

Supporting Information

Tuning Reactivity of Yttrium Complex Bearing a Functionalized Silylamido Ligand Using Solvated KCl

Qing You,^{‡a} Jiamin Cai,^{‡a} Jie Zhang^{*a} and Xigeng Zhou^{*a}

^a Department of Chemistry, Fudan University Handan Road No 220, Shanghai
200433 (China)

E-mail: zhangjie@fudan.edu.cn; xgzhou@fudan.edu.cn

[‡] These authors contributed equally to this work.

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1. Experimental Procedures

General Procedures and Materials. All reactions were carried out under a dry and oxygen-free nitrogen atmosphere in a Vigor (SG1200/750TS-F) glovebox. Anhydrous THF, toluene, and hexane were purified using an MB SPS-800 Solvent Purification System and dried over fresh Na chips in glovebox. C_6D_6 , $CDCl_3$, and d_8 -THF were purchased from J&K and transferred under vacuum, dried over Na/K alloy, and stored in the glovebox. Organometallic samples for NMR spectroscopic measurements were prepared in the glovebox using J-Young valve NMR tubes. 1H , ^{13}C and ^{13}C - 1H HSQC spectra were recorded on a Bruker Advance 400 MHz spectrometer. All chemical shifts were reported in δ units with reference to the residual solvent resonance of the deuterated solvents for proton and chemical shifts. High-resolution mass spectra (HRMS) were obtained on a micro TOF II instrument using ESI ionization sources. Elemental analyses for C, H, and N were carried out on a vario EL III elemental analyzer. Organic molecules were identified and quantified by gas chromatography (Shimadzu 2010 Plus, 0.25 mm \times 30 m Rtx-5 capillary column), and then detected by an Agilent Technologies 7890A gas chromatograph and an Agilent Technologies 5975C mass spectrometer. Anhydrous YCl_3 were prepared according to literature procedures. **1** was prepared according to our previous report². $PhSiH_3$, 4-methylphenyl isothiocyanate, phenyl isothiocyanate, tert-butyl isocyanide, S_8 , and KCl were purchased from J&K and dried with a vacuum drying oven. Liquid reagents were additionally dried with 4 Å sieves. Other commercially available reagents were purchased and used without further purification.

Preparation Details for Complexes 2-9

Synthesis of 2-4. Complex **1** (0.723 g, 1.0 mmol) and KCl (0.037g, 0.5 mmol) were placed in a Schlenk reaction flask with a Teflon-sealed stopcock, and 10 mL of THF solution was added to dissolve. After stirred for 24 h at 60 °C, a THF solution of S_8 (0.064g, 0.25 mmol) was added dropwise and stirred for 12 h. The resulting pale-yellow turbid solution was filtered, and the filtrate was collected and concentrated to dryness under vacuum. Then, 10 mL of n-hexane was added, stirred, and dried by suction. This operation was repeated three times, and the final n-hexane mixture was filtered through a sintered glass funnel to obtain a pale-yellow solid powder. The solid powder was redissolved in a toluene solution, and the insoluble material was filtered off. The clear filtrate was concentrated to saturation and left to stand at room temperature for several days, yielding colorless transparent block-shaped crystals **2**, which is suitable for X-ray single-crystal diffraction analysis. Crude samples of **3** were collected from the insoluble material after the pale yellow solid powder redissolved in a toluene solution. and were redissolved in a THF solution, concentrated to saturation, and left to stand at room temperature for several days, could yield colorless transparent plate-shaped crystals **3**, which is suitable for X-ray single-crystal diffraction analysis. The crystals of **4** could obtained from mother liquid of **2** by n-hexane diffusion.

For **2**, Yield: 0.103 g (23% based on Y metal). 1H NMR (400 MHz, d_8 -THF, 25 °C): δ [ppm] 1.77 (br s, 4H, THF), 2.38 (s, 36H, CH_3 -Tp^{Me2}), 2.51 (s, 18H, CH_3 -Tp^{Me2}), 3.61 (br s, 4H, THF), 5.68 (overlap s, 2H, CH-Tp^{Me2}), 5.70 (overlap s, 5H, CH-Tp^{Me2}), 5.76 (br s, 2H, CH-Tp^{Me2}), 7.07–7.13 (m, 5H, H-Ar), 7.17 (d, J = 7.2 Hz, 3H, H-Ar), 8.05 (d, J = 7.6 Hz, 2H, H-Ar). ^{13}C NMR (100 MHz, d_8 -THF, 25 °C): δ [ppm] 11.9 (CH_3 -Tp^{Me2}), 12.1 (CH_3 -Tp^{Me2}), 15.2 (CH_3 -Tp^{Me2}), 29.6 (THF), 66.9 (THF), 105.4 (CH-Tp^{Me2}), 105.6 (CH-Tp^{Me2}), 105.6 (CH-Tp^{Me2}), 125.0 (C-Ar), 125.8 (C-Ar), 126.1 (C-Ar), 126.8 (C-Ar), 127.8 (C-Ar), 128.6 (C-Ar), 130.7 (C-Ar), 133.7 (C-Ar), 144.5 (C-Tp^{Me2}), 150.3 (C-Tp^{Me2}). Anal. Calcd for $C_{61}H_{84}B_3ClN_{18}OS_8Si_2Y_4$ (1820.06): C, 40.22; H, 4.65; N, 13.84. Found: C, 40.35; H, 4.46; N, 14.01.

For **3**, Yield: 0.311 g (47% based on Y metal). 1H NMR (400 MHz, d_8 -THF, 25 °C): δ [ppm] 1.69 (br s, 8H, THF), 1.79 (s, 18H, CH_3 -Tp^{Me2}), 2.24 (d, J = 6.0 Hz, 18H, CH_3 -Tp^{Me2}), 2.33 (s, 18H, CH_3 -Tp^{Me2}), 2.49 (s, 18H, CH_3 -Tp^{Me2}), 2.77 (s, 18H, CH_3 -Tp^{Me2}), 3.55 (br s, 8H, THF), 5.37 (s, 6H, CH-Tp^{Me2}), 5.40 (s, 3H, CH-Tp^{Me2}), 5.96 (s, 6H, CH-Tp^{Me2}), 6.49 (t, J = 7.6 Hz, 6H, H-Ar), 6.49 (t, J = 7.6 Hz, 3H, H-Ar), 7.32 (d, J = 6.8 Hz, 6H, H-Ar). ^{13}C NMR (100 MHz, d_8 -THF, 25 °C): δ [ppm] 11.6 (CH_3 -Tp^{Me2}), 12.0 (CH_3 -Tp^{Me2}), 12.2 (CH_3 -Tp^{Me2}), 14.9 (CH_3 -Tp^{Me2}), 15.1 (CH_3 -Tp^{Me2}), 24.8 (THF), 66.9 (THF), 104.4 (CH-Tp^{Me2}), 104.9 (CH-Tp^{Me2}), 106.4 (CH-Tp^{Me2}), 124.4 (C-Ar), 124.8 (C-Ar), 133.4 (C-Ar), 133.5 (C-Ar), 142.8 (C-Tp^{Me2}), 143.1 (C-Tp^{Me2}), 147.6 (C-Tp^{Me2}), 148.8 (C-Tp^{Me2}), 150.4 (C-Tp^{Me2}), 150.5 (C-Tp^{Me2}), 150.6 (C-Tp^{Me2}). Anal. Calcd for $C_{101}H_{141}B_5K_2N_{30}O_2S_9Si_3Y_4$ (2668.12): C, 47.47; H, 5.33; N, 15.75. Found: C, 47.28; H, 5.44; N, 15.63.

For **4**, Yield: 0.072 g (11% based on Y metal). No valuable NMR spectra data were obtained due to its poor solubility in d_8 -THF. Anal. Calcd for $C_{72}H_{124}B_4Cl_4KN_{26}Si_4Y_3$ (1957.19): C, 44.19; H, 6.39; N, 18.61. Found: C, 44.28; H, 6.45; N, 18.47.

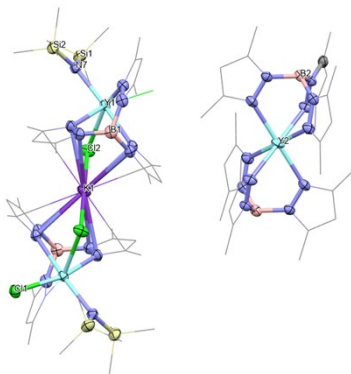


Figure S1. Molecular structure of **4** with ellipsoids set at 30% probability. All hydrogen atoms are omitted for clarity. Selected bond lengths [Å] and angles (°): Y1–Cl1 2.590(7), Y1–Cl2 2.654(7), Y1–N7 2.276(2), K1–Cl2 3.112(7); Cl1–Y1–Cl2 104.2(2), N7–Y1–Cl1 101.2(6), Cl2–K1–Cl2A 180.

Synthesis of 5 and 6. At room temperature, the complex **1** (0.723 g, 1.0 mmol) was placed in a Schlenk reaction flask with a Teflon-sealed stopcock, and 5 mL of THF solution was added to dissolve. Subsequently, a THF solution of S₈ (0.032g, 0.125 mmol) was added dropwise, and the reaction flask was placed in a 60 °C oil bath and heated for 12 h. The resulting pale-yellow solution was concentrated to dryness under vacuum and washed (15 ml × 2) with hexane to give the pale-yellow powder **5**. Colorless single crystals suitable for X-ray diffraction analysis were obtained by a slow solvent evaporation method from a toluene (1 mL) solution of **5**. Yield: 0.503 g (88%). ¹H NMR (400 MHz, C₆D₆, 25 °C): δ [ppm] : δ 8.12 (d, J = 7.2 Hz, 2H, *H*-Ar), 7.24 (d, J = 6.5 Hz, 3H, *H*-Ar), 5.57 (s, 1H, *CH*-Tp^{Me2}), 5.52 (s, 1H, *CH*-Tp^{Me2}), 5.46 (s, 1H, *CH*-Tp^{Me2}), 5.30 (s, 1H, SiH), 5.18 (s, 1H, SiH), 3.63 (s, 4H, THF), 2.69 (s, 3H, CH₃-Tp^{Me2}), 2.40 (s, 6H, CH₃-Tp^{Me2}), 2.09 (s, 10H, CH₃-Tp^{Me2} & SCH), 1.23 (s, 4H, THF), 0.82 (s, 3H, SiCH₃), 0.56 (s, 3H, SiCH₃), 0.10 (s, 9H, Si(CH₃)₃). ¹³C NMR (100 MHz, C₆D₆, 25 °C): δ [ppm]: δ 150.9 (C-Tp^{Me2}), 149.9 (C-Tp^{Me2}), 146.0 (C-Tp^{Me2}), 145.7 (C-Tp^{Me2}), 144.8 (C-Tp^{Me2}), 136.6 (C-Ar), 129.3 (C-Ar), 106.7 – 106.0 (CH-Tp^{Me2}), 70.7 (THF), 25.3 (THF), 15.2 (CH₃-Tp^{Me2}), 13.0 (CH₃-Tp^{Me2}), 6.2 (SCH), 5.6 (Si(CH₃)₃). Anal. Calcd for C₃₁H₅₃BN₇OSSi₃Y (755.85): C, 49.26; H, 7.07; N, 12.97. Found: C, 49.16; H, 7.10; N, 12.93.

Additionally, complex **5** could further convert into known yttrium disulfide **6** (0.259 g, 57%) and unidentified organic products by reacting with S₈ (0.032g, 0.125 mmol) after heating for 12 h. Complex **6** could be also obtained by the reaction of **1** (0.723 g, 1.0 mmol) and S₈ (0.064 g, 0.25 mmol) directly after heating for 12 h. The crystal structure of **6** has also been confirmed by XRD analysis.

Synthesis of 7. Complex **1** (0.723 g, 1.0 mmol) and KCl (0.037 g, 0.5 mmol) were placed in a Schlenk reaction flask with a Teflon-sealed stopper. 10 mL of THF solution was added to dissolve the reactants. After stirred for 24 h at 60 °C, a THF solution of 4-methylphenyl isothiocyanate (0.149 g, 1.0 mmol) was added dropwise and stirred for 5 h. The resulting pale-yellow transparent solution was concentrated under reduced pressure to dryness. 10 mL of hexane was added and the mixture was stirred and dried. This operation was repeated three times, and the final hexane mixture was filtered through a sintered glass funnel to obtain a pale-yellow solid powder **7**. The solid powder was then redissolved in toluene, concentrated to saturation, and left to stand at room temperature for several days, yielding pale yellow transparent block-shaped crystals **7**, which is suitable for X-ray single-crystal diffraction analysis. Yield: 0.531 g (78%). ¹H NMR (400 MHz, C₆D₆, 25 °C): δ [ppm] –0.05 (s, 9H, –Si(CH₃)₃), 1.26 (s, 3H, –Si(CH₃)₂–), 1.30 (s, 3H, –Si(CH₃)₂–), 1.87 (s, 3H, CH₃Ph–), 1.89 (s, 3H, CH₃Ph–), 1.93 (s, 3H, CH₃-Tp^{Me2}), 2.01 (s, 3H, CH₃-Tp^{Me2}), 2.03 (s, 3H, CH₃-Tp^{Me2}), 2.09 (overlap s, 9H, CH₃-Tp^{Me2}), 2.10 (overlap s, 3H, CH₃-Tp^{Me2}), 2.47 (s, 3H, CH₃-Tp^{Me2}), 2.53 (s, 3H, CH₃-Tp^{Me2}), 2.83 (s, 3H, CH₃-Tp^{Me2}), 3.01 (s, 3H, CH₃-Tp^{Me2}), 4.73 (br s, 2H, BH-Tp^{Me2}), 5.28 (s, 1H, CH-Tp^{Me2}), 5.38 (overlap s, 1H, CH-Tp^{Me2}), 5.39 (overlap s, 1H, CH-Tp^{Me2}), 5.48 (s, 1H, CH-Tp^{Me2}), 5.50 (s, 1H, CH-Tp^{Me2}), 5.54 (s, 1H, CH-Tp^{Me2}), 6.56 (s, 1H, –(CH₃)₂SiCHC–), 6.66 (d, J = 7.6 Hz, 2H, *H*-Ar), 6.71 (d, J = 7.6 Hz, 2H, *H*-Ar), 7.26 (d, J = 7.6 Hz, 2H, *H*-Ar), 7.50 (d, J = 7.6 Hz, 2H, *H*-Ar). ¹³C NMR (100 MHz, C₆D₆, 25 °C): δ [ppm] 2.3 (–Si(CH₃)₂–), 3.6 (–Si(CH₃)₂–), 4.5 (–Si(CH₃)₃), 12.4 (CH₃-Tp^{Me2}), 12.5 (CH₃-Tp^{Me2}), 12.6 (CH₃-Tp^{Me2}), 12.6 (CH₃-Tp^{Me2}), 12.7 (CH₃-Tp^{Me2}), 12.8 (CH₃-Tp^{Me2}), 13.1 (CH₃-Tp^{Me2}), 13.6 (CH₃-Tp^{Me2}), 15.0 (CH₃-Tp^{Me2}), 15.4 (CH₃-Tp^{Me2}), 16.2 (CH₃-Tp^{Me2}), 16.6 (CH₃-Tp^{Me2}), 20.3 (CH₃Ph–), 20.4 (CH₃Ph–), 73.7 (–(CH₃)₂SiCHC–), 105.6 (CH-Tp^{Me2}), 105.7 (CH-Tp^{Me2}), 106.0 (CH-Tp^{Me2}), 106.2 (CH-Tp^{Me2}), 106.3 (CH-Tp^{Me2}), 123.2 (C-Ar), 123.8 (C-Ar), 129.0 (C-Ar), 129.4 (C-Ar), 133.9 (C-Ar), 134.1 (C-Ar), 144.4 (C-Ar), 145.1 (–N=CS), 145.1 (–N=CS), 145.2 (C-Ar), 145.4 (C-Tp^{Me2}), 146.1 (C-Tp^{Me2}), 146.2 (C-Tp^{Me2}), 146.9 (C-Tp^{Me2}), 150.4 (C-Tp^{Me2}), 150.7 (C-Tp^{Me2}), 151.0 (C-Tp^{Me2}), 151.0 (C-Tp^{Me2}), 151.5 (C-Tp^{Me2}), 151.8 (C-Tp^{Me2}), 194.7 (C-Tp^{Me2}), 196.4 (C-Tp^{Me2}). Anal. Calcd for C₅₉H₈₂B₂ClN₁₅S₂Si₂Y₂ (1355.38): C, 52.24; H, 6.09; N, 15.49. Found: C, 52.11; H, 5.98; N, 15.72.

Hydrolyzing the hexane solution of reaction concentration, we detected the hydrolysis product by GC-MS analysis, mainly as the silylamine organic compound [(PhSiH₂)₂CHSi(Me)₂]NHSiMe₃ (**II**), which is the hydrolysis product of KNSiMe₃Si(Me)₂CH(SiH₂Ph)₂ (**I**). The **II** was further purified by vacuum distillation at 150 °C to obtain a pure, colorless, oily liquid. ¹H NMR (400 MHz, CDCl₃, 25 °C): δ [ppm] -0.09 (br s, 1H, (-SiH₂)₂CHSi(CH₃)₂-), -0.01 (s, 9H, -Si(CH₃)₃), 0.14 (s, 6H, -Si(CH₃)₂-), 4.46-4.48 (m, 2H, -SiH₂-), 4.52 (m, 2H, -SiH₂-), 7.30-7.33 (m, 4H, *H*-Ar), 7.37 (d, *J* = 6.8 Hz, 2H, *H*-Ar), 7.53 (d, *J* = 7.2 Hz, 4H, *H*-Ar). ¹³C NMR (100 MHz, CDCl₃, 25 °C): δ [ppm] -5.2 (-SiH₂)₂CHSi(CH₃)₂-, 2.4 (-Si(CH₃)₃), 2.5 (-Si(CH₃)₂-), 127.9 (*C*-Ar), 129.6 (*C*-Ar), 133.5 (*C*-Ar), 135.3 (*C*-Ar). HRMS Calcd for C₁₈H₃₂NSi₄ [M+H]⁺: 374.1612; Found: 374.1621.

Synthesis of 8. Complex **1** (0.723 g, 1.0 mmol) was placed in a Schlenk reaction flask with a Teflon-sealed stopcock, and 5 mL of THF solution was added to dissolve. Subsequently, a THF solution of phenyl isothiocyanate (0.135 g, 1 mmol) was added dropwise, and the reaction flask was placed in a 60 °C oil bath and heated for 12 h. The resulting pale-yellow solution was concentrated to dryness under vacuum and washed (15 ml × 2) with hexane to give the pale-yellow powder **8**. Colorless single crystals suitable for X-ray diffraction analysis were obtained by a slow solvent evaporation method from a toluene (1 mL) solution of **8**. Yield: 0.738 g (86%). ¹H NMR (400 MHz, C₆D₆, 25 °C): δ [ppm] : δ 7.36 (s, 1H, *H*-Ar), 7.12 (s, 2H, *H*-Ar), 7.02 (s, 6H, *H*-Ar), 6.96 (s, 1H, *H*-Ar), 5.64 (s, 1H, *CH*-Tp^{Me2}), 5.57 (s, 1H, *SiH*), 5.53 (s, 2H, *CH*-Tp^{Me2}), 5.43 (s, 1H, *SiH*), 2.56 (s, 4H, *THF*), 2.20 (s, 3H, CH₃-Tp^{Me2}), 2.18 (s, 6H, CH₃-Tp^{Me2}), 2.11 (s, 6H, CH₃-Tp^{Me2}), 2.09 (s, 2H, CH₃-Tp^{Me2}), 1.97 (s, 4H, CH₃-Tp^{Me2}), 1.53 (s, 1H, *CCH*), 1.38 (s, 4H, *THF*), 0.71 (s, 6H, SiCH₃), 0.54 & 0.10 (s, 3H, Si(CH₃)₃), -0.18 (s, 6H, Si(CH₃)₃). ¹³C NMR (100 MHz, C₆D₆, 25 °C): δ [ppm]: δ 150.5 (*C*-Tp^{Me2}), 149.9 (*C*-Tp^{Me2}), 149.8 (*C*-Tp^{Me2}), 146.1 (*C*-Tp^{Me2}), 144.5 (*C*-Tp^{Me2}), 129.4 (*C*-Ar), 106.5-106.1 (*CH*-Tp^{Me2}), 14.7 (CH₃-Tp^{Me2}), 13.1 (CH₃-Tp^{Me2}), 12.0 (CH₃-Tp^{Me2}), 11.8 (CH₃-Tp^{Me2}), 9.2 (SCH), 6.6 (Si(CH₃)₃). Anal. Calcd for C₃₈H₅₈BN₈OSSi₃Y (858.97): C, 53.13; H, 6.81; N, 13.04. Found: C, 52.98; H, 6.79; N, 13.00.

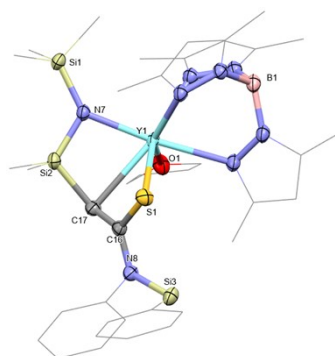


Figure S2. Molecular structure of **8** with ellipsoids set at 30% probability. All hydrogen atoms are omitted for clarity. Selected bond lengths [Å] and angles (°): Y1-N7 2.2579(17), Y1-Si1, 2.7620(6) Y1-C17 2.732(2), Y1-C16 2.976(2), C17-C16 1.374(3), C16-S1 1.736(2), C16-N8 1.396(3); Y1-Si1-C16 79.27(7), C17-C16-N8 123.7(2).

Synthesis of 9. In the glove box, complex **1** (0.723 g, 1.0 mmol) was placed in a Schlenk reaction flask with a Teflon-sealed stopper, and 10 mL of THF solution was added to dissolve it. Then, a THF solution of tert-butyl isocyanide (0.04 g, 0.5 mmol) was added dropwise. The reaction flask was sealed and removed, and CO₂ (1.12 mL, 0.5 mmol) was bubbled through the solution. The reaction flask was then placed in a 60 °C oil bath and heated for 12 h. The resulting pale yellow, clear solution was concentrated under vacuum to dryness. Then, 10 mL of hexane was added, and the mixture was stirred and dried. This operation was repeated three times, and the final hexane mixture was filtered through a sintered glass funnel to obtain a pale yellow solid powder **9**. The solid powder was redissolved in toluene, concentrated to saturation, and left to stand at room temperature for several days, yielding colorless block-shaped crystals **9**, which is suitable for X-ray single-crystal diffraction analysis. Yield: 0.252 g (35%). ¹H NMR (400 MHz, C₆D₆, 25 °C): δ [ppm] -0.82 (s, 3H, -Si(CH₃)₂-), -0.22 (s, 9H, -Si(CH₃)₃), 0.07 (s, 3H, -Si(CH₃)₂-), 0.18 (s, 9H, -Si(CH₃)₃), 0.68 (s, 3H, -Si(CH₃)₂-), 0.90 (s, 9H, CH₃-^tBu), 0.98 (s, 3H, -Si(CH₃)₂-), 1.95 (s, 3H, CH₃-Tp^{Me2}), 2.05 (s, 3H, CH₃-Tp^{Me2}), 2.10 (s, 3H, CH₃-Tp^{Me2}), 2.18 (s, 3H, CH₃-Tp^{Me2}), 2.23 (s, 3H, CH₃-Tp^{Me2}), 2.26 (s, 3H, CH₃-Tp^{Me2}), 2.38 (s, 3H, CH₃-Tp^{Me2}), 2.48 (s, 3H, CH₃-Tp^{Me2}), 2.64 (s, 3H, CH₃-Tp^{Me2}), 2.77 (s, 3H, CH₃-Tp^{Me2}), 2.90 (s, 3H, CH₃-Tp^{Me2}), 2.92 (s, 3H, CH₃-Tp^{Me2}), 3.90 (d, *J* = 7.6 Hz, 1H, -Si(CH₃)₂CH-), 5.18 (d, *J* = 6.0 Hz, 1H, PhSiH₂-), 5.25 (d, *J* = 5.6 Hz, 1H, PhSiH₂-), 5.36 (s, 1H, *CH*-Tp^{Me2}), 5.58 (s, 2H, *CH*-Tp^{Me2}), 5.60 (s, 1H, *CH*-Tp^{Me2}), 5.64 (s, 1H, *CH*-Tp^{Me2}), 5.68 (s, 1H, *CH*-Tp^{Me2}), 5.77 (s, 1H, PhSiH₂-), 5.89 (s, 1H, PhSiH₂-), 7.13 (d, *J* = 2.4 Hz, 2H, *H*-Ar), 7.30 (d, *J* = 7.2 Hz, 1H, *H*-Ar), 7.35-7.40 (m, 3H, *H*-Ar), 7.75-7.77 (m, 2H, *H*-Ar), 8.12 (d, *J* = 6.4 Hz, 2H, *H*-Ar), 8.52 (d, *J* = 7.2 Hz, 1H, ^tBuN=CH-). ¹³C NMR (100 MHz, C₆D₆, 25 °C): δ [ppm] -0.3 (-Si(CH₃)₂-), 3.4 (-Si(CH₃)₂-), 5.0 (-Si(CH₃)₃), 5.3

(-Si(CH₃)₃), 8.5 (-Si(CH₃)₂-), 8.8 (-Si(CH₃)₂-), 12.6 (CH₃-Tp^{Me2}), 12.7 (CH₃-Tp^{Me2}), 12.9 (CH₃-Tp^{Me2}), 12.9 (CH₃-Tp^{Me2}), 13.0 (CH₃-Tp^{Me2}), 14.0 (CH₃-Tp^{Me2}), 15.2 (CH₃-Tp^{Me2}), 15.9 (CH₃-Tp^{Me2}), 16.2 (CH₃-Tp^{Me2}), 16.3 (CH₃-Tp^{Me2}), 16.6 (CH₃-Tp^{Me2}), 17.2 (CH₃-Tp^{Me2}), 29.5 (CH₃-^tBu), 30.5 (CH₃-^tBu), 32.0 (CH₃-^tBu), 58.2 (CH-^tBu), 59.1 (-Si(CH₃)₂CH-), 105.4 (CH-Tp^{Me2}), 105.5 (CH-Tp^{Me2}), 105.7 (CH-Tp^{Me2}), 105.9 (CH-Tp^{Me2}), 105.9 (CH-Tp^{Me2}), 106.2 (CH-Tp^{Me2}), 121.5 (C-Ar), 121.8 (C-Ar), 125.1 (C-Ar), 126.2 (C-Ar), 127.2 (C-Ar), 127.7 (C-Ar), 128.4 (C-Ar), 135.1 (C-Ar), 136.0 (C-Ar), 138.2 (C-Ar), 143.8 (C-Tp^{Me2}), 143.9 (C-Tp^{Me2}), 144.4 (C-Tp^{Me2}), 145.3 (C-Tp^{Me2}), 145.6 (C-Tp^{Me2}), 146.0 (C-Tp^{Me2}), 146.7 (C-Tp^{Me2}), 148.8 (C-Tp^{Me2}), 149.3 (C-Tp^{Me2}), 150.2 (C-Tp^{Me2}), 150.4 (C-Tp^{Me2}), 151.2 (C-Tp^{Me2}), 151.3 (C-Tp^{Me2}), 174.3 (^tBuN=CH-), 175.7 (-CO₂). Anal. Calcd for C₆₀H₉₉B₂N₁₅O₂Si₆Y₂ (1430.47): C, 50.38; H, 6.98; N, 14.69. Found: C, 50.72; H, 6.79; N, 14.81.

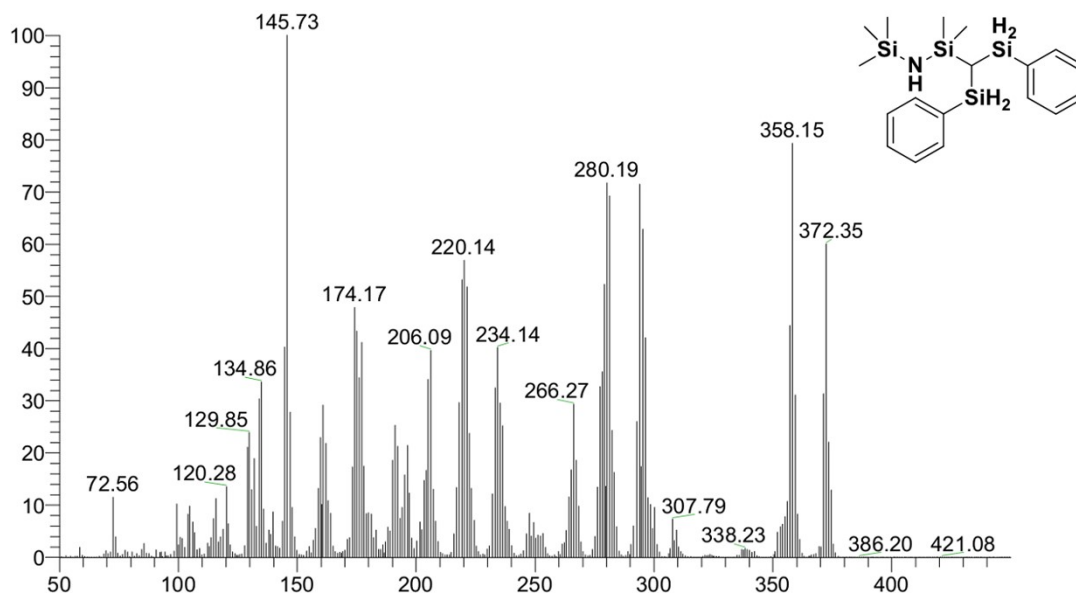


Figure S3. GC-MS detected hydrolysis product HNSiMe₃Si(Me₂)CH(SiH₂Ph)₂ (II).

X-ray Data Collection, Structure Determination, and Refinement. Data collections were performed on Bruker D8 VENTURE system diffractometers (173 K, Ga K α radiation, ω -scan technique, $\lambda = 1.34138$ Å). Diffraction data were collected over the full sphere and corrected for absorption. Structure solutions were found with SHELXS³ package using direct methods and were refined with SHELXTL program⁴ against F^2 using first isotropic and late anisotropic thermal parameters for all non-hydrogen atoms. Hydrogen atoms were placed at calculated positions and included in the structure calculation without further refinement of the parameters. The residual electron densities were of no chemical significance. Details of SQUEEZE are given in the cif files..

2. Computational Details

The optimizations of reactant, intermediates, transition states, IRC, and product were carried out by employing DFT hybrid functional (B3PW91)⁵ along with small core pseudopotential Stuttgart basis set⁶ for yttrium, potassium atoms, and Pople basis set⁷ (6-31G**) for the rest of atoms. Frequency calculations were performed to locate saddle points for transition state structures, minima for the rest of the structures, and for obtaining thermal corrections over the energies. Dispersion corrections were included in our calculations by employing the D3 version of Grimme's dispersion with Becke-Johnson damping⁸. Solvent corrections using the SMD model⁹ were included by considering the reaction in toluene. All the calculations were performed using the Gaussian 16 package¹⁰.

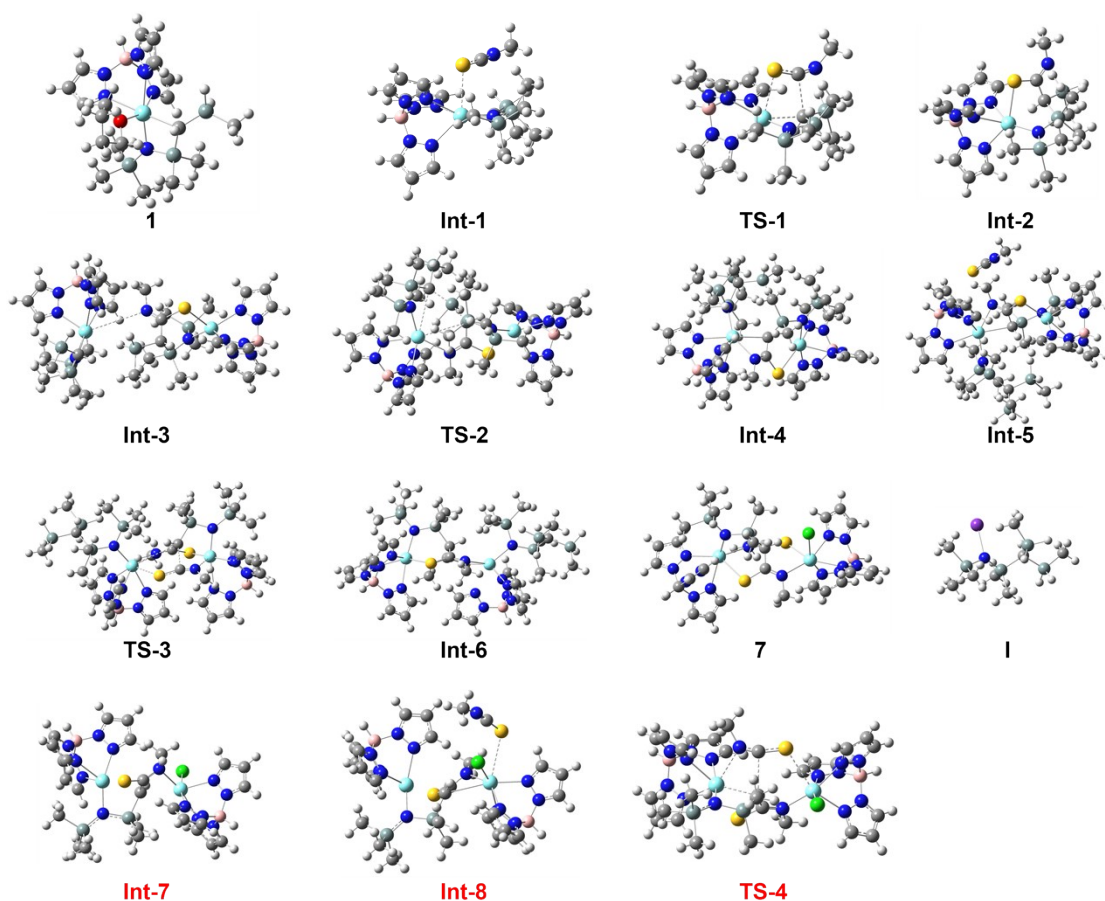


Figure S4. The optimized atomic structures of reactant, intermediates, transition states, and product. For clarity, Me in Tp^{Me_2} and Ph in total molecules were simplified in H and CH_3 , respectively.

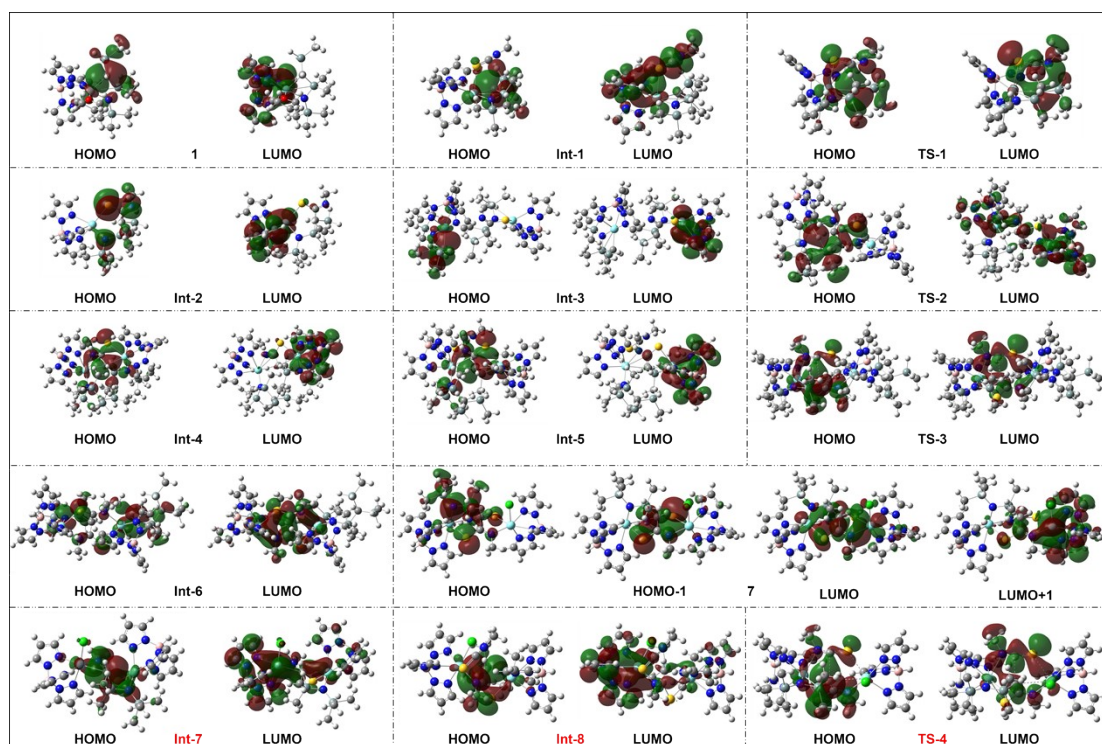


Figure S5. Molecular orbitals for reactant, intermediates, transition states, and product (isovalue = 0.02). For clarity, Me in Tp^{Me_2} and Ph in total molecules were simplified in H and CH_3 , respectively.

3. X-ray Crystallographic Analysis of All new Complexes

Table S1. Crystal data and structure refinement for **2**, **3** and **4**

	2	3	4
Formula	$C_{61}H_{84}B_3ClN_{18}OS_8Si_2Y_4$	$C_{101}H_{141}B_5K_2N_{30}O_2S_9Si_3Y_4$	$C_{72}H_{124}B_4Cl_4KN_{26}Si_4Y_3$
Formula weight	1821.64	2668.13	1957.19
Temperature (K)	173(2)	173(2)	173(2)
Wavelength	1.34138	1.34138	1.34138
Crystal system	Triclinic	Triclinic	Triclinic
Space group	<i>P</i> -1	<i>P</i> -1	<i>P</i> -1
a(Å)	13.1824(8)	14.1551(10)	12.1010(12)
b(Å)	19.7505(13)	19.7674(14)	14.5774(14)
c(Å)	20.5607(13)	32.281(2)	16.2856(17)
α(deg)	94.847(3)	73.351(2)	97.075(3)
β(deg)	97.001(2)	89.229(2)	106.057(3)
γ(deg)	104.799(2)	71.840(2)	93.058(4)
V(Å ³)	5099.6(6)	8194.1(10)	2728.2(5)
Z	2	2	1
D _c (g/m ³)	1.186	1.081	1.191
μ (mm ⁻¹)	3.513	2.597	2.748
F(000)	1856	2756	1018
Crystal size (mm)	0.060 x 0.060 x 0.040	0.160 x 0.150 x 0.120	0.120 x 0.080 x 0.080
θ range (°)	3.344 to 52.321	3.957 to 53.000	3.320 to 52.996
h, k, l range	-15<=h<=15 -23<=k<=23 -24<=l<=24	-16<=h<=16 -23<=k<=23 -38<=l<=38	-14<=h<=14 -17<=k<=17 -19<=l<=19
Refinement method	Full-matrix least-squares on F ²	Full-matrix least-squares on F ²	Full-matrix least-squares on F ²
Data / restraints / parameters	17383 / 738 / 910	28922 / 1562 / 1490	9610 / 0 / 543
Goodness-of-fit on F ²	1.092	1.018	1.022
Final R indices [<i>I</i> >2σ(<i>I</i>)]	R1 = 0.0611 wR2 = 0.1800	R1 = 0.0478 wR2 = 0.1348	R1 = 0.0400 wR2 = 0.1470
R indices (all data)	R1 = 0.0741 wR2 = 0.1904	R1 = 0.0597 wR2 = 0.1422	R1 = 0.0446 wR2 = 0.1550
Largest diff. peak and hole (e. Å ⁻³)	2.204 and -0.800	0.691 and -0.678	2.033 and -0.652

Table S2. Crystal data and structure refinement for **5** and **7-toluene**

	5	7-toluene
Formula	C ₃₁ H ₅₃ BN ₇ OSSi ₃ Y	C ₅₉ H ₈₂ B ₂ CIN ₁₅ S ₂ Si ₂ Y ₂
Formula weight	755.85	1356.58
Temperature (K)	173	173(2)
Wavelength	1.34139	1.34138
Crystal system	monoclinic	Monoclinic
Space group	P2 ₁ /c	P2 ₁ /c
a(Å)	14.1492(6)	25.1705(5)
b(Å)	29.6721(12)	13.2786(3)
c(Å)	9.7824(4)	20.5853(4)
α(deg)	90	90
β(deg)	107.0320(10)	91.8010(10)
γ(deg)	90	90
V(Å ³)	3926.9(3)	6876.8(2)
Z	4	4
D _c (g/m ³)	1.278	1.310
μ (mm ⁻¹)	2.472	2.586
F(000)	1592	2824
Crystal size (mm)	0.420 × 0.360 × 0.240	0.210 × 0.200 × 0.180
θ range (°)	7.694 to 106.276	3.274 to 52.999
h, k, l range	-16 ≤ h ≤ 16 -35 ≤ k ≤ 35, -11 ≤ l ≤ 11	-29 ≤ h ≤ 29 -15 ≤ k ≤ 12 -24 ≤ l ≤ 24
Data / restraints / parameters	6888/36/423	12130 / 0 / 776
Goodness-of-fit on F ²	1.04	0.979
Final R indices [I>2σ(I)]	R1 = 0.0471 wR2 = 0.1206	R1 = 0.0314 wR2 = 0.0974
R indices (all data)	R1 = 0.0495 wR2 = 0.1230	R1 = 0.0392 wR2 = 0.1056
Largest diff. peak and hole (e. Å ³)	1.08 and -0.67	0.469 and -0.552

Table S3. Crystal data and structure refinement for **8** and **9**

	8	9
Formula	C ₃₈ H ₅₆ BN ₈ OSSi ₃ Y	C ₆₀ H ₉₉ B ₂ N ₁₅ O ₂ Si ₆ Y ₂
Formula weight	858.97	1430.52
Temperature (K)	173	173(2)
Wavelength	1.34138	1.34138
Crystal system	monoclinic	Triclinic
Space group	P21/n	<i>P</i> -1
a(Å)	10.6116(13)	14.6139(13)
b(Å)	31.558(4)	15.8993(14)
c(Å)	13.2103(17)	18.6213(16)
α(deg)	90	77.834(3)
β(deg)	93.169(4)	82.261(3)
γ(deg)	90	86.714(3)
V(Å ³)	4417.2(10)	4189.1(6)
Z	4	2
D _c (g/m ³)	1.292	1.134
μ (mm ⁻¹)	2.244	2.003
F(000)	1808	1504
Crystal size (mm)	0.230 × 0.120 × 0.080	0.250 × 0.200 × 0.200
h, k, l range	-13 ≤ h ≤ 13 -40 ≤ k ≤ 40 -16 ≤ l ≤ 16	-17 ≤ h ≤ 17 -18 ≤ k ≤ 18 -22 ≤ l ≤ 22
Refinement method	Full-matrix least-squares on F ²	Full-matrix least-squares on F ²
Data / restraints / parameters	9753 / 6 / 496	14716 / 0 / 833
Goodness-of-fit on F ²	1.022	1.028
Final R indices [I > 2σ(I)]	R1 = 0.0456 wR2 = 0.1246	R1 = 0.0415 wR2 = 0.1345
R indices (all data)	R1 = 0.0487 wR2 = 0.1288	R1 = 0.0466 wR2 = 0.1400
Largest diff. peak and hole (e. Å ³)	0.81 and -1.26	0.626 and -0.612

4. NMR Spectra of All New Compounds

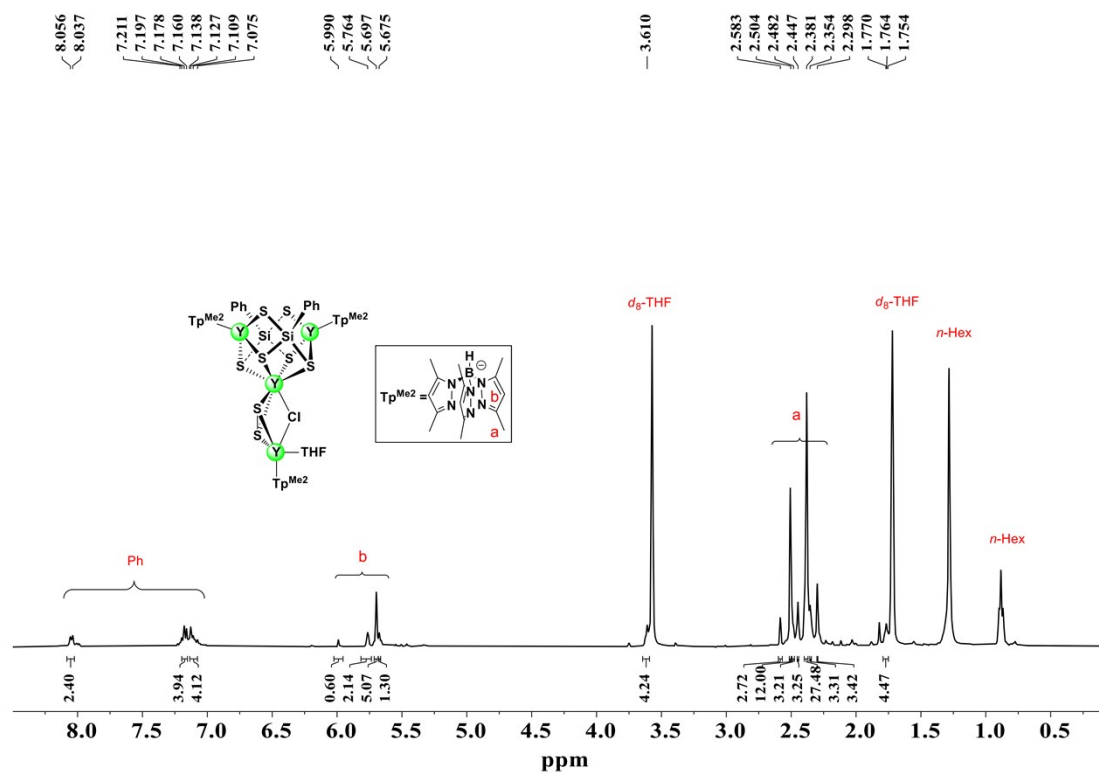


Figure S6. ^1H NMR spectrum of **2** (25 °C, 400 MHz, d_8 -THF).

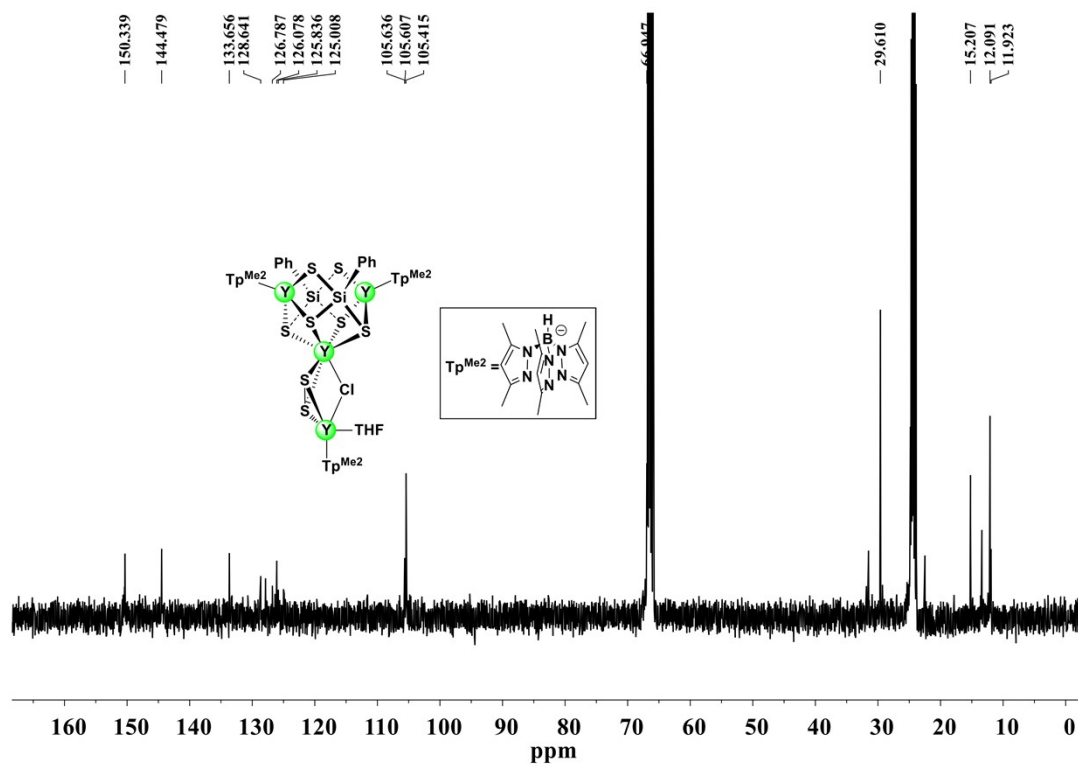


Figure S7. ^{13}C NMR spectrum of **2** (25 °C, 100 MHz, d_8 -THF).

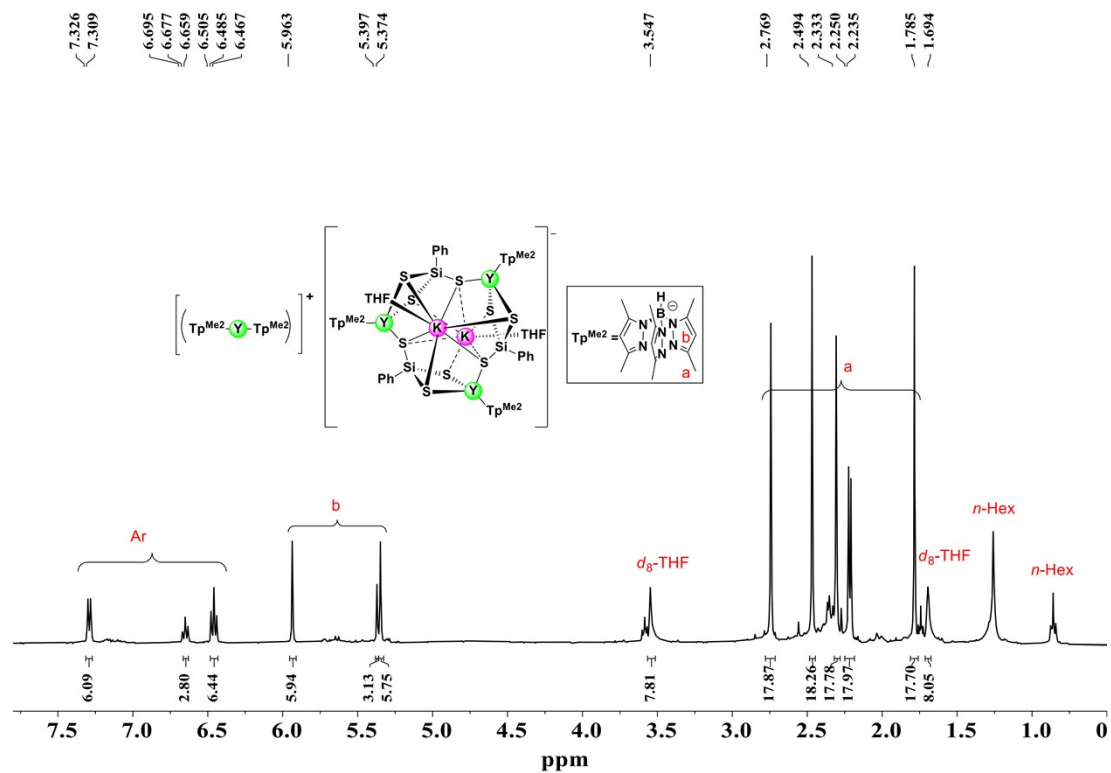


Figure S8. ^1H NMR spectrum of **3** (25 °C, 400 MHz, d_8 -THF).

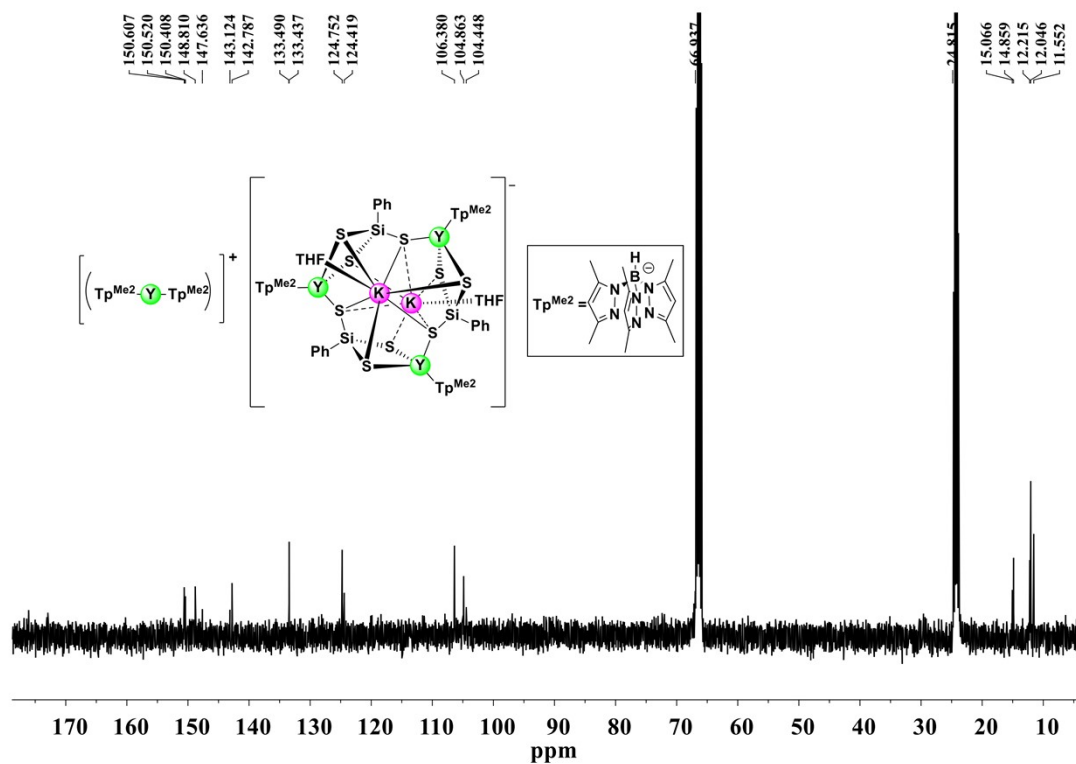


Figure S9. ^{13}C NMR spectrum of **3** (25 °C, 100 MHz, d_8 -THF).

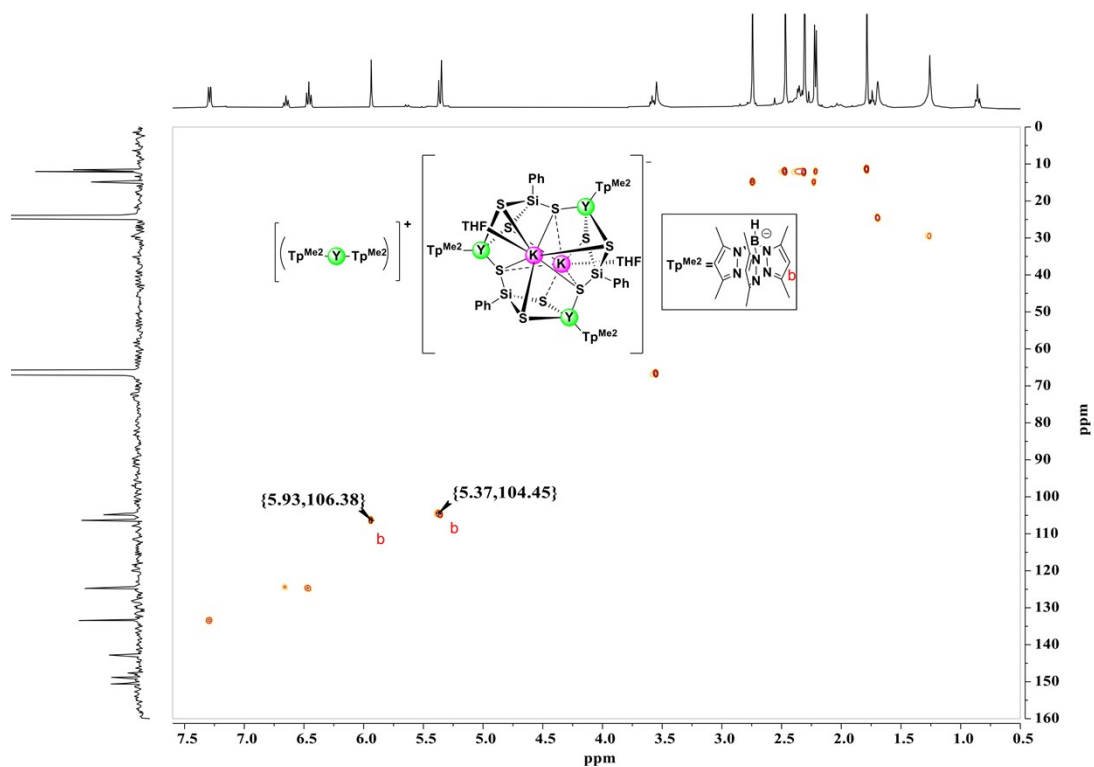


Figure S10. HSQC (^1H NMR- ^{13}C NMR) Spectrum of **3** (25 $^\circ\text{C}$, d_8 -THF).

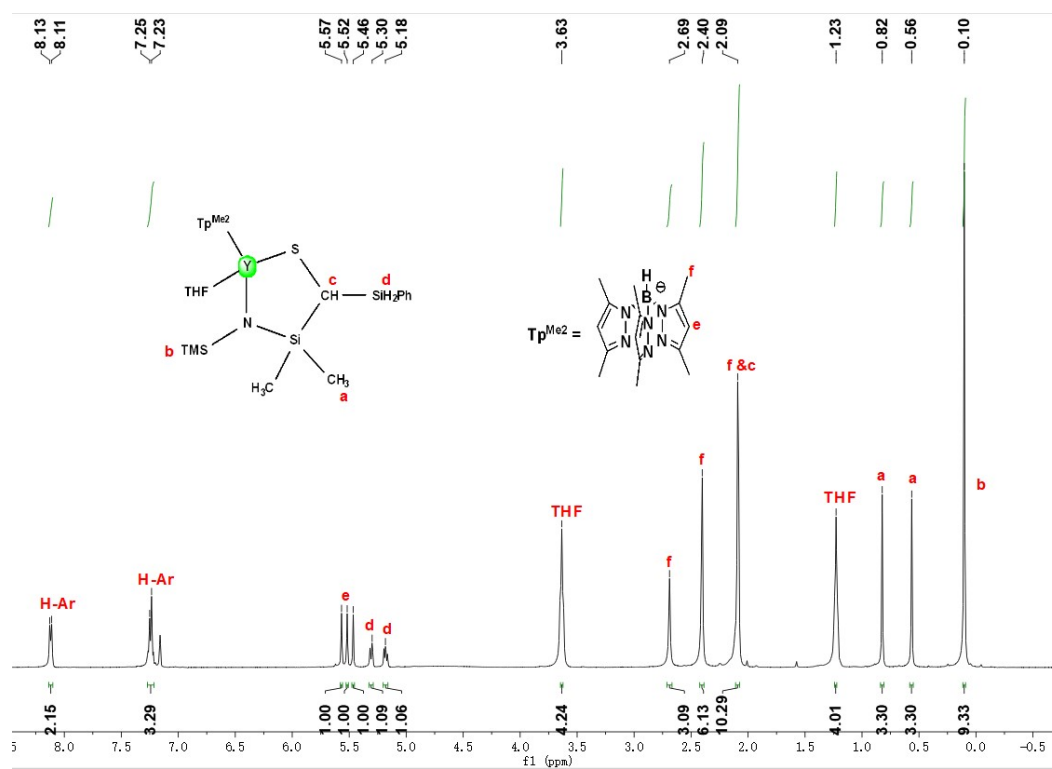
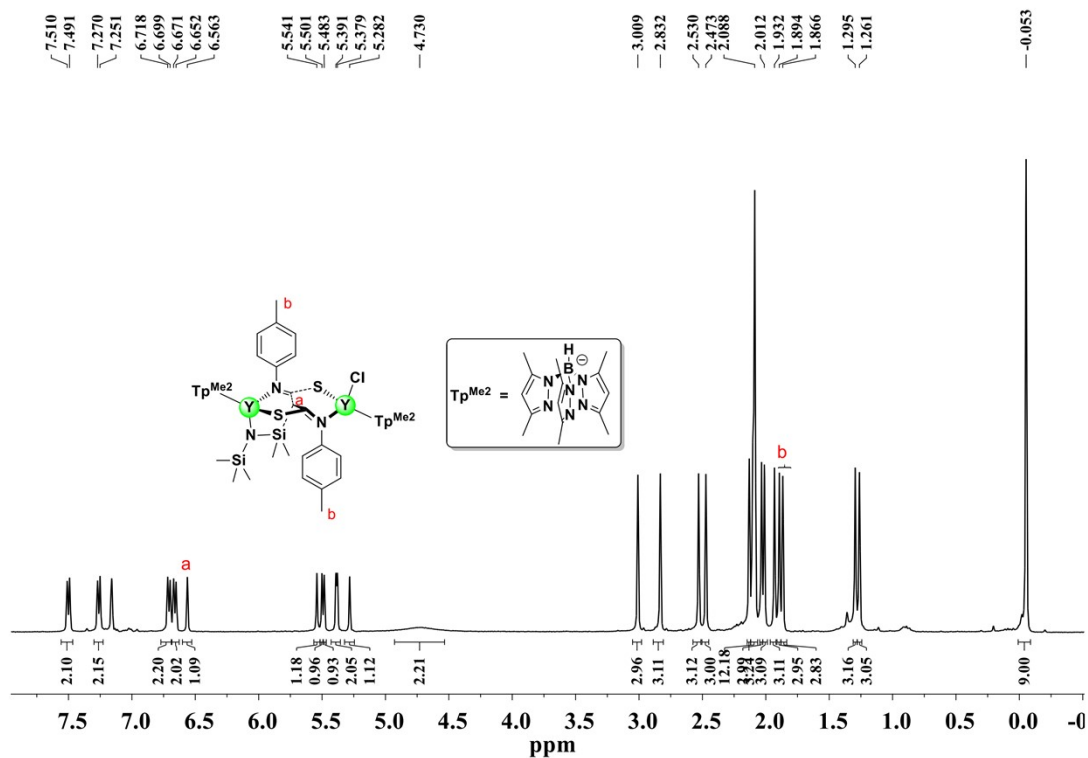
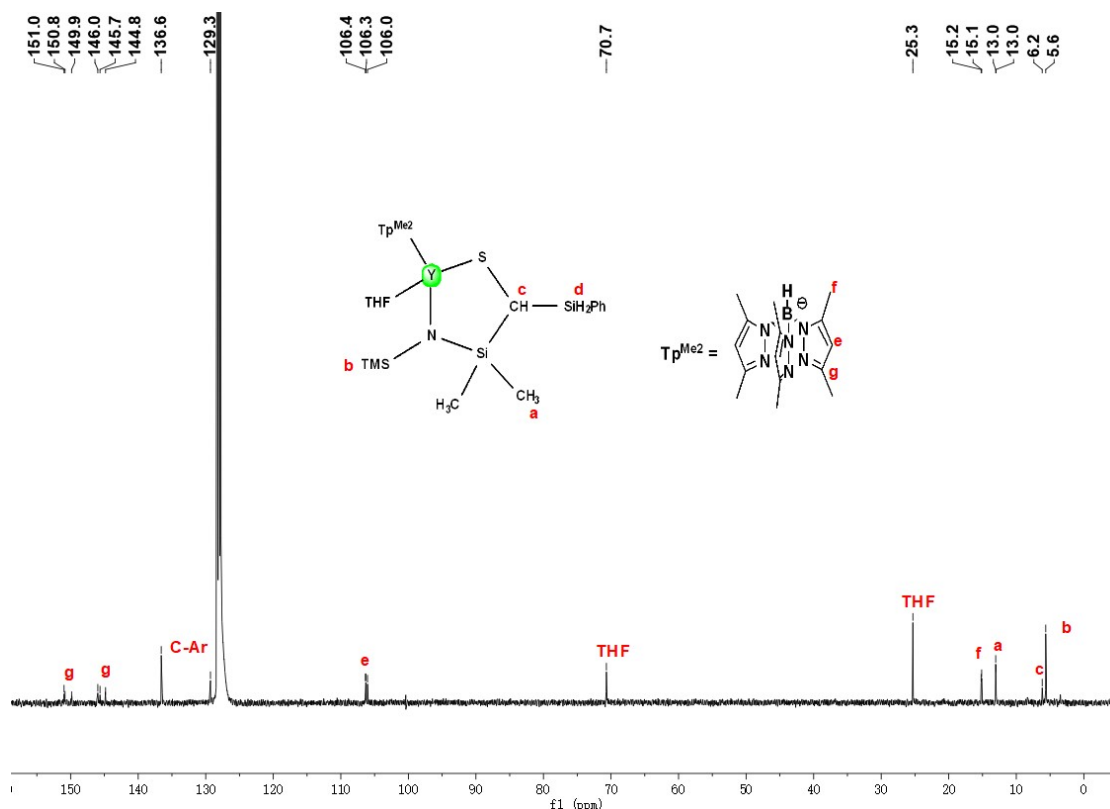


Figure S11. ^1H NMR spectrum of **5** (25 $^\circ\text{C}$, 400 MHz, C_6D_6).



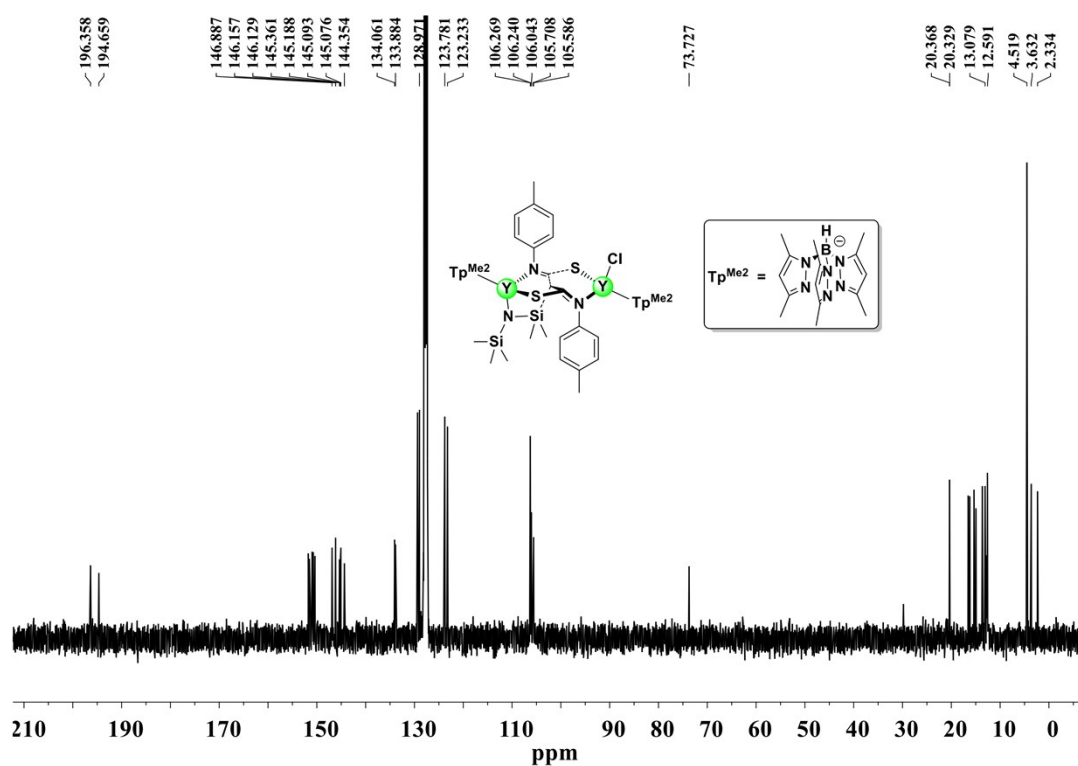


Figure S14. ^{13}C NMR spectrum of **7** (25 °C, 100 MHz, C_6D_6).

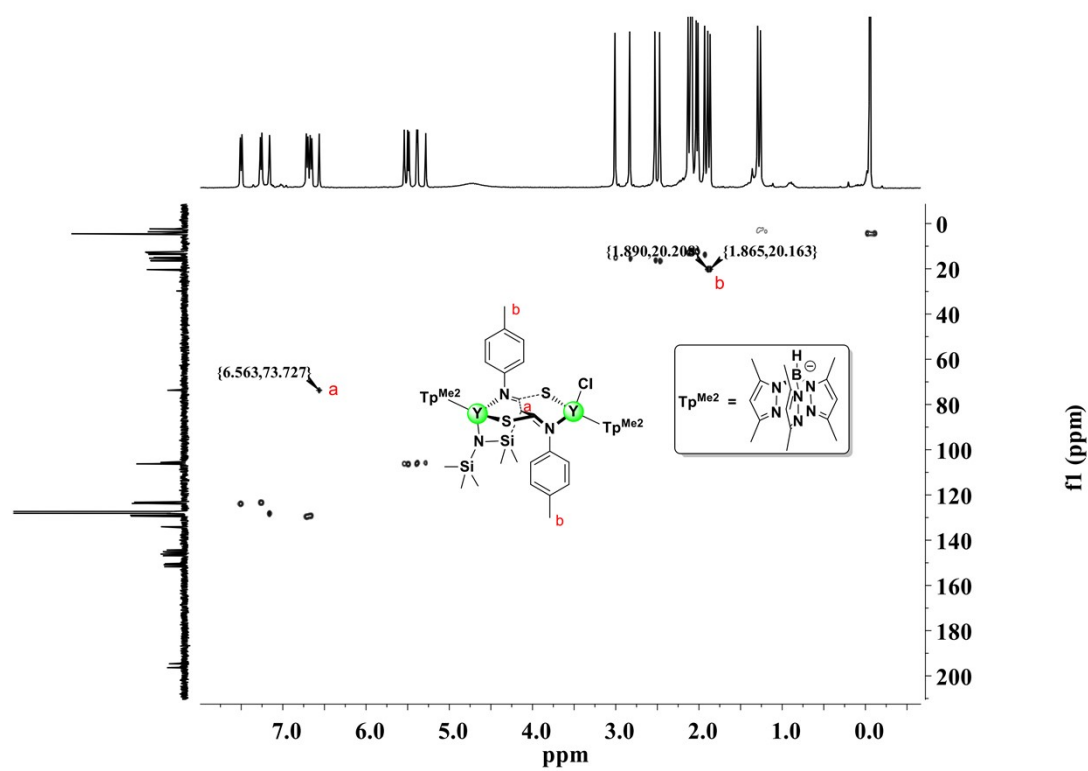


Figure S15. HSQC (^1H NMR- ^{13}C NMR) Spectrum of **7** (25 °C, C_6D_6).

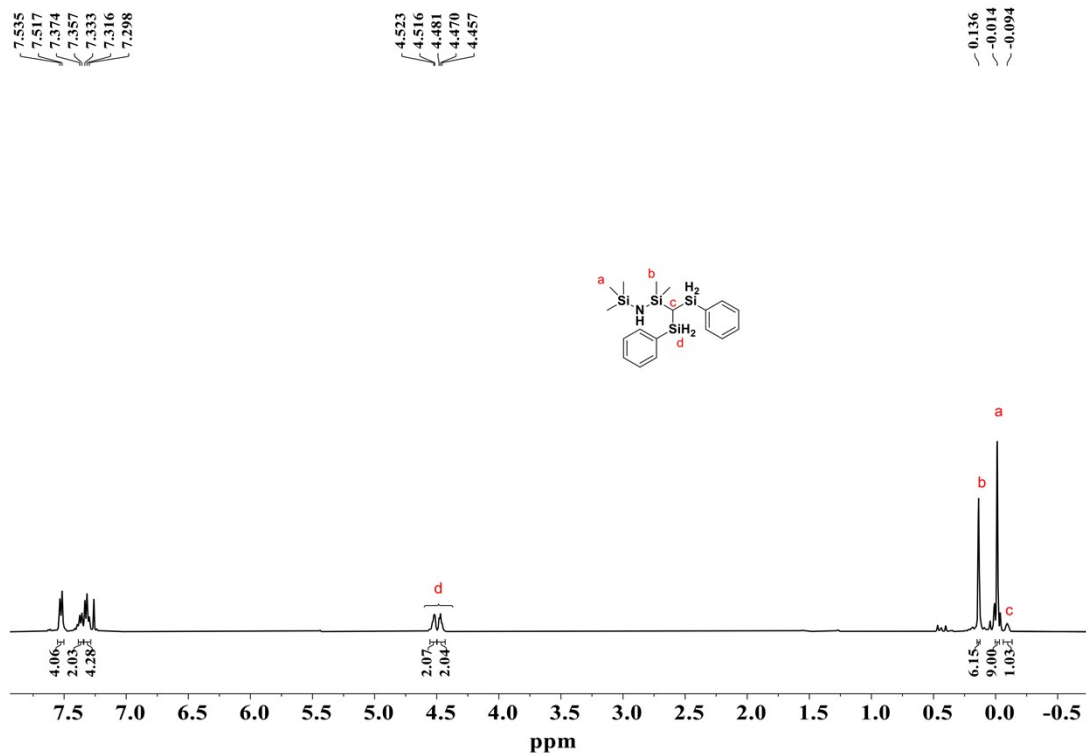


Figure S16. ¹H NMR spectrum of II (25 °C, 400 MHz, CDCl₃).

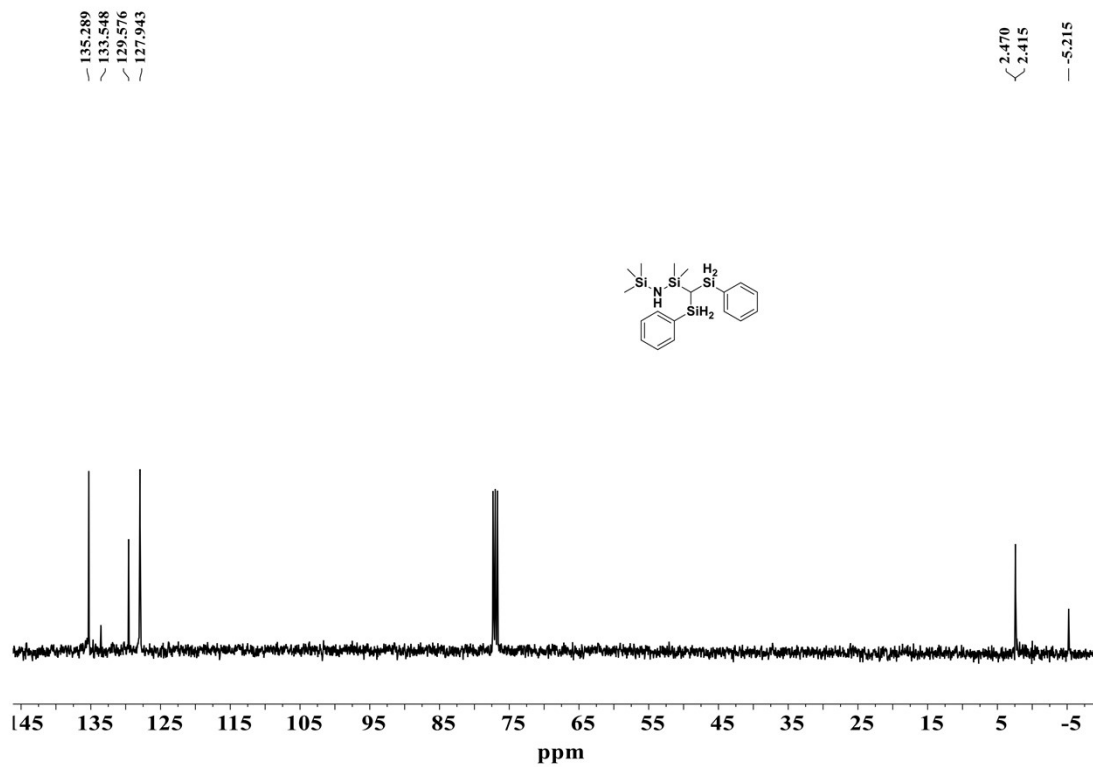


Figure S17. ¹³C NMR spectrum of II (25 °C, 100 MHz, CDCl₃).

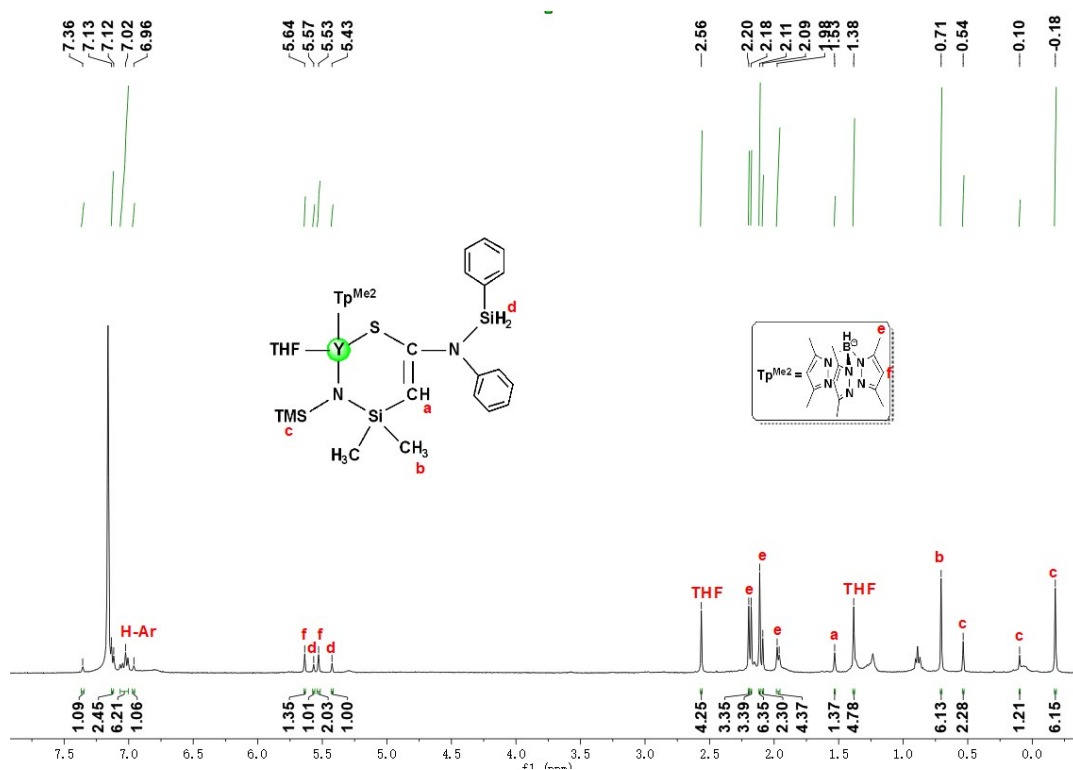


Figure S18. ¹H NMR spectrum of **8** (25 °C, 400 MHz, C₆D₆).

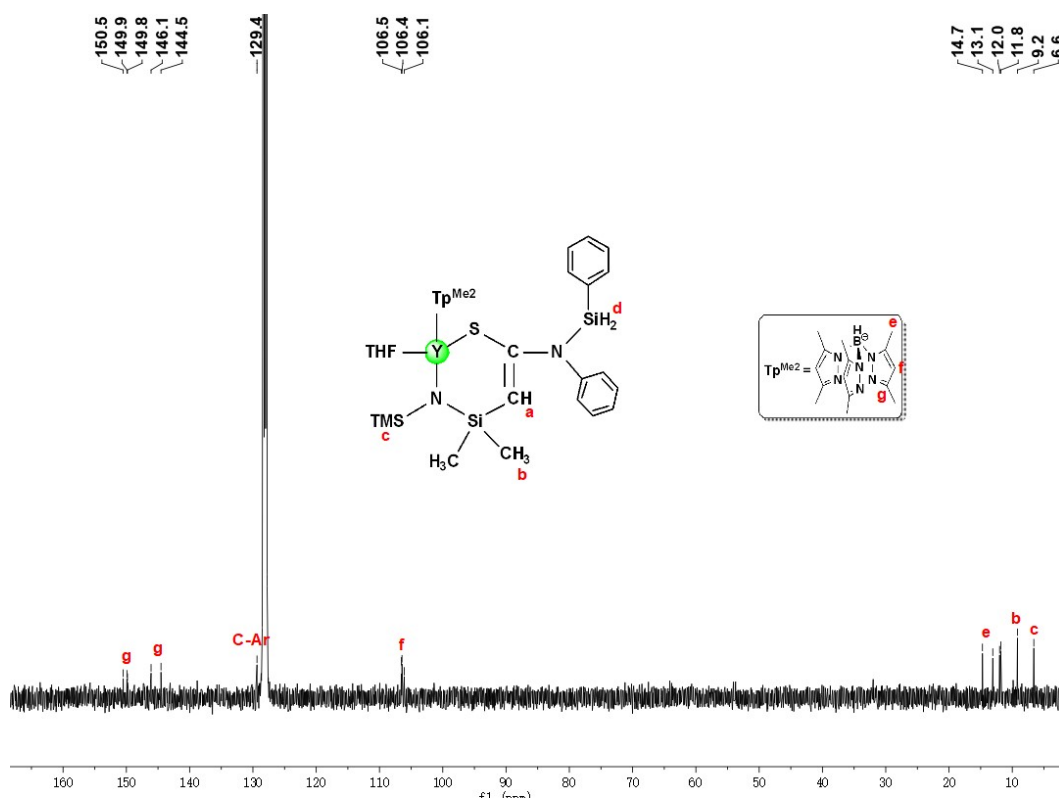


Figure S19. ¹³C NMR spectrum of **8** (25 °C, 100 MHz, C₆D₆).

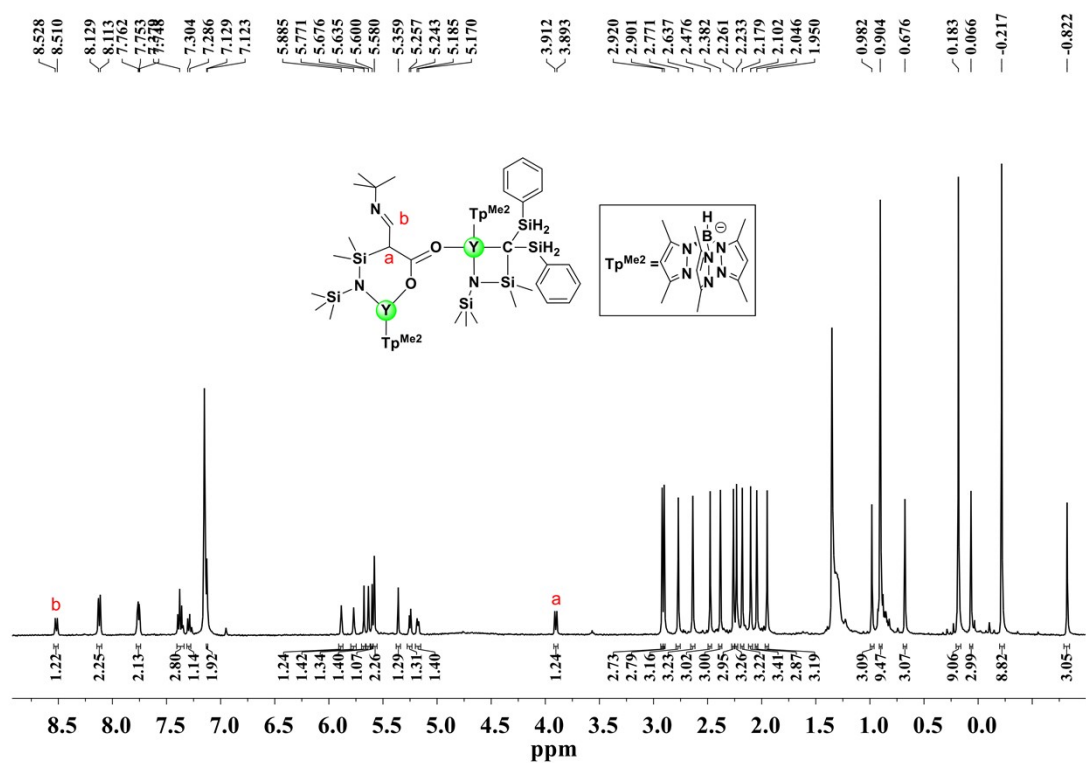


Figure S20. ^1H NMR spectrum of **9** (25 °C, 400 MHz, C_6D_6).

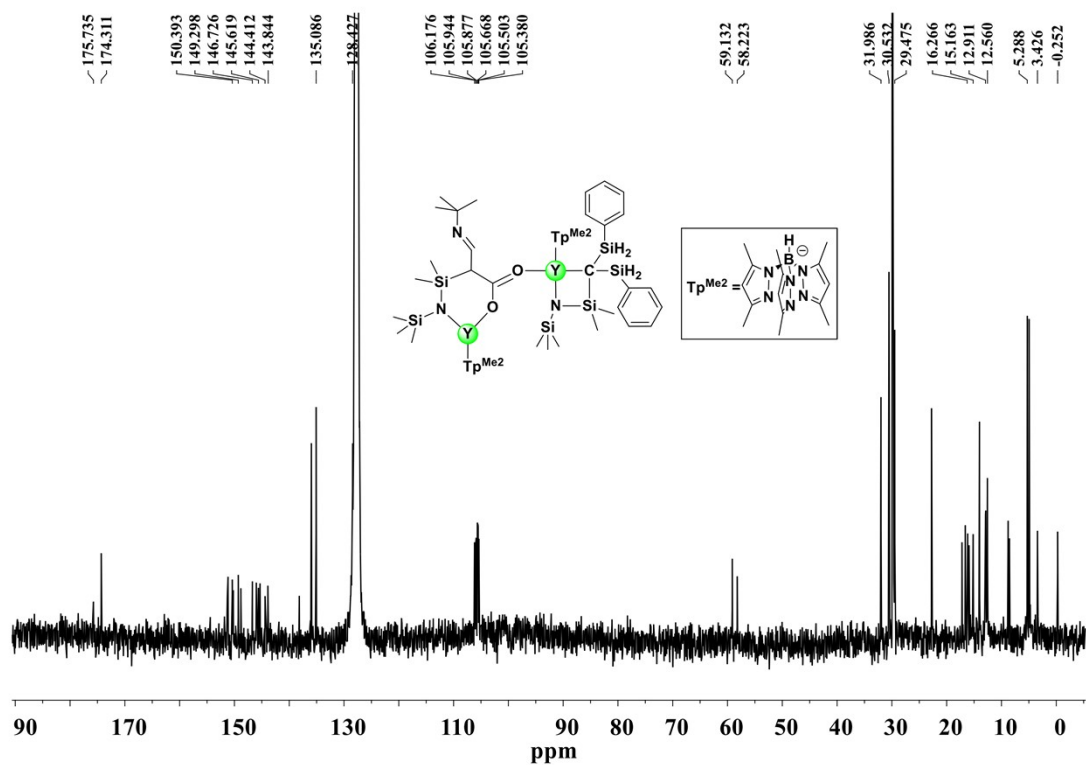


Figure S21. ^{13}C NMR spectrum of **9** (25 °C, 100 MHz, C_6D_6).

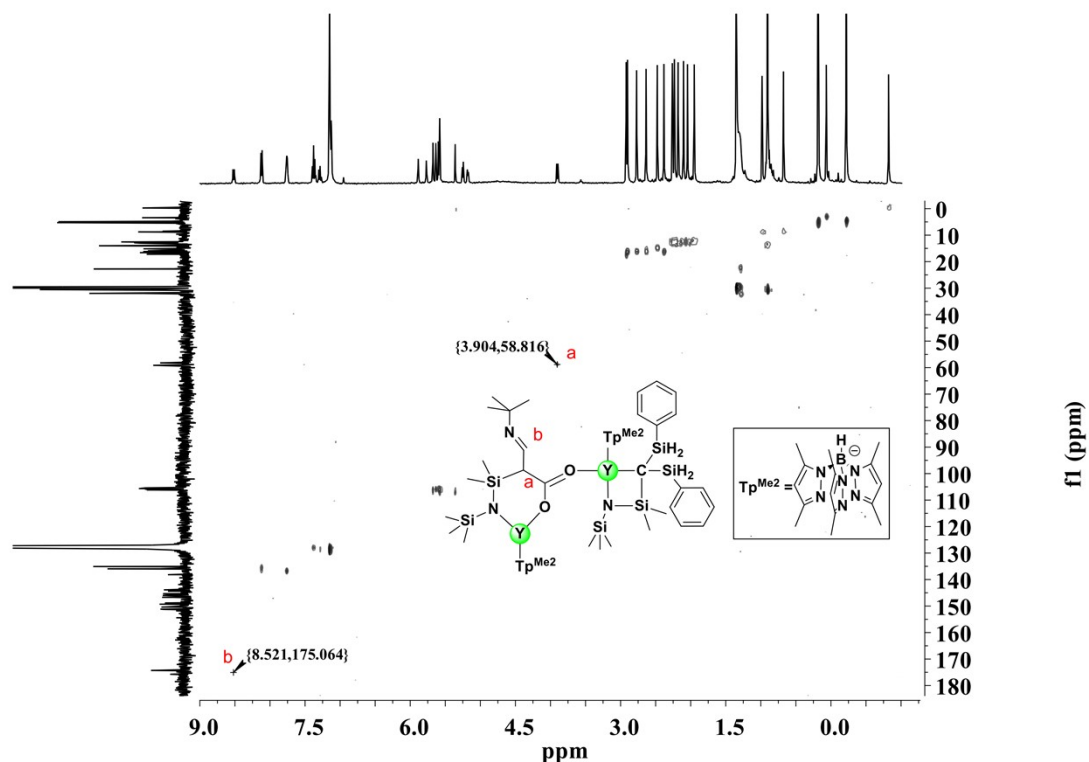


Figure S22. HSQC (^1H NMR- ^{13}C NMR) Spectrum of **9** (25 °C, C_6D_6).

5. Optimized Geometries

Atom	x	y	z
1			
Y	-0.04780200	0.06831200	0.17979700
B	-3.36513200	0.31519500	-1.13195500
N	-2.33750000	0.86564800	-2.16014300
N	-0.97334800	0.89223900	-1.90629100
N	-3.28851500	1.14584800	0.18152100
N	-2.12095000	1.26400000	0.92176100
N	-3.05387900	-1.18645400	-0.84011400
N	-1.83546500	-1.61607000	-0.34019300
N	1.92596400	-0.63532900	-0.55307400
Si	2.35389200	-2.04449500	-1.47405400
Si	2.90593200	0.71814800	0.04717000
Si	1.33862800	3.54506000	0.66660200
O	-0.09017200	-1.11512400	2.20343000
C	-2.56024700	1.37254500	-3.38338100
C	-1.35910800	1.73696000	-3.94725500
H	-1.19477300	2.17001600	-4.90441100
C	-0.39989300	1.41432900	-2.98162100
C	-4.23693700	1.92058100	0.73373400
C	-3.71470500	2.55438100	1.83761100
H	-4.20394300	3.24062600	2.48619800

C	-2.38753200	2.11479700	1.90452900
C	-3.84117700	-2.25219900	-1.05423100
C	-3.15896100	-3.39494400	-0.70088900
H	-3.50027300	-4.40062500	-0.75763400
C	-1.91081300	-2.93992500	-0.26488000
C	1.09498800	-2.37328900	-2.89129200
H	1.15167300	-1.58651400	-3.63905600
H	1.30670200	-3.31923600	-3.38378400
H	0.07100300	-2.40360400	-2.53054000
C	4.08534300	-1.98022600	-2.30670400
H	4.87934000	-1.80953700	-1.58522300
H	4.29085800	-2.92235000	-2.80945700
H	4.13280800	-1.19013600	-3.05036900
C	2.36168000	-3.63849100	-0.38133000
H	1.40341800	-3.79219100	0.11095400
H	2.57022500	-4.52015600	-0.98196500
H	3.12576700	-3.57148000	0.38980600
C	3.73825000	1.70602600	-1.37990700
H	3.00125600	2.12460700	-2.05988500
H	4.32593900	2.52846200	-0.98091500
H	4.40386800	1.07273800	-1.95894800
C	4.35294500	0.13946200	1.18168200
H	5.03878300	-0.51572800	0.65045100
H	4.91615900	1.00051500	1.53263000
H	3.98852500	-0.39719500	2.05326400
C	1.60229400	1.72733100	0.98356000
H	1.69508100	1.56486500	2.06354700
C	1.14854100	-1.49915900	2.92057100
H	1.78346500	-2.01305200	2.22208000
H	1.62133300	-0.59251500	3.25893200
C	0.65796400	-2.36008600	4.09102200
H	0.54595800	-3.39130000	3.78046200
H	1.33670300	-2.31479700	4.93047100
C	-0.72232100	-1.74633800	4.40306800
H	-1.36141100	-2.41309900	4.96400500
H	-0.60215700	-0.82133500	4.95285900
C	-1.28167100	-1.46640200	3.00411500
H	-1.96553700	-0.63860800	2.95461100
H	-1.72882400	-2.34401300	2.56882200
H	-4.47034600	0.40020900	-1.58723500
H	0.97373300	3.79997800	-0.77041100
H	0.17852200	4.06517700	1.47737200
H	-1.63002000	2.39587700	2.59888000
H	-5.21210200	1.97995800	0.31025600
H	0.65686100	1.54027800	-3.02642000
H	-3.54741500	1.44379300	-3.77611800
H	-1.08235000	-3.51443800	0.08062700

H	-4.82548100	-2.13777000	-1.44352300
C	2.78569400	4.76090800	1.06084000
H	3.65646800	4.54585600	0.44916700
H	2.48302500	5.78730300	0.87102200
H	3.07998300	4.68154900	2.10395200

Int-1

Y	-0.25724000	0.37495500	0.19471900
B	-3.78677800	-0.43412300	0.16955200
N	-3.46701400	0.46460400	1.38030900
N	-2.20985800	0.88438000	1.65004700
N	-2.98396600	-1.74091000	0.26526300
N	-1.63088800	-1.74847200	0.32607900
N	-3.41680000	0.30747900	-1.13228600
N	-2.16325900	0.75463500	-1.37239600
N	1.65004100	1.56624700	-0.03283100
Si	1.93190200	3.22803700	-0.29838500
Si	2.78237700	0.34453700	0.44414000
Si	2.44699300	-2.61682200	1.37794600
C	-4.32667700	0.96022100	2.29314200
C	-3.60824900	1.73346400	3.19479300
H	-3.98929500	2.27040800	4.05101300
C	-2.28434500	1.65301500	2.74469300
C	-3.45915300	-3.00371300	0.25529000
C	-2.37835700	-3.87222400	0.31148300
H	-2.40194800	-4.95228800	0.32212400
C	-1.25619600	-3.03258900	0.35185400
C	-4.22711200	0.62077600	-2.16339400
C	-3.47864700	1.29930100	-3.11562000
H	-3.81851300	1.69493500	-4.06140600
C	-2.19054700	1.35872300	-2.56873400
C	0.50609300	3.94123400	-1.32032900
H	0.46887300	3.47704600	-2.31326300
H	0.60036900	5.02504600	-1.46140400
H	-0.45775800	3.75319400	-0.83060600
C	2.01117100	4.21665100	1.31670200
H	1.08343600	4.09367300	1.88937000
H	2.15528300	5.28943900	1.13764700
H	2.83744200	3.86878300	1.94779300
C	3.54349000	3.57071300	-1.23181200
H	4.41217300	3.22596700	-0.65884400
H	3.67808600	4.64232000	-1.42492600
H	3.55580700	3.05255400	-2.19797800
C	3.97760400	0.95121900	1.79271900
H	4.57092300	1.81403200	1.45974200
H	4.68023200	0.15846300	2.08006200
H	3.42726200	1.25241800	2.69303000

C	3.89066000	-0.17375200	-1.00399100
H	3.29624900	-0.42822400	-1.89098700
H	4.52533100	-1.03479600	-0.75537400
H	4.55191900	0.66123600	-1.27786400
C	1.66167900	-1.00890500	1.03689900
H	1.27970700	-0.68278000	2.02954200
H	-4.96027800	-0.68375100	0.15878800
H	1.68349200	-3.84799000	0.94917000
H	3.75619000	-2.79122400	0.66408200
S	0.23449700	-1.02497100	-2.43202400
C	1.33057100	-2.16233700	-2.09429300
N	2.08225900	-3.05138500	-1.92527300
H	-0.20584600	-3.28452500	0.39937200
H	-4.52247200	-3.19244600	0.21013400
H	-5.38090400	0.72845100	2.23882700
H	-1.38880400	2.10505800	3.15113400
H	-5.27209900	0.34589700	-2.14492600
H	-1.29114200	1.80413800	-2.97335800
C	3.17232300	-3.94225100	-1.92358300
H	3.01818100	-4.72341100	-1.18316500
H	3.25951900	-4.39891700	-2.90970400
H	4.08778700	-3.38040600	-1.68562400
C	2.79791300	-2.87473100	3.22233600
H	3.25812000	-3.85068500	3.42569200
H	3.47300100	-2.09494700	3.59594200
H	1.86923600	-2.81523800	3.80340600

TS-1

Y	-0.26514600	0.37155000	0.14359500
B	-3.79205400	-0.39181000	0.16463000
N	-3.45180700	0.48673600	1.38386400
N	-2.18705600	0.89073800	1.64201800
N	-3.00208600	-1.70990300	0.23785100
N	-1.64917600	-1.73849300	0.29585500
N	-3.42395100	0.36808400	-1.12670800
N	-2.17048000	0.81846900	-1.35730600
N	1.68353200	1.52213300	0.02555100
Si	1.97951900	3.18348100	-0.24251100
Si	2.80137900	0.26284100	0.39834300
Si	2.48585000	-2.73406500	1.29089700
C	-4.29638200	0.98739000	2.30781300
C	-3.55961500	1.74750200	3.20587200
H	-3.92550200	2.28593700	4.06769800
C	-2.24136800	1.65435700	2.74153300
C	-3.49569800	-2.96575000	0.23407700
C	-2.42806400	-3.85020300	0.29388100
H	-2.46808000	-4.92960300	0.31188900

C	-1.29338200	-3.02773800	0.33029900
C	-4.22676900	0.68149100	-2.16359500
C	-3.47190800	1.36374100	-3.10845300
H	-3.80515900	1.75908400	-4.05674300
C	-2.18778400	1.42326900	-2.55273100
C	0.56201100	3.90431800	-1.26930400
H	0.52105400	3.43091500	-2.25768800
H	0.67087500	4.98521300	-1.42027200
H	-0.40475500	3.73322200	-0.77938500
C	2.06303500	4.16465900	1.37492700
H	1.12427400	4.06634100	1.93410000
H	2.24054800	5.23334600	1.20219400
H	2.86991800	3.78950700	2.01571300
C	3.59629000	3.50522100	-1.17208500
H	4.45977400	3.16191000	-0.59021800
H	3.73798300	4.57372300	-1.37583100
H	3.61082900	2.97553200	-2.13169100
C	3.93158400	0.71383000	1.85489000
H	4.53272100	1.60342500	1.62687000
H	4.62630300	-0.10016400	2.09692900
H	3.34026000	0.93051700	2.75232500
C	3.95837500	-0.16188800	-1.03761400
H	3.40698600	-0.25966500	-1.97813300
H	4.49567800	-1.10032100	-0.85907900
H	4.70507200	0.63016300	-1.16694300
C	1.66361800	-1.17117200	0.78644200
H	1.09857600	-0.92515400	1.71094500
H	-4.96768400	-0.63069400	0.15887800
H	1.73170000	-3.98761500	0.94996200
H	3.85115800	-2.92688500	0.70320500
S	0.29998800	-0.98044800	-2.36253900
C	1.33332000	-1.98425400	-1.57096000
N	2.08850500	-2.91170300	-1.47274900
H	-0.24669900	-3.29455900	0.37603100
H	-4.56177800	-3.13885700	0.19202700
H	-5.35388100	0.76907900	2.26224400
H	-1.33663700	2.09522200	3.13970600
H	-5.27049200	0.40147000	-2.15566000
H	-1.28416200	1.86575300	-2.95087400
C	2.85098500	-3.79719300	-2.30243300
H	2.65794700	-4.83000500	-2.00192500
H	2.59844800	-3.66779100	-3.35972300
H	3.91550100	-3.59596300	-2.15250100
C	2.70216100	-2.76927600	3.17429500
H	3.17564100	-3.69649900	3.51687000
H	3.31755300	-1.92783600	3.51126800
H	1.72788300	-2.68685600	3.67110200

Int-2

Y	0.36785000	-0.74976600	-0.10014600
B	3.94971300	-0.14729200	-0.21422300
N	3.21014300	0.71734700	-1.25499700
N	1.88817100	0.56925500	-1.50284800
N	3.74152600	-1.62560300	-0.57183200
N	2.49631500	-2.14379500	-0.62958200
N	3.38245500	0.10489800	1.19968300
N	2.10042400	-0.17793700	1.52279200
N	-0.86666800	1.13743800	0.27465900
Si	-0.29755400	2.76127400	0.54796900
Si	-2.57953400	0.88023500	0.41136100
Si	-4.56326900	-0.55104500	-1.69898500
C	3.72460000	1.67423700	-2.05285600
C	2.70451100	2.16899300	-2.85538900
H	2.77478000	2.94072000	-3.60759400
C	1.57214000	1.44258000	-2.46834700
C	4.65871900	-2.57151200	-0.86140800
C	3.98739100	-3.75840100	-1.11897900
H	4.41671800	-4.71377900	-1.38308600
C	2.63237400	-3.43399500	-0.95879600
C	4.04096800	0.55406400	2.28526900
C	3.15971400	0.56445600	3.35959100
H	3.36427500	0.86848200	4.37543400
C	1.95267600	0.09880400	2.82561400
C	1.56037100	2.93137700	0.83595000
H	1.88555100	2.43764500	1.75534600
H	1.77345000	4.00274600	0.94414600
H	2.16935600	2.55809800	0.01105800
C	-0.65799300	3.92018400	-0.90643100
H	-0.22045100	3.52890700	-1.83134200
H	-0.20734500	4.90299900	-0.71966200
H	-1.72704200	4.07171500	-1.07812300
C	-1.04846400	3.54031700	2.10584300
H	-2.13842200	3.63122000	2.07836100
H	-0.63740100	4.54738000	2.25015900
H	-0.78535800	2.94775900	2.99025000
C	-3.63051200	2.32083300	-0.21813100
H	-3.47475800	3.21251800	0.39712100
H	-4.69459000	2.06645600	-0.15301100
H	-3.40908200	2.59039400	-1.25368500
C	-3.13581400	0.58695300	2.18958300
H	-2.64087600	-0.29355100	2.61272300
H	-4.21860000	0.43547600	2.25461400
H	-2.87925700	1.45346000	2.80800300
C	-3.03912300	-0.70728100	-0.59853500

H	-2.22067300	-0.86963400	-1.31549000
H	5.11695600	0.12622000	-0.22604300
H	-4.98455600	-1.90695900	-2.16465000
H	-5.73940700	0.05419700	-1.01163800
S	-1.64964200	-2.65768000	0.85772700
C	-3.15614900	-1.88692700	0.32434500
N	-4.33281500	-2.25019900	0.70141900
H	1.75719400	-4.06241500	-1.06293700
H	5.71334800	-2.33520500	-0.86428200
H	4.77316200	1.93004100	-1.99865000
H	0.55408100	1.50620300	-2.82757200
H	5.08499000	0.82575000	2.22118500
H	0.99142300	-0.03819800	3.30319300
C	-4.45500800	-3.32653500	1.66011600
H	-5.51151200	-3.49871100	1.88698800
H	-4.03014500	-4.26837100	1.28641400
H	-3.93587100	-3.09905100	2.60162600
C	-4.14284500	0.45083500	-3.23883900
H	-4.99282700	0.48037300	-3.92937300
H	-3.86395600	1.48133900	-3.00310700
H	-3.30083200	-0.01423200	-3.76470300

Int-3

Y	-4.00110900	0.09219800	0.17774500
B	-4.54238100	3.56231000	-0.19184400
N	-5.87895600	2.78037700	-0.36416200
N	-5.94786900	1.39710200	-0.27716700
N	-3.96483300	3.31178300	1.22544800
N	-3.65261200	2.03807800	1.68398200
N	-3.51238100	3.09227200	-1.26629800
N	-3.03727200	1.78822500	-1.35345800
N	-4.68855500	-1.73237800	-0.84665100
Si	-4.99472500	-2.13717000	-2.51428800
Si	-5.03024600	-2.71111100	0.60256100
Si	-5.67226900	-1.02206400	3.34357600
C	-7.10997600	3.25955300	-0.59197200
C	-8.00063900	2.21022100	-0.65774100
H	-9.04954000	2.25750400	-0.82564300
C	-7.22228200	1.06845200	-0.45421800
C	-3.69131400	4.20316800	2.19249800
C	-3.19833300	3.53846800	3.29092600
H	-2.89097200	3.95435400	4.22012700
C	-3.19874800	2.18795800	2.92005600
C	-2.91087400	3.83778600	-2.20511800
C	-2.03592100	3.04954700	-2.91872900
H	-1.40791300	3.33715900	-3.72705300
C	-2.15454200	1.78131700	-2.34332900

C	-3.82243700	-1.17901700	-3.69943600
H	-3.95479800	-0.10430100	-3.61715200
H	-4.02575600	-1.45823000	-4.73035300
H	-2.78065700	-1.41339300	-3.49264100
C	-6.78181100	-1.70780500	-3.08964800
H	-7.52568900	-2.20907100	-2.47601300
H	-6.93388800	-2.02044900	-4.12009000
H	-6.96682100	-0.63828200	-3.03550300
C	-4.74511800	-4.00007000	-2.92432300
H	-3.74028800	-4.32593300	-2.67099100
H	-4.89692000	-4.16978800	-3.98767300
H	-5.44602000	-4.63175100	-2.38562100
C	-6.88682300	-3.21919100	0.67732800
H	-7.53956400	-2.35646500	0.77949700
H	-7.07023100	-3.87828900	1.52147900
H	-7.17890700	-3.75013900	-0.22587100
C	-4.04440700	-4.36231300	0.65311000
H	-4.40683500	-5.06940600	-0.08660400
H	-4.14472000	-4.81976700	1.63439700
H	-2.98835000	-4.19513700	0.46512900
C	-4.49934600	-1.51644700	1.97635900
H	-3.56328400	-1.85499000	2.42911600
H	-4.75009700	4.73319600	-0.34016500
H	-6.89405100	-0.34105400	2.78858300
H	-5.03321400	-0.02267600	4.26955100
Y	4.72030300	0.30685100	0.02358400
B	7.95776200	-0.56678400	0.93626300
N	7.49903000	-1.49284100	-0.22146200
N	6.22223600	-1.39815400	-0.75450900
N	7.00233700	-0.75291800	2.15241700
N	5.63708700	-0.48829500	2.08120500
N	7.92283100	0.92758300	0.46449100
N	6.77997600	1.56758300	-0.01315400
N	3.13295900	-0.43075600	-1.31119300
Si	3.15413600	0.36288600	-2.86773100
Si	1.87585100	-1.42674900	-0.60622000
Si	-0.53247800	-1.08053100	1.59196700
C	8.14656400	-2.50209300	-0.82052000
C	7.31198900	-3.08394600	-1.75082500
H	7.52590700	-3.90739900	-2.38862900
C	6.12133200	-2.35889600	-1.66695000
C	7.30642800	-1.10166700	3.41074300
C	6.16380900	-1.07286500	4.18016600
H	6.07300400	-1.29371300	5.21617200
C	5.15197600	-0.67511900	3.30463900
C	8.93655700	1.80320600	0.46322000
C	8.49091300	3.02005100	-0.00723400

H	9.05142300	3.91543700	-0.12725300
C	7.14095300	2.81844700	-0.28812200
C	4.55222900	1.69949200	-2.74100600
H	4.33383400	2.44918600	-1.97766800
H	4.60037400	2.24021300	-3.68245000
H	5.55132800	1.29700200	-2.57862900
C	3.61068800	-0.76383100	-4.34981700
H	4.61898100	-1.15726900	-4.25913000
H	3.55602100	-0.20410800	-5.28019500
H	2.92773100	-1.60530500	-4.43194800
C	1.55925600	1.31280600	-3.33205200
H	0.81264600	0.64854800	-3.75644800
H	1.78123900	2.07563600	-4.07435600
H	1.12840100	1.79800800	-2.46218100
C	2.61019300	-3.11947400	-0.07160800
H	2.90278300	-3.69733600	-0.94460300
H	1.89478700	-3.70993300	0.49190100
H	3.49666700	-2.99850300	0.54871400
C	0.41351000	-1.76852600	-1.79128500
H	-0.17229200	-0.87139100	-1.95362100
H	-0.25086700	-2.52682000	-1.38637900
H	0.76576300	-2.12609200	-2.75508300
C	1.23389900	-0.59056000	1.03094000
H	1.89744800	-0.92405200	1.82665300
H	9.07562600	-0.84088200	1.26165300
H	-0.91559500	-0.27088100	2.77554600
H	-1.57657700	-0.84462500	0.53989000
S	2.88056400	1.71066400	1.50229200
C	1.27780700	0.92094800	0.95929400
N	0.24546600	1.53666600	0.60112500
H	-7.52646000	0.04827400	-0.43367600
H	-7.28072200	4.30562000	-0.69366800
H	-3.86422700	5.24353000	2.04455600
H	-2.90168600	1.34381700	3.49613900
H	5.21545800	-2.49072400	-2.20941100
H	9.14737700	-2.74909500	-0.55345700
H	4.12254100	-0.49455900	3.50972300
H	8.30642700	-1.34269700	3.68634000
H	6.43570500	3.51942800	-0.67168900
H	9.90755400	1.51668800	0.79292900
C	-0.60242000	-2.93474300	2.07118600
H	-0.46101800	-3.58481800	1.21397000
H	0.17283100	-3.16254400	2.79790000
H	-1.56062700	-3.18006700	2.51416500
C	0.13839700	2.99924900	0.52434500
H	-0.55296500	3.32564600	1.29074000
H	1.08931800	3.49498500	0.66466700

H	-0.28160500	3.26157800	-0.43615700
C	-6.33242400	-2.41106800	4.51041900
H	-6.96222300	-1.98601300	5.28749900
H	-6.91812400	-3.14131400	3.96102100
H	-5.50816100	-2.93227700	4.98990000
H	-1.64284400	0.88888000	-2.61265700
H	-3.13553700	4.87349800	-2.30805300

TS-2

Y	-2.83302200	-0.45892600	-0.10580300
B	-4.91194400	-3.14328700	-1.34560100
H	-5.60454300	-4.02995500	-1.76330700
N	-5.78421800	-1.92704100	-0.98996100
C	-7.12473500	-1.80646900	-1.07484100
H	-7.72943100	-2.62368000	-1.44186800
C	-7.47516000	-0.53728500	-0.63325800
H	-8.46638200	-0.11207000	-0.57368900
C	-6.25717900	0.06275800	-0.28744200
H	-6.04927800	1.05062300	0.09574000
N	-5.24351100	-0.78511900	-0.50583100
N	-3.89159800	-2.73422400	-2.42398100
C	-3.57690200	-3.40308600	-3.55205700
H	-4.11129300	-4.30148700	-3.82746200
C	-2.54880600	-2.72059700	-4.18815300
H	-2.06883200	-2.97517000	-5.12177300
C	-2.28596600	-1.62725100	-3.35273400
H	-1.55284400	-0.83886700	-3.45453100
N	-3.09919800	-1.64396400	-2.28924600
N	-4.16988800	-3.63566100	-0.08550600
C	-4.27633800	-4.83186900	0.52889800
H	-4.92122400	-5.60146400	0.12892700
C	-3.45575200	-4.81817200	1.64822400
H	-3.30219300	-5.61469900	2.36152300
C	-2.87435900	-3.54227600	1.63990600
H	-2.16404200	-3.10637800	2.32964700
N	-3.30976100	-2.83938700	0.58831200
N	-3.38046400	1.61885100	0.79108600
Si	-4.05852100	1.69511600	2.37615800
C	-4.49604500	-0.05364600	2.96953500
H	-5.20576500	-0.54223600	2.29313600
H	-4.96125300	-0.00530400	3.96207800
H	-3.61304300	-0.69744700	3.05651700
C	-5.65667200	2.70797200	2.50790300
H	-5.51968100	3.74178900	2.17387800
H	-5.98599100	2.74138400	3.55411500
H	-6.47117000	2.27147900	1.91940200
C	-2.91276500	2.40643100	3.70918700

H	-2.63261800	3.44459100	3.50462600
H	-1.99151300	1.82535500	3.80567100
H	-3.42292600	2.38433500	4.68088100
Si	-3.28171000	3.07119400	-0.14492400
C	-2.06476700	2.89379700	-1.58062100
H	-2.63191700	2.27963000	-2.30126500
C	-4.95965100	3.46901500	-0.93956200
H	-5.27017100	2.64074500	-1.58826200
H	-4.91265700	4.37520400	-1.55455700
H	-5.74289600	3.61415300	-0.18784100
C	-2.80178100	4.60230600	0.86535100
H	-3.42424400	4.71783300	1.75865500
Y	3.82362900	-0.04355100	0.52077300
B	6.59187800	-0.26663800	-1.74225000
H	7.49415600	-0.35003900	-2.52853500
N	7.03855100	0.52240000	-0.50221500
C	8.13388100	1.29053300	-0.33815000
H	8.90132500	1.32515300	-1.09854800
C	8.04107800	1.92068400	0.89585600
H	8.75533800	2.59419400	1.34616600
C	6.82282700	1.47392500	1.42492000
H	6.35608600	1.70538400	2.37359700
N	6.22628200	0.63061100	0.57172700
N	5.40836600	0.48216100	-2.39345500
C	5.22390800	0.72195500	-3.70612900
H	5.96831600	0.42104900	-4.42963000
C	4.01202800	1.38058100	-3.86411900
H	3.56777200	1.73140700	-4.78402100
C	3.51012200	1.50344700	-2.56452500
H	2.58342000	1.94835400	-2.23055600
N	4.35910200	0.96317300	-1.67707300
N	6.15926600	-1.68358900	-1.31728300
C	6.73432200	-2.85828700	-1.64596800
H	7.58441400	-2.88706900	-2.31267500
C	6.04203700	-3.87640500	-1.00439100
H	6.23598400	-4.93779100	-1.05464600
C	5.03358000	-3.21710300	-0.28989000
H	4.25444600	-3.62486900	0.33982100
N	5.11398400	-1.89493200	-0.48539000
N	2.22962400	0.07627000	2.18250100
Si	2.52517000	-0.61227900	3.73930400
C	4.40444500	-0.77120400	4.01545500
H	4.76262000	0.00081200	4.70724800
H	5.00200600	-0.66066400	3.10441600
H	4.64512100	-1.75011900	4.44864800
C	1.88352800	0.44160300	5.17583600
H	2.40406400	1.40583400	5.21464100

H	2.05453500	-0.06840200	6.13257000
H	0.81023900	0.64427900	5.09787900
C	1.74915400	-2.34222300	3.91220600
H	2.38318900	-3.00653700	4.51129400
H	1.61672600	-2.80497400	2.92749900
H	0.76476000	-2.30421100	4.39273400
Si	0.65350800	0.67993400	1.78655300
C	0.42038400	2.46541000	2.34306000
H	0.37011600	2.51237100	3.43660600
H	-0.50188400	2.89447900	1.94134800
H	1.25974200	3.08815000	2.01793600
C	-0.69046100	-0.35861800	2.60650800
H	-0.68353700	-1.37802800	2.21182600
H	-1.67052400	0.08559400	2.42104200
H	-0.56269900	-0.40835700	3.69175700
C	0.51735900	0.55074300	-0.11133400
H	1.51323800	0.91969000	-0.39504200
C	0.48981800	-0.88470800	-0.50867100
S	2.04101600	-1.61922100	-0.94185900
N	-0.62734800	-1.55820000	-0.52013800
C	-0.57815600	-2.95917300	-0.90595500
H	-1.59019100	-3.34596400	-1.01779400
H	-0.04145000	-3.10180200	-1.85105000
H	-0.06159400	-3.56119900	-0.14616100
H	-2.92958300	5.50868500	0.26085300
H	-1.75545800	4.56517900	1.18735400
Si	-1.76518700	4.50755000	-2.46908300
H	-1.07864600	5.52160100	-1.61320700
H	-3.06668000	5.16084800	-2.83875700
Si	-0.47126300	1.80834400	-1.30768900
H	-1.58352000	0.54970400	-1.46788600
H	0.05954200	1.43290200	-2.67498200
C	0.73190700	3.29716200	-0.87151700
H	1.72153000	2.99155400	-0.51194500
H	0.89473700	3.93001800	-1.75396600
H	0.29065600	3.93938200	-0.10171800
C	-0.79683400	4.29533600	-4.07752900
H	0.04666500	3.61066400	-3.94460100
H	-1.44362900	3.87780500	-4.85737600
H	-0.40557400	5.25116400	-4.44251900

Int-4

Y	-2.56878700	-0.53826100	0.31682700
B	-5.29058300	-2.71556200	-0.79356200
N	-5.71300800	-1.26320500	-1.04678400
N	-4.88809400	-0.23213100	-0.74730800
N	-4.01526700	-3.00297700	-1.60775900

N	-2.92638100	-2.20525500	-1.53181400
N	-5.03828000	-2.89249000	0.71632100
N	-4.22547700	-2.06082800	1.40172100
N	-2.58613300	1.83197600	0.19460700
Si	-3.51194200	2.75210000	1.32627200
Si	-1.92434900	2.58917100	-1.20052700
Si	0.51537200	3.98245500	0.23575100
C	-6.87040700	-0.80554200	-1.56826200
C	-6.80323100	0.57977500	-1.61441600
H	-7.55546800	1.26466900	-1.97807400
C	-5.53909600	0.88400300	-1.08854800
C	-3.81923200	-3.96969100	-2.52878700
C	-2.55526300	-3.79842900	-3.07581400
H	-2.08192000	-4.39695100	-3.84038000
C	-2.03681400	-2.67611800	-2.41283100
C	-5.59715600	-3.79222900	1.55186800
C	-5.13140500	-3.53921300	2.83523500
H	-5.38133000	-4.06899900	3.74280700
C	-4.27140300	-2.44206600	2.68313200
C	-4.50531400	1.54392200	2.39130400
H	-5.23440100	0.98386900	1.79618000
H	-5.04933900	2.07075300	3.18452700
H	-3.84104500	0.81799500	2.87821800
C	-4.71206600	4.01315600	0.56083900
H	-4.16678600	4.75575700	-0.03382600
H	-5.21353500	4.55611600	1.37219900
H	-5.49244600	3.58554100	-0.07487400
C	-2.56550500	3.84469500	2.55323800
H	-1.83169900	3.29304200	3.14488000
H	-3.29213600	4.28810100	3.24667700
H	-2.04551500	4.66918800	2.05574000
C	-0.72397700	1.41400800	-2.07646600
H	0.27164700	1.39629500	-1.62364000
H	-0.61194700	1.69335500	-3.12926600
H	-1.11832800	0.38981500	-2.05376900
C	-3.21384300	2.96635300	-2.54092300
H	-3.71301300	2.03722700	-2.83908500
H	-2.74006200	3.38206700	-3.43824200
H	-3.98343500	3.67184700	-2.21207900
C	-1.02617100	4.22833800	-0.81229200
H	-6.15844600	-3.46979400	-1.13945300
H	0.89793000	2.54140900	0.28223600
H	0.23771100	4.37420300	1.64590000
Y	2.70469600	-1.09953800	0.03363000
B	5.91144300	-0.79442000	-1.65031600
N	5.33622200	0.60086800	-1.34001300
N	4.08279000	0.75352400	-0.85651100

N	4.93604200	-1.53717100	-2.57894600
N	3.66151700	-1.80351300	-2.20731100
N	6.08244700	-1.59391700	-0.34251900
N	5.02419500	-1.94140600	0.42211600
N	2.40896400	0.05163500	1.96447500
Si	3.45711100	0.97533200	2.96485400
Si	0.72116700	-0.20151000	2.27432000
Si	-0.72205400	5.29025300	-2.32334200
C	5.92754000	1.80463900	-1.48012000
C	5.02519200	2.78220600	-1.07836500
H	5.17297900	3.85192000	-1.06898300
C	3.88412500	2.06669100	-0.69389600
C	5.16372600	-1.99022500	-3.82911400
C	3.99597000	-2.57528200	-4.29746500
H	3.83151500	-3.03821800	-5.25953100
C	3.08594000	-2.43209800	-3.24064600
C	7.22277700	-2.05838200	0.20654100
C	6.89941100	-2.73795600	1.37390500
H	7.57484900	-3.23301000	2.05606400
C	5.50541300	-2.63218700	1.46334500
C	5.27405100	0.76579600	2.48579300
H	5.62280700	-0.26031700	2.63875700
H	5.89758300	1.42763800	3.10020000
H	5.44478500	1.02618800	1.43602900
C	3.11561700	2.83581200	2.87595700
H	3.34669100	3.21841300	1.87665500
H	3.74040100	3.38486500	3.59174900
H	2.06932000	3.07150800	3.09401300
C	3.31343100	0.48111800	4.78913200
H	2.30417000	0.66513600	5.17552100
H	4.01547200	1.04815800	5.41305700
H	3.53159100	-0.58495300	4.92470800
C	-0.15017600	1.27686900	3.04897000
H	0.28562500	1.52852600	4.02337200
H	-1.20842100	1.03745400	3.20550100
H	-0.09602100	2.16119300	2.41288100
C	0.45587200	-1.61587500	3.50708800
H	0.84127500	-2.56382100	3.11335200
H	-0.59982100	-1.76004800	3.76221700
H	0.99703400	-1.39383000	4.43444900
C	0.03759600	-0.74073700	0.62347100
H	0.38178100	-0.20845500	-0.26996200
H	6.97938300	-0.67730500	-2.18429000
S	0.88601500	-3.17027200	-0.50142700
C	-0.24514700	-2.15874400	0.41609600
N	-1.35957500	-2.60115300	0.93917100
H	-1.72706300	4.80880900	-0.19378800

H	-0.00901300	6.54843900	-1.94106500
H	-2.02401600	5.74555300	-2.89865100
H	-5.05775500	1.83616900	-0.94471200
H	-7.65020500	-1.49171300	-1.86750500
H	-6.28696600	-4.53598500	1.17890700
H	-3.68144100	-1.92250200	3.42695800
H	-4.58998900	-4.69919700	-2.73330500
H	-1.06865500	-2.20564500	-2.51111900
H	4.83139700	-3.00858400	2.22182100
H	8.17588600	-1.88061200	-0.27109800
H	6.13254500	-1.86648800	-4.29214900
H	2.05443900	-2.75006200	-3.16680100
H	6.93688700	1.88141400	-1.85887600
H	2.93881800	2.41677500	-0.30862300
C	2.01696500	4.96906900	-0.33612800
H	1.80805100	6.04332000	-0.31512800
H	2.86383100	4.78192200	0.33238800
H	2.32448300	4.70471000	-1.35286300
C	0.27292600	4.42264100	-3.66318000
H	-0.33934000	3.68514900	-4.19050200
H	0.64241300	5.14313200	-4.40058100
H	1.13619400	3.90122400	-3.23676700
C	-1.69708600	-4.00312600	0.86444500
H	-2.62962200	-4.18103000	1.40604900
H	-1.83121500	-4.33366500	-0.17433600
H	-0.91368000	-4.63330400	1.30638200

Int-5

Y	-2.48814100	-0.18464000	0.18044200
B	-5.36308000	0.62394600	2.07934800
N	-5.72381500	-0.62494900	1.25819800
N	-4.78032300	-1.20070900	0.42336000
N	-4.16612200	0.25770700	3.01826000
N	-2.97295200	-0.30807900	2.57704400
N	-5.01188200	1.77845400	1.09361100
N	-4.10880900	1.65190400	0.04040900
N	-2.24719100	-2.10517400	-1.09436200
Si	-2.72744200	-1.91332200	-2.76820400
Si	-1.63950400	-3.57019100	-0.35353000
Si	1.49539500	-3.68392500	-1.30272600
C	-6.85679200	-1.34223400	1.21826600
C	-6.67927500	-2.40087400	0.35887300
H	-7.38094500	-3.15839000	0.10389700
C	-5.36531200	-2.26580100	-0.10621300
C	-4.13369200	0.34409400	4.35694900
C	-2.93368500	-0.14811900	4.81646400
H	-2.59835300	-0.21473900	5.82338000

C	-2.24454100	-0.53572300	3.66459800
C	-5.58946800	2.99076800	1.02400800
C	-5.08095000	3.67590500	-0.05360500
H	-5.32395500	4.65478300	-0.38947700
C	-4.16061300	2.79582600	-0.63092900
C	-3.22101800	-0.06467700	-3.00959900
H	-4.08045400	0.21027900	-2.40129600
H	-3.51241100	0.09823800	-4.04420700
H	-2.40853100	0.62879400	-2.81047900
C	-4.26985900	-2.90962600	-3.35595100
H	-4.21952500	-3.95615700	-3.06542000
H	-4.30710500	-2.87798700	-4.44260900
H	-5.20197000	-2.49736400	-2.98559100
C	-1.40894800	-2.38040100	-4.09060600
H	-0.39619700	-2.19660100	-3.75896900
H	-1.57437800	-1.80290000	-4.99715600
H	-1.49757200	-3.43048200	-4.35717200
C	-0.97284000	-3.16223500	1.40655800
H	-0.32172400	-2.29300400	1.41856900
H	-0.40608500	-4.00070400	1.80142000
H	-1.79901200	-2.98222700	2.08922100
C	-3.02206300	-4.87250500	-0.02341600
H	-3.77268900	-4.45707100	0.64103100
H	-2.62819600	-5.76418700	0.45360100
H	-3.51892100	-5.18758000	-0.93677800
C	-0.24885300	-4.47226500	-1.35939000
H	-6.28327800	0.97142400	2.76368500
H	2.28393400	-4.29570900	-0.19049100
H	1.45035800	-2.22255500	-1.02536800
Y	2.90759100	0.61997000	0.52896300
B	5.92275200	-1.09795900	1.12092800
N	5.66531700	-1.02218000	-0.40776900
N	4.51841200	-0.43937300	-0.92186200
N	4.77634000	-1.88978400	1.80229000
N	3.45040700	-1.47613000	1.73742400
N	5.97577300	0.34765700	1.73231900
N	4.90752000	1.23820700	1.69899100
N	2.30679600	1.96103200	-1.10039500
Si	3.18355400	3.29917000	-1.80656600
Si	0.67284400	1.42102400	-1.52973200
Si	-0.12128800	-6.36475400	-1.08079200
C	6.42122600	-1.46626700	-1.42163400
C	5.78708400	-1.18527900	-2.61305000
H	6.12509700	-1.40653300	-3.59683900
C	4.60418200	-0.53867200	-2.24421700
C	4.85958800	-2.96397000	2.60414500
C	3.60538800	-3.27224100	3.07591100

H	3.33274400	-4.06585800	3.72907300
C	2.76493900	-2.30794000	2.50959500
C	6.96825500	0.89626500	2.44540800
C	6.57855300	2.14160500	2.89116800
H	7.13930400	2.82543600	3.48153500
C	5.28328100	2.30348800	2.40132300
C	5.06568400	3.20667300	-1.43243900
H	5.28190300	3.23296700	-0.36934500
H	5.56447500	4.05798900	-1.88948100
H	5.51225500	2.30333000	-1.83510300
C	3.03163000	3.40641400	-3.72043000
H	3.44402100	2.51972900	-4.19497400
H	3.58474800	4.26657500	-4.08943900
H	2.00187000	3.51136000	-4.04949800
C	2.60580700	5.00210100	-1.11414100
H	1.56571000	5.19703700	-1.35664900
H	3.20671800	5.80724800	-1.52977300
H	2.71030800	5.02687800	-0.03137400
C	0.73640200	0.41611300	-3.15925100
H	1.20911000	1.00669400	-3.93911500
H	-0.25128000	0.14189400	-3.50517800
H	1.30905900	-0.49878600	-3.04044400
C	-0.51017100	2.89544600	-1.83011700
H	-0.77097500	3.38457200	-0.89976200
H	-1.42809400	2.57574000	-2.31143500
H	-0.04823900	3.62672100	-2.48685200
C	0.12841900	0.33536700	-0.05508800
H	0.58778500	-0.64009800	0.08059900
H	6.97055100	-1.63807400	1.32879000
S	1.07322000	1.20063000	2.55082100
C	-0.14763600	1.10007800	1.17678800
N	-1.29510400	1.68097800	1.21122700
H	-0.55749400	-4.37946700	-2.40274500
H	1.00570100	-6.90610600	-1.90653100
H	-1.35751400	-7.05179700	-1.55641900
H	-4.83481700	-2.88717800	-0.77841100
H	-7.70619400	-1.06202100	1.79636200
H	-6.32793300	3.28395600	1.73300800
H	-3.55259700	2.96651800	-1.48730700
H	-4.95975500	0.74200100	4.89822000
H	-1.26127100	-0.93726200	3.59368300
H	4.62353400	3.13113300	2.53119700
H	7.88384700	0.37520000	2.59986700
H	5.79518300	-3.43636900	2.79272700
H	1.71670100	-2.18649600	2.64345600
H	7.35298900	-1.94941700	-1.24207400
H	3.83629700	-0.14443900	-2.86760100

C	2.45447300	-3.95089100	-2.94148100
H	1.93239600	-3.49014200	-3.77463000
H	3.44557600	-3.51286500	-2.87710600
H	2.56216200	-5.00925600	-3.15559800
C	0.22440700	-6.88296100	0.73484100
H	-0.59248300	-6.61433800	1.39548200
H	0.36066500	-7.95880100	0.78908100
H	1.12982700	-6.41047300	1.10236900
C	-1.65991200	2.62711000	2.27559900
H	-2.63348200	3.02954600	2.04772700
H	-1.68560800	2.14370100	3.24278100
H	-0.93725300	3.43216500	2.33243500
N	-1.36980200	6.44947300	-0.20309200
S	-3.28921200	6.44028300	-2.27366000
C	-2.14927100	6.44220600	-1.04664100
C	-0.39509100	6.44963200	0.85510900
H	0.48693500	6.97503800	0.52216500
H	-0.81547500	6.94035700	1.72054100
H	-0.13882600	5.42995300	1.09766900

TS-3

Y	3.69056100	0.18316800	-0.07988700
Y	-2.35554100	-0.57593700	-0.12111600
B	6.53695000	-2.02313000	-0.11156500
B	-3.41456200	-3.96311100	-0.20477200
N	6.67818800	-1.00025500	1.05690500
N	5.71015400	-0.04533600	1.32358200
N	6.41704600	-1.27636500	-1.46205700
N	5.36178900	-0.41956900	-1.73883400
N	5.26091500	-2.88510000	0.12307800
N	3.99316300	-2.33064300	0.22669000
N	-3.53442500	-3.39380100	1.24292800
N	-3.09083000	-2.12725200	1.60195400
N	-1.93719900	-3.94262800	-0.64703000
N	-1.26321000	-2.73982500	-0.78141900
N	-4.23267600	-3.09429700	-1.21821300
N	-3.95146000	-1.75891400	-1.48692200
N	3.88721600	2.37897300	-0.07369100
N	2.61180200	-0.48540500	2.20868400
N	-0.55780500	0.21058200	-1.37120300
Si	5.25041200	3.47574600	-0.14308900
Si	2.18866500	2.83025900	-0.15803800
S	-0.15317000	-1.01918800	2.15089800
S	2.00683600	0.10563500	-2.38858200
C	7.69179300	-0.85136100	1.92300100
C	7.40784400	0.19533000	2.77304200
H	8.00995200	0.57243100	3.56459800

C	6.16170600	0.66592200	2.35049900
C	7.19402800	-1.37600600	-2.55409700
C	6.66603200	-0.59466200	-3.55461800
H	7.04220700	-0.45711300	-4.53973200
C	5.51884800	-0.02097500	-2.99283100
C	5.16954100	-4.21991000	0.23537000
C	3.85051100	-4.56608000	0.41764100
H	3.44235400	-5.54068800	0.53871600
C	3.16000600	-3.34934900	0.40343500
C	-4.00701500	-4.01248500	2.33490900
C	-3.88402900	-3.17451400	3.42125600
H	-4.16724500	-3.36841900	4.42770300
C	-3.30832300	-2.01111300	2.90898800
C	-1.13880000	-4.94645000	-1.04692100
C	0.06638800	-4.42090600	-1.44817900
H	0.91325500	-4.94138800	-1.82666800
C	-0.06582500	-3.03663900	-1.26674100
C	-5.20007100	-3.50577800	-2.04912200
C	-5.56915400	-2.46428200	-2.87273200
H	-6.30877200	-2.46790600	-3.63665000
C	-4.75919500	-1.39915000	-2.47998500
C	6.85604300	2.66328900	-0.81025600
H	6.78476800	2.48595900	-1.87877300
H	7.69489900	3.33430100	-0.63908800
H	7.07808400	1.71624200	-0.33399000
C	4.95823900	5.00070000	-1.28210700
H	4.19264500	5.66633200	-0.89340200
H	5.88161400	5.57053100	-1.35767900
H	4.66571200	4.70129300	-2.28374500
C	5.69133200	4.25028100	1.57140500
H	6.28397900	5.15015200	1.42369500
H	4.79611500	4.52821100	2.12095900
H	6.27562900	3.57732700	2.19069800
C	1.68903000	3.77699200	-1.74570600
H	2.03851000	3.25169400	-2.62718000
H	0.61014300	3.86494700	-1.81061900
H	2.10728900	4.77791700	-1.75340200
C	1.64195300	3.89263500	1.34319400
H	2.22731100	4.80678700	1.40211900
H	0.59632800	4.17086100	1.26356700
H	1.77823000	3.35158400	2.27620100
C	1.19754400	1.16604800	0.02259000
H	0.40704600	1.37018900	0.73164300
C	1.43932500	-0.54683600	2.01929000
C	0.70666600	0.54312200	-1.16611800
H	-3.84492500	-5.08032500	-0.21735400
H	7.49951700	-2.73700200	-0.12701600

N	-3.73908400	1.07775400	0.56344400
Si	-3.00489900	2.66915000	0.90502100
Si	-5.43558100	0.84454700	1.04067100
Si	-6.34901900	2.40402900	-1.67140600
C	-1.92207400	2.57770900	2.49333700
H	-2.53656000	2.29196400	3.34380100
H	-1.48437100	3.54807900	2.71055700
H	-1.11281900	1.86039800	2.42119400
C	-4.20274600	4.13483700	1.25697400
H	-4.76146800	4.42176000	0.37327100
H	-3.58405800	4.98492600	1.53707900
H	-4.90065000	3.96187100	2.06782100
C	-1.96259800	3.30472400	-0.56516900
H	-1.21277200	2.60067400	-0.89591700
H	-1.46457600	4.23081200	-0.29093800
H	-2.61546300	3.51711600	-1.40740200
C	-6.16690400	-0.89763700	0.71738300
H	-6.40342900	-1.05704500	-0.32684800
H	-7.09081900	-0.97820900	1.28570700
H	-5.52083100	-1.69912800	1.03985000
C	-5.64116700	1.11172300	2.93896000
H	-5.23817900	0.25737600	3.47635800
H	-6.68789400	1.20303700	3.21159300
H	-5.12410800	1.99731000	3.29198300
C	-6.68210800	2.06004300	0.17739100
Si	-8.53315800	1.66496900	0.49302500
H	-6.54026700	3.02284500	0.66833200
C	-7.50539100	3.75264500	-2.39969000
H	-7.37544900	4.69281000	-1.87200600
H	-7.27377900	3.92028400	-3.44718700
H	-8.55104800	3.47192900	-2.32555900
H	-6.54283100	1.15661500	-2.47396600
H	-4.94525600	2.84118300	-1.90892000
H	-9.30624200	2.94593000	0.46561700
H	-8.74245500	1.07619300	1.84903800
H	-4.39706900	-5.00152200	2.27777000
H	-3.05400700	-1.11491000	3.42622000
H	-1.47470700	-5.95696900	-1.02888300
H	0.64405800	-2.27452700	-1.48984700
H	6.03676800	-4.83518900	0.17940100
H	2.11114600	-3.19582800	0.50620100
H	8.54531100	-1.48675100	1.88317000
H	5.59410200	1.48041000	2.73469700
H	8.06173400	-1.99339900	-2.55543000
H	4.81611600	0.64202200	-3.44150800
H	-4.74879700	-0.40522500	-2.86228000
H	-5.56295500	-4.50611000	-2.01299700

C	3.42581100	-1.07459000	3.32866700
H	3.85507800	-0.25759100	3.88115900
H	2.78542400	-1.67303600	3.95894300
H	4.19824300	-1.66724000	2.87646800
C	-0.95470100	-0.13728000	-2.76949500
H	-0.41739600	-0.98571000	-3.16276300
H	-2.01585600	-0.37238800	-2.79190300
H	-0.78992800	0.70811700	-3.42348300
C	-9.34026200	0.48248300	-0.78713700
H	-8.84421700	-0.48141200	-0.80190100
H	-10.38268600	0.32370200	-0.52740700
H	-9.30468000	0.89485400	-1.79035500

Int-6

Y	-4.28278100	-0.09290000	0.40962000
Y	2.29836200	0.36697400	0.12999400
B	-6.84779500	1.74857600	-1.46803800
B	3.35635400	3.77019100	0.80188800
N	-7.45731200	1.26657700	-0.13672200
N	-6.72734100	0.56281200	0.75517900
N	-6.35507100	0.52828400	-2.26732300
N	-5.39715500	-0.30078800	-1.79406100
N	-5.67089300	2.69174200	-1.16271300
N	-4.63083700	2.28890400	-0.40090400
N	3.67929300	2.85218300	1.99465500
N	3.29963000	1.55647400	2.00844000
N	1.83760900	3.77551700	0.56050300
N	1.17644600	2.65702400	0.17933200
N	4.04008500	3.23902700	-0.47185300
N	3.72658000	2.02575900	-0.97180200
N	-3.62571300	-2.28525000	0.43503500
N	-2.26641000	0.29667000	1.75096000
N	0.36478500	0.11215400	-1.38591600
Si	-4.68828200	-3.58645800	0.84445100
Si	-1.95708800	-2.60757300	0.21438300
S	0.35058500	0.33263900	2.40490100
S	-2.31218100	0.30109000	-1.62544500
C	-8.70333000	1.47052500	0.33760200
C	-8.79430200	0.87654200	1.58916700
H	-9.65180400	0.85183700	2.24565100
C	-7.52536600	0.32038000	1.80274800
C	-6.79760800	0.09119100	-3.46404900
C	-6.10410100	-1.06795900	-3.78641100
H	-6.21097700	-1.67292300	-4.67485200
C	-5.23689900	-1.26916900	-2.70445800
C	-5.52565100	3.99058800	-1.50053300
C	-4.34451100	4.45481900	-0.93698200

H	-3.92669000	5.44834300	-1.00942800
C	-3.82335700	3.34494300	-0.25672700
C	4.35347100	3.14941500	3.12428100
C	4.41040300	2.00414400	3.90900100
H	4.87500900	1.89309900	4.87767900
C	3.73295000	1.03203100	3.16093000
C	0.98280300	4.81369800	0.66799000
C	-0.28790200	4.35949400	0.34323400
H	-1.20371800	4.93170700	0.31769100
C	-0.11003700	3.00003400	0.04599100
C	4.87847500	3.88126400	-1.30904200
C	5.11745000	3.05731400	-2.40258000
H	5.74517000	3.26266500	-3.25706500
C	4.36438700	1.90470400	-2.14183200
C	-6.46120300	-3.12526300	0.37815100
H	-6.55950900	-2.97411100	-0.70282600
H	-7.15878900	-3.91898300	0.67269400
H	-6.78353400	-2.20226800	0.87288200
C	-4.29574400	-5.20321500	-0.05413600
H	-3.30203600	-5.59130200	0.19356300
H	-5.02832000	-5.97320900	0.21783800
H	-4.34222000	-5.06738000	-1.14058500
C	-4.68395200	-3.93830200	2.70343400
H	-4.96181600	-3.03384200	3.25892700
H	-5.39647600	-4.72852100	2.97028000
H	-3.69210900	-4.24792900	3.05079300
C	-1.54950000	-3.34813900	-1.47159900
H	-1.99430600	-2.73662500	-2.26347300
H	-0.46810800	-3.39417300	-1.64126600
H	-1.94844800	-4.36413700	-1.55933900
C	-1.18741700	-3.69744900	1.55405000
H	-1.67920600	-4.67211200	1.63640300
H	-0.12760800	-3.87561200	1.33555400
H	-1.24929900	-3.20496000	2.53162400
C	-0.84502300	-1.03884700	0.32693500
H	0.14658800	-1.49064500	0.44108000
C	-1.06136000	-0.13659700	1.51910300
C	-0.81826400	-0.20350100	-0.92897100
H	3.74215200	4.88151900	1.03652800
H	-7.68064100	2.33321400	-2.10424100
N	4.10034300	-1.12209200	0.27978000
Si	3.60706600	-2.78414200	0.43697500
Si	5.77090900	-0.80135300	0.58401900
Si	6.20589200	-1.72381900	-2.41586100
C	2.82460200	-3.04257100	2.14322100
H	3.55716700	-2.85286100	2.93734400
H	2.43494800	-4.05905700	2.27808700

H	1.99529900	-2.33747800	2.28649000
C	4.88344100	-4.16255900	0.21697300
H	5.28291800	-4.20092900	-0.80075500
H	4.36385600	-5.11217700	0.40032300
H	5.72207600	-4.10984200	0.91708200
C	2.25903200	-3.13763000	-0.84273400
H	1.50903900	-2.33902300	-0.86322000
H	1.73930900	-4.07956300	-0.63254800
H	2.68874400	-3.20344700	-1.84941600
C	6.27153900	1.01561900	0.57826700
H	6.19322800	1.47693500	-0.40794300
H	7.31733200	1.08611100	0.90227900
H	5.67517000	1.60299700	1.27793500
C	6.32633300	-1.43998900	2.28143700
H	5.81315400	-0.88849800	3.07726200
H	7.40476800	-1.29432700	2.41780900
H	6.11361500	-2.50481200	2.42138800
C	6.91074100	-1.66940000	-0.68594500
Si	8.65628200	-0.99618900	-0.72507100
H	6.99592400	-2.71531900	-0.36062100
C	7.32455500	-2.65771100	-3.61189900
H	7.50117600	-3.67764000	-3.25221100
H	6.86802800	-2.72553800	-4.60557800
H	8.29842800	-2.16917300	-3.72225100
H	6.01836800	-0.33541000	-2.92551100
H	4.86368400	-2.37080200	-2.44864600
H	9.60124100	-2.05968700	-1.19328000
H	9.12176200	-0.63432200	0.64941600
H	4.73794300	4.14572400	3.29013000
H	3.54294000	-0.00838700	3.38649800
H	1.33760600	5.79264700	0.95775800
H	-0.84426400	2.26572200	-0.25712700
H	-6.26789400	4.48888000	-2.10794000
H	-2.91926200	3.25529900	0.32758000
H	-9.43103600	2.01975400	-0.24286200
H	-7.15227800	-0.23788600	2.65171200
H	-7.56675300	0.63172600	-3.99723600
H	-4.50713900	-2.04954800	-2.53744600
H	4.26246100	1.00020500	-2.72397900
H	5.23733600	4.87347300	-1.07511900
C	-2.47407900	1.29892000	2.78086500
H	-2.25323900	0.90750200	3.78187300
H	-1.83352300	2.17586800	2.62281300
H	-3.52180400	1.61832000	2.76397600
C	0.46102100	0.90596600	-2.59952500
H	-0.09983800	1.84551000	-2.52146400
H	1.51217800	1.13933500	-2.79236700

H	0.06443500	0.35815400	-3.46371400
C	8.86218300	0.49546500	-1.85502200
H	8.13784300	1.27979000	-1.61663500
H	9.86824200	0.91708100	-1.75579700
H	8.72072300	0.21462900	-2.90397900

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Y	-2.91692700	0.27606600	0.61345900
Y	3.55344600	-0.03860100	-0.61081800
B	-5.90570600	2.02250600	-0.57566300
B	6.81007400	0.84414200	0.71328000
N	-6.19327400	1.37094600	0.79158200
N	-5.22460300	0.72940600	1.47917200
N	-5.49257100	0.93291200	-1.57970400
N	-4.39491500	0.16923900	-1.37986900
N	-4.75823500	3.03525500	-0.41701000
N	-3.53368700	2.65544000	0.01266000
N	6.24171000	-0.34747500	1.50003900
N	5.03546200	-0.88692400	1.20300200
N	5.84879600	2.03925600	0.84816600
N	4.55831400	1.94294200	0.45992200
N	6.92516100	0.44628000	-0.77084600
N	5.84516400	0.03181100	-1.46969800
N	-2.57086500	-1.91323500	0.12122700
N	-0.70292900	0.26486300	1.73394000
N	1.43313300	0.54485800	-1.68851300
Si	-3.70583000	-3.19584400	0.36137300
Si	-0.97613900	-2.29826900	-0.36695200
S	1.99996100	0.03167700	1.80049900
S	-1.22661100	0.99844600	-1.58404500
C	-7.35635900	1.32250800	1.47103500
C	-7.14206700	0.62218600	2.65123200
H	-7.86134200	0.40245400	3.42646800
C	-5.78649500	0.27153200	2.60613100
C	-6.10860000	0.57325700	-2.72466000
C	-5.38333700	-0.46421600	-3.29686400
H	-5.59949800	-0.98776100	-4.21682900
C	-4.31847500	-0.67907900	-2.41069300
C	-4.77807900	4.36222900	-0.65925300
C	-3.51891300	4.87306400	-0.37611500
H	-3.18967900	5.89823700	-0.46252100
C	-2.77661800	3.75860500	0.03906500
C	6.81442600	-1.01766700	2.51990100
C	5.95265100	-2.03445100	2.90761300
H	6.10096800	-2.75855100	3.69523300
C	4.85297500	-1.90752500	2.04935400
C	6.08942000	3.26365600	1.35640300

C	4.91232600	3.99881700	1.29634400
H	4.75555800	5.01707600	1.62048200
C	3.98118900	3.12236200	0.72601400
C	8.02066500	0.41929000	-1.55386800
C	7.64564200	-0.02730800	-2.81468800
H	8.27854200	-0.16706300	-3.67859500
C	6.26905600	-0.25633800	-2.70867000
C	-5.49509300	-2.60466200	0.22750500
H	-5.73656600	-2.27007300	-0.78614700
H	-6.17143000	-3.42974200	0.48412000
H	-5.70421300	-1.77732100	0.91287700
C	-3.52455300	-4.59841800	-0.89522100
H	-2.54271500	-5.08159400	-0.85032700
H	-4.28151700	-5.37032200	-0.70899500
H	-3.67098600	-4.22785700	-1.91624000
C	-3.53328700	-3.94110300	2.09354900
H	-3.69025600	-3.16460900	2.85292500
H	-4.26835200	-4.73589500	2.27082700
H	-2.53515000	-4.36295300	2.25383500
C	-0.77468800	-2.73616900	-2.19069200
H	-1.18786300	-1.94060600	-2.81967100
H	0.28853700	-2.84759900	-2.43657700
H	-1.28075600	-3.67260000	-2.44484900
C	-0.16231400	-3.65247500	0.66960500
H	-0.70231400	-4.60316100	0.61085300
H	0.86552100	-3.82387100	0.32802500
H	-0.12219100	-3.35273200	1.72351100
C	0.28165100	-0.86007300	-0.15699300
H	1.20615500	-1.42913900	-0.30923000
C	0.38552100	-0.18266200	1.18519600
C	0.26382600	0.22724300	-1.19971300
H	7.89085800	1.14160300	1.13850200
H	-6.89203200	2.58195300	-0.96871200
Cl	3.33282100	-2.65311000	-1.07667500
C	1.52905600	1.61554800	-2.66504700
H	0.97841900	1.37513300	-3.58260800
H	1.12087100	2.55580500	-2.27321200
H	2.58002500	1.77162000	-2.92726700
C	-0.61904600	1.02981900	2.96484600
H	-0.22037500	0.42631400	3.78913400
H	0.03384000	1.90447700	2.85136100
H	-1.62012400	1.37200900	3.24447000
H	7.07198500	3.52386700	1.72364700
H	2.93422100	3.27632300	0.50043500
H	-5.67799300	4.84438700	-1.01399300
H	-1.74083400	3.69612000	0.34496800
H	-8.24645400	1.78892600	1.07324800

H	-5.19447100	-0.28742000	3.31938300
H	-7.00841700	1.07696900	-3.04863100
H	-3.51328800	-1.39893500	-2.44603900
H	3.94579600	-2.49228500	1.99903200
H	7.78601400	-0.72613200	2.89293800
H	8.98363300	0.71574800	-1.16299900
H	5.56828600	-0.61353500	-3.45203700

Int-7

Y	-2.71453800	-0.66321000	-0.33865800
B	-5.88235200	0.58942400	0.44846600
N	-5.40072300	1.20853500	-0.89996400
N	-4.16531000	0.91298900	-1.46769600
N	-5.94277700	-0.96799600	0.30402500
N	-4.82362800	-1.73782400	0.00790100
N	-4.89626900	0.95784700	1.58428700
N	-3.55964200	0.58038400	1.54380300
C	-6.08682100	1.99188500	-1.74449200
C	-5.32753900	2.22224200	-2.87035100
H	-5.58819500	2.80048000	-3.72360100
C	-4.14190600	1.51909900	-2.64986100
C	-7.01133200	-1.77308300	0.37169400
C	-6.62049500	-3.07187700	0.12402100
H	-7.23205400	-3.94131700	0.10166200
C	-5.24619200	-2.99267300	-0.10396400
C	-5.13269400	1.59341300	2.74090200
C	-3.96803900	1.64517600	3.47365400
H	-3.82096300	2.08390600	4.43092400
C	-3.01556700	0.99693800	2.68353400
H	-6.97659600	1.00124000	0.70417100
Y	2.48077800	0.06325700	0.28529100
B	4.99346400	-2.24441100	-0.46028000
N	5.03231000	-1.09568100	-1.51038400
N	4.12282900	-0.05048200	-1.47571000
N	3.61471500	-2.95698000	-0.54616800
N	2.40468000	-2.28821100	-0.37149300
N	5.21325100	-1.65908400	0.97344400
N	4.37072100	-0.71807000	1.55460400
N	1.97919100	2.15318300	-0.16714700
Si	2.98997800	3.56095100	0.02229900
Si	0.25413800	2.01679900	-0.45488500
C	5.81918700	-0.95179900	-2.58588100
C	5.44291000	0.18312900	-3.27195900
H	5.86789400	0.57272100	-4.16539100
C	4.37791800	0.70818200	-2.53641100
C	3.35784700	-4.24190300	-0.84036900
C	1.99695700	-4.43862200	-0.86299400

H	1.47240100	-5.33960100	-1.07138200
C	1.44762500	-3.18773400	-0.56431300
C	6.16605700	-1.98650500	1.85743800
C	5.97108100	-1.27663600	3.02250100
H	6.55378400	-1.31280300	3.91112300
C	4.83474700	-0.50357100	2.78081200
C	4.73908600	3.02135300	0.61602600
H	4.70359800	2.58689000	1.61294600
H	5.39673900	3.88547700	0.66534000
H	5.19748200	2.29464800	-0.04777600
C	3.22356600	4.57118300	-1.59794100
H	3.68742400	3.97977100	-2.38204500
H	3.85772700	5.43539100	-1.41540700
H	2.27138900	4.93389800	-1.97670300
C	2.35463600	4.80857000	1.33797900
H	1.44674900	5.31141400	1.01962000
H	3.10854600	5.57012500	1.52332200
H	2.14309500	4.30704000	2.27834500
C	-0.22519800	2.36366200	-2.28137200
H	0.21006300	3.29924900	-2.62146500
H	-1.30264300	2.44612100	-2.39257900
H	0.12697900	1.57580700	-2.94235200
C	-0.83630200	3.16049100	0.62301200
H	-0.69495400	4.20099200	0.34384400
H	-0.59445300	3.05770500	1.67483200
H	-1.88876300	2.92450800	0.49202000
C	-0.14626000	0.16695600	-0.18882100
H	-0.24776300	-0.44723700	-1.08289600
H	5.86561400	-3.03106300	-0.69258200
S	0.69649400	-0.05609000	2.50524400
C	-0.30606300	-0.54915000	1.05525100
N	-1.17120000	-1.54203800	1.10402800
H	-3.29928100	1.42439400	-3.29502400
H	-7.06603100	2.33275100	-1.50217900
H	-6.10306400	1.96495300	2.97407200
H	-1.98391800	0.82965500	2.89346700
H	-7.97866200	-1.38286500	0.58575500
H	-4.56747300	-3.77549500	-0.35457200
H	4.34441400	0.17732400	3.43839500
H	6.91798500	-2.69948700	1.61281600
H	4.14961300	-4.93144700	-1.01855600
H	0.42053000	-2.91948400	-0.47890000
H	6.58860200	-1.65548000	-2.80173800
H	3.80296700	1.58442600	-2.72262400
C	-1.25273800	-2.43683200	2.27030600
H	-1.97020600	-3.21479600	2.04553800
H	-0.29225300	-2.89100600	2.47743200

H	-1.57076000	-1.90894100	3.16124700
Cl	-2.22881700	-2.08677500	-2.51362100

Int-8

Y	-2.62969100	-0.30648600	-0.33940200
Y	2.76964400	0.48607600	-0.02823500
B	-4.95669700	2.30722500	0.02615100
B	5.48560500	-1.74070800	-0.23442600
N	-4.98848100	1.41000100	1.29588900
N	-4.15848700	0.30844300	1.43090500
N	-5.30095500	1.45679600	-1.23893700
N	-4.54016800	0.37206400	-1.66024700
N	-3.53499500	2.92313300	-0.12695200
N	-2.39001600	2.13896800	-0.20728900
N	4.77526000	-1.91973600	1.13499200
N	3.68997900	-1.13432300	1.50676800
N	5.99120400	-0.26533700	-0.34704300
N	5.14966000	0.84683800	-0.31873000
N	4.49930700	-2.03124000	-1.38682400
N	3.32580500	-1.30360200	-1.54305800
N	-2.29705500	-2.31737600	0.46418300
N	1.47679700	4.86811500	1.37516900
N	1.07236800	0.85264300	-1.49301800
Si	-3.42909300	-3.63506900	0.57586800
Si	-0.54978100	-2.28562600	0.67873700
S	3.06091300	3.84283300	-0.73614800
S	-0.91836800	-0.76161900	-2.55242700
C	-5.71619800	1.54539800	2.41459900
C	-5.37734900	0.54326800	3.29728700
H	-5.77343100	0.37213300	4.26916900
C	-4.39916800	-0.20226600	2.63271700
C	-6.29095300	1.65650300	-2.12161700
C	-6.20081400	0.71963100	-3.12715800
H	-6.83446500	0.61140300	-3.97410300
C	-5.08789400	-0.05449100	-2.79192700
C	-3.18231700	4.21484700	-0.21637900
C	-1.81503100	4.30064100	-0.35393600
H	-1.22714500	5.17946700	-0.47069800
C	-1.36862900	2.97227300	-0.34297100
C	5.13743300	-2.67958900	2.17843600
C	4.30836900	-2.40973900	3.24416800
H	4.33434500	-2.84382200	4.21448100
C	3.42895300	-1.43012200	2.77509100
C	7.25887200	0.15293900	-0.43593300
C	7.28442700	1.53025600	-0.46655700
H	8.13514300	2.16454000	-0.53323500
C	5.94701400	1.91246800	-0.38765600

C	4.57427700	-2.95314200	-2.35612800
C	3.46082900	-2.85298300	-3.15948700
H	3.21460300	-3.44447100	-4.00795300
C	2.71125200	-1.81181900	-2.60878600
C	-5.15358400	-3.05843200	-0.05753500
H	-5.13336300	-2.84246000	-1.12345100
H	-5.88883200	-3.84375300	0.09870300
H	-5.50608800	-2.16859300	0.45609600
C	-2.96347700	-5.16467500	-0.48961300
H	-2.08901100	-5.67861300	-0.10235700
H	-3.78708300	-5.87477000	-0.50540800
H	-2.74827800	-4.87233200	-1.51364100
C	-3.68818700	-4.29663000	2.36472300
H	-4.05713500	-3.52292800	3.03217200
H	-4.41261500	-5.10766700	2.36440200
H	-2.76148400	-4.68077000	2.78278100
C	0.40959900	-3.66382000	-0.23492300
H	0.16471400	-3.67806900	-1.29062300
H	1.47896400	-3.49826400	-0.13610300
H	0.18286100	-4.64095900	0.18274600
C	-0.06983600	-2.40114800	2.53340600
H	-0.65813500	-3.17016900	3.02637800
H	0.97698700	-2.65802300	2.65263700
H	-0.25327600	-1.46209500	3.04985800
C	-0.03945600	-0.53136400	0.10379700
H	0.28547000	0.14364600	0.88850600
C	2.12186200	4.45756800	0.52675700
C	0.16021100	-0.08193700	-1.22461900
H	6.42511800	-2.48025300	-0.30069300
H	-5.76342700	3.18625400	0.13303000
Cl	2.01707000	1.72268000	2.27052000
C	1.10336500	1.50217700	-2.81974100
H	1.35929200	0.80433400	-3.60780400
H	0.14113000	1.93293600	-3.06551700
H	1.83806400	2.29220200	-2.79073600
C	0.67912300	5.08558900	2.56153900
H	0.85441000	4.24757700	3.21898500
H	0.98003000	6.01337400	3.02232700
H	-0.35958800	5.12384600	2.27226300
H	8.06276000	-0.54441800	-0.47063200
H	5.54176700	2.89512800	-0.37500400
H	-3.91476100	4.98718000	-0.18033000
H	-0.37682200	2.59569100	-0.43991000
H	-6.42258300	2.33545300	2.51793900
H	-3.87636300	-1.06870600	2.96370600
H	-6.99241600	2.44631000	-1.98813500
H	-4.67127700	-0.88033000	-3.32193800

H	2.64908400	-0.92809500	3.29610800
H	5.95874200	-3.35363200	2.10616000
H	5.40297900	-3.61925500	-2.41604100
H	1.76406700	-1.44701400	-2.92702400

TS-4

Y	2.47464000	-0.07423900	-0.09482400
Y	-3.32927100	0.55278600	-0.01757300
B	5.03068200	-2.60648600	-0.10091500
B	-6.39360800	-1.16948100	-0.06929000
N	5.19438800	-1.69273200	1.15282500
N	4.35402900	-0.61942900	1.40353000
N	5.11858300	-1.75216400	-1.38971300
N	4.20416000	-0.74676000	-1.67094600
N	3.64404700	-3.31756800	-0.05114600
N	2.45196300	-2.61087200	-0.02913600
N	-6.11736600	-0.65562700	1.37302200
N	-4.94729200	0.01367600	1.71302400
N	-5.26147600	-2.14403200	-0.49034900
N	-3.94165300	-1.72750500	-0.54937100
N	-6.41966000	0.04222400	-1.05819700
N	-5.32850500	0.88301500	-1.24811600
N	2.83358000	2.09637600	0.06671400
N	1.20347800	-0.88348200	2.12583800
N	-1.64378900	0.29035100	-1.52677500
Si	4.27354300	3.08978700	0.10939500
Si	1.17111000	2.67704600	0.00443400
S	-1.62212400	-0.90391300	2.06550700
S	0.93435800	0.08314900	-2.47045100
C	6.15416600	-1.72545100	2.08999600
C	5.96017600	-0.68366000	2.97072200
H	6.55185700	-0.42832500	3.81685100
C	4.82723000	-0.02086300	2.49116100
C	5.95950200	-1.87792700	-2.43115300
C	5.61358100	-0.96767800	-3.40126400
H	6.07955600	-0.81351800	-4.34463800
C	4.50678700	-0.28861200	-2.87620200
C	3.37546600	-4.63177400	-0.12405500
C	2.01127500	-4.81077400	-0.14596000
H	1.47603400	-5.72802300	-0.20348000
C	1.48414100	-3.51573000	-0.08930400
C	-6.91352200	-0.70898800	2.45150800
C	-6.28938500	-0.08341000	3.50722500
H	-6.65777500	0.04601200	4.49611600
C	-5.06748800	0.35527400	2.99033100
C	-5.32753500	-3.43663200	-0.83830000
C	-4.05882100	-3.88913400	-1.13039200

H	-3.77307600	-4.86516800	-1.44088600
C	-3.23166100	-2.78072000	-0.93481900
C	-7.43957300	0.49151800	-1.80069300
C	-7.04442500	1.62208800	-2.48462300
H	-7.62333600	2.21338700	-3.15204500
C	-5.72022700	1.82710300	-2.09920600
C	5.85332200	2.16391100	-0.46812600
H	5.84876100	2.02160200	-1.54412800
H	6.72926100	2.75691100	-0.21484300
H	5.96124200	1.18878800	-0.00855500
C	4.16423300	4.65027500	-1.01173800
H	3.44160100	5.37179600	-0.64136700
H	5.13379300	5.14199400	-1.04458700
H	3.88444200	4.38894500	-2.02800900
C	4.65628900	3.78682800	1.86816900
H	4.99799000	3.01709700	2.55348500
H	5.44091700	4.53734400	1.80414100
H	3.77908400	4.25747700	2.30295700
C	0.70901200	3.79756200	-1.47463500
H	0.96515800	3.32398500	-2.41591000
H	-0.36365500	3.97365600	-1.45829900
H	1.20657600	4.76032500	-1.42538300
C	0.64299800	3.58037100	1.60838500
H	1.20150900	4.50404500	1.73830000
H	-0.41384100	3.82543000	1.57792000
H	0.82526600	2.95997300	2.48321700
C	0.09036700	1.06472300	-0.02457000
H	-0.71103500	1.29086200	0.66664500
C	0.04654700	-0.73180800	1.93233300
C	-0.36973500	0.53214500	-1.27433000
H	-7.45203600	-1.72700000	-0.10296400
H	5.89818800	-3.43319400	-0.09933300
Cl	-3.20132500	3.05083000	0.77826500
C	-2.02833300	-0.19977400	-2.87466600
H	-1.70089200	0.49163800	-3.63953900
H	-1.59261600	-1.16564400	-3.09294500
H	-3.10753800	-0.28528200	-2.91664700
C	1.94344500	-1.67445500	3.16827700
H	2.46960400	-0.97490100	3.79267100
H	1.23408000	-2.25073900	3.74248200
H	2.63746000	-2.30616800	2.64765100
H	-6.25831600	-3.95335200	-0.85928300
H	-2.17760000	-2.70402900	-1.06345800
H	4.15976500	-5.35103900	-0.15957800
H	0.45983100	-3.22119500	-0.09692300
H	6.91248100	-2.47274000	2.07261100
H	4.35589200	0.85294400	2.87608000

H	6.74002100	-2.60239000	-2.42155500
H	3.93009200	0.48983700	-3.31943900
H	-4.29623500	0.90181600	3.48232400
H	-7.86730500	-1.18033600	2.40606100
H	-8.37958000	-0.00863700	-1.79975900
H	-5.05715900	2.61002800	-2.38931800

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