, Multiplicity=1

Yb	-1.87026300	-0.10583700	-0.71430300
N	-2.60428500	-0.29556400	1.49555700
N	-1.73757400	2.17384300	-0.06827400
N	-0.05159600	0.87971000	-2.11888300
N	-0.35172100	-2.02727700	-1.42732000
N	-5.32040700	-0.26425400	-1.82561400
C	-4.03526200	0.34044400	3.39895100

H	-4.83909500	-0.37823400	3.21096300
H	-4.46915100	1.23232500	3.85610200
H	-3.36134600	-0.12771000	4.12343100
C	-3.28733400	0.67357200	2.11540800
C	-3.38325700	2.00887200	1.67862500
H	-4.06237000	2.58696000	2.28191900
C	-2.61385700	2.76323900	0.74159100
C	-2.83206600	4.31771000	0.84507100
C	-0.67101100	2.90212000	-0.76993300
H	-0.19009100	3.64700000	-0.13430300
H	-1.05116600	3.43547200	-1.64727500
C	0.44609300	1.95961300	-1.22061600
H	1.23738200	2.54918700	-1.70816800
H	0.90657700	1.48326400	-0.34845000
C	0.99115000	-0.13751600	-2.40052900
H	1.69757800	-0.15552300	-1.56189400
H	1.58234600	0.14026100	-3.28474500
C	0.37749700	-1.52194400	-2.62070700
H	-0.34773300	-1.48354700	-3.44412300
H	1.16446900	-2.23043900	-2.92006200
C	0.56897300	-2.39478000	-0.32495300
H	1.22049800	-1.55680100	-0.05760600
H	1.20931100	-3.24201100	-0.60715200
H	-0.02413200	-2.67421400	0.54992700
C	-1.16334500	-3.20196900	-1.78761000
H	-1.67517500	-3.57422200	-0.89522700
H	-0.54746600	-4.01731500	-2.20017000
H	-1.91659700	-2.92507700	-2.53532300
C	-0.60905300	1.41636700	-3.37106800
H	-0.89650800	0.59180100	-4.03053900
H	0.11992200	2.04925400	-3.90167000
H	-1.50573200	2.01162700	-3.17326000
C	-1.87523800	4.85238400	1.93502500
H	-1.99037500	5.93807400	2.04521600
H	-0.83113900	4.64653600	1.68895000
H	-2.08944700	4.38043400	2.89975500
C	-4.28512800	4.66934400	1.26730400
H	-5.02161900	4.19581700	0.60758500
H	-4.42287200	5.75400900	1.20459500
H	-4.51654600	4.38746100	2.29722000
C	-2.59989600	5.08235200	-0.48303300
H	-1.54626800	5.23493800	-0.71447200
H	-3.04929700	6.07836800	-0.40884300
H	-3.07282200	4.56932800	-1.32891900
C	-2.45976900	-1.57432800	2.11030000
C	-1.24782500	-1.86476800	2.79493500
C	-1.10071600	-3.13197900	3.37105100

H	-0.19102800	-3.37063300	3.91098000
C	-2.09127400	-4.10708100	3.25213200
H	-1.94998000	-5.08418300	3.70629600
C	-3.24857200	-3.82944400	2.53314500
H	-4.00774400	-4.59982800	2.42154400
C	-3.45576100	-2.57022300	1.95437000
C	-4.72645900	-2.32112600	1.14573400
H	-4.74770200	-1.26078400	0.87682400
C	-4.70968900	-3.12958200	-0.16551700
H	-3.86988600	-2.83612000	-0.80520700
H	-5.63722400	-2.97239200	-0.72779000
H	-4.61295000	-4.20237300	0.03599600
C	-6.01595800	-2.62989400	1.92965600
H	-6.11366500	-3.70232300	2.13344800
H	-6.89464200	-2.31942700	1.35094000
H	-6.03868800	-2.10916000	2.89217900
C	-0.11667500	-0.83604000	2.85723500
H	-0.05899500	-0.36113700	1.86732400
C	-0.38225600	0.30073500	3.86441000
H	-1.26169400	0.89119100	3.59909800
H	0.47751400	0.97909100	3.87804200
H	-0.52062600	-0.10325600	4.87505300
C	1.25767900	-1.46020900	3.14179900
H	1.35685500	-1.74832800	4.19612800
H	2.04722400	-0.74180400	2.90881900
H	1.43999500	-2.35035300	2.53382600
C	-4.15421700	-0.15896400	-1.85346100
C	-6.68459000	-0.43180900	-1.65862700
C	-7.32490500	0.32796800	-0.65770200
C	-8.68948600	0.09599000	-0.46730900
H	-9.21640400	0.65918100	0.29741600
C	-9.37511000	-0.84089500	-1.24176300
H	-10.43549000	-1.00544900	-1.07392700
C	-8.71111000	-1.56591300	-2.23282000
H	-9.25435600	-2.28925400	-2.83395800
C	-7.34768500	-1.37715400	-2.46636500
C	-6.60075400	-2.14468500	-3.52674300
H	-5.78398500	-2.73263700	-3.09127200
H	-6.15108900	-1.46854100	-4.26407000
H	-7.26851900	-2.82943600	-4.05579300
C	-6.55997400	1.33800300	0.15473500
H	-5.70945800	0.89179200	0.68106100
H	-7.20621100	1.81382000	0.89679600
H	-6.13789300	2.12428100	-0.48316100
Si	3.83340900	0.04277000	0.27108600
Si	5.01155800	-2.75135300	-0.35134300
Si	7.05850000	-0.79139200	0.96136100

Si	6.08707600	-0.31050200	-1.97668200
C	4.46572400	1.89820400	0.46041400
H	5.50875700	2.00327900	0.17489200
C	4.24289700	1.22767500	1.82017900
H	5.11964700	0.97687800	2.41317500
C	3.14186600	1.76837600	2.61466900
H	2.96999500	1.32711400	3.59642300
C	2.34738700	2.78776900	2.20781700
H	1.53646500	3.14164500	2.84272400
C	2.61376600	3.52647200	0.97325500
C	1.90840700	4.69367100	0.64806300
H	1.15929400	5.06171400	1.34636500
C	2.16389100	5.40517800	-0.52875300
H	1.59162900	6.29995800	-0.76235800
C	3.17300800	4.96033200	-1.38421900
H	3.38918100	5.49712200	-2.30525900
C	3.92595300	3.83090600	-1.04409700
H	4.72967300	3.50221400	-1.70034900
C	3.66609200	3.09279100	0.11971000
C	5.59348400	-0.93779800	-0.24569800
C	3.96336200	-3.32346100	1.13109100
H	4.46485000	-3.18908600	2.09311800
H	3.73796900	-4.39247900	1.01368400
H	3.01892600	-2.77657500	1.17645300
C	6.37756600	-4.07242200	-0.49478400
H	7.07933500	-3.88015600	-1.31152100
H	5.90095100	-5.04377100	-0.68440600
H	6.95400100	-4.16897100	0.43222500
C	3.86849000	-3.05311000	-1.85183900
H	3.07384200	-2.30330900	-1.86498900
H	3.40434800	-4.04416100	-1.75973400
H	4.38747600	-3.01448200	-2.81468900
C	6.68059800	-1.63296700	2.62739100
H	5.70542800	-1.32424200	3.02022100
H	7.44605100	-1.35213900	3.36200400
H	6.68255900	-2.72655700	2.55274700
C	8.67527500	-1.57617600	0.31192000
H	8.57698200	-2.61912100	0.00216900
H	9.42993600	-1.53301700	1.10885700
H	9.07383100	-1.01183100	-0.53945900
C	7.66547900	0.96107400	1.41350900
H	8.04931600	1.50844200	0.54871800
H	8.50680700	0.82423800	2.10708100
H	6.93165500	1.59850000	1.91119600
C	7.22054200	1.22178600	-2.01404000
H	6.82374600	2.07684400	-1.45936300
H	7.32155500	1.52716500	-3.06427300

H	8.22843200	1.01245400	-1.64004700
C	7.07100000	-1.58217200	-3.00862500
H	7.98490400	-1.89945900	-2.49510500
H	7.36979600	-1.11301700	-3.95562300
H	6.50049600	-2.48362100	-3.25423600
C	4.60816100	0.19648500	-3.06844900
H	4.07492500	1.05420300	-2.64449500
H	3.88898000	-0.61537100	-3.20796600
H	4.98699100	0.48456100	-4.05856400

IM0_1

Charge=0, Multiplicity=1

Yb	-1.20247700	-0.59594100	0.39852900
N	-3.18315800	0.50819600	-0.79535300
N	-3.15323200	-2.12700100	0.55914600
N	-0.71047800	-2.71211400	2.12191800
N	-0.35470800	0.23185400	2.92955300
C	-4.95923200	0.45668300	-2.55342800
H	-5.17985400	1.48836900	-2.27768900
H	-5.90158600	-0.09527900	-2.59922600
H	-4.53187900	0.46198100	-3.56289500
C	-3.99233500	-0.20926600	-1.57316900
C	-4.10892800	-1.61847300	-1.55890400
H	-4.69085600	-1.99430000	-2.38367000
C	-3.92797800	-2.49241100	-0.45843700
C	-4.80353400	-3.80315600	-0.50175900
C	-3.16924300	-2.79389500	1.85166300
H	-4.03757200	-3.42863100	2.03777800
H	-3.22270100	-2.01392100	2.62871600
C	-1.88528800	-3.60444200	2.04815900
H	-1.94516500	-4.24717900	2.94428300
H	-1.74957700	-4.25359500	1.18244100
C	-0.55430900	-2.21231500	3.49997300
H	-0.07921100	-2.98108700	4.13411800
H	-1.54638900	-2.03777900	3.92484600
C	0.27152800	-0.93968500	3.57906600
H	0.48256800	-0.71539300	4.64045000
H	1.23222000	-1.09801100	3.08181500
C	-1.56637700	0.67760900	3.63203000
H	-1.94730800	1.57260200	3.13524600
H	-1.37354800	0.91757800	4.69247700
H	-2.35053600	-0.08260400	3.58634100
C	0.64422300	1.31703500	2.95181500
H	1.46260900	1.06020600	2.28020400
H	1.03996800	1.47583600	3.96924200
H	0.19175400	2.24526800	2.61096200
C	0.50451000	-3.43178800	1.69831000
H	1.34984400	-2.74508900	1.67031600

H	0.36375500	-3.81710300	0.68904400
H	0.73502300	-4.27223700	2.37534600
C	-4.06798200	-5.06888000	0.00916700
H	-3.08986700	-5.17139200	-0.46837100
H	-4.65744100	-5.95753800	-0.24306200
H	-3.92020400	-5.09622800	1.08829200
C	-6.09355500	-3.55040000	0.31610600
H	-5.89394800	-3.35459700	1.37342000
H	-6.75785400	-4.42214400	0.25678300
H	-6.62842300	-2.68253500	-0.08517400
C	-5.25148200	-4.16584000	-1.94242800
H	-5.94962900	-3.43944700	-2.36640400
H	-5.77196200	-5.12968300	-1.92078700
H	-4.39649000	-4.26303600	-2.62076800
C	-3.42051700	1.90843100	-0.65840600
C	-3.00152400	2.86020000	-1.62326100
C	-3.19837200	4.22262600	-1.35717000
H	-2.86642100	4.95723400	-2.08614100
C	-3.83250000	4.65464100	-0.19858400
H	-3.98437300	5.71568600	-0.01900100
C	-4.27889500	3.71334200	0.72821300
H	-4.78733000	4.05842100	1.62279500
C	-4.07078700	2.34421700	0.53137000
C	-4.58309100	1.32510300	1.54935600
H	-3.83382300	0.52685000	1.62008400
C	-5.88639800	0.64807700	1.07453500
H	-6.66884500	1.39840600	0.90743900
H	-6.24685900	-0.05755300	1.83357400
H	-5.73604000	0.08881600	0.14968900
C	-4.79967100	1.90511600	2.95667800
H	-3.93841700	2.48279500	3.30922300
H	-4.98089200	1.09318400	3.67048800
H	-5.67540600	2.56423500	2.99016900
C	-2.40784300	2.46497000	-2.97522200
H	-2.37155300	1.37257800	-3.02158700
C	-3.27616100	2.97865200	-4.14463900
H	-4.32876100	2.70872900	-4.03285200
H	-2.91462300	2.56717900	-5.09483600
H	-3.22239600	4.07126500	-4.21783500
C	-0.97245800	2.97905300	-3.16572000
H	-0.92339500	4.07036100	-3.07134600
H	-0.59704400	2.71069800	-4.16086000
H	-0.30027500	2.55059700	-2.42573500
C	1.30185700	4.83386000	-0.81239900
C	1.60060400	6.19969400	-0.77081900
C	0.98728400	7.04715000	0.14782100
C	0.06458200	6.53780400	1.06161500

C	-0.26671300	5.18214600	1.07260800
C	0.35555800	4.35062300	0.11412600
H	2.32931400	6.59481100	-1.47367400
H	1.23240200	8.10548700	0.15772400
H	-0.40674900	7.19867100	1.78407700
C	-1.22549600	4.63588300	2.09946100
H	-1.82315800	3.81103500	1.70741500
H	-0.68225400	4.27771500	2.98358100
H	-1.91699800	5.41505000	2.43264600
C	1.98493500	3.95083400	-1.82440500
H	1.88898900	2.89089200	-1.58597000
H	1.56710400	4.10991100	-2.82480500
H	3.05200600	4.18493100	-1.87256000
N	0.00896000	3.00754300	0.09530800
C	-0.34864700	1.89074900	0.10318000
Si	2.53490900	-0.74495300	-0.18541400
Si	4.66253900	0.94678100	1.29928700
Si	5.48340300	0.14179500	-1.61803900
Si	5.32862600	-2.03852100	0.61094700
C	2.39512800	-2.00645400	-1.67714100
H	3.36287900	-2.31536900	-2.06084800
C	1.96427000	-0.59885400	-2.11705600
H	2.61234900	-0.03613700	-2.78446400
C	0.54963000	-0.42195100	-2.36320900
H	0.21712700	0.54067400	-2.74258500
C	-0.38825900	-1.39655400	-2.15060200
H	-1.43165700	-1.21530600	-2.41211400
C	0.00926700	-2.78662900	-1.87766500
C	-0.93606900	-3.82296600	-1.85707500
H	-1.98437800	-3.56813700	-1.98711700
C	-0.54308900	-5.15445800	-1.69526300
H	-1.28679200	-5.94690800	-1.68641200
C	0.81482000	-5.45793700	-1.57395800
H	1.13703000	-6.48931100	-1.45359400
C	1.76552800	-4.43341900	-1.60662300
H	2.82171000	-4.67594300	-1.51066000
C	1.38963400	-3.08886600	-1.72802900
C	4.55261500	-0.41528700	-0.04455600
C	3.50624000	2.42261600	0.95878800
H	3.96125500	3.13338600	0.26300800
H	3.30647500	2.96026700	1.89470800
H	2.54728800	2.11120000	0.53875800
C	6.36969300	1.75517500	1.53377400
H	7.16617800	1.03648400	1.74610800
H	6.30731200	2.44563700	2.38559600
H	6.66754400	2.34334500	0.65889300
C	4.18681300	0.29162500	3.02602700

H	3.21939900	-0.21655000	3.02087100
H	4.11915600	1.13592000	3.72429400
H	4.92552600	-0.41051800	3.42522700
C	4.98417100	1.89648500	-2.15114700
H	3.89655600	1.97956800	-2.22275700
H	5.40619500	2.11113300	-3.14099900
H	5.33849500	2.67206700	-1.46381100
C	7.38194700	0.15551900	-1.42326200
H	7.74126400	0.72335400	-0.56165000
H	7.81409000	0.60901300	-2.32534800
H	7.78881600	-0.85942600	-1.34771300
C	5.25871000	-0.90575700	-3.19635100
H	5.54954900	-1.95140100	-3.06934700
H	5.93195100	-0.47305000	-3.94914400
H	4.25016800	-0.88949200	-3.61666200
C	5.83490700	-3.29053500	-0.72959100
H	5.00599300	-3.57118800	-1.38594300
H	6.17262500	-4.20157500	-0.21820000
H	6.66255300	-2.94221600	-1.35539300
C	6.93360300	-1.77325500	1.60705700
H	7.70094400	-1.25460800	1.02356100
H	7.33632300	-2.75696200	1.88251200
H	6.78410900	-1.21070300	2.53429100
C	4.17162800	-3.04548700	1.73855000
H	3.69224100	-2.45729300	2.52673600
H	4.76092700	-3.83567200	2.22291500
H	3.38613400	-3.53193400	1.15055400

TS1_1'

Charge=0, Multiplicity=1

Yb	-0.72290000	-0.35660000	0.21220000
N	-2.72360000	0.93670000	0.51740000
N	-1.19120000	-0.49900000	2.55730000
N	-1.22880000	-2.91410000	0.78310000
N	-4.17130000	-3.22770000	-1.57260000
C	-3.21130000	3.26180000	1.19410000
H	-2.93710000	3.66880000	0.21440000
H	-2.93420000	3.98660000	1.96340000
H	-4.30060000	3.15180000	1.19870000
C	-2.52840000	1.91830000	1.41650000
C	-1.75210000	1.80430000	2.58660000
H	-1.63740000	2.73130000	3.12430000
C	-1.36270000	0.60880000	3.26350000
C	-1.24260000	0.69150000	4.81890000
C	-1.17560000	-1.85330000	3.08960000
H	-1.69750000	-1.96070000	4.04530000
H	-0.14490000	-2.19560000	3.25470000
C	-1.88530000	-2.79380000	2.10900000

H	-1.97700000	-3.79520000	2.56590000
H	-2.89700000	-2.41040000	1.94630000
C	-2.14780000	-3.60840000	-0.15640000
H	-2.79600000	-4.31570000	0.38280000
H	-1.53700000	-4.18690000	-0.84970000
C	-3.01520000	-2.61310000	-0.93320000
H	-3.39230000	-1.84140000	-0.25190000
H	-2.36700000	-2.09370000	-1.67670000
C	-3.82200000	-4.27740000	-2.52120000
H	-3.24250000	-5.07000000	-2.03950000
H	-3.24130000	-3.89660000	-3.38560000
H	-4.74040000	-4.72810000	-2.91220000
C	-5.00130000	-2.21670000	-2.22210000
H	-5.91150000	-2.68550000	-2.61170000
H	-4.48360000	-1.71710000	-3.06430000
H	-5.28980000	-1.45020000	-1.50370000
C	0.04080000	-3.66220000	0.89870000
H	0.49220000	-3.76720000	-0.08720000
H	-0.11740000	-4.66410000	1.33110000
H	0.74870000	-3.11030000	1.51930000
C	-0.04500000	-0.12240000	5.36230000
H	-0.12980000	-1.19700000	5.20610000
H	0.04410000	0.03790000	6.44300000
H	0.88620000	0.21250000	4.89580000
C	-2.57600000	0.20330000	5.43710000
H	-3.41010000	0.80210000	5.05590000
H	-2.54540000	0.30900000	6.52870000
H	-2.79090000	-0.84540000	5.21240000
C	-1.01910000	2.14210000	5.31260000
H	-0.13920000	2.59540000	4.84290000
H	-0.85220000	2.12810000	6.39560000
H	-1.88390000	2.78500000	5.12720000
C	-3.93760000	0.97970000	-0.22710000
C	-5.10690000	0.45270000	0.38270000
C	-6.32340000	0.54020000	-0.30260000
H	-7.22930000	0.16730000	0.16850000
C	-6.38840000	1.07380000	-1.58940000
H	-7.33890000	1.12430000	-2.11390000
C	-5.22310000	1.52520000	-2.20410000
H	-5.27410000	1.92490000	-3.21320000
C	-3.99050000	1.50280000	-1.53790000
C	-2.73980000	2.03430000	-2.22440000
H	-1.95760000	2.14330000	-1.46500000
C	-2.22570000	1.02460000	-3.26510000
H	-1.98720000	0.06220000	-2.79690000
H	-1.32000000	1.40270000	-3.75160000
H	-2.98080000	0.83640000	-4.03800000

C	-2.94540000	3.41440000	-2.86840000
H	-3.65870000	3.37150000	-3.70020000
H	-1.99660000	3.79300000	-3.25690000
H	-3.32510000	4.13820000	-2.13930000
C	-5.04190000	-0.20370000	1.75890000
H	-3.98330000	-0.35840000	1.98890000
C	-5.61870000	0.71240000	2.85420000
H	-5.05620000	1.64930000	2.91910000
H	-5.57020000	0.22190000	3.83440000
H	-6.66840000	0.95730000	2.64940000
C	-5.73250000	-1.58100000	1.78010000
H	-6.81800000	-1.49600000	1.65110000
H	-5.55830000	-2.07510000	2.74430000
H	-5.35810000	-2.23850000	0.98660000
C	0.24270000	4.27170000	-1.10680000
C	-0.21900000	5.49520000	-1.60280000
C	-0.12540000	5.82110000	-2.95440000
C	0.44120000	4.90400000	-3.83690000
C	0.92480000	3.67070000	-3.38990000
C	0.82330000	3.34780000	-2.01340000
H	-0.66270000	6.20370000	-0.90690000
H	-0.49260000	6.77770000	-3.31540000
H	0.51840000	5.14450000	-4.89470000
C	1.52840000	2.70400000	-4.37890000
H	1.82590000	3.22010000	-5.29740000
H	2.40540000	2.20010000	-3.96270000
H	0.81740000	1.91890000	-4.66680000
C	0.15620000	3.99850000	0.37460000
H	-0.20120000	2.99280000	0.59630000
H	1.13700000	4.10460000	0.85380000
H	-0.52290000	4.70830000	0.85650000
N	1.42760000	2.15090000	-1.58280000
C	1.01750000	1.20730000	-0.87230000
Si	2.26310000	-0.43130000	-0.28090000
Si	3.53010000	0.38950000	2.32060000
Si	4.85430000	1.69040000	-0.21800000
Si	5.28360000	-1.35640000	0.45010000
C	2.85960000	-2.09360000	-2.13210000
H	3.90400000	-2.22760000	-1.89120000
C	2.37410000	-0.79670000	-2.47900000
H	3.06730000	-0.01210000	-2.76470000
C	1.02940000	-0.72470000	-3.01370000
H	0.65550000	0.23240000	-3.34430000
C	0.23220000	-1.83160000	-3.09840000
H	-0.76700000	-1.74810000	-3.51890000
C	0.71780000	-3.14220000	-2.75180000
C	-0.05700000	-4.30340000	-2.93530000

H	-1.05780000	-4.20400000	-3.34550000
C	0.44030000	-5.55660000	-2.60480000
H	-0.17260000	-6.44210000	-2.74760000
C	1.74890000	-5.67650000	-2.09570000
H	2.14110000	-6.65700000	-1.83970000
C	2.54290000	-4.55490000	-1.93280000
H	3.55570000	-4.65260000	-1.55470000
C	2.05390000	-3.26110000	-2.25060000
C	4.03040000	0.09920000	0.48130000
C	1.96420000	1.45100000	2.46670000
H	1.87220000	2.19270000	1.67360000
H	1.97170000	1.98780000	3.42450000
H	1.06110000	0.83670000	2.45550000
C	4.84500000	1.29830000	3.35120000
H	5.81340000	0.79270000	3.37130000
H	4.47470000	1.34990000	4.38390000
H	5.00760000	2.32600000	3.01210000
C	3.15300000	-1.22630000	3.24890000
H	2.44090000	-1.84250000	2.69000000
H	2.70160000	-0.98340000	4.21840000
H	4.04400000	-1.83040000	3.44560000
C	3.99920000	3.30740000	0.29230000
H	3.00240000	3.37410000	-0.14630000
H	4.59230000	4.13830000	-0.11140000
H	3.91820000	3.45700000	1.37330000
C	6.66320000	1.92540000	0.34090000
H	6.77420000	1.94190000	1.42900000
H	6.99620000	2.90080000	-0.03760000
H	7.35140000	1.17330000	-0.05690000
C	4.88260000	1.75000000	-2.11090000
H	5.27150000	0.84290000	-2.58330000
H	5.51510000	2.58800000	-2.43060000
H	3.86940000	1.94170000	-2.47460000
C	6.27340000	-1.43860000	-1.18100000
H	5.67930000	-1.38970000	-2.09800000
H	6.83010000	-2.38470000	-1.19880000
H	7.00930000	-0.62990000	-1.23510000
C	6.65000000	-1.29010000	1.77510000
H	7.23790000	-0.36960000	1.75310000
H	7.33410000	-2.12610000	1.57650000
H	6.26300000	-1.42460000	2.79020000
C	4.47630000	-3.06360000	0.73340000
H	4.53020000	-3.33960000	1.79150000
H	5.03100000	-3.82620000	0.17150000
H	3.42740000	-3.11360000	0.43130000

TS1_1

Charge=0, Multiplicity=1

Yb	1.08780000	0.16800000	-0.36100000
N	2.90640000	0.81710000	0.96340000
N	2.19720000	1.77590000	-1.72550000
N	1.79300000	-1.00000000	-2.52400000
N	4.00660000	-3.58600000	-0.88860000
C	3.20560000	2.67860000	2.55150000
H	2.65310000	2.16160000	3.34360000
H	3.02000000	3.75190000	2.63500000
H	4.26910000	2.49460000	2.73690000
C	2.79860000	2.13680000	1.18930000
C	2.34290000	3.08450000	0.24520000
H	2.22200000	4.07450000	0.65440000
C	2.32350000	2.97430000	-1.18630000
C	2.52500000	4.28910000	-2.00060000
C	2.40230000	1.38990000	-3.10880000
H	3.19920000	1.94320000	-3.62010000
H	1.48840000	1.54490000	-3.69940000
C	2.78950000	-0.09440000	-3.15320000
H	2.96400000	-0.40120000	-4.19870000
H	3.73020000	-0.21630000	-2.60720000
C	2.38830000	-2.35080000	-2.34100000
H	3.12010000	-2.56440000	-3.13380000
H	1.58440000	-3.08260000	-2.43400000
C	3.06390000	-2.47860000	-0.96960000
H	3.61950000	-1.55840000	-0.75150000
H	2.26870000	-2.56420000	-0.19390000
C	3.37670000	-4.88620000	-1.09500000
H	2.88950000	-4.93440000	-2.07330000
H	2.62320000	-5.12670000	-0.32000000
H	4.14590000	-5.66530000	-1.06980000
C	4.72210000	-3.56540000	0.38580000
H	5.48210000	-4.35430000	0.38880000
H	4.05590000	-3.72430000	1.25460000
H	5.22190000	-2.60520000	0.52270000
C	0.54840000	-1.08370000	-3.31780000
H	-0.18170000	-1.70950000	-2.79990000
H	0.72280000	-1.50240000	-4.32070000
H	0.10000000	-0.09390000	-3.43260000
C	1.56920000	4.36800000	-3.21300000
H	1.76710000	3.61610000	-3.97660000
H	1.67020000	5.34660000	-3.69600000
H	0.52720000	4.26190000	-2.89050000
C	4.00370000	4.34490000	-2.45670000
H	4.67060000	4.30240000	-1.58850000
H	4.19650000	5.28190000	-2.99360000
H	4.27150000	3.52030000	-3.12320000
C	2.25540000	5.56020000	-1.16120000

H	1.24180000	5.56270000	-0.74430000
H	2.35290000	6.44070000	-1.80610000
H	2.97060000	5.67920000	-0.34240000
C	3.86520000	0.07210000	1.70540000
C	5.20660000	0.08550000	1.24120000
C	6.17590000	-0.61380000	1.96770000
H	7.21160000	-0.58820000	1.63880000
C	5.83260000	-1.36220000	3.09340000
H	6.59640000	-1.90640000	3.64230000
C	4.50150000	-1.42290000	3.49820000
H	4.23300000	-2.02590000	4.36180000
C	3.50150000	-0.70940000	2.82490000
C	2.05580000	-0.79780000	3.29630000
H	1.47750000	-0.06800000	2.72130000
C	1.46460000	-2.19190000	3.01540000
H	1.48700000	-2.43150000	1.94730000
H	0.42030000	-2.24650000	3.34170000
H	2.02830000	-2.96970000	3.54450000
C	1.88860000	-0.42730000	4.78070000
H	2.37640000	-1.15810000	5.43640000
H	0.82510000	-0.40160000	5.04700000
H	2.32050000	0.55540000	4.99960000
C	5.58240000	0.83460000	-0.03570000
H	4.64810000	1.09690000	-0.54120000
C	6.32410000	2.14900000	0.27050000
H	5.70660000	2.81860000	0.87790000
H	6.57740000	2.67550000	-0.65820000
H	7.25630000	1.95810000	0.81660000
C	6.39860000	-0.03950000	-1.00620000
H	7.38540000	-0.29430000	-0.60220000
H	6.56170000	0.49670000	-1.94940000
H	5.88320000	-0.97970000	-1.23470000
C	-2.40940000	-3.80610000	1.95700000
C	-3.02390000	-5.03870000	2.20560000
C	-2.85950000	-6.12420000	1.34850000
C	-2.03710000	-6.00160000	0.22700000
C	-1.38260000	-4.80250000	-0.05020000
C	-1.59870000	-3.69750000	0.80650000
H	-3.65260000	-5.13640000	3.08770000
H	-3.35780000	-7.06630000	1.55990000
H	-1.88880000	-6.85050000	-0.43580000
C	-0.45730000	-4.66490000	-1.22890000
H	-0.84280000	-3.94110000	-1.95560000
H	0.52450000	-4.30990000	-0.89920000
H	-0.32380000	-5.62300000	-1.74160000
C	-2.64750000	-2.65260000	2.89640000
H	-2.73080000	-3.00480000	3.93090000

H	-1.85470000	-1.90350000	2.84250000
H	-3.57810000	-2.13690000	2.63870000
N	-0.94040000	-2.52460000	0.48540000
C	-0.88670000	-1.32660000	0.28270000
Si	-3.17190000	-0.04830000	0.33330000
Si	-2.54000000	2.06450000	2.44400000
Si	-5.26580000	2.48740000	0.95410000
Si	-2.59460000	2.91380000	-0.60240000
C	-4.10410000	-0.34340000	-1.35080000
H	-4.57300000	0.55220000	-1.75270000
C	-4.84160000	-0.96210000	-0.14890000
H	-5.77520000	-0.49450000	0.16010000
C	-4.86880000	-2.42790000	-0.10950000
H	-5.39480000	-2.89760000	0.72030000
C	-4.25810000	-3.20920000	-1.02660000
H	-4.27410000	-4.29070000	-0.92020000
C	-3.60730000	-2.65510000	-2.21380000
C	-3.06360000	-3.48560000	-3.20490000
H	-3.08720000	-4.56300000	-3.05210000
C	-2.51090000	-2.96010000	-4.37640000
H	-2.09310000	-3.62430000	-5.12870000
C	-2.52200000	-1.57830000	-4.57740000
H	-2.11220000	-1.15280000	-5.49070000
C	-3.06390000	-0.73760000	-3.59920000
H	-3.07220000	0.33970000	-3.75790000
C	-3.58940000	-1.24680000	-2.40460000
C	-3.45310000	1.91410000	0.76610000
C	-3.14330000	0.79290000	3.73390000
H	-3.64340000	1.29780000	4.56880000
H	-2.29250000	0.23660000	4.14530000
H	-3.84230000	0.06230000	3.32060000
C	-2.68020000	3.74810000	3.31910000
H	-2.42450000	4.60330000	2.68770000
H	-1.99340000	3.74670000	4.17600000
H	-3.68970000	3.90750000	3.71430000
C	-0.67530000	1.72030000	2.25670000
H	-0.14050000	2.42230000	1.60830000
H	-0.55050000	0.69890000	1.87620000
H	-0.19580000	1.75840000	3.24270000
C	-6.10490000	1.69840000	2.46450000
H	-6.03130000	0.60560000	2.43790000
H	-7.16960000	1.96370000	2.46190000
H	-5.68150000	2.03780000	3.41570000
C	-5.40110000	4.37920000	1.15610000
H	-4.79350000	4.77950000	1.97120000
H	-6.44790000	4.64080000	1.35950000
H	-5.11130000	4.90420000	0.23820000

C	-6.44220000	2.14230000	-0.50360000
H	-6.15410000	2.66230000	-1.42060000
H	-7.42440000	2.53420000	-0.20610000
H	-6.57550000	1.08590000	-0.74740000
C	-3.64140000	3.34400000	-2.12800000
H	-4.08860000	2.46880000	-2.60760000
H	-2.97470000	3.81990000	-2.85950000
H	-4.44190000	4.05710000	-1.90690000
C	-1.85540000	4.57790000	-0.04230000
H	-2.61110000	5.25400000	0.37120000
H	-1.40290000	5.07450000	-0.91150000
H	-1.06830000	4.45040000	0.70930000
C	-1.08060000	1.98520000	-1.30360000
H	-0.26240000	2.15520000	-0.59520000
H	-0.75730000	2.41530000	-2.25680000
H	-1.29540000	0.92090000	-1.45400000

TS1_2

Charge=0, Multiplicity=1

Yb	1.34440000	0.48780000	-0.61320000
N	3.12190000	-0.00340000	0.91660000
N	1.76360000	2.60900000	0.40690000
N	1.74830000	2.27140000	-2.51010000
N	2.09160000	-0.72300000	-2.79630000
N	-0.22640000	-2.04230000	0.95280000
C	3.67020000	-0.21730000	3.31940000
H	3.19690000	-1.17300000	3.56510000
H	3.66010000	0.40830000	4.21480000
H	4.70950000	-0.43230000	3.05410000
C	2.93930000	0.44820000	2.16040000
C	2.10520000	1.53640000	2.51280000
H	1.95190000	1.61770000	3.57620000
C	1.71680000	2.66640000	1.73600000
C	1.35270000	3.95640000	2.54790000
C	1.77720000	3.75860000	-0.48650000
H	2.33220000	4.61680000	-0.08910000
H	0.76340000	4.12000000	-0.70040000
C	2.45450000	3.36860000	-1.80620000
H	2.54270000	4.25340000	-2.46030000
H	3.46520000	3.02040000	-1.58010000
C	2.62830000	1.60530000	-3.49480000
H	3.60960000	1.47180000	-3.02890000
H	2.77780000	2.23990000	-4.38550000
C	2.08180000	0.24330000	-3.92020000
H	1.05500000	0.33820000	-4.28110000
H	2.67310000	-0.14230000	-4.76620000
C	3.41100000	-1.37420000	-2.69010000
H	4.19350000	-0.62970000	-2.52670000

H	3.64650000	-1.94760000	-3.60180000
H	3.42910000	-2.04840000	-1.83370000
C	1.03230000	-1.73630000	-2.97510000
H	1.03600000	-2.42250000	-2.12510000
H	1.16520000	-2.31440000	-3.90150000
H	0.05360000	-1.25330000	-3.01640000
C	0.53200000	2.77990000	-3.17120000
H	-0.06150000	1.95690000	-3.57240000
H	0.78390000	3.47190000	-3.99270000
H	-0.09040000	3.30650000	-2.44960000
C	2.62020000	4.83910000	2.65250000
H	2.41480000	5.72090000	3.27230000
H	2.96940000	5.19420000	1.67850000
H	3.43760000	4.27530000	3.11530000
C	0.89840000	3.63800000	3.99510000
H	0.07680000	2.91490000	4.01110000
H	0.54660000	4.56130000	4.46870000
H	1.71190000	3.25370000	4.61690000
C	0.18740000	4.74880000	1.90870000
H	0.45680000	5.24550000	0.97680000
H	-0.14220000	5.53390000	2.59820000
H	-0.66970000	4.09740000	1.71340000
C	4.26760000	-0.79210000	0.59640000
C	5.38790000	-0.10960000	0.04750000
C	6.49880000	-0.85060000	-0.36580000
H	7.36220000	-0.33930000	-0.78130000
C	6.51990000	-2.24050000	-0.25350000
H	7.39060000	-2.80300000	-0.58000000
C	5.42030000	-2.89930000	0.28480000
H	5.44060000	-3.98210000	0.37740000
C	4.28270000	-2.20130000	0.71640000
C	3.10940000	-2.98930000	1.28820000
H	2.32760000	-2.27840000	1.56690000
C	2.50900000	-3.94640000	0.24260000
H	2.09000000	-3.39490000	-0.60400000
H	1.70460000	-4.53990000	0.68590000
H	3.26550000	-4.63720000	-0.14740000
C	3.50490000	-3.78920000	2.54580000
H	4.19490000	-4.60420000	2.29540000
H	2.61230000	-4.23210000	3.00250000
H	3.99970000	-3.15830000	3.29060000
C	5.37970000	1.41180000	-0.05610000
H	4.33160000	1.71730000	-0.13390000
C	5.92500000	2.06060000	1.23190000
H	5.32910000	1.77150000	2.10190000
H	5.89610000	3.15490000	1.15520000
H	6.96390000	1.75690000	1.41030000

C	6.13220000	1.94890000	-1.28400000
H	7.21630000	1.81150000	-1.19620000
H	5.95400000	3.02520000	-1.39620000
H	5.81140000	1.45110000	-2.20730000
C	-0.47240000	-1.12000000	0.20380000
C	-0.48260000	-3.15590000	1.72780000
C	-0.18300000	-3.11020000	3.10810000
C	-0.37460000	-4.27130000	3.86250000
H	-0.15540000	-4.24390000	4.92730000
C	-0.83110000	-5.44980000	3.27550000
H	-0.97030000	-6.34250000	3.87870000
C	-1.10050000	-5.47940000	1.90630000
H	-1.44740000	-6.39890000	1.44130000
C	-0.93400000	-4.34660000	1.10840000
C	-1.17570000	-4.39040000	-0.37610000
H	-0.23610000	-4.26830000	-0.93190000
H	-1.84110000	-3.59230000	-0.70380000
H	-1.61830000	-5.34580000	-0.67380000
C	0.30030000	-1.84520000	3.76940000
H	0.79190000	-1.17010000	3.06460000
H	1.00050000	-2.07450000	4.57990000
H	-0.53800000	-1.28960000	4.20430000
Si	-3.01850000	-0.72250000	-0.38010000
Si	-3.55390000	0.28830000	2.48260000
Si	-5.98850000	0.54700000	0.50330000
Si	-3.45900000	2.35420000	0.13480000
C	-3.57910000	-0.47200000	-2.23070000
H	-4.27020000	0.36060000	-2.34020000
C	-4.20400000	-1.72900000	-1.58580000
H	-5.26300000	-1.68950000	-1.33830000
C	-3.80640000	-3.00790000	-2.17570000
H	-4.24900000	-3.90860000	-1.75210000
C	-2.93610000	-3.12340000	-3.20450000
H	-2.66960000	-4.10530000	-3.59030000
C	-2.39240000	-1.95660000	-3.89480000
C	-1.60190000	-2.09330000	-5.04620000
H	-1.36000000	-3.09480000	-5.39760000
C	-1.13180000	-0.98010000	-5.74680000
H	-0.51970000	-1.11130000	-6.63550000
C	-1.47140000	0.29960000	-5.30150000
H	-1.13120000	1.17880000	-5.84440000
C	-2.27110000	0.45110000	-4.16180000
H	-2.55220000	1.44900000	-3.82950000
C	-2.73320000	-0.65400000	-3.43320000
C	-4.08560000	0.64170000	0.66900000
C	-3.56380000	-1.55990000	2.91510000
H	-4.56220000	-1.99890000	2.83100000

H	-3.23100000	-1.68300000	3.95460000
H	-2.89060000	-2.14590000	2.28370000
C	-4.63390000	1.11690000	3.81330000
H	-4.69590000	2.20360000	3.69790000
H	-4.18230000	0.91210000	4.79290000
H	-5.65420000	0.71970000	3.83550000
C	-1.79040000	0.90520000	2.86160000
H	-1.02400000	0.40660000	2.26270000
H	-1.57280000	0.69300000	3.91590000
H	-1.67380000	1.98330000	2.72340000
C	-6.67460000	-1.04810000	1.27640000
H	-6.12490000	-1.92980000	0.92880000
H	-7.72680000	-1.17070000	0.99020000
H	-6.63070000	-1.03630000	2.37110000
C	-6.88870000	2.01450000	1.32640000
H	-6.60460000	2.19780000	2.36450000
H	-7.96800000	1.81250000	1.30520000
H	-6.72630000	2.94230000	0.76490000
C	-6.71530000	0.61640000	-1.25930000
H	-6.46870000	1.54570000	-1.77930000
H	-7.80730000	0.59460000	-1.14050000
H	-6.44370000	-0.21420000	-1.91460000
C	-4.29170000	3.12010000	-1.39610000
H	-4.27880000	2.46730000	-2.27360000
H	-3.73620000	4.03220000	-1.65390000
H	-5.32910000	3.41770000	-1.21030000
C	-3.65180000	3.71670000	1.45460000
H	-4.70570000	3.86390000	1.71360000
H	-3.27660000	4.66420000	1.04590000
H	-3.10950000	3.52180000	2.38420000
C	-1.61740000	2.29860000	-0.33960000
H	-1.48550000	1.68590000	-1.23950000
H	-0.99590000	1.89840000	0.46480000
H	-1.27160000	3.31540000	-0.55470000

TS2

Charge=0, Multiplicity=1

Yb	-1.24390000	-0.53220000	0.02460000
N	-3.15570000	0.93800000	0.44110000
N	-1.41100000	-0.36670000	2.46780000
N	-1.57550000	-2.91740000	1.06380000
N	-2.27870000	-2.26050000	-1.79680000
N	0.17330000	0.89240000	-1.35120000
C	-3.90360000	3.15350000	1.23100000
H	-3.70090000	3.69230000	0.30020000
H	-3.74750000	3.83780000	2.06810000
H	-4.96130000	2.87210000	1.20640000
C	-3.01590000	1.91930000	1.33690000

C	-2.09730000	1.91950000	2.41030000
H	-2.03110000	2.87150000	2.91060000
C	-1.49580000	0.81410000	3.07430000
C	-1.06300000	1.07530000	4.56160000
C	-1.27290000	-1.62790000	3.18800000
H	-1.68220000	-1.60120000	4.20330000
H	-0.22020000	-1.92060000	3.28420000
C	-2.04310000	-2.72910000	2.45140000
H	-1.97320000	-3.67670000	3.01560000
H	-3.09730000	-2.44310000	2.41440000
C	-2.57120000	-3.64370000	0.25760000
H	-3.54240000	-3.16570000	0.41540000
H	-2.66480000	-4.69180000	0.59550000
C	-2.22460000	-3.62720000	-1.22900000
H	-1.21880000	-4.02550000	-1.37930000
H	-2.91220000	-4.29650000	-1.77240000
C	-3.66400000	-1.92700000	-2.17550000
H	-4.32010000	-1.97890000	-1.30530000
H	-4.04260000	-2.61550000	-2.95020000
H	-3.71540000	-0.90640000	-2.55340000
C	-1.39990000	-2.17050000	-2.97530000
H	-1.46660000	-1.16920000	-3.40330000
H	-1.67520000	-2.90340000	-3.75330000
H	-0.36520000	-2.34650000	-2.67260000
C	-0.28160000	-3.61710000	1.04340000
H	0.19200000	-3.53100000	0.06680000
H	-0.39370000	-4.68600000	1.28670000
H	0.39600000	-3.16540000	1.76340000
C	-2.25500000	0.73390000	5.48850000
H	-2.00010000	0.95810000	6.53220000
H	-2.54060000	-0.32120000	5.43600000
H	-3.13190000	1.32930000	5.21140000
C	-0.70500000	2.56380000	4.81040000
H	0.04840000	2.91940000	4.10100000
H	-0.29630000	2.66890000	5.82160000
H	-1.57520000	3.22310000	4.75200000
C	0.19470000	0.27070000	4.97470000
H	0.00510000	-0.79150000	5.12620000
H	0.58130000	0.65830000	5.92400000
H	0.98860000	0.36570000	4.22850000
C	-4.36450000	0.85270000	-0.30970000
C	-5.40640000	0.03700000	0.21180000
C	-6.57770000	-0.12690000	-0.53360000
H	-7.38170000	-0.74350000	-0.14250000
C	-6.73070000	0.47920000	-1.78060000
H	-7.64660000	0.33870000	-2.34880000
C	-5.70060000	1.26250000	-2.29060000

H	-5.81730000	1.73060000	-3.26500000
C	-4.51190000	1.46560000	-1.57590000
C	-3.40940000	2.31820000	-2.18910000
H	-2.61130000	2.40060000	-1.45030000
C	-2.80200000	1.65090000	-3.43610000
H	-2.26570000	0.73760000	-3.16090000
H	-2.08130000	2.31800000	-3.91750000
H	-3.57680000	1.39010000	-4.16740000
C	-3.88550000	3.74050000	-2.53730000
H	-4.60580000	3.73050000	-3.36420000
H	-3.02970000	4.35140000	-2.84750000
H	-4.37110000	4.22770000	-1.68520000
C	-5.23000000	-0.65690000	1.55840000
H	-4.15270000	-0.81030000	1.68300000
C	-5.68500000	0.23150000	2.73380000
H	-5.09740000	1.15040000	2.79030000
H	-5.56100000	-0.29980000	3.68600000
H	-6.74340000	0.50080000	2.62910000
C	-5.93190000	-2.02310000	1.63870000
H	-7.02170000	-1.91980000	1.70100000
H	-5.60920000	-2.56160000	2.53790000
H	-5.71150000	-2.65010000	0.76690000
C	1.08240000	0.09030000	-0.87360000
C	0.28910000	2.01510000	-2.23130000
C	-0.09810000	3.30010000	-1.78120000
C	-0.05690000	4.37830000	-2.67050000
H	-0.33860000	5.36340000	-2.30440000
C	0.33690000	4.21540000	-3.99600000
H	0.37070000	5.06590000	-4.67130000
C	0.66130000	2.94030000	-4.44610000
H	0.92850000	2.78430000	-5.48930000
C	0.62330000	1.82970000	-3.59400000
C	0.82050000	0.47160000	-4.21870000
H	-0.01910000	0.24610000	-4.89120000
H	0.88610000	-0.33030000	-3.48940000
H	1.73120000	0.44820000	-4.82620000
C	-0.53740000	3.57510000	-0.36660000
H	-0.78650000	2.67130000	0.18470000
H	-1.41770000	4.22740000	-0.35930000
H	0.24740000	4.09110000	0.19490000
Si	3.01130000	0.24820000	-1.20350000
Si	3.32650000	2.49300000	0.86330000
Si	5.92160000	0.96850000	-0.03980000
Si	3.90080000	-0.37840000	1.97400000
C	3.74630000	-2.29070000	-1.10540000
H	4.49080000	-2.20390000	-0.33210000
C	3.82830000	-1.39260000	-2.23930000

H	4.81720000	-1.01940000	-2.48960000
C	3.04760000	-1.80400000	-3.41740000
H	3.17490000	-1.23320000	-4.33170000
C	2.19570000	-2.85410000	-3.38830000
H	1.63730000	-3.12410000	-4.28310000
C	2.05270000	-3.69810000	-2.21980000
C	1.25480000	-4.85440000	-2.23080000
H	0.64660000	-5.06070000	-3.11010000
C	1.27030000	-5.75410000	-1.16780000
H	0.66210000	-6.65350000	-1.19990000
C	2.09550000	-5.49180000	-0.05820000
H	2.12280000	-6.19410000	0.77140000
C	2.86300000	-4.33960000	-0.00390000
H	3.49080000	-4.14690000	0.86190000
C	2.87450000	-3.40820000	-1.07910000
C	4.05780000	0.74960000	0.41350000
C	3.06640000	3.59730000	-0.66100000
H	4.02430000	3.98740000	-1.01600000
H	2.45400000	4.45790000	-0.36460000
H	2.56760000	3.12460000	-1.50960000
C	4.40950000	3.59310000	1.97410000
H	4.72190000	3.13350000	2.91420000
H	3.80300000	4.47480000	2.22200000
H	5.30180000	3.95490000	1.45260000
C	1.68420000	2.30330000	1.79020000
H	0.95560000	1.69700000	1.24970000
H	1.24110000	3.29180000	1.94970000
H	1.82210000	1.85020000	2.77330000
C	6.20360000	2.34630000	-1.31700000
H	5.48210000	2.29940000	-2.14060000
H	7.20860000	2.23230000	-1.74300000
H	6.14740000	3.34680000	-0.87490000
C	7.01010000	1.39420000	1.46500000
H	6.66100000	2.24790000	2.04760000
H	8.01020000	1.64060000	1.08380000
H	7.12840000	0.54800000	2.14970000
C	6.79240000	-0.55730000	-0.77990000
H	6.51150000	-1.51490000	-0.33520000
H	7.86790000	-0.42150000	-0.60550000
H	6.65700000	-0.63500000	-1.86340000
C	5.19790000	-1.77200000	2.14330000
H	5.13170000	-2.57790000	1.40940000
H	5.02630000	-2.22480000	3.12910000
H	6.22740000	-1.40300000	2.13670000
C	4.18940000	0.52870000	3.62920000
H	5.21470000	0.90690000	3.70140000
H	4.05900000	-0.21150000	4.42970000

H	3.51150000	1.35780000	3.84190000
C	2.22020000	-1.23020000	2.05600000
H	2.08930000	-1.87310000	1.18280000
H	1.38040000	-0.53100000	2.06920000
H	2.17350000	-1.84950000	2.96130000

TS0_3

Charge=0, Multiplicity=1

Yb	-0.81598000	-0.79245900	-0.09927400
N	-2.69567000	-0.27601800	-1.56328100
N	-2.77741400	-1.79279700	0.91450300
N	-0.40032300	-1.25495700	2.50203800
N	0.43433400	1.48285000	5.01763700
C	-4.27923700	-1.20033700	-3.22474700
H	-5.00599300	-0.38268500	-3.15489100
H	-4.82485800	-2.12496400	-3.42740500
H	-3.63837000	-0.97651700	-4.08332300
C	-3.47358700	-1.29880900	-1.93437400
C	-3.67272800	-2.47747300	-1.17813300
H	-4.21249300	-3.24586900	-1.70684400
C	-3.55935900	-2.62147800	0.23552300
C	-4.45781000	-3.72434900	0.89585600
C	-2.86946500	-1.51598000	2.33977800
H	-3.72640100	-1.96009700	2.85174400
H	-2.99861900	-0.42677000	2.45251400
C	-1.58652200	-1.93634300	3.06287400
H	-1.67893600	-1.75640900	4.14648400
H	-1.44531300	-3.01019600	2.91954400
C	-0.18542000	0.08351800	3.09086100
H	-1.15848600	0.58061500	3.14995500
H	0.41608800	0.67794500	2.39727900
C	0.51555700	0.13014800	4.45936700
H	0.09901000	-0.62350500	5.15237000
H	1.57006200	-0.12540100	4.32059800
C	-0.78615400	1.67492500	5.79046800
H	-0.87646500	2.72479200	6.08886100
H	-0.81779300	1.05045400	6.70467800
H	-1.66136800	1.42582300	5.18149400
C	1.61763500	1.84702400	5.78903200
H	2.50545000	1.77618700	5.15257100
H	1.77157200	1.20930000	6.68083200
H	1.52615900	2.88492500	6.12843500
C	0.79559900	-2.10950600	2.59582900
H	1.64204000	-1.58361600	2.15633100
H	0.63125500	-3.01975800	2.01810300
H	1.03985000	-2.39440600	3.63057000
C	-3.72004300	-4.47829800	2.03139400
H	-2.72744900	-4.80310000	1.70453300

H	-4.29179800	-5.36986600	2.31285300
H	-3.59556300	-3.88994000	2.94061600
C	-5.75657100	-3.06605100	1.42111500
H	-5.56783800	-2.31095000	2.18906700
H	-6.41774400	-3.82754900	1.85422500
H	-6.28974500	-2.57489900	0.59973600
C	-4.88635700	-4.81643400	-0.11609600
H	-5.55539000	-4.43151600	-0.89055200
H	-5.43216400	-5.60281100	0.41742700
H	-4.02192400	-5.28064800	-0.60398700
C	-2.97116200	1.00526600	-2.12699400
C	-2.38104100	1.43717300	-3.33645500
C	-2.74612300	2.68428800	-3.86006200
H	-2.30720500	3.01801700	-4.79630700
C	-3.65087400	3.50884900	-3.19637000
H	-3.92735600	4.47098400	-3.61967200
C	-4.16842500	3.10959800	-1.96450300
H	-4.84128000	3.77508800	-1.43162100
C	-3.83609100	1.87088500	-1.40584800
C	-4.38687200	1.44538600	-0.04774000
H	-3.65228800	0.75768300	0.38466100
C	-5.70409700	0.65633300	-0.18360900
H	-6.47288000	1.26633500	-0.67435500
H	-6.08078000	0.36485800	0.80507300
H	-5.56156900	-0.25754100	-0.76569400
C	-4.56967900	2.62026100	0.92753900
H	-3.67876300	3.25521100	0.96987600
H	-4.77115900	2.23998500	1.93655700
H	-5.41825100	3.25770400	0.65084900
C	-1.32419500	0.59168400	-4.03250700
H	-1.39968300	-0.42086400	-3.62532000
C	-1.51179100	0.49894500	-5.55585300
H	-2.52458200	0.17258000	-5.81704800
H	-0.80019300	-0.21863600	-5.98121100
H	-1.33462200	1.46230400	-6.04831400
C	0.08122400	1.12198900	-3.68886600
H	0.18563200	2.17131500	-3.98964600
H	0.85809100	0.54300200	-4.20083400
H	0.28197400	1.05965600	-2.61342500
C	-0.82332400	5.11867900	-0.36181000
C	-0.87916500	6.49388100	-0.11967700
C	-1.10220400	6.99139600	1.16402200
C	-1.28024100	6.11976100	2.23915600
C	-1.23437000	4.73620800	2.05639500
C	-1.00068700	4.26715800	0.74736400
H	-0.74802500	7.17822000	-0.95322900
H	-1.14283500	8.06474400	1.32736100

H	-1.46041300	6.51366000	3.23556800
C	-1.42654100	3.77288900	3.19634600
H	-2.23010200	3.05902800	2.97716900
H	-0.52289900	3.18368000	3.39886300
H	-1.69140700	4.30686600	4.11337100
C	-0.58055000	4.56049800	-1.73694000
H	0.43632300	4.16240000	-1.82226100
H	-1.26840900	3.74318100	-1.96368300
H	-0.71164200	5.33427100	-2.49853200
N	-0.95790400	2.89841700	0.54410500
C	-0.92459400	1.74365100	0.35498700
Si	2.34436200	-0.79345100	-0.61371400
Si	3.73853000	1.78537700	0.22126800
Si	5.01136400	0.25164200	-2.22003300
Si	5.28795400	-0.90805000	0.66748600
C	2.62635600	-2.68546200	-1.02527100
H	3.66995000	-2.98510700	-1.07973600
C	2.12307300	-1.91644300	-2.25469400
H	2.79974100	-1.77261900	-3.09071300
C	0.73899000	-2.14798900	-2.61885300
H	0.37268200	-1.67895000	-3.52821500
C	-0.12348200	-2.89788600	-1.87198600
H	-1.15673300	-3.02764300	-2.18912900
C	0.36126800	-3.74560700	-0.77138500
C	-0.49606200	-4.63781400	-0.11173300
H	-1.55116400	-4.62977300	-0.37409000
C	-0.00812800	-5.53192600	0.84625500
H	-0.68630500	-6.21535500	1.35045700
C	1.36006200	-5.55608700	1.12334000
H	1.75843600	-6.25731100	1.85233000
C	2.22478800	-4.66884000	0.47153200
H	3.28847100	-4.68933500	0.69892100
C	1.74644500	-3.72325900	-0.44383700
C	4.14974700	0.06680600	-0.52722100
C	2.31672500	2.67566100	-0.66991600
H	2.63299700	3.07420000	-1.63845500
H	1.98842500	3.51960600	-0.04888800
H	1.45514000	2.02671400	-0.83757900
C	5.13322000	3.07927100	0.19264700
H	6.08156900	2.73221600	0.60946000
H	4.80217900	3.94202400	0.78620100
H	5.32004000	3.44061000	-0.82472000
C	3.19633900	1.63332100	2.04349900
H	2.46003100	0.83537800	2.17062700
H	2.72875800	2.57123800	2.36944100
H	4.03581100	1.42572700	2.71610900
C	4.03829500	1.39453300	-3.38550100

H	2.96971900	1.15616500	-3.38544200
H	4.41248900	1.27525100	-4.41022400
H	4.14932100	2.45092600	-3.11730100
C	6.76811100	0.98200700	-2.09761900
H	6.82029800	1.94849500	-1.59054300
H	7.15275600	1.11962700	-3.11733500
H	7.45465700	0.29784100	-1.58572900
C	5.29273700	-1.38282600	-3.17795100
H	6.36389100	-1.50078400	-3.38208100
H	4.78162300	-1.35129600	-4.14780200
H	4.96360200	-2.28569200	-2.66095600
C	6.29011000	-2.31355500	-0.13866300
H	5.67049200	-3.12064400	-0.54093600
H	6.92132300	-2.74877600	0.64736800
H	6.95357100	-1.97225100	-0.93940800
C	6.62699800	0.17245000	1.48852800
H	7.25302600	0.68883500	0.75400200
H	7.28086900	-0.48179400	2.07995000
H	6.21700600	0.92546800	2.16976300
C	4.37465900	-1.74609200	2.10792200
H	3.83480300	-1.03474200	2.74031600
H	5.11888700	-2.24936800	2.73931800
H	3.66575200	-2.50238700	1.75858100

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