Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Straightforward Construction of Rare Earth Diphosphanato Complex from White Phosphorus: Synthesis and Reactivity**

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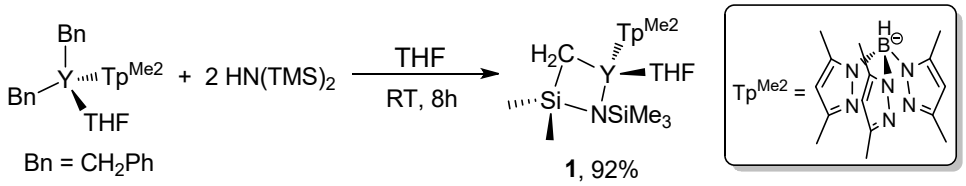
Table of Contents

Experimental Procedures

All manipulations involving air- and moisture-sensitive compounds were carried out with rigorous exclusion of air and water, using standard Schlenk techniques or a Vigor glovebox under an atmosphere of dinitrogen. THF, toluene and hexane were purified using an Mbraun SPS-800 Solvent Purification System, dried over fresh Na chips and stored in the glovebox in the glovebox. C_6D_6 and THF-d_8 were obtained from Cambridge Isotope and dried over Na/K alloy prior to use. (Tp^{Me2})YBn_2(THF) and KBn were prepared according to literature procedure[1,2]. $(CH_3)_3SiCl$, CH_3OH, $^iPr_2NH$, and $HPPh_2$ were purchased from J&K and dried with 4Å sieves. Other commercially available reagents were purchased and used without purification. P_4 was prepared by sublimation of red phosphorus at 450 °C in quartz tube under vacuum condition and stored in the refrigerator of the glovebox. Organometallic samples for NMR spectroscopic measurements were prepared in the glovebox using J. Young valve NMR tubes. ^1H NMR, ^{13}C NMR and ^{31}P NMR spectra were recorded on a Bruker Avance 400 MHz spectrometer (FT, 400 MHz for ^1H; 100 MHz for ^{13}C; 161 MHz for ^{31}P) at room temperature. Chemical shifts for ^1H and ^{13}C NMR were quoted in ppm referenced to the residual resonance of the deuterated solvents. H_3PO_4 (85%) sealed in a capillary was used as an external standard in the ^{31}P NMR analysis. Elemental analyses for C, H and N were carried out on a Vario EL III elemental analyzer. *The resonances of B-H bond in the Tp^{Me2} ligand are too broad to be observed in their ^1H NMR spectra.* ***Caution:*** P_4 is light-sensitive and highly flammable upon exposure to air. It should be handled carefully.

2. Synthesis and characterization of complexes 1-10.

2.1 Synthesis and characterization of (Tp^{Me2})Y[η^2-*C,N*-$CH_2Si(CH_3)_2NSi(CH_3)_3$](THF) (1).



Bn = CH_2Ph

1, 92%

A THF solution of $HN[Si(CH_3)_3]_2$ (3.22 g, 20.0 mmol) was added slowly to a stirred THF solution (50 mL) of $Tp^{Me2}YBn_2$(THF) (6.40 g, 10.0 mmol) at room temperature. After stirring for 8 hours, all the volatiles were removed under vacuum. The residue was washed by *n*-hexane two times (10 mL×2) and dried under vacuum to give **1** as a white powder (5.67 g, 92% yield). Recrystallization of the white powder in a mixed solvent of THF and *n*-hexane afforded colorless crystals of **1** suitable for X-ray diffraction analysis. ^{1}H NMR (400 MHz, C_6D_6, 25 °C): δ (ppm) 5.56 (s, 3H, 4-*H*-Tp^{Me2}), 3.56 (m, 4H, *THF*), 2.50 (s, 9H, 3-CH_3-Tp^{Me2}), 2.10 (s, 9H, 5-CH_3-Tp^{Me2}), 1.14 (m, 4H, *THF*), 0.79 (s, 6H, $Si(CH_3)_2$), 0.33 (s, 9H, $Si(CH_3)_3$), 0.13 (d, $^2J_{YH}$ = 1.6 Hz, 2H, $SiCH_2Y$); $^{13}C\{^1H\}$ NMR (100 MHz, C_6D_6, 25 °C): δ (ppm) 150.13 (Tp^{Me2}), 145.49 (Tp^{Me2}), 105.91 (4-*C*-Tp^{Me2}), 71.27 (*THF*), 26.90 (d, $^1J_{YC}$ = 30.81 Hz, $SiCH_2Y$), 25.29 (*THF*), 14.73 (CH_3-Tp^{Me2}), 13.07 (CH_3-Tp^{Me2}), 8.33 (s, $Si(CH_3)_2$), 8.32 (s, $Si(CH_3)_2$), 5.74 ($Si(CH_3)_3$). Elemental Analysis: Calcd. (%) for $C_{25}H_{47}N_7BOSi_2Y$: C, 48.62; H, 7.67; N, 15.88. Found: C, 48.04; H, 7.74; N, 16.17.

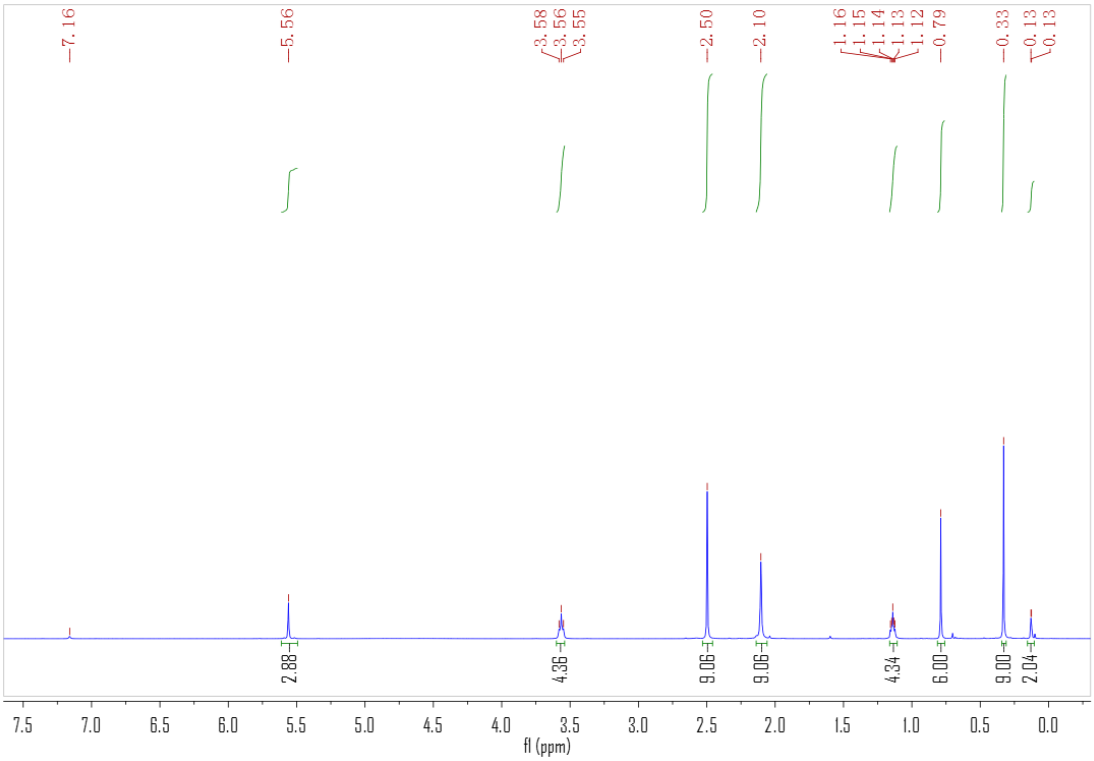


Figure S1. ^{1}H NMR spectrum of complex **1** in C_6D_6 at room temperature.

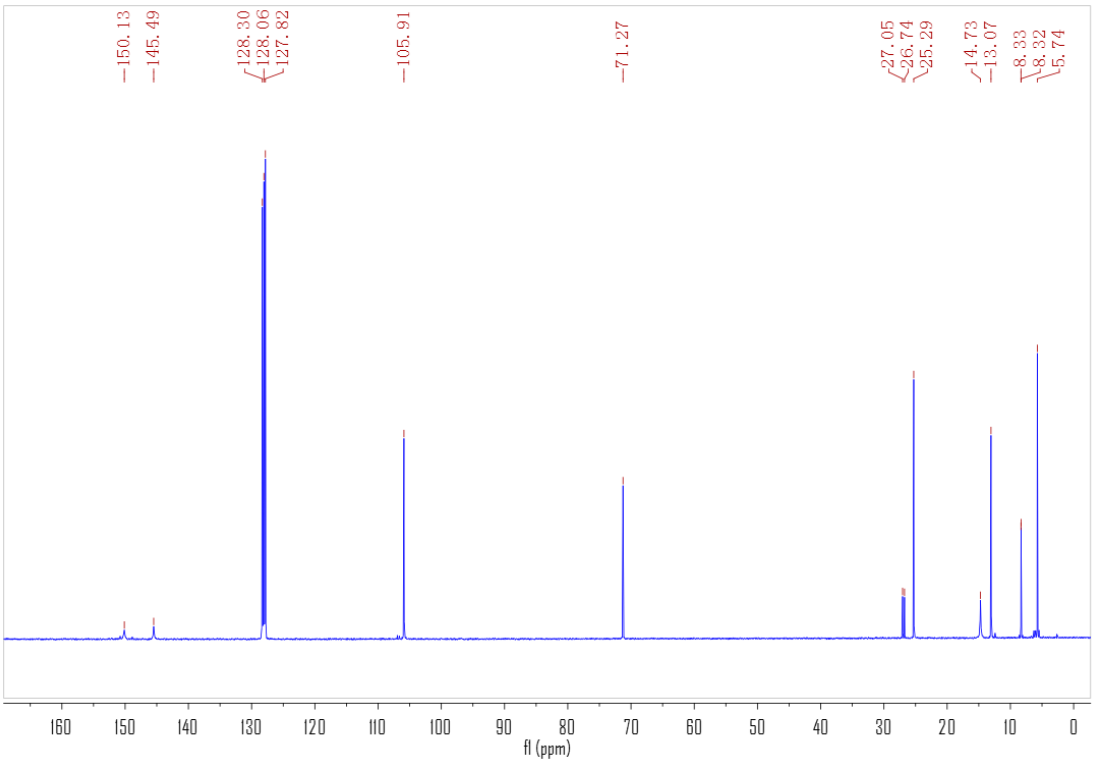
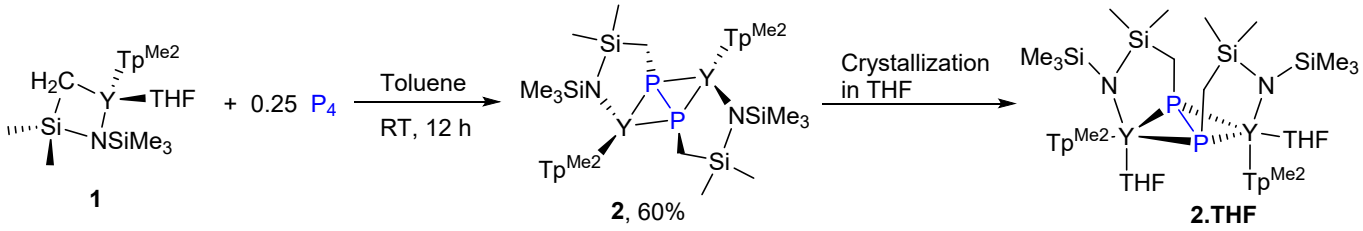


Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of complex **1** in C_6D_6 at room temperature.

2.2 Synthesis and characterization of diphosphanato yttrium complex 2 and 2·THF.



P_4 (31.0 mg, 0.25 mmol) was added to a stirred toluene solution (2 mL) of **1** (617 mg, 1.0 mmol) at ambient temperature. The reaction mixture gradually changed from light yellow to reddish brown. After a half hour, a pale solid began to precipitate out. The mixture was continued to stir for overnight, the precipitation was filtered under reduced pressure and washed by 2 mL *n*-hexane and dried under vacuum to give **2** as a light yellow powder (342 mg, 60% yield). Yellow crystals of **2** suitable for X-ray single crystal diffraction analysis were obtained by evaporation of the solvent of the solution of **2** in 30:1 toluene and THF mixture. ^{1}H NMR (400 MHz, THF-d_8, 25 °C): δ (ppm) 5.76 (s, 2H, 4-*H*-Tp^{Me2}), 5.74 (s, 2H, 4-*H*-Tp^{Me2}), 5.25 (s, 2H, 4-*H*-Tp^{Me2}), 2.67 (s, 6H, C*H*$_3$-Tp^{Me2}), 2.59 (s, 6H, C*H*$_3$-Tp^{Me2}), 2.38-2.33 (m, 24H, C*H*$_3$-Tp^{Me2}), 1.29 (s, 4H, SiC*H*$_2$P), 0.27 (s, 12H, Si(C*H*$_3$)$_2$), 0.15 (s, 18H, Si(C*H*$_3$)$_3$); ^{13}C{^{1}H} NMR (100 MHz, THF-d_8, 25 °C): δ (ppm) 152.66 (Tp^{Me2}), 151.79 (Tp^{Me2}), 150.55 (Tp^{Me2}), 145.46 (Tp^{Me2}), 145.35 (Tp^{Me2}), 144.63 (Tp^{Me2}), 106.80 (4-*C*-Tp^{Me2}), 106.20 (4-*C*-Tp^{Me2}), 19.22 (*C*H$_3$-Tp^{Me2}), 15.65 (*C*H$_3$-Tp^{Me2}), 14.67 (m, Si*C*H$_2$P), 13.31 (*C*H$_3$-Tp^{Me2}), 13.18 (*C*H$_3$-Tp^{Me2}), 13.06 (*C*H$_3$-Tp^{Me2}), 8.43 (Si(*C*H$_3$)$_2$), 8.15 (Si(*C*H$_3$)$_2$), 6.15 (Si(*C*H$_3$)$_3$); ^{31}P NMR (161 MHz, THF-d_8, 25 °C): δ (ppm) -97.10 (t, $^1J_{YP}$ = 30 Hz). Elemental Analysis: Calcd. (%) for $C_{42}H_{78}N_{14}B_2Si_4P_2Y_2$: C, 43.76; H, 6.82; N, 17.00. Found: C, 42.86; H, 6.69; N, 17.33. It is noted that recrystallization of **2** in THF afforded **2·THF** as yellow crystals. Elemental Analysis: Calcd. (%) for $C_{50}H_{94}N_{14}B_2O_2Si_4P_2Y_2$: C, 46.30; H, 7.30; N, 15.12. Found: C, 45.66; H, 7.14; N, 15.37. However, the difficulty in redissolving the isolated crystals of **2·THF** prevented its characterization by NMR spectroscopy.

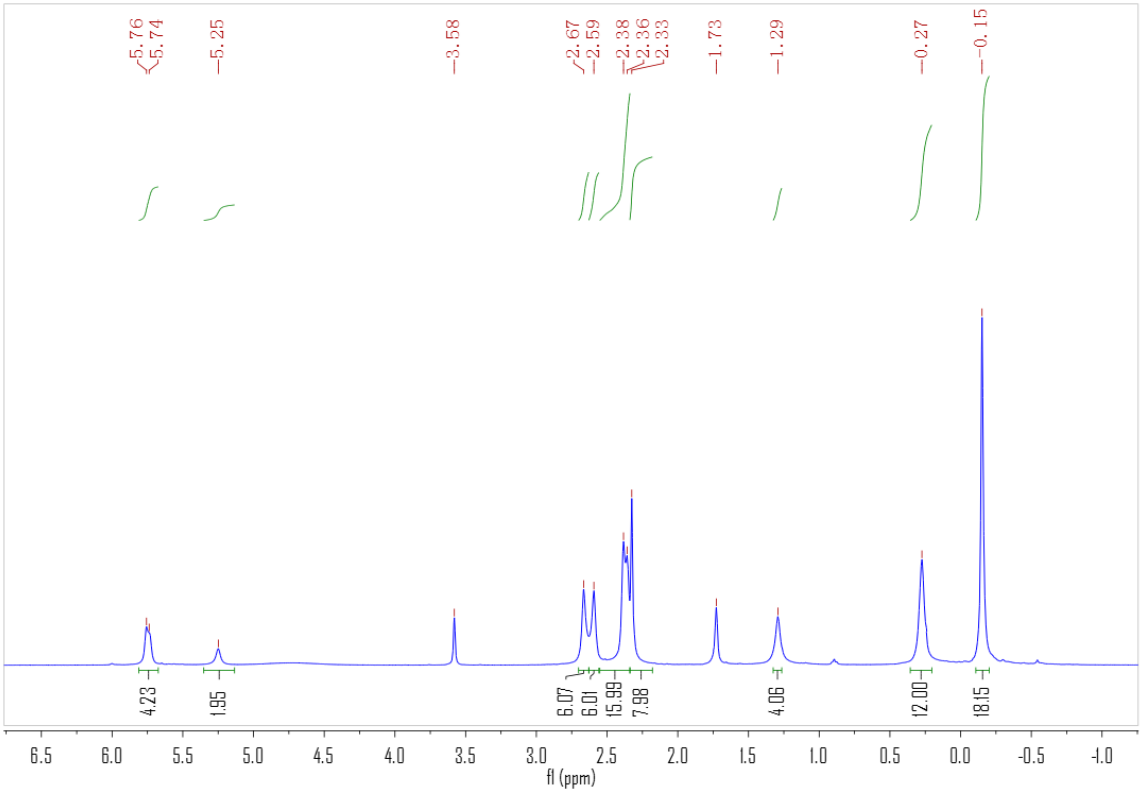


Figure S3. ^{1}H NMR spectrum of complex **2** in THF-d_8 at room temperature.

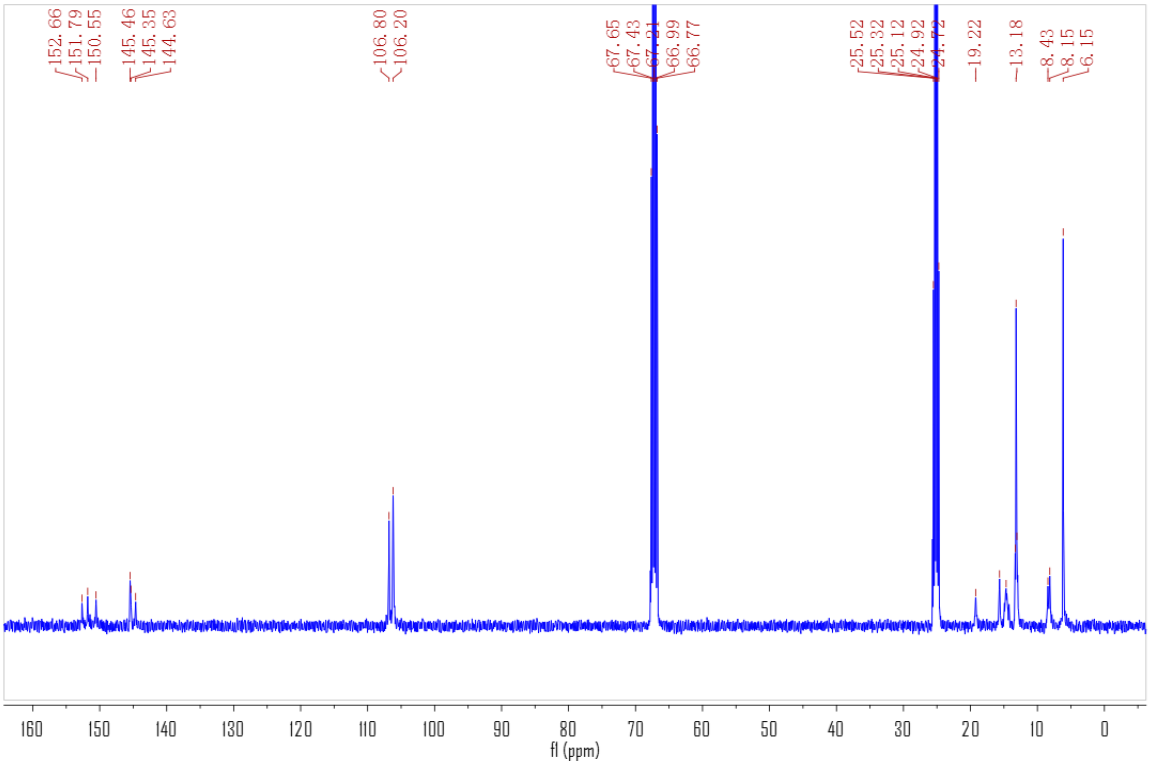


Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum of complex **2** in THF-d_8 at room temperature.

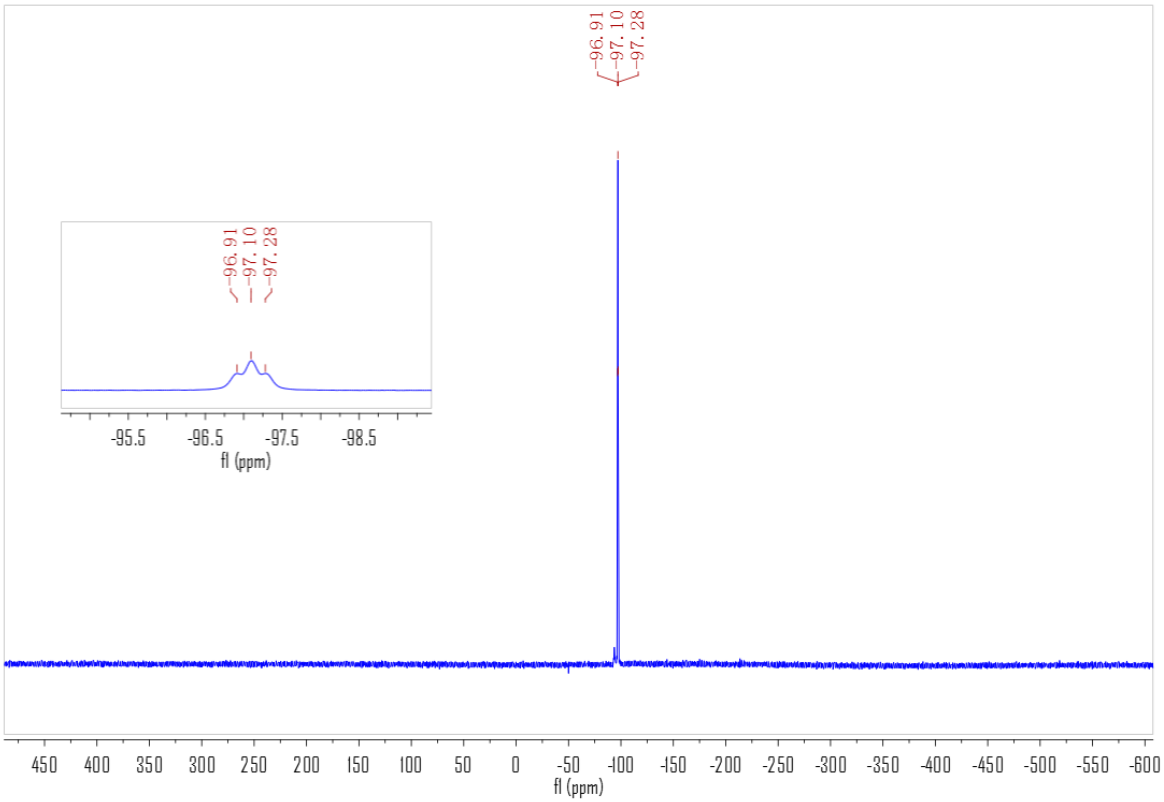
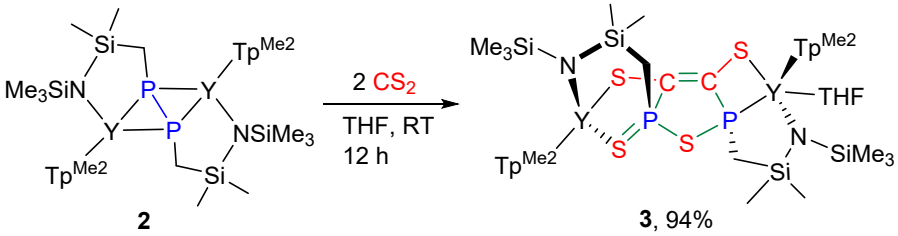


Figure S5. ^{31}P NMR spectrum of complex **2** in THF-d_8 at room temperature.

2.3 Synthesis and characterization of complex 3.



A cooled THF solution (5 mL) of CS_2 (30.3 mg, 0.40 mmol) was added slowly to a stirred THF solution (10 mL) of **2** (230 mg, 0.20 mmol) at ambient temperature. The mixture gradually changed from yellow to reddish brown. After stirring for 1 hour, the solvent was removed under vacuum and the residue was washed by *n*-hexane two times (10 mL×2) and dried under vacuum to give **3** as a yellow powder (260 mg, 94% yield). Crystals suitable for X-ray analysis were obtained by recrystallization of **3** in toluene. ^{1}H NMR (400 MHz, THF-d_8, 25 °C): δ (ppm) 5.82 (s, 1H, 4-*H*-Tp^{Me2}), 5.81 (s, 1H, 4-*H*-Tp^{Me2}), 5.79 (s, 1H, 4-*H*-Tp^{Me2}), 5.76 (s, 1H, 4-*H*-Tp^{Me2}), 5.68 (s, 1H, 4-*H*-Tp^{Me2}), 5.57 (s, 1H, 4-*H*-Tp^{Me2}), 3.62 (m, *THF*), 2.65 (s, 3H, C*H*$_3$-Tp^{Me2}), 2.51 (s, 3H, C*H*$_3$-Tp^{Me2}), 2.47 (s, 3H, C*H*$_3$-Tp^{Me2}), 2.41-2.40 (m, 18H, C*H*$_3$-Tp^{Me2}), 2.37 (s, 3H, C*H*$_3$-Tp^{Me2}), 2.28 (s, 3H, C*H*$_3$-Tp^{Me2}), 2.22 (s, 3H, C*H*$_3$-Tp^{Me2}), 1.94-1.81(m, 4H, SiC*H*$_2$P), 1.77 (m, *THF*), 0.48 (s, 3H, Si(C*H*$_3$)$_2$), 0.45 (s, 3H, Si(C*H*$_3$)$_2$), 0.30 (s, 3H, Si(C*H*$_3$)$_2$), 0.24 (s, 3H, Si(C*H*$_3$)$_2$), 0.00 (s, 9H, Si(C*H*$_3$)$_3$), -0.50 (s, 9H, Si(C*H*$_3$)$_3$); ^{13}C{^{1}H} NMR (100 MHz, THF-d_8, 25 °C): δ (ppm) 152.67 (q, $^1J_{PC}$ = 3.21 Hz, $^2J_{YC}$ = 1.56 Hz, *S*CPS), 152.38 (Tp^{Me2}), 152.22 (d, $^1J_{PC}$ = 1.99 Hz, *S*CPS$_2$), 151.70 (Tp^{Me2}), 151.28 (Tp^{Me2}), 150.69 (Tp^{Me2}), 150.66 (Tp^{Me2}), 150.08 (Tp^{Me2}), 147.16 (Tp^{Me2}), 146.76 (Tp^{Me2}), 146.16 (Tp^{Me2}), 145.42 (Tp^{Me2}), 144.32 (Tp^{Me2}), 106.82 (4-*C*-Tp^{Me2}), 106.68 (4-*C*-Tp^{Me2}), 106.58 (4-*C*-Tp^{Me2}), 106.45 (4-*C*-Tp^{Me2}), 106.37 (4-*C*-Tp^{Me2}), 106.27 (4-*C*-Tp^{Me2}), 68.02 (*THF*), 41.11 (d, $^1J_{PC}$ = 44.71 Hz, Si*C*H$_2$P), 32.69 (d, $^1J_{PC}$ = 34.45 Hz, Si*C*H$_2$P), 26.17 (*THF*), 16.52 (*C*H$_3$-Tp^{Me2}), 16.15 (*C*H$_3$-Tp^{Me2}), 15.58 (*C*H$_3$-Tp^{Me2}), 15.50 (*C*H$_3$-Tp^{Me2}), 14.49 (*C*H$_3$-Tp^{Me2}), 14.36 (*C*H$_3$-Tp^{Me2}), 13.18 (*C*H$_3$-Tp^{Me2}), 13.09 (*C*H$_3$-Tp^{Me2}), 13.04 (*C*H$_3$-Tp^{Me2}), 12.93 (*C*H$_3$-Tp^{Me2}), 12.85 (*C*H$_3$-Tp^{Me2}), 12.77 (*C*H$_3$-Tp^{Me2}), 9.27 (d, $^3J_{PC}$ = 7.28 Hz, Si(*C*H$_3$)$_2$), 8.66 (d, $^3J_{PC}$ = 11.6 Hz, Si(*C*H$_3$)$_2$), 6.41 (Si(*C*H$_3$)$_2$), 6.38 (Si(*C*H$_3$)$_3$), 6.25 (Si(*C*H$_3$)$_2$), 4.76 (Si(*C*H$_3$)$_3$); ^{31}P NMR (161 MHz, THF-d_8, 25 °C): δ (ppm) 92.43 (q, $^1J_{YP}$ =17.6 Hz), 47.88 (s). Elemental Analysis: Calcd. (%) for $C_{48}H_{86}N_{14}B_2OSi_4P_2S_4Y_2$: C, 41.86; H, 6.29; N, 14.24. Found: C, 41.14; H, 6.16; N, 14.45.

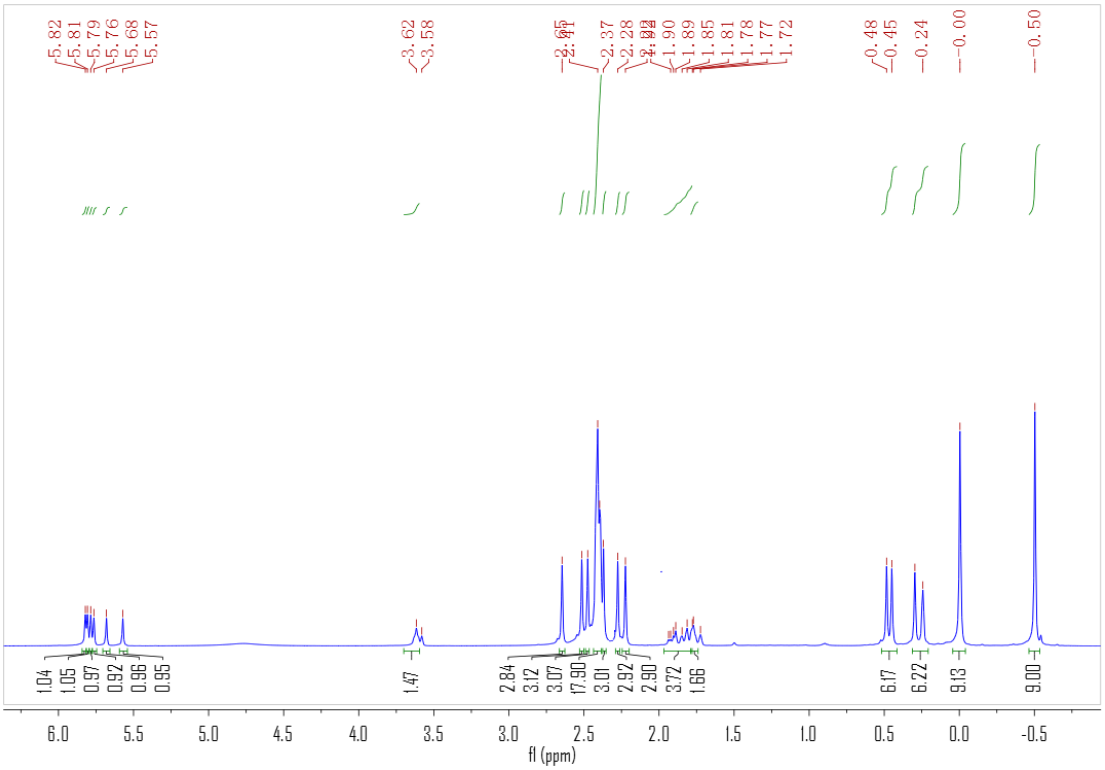


Figure S6. ^{1}H NMR spectrum of complex **3** in THF-d_8 at room temperature.

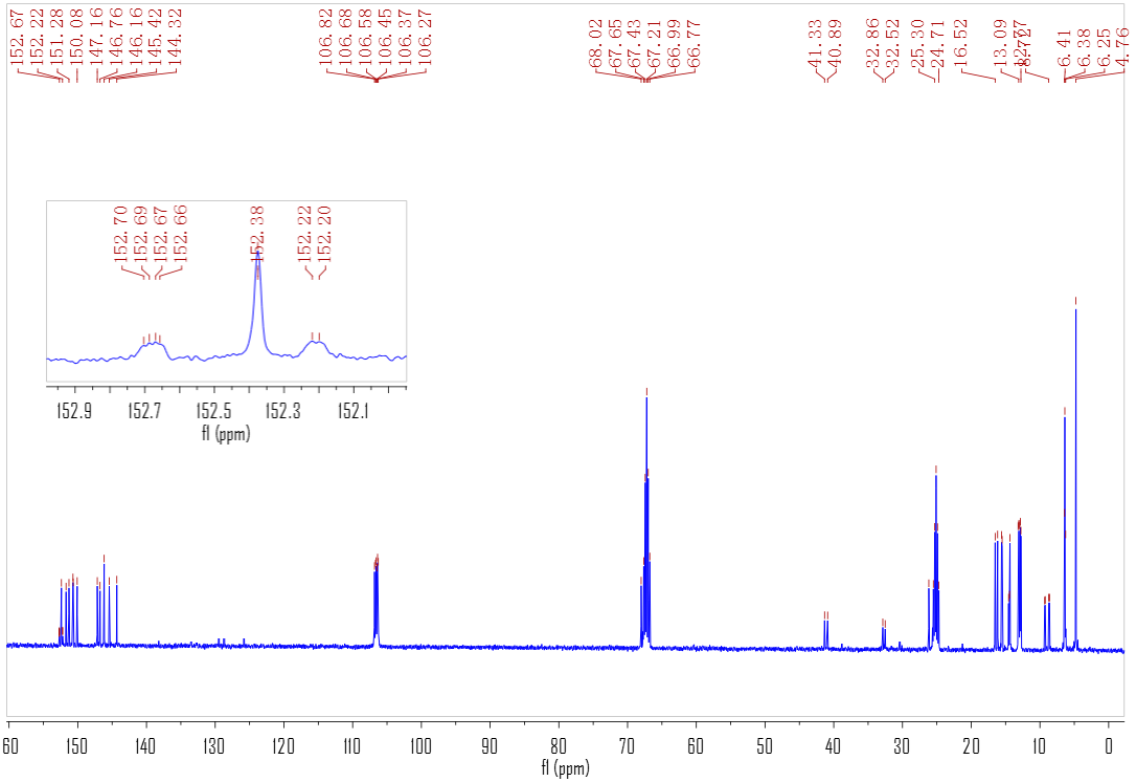


Figure S7. $^{13}C\{^{1}H\}$ NMR spectrum of complex **3** in THF-d_8 at room temperature.

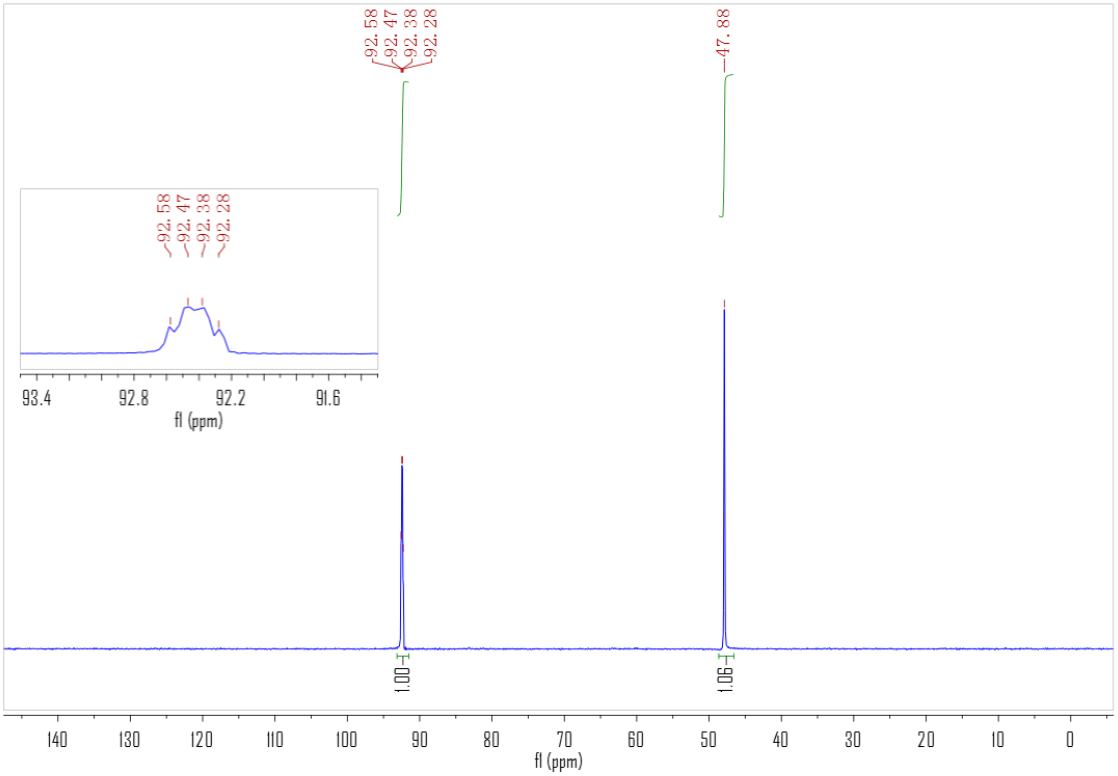
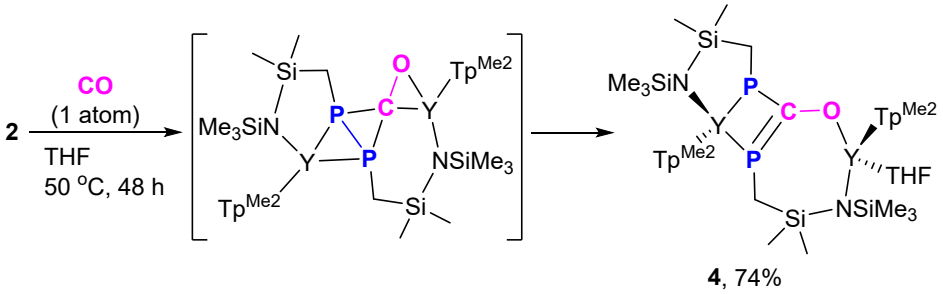


Figure S8. ^{31}P NMR spectrum of complex **3** in THF-d_8 at room temperature.

2.4 Synthesis and characterization of $(Tp^{Me2})_2Y_2[\mu\text{-}\eta^3\text{:}\eta^2\text{-}OC(PCH_2SiMe_2NSiMe_3)_2](THF)$ (4).



A THF solution (10 mL) of **2** (230 mg, 0.20 mmol) was degassed by freeze-pump-thaw and then exposed to excess 1.0 atm of CO. The reaction mixture gradually changed from yellow to orange. After stirring at 50 °C for two days, the solvent was removed under vacuum to give an orange solid. The residue was washed by hexane two times (5 mL×2) and dried under vacuum, giving **4** as an orange powder (185 mg, 74% yield). The orange single crystals of **4** for X-ray diffraction analysis were obtained by solvent evaporation of concentrated toluene solution (ca 2 mL) of **4**. ^{1}H NMR (400 MHz, toluene-d_8, 25 °C): δ (ppm) 5.61 (s, 2H, 4-*H*-Tp^{Me2}), 5.57 (s, 1H, 4-*H*-Tp^{Me2}), 5.50 (s, 2H, 4-*H*-Tp^{Me2}), 5.46 (s, 1H, 4-*H*-Tp^{Me2}), 3.67 (s, 4H, *THF*), 3.01 (s, 3H, C*H*$_3$-Tp^{Me2}), 2.93 (s, 3H, C*H*$_3$-Tp^{Me2}), 2.75 (s, 3H, C*H*$_3$-Tp^{Me2}), 2.64 (s, 3H, C*H*$_3$-Tp^{Me2}), 2.51 (s, 3H, C*H*$_3$-Tp^{Me2}), 2.43 (s, 3H, C*H*$_3$-Tp^{Me2}), 2.15-2.21 (m, 15H, C*H*$_3$-Tp^{Me2}), 2.06 (s, 3H, C*H*$_3$-Tp^{Me2}), 1.29-1.37 (m, 2H, SiC*H*$_2$P), 1.33 (s, 4H, *THF*), 1.08-1.22 (m, 4H, SiC*H*$_2$P), 0.66 (s, 3H, Si(C*H*$_3$)$_2$), 0.49 (s, 3H, Si(C*H*$_3$)$_2$), 0.41 (s, 6H, Si(C*H*$_3$)$_2$), -0.18 (s, 9H, Si(C*H*$_3$)$_3$), -0.22 (s, 9H, Si(C*H*$_3$)$_3$); ^{31}P NMR (161 MHz, toluene-d_8, 25 °C): δ (ppm) 65.01 (d, $^1J_{YP}$ =136.4 Hz), -11.89 (d, $^1J_{YP}$ = 120.3 Hz). ^{1}H NMR (400 MHz, C_6D_6, 25 °C): δ (ppm) 5.64 (s, 3H, 4-*H*-Tp^{Me2}), 5.53 (s, 2H, 4-*H*-Tp^{Me2}), 5.46 (s, 1H, 4-*H*-Tp^{Me2}), 3.78 (m, 4H, *THF*), 3.15 (s, 3H, C*H*$_3$-Tp^{Me2}), 2.96 (s, 3H, C*H*$_3$-Tp^{Me2}), 2.81 (s, 3H, C*H*$_3$-Tp^{Me2}), 2.67 (s, 3H, C*H*$_3$-Tp^{Me2}), 2.56 (s, 3H, C*H*$_3$-Tp^{Me2}), 2.49 (s, 3H, C*H*$_3$-Tp^{Me2}), 2.11-2.21 (m, 15H, C*H*$_3$-Tp^{Me2}), 2.05 (s, 3H, C*H*$_3$-Tp^{Me2}), 1.29-1.37 (m, 2H, SiC*H*$_2$P), 1.17 (m, 2+4H, SiC*H*$_2$P+*THF*), 0.74 (s, 3H, Si(C*H*$_3$)$_2$), 0.57 (s, 3H, Si(C*H*$_3$)$_2$), 0.45 (s, 6H, Si(C*H*$_3$)$_2$), -0.09 (s, 9H, Si(C*H*$_3$)$_3$), -0.13 (s, 9H, Si(C*H*$_3$)$_3$); ^{13}C NMR (100 MHz, C_6D_6, 25 °C): δ (ppm) 151.55 (*C*O), 151.42 (Tp^{Me2}), 150.31 (Tp^{Me2}), 150.22 (Tp^{Me2}), 150.10 (Tp^{Me2}), 149.65 (Tp^{Me2}), 146.79 (Tp^{Me2}), 146.24 (Tp^{Me2}), 145.79 (Tp^{Me2}), 144.71 (Tp^{Me2}), 144.54 (Tp^{Me2}), 106.64 (4-*C*-Tp^{Me2}), 106.40 (4-*C*-Tp^{Me2}), 106.09 (4-*C*-Tp^{Me2}), 105.86 (4-*C*-Tp^{Me2}), 72.51 (*THF*), 25.14 (*THF*), 19.72 (d, $^1J_{PC}$ = 49.66 Hz, Si*C*H$_2$P), 15.84 (d, $^1J_{PC}$ = 12.42 Hz, Si*C*H$_2$P), 15.47 (*C*H$_3$-Tp^{Me2}), 15.33 (*C*H$_3$-Tp^{Me2}), 15.25 (*C*H$_3$-Tp^{Me2}), 15.07 (*C*H$_3$-Tp^{Me2}), 14.84 (*C*H$_3$-Tp^{Me2}), 14.71 (*C*H$_3$-Tp^{Me2}), 14.62 (*C*H$_3$-Tp^{Me2}), 13.21 (*C*H$_3$-Tp^{Me2}), 13.04 (*C*H$_3$-Tp^{Me2}), 12.98 (*C*H$_3$-Tp^{Me2}), 9.00 (Si(*C*H$_3$)$_2$), 8.44 (s, Si(*C*H$_3$)$_2$), 8.24 (s, Si(*C*H$_3$)$_2$), 5.81 (Si(*C*H$_3$)$_3$), 4.80 (Si(*C*H$_3$)$_3$), 1.43 (Si(*C*H$_3$)$_2$); ^{31}P NMR (161 MHz, C_6D_6, 25 °C): *δ* (ppm) 66.56 (br s), -11.81 (br s); Elemental Analysis: Calcd. (%) for $C_{47}H_{86}N_{14}B_2O_2Si_4P_2Y_2$: C, 45.05; H, 6.92; N, 15.65. Found: C, 44.33; H, 6.77; N, 15.75.

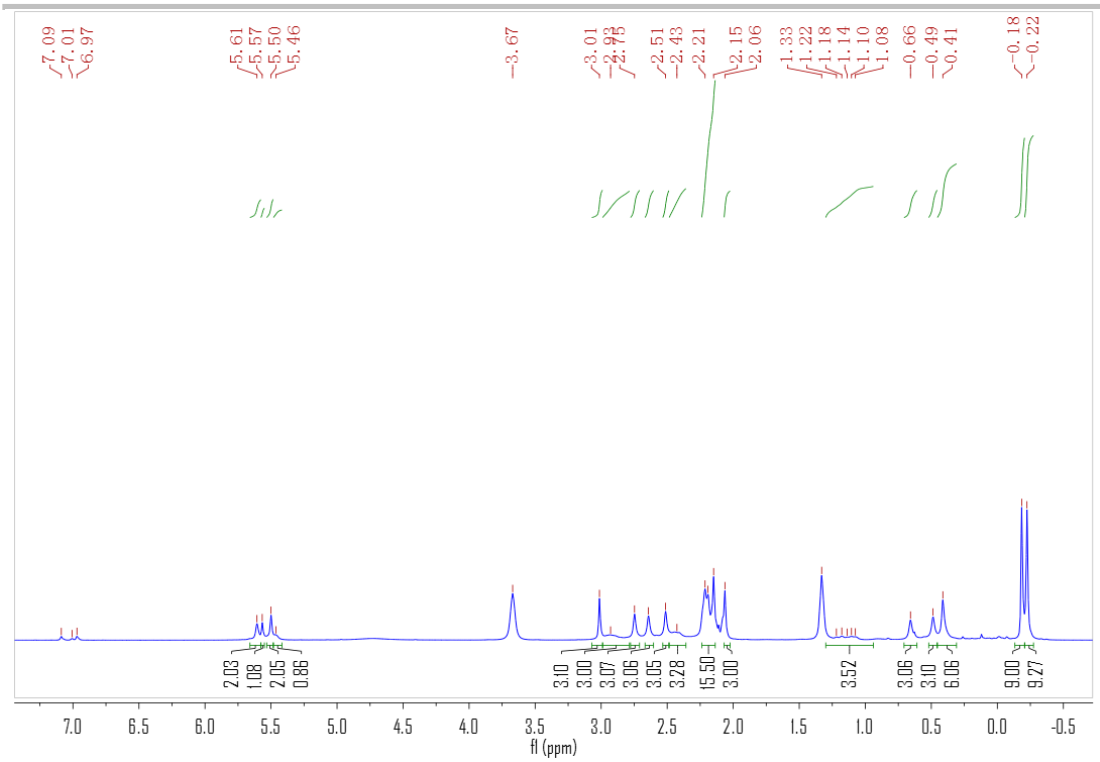


Figure S9. ^{1}H NMR spectrum of **4** in Toluene-d_8 at room temperature.

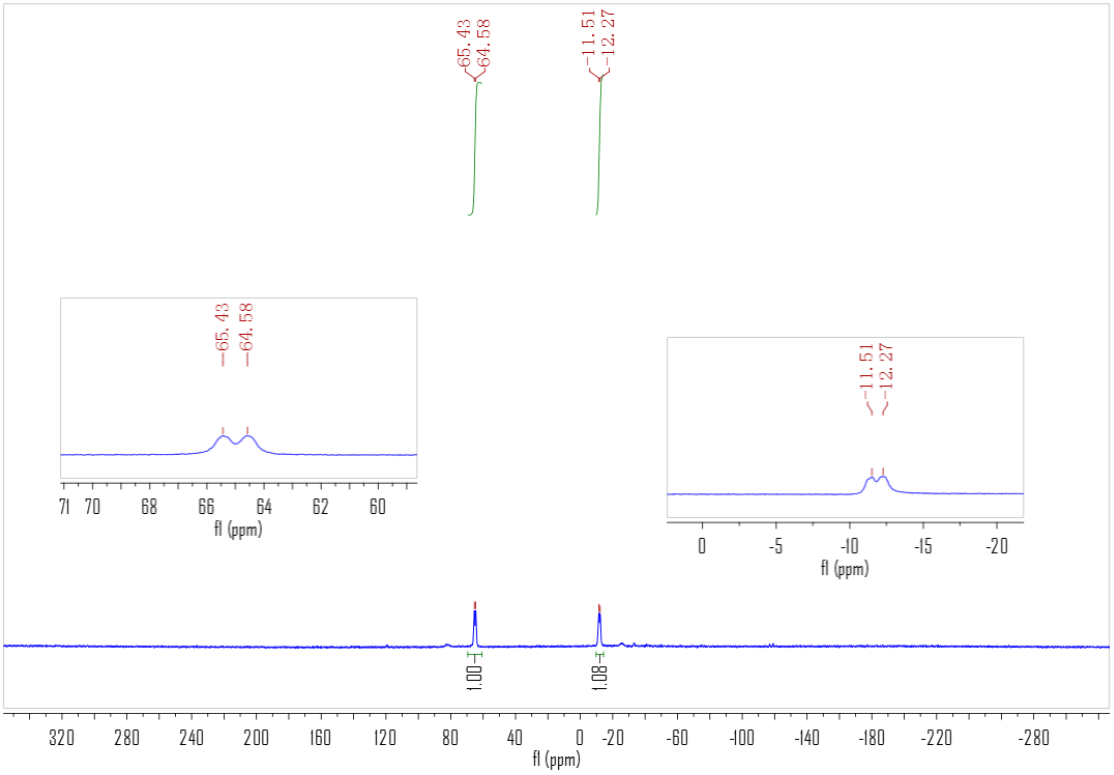


Figure S10. ^{31}P NMR spectrum of **4** in toluene-d_8 at room temperature.

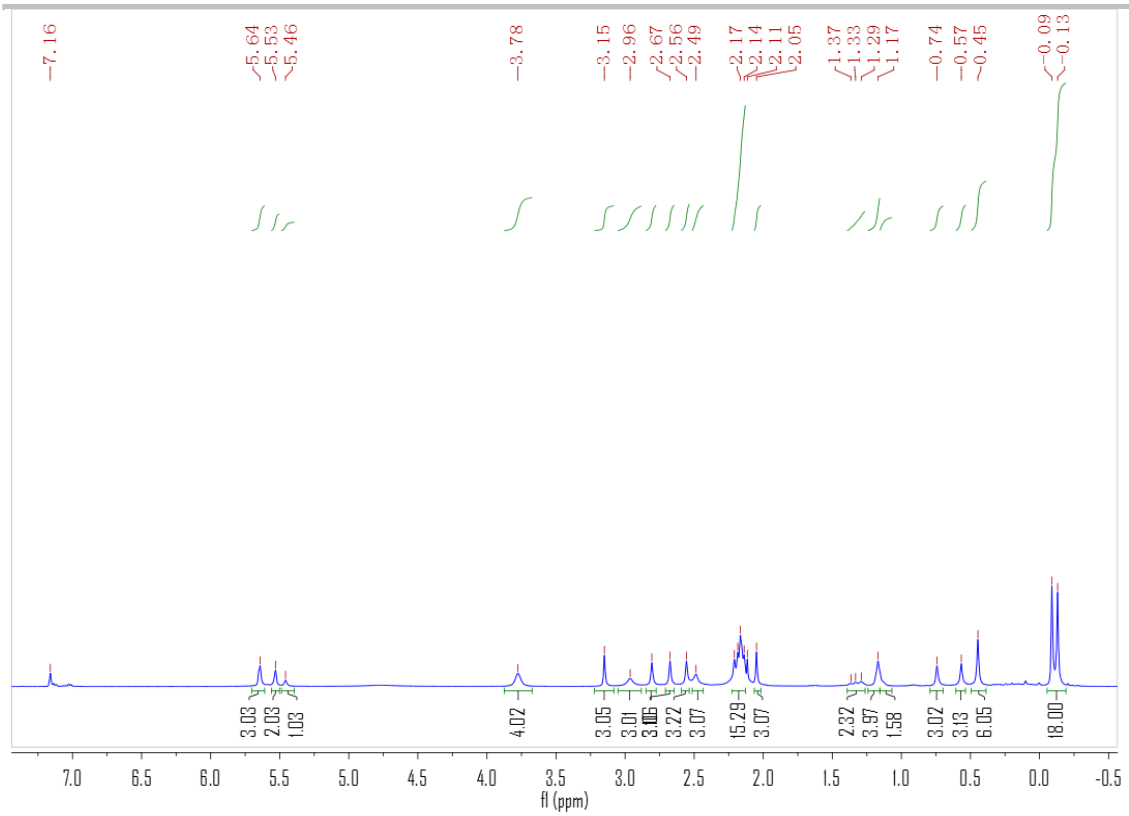


Figure S11. ^{1}H NMR spectrum of **4** in C_6D_6 at room temperature.

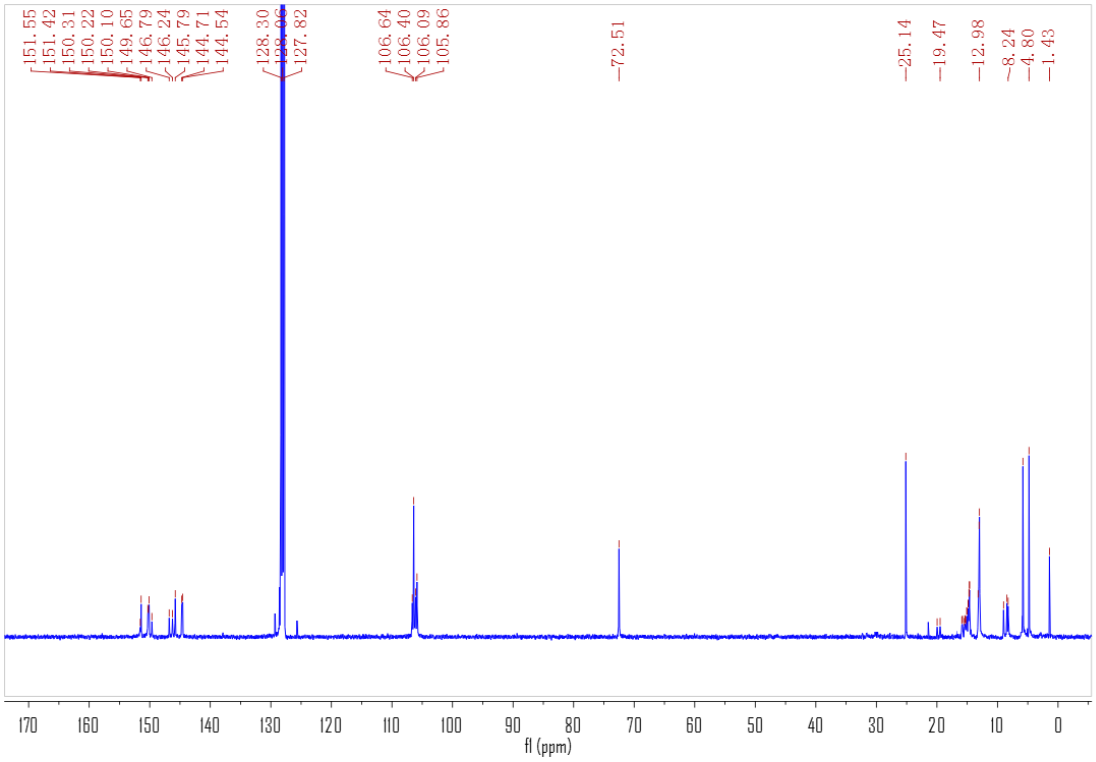


Figure S12. $^{13}C\{^{1}H\}$ NMR spectrum of **4** in C_6D_6 at room temperature.

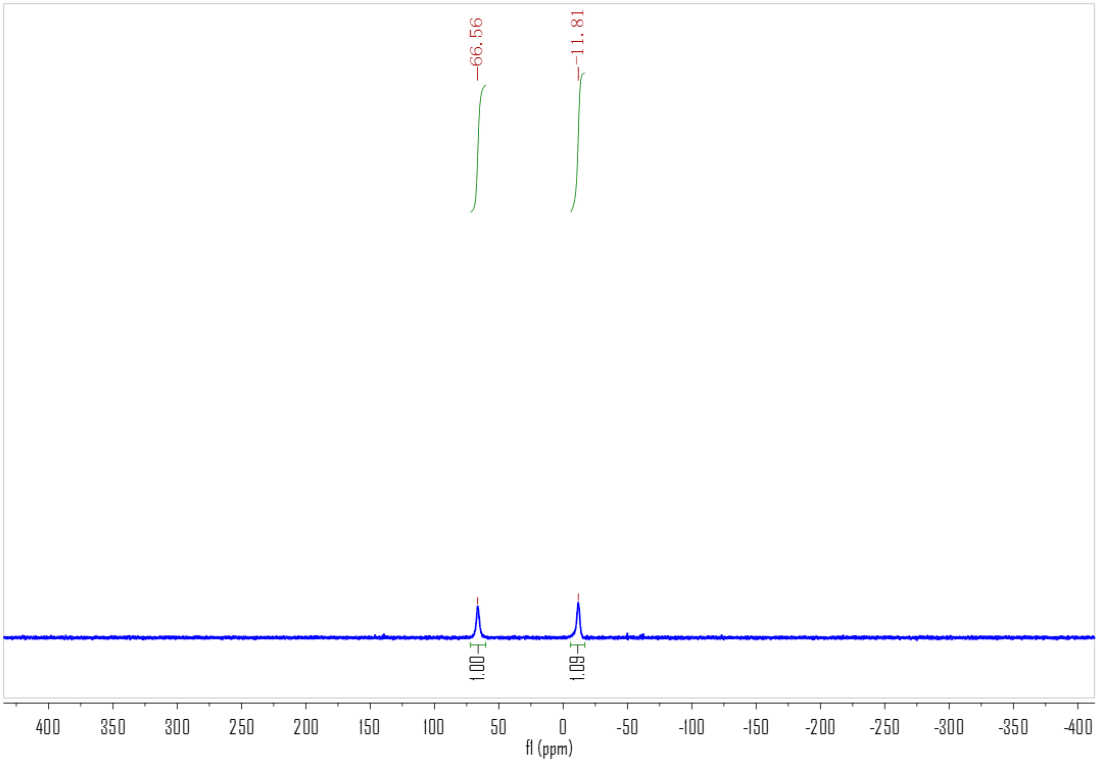
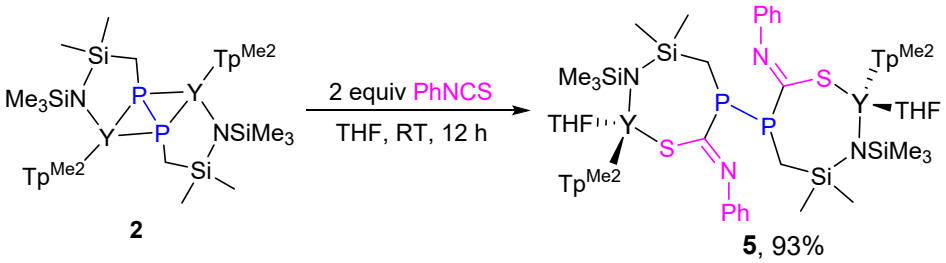


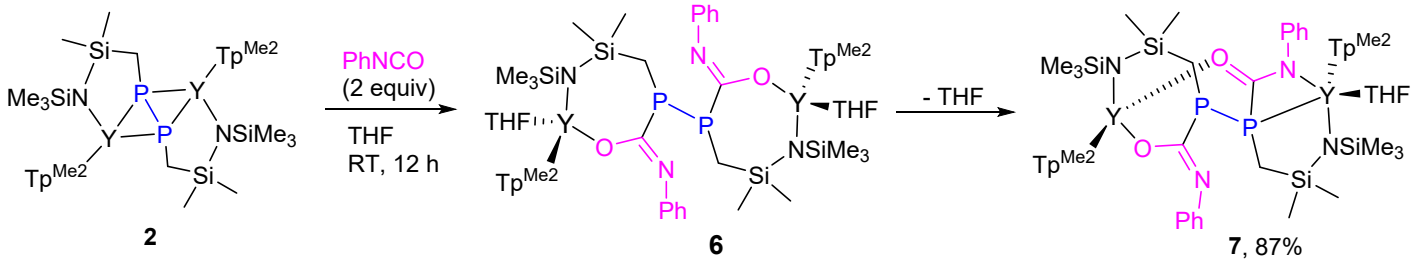
Figure S13. ^{31}P NMR spectrum of **4** in C_6D_6 at room temperature.

2.5 Synthesis and characterization of complex 5.



A cooled THF solution (3 mL) of PhNCS (27.5 mg, 0.20 mmol) was added slowly to a stirred THF solution (10 mL) of **2** (115.2 mg, 0.10 mmol) at ambient temperature. After stirring for 5 min, the reaction solution was stood at room temperature for 2 days to give **5** as colorless crystals (145 mg, 93% yield). Regrettably, the low solubility of **5** precluded the acquisition of its NMR spectra. Elemental Analysis: Calcd. (%) for $C_{64}H_{102}N_{16}B_2O_2Si_4P_2S_2Y_2$: C, 49.10; H, 6.57; N, 14.32. Found: C, 49.74; H, 6.52; N, 14.59.

2.6 Synthesis and characterization of diphosphine complexes 6 and 7.



A cooled THF solution (5 mL) of PhNCO (47.6 mg, 0.40 mmol) was added slowly to a stirred THF solution (10 mL) of **2** (230 mg, 0.20 mmol) at ambient temperature. The reaction solution gradually changed from yellow to colorless. After stirring at ambient temperature for 12 h, the solution was concentrated to ca 3 mL under reduced pressure. After standing at room temperature for several days, colorless crystals of complex **6** were obtained (169 mg, 55% yield). However, if the reaction mixture was directly evaporated to dryness under vacuum, washing the residue with hexane three times (10 mL×3) followed by crystallization in THF/hexane would lead to the loss of one coordinated THF, affording **7** as crystalline solid (267 mg, 87% yield). Crystals suitable to the X-ray diffraction analysis were obtained by gas phase diffusion of hexane into the THF solution of **7**. Notably, retransformation of **7** into **6** is quite difficult to perform in THF at room temperature, whereas transformation of compound **6** into compound **7** occurred slowly under vacuum condition or exposure to nitrogen gas too. For example, the ^{31}P NMR monitoring data indicate the formation of a small amount of **7** after storing a solution of **6** in THF-d_8 at room temperature for 1 week (***Figure S14***). Therefore, compound **6** is not characterized by EA and NMR spectra. For compound **7:** ^{1}H NMR (400 MHz, THF-d_8, 25 °C): δ (ppm) 7.32 (d, 2H, $^3J_{HH}$ = 7.72 Hz, *Ph*), 7.03 (t, 2H, $^3J_{HH}$ = 7.32 Hz, *Ph*), 6.73 (t, 1H, $^3J_{HH}$ = 7.2 Hz, *Ph*), 6.27 (t, 1H, $^3J_{HH}$ = 7.08 Hz, *Ph*), 5.91 (m, 2H, *Ph*), 5.89 (s, 1H, 4-*H*-Tp^{Me2}), 5.82 (s, 1H, 4-*H*-Tp^{Me2}), 5.74 (s, 1H, 4-*H*-Tp^{Me2}), 5.59 (m, 2H, *Ph*), 5.54(s, 1H, 4-*H*-Tp^{Me2}), 5.27 (s, 1H, 4-*H*-Tp^{Me2}), 5.27 (s, 1H, 4-*H*-Tp^{Me2}), 3.62 (m, 4H, *THF*), 2.57 (s, 6H, C*H*$_3$-Tp^{Me2}), 2.49 (s, 3H, C*H*$_3$-Tp^{Me2}), 2.45 (s, 3H, C*H*$_3$-Tp^{Me2}), 2.35 (s, 12H, C*H*$_3$-Tp^{Me2}), 2.31 (s, 3H, C*H*$_3$-Tp^{Me2}), 2.24 (s, 3H, C*H*$_3$-Tp^{Me2}), 2.04 (s, 3H, C*H*$_3$-Tp^{Me2}), 1.89-1.86 (m, 2H, SiC*H*$_2$P), 1.77 (m, 4H, *THF*), 1.61-1.54 (m, 2H, SiC*H*$_2$P), 1.47 (s, 3H, C*H*$_3$-Tp^{Me2}), 0.46 (s, 3H, Si(C*H*$_3$)$_2$), 0.44 (s, 3H, Si(C*H*$_3$)$_2$), 0.36 (s, 3H, Si(C*H*$_3$)$_2$), 0.21 (s, 3H, Si(C*H*$_3$)$_2$), -0.45 (s, 9H, Si(C*H*$_3$)$_3$), -0.67 (s, 9H, Si(C*H*$_3$)$_3$); ^{13}C{^{1}H} NMR (100 MHz, THF-d_8, 25 °C): δ (ppm) 181.61 (t, $^1J_{PC}$ = 5.0 Hz, P*C*=O), 165.83 (q, $^1J_{PC}$ = 3.0 Hz, P*C*=N), 151.38 (Tp^{Me2}), 150.44 (Tp^{Me2}), 150.42 (Tp^{Me2}), 149.96 (Tp^{Me2}), 149.69 (Tp^{Me2}), 149.54 (Tp^{Me2}), 146.34 (Tp^{Me2}), 146.04 (Tp^{Me2}), 144.88 (Tp^{Me2}), 144.49 (Tp^{Me2}), 128.11 (*Ph*), 127.44 (*Ph*), 126.72 (*Ph*), 125.34 (*Ph*), 124.84 (*Ph*), 123.61 (*Ph*), 122.27 (*Ph*), 121.01 (*Ph*), 106.71 (4-*C*-Tp^{Me2}), 106.48 (4-*C*-Tp^{Me2}), 106.24 (4-*C*-Tp^{Me2}), 105.82 (4-*C*-Tp^{Me2}), 105.20 (4-*C*-Tp^{Me2}), 104.74 (4-*C*-Tp^{Me2}), 68.02 (*THF*), 26.16 (*THF*), 15.43 (*C*H$_3$-Tp^{Me2}), 15.39 (*C*H$_3$-Tp^{Me2}), 15.06 (*C*H$_3$-Tp^{Me2}), 14.96 (*C*H$_3$-Tp^{Me2}),

14.33 (CH_3-Tp^{Me2}), 14.13 (CH_3-Tp^{Me2}), 14.06 (d, $^1J_{PC}$ = 27.45 Hz, SiCH_2P), 13.06 (d, $^1J_{PC}$ = 4.23 Hz, SiCH_2P), 12.93 (CH_3-Tp^{Me2}), 12.91 (CH_3-Tp^{Me2}), 12.87 (CH_3-Tp^{Me2}), 12.69 (CH_3-Tp^{Me2}), 9.64 (d, $^3J_{PC}$ = 5.09 Hz, Si(CH_3)$_2$), 7.59 (d, $^3J_{PC}$ = 10.91 Hz, Si(CH_3)$_2$), 6.31 (Si(CH_3)$_3$), 6.17 (Si(CH_3)$_2$), 4.68 (Si(CH_3)$_3$), 3.81 (d, $^3J_{PC}$ = 4.28 Hz, Si(CH_3)$_2$); ^{31}P NMR (161 MHz, THF-d_8, 25 °C): δ (ppm) -26.71 (dm, $^1J_{PP}$ = 374 Hz, PY), -39.64 (dd, J_{PP} =374, 12.8 Hz, free P). Elemental Analysis: Calcd. (%) for $C_{60}H_{94}N_{16}B_2O_3Si_4P_2Y_2$: C, 49.32; H, 6.48; N, 15.34. Found: C, 49.59; H, 6.34; N, 15.57.

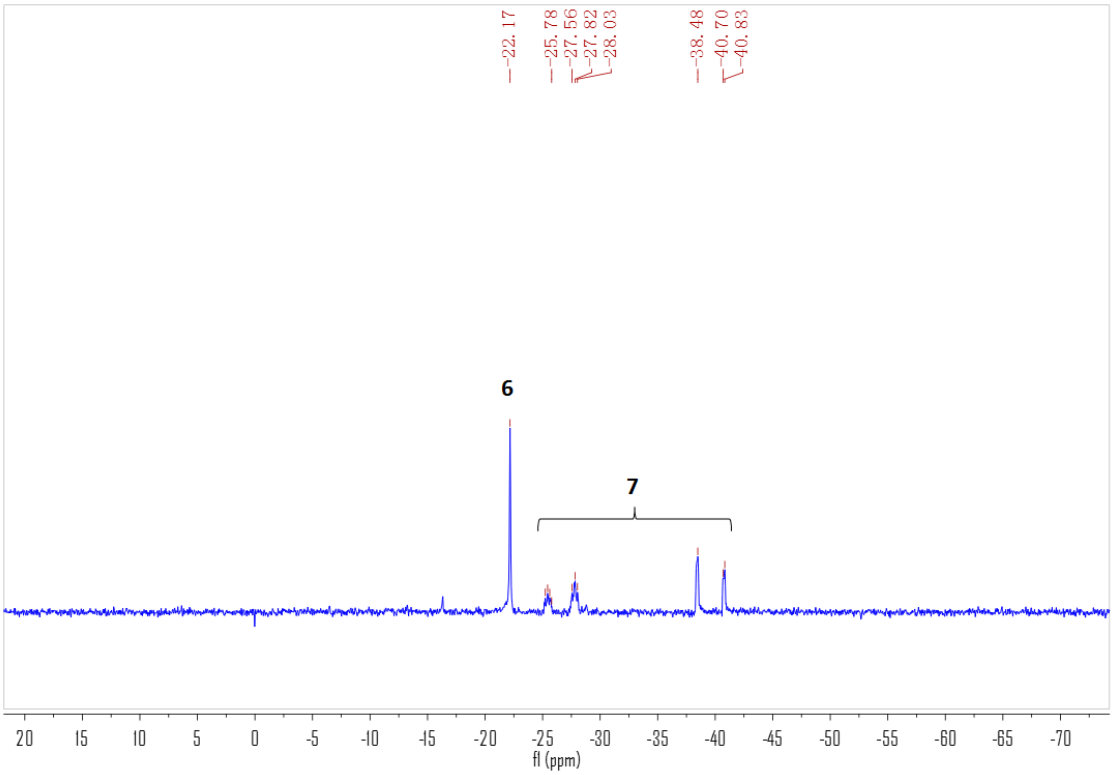


Figure S14. ^{31}P NMR spectrum of **6** after storing in THF-d_8 at room temperature for 1 week.

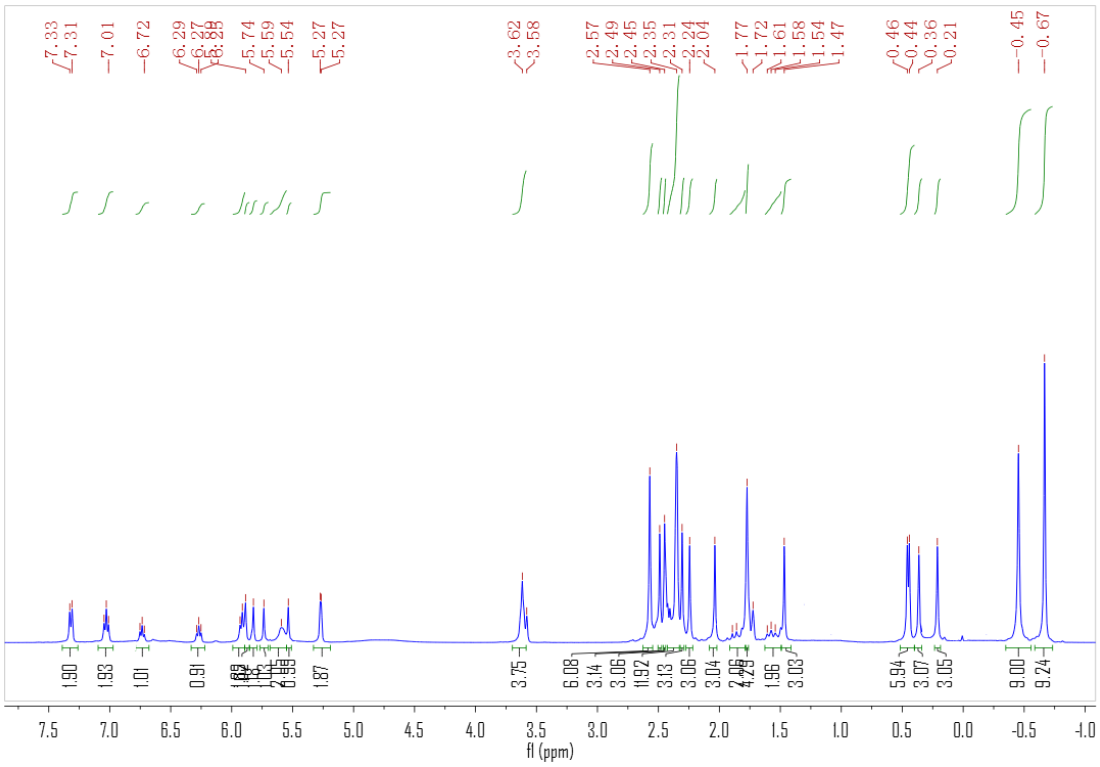


Figure S15. ^{1}H NMR spectrum of **7** in THF-d_8 at room temperature.

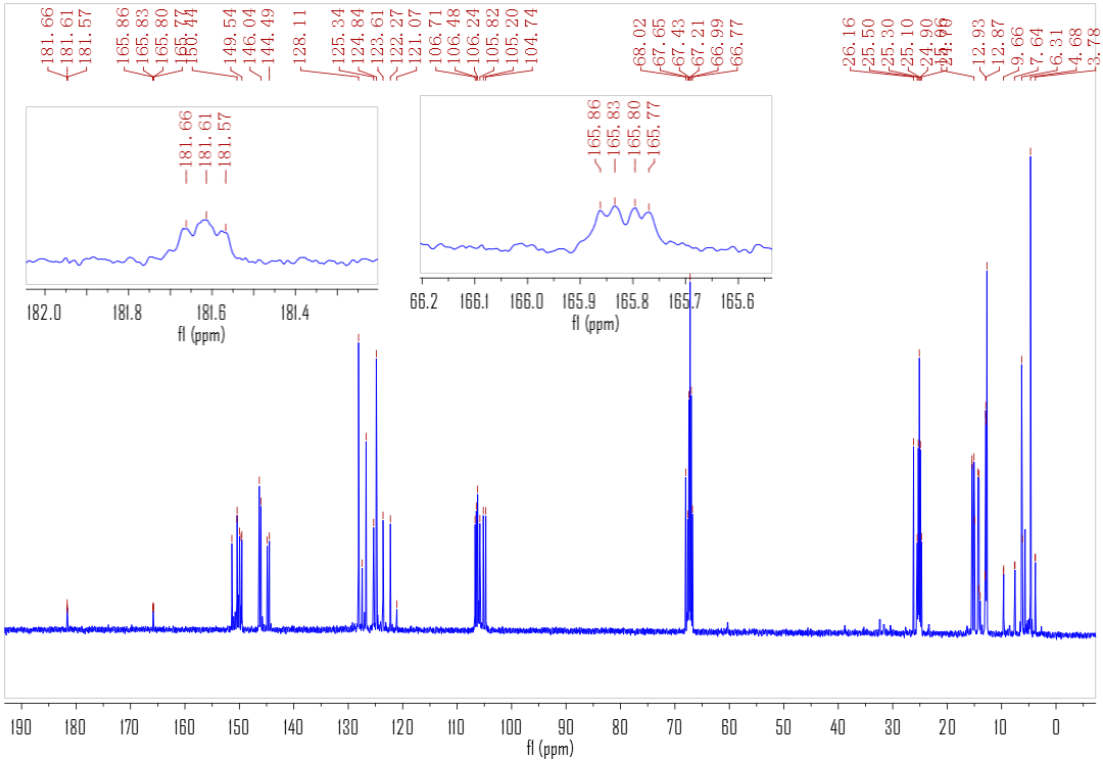


Figure S16. $^{13}C\{^{1}H\}$ NMR spectrum of compound **7** in THF-d_8 at room temperature.

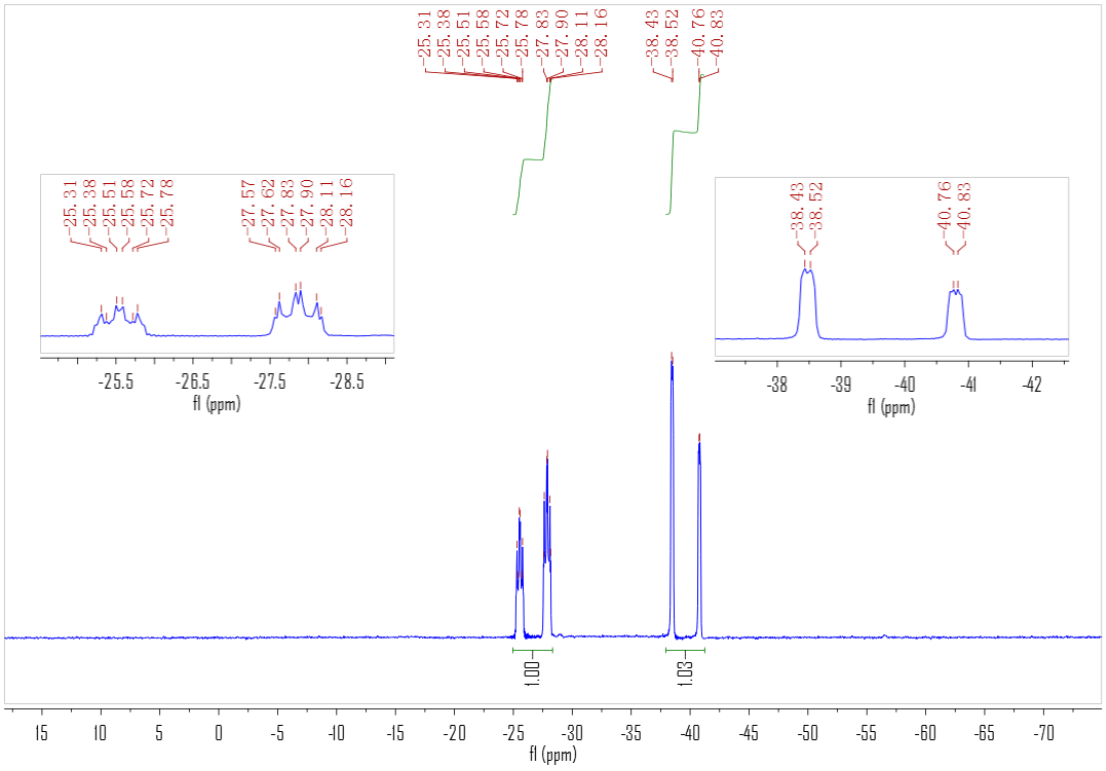
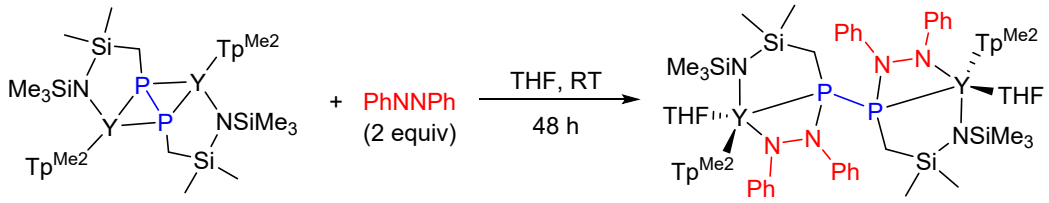


Figure S17. ^{31}P NMR spectrum of compound **7** in THF-d_8 at room temperature.

2.7 Synthesis and characterization of complex 8.



A THF solution (5 mL) of PhNNPh (39.6 mg, 0.20 mmol) was added slowly to a stirred THF solution (10 mL) of **2** (115 mg, 0.10 mmol) at ambient temperature. The color of the reaction mixture gradually changed from yellow to greenish black. After stirring for 2 days, the solvent was removed under vacuum and the solid residue was washed by n-hexane two times (5 mL×2) and dried under vacuum to give a yellow powder of **8** (141 mg, 85% yield). Yellow crystals suitable for X-ray diffraction analysis were obtained by solvent evaporation of concentrated THF solution (ca 2 mL) of **8**. No satisfied ^{13}C NMR data of **8** was obtained due to its poor solubility. ^{1}H NMR (400 MHz, THF-d_8, 25 °C): δ (ppm) 7.31 (d, 4H, $^{3}J_{HH}$ = 7.92 Hz, -C$_6$*H*$_5$), 6.97 (t, $^{3}J_{HH}$ = 7.88 Hz, 6H,-C$_6$*H*$_5$), 6.70 (br, 2H, -C$_6$*H*$_5$), 6.63 (t, $^{3}J_{HH}$ = 7.12 Hz, 2H, -C$_6$*H*$_5$), 6.30 (br, 2H, -C$_6$*H*$_5$), 6.13 (t, $^{3}J_{HH}$ = 6.4 Hz, 4H, -C$_6$*H*$_5$), 5.87(s, 2H, 4-*H*-Tp^{Me2}), 5.82 (s, 2H, 4-*H*-Tp^{Me2}), 5.60 (s, 2H, 4-*H*-Tp^{Me2}), 3.60 (m, 4H, *THF*), 2.64 (s, 6H, C*H*$_3$-Tp^{Me2}), 2.52 (s, 6H, C*H*$_3$-Tp^{Me2}), 2.48 (s, 6H, C*H*$_3$-Tp^{Me2}), 2.46 (s, 6H, C*H*$_3$-Tp^{Me2}), 2.45 (s, 6H, C*H*$_3$-Tp^{Me2}), 2.39-2.41 (m, 4H, SiC*H*$_2$P), 2.11 (s, 6H, C*H*$_3$-Tp^{Me2}), 1.77 (m, 4H, *THF*), 0.14 (s, 6H, Si(C*H*$_3$)$_2$), -0.38 (s, 18H, Si(C*H*$_3$)$_3$), -0.56 (s, 6H, Si(C*H*$_3$)$_2$); ^{31}P NMR (161 MHz, THF-d_8, 25 °C): δ (ppm) 50.66 (s); Elemental Analysis: Calcd. (%) for $C_{74}H_{112}N_{18}B_2O_2Si_4P_2Y_2$: C, 53.56; H, 6.80; N, 15.19. Found: C, 53.27; H, 6.73; N, 15.27.

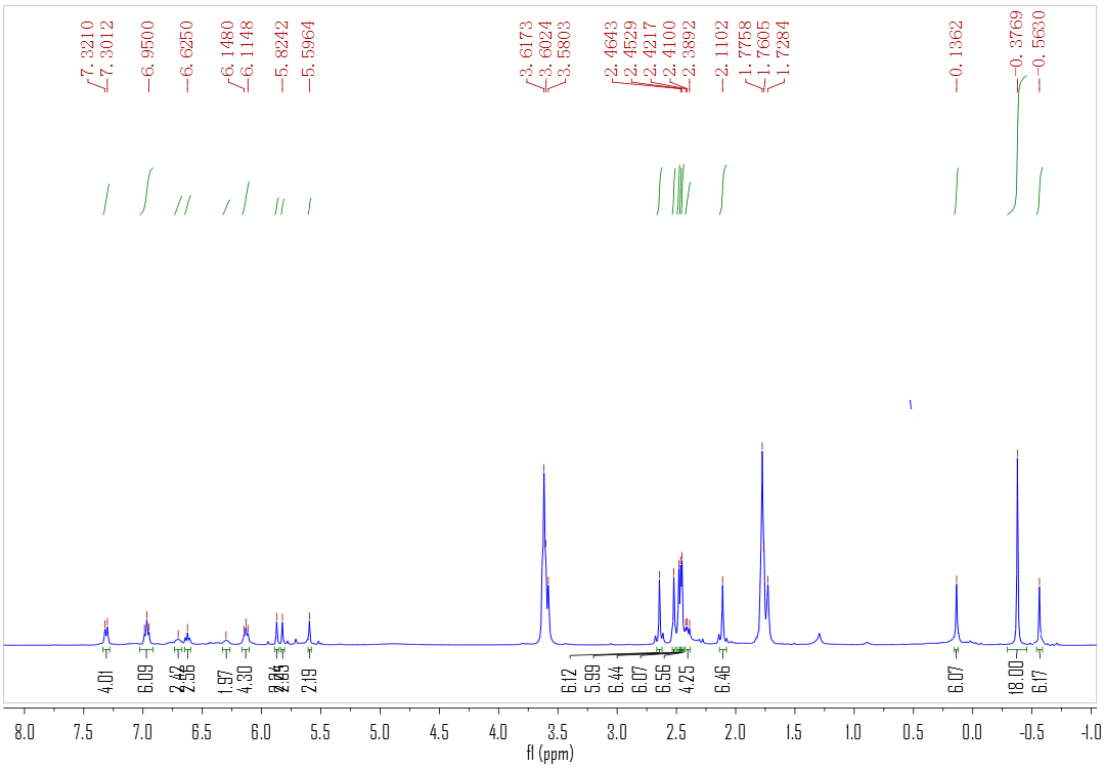


Figure S18. ^{1}H NMR spectrum of **8** in THF-d_8 at room temperature.

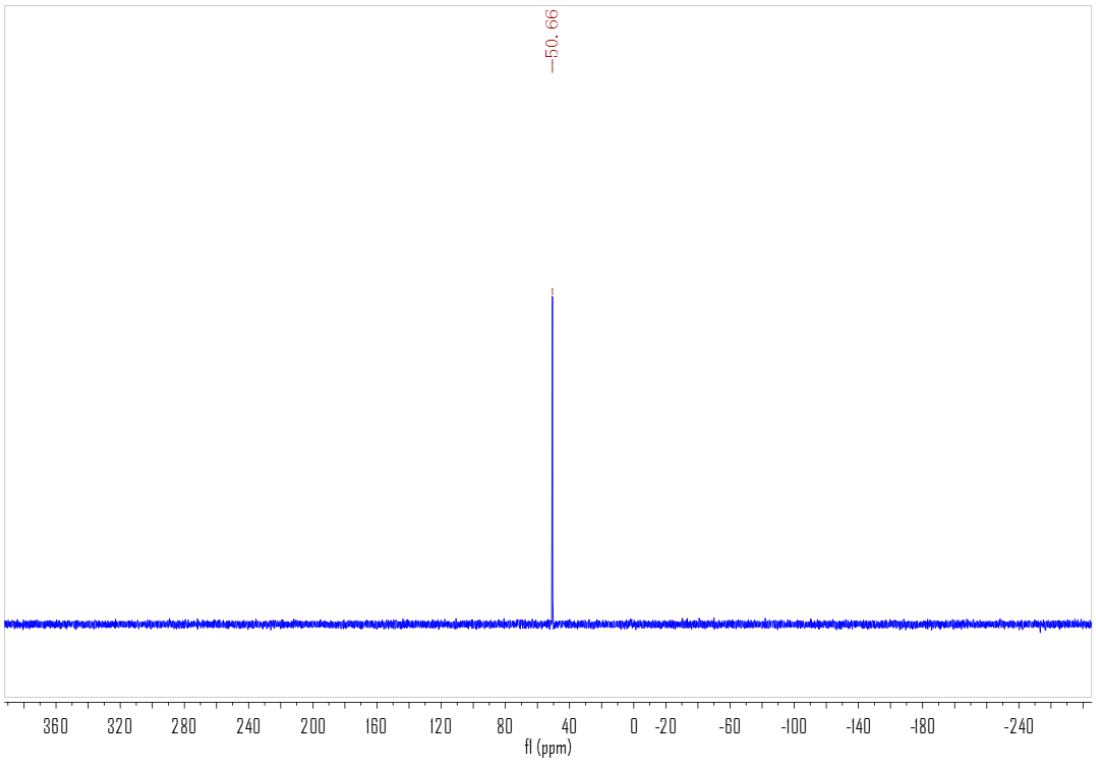
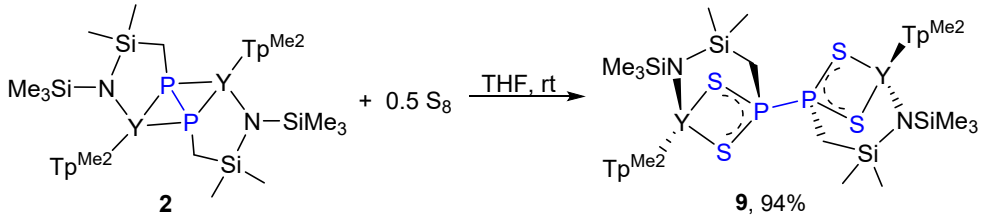


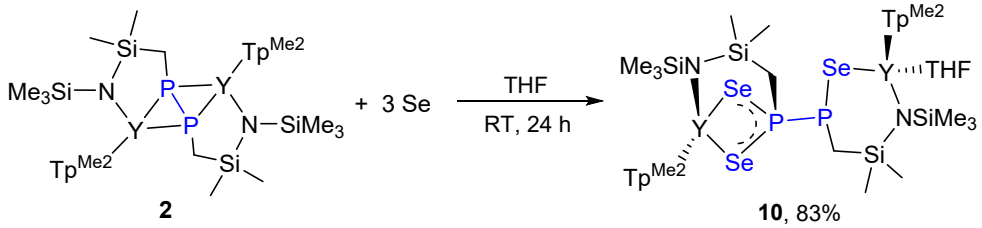
Figure S19. ^{31}P NMR spectrum of **8** in THF-d_8 at room temperature.

2.8 Synthesis and characterization of complex 9.



A THF solution (5 mL) of S_8 (12.8 mg, 0.050 mmol) was added slowly to a stirred THF solution (10 mL) of **2** (115 mg, 0.10 mmol) at ambient temperature. After stirring for 5 min, the reaction solution was stood at room temperature for three days to give **9** as colorless crystals (120 mg, 94% yield). No satisfied NMR data of **9** was obtained due to its poor solubility even in heating THF-d_8. Elemental Analysis: Calcd. (%) for $C_{42}H_{78}N_{14}B_2S_4Si_4P_2Y_2$: C, 39.37; H, 6.14; N, 15.31. Found: C, 38.53; H, 6.03; N, 15.26.

2.10 Synthesis and characterization of complex 10.



Se power (23.7 mg, 0.30 mmol) was added to a stirred THF solution (10 mL) of **2** (230 mg, 0.20 mmol) at ambient temperature. The mixture gradually changed from greenish black to colorless. After stirring for overnight, removing solvent gave colorless solid, which was washed by hexane two times (10 mL×2) and dried under vacuum to give **10** as a colorless powder (243 mg, 83% yield). Colorless crystals for X-ray diffraction analysis were obtained by gas-phase diffusing hexane into a concentrated THF solution (ca 2 mL) of **10**. ^{1}H NMR (400 MHz, THF-d_8, 25 ^{o}C): δ (ppm) 5.86 (s, 1H, 4-*H*-Tp^{Me2}), 5.83(s, 3H, 4-*H*-Tp^{Me2}), 5.71 (s, 1H, 4-*H*-Tp^{Me2}), 5.60 (s, 1H, 4-*H*-Tp^{Me2}), 3.61 (m, 4H, *THF*), 2.75 (s, 3H, C*H*$_3$-Tp^{Me2}), 2.63 (s, 6H, C*H*$_3$-Tp^{Me2}), 2.60 (s, 3H, C*H*$_3$-Tp^{Me2}), 2.50 (s, 3H, C*H*$_3$-Tp^{Me2}), 2.44 (s, 12H, C*H*$_3$-Tp^{Me2}), 2.42 (s, 3H, C*H*$_3$-Tp^{Me2}), 2.34 (s, 3H, C*H*$_3$-Tp^{Me2}), 2.30 (s, 3H, C*H*$_3$-Tp^{Me2}), 2.12-2.27 (m, 4H, SiC*H*$_2$P), 1.77 (m, 4H, *THF*), 1.47 (s, 3H, C*H*$_3$-Tp^{Me2}), 0.42 (s, 3H, Si(C*H*$_3$)$_2$), 0.32 (s, 3H, Si(C*H*$_3$)$_2$), 0.30 (s, 6H, Si(C*H*$_3$)$_2$), -0.40 (s, 9H, Si(C*H*$_3$)$_3$), -0.50 (s, 9H, Si(C*H*$_3$)$_3$); ^{13}C NMR (100 MHz, THF-d_8, 25 ^{o}C): δ (ppm) 151.65 (Tp^{Me2}), 151.50 (Tp^{Me2}), 151.35 (Tp^{Me2}), 151.05 (Tp^{Me2}), 150.95 (Tp^{Me2}), 150.14 (Tp^{Me2}), 147.03 (Tp^{Me2}), 146.97 (Tp^{Me2}), 146.95 (Tp^{Me2}), 146.47 (Tp^{Me2}), 145.60 (Tp^{Me2}), 144.60 (Tp^{Me2}), 106.90 (4-*C*-Tp^{Me2}), 106.84 (4-*C*-Tp^{Me2}), 106.73 (4-*C*-Tp^{Me2}), 106.66 (4-*C*-Tp^{Me2}), 106.17 (4-*C*-Tp^{Me2}), 68.02 (*THF*), 34.68 (d, $^1J_{PC}$ = 5.34 Hz, Si*C*H$_2$P), 34.49 (d, $^1J_{PC}$ = 5.87 Hz, Si*C*H$_2$P), 26.16 (*THF*), 17.51 (C*H*$_3$-Tp^{Me2}), 17.28 (C*H*$_3$-Tp^{Me2}), 16.76 (C*H*$_3$-Tp^{Me2}), 15.59 (C*H*$_3$-Tp^{Me2}), 15.48 (C*H*$_3$-Tp^{Me2}), 14.77 (C*H*$_3$-Tp^{Me2}), 12.97 (C*H*$_3$-Tp^{Me2}), 12.89 (C*H*$_3$-Tp^{Me2}), 12.86 (C*H*$_3$-Tp^{Me2}), 7.54 (d, $^3J_{PC}$ = 3.81 Hz,Si(*C*H$_3$)$_2$), 7.46 (overlap d, Si(*C*H$_3$)$_2$), 7.42 (d, $^3J_{PC}$ = 3.65 Hz, Si(*C*H$_3$)$_2$), 6.80 (d, $^3J_{PC}$ = 5.19 Hz, Si(*C*H$_3$)$_2$), 5.53 (Si(*C*H$_3$)$_3$), 4.98 (s, Si(*C*H$_3$)$_3$); ^{31}P NMR (161 MHz, THF-d_8, 25 ^{o}C): δ (ppm) 29.97 (d, $^1J_{PP}$ = 390 Hz), 23.68 (d, $^1J_{PP}$ = 390 Hz); Elemental Analysis: Calcd. (%) for $C_{46}H_{86}N_{14}B_2OSe_3Si_4P_2Y_2$: C, 37.79; H, 5.93; N, 13.41. Found: C, 37.53; H, 5.81; N, 13.29.

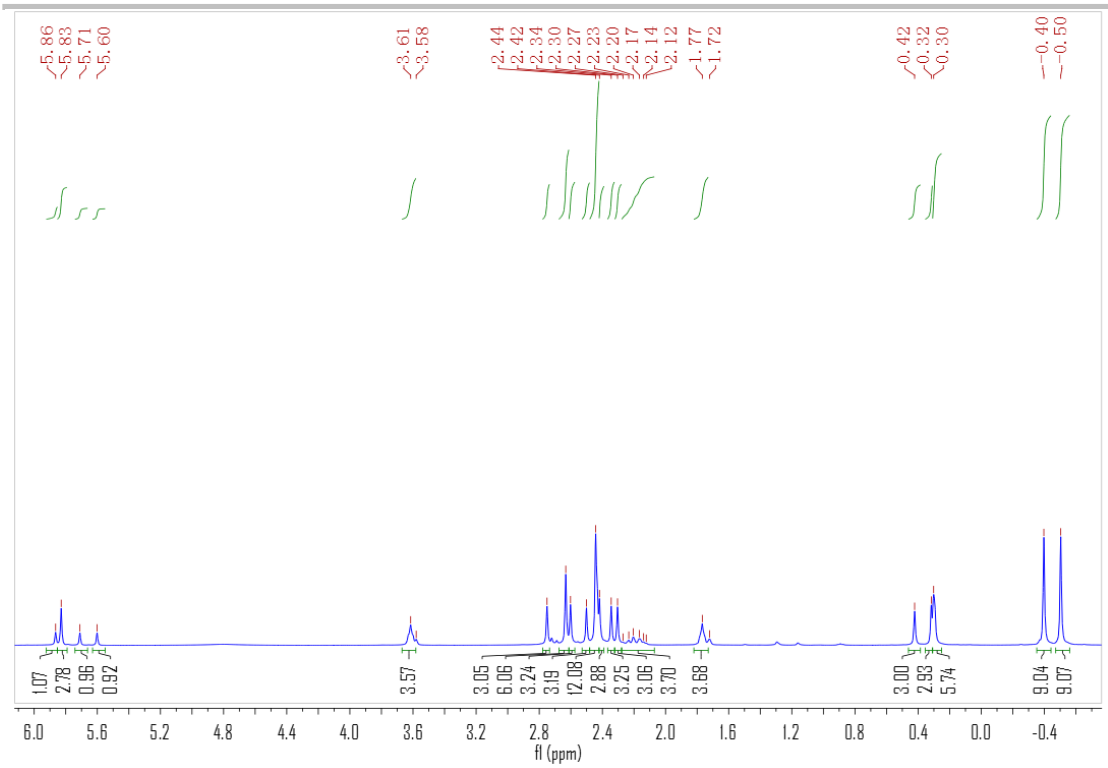


Figure S20. ^{1}H NMR spectrum of compound **10** in THF-d_8 at room temperature.

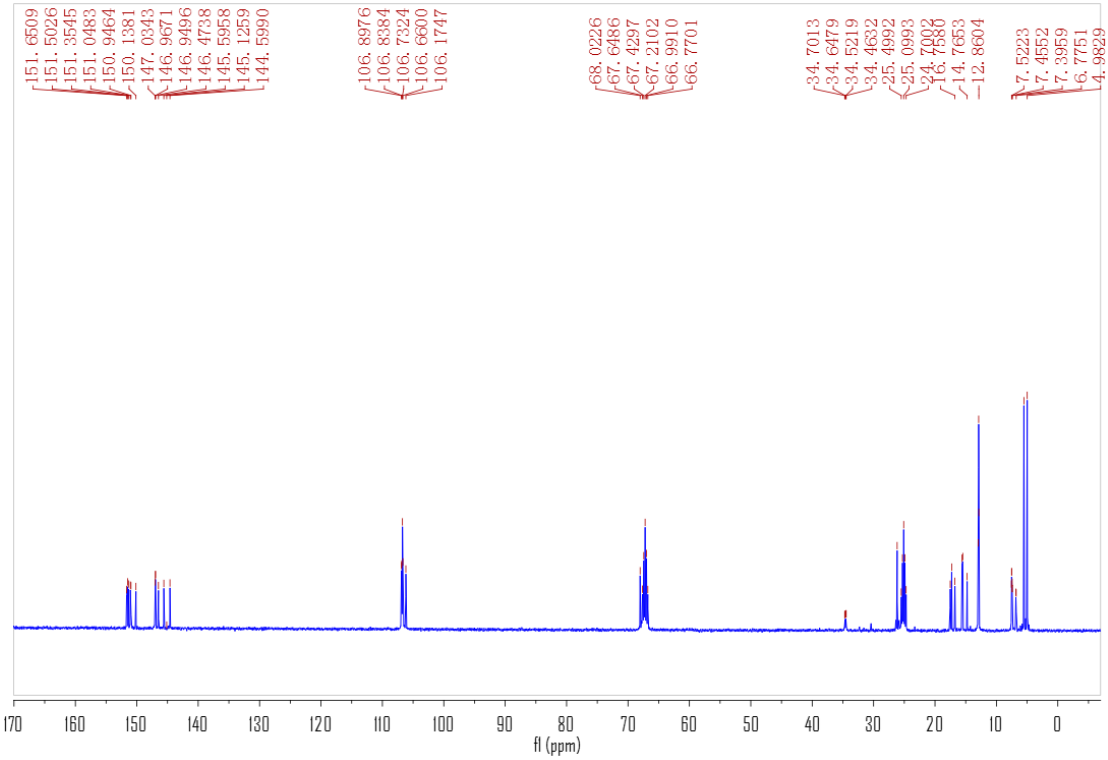


Figure S21. ^{13}C{^{1}H} NMR spectrum of compound **10** in THF-d_8 at room temperature.

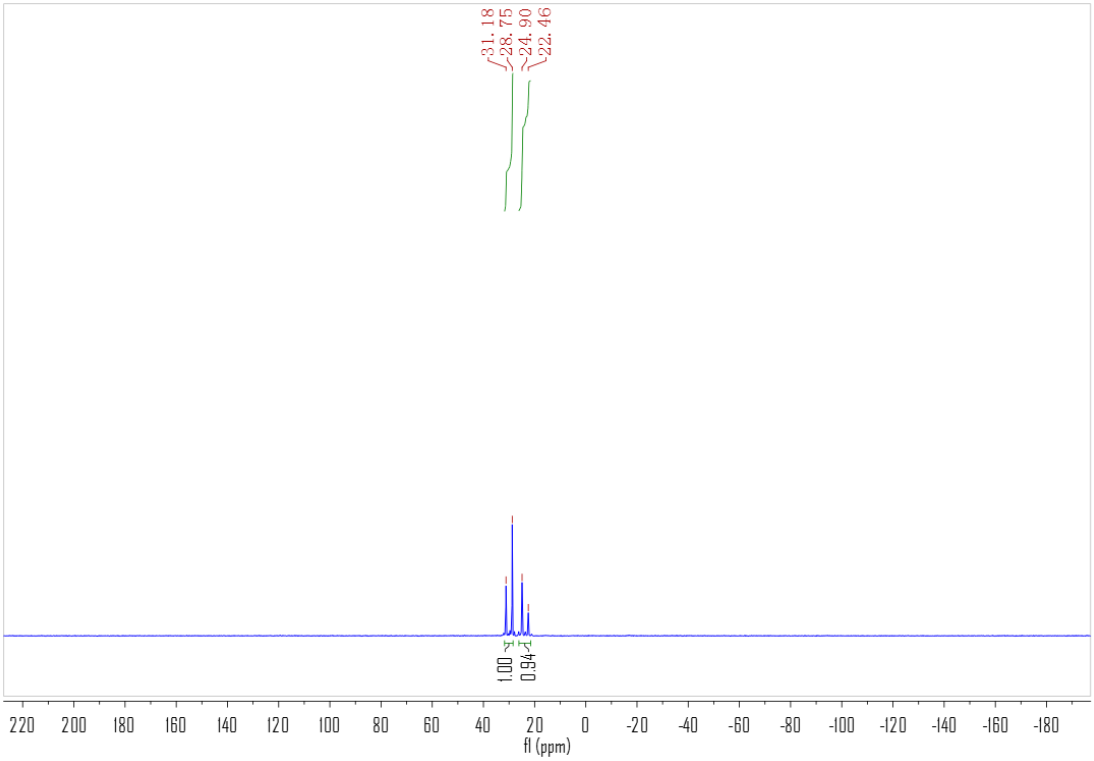


Figure S22. ^{31}P NMR spectrum of compound **10** in THF-d_8 at room temperature.

3. X-ray Crystallographic Analyses of Complexes 1-10

Suitable crystals were wrapped in mineral oil and then were frozen at 173 or 223 K. Data collections were performed on a Bruker SMART APEX (at 293 K) or Bruker SMART APEX (II) (at 173 or 293 K) diffractometer with CCD area detector using graphite-monochromated Mo Kα radiation (λ= 0.71073 Å). The determination of crystal class and unit cell was carried out by SMART program package. The raw frame data were processed using SAINT[3] and SADABS[4] to yield the reflection data file. All structures were solved by using SHELXTL program[5] and refined on *F*2 by full-matrix least-squares techniques with anisotropic thermal parameters for non-hydrogen atoms. Hydrogen atoms were placed at the 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 cif files. Calculations were carried out using the *SHELXL-2008* or *SHELXL-2014* program. Unfortunately, the precision of compounds **5** and **6** was limited by the poor quality of their crystals. CCDC 1879573 (**1**), 1879574 (**2**), 1879577 (**2·THF**), 1879583 (**3**), 1879582 (**4**), 1879576 (**5**), 1879581 (**6**), 1879575 (**7**·0.5C_6H_{14}), 1879580 (**8**), 1879579 (**9**), and 1879578 (**10**), contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/conts/retrieving.html (or from The Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK; fax: (+44)-1223-336033; or deposit@ccdc.cam.ac.uk).

Table S1. Crystal data and collection parameters of complexes **1**, **2** and **2·THF**

Identification code	**1**	**2**	**2·THF**
Formula	$C_{25}H_{47}BN_7OSi_2Y$	$C_{42}H_{78}B_2N_{14}P_2Si_4Y_2$	$C_{50}H_{94}B_2N_{14}O_2P_2Si_4Y_2$
Formula weight	617.59	1152.92	1297.13
Temperature (K)	298(2)	173(2)	173(2)
Wavelength (Å)	0.71073	0.71073	0.71073
Crystal system	Orthorhombic	Triclinic	Monoclinic
Space group	*P*2(1)2(1)2(1)	*P*-1	*C*2/c
a (Å)	11.632(2)	10.966(17)	34.357(4)
b (Å)	15.388(3)	11.122(17)	13.674(18)
c (Å)	18.887(4)	13.834(2)	16.179(2)
α (deg)	90	81.500(2)	90
β (deg)	90	87.739(3)	106.458(2)
γ (deg)	90	70.796(2)	90
V (Å ^{3})	3380.7(12)	4153.5(13)	7289.1(16)
Z	4	1	4
Dc (g/m^3)	1.213	1.215	1.182
μ (mm^{-1})	1.824	1.998	1.737
F(000)	1304	602	2728
Crystal size (mm)	0.50 x 0.38 x 0.36	0.44 x 0.24 x 0.22	0.24 x 0.22 x 0.18
ϑ range (°)	1.707 to 25.047	1.488 to 25.05	1.236 to 25.05
	-13<=h<=13	-13<=h<=9	-40<=h<=40
h, k, l range	-18<=k<=11	-13<=k<=12	-16<=k<=16
	-22<=l<=21	-16<=l<=16	-12<=l<=19
Reflections collected / unique	16505 / 5909	9491 / 5529	19112 / 6231
	[*R*(int) = 0.0417]	[*R*(int) = 0.0201]	[*R*(int) = 0.0438]
Completeness to *ϑ*	99.9 % (*ϑ* = 25.10)	98.7 % (*ϑ* = 25.10)	96.6 % (*ϑ* = 25.10)
Max. and min. transmission	0.7456 and 0.3383	0.7456 and 0.6028	0.7456 and 0.5915
Refinement method	Full-matrix least-squares on	Full-matrix least-squares on	Full-matrix least-squares on F^2
	F^2	F^2	
Data / restraints / parameters	5909 /0 / 344	5529 / 0 / 309	6231 / 0 / 354
Goodness-of-fit on F^2	0.978	1.011	1.04
Final *R* indices [*I*>2sigma(*I*)]	R_1 = 0.0347	R_1 = 0.0463	R_1 = 0.0682
	wR_2 = 0.0719	wR_2 = 0.1565	wR_2 = 0.2132
R indices (all data)	R_1 = 0.0552	R_1 = 0.0542	R_1 = 0.0826
	wR_2 = 0.0773	wR_2 = 0.1697	wR_2 = 0.2340
Largest diff. peak and hole (e·Å^{-3})	0.299 and -0.30	0.738 and -0.883	1.154 and -1.565

Table S2. Crystal data and collection parameters of complexes **3** and **4**

Identification code	**3**	**4**
Formula	$C_{48}H_{86}B_2N_{14}OP_2S_4Si_4Y_2$	$C_{47}H_{86}B_2N_{14}P_2O_2Si_4Y_2$
Formula weight	1377.28	1253.03
Temperature (K)	203(2)	203(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic
Space group	*P*2(1)/*c*	*P*2(1)/*c*
a (Å)	15.293(3)	18.2262(19)
b (Å)	38.01(6)	27.133(3)
c (Å)	17.798(3)	17.7123(19)
α (deg)	90	90
β (deg)	109.192(3)	113.322(2)
γ (deg)	90	90
V (Å ^{3})	9770(1)	8043.7(15)
Z	4	4
*D*c (g/m^3)	0.936	1.035
μ (mm^{-1})	1.380	1.572
F(000)	2872	2624
Crystal size (mm)	0.32 x 0.22 x 0.08	0.28 x 0.23 x 0.20
ϑ range (°)	1.071to 25.049	1.217 to 25.048
	-18<=h<=18	-21<=h<=21
h, k, l range	-45<=k<=37	-32<=k<=32
	-20<=l<=21	-19<=l<=21
Reflections collected / unique	58673 / 17248	48604 / 14238
	[*R*(int) = 0.0967]	[*R*(int) = 0.059]
Completeness to *ϑ*	99.7 % (*ϑ* = 25.10)	99.4% (*ϑ* = 25.10)
Max. and min. transmission	0.7456 and 0.5633	0.7456 and 0.6786
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	17248 / 1 / 716	14238 / 0 / 680
Goodness-of-fit on F^2	1.01	1.031
Final *R* indices [*I*>2sigma(I)]	R_1 = 0.0590	R_1 = 0.0433
	wR_2 = 0.1465	wR_2 = 0.1127
R indices (all data)	R_1 = 0.1136	R_1 = 0.0675
	wR_2 = 0.1580	wR_2 = 0.1198
Largest diff. peak and hole (e·Å^{-3})	1.063 and -0.355	0.408 and -0.384

Table S3. Crystal data and collection parameters of complexes **5** and **6**

Identification code	**5**	**6**
Formula	$C_{64}H_{102}B_2N_{16}O_2P_2S_2Si_4Y_2$	$C_{64}H_{102}B_2N_{16}O_4P_2Si_4Y_2$
Formula weight	1565.47	1533.35
Temperature (K)	173(2)	298(2)
Wavelength (Å)	0.71073	1.3414
Crystal system	Triclinic	Triclinic
Space group	*P*-1	*P*-1
a (Å)	12.934(6)	10.799(5)
b (Å)	13.333(6)	13.614(8)
c (Å)	14.362(7)	16.654(5)
α (deg)	90.678(8)	95.00(3)
β (deg)	101.070(8)	90.66(3)
γ (deg)	114.517(7)	106.51(3)
V (Å ^{3})	2199.9(18)	2336.9(18)
Z	1	1
Dc (g/m^3)	1.182	1.090
μ (mm^{-1})	1.496	1.879
F(000)	820	804
Crystal size (mm)	0.18 x 0.17 x 0.16	0. 2 x 0.05 x 0.03
ϑ range (°)	1.688 to 25.05	2.959 to 48.498
	-15<=h<=13	-12<=h<=12
h, k, l range	-15<=k<=15	-15<=k<=15
	-16<=l<=17	-18<=l<=18
Reflections collected / unique	12924 / 7597	47301 / 6566
	[*R*(int) = 0.0438]	[*R*(int) = 0.1858]
Completeness to *ϑ*	97.7 % (*ϑ* = 25.10)	96.4 % (*ϑ* = 48.5)
Max. and min. transmission	0.7456 and 0.5516	0.7519 and 0.3592
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	7597 / 18 / 435	6566 / 24 / 435
Goodness-of-fit on F^2	1.064	1.064
Final *R* indices [*I*>2sigma(*I*)]	R_1 = 0.1003	R_1 = 0.1277
	wR_2 = 0.3027	wR_2 = 0.3316
R indices (all data)	R_1 = 0.1334	R_1 = 0.1608
	wR_2 = 0.3413	wR_2 = 0.3577
Largest diff. peak and hole (e·Å^{-3})	1.960 and -1.025	1.049 and -1.531

Table S4. Crystal data and collection parameters of complexes **7**·**0.5C$_6$H$_{14}$** and **8**

Identification code	**7·0.5C$_6$H$_{14}$**	**8**
Formula	$C_{63}H_{101}B_2N_{16}O_3P_2Si_4Y_2$	$C_{74}H_{112}B_2N_{18}O_2P_2Si_4Y_2$
Formula weight	1504.33	1659.55
Temperature (K)	173(2)	203(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	Triclinic	Monoclinic
Space group	*P*-1	*P*2(1)/c
a (Å)	13.145(12)	14.031(2)
b (Å)	17.265(16)	13.510(2)
c (Å)	19.436(18)	28.504(5)
α (deg)	98.426(2)	90
β (deg)	106.504(2)	98.218(3)
γ (deg)	111.624(2)	90
V (Å ^{3})	3849.6(6)	5348(16)
Z	2	2
Dc (g/m^3)	1.298	1.031
μ (mm^{-1})	1.656	1.197
F(000)	1578	1744
Crystal size (mm)	0.40 x 0.30 x 0.28	0.32 x 0.28 x 0.26
ϑ range (°)	1.756 to 25.05	1.444to 25.05
h, k, l range	-15<=h<=15 -20<=k<=20 -16<=l<=23	-16<=h<=10 -16<=k<=15 -33<=l<=33
Reflections collected / unique	23151 / 13414 [R(int) = 0.0287]	31246 / 9423 [*R*(int) = 0.0356]
Completeness to *ϑ*	98.5 % (*ϑ* = 25.10)	99.6 % (*ϑ* = 25.10)
Max. and min. transmission	0.7456 and 0.6871	0.7456 and 0.6680
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	13414 / 0 / 852	9423 / 0 / 480
Goodness-of-fit on F^2	1.001	1.058
Final R indices [*I*>2sigma(*I*)]	R_1 = 0.0465 wR_2 = 0.1347	R_1 = 0.0514 wR_2 = 0.1868
R indices (all data)	R_1 = 0.0699 wR_2 = 0.1545	R_1 = 0.0637 wR_2 = 0.1999
Largest diff. peak and hole (e·Å^{-3})	0.863 and -0.571	0.826 and -0.351

Table S5. Crystal data and collection parameters of complexes **9** and **10**

Identification code	**9**	**10**
Formula	$C_{42}H_{78}B_2N_{14}P_2S_4Si_4Y_2$	$C_{46}H_{86}B_2N_{14}OP_2Se_3Si_4Y_2$
Formula weight	1281.16	1461.90
Temperature (K)	173(2)	173(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	Monoclinic	Triclinic
Space group	*P*2(1)/c	*P*-1
a (Å)	11.1809(12)	13.6391(14)
b (Å)	20.007(2)	14.3186(14)
c (Å)	18.356(2)	20.338(2)
α (deg)	90	78.382(2)
β (deg)	106.077(2)	77.425(2)
γ (deg)	90	87.151(2)
V (Å ^{3})	3945.6(7)	3797.2(7)
Z	2	2
*D*c (g/m^3)	1.078	1.279
μ (mm^{-1})	1.704	3.102
F(000)	1332	1488
Crystal size (mm)	0.16 x 0.14 x 0.10	0.50 x 0.32 x 0.29
ϑ range (°)	2.036 to 25.05	1.615 to 25.048
h, k, l range	-13<=h<=10 -23<=k<=23 -21<=l<=21	-16<=h<=16 -16<=k<=17 -24<=l<=21
Reflections collected / unique	23586 / 6947 [*R*(int) = 0.0591]	22793 / 13230 [R(int) = 0.0263]
Completeness to *ϑ*	99.3 % (*ϑ* = 25.10)	98.6 % (*ϑ* = 25.10)
Max. and min. transmission	0.7456 and 0.6564	0.7455 and 0.5269
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	6947 / 0 / 327	13252 / 0 / 689
Goodness-of-fit on F^2	1.029	1.013
Final *R* indices [*I*>2sigma(I)]	R_1 = 0.0460 wR_2 = 0.1430	R_1 = 0.0417 wR_2 = 0.1312
R indices (all data)	R_1 = 0.0706 wR_2 = 0.1545	R_1 = 0.0577 wR_2 = 0.1445
Largest diff. peak and hole (e·Å^{-3})	0.433 and -0.414	0.744 and -0.643

4. Molecular structures and important bond parameters of Complexes 1-10

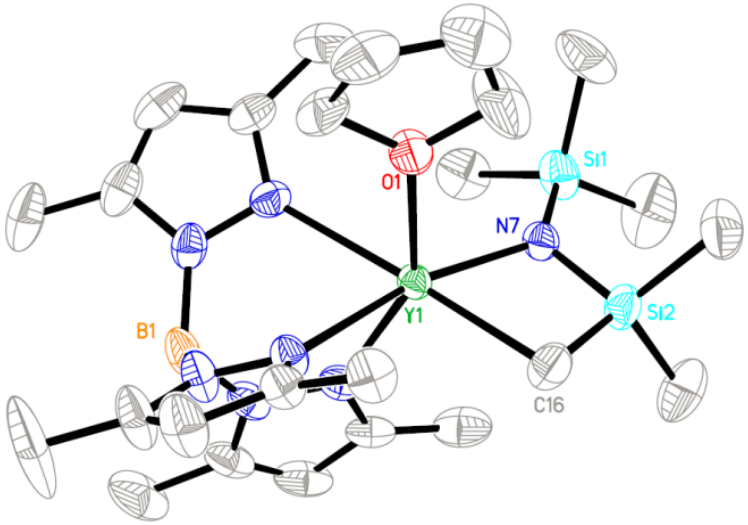


Figure S23. Molecular structure of **1** with ellipsoids set at 30% probability. All hydrogen atoms are omitted for clarity.

Table S6. Selected bond lengths (Å) and bond angles (°) of **1**

Bond length (Å)			
Y1-N7	2.241(3)	Si2-C16	1.788(6)
Y1-O1	2.348(3)	Si1-N7	1.683(4)
Y1-C16	2.402(5)	Si2-N7	1.743(4)
Bond Angle (°)			
N7-Y1-C16	72.13(17)	Si1-N7-Si2	127.9(2)
N7-Y1-O1	98.65(12)	Si1-N7-Y1	135.6(2)
Si2-C16-Y1	89.8(2)	N7-Si2-C16	101.6(2)
Si2-N7-Y1	96.44(16)		

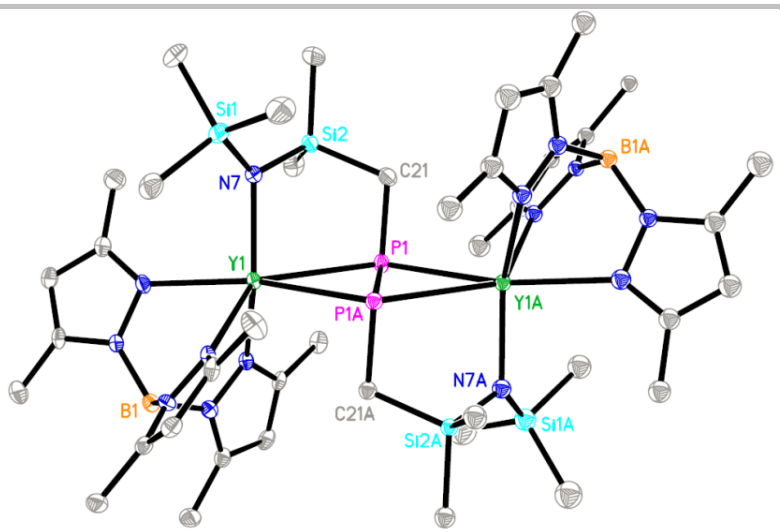


Figure S24. Molecular structure of **2** with ellipsoids set at 30% probability. All hydrogen atoms are omitted for clarity.

Table S7. Selected bond lengths (Å) and bond angles (°) of **2**

Bond length (Å)			
Y1-N7	2.252(4)	P1-C21	1.901(5)
Y1-P1	2.8874(12)	N7-Si1	1.706(4)
Y1-P1A	2.8349 (12)	N7-Si2	1.717(4)
P1-P1A	2.213(2)	Si2-C21	1.867(5)
Bond Angle (°)			
P1A-Y1-P1	45.48(4)	Y1A-P1-Y1	134.52(4)
N7-Y1-P1A	96.20(10)	C21-P1-Y1A	90.17(15)
N7-Y1-P1	83.84(10)	Si2-C21-P1	107.1(2)
P1A-P1-Y1	66.01(5)	Si1-N7-Si2	123.3(2)
P1A-P1-Y1A	68.51(5)	Si1-N7-Y1	120.8(2)
C21-P1-P1A	100.01(17)	Si2-N7-Y1	112.10(19)
C21-P1-Y1	97.49 (15)	N7-Si2-C21	109.4(2)

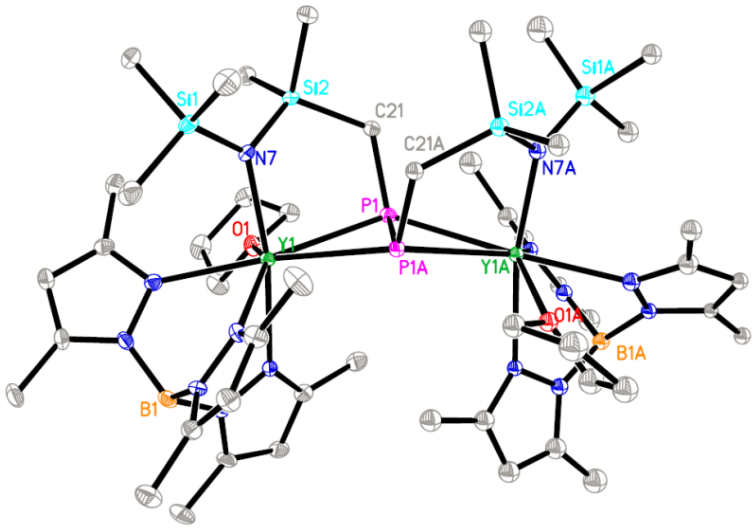


Figure S25. Molecular structure of **2·THF** with ellipsoids set at 30% probability. All hydrogen atoms are omitted for clarity.

Table S8. S Selected bond lengths (Å) and bond angles (°) of **2·THF**

Bond length (Å)			
Y1-O1	2.567(4)	P1-P1A	2.190(3)
Y1-N7	2.303(4)	P1-Y1A	2.9097(15)
Y1-P1	2.8501(14)	Si1-N7	1.720(4)
Y1-P1A	2.9097(15)	Si2-N7	1.712(4)
P1-C21	1.869(5)	Si2-C21	1.906(5)
Bond Angle (°)			
P1-Y1-P1A	44.69(5)	C21-P1-Y1	97.40(17)
N7-Y1-P1	86.71(11)	C21-P1-Y1A	115.85(18)
N7-Y1-P1A	88.43(11)	P1-C21-Si2	120.0(3)
C21-P1-P1A	105.47 (18)	Si2-N7-Si1	118.6(3)
P1A-P1-Y1	69.10(7)	Si2-N7-Y1	114.8(2)
P1A-P1-Y1A	66.22(7)	Si1-N7-Y1	126.5(2)
Y1-P1-Y1A	129.57(5)	N7-Si2-C21	113.4(2)

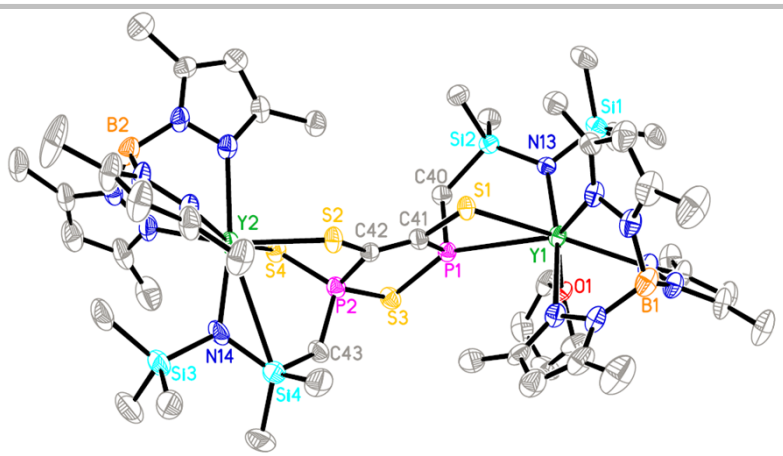


Figure S26. Molecular structure of **3** with ellipsoids set at 30% probability. All hydrogen atoms are omitted for clarity.

Table S9. Selected bond lengths (Å) and bond angles (°) of **3**

Bond length (Å)			
Y1-S1	2.8319(14)	P2-S4	1.999(2)
Y1-P1	3.1242(15)	P2-S3	2.100(2)
Y1-O1	2.364(4)	S1-C41	1.737(6)
Y1-N13	2.296(4)	S2-C42	1.749(5)
Y2-S2	2.7266(15)	C41-C42	1.332(6)
Y2-S4	2.8045(17)	Si1-N13	1.744(4)
Y2-N14	2.286(5)	Si2-N13	1.725(4)
P1-C41	1.790(6)	Si3-N14	1.729(4)
P1-C40	1.809(5)	Si4-N14	1.719(5)
P1-S3	2.157(2)	Si2-C40	1.895(5)
P2-C42	1.792(6)	Si4-C43	1.914(6)
P2-C43	1.800(5)		
Bond Angle (°)			
N13-Y1-S1	89.94(10)	C42-P2-S3	103.73(18)
S1-Y1-P1	56.78(4)	C43-P2-S3	104.6(2)
N14-Y2-S2	95.09(12)	S4-P2-S3	113.55(9)
N14-Y2-S4	97.31(13)	C41-S1-Y1	101.6(2)
S2-Y2-S4	84.89(4)	C42-S2-Y2	105.05(18)
C41-P1-C40	106.4(3)	P2-S3-P1	95.06(8)
C41-P1-S3	99.63(19)	P2-S4-Y2	91.41(7)
C40-P1-S3	103.74(18)	C42-C41-S1	129.1(5)
C41-P1-Y1	90.28(17)	C42-C41-P1	123.4(4)
C40-P1-Y1	99.17(17)	S1-C41-P1	107.5(3)
S3-P1-Y1	151.20(8)	C41-C42-S2	127.9(4)
C42-P2-C43	112.2(3)	C41-C42-P2	117.2(4)
C42-P2-S4	111.96(18)	S2-C42-P2	114.9(3)
C43-P2-S4	110.41(19)	P2-C43-Si4	126.8(4)

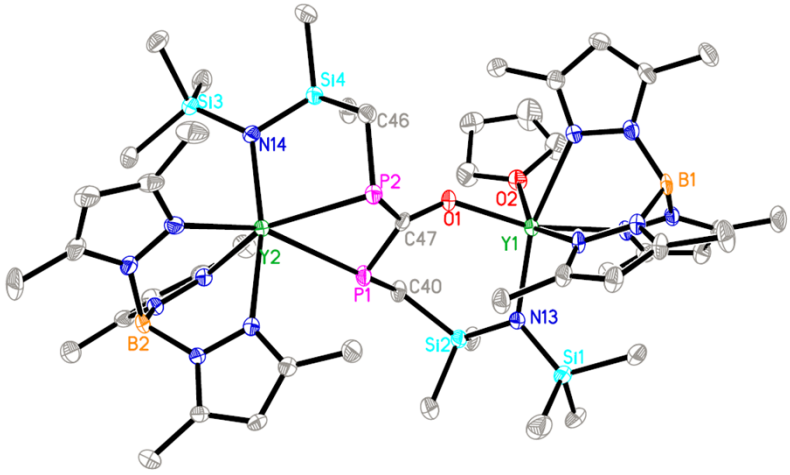


Figure S27. Molecular structure of **4** with ellipsoids set at 30% probability. All hydrogen atoms are omitted for clarity. Selected bond lengths (Å) and bond angles (°):

Table S10. Selected bond lengths (Å) and bond angles (°) of **4**

Bond length (Å)			
Y1-O1	2.153(2)	P2-C47	1.828(4)
Y1-N13	2.295(3)	P2-C46	1.877(4)
Y1-O2	2.405(3)	O1-C47	1.320(4)
Y2-N14	2.286(3)	Si1-N13	1.728(3)
Y2-P2	2.8306(10)	Si3-N14	1.715(3)
Y2-P1	2.9128(10)	Si2-N13	1.728(3)
P1-C47	1.713(4)	Si4-N14	1.730(3)
P1-C40	1.847(4)		
Bond Angle (°)			
O1-Y1-N13	101.03(9)	P1-C40-Si2	121.2(2)
O1-Y1-O2	88.80(9)	Si4-C46-P2	117.2(2)
N13-Y1-O2	109.84(10)	O1-C47-P1	124.7(3)
N14-Y2-P2	86.77(7)	O1-C47-P2	122.2(3)
N14-Y2-P1	110.07(7)	P1-C47-P2	113.08(19)
P2-Y2-P1	61.91(3)	Si2-N13-Si1	114.92(17)
C47-P1-C40	105.22(17)	Si2-N13-Y1	118.36(15)
C47-P1-Y2	87.62(11)	Si1-N13-Y1	126.57(15)
C40-P1-Y2	148.37(12)	Si3-N14-Si4	119.31(17)
C47-P2-C46	100.61(17)	Si3-N14-Y2	125.12(15)
C47-P2-Y2	88.07(12)	Si4-N14-Y2	114.96(14)
C46-P2-Y2	97.08(11)	N13-Si2-C40	115.51(16)
C47-O1-Y1	138.4(2)	N14-Si4-C46	111.04(16)

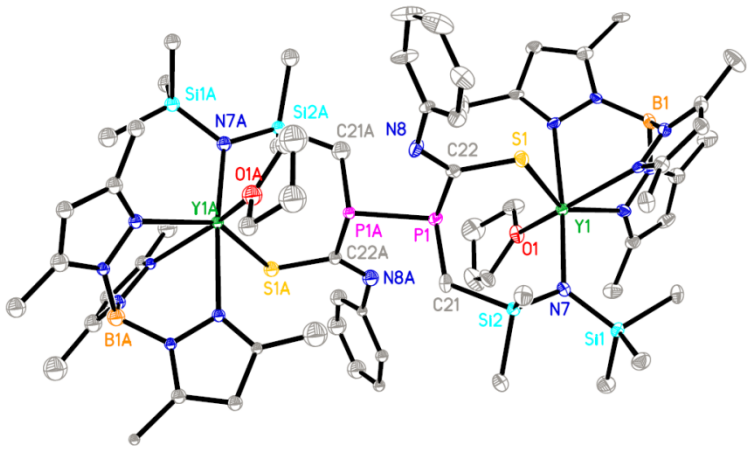


Figure S28. Molecular structure of **5** with ellipsoids set at 30% probability. All hydrogen atoms are omitted for clarity.

Table S11. Selected bond lengths (Å) and bond angles (°) of **5**

Bond length (Å)			
Y1-S1	2.742(3)	Si1-N7	1.723(8)
Y1-O1	2.368(6)	Si2-N7	1.701(7)
Y1-N7	2.321 (8)	Si2-C21	1.882(9)
P1-C21	1.827(11)	S1-C22	1.724(8)
P1-C22	1.842(9)	N8-C22	1.251(11)
P1-P1A	2.235(4)		
Bond Angle (°)			
S1-Y1-N7	91.7(2)	Si2-N7-Y1	121.2(4)
C21-P1-C22	103.6(4)	P1-C21-Si2	123.2(5)
C21-P1-P1A	100.6(3)	N8-C22-S1	128.9(7)
C22-P1-P1A	99.5(3)	N8-C22-P1	118.3(7)
C22-S1-Y1	108.2(3)	S1-C22-P1	112.4(4)

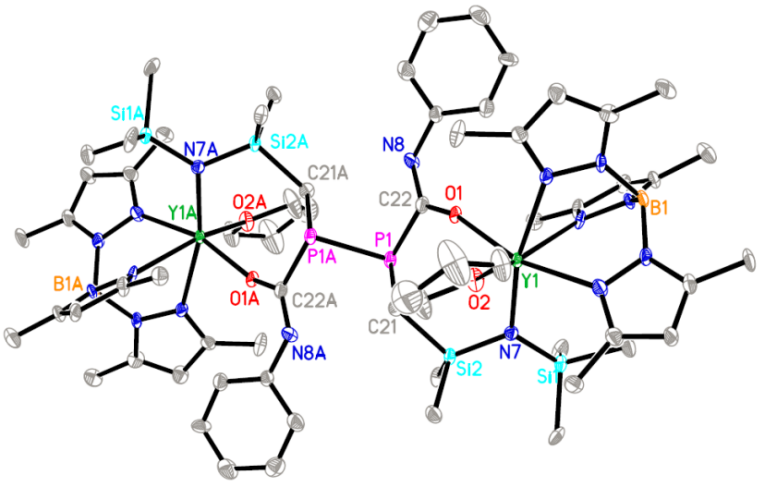


Figure S29. Molecular structure of **6** with ellipsoids set at 30% probability. All hydrogen atoms are omitted for clarity.

Table S12. Selected bond lengths (Å) and bond angles (°) of **6**

Bond length (Å)			
Y1-O2	2.409(7)	Si1-N7	1.715(9)
Y1-O1	2.117(7)	Si2-N7	1.716(9)
Y1-N7	2.279(9)	Si2-C21	1.898(11)
P1-C21	1.826(11)	O1-C22	1.305(13)
P1-C22	1.851(12)	N8-C22	1.305(15)
P1-P1A	2.209(5)		
Bond Angle (°)			
O1-Y1-N7	100.9(3)	Si2-N7-Y1	115.5(4)
C21-P1-C22	99.5(5)	P1-C21-Si2	115.0(6)
C21-P1-P1A	100.2(4)	N8-C22-O1	128.1(10)
C22-P1-P1A	98.8(4)	N8-C22-P1	115.1(8)
C22-O1-Y1	153.1(7)	O1-C22-P1	116.7(8)

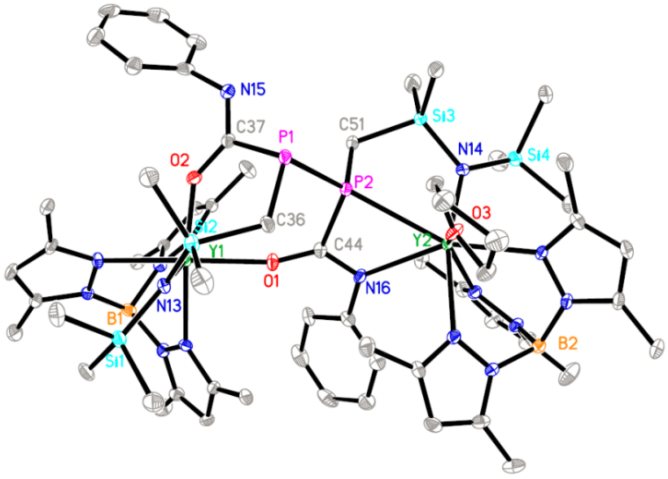


Figure S30. Molecular structure of **7** with ellipsoids set at 30% probability. All hydrogen atoms are omitted for clarity.

Table S13. Selected bond lengths (Å) and bond angles (°) of **7**

Bond length (Å)			
Y1-O1	2.227(3)	P2-C44	1.870(5)
Y1-O2	2.172(3)	O1-C44	1.262(6)
Y1-N13	2.299(4)	O2-C37	1.318(6)
Y2-O3	2.498(4)	N16-C44	1.332(6)
Y2-N16	2.552(4)	N15-C37	1.261(7)
Y2-P2	2.9417(14)	N16-C44	1.332(6)
P1-C36	1.847(6)	Si1-N13	1.718(4)
P1-C37	1.874(5)	Si2-N13	1.717(4)
P1-P2	2.1946 (19)	Si3-N14	1.726(4)
P2-C51	1.848(6)	Si4-N14	1.743(5)
Bond Angle (°)			
O2-Y1-O1	86.18(13)	C44-O1-Y1	162.8(3)
O2-Y1-N13	90.81(14)	C37-O2-Y1	144.6(3)
O1-Y1-N13	104.60(14)	C44-N16-Y2	111.0(3)
N14-Y2-N16	104.90(15)	N16-C44-P2	108.2(4)
N14-Y2-P2	81.72(11)	P1-C36-Si2	122.4(3)
N16-Y2-P2	56.25(9)	P2-C51-Si3	111.0(3)
C36-P1-P2	97.14(19)	N15-C37-O2	128.4(5)
C37-P1-P2	103.55(17)	N15-C37-P1	111.3(4)
C36-P1-C37	107.3(2)	O2-C37-P1	120.1(4)
C51-P2-C44	104.9(2)	O1-C44-N16	128.5(5)
C51-P2-P1	108.76(18)	O1-C44-P2	123.3(4)
C44-P2-P1	108.79(17)	N16-C44-P2	108.2(4)
C51-P2-Y2	98.08(17)	Si2-N13-Si1	118.2(2)
C44-P2-Y2	82.56(16)	Si3-N14-Si4	114.5(2)
P(1)-P(2)-Y(2)	146.29(7)		

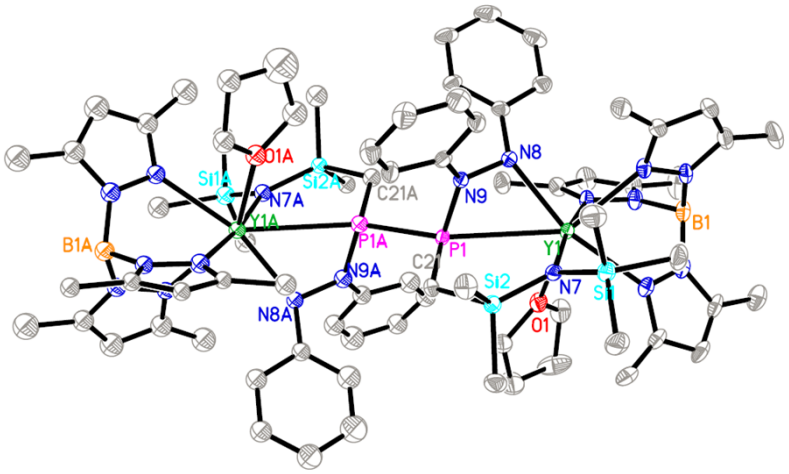


Figure S31. Molecular structure of **8** with ellipsoids set at 30% probability. All hydrogen atoms are omitted for clarity.

Table S14. Selected bond lengths (Å) and bond angles (°) of **8**

Bond length (Å)			
Y1-N7	2.317(3)	P1-P1A	2.2955(18)
Y1-N8	2.342(3)	Si1-N7	1.740(3)
Y1-O1	2.501(3)	Si2-N7	1.724(3)
Y1-P1	3.1503(10)	Si2-C21	1.906(4)
P1-N9	1.699(3)	N8-N9	1.442(4)
P1-C21	1.820(4)	N9-C28	1.399(5)
Bond Angle (°)			
N7-Y1-N8	96.49(11)	P1A-P1-Y1	157.13(6)
N7-Y1-P1	77.30(8)	P1-C21-Si2	117.2(2)
N8-Y1-P1	53.95(8)	N7-Si2-C21	115.18(16)
N9-P1-C21	105.37(17)	Si2-N7-Si1	113.12(19)
N9-P1-P1A	106.88(12)	Si2-N7-Y1	125.65(16)
C21-P1-P1A	101.89(13)	Si1-N7-Y1	121.13(16)
N9-P1-Y1	71.84(11)	N9-N8-Y1	106.4(2)
C21-P1-Y1	100.37(12)	N8-N9-P1	111.1(2)

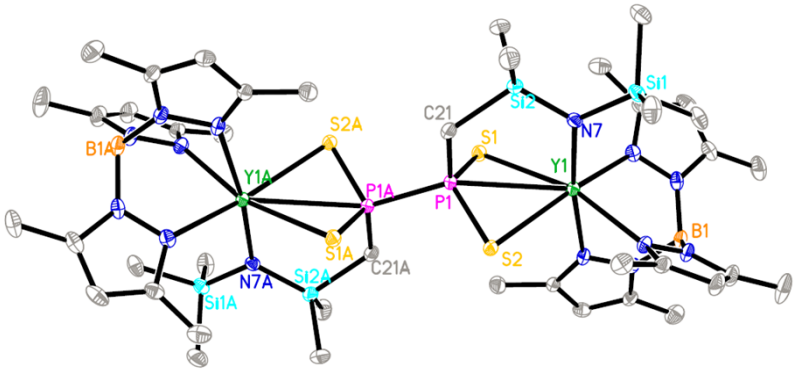


Figure S32. Molecular structure of **9** with ellipsoids set at 30% probability. All hydrogen atoms are omitted for clarity.

Table S15. Selected bond lengths (Å) and bond angles (°) of **9**

Bond length (Å)			
Y1-N7	2.275(4)	P1-S1	2.0097(17)
Y1-S2	2.7847(13)	P1-P1A	2.211(2)
Y1-S1	2.8120(13)	Si1-N7	1.728(4)
Y1-P1	3.1365(12)	Si2-N7	1.722(4)
P1-C21	1.777(5)	Si2-C21	1.932(5)
P1-S2	2.0041(16)		
Bond Angle (°)			
N7-Y1-S2	95.02(10)	C21-P1-Y1	99.59(15)
N7-Y1-S1	91.81(10)	S2-P1-Y1	60.98(4)
S2-Y1-S1	73.46(4)	S1-P1-Y1	61.74(4)
N7-Y1-P1	80.11(9)	P1A-P1-Y1	153.83(8)
S2-Y1-P1	39.00(3)	P1-S1-Y1	79.25(5)
S1-Y1-P1	39.01(3)	P1-S2-Y1	80.03(5)
C21-P1-S2	110.30(17)	P1-C21-Si2	116.3(3)
C21-P1-S1	110.62(18)	Si2-N7-Si1	116.1(2)
S2-P1-S1	113.01(7)	Si2-N7-Y1	121.83(19)
C21-P1-P1A	106.56(17)	Si1-N7-Y1	121.86(19)
S2-P1-P1A	107.59(8)	N7-Si2-C21	114.91(19)
S1-P1-P1A	108.49(9)		

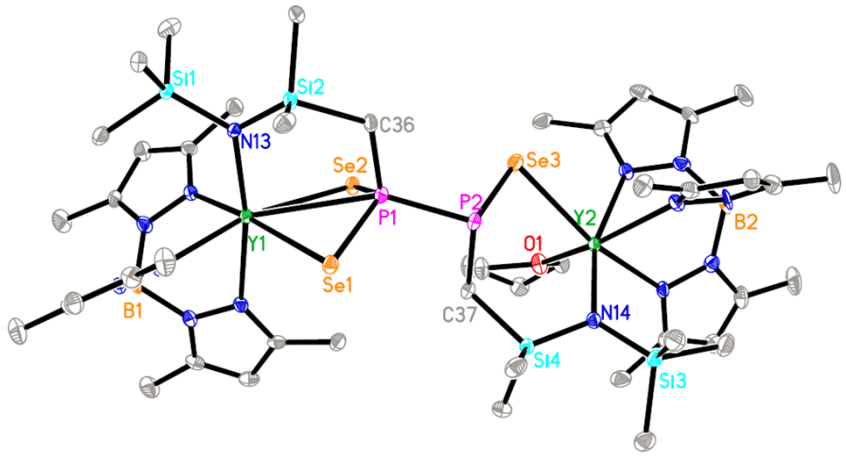


Figure S33. Molecular structure of **10** with ellipsoids set at 30% probability. All hydrogen atoms are omitted for clarity.

Table S16. Selected bond lengths (Å) and bond angles (°) of **10**

Bond length (Å)			
Y1-N13	2.272(4)	P1-Se1	2.2008(14)
Y1-Se1	2.8738(7)	P1-P2	2.2089(19)
Y1-Se2	2.8867(7)	P2-C37	1.835(5)
Y1-P1	3.2272(14)	P2-Se3	2.2292(14)
Y2-N14	2.265(4)	Si2-C36	1.919(5)
Y2-O1	2.397(3)	Si4-C37	1.887(5)
Y2-Se3	2.8539(8)	Si2-N13	1.715(4)
P1-C36	1.803(5)	Si4-N14	1.707(4)
P1-Se2	2.1837(14)		
Bond Angle (°)			
N13-Y1-Se1	92.57(10)	C36-P1-Y1	96.03(17)
N13-Y1-Se2	95.93(11)	Se2-P1-Y1	60.92(3)
Se1-Y1-Se2	78.557(19)	Se1-P1-Y1	60.48(3)
N13-Y1-P1	80.59(11)	P2-P1-Y1	154.95(7)
Se1-Y1-P1	41.79(3)	C37-P2-P1	97.12(17)
Se2-Y1-P1	41.38(3)	C37-P2-Se3	103.70(17)
N14-Y2-Se3	105.65(11)	P1-P2-Se3	101.08(6)
C36-P1-Se2	107.27(19)	P1-Se1-Y1	77.73(4)
C36-P1-Se1	109.08(18)	P1-Se2-Y1	77.70(4)
Se2-P1-Se1	112.56(6)	P2-Se3-Y2	95.20(4)
C36-P1-P2	107.88(18)	P1-C36-Si2	118.6(3)
Se2-P1-P2	116.43(7)	P2-C37-Si4	114.9(3)
Se1-P1-P2	103.38(6)		

5. Computational Details

All DFT calculations were performed with Gaussian 09.[6] Geometries were fully optimized in gas phase without symmetry constraints, employing the B3PW91 functional[7] and the Stuttgart effective core potential for Y[8] and Si[9] augmented with a polarization functions (ζ_f = 1.000 for Y and ζ_d = 0.284 for Si). For the other elements (H, P, C, N, O, B and S), Pople's double-ζ basis set 6-31G(d,p) [10] was used. Calculations of vibrational frequencies were systematically done in order to characterize the nature of stationary points. The electron density and partial charge distribution were examined in terms of localized electron-pair bonding units using the NBO program[11] available in Gaussian 09.

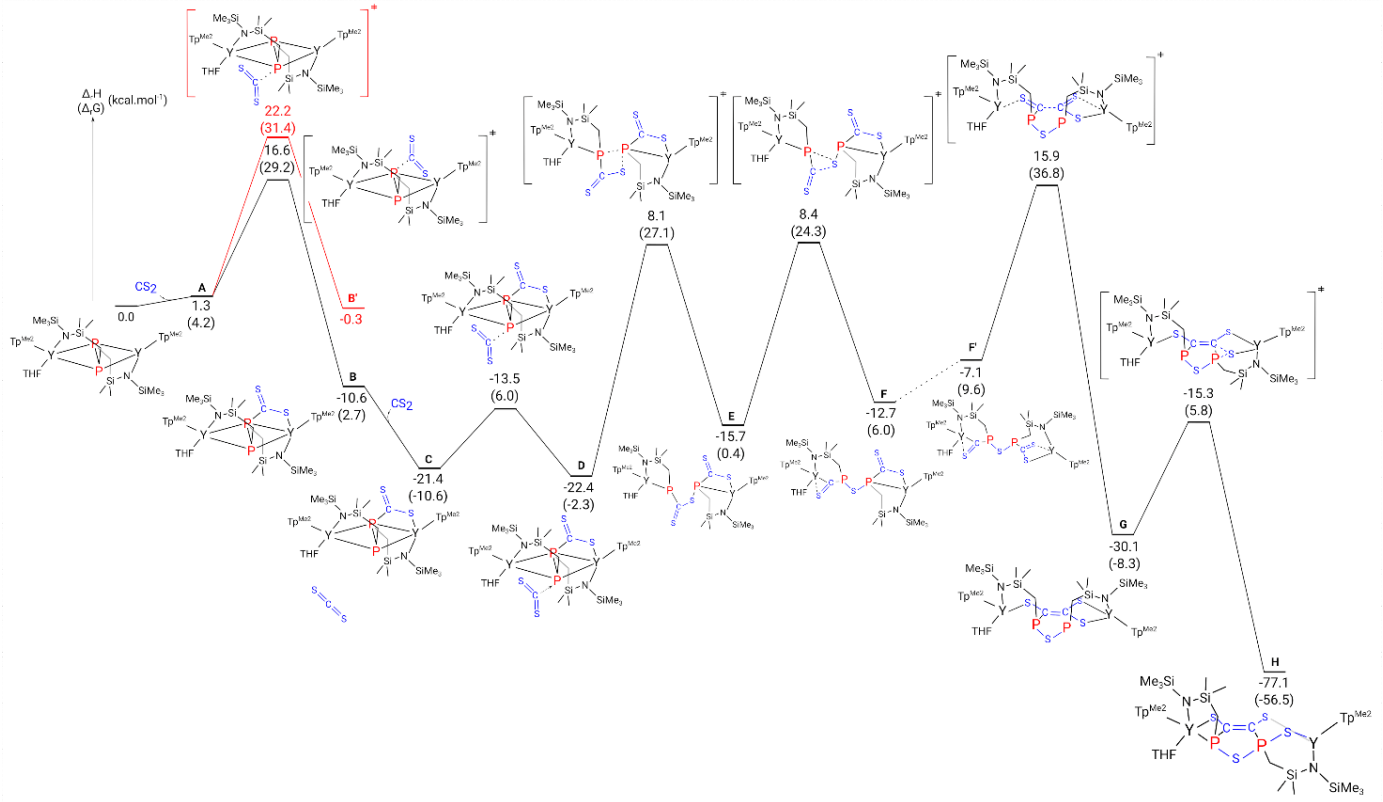


Figure S34. Computed (DFT) Gibbs Free energy pathway at room temperature

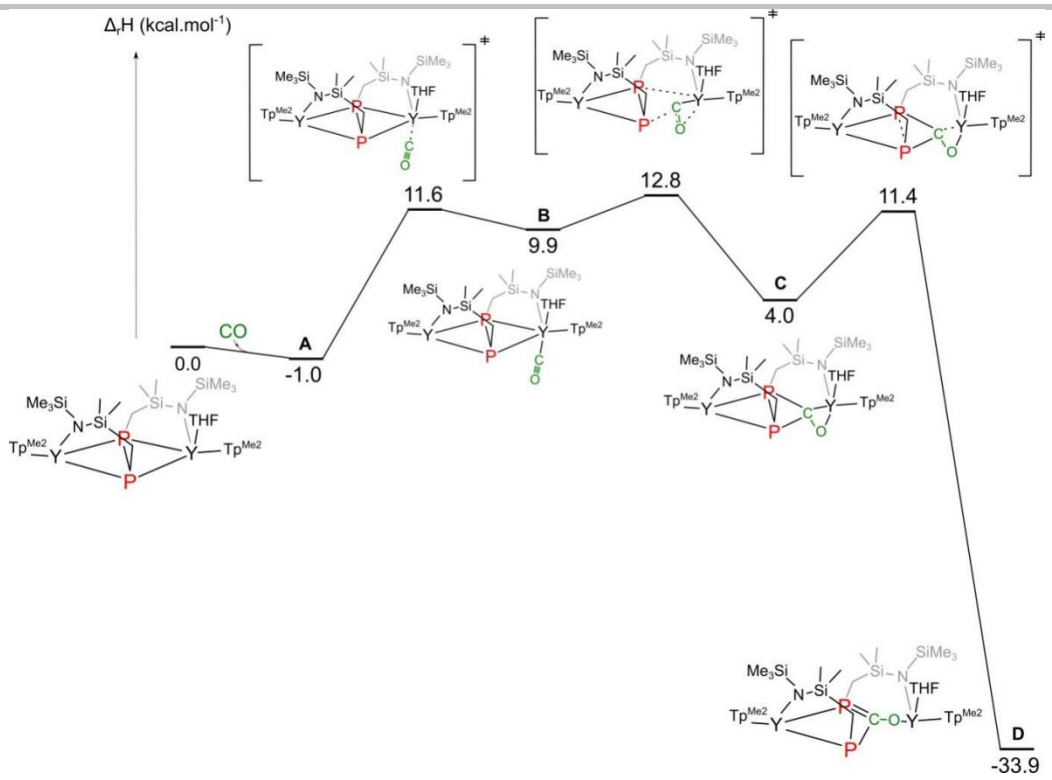


Figure S35. Computed enthalpy profile for the CO insertion reaction

Cartesian coordinates of all optimized structures

2
CO
C -0.99845 -0.42113 -2.23926
O -0.45507 -0.68047 -3.20376
157
CO insertion Y Dimer
C -2.33986 -2.54625 -1.24099
N -2.71743 -1.25926 -1.36408
N -3.61119 -1.20220 -2.39638
C -3.80465 -2.43910 -2.91227
C -3.00665 -3.32001 -2.19758
Y -2.40675 0.66862 0.10718
Si -2.45654 -0.21240 3.45921
C -2.12730 -1.81201 4.44434
B -4.18501 0.12961 -2.93184
N -5.14882 0.79202 -1.92416
N -4.76760 1.08562 -0.65308
C -5.82712 1.64361 -0.04568
C -6.89743 1.72504 -0.94757
C -6.43380 1.16980 -2.13094
C -5.81611 2.05612 1.38963
C -7.16832 0.98900 -3.41854
C -4.73431 -2.74509 -4.04032
C -1.33339 -3.02034 -0.24725
N -3.32897 -0.38536 1.93972
Si -4.63610 -1.58545 1.99707
C -5.83031 -1.61446 0.52050
O -2.91838 3.06375 0.66863
C -2.57374 3.70292 1.91470
C -2.42975 5.17850 1.58283
C -3.52730 5.35992 0.53243
C -3.46096 4.05286 -0.25188

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N	-3.04907	1.10311	-3.29748
C	-2.74915	1.57060	-4.53404
C	-1.74616	2.51186	-4.38514
C	-1.47514	2.56454	-3.00997
C	-3.41073	1.11580	-5.79376
C	-0.46308	3.45949	-2.37180
C	-5.76881	-1.35260	3.52094
C	-4.03350	-3.39776	2.05127
C	-0.70260	0.47775	3.13308
P	0.02746	-0.17123	1.52167
P	0.39403	1.55265	0.19749
C	1.14864	3.03618	1.09158
Si	2.61543	2.86146	2.32414
C	3.52139	4.53596	2.18154
Y	2.70265	-0.06987	0.57902
N	3.62154	1.47705	1.92863
Si	5.22101	1.37474	2.67756
C	5.94484	-0.37985	2.64155
N	3.36779	-2.18797	1.51747
C	3.23087	-2.72371	2.74177
C	4.02106	-3.87432	2.83625
C	4.64757	-4.00557	1.60430
N	4.23980	-2.97615	0.82491
C	2.37365	-2.10312	3.79290
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N	3.26717	-2.69253	-1.51751
N	2.41823	-1.62283	-1.46176
C	1.57878	-1.73941	-2.50078
C	1.86903	-2.91205	-3.21697
C	2.94740	-3.48900	-2.56952
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C	5.54748	0.70388	-1.32292
C	7.41091	-2.40755	-1.99663
C	5.14298	2.14093	-1.38242
C	1.89506	2.82260	4.08458
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H	6.22224	1.66986	4.93607

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H 2.81805 5.35635 2.36934
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CO coordination adduct
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O -2.97742 3.05373 0.64029
C -2.57508 3.71275 1.85772
C -2.41507 5.17627 1.48417
C -3.55788 5.35744 0.48323
Y -2.45125 0.65824 0.10497
N -3.32329 -0.38878 1.96643
Si -2.42588 -0.18522 3.46704
C -0.67897 0.50365 3.10006
P 0.02145 -0.14028 1.47429
P 0.34172 1.58064 0.13440
C 1.12469 3.07112 0.99387
Si 2.60026 2.90518 2.21734
N 3.60243 1.51645 1.82564
Si 5.19992 1.40922 2.57961
C 6.52092 2.50428 1.74911
Y 2.66581 -0.02433 0.47793
N 3.32501 -2.12700 1.43961
N 4.16321 -2.95236 0.75005
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C 3.18369 -2.63912 2.67279
B 4.49397 -2.73374 -0.74618
N 3.20659 -2.67160 -1.59773
N 2.35583 -1.60374 -1.53479
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N 4.73411 -0.20580 -0.83234
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N 5.30529 -1.43062 -1.00210
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C 7.38247 -2.44187 -1.99944
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N -2.76828 -1.29079 -1.33731
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C	-4.83046	-2.83404	-3.94562
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H	1.27112	-3.27868	-4.14907
H	0.49220	0.12184	-2.16249
H	-0.54356	-1.13467	-2.85333
H	0.62164	-0.29661	-3.87838
H	5.05116	-5.65415	0.27455
H	5.63436	-5.75972	1.94217
H	6.43694	-4.68853	0.78520
H	4.03675	-4.45340	3.64141
H	2.54505	-2.43452	4.69580
H	1.27517	-2.11372	3.49667
H	2.53513	-0.91430	3.77928
H	7.63992	-3.03853	-1.11936

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H 6.91913 -3.11291 -2.72944
H 7.51822 0.50433 -2.41850
H 4.53116 2.32967 -2.34466
H 6.04971 2.77704 -1.55846
H 4.61581 2.44570 -0.57206
H -2.94626 4.05454 -1.16728
H -4.56248 3.68490 -0.54411
H -4.50458 5.50971 1.01343
H -3.41148 6.20545 -0.19096
H -1.44556 5.34175 1.00231
H -2.48735 5.83813 2.35132
H -1.65736 3.23658 2.20710
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H -4.17957 0.62882 5.09360
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H -1.52454 -1.47316 5.38357
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H 6.94131 -0.29566 2.94741
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H 1.43229 1.92559 4.22445
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H 2.67254 3.08362 4.72268
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159
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N 5.84187 -1.34326 -0.67439
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C 6.72771 0.28783 -1.88502
Y 2.83346 -0.54154 0.46832
N 3.11220 -2.79536 -0.85367
N 4.35778 -3.34911 -0.89206
C 4.35999 -4.47225 -1.65059
C 3.07104 -4.65529 -2.11850
C 2.32621 -3.58854 -1.59364

B	5.51840	-2.74722	-0.09047
N	5.13382	-2.73902	1.41429
N	4.02304	-2.09896	1.87443
C	3.88387	-2.41151	3.17046
C	4.91917	-3.27074	3.55454
C	5.69408	-3.45775	2.41612
C	2.76453	-1.85948	3.99015
C	6.92916	-4.28354	2.26727
C	0.87523	-3.33236	-1.78811
C	5.56877	-5.31454	-1.89449
C	8.25852	-1.71469	-1.26801
C	4.56825	1.75909	-2.00398
P	0.02679	-0.84648	0.98722
P	0.41631	0.83715	-0.40960
C	1.02959	2.41005	0.44506
Si	2.33765	2.52239	1.83767
C	1.52087	2.53689	3.55905
Y	-2.53709	0.44833	-0.27133
N	-2.59153	1.83864	-2.56567
N	-3.64615	1.60984	-3.40385
C	-3.44984	2.21312	-4.60090
C	-2.23036	2.86444	-4.53820
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C	-6.66401	2.23099	-1.57671
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C	-7.58963	2.49555	-2.71847
C	-4.40651	2.15052	-5.74632
C	-0.41836	3.09511	-2.73552
N	-3.64877	-1.04159	-1.85489
C	-3.57752	-2.37741	-1.96957
C	-4.53888	-2.82035	-2.88602
C	-5.18942	-1.67891	-3.32972
N	-4.63314	-0.61788	-2.69609
C	-2.54784	-3.18756	-1.26223
C	-6.30955	-1.57840	-4.31202
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Si	-4.92449	-1.60981	1.66431
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O	-2.43802	2.83847	0.66564
C	-2.15075	3.27096	2.01956
C	-2.19411	4.79455	1.99548
C	-3.18195	5.07800	0.86292
C	-2.84003	3.98354	-0.13398
C	-0.80437	-0.57144	-2.95731
O	-0.30274	-0.44561	-3.97329
Si	-2.39997	-0.81633	2.96774
C	-2.97281	0.17894	4.49691
C	-2.09422	-2.59701	3.57023
C	-0.66780	-0.13680	2.58481
C	-6.33008	-1.16377	0.46749
C	-5.74384	-1.48970	3.38926
C	2.97254	4.31171	1.60853
N	3.54006	1.25829	1.63893
Si	5.13237	1.62345	2.33338
C	5.02122	2.36312	4.09052
C	6.27779	0.12924	2.53833

C	6.14337	2.84549	1.27662
H	-5.73559	0.95780	-3.81140
H	6.49262	-3.43066	-0.21719
H	-4.59012	1.12051	-6.06722
H	-3.98862	2.69727	-6.59494
H	-5.37622	2.59468	-5.50128
H	-1.76161	3.44670	-5.31885
H	-0.41794	3.18832	-1.65071
H	-0.18365	4.06819	-3.17896
H	0.39143	2.40348	-2.99277
H	-8.45406	3.05873	-2.35891
H	-7.95408	1.56945	-3.17317
H	-7.10955	3.08211	-3.50808
H	-7.64394	3.12944	0.18952
H	-5.13807	3.14857	2.21325
H	-4.62932	1.43535	2.14801
H	-6.32222	1.86650	2.42561
H	-7.19783	-1.11752	-3.86936
H	-6.58265	-2.58045	-4.65066
H	-6.03520	-0.98662	-5.19064
H	-4.73612	-3.83890	-3.18816
H	-1.69557	-3.35598	-1.92504
H	-2.94738	-4.16469	-0.98101
H	-2.17800	-2.69265	-0.35933
H	6.37149	-4.74732	-2.37625
H	5.30394	-6.14694	-2.55061
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H	2.71471	-5.45664	-2.75007
H	0.48974	-2.61987	-1.05451
H	0.31782	-4.26711	-1.67419
H	0.67246	-2.94863	-2.79356
H	6.78503	-5.11418	1.56931
H	7.20288	-4.70279	3.23818
H	7.77355	-3.69065	1.90371
H	5.09007	-3.69815	4.53217
H	2.89089	-2.13096	5.04098
H	1.79761	-2.24515	3.64992
H	2.73409	-0.76671	3.91881
H	8.58883	-1.93277	-0.24800
H	9.04234	-1.13475	-1.76058
H	8.16228	-2.66995	-1.79345
H	7.42419	0.88921	-2.45156
H	3.75555	1.46814	-2.67881
H	5.18784	2.49751	-2.51817
H	4.12468	2.23774	-1.12440
H	-1.99583	4.27475	-0.76602
H	-3.66989	3.67165	-0.76721
H	-4.21540	4.97734	1.20893
H	-3.06528	6.07515	0.42964
H	-1.20734	5.20323	1.75135
H	-2.50228	5.20943	2.95885
H	-1.17595	2.87758	2.31092
H	-2.91185	2.85030	2.68134
H	-6.81340	-0.21241	0.70045
H	-7.08299	-1.95620	0.56655
H	-6.00612	-1.13826	-0.57466
H	-5.15753	-1.96566	4.18113
H	-6.70987	-2.00724	3.34453
H	-5.93560	-0.45392	3.68617
H	-5.45837	-4.03485	1.90075
H	-3.70818	-3.85589	1.69944

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H -0.66951 0.95503 2.54396
H -0.01368 -0.39969 3.42509
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H 7.22709 0.50360 2.94118
H 6.49106 -0.36483 1.58816
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H 7.09091 3.06204 1.78488
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H 3.42522 4.45618 0.62209
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159
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Y -2.52986 0.43625 -0.33300
Si -2.40714 -0.87818 2.91744
C -2.06274 -2.66521 3.48067
B -4.97487 0.95340 -2.95419
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C -6.66878 2.30222 -1.53102
C -5.39094 2.07212 1.90514
C -7.60313 2.61910 -2.65216
C -6.42796 -1.44843 -4.36781
C -2.62349 -3.18294 -1.43890
N -3.41442 -0.71460 1.47944
Si -4.90592 -1.67787 1.58317
C -6.32388 -1.19529 0.41539
O -2.41492 2.82016 0.65509
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C -2.24850 4.77077 2.00858
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C -2.80173 3.96708 -0.14652
C -1.00192 -0.42510 -2.24009
O -0.45631 -0.68871 -3.21141
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N -3.69331 1.66271 -3.43348
C -3.50033 2.25923 -4.63432
C -2.26091 2.87460 -4.59473
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C	-4.47885	2.22693	-5.76234
C	-0.41282	3.05647	-2.82092
C	-5.72415	-1.61631	3.31301
C	-4.65315	-3.54244	1.23958
C	-0.68720	-0.13875	2.58896
P	0.06098	-0.78621	0.99546
P	0.48844	0.90869	-0.36182
C	1.04754	2.49442	0.48648
Si	2.36814	2.56934	1.86850
C	2.99566	4.36645	1.68527
Y	2.87267	-0.52624	0.50578
N	3.56988	1.30912	1.63048
Si	5.17593	1.68663	2.28802
C	6.34369	0.20460	2.45493
N	4.07976	-2.04893	1.93230
C	3.96788	-2.32689	3.23881
C	5.01207	-3.17476	3.62367
C	5.76271	-3.39217	2.47412
N	5.18059	-2.70110	1.46542
C	2.86287	-1.75554	4.06513
B	5.52785	-2.75535	-0.04858
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C	4.32806	-4.53958	-1.50323
C	6.99462	-4.22188	2.32114
C	0.83587	-3.41698	-1.59437
C	5.53085	-5.39017	-1.74830
N	4.86886	-0.43645	-0.86752
N	5.84332	-1.36990	-0.67932
C	6.97534	-0.98261	-1.31623
C	6.71677	0.23580	-1.93238
C	5.38464	0.53952	-1.62725
C	8.24461	-1.76890	-1.31577
C	4.56505	1.72030	-2.03401
C	1.55780	2.51751	3.59060
C	-3.01126	0.07228	4.46373
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C	5.10126	2.40578	4.05589
H	-5.80552	1.06918	-3.80812
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H	-4.69036	1.20391	-6.08846
H	-4.06463	2.77187	-6.61395
H	-5.43401	2.68956	-5.49562
H	-1.79119	3.44496	-5.38356
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H	-0.15732	4.02101	-3.27116
H	0.37547	2.34311	-3.08546
H	-8.44850	3.19307	-2.26529
H	-7.99661	1.71449	-3.12577
H	-7.12001	3.21480	-3.43300
H	-7.61757	3.15043	0.27618
H	-5.11991	3.06424	2.28104
H	-4.59983	1.35699	2.13963
H	-6.29239	1.76499	2.44550
H	-7.30139	-0.98613	-3.89792
H	-6.72170	-2.43726	-4.72741
H	-6.16003	-0.83821	-5.23583
H	-4.85253	-3.75663	-3.34434
H	-1.76263	-3.29653	-2.10426

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H	-2.27093	-2.74746	-0.49962
H	6.31838	-4.84182	-2.27480
H	5.24839	-6.24760	-2.36358
H	5.96270	-5.77129	-0.81745
H	2.65062	-5.57973	-2.49741
H	0.45132	-2.71999	-0.84509
H	0.28916	-4.35930	-1.49200
H	0.62074	-3.01484	-2.58977
H	6.83475	-5.07275	1.65157
H	7.29127	-4.61224	3.29732
H	7.82970	-3.63988	1.92047
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H	3.00610	-2.00449	5.11931
H	1.89009	-2.14843	3.75055
H	2.83117	-0.66454	3.97142
H	8.59882	-1.96674	-0.29965
H	9.01993	-1.20610	-1.84056
H	8.12800	-2.73474	-1.81713
H	7.40632	0.82226	-2.52255
H	3.75640	1.42649	-2.71234
H	5.18548	2.45991	-2.54551
H	4.11516	2.19767	-1.15696
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H	-3.59607	3.64789	-0.82027
H	-4.24983	4.89875	1.15983
H	-3.11090	6.04455	0.43250
H	-1.26895	5.21453	1.79920
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H	-5.13642	-2.11237	4.09143
H	-6.68519	-2.14106	3.24833
H	-5.92726	-0.59237	3.64165
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H	-1.40162	-2.64323	4.35548
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H	-0.72532	0.95304	2.57502
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H	6.37128	2.48178	0.23510
H	7.10428	3.15021	1.69699
H	5.62153	3.86725	1.05119
H	4.59803	3.37453	4.12482
H	6.12428	2.54319	4.42603
H	4.59506	1.71305	4.73715
H	3.73848	4.65390	2.43455
H	2.14092	5.04556	1.79655
H	3.42718	4.54125	0.69428
H	1.10186	1.54927	3.80839

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159
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C	-4.54394	-2.55527	-3.36596
C	-3.58060	-2.07868	-2.46833
C	-2.36392	-2.78449	-1.97482
C	-6.62136	-1.46094	-4.46248
C	-0.54045	0.28827	1.80726
Si	-2.01363	-0.72378	2.48391
C	-2.51104	0.13140	4.11804
C	-1.33949	-2.43244	2.96184
C	-4.05922	-3.69500	1.00825
C	-6.15069	-1.59812	0.49055
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Si	5.25624	1.73121	2.35997
C	6.56776	2.72537	1.39791
C	3.46452	4.45736	0.88046
C	4.99415	2.66878	4.00324
C	6.14232	0.13072	2.86312
H	-6.39693	1.07244	-3.65915
H	6.36932	-3.96108	0.30793
H	-5.49907	1.68898	-5.97643
H	-5.07421	3.36805	-6.32948
H	-6.32993	3.00019	-5.13761
H	-2.71608	4.01795	-5.23272
H	-0.95067	3.20749	-1.74809
H	-0.99405	4.50886	-2.95617
H	-0.32331	2.92422	-3.36117
H	-9.24561	2.47624	-1.65917
H	-8.62494	1.16009	-2.66595
H	-8.08801	2.81582	-2.95347
H	-8.10962	2.52209	0.76698
H	-5.19349	2.83741	2.36580
H	-4.67820	1.13952	2.18681
H	-6.31533	1.53397	2.73944
H	-7.52368	-1.20088	-3.90064
H	-6.77321	-2.44612	-4.90910
H	-6.51738	-0.73382	-5.27369
H	-4.59708	-3.54092	-3.80556
H	-1.54916	-2.65562	-2.69324
H	-2.55502	-3.85512	-1.86685
H	-2.01653	-2.39497	-1.01382
H	6.26138	-5.50254	-1.61203
H	4.91302	-6.58207	-1.99313
H	5.29580	-6.19965	-0.30940
H	2.79052	-5.22062	-2.92102
H	0.67084	-2.40407	-1.74092
H	1.00841	-3.22999	-3.27661
H	1.68112	-1.62587	-2.95486
H	6.33164	-5.42316	2.24313
H	6.58331	-4.94012	3.92732
H	7.43145	-4.09679	2.62381
H	4.48547	-3.58020	4.87899
H	2.09017	-2.07218	4.78201
H	1.66733	-1.39187	3.19670
H	2.81954	-0.54946	4.24647
H	8.72308	-2.94463	0.38633
H	9.45860	-2.30284	-1.08968
H	8.28152	-3.62087	-1.18258
H	8.35813	-0.01796	-1.96077
H	5.14433	1.23822	-2.75768
H	6.50553	2.11436	-2.04251

H 5.01623 1.88111 -1.11007
H -2.67843 4.52843 -0.90516
H -4.24367 3.71451 -0.67969
H -4.61573 4.86404 1.43489
H -3.77331 6.13236 0.53083
H -1.61493 5.48750 1.47640
H -2.67154 5.28907 2.88285
H -1.18559 3.18141 1.91667
H -2.81517 2.90461 2.56879
H -6.69911 -0.71693 0.83239
H -6.80227 -2.47161 0.61735
H -5.94908 -1.48368 -0.57735
H -4.39329 -2.41447 3.98605
H -6.01904 -2.70419 3.36488
H -5.48233 -1.04987 3.68776
H -4.76795 -4.41047 1.44234
H -3.05648 -3.96116 1.35027
H -4.09280 -3.81724 -0.07773
H -2.92277 1.13258 3.95266
H -1.62878 0.23857 4.76064
H -3.25755 -0.44432 4.67212
H -2.10945 -3.07629 3.39692
H -0.54763 -2.31501 3.70979
H -0.91077 -2.94090 2.09314
H -0.87534 1.28122 1.47646
H 0.13386 0.50097 2.64564
H 5.56817 -0.46845 3.57529
H 7.08435 0.41485 3.34827
H 6.38829 -0.49973 2.00495
H 6.98692 2.12831 0.58245
H 7.39172 2.98005 2.07554
H 6.17891 3.65685 0.97836
H 4.67862 3.70721 3.86213
H 5.94483 2.68803 4.54944
H 4.25522 2.17144 4.64025
H 4.16692 4.80632 1.64369
H 2.69263 5.22859 0.76667
H 4.00489 4.38610 -0.06979
H 1.11048 2.28487 3.28721
H 0.99128 3.98672 2.79792
H 2.36163 3.43639 3.76359
H 1.55442 3.28075 -0.82576
H 0.34165 2.85703 0.36013
159
CO insertion product
Y -2.90800 0.64044 -0.48762
Y 3.41472 -0.22007 0.53744
B -5.46751 0.50629 -2.99969
H -6.32492 0.43091 -3.83346
B 5.16875 -3.09303 -0.14993
H 5.80621 -4.08646 -0.34340
P 0.51394 -0.20906 1.00467
P 1.26075 1.41215 -0.34418
Si -4.28696 -1.85058 1.81758
Si -2.00028 -0.33780 2.88648
Si 5.48537 1.61563 2.73062
Si 2.92945 2.98303 1.90899
O -0.98801 0.10768 -1.41176
O -3.12981 3.08860 0.15560
N -4.41263 1.53825 -3.46453
N -3.30888 1.79199 -2.71412

N	-6.11976	0.96689	-1.67600
N	-5.38526	1.15403	-0.54840
N	-4.80031	-0.88265	-2.85750
N	-3.71557	-1.07938	-2.05648
N	3.96206	-3.07074	-1.11342
N	3.20454	-1.94370	-1.29389
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N	3.86710	-2.16377	1.83492
N	6.07593	-1.86726	-0.47414
N	5.57232	-0.59992	-0.48723
N	-3.08105	-0.58308	1.52778
N	3.98017	1.56524	1.78514
C	-5.38101	2.11907	-5.71489
H	-5.48345	1.10846	-6.12329
H	-5.10968	2.78664	-6.53631
H	-6.36461	2.42179	-5.34270
C	-4.33405	2.18821	-4.65180
C	-3.13507	2.88704	-4.66305
H	-2.75508	3.51127	-5.45965
C	-2.52077	2.60022	-3.43448
C	-1.18125	3.04350	-2.94354
H	-1.22374	3.38643	-1.90479
H	-0.79656	3.85759	-3.56398
H	-0.47200	2.21033	-2.96871
C	-8.49976	1.17242	-2.47391
H	-9.45328	1.46237	-2.02604
H	-8.60171	0.15202	-2.85565
H	-8.31622	1.82583	-3.33257
C	-7.41907	1.27656	-1.44829
C	-7.52402	1.68086	-0.12450
H	-8.42373	1.98530	0.39159
C	-6.22797	1.58621	0.40142
C	-5.76976	1.89207	1.78942
H	-5.49837	2.94844	1.90146
H	-4.90026	1.28181	2.05121
H	-6.56737	1.68349	2.50821
C	-6.17129	-2.13515	-4.55899
H	-7.14262	-1.94992	-4.09007
H	-6.18007	-3.14995	-4.96382
H	-6.07397	-1.43798	-5.39728
C	-5.04818	-2.00144	-3.58343
C	-4.09125	-2.94370	-3.23918
H	-4.00149	-3.94853	-3.62710
C	-3.27006	-2.32154	-2.28696
C	-2.05047	-2.87462	-1.62597
H	-1.15687	-2.63360	-2.20874
H	-2.12254	-3.96303	-1.54413
H	-1.90334	-2.45780	-0.62757
C	4.27169	-5.35104	-2.13580
H	5.34522	-5.29760	-2.34301
H	3.80053	-5.91807	-2.94184
H	4.14344	-5.91642	-1.20733
C	3.64504	-3.99829	-2.05119
C	2.66874	-3.45041	-2.86604
H	2.19648	-3.91789	-3.71820
C	2.43025	-2.16078	-2.36882
C	1.51501	-1.13114	-2.94130
H	0.61384	-0.95428	-2.34018
H	1.19201	-1.44449	-3.93797
H	2.02450	-0.16775	-3.04120
C	5.82554	-5.24272	2.05914

H	5.44487	-5.89439	1.26686
H	5.87521	-5.82503	2.98185
H	6.84457	-4.95333	1.78553
C	4.94862	-4.05320	2.27117
C	4.25021	-3.69384	3.41802
H	4.23024	-4.22680	4.35764
C	3.58607	-2.50511	3.10256
C	2.68983	-1.67580	3.96062
H	2.89253	-1.86548	5.01788
H	1.63702	-1.90823	3.77149
H	2.83657	-0.60741	3.77119
C	8.13931	-3.09766	-1.22069
H	8.29991	-3.60691	-0.26602
H	9.11483	-2.81786	-1.62465
H	7.68392	-3.81887	-1.90666
C	7.29783	-1.87474	-1.06271
C	7.58046	-0.57739	-1.46980
H	8.47368	-0.23736	-1.97399
C	6.46514	0.18672	-1.10391
C	6.17138	1.62322	-1.39167
H	5.68888	1.72591	-2.37098
H	7.08925	2.21600	-1.41224
H	5.50755	2.05205	-0.63521
C	-3.92491	4.08763	-0.53819
H	-3.48502	4.23774	-1.52801
H	-4.93450	3.69251	-0.66170
C	-3.84644	5.34645	0.31912
H	-4.64993	5.36284	1.06407
H	-3.92647	6.25601	-0.28234
C	-2.48919	5.18981	1.00783
H	-1.67688	5.46926	0.32756
H	-2.39188	5.78235	1.92151
C	-2.46284	3.69408	1.27953
H	-1.46409	3.25927	1.33367
H	-3.01053	3.44598	2.19769
C	-5.77464	-1.84628	0.63559
H	-6.45153	-1.00581	0.80797
H	-6.33297	-2.77160	0.82674
H	-5.48465	-1.84339	-0.41710
C	-5.10516	-1.74165	3.54577
H	-4.40975	-1.86563	4.38097
H	-5.86170	-2.53129	3.62852
H	-5.61680	-0.78176	3.67510
C	-3.59065	-3.62224	1.66075
H	-4.31091	-4.33519	2.08031
H	-2.63707	-3.76442	2.17415
H	-3.44906	-3.88256	0.60781
C	-2.71381	0.80917	4.23862
H	-2.97863	1.78841	3.82548
H	-1.97694	0.97229	5.03423
H	-3.61381	0.38680	4.69459
C	-1.41790	-1.91782	3.79032
H	-2.23237	-2.52774	4.18879
H	-0.78570	-1.62288	4.63692
H	-0.82075	-2.55074	3.12453
C	-0.31569	0.52046	2.47797
H	-0.48345	1.58670	2.31012
H	0.30596	0.41693	3.37563
C	6.22956	-0.11143	3.00353
H	5.61404	-0.73780	3.65491
H	7.20006	0.02663	3.49594

H 6.41136 -0.65730 2.07335
C 6.87726 2.62915 1.91471
H 7.33730 2.07158 1.09388
H 7.66039 2.82534 2.65670
H 6.53468 3.59176 1.52621
C 5.26833 2.33417 4.48143
H 5.04321 3.40514 4.47977
H 6.20773 2.19993 5.03099
H 4.47930 1.82018 5.03905
C 3.84319 4.62384 1.58953
H 4.60219 4.83590 2.34918
H 3.12653 5.45366 1.60066
H 4.33549 4.62001 0.61093
C 2.06200 3.16472 3.59215
H 1.52198 2.25304 3.86139
H 1.33250 3.98191 3.53711
H 2.75947 3.39795 4.39967
C 1.49568 2.97229 0.61277
H 1.70018 3.75209 -0.13340
H 0.56816 3.26002 1.11914
C -0.51224 0.72860 -0.33165
159
CO P-P activation TS
Y -0.51842 5.63885 5.48472
Y 5.72309 4.71430 6.55528
B -3.16922 6.17294 3.10554
H -4.05837 6.31604 2.31610
B 7.88642 2.00439 6.44238
H 8.67202 1.10204 6.45214
P 2.88986 4.74936 6.99506
P 3.68490 6.17445 5.18313
Si -2.16769 2.97839 7.32857
Si 0.21115 4.12025 8.64766
Si 7.87724 7.05775 8.18687
Si 5.13338 8.02060 7.42268
O 1.29037 4.86689 4.57689
O -0.42191 7.99542 6.47155
N -2.00506 7.10777 2.70915
N -0.85043 7.14803 3.42846
N -3.70846 6.53703 4.50437
N -2.93649 6.41821 5.61687
N -2.68929 4.70524 3.04058
N -1.56257 4.28636 3.68736
N 6.63937 1.59030 5.63926
N 5.64036 2.48210 5.37401
N 7.49546 2.31132 7.91461
N 6.51484 3.20315 8.23232
N 8.54988 3.21699 5.72799
N 7.83642 4.34121 5.43767
N -0.87558 4.20085 7.27358
N 6.32024 6.71314 7.40819
C -2.97919 8.04181 0.58217
H -3.20952 7.10048 0.07284
H -2.65895 8.76262 -0.17393
H -3.90884 8.40803 1.02821
C -1.89591 7.87492 1.59689
C -0.62702 8.43435 1.60202
H -0.20651 9.09961 0.86114
C -0.00572 7.94500 2.75951
C 1.38937 8.19849 3.22283
H 1.43624 8.35125 4.30451

H	1.80048	9.08478	2.73161
H	2.03904	7.34649	2.99574
C	-6.04140	7.22368	3.84647
H	-6.92917	7.58204	4.37302
H	-6.31232	6.30912	3.31024
H	-5.76727	7.97276	3.09711
C	-4.94339	6.98847	4.83139
C	-4.96768	7.16856	6.20684
H	-5.80410	7.50608	6.80261
C	-3.69399	6.79663	6.65857
C	-3.19266	6.77512	8.06436
H	-2.84222	7.76217	8.38677
H	-2.37319	6.05823	8.16643
H	-3.99463	6.47987	8.74755
C	-4.35844	3.85416	1.35723
H	-5.24678	4.08780	1.95203
H	-4.53597	2.90642	0.84345
H	-4.25666	4.63614	0.59802
C	-3.13740	3.73277	2.20842
C	-2.27024	2.65792	2.31762
H	-2.33415	1.71535	1.79272
C	-1.29180	3.05038	3.24198
C	-0.07514	2.28572	3.64234
H	0.76940	2.57966	3.01275
H	-0.24432	1.21243	3.51781
H	0.21635	2.48321	4.67403
C	7.30558	-0.76940	5.07350
H	8.30237	-0.56133	4.67163
H	6.87337	-1.58851	4.49428
H	7.43235	-1.11577	6.10405
C	6.40825	0.42147	4.99298
C	5.22643	0.56663	4.28390
H	4.74969	-0.17319	3.65687
C	4.78229	1.87081	4.54442
C	3.57006	2.54661	4.00171
H	2.84512	2.79399	4.78233
H	3.07821	1.89545	3.27592
H	3.81908	3.48459	3.49530
C	9.01011	0.66279	9.06226
H	8.72879	-0.22953	8.49481
H	9.19989	0.36174	10.09494
H	9.94735	1.03854	8.64129
C	7.93614	1.69975	9.03863
C	7.21640	2.21490	10.11083
H	7.32152	1.94354	11.15140
C	6.33675	3.15237	9.56149
C	5.32188	4.00435	10.24910
H	5.53848	4.06916	11.31832
H	4.31640	3.58633	10.13257
H	5.31290	5.02004	9.84002
C	10.79069	2.20001	5.20434
H	11.05844	1.99010	6.24405
H	11.69367	2.52108	4.68025
H	10.45489	1.26026	4.75484
C	9.75209	3.26780	5.10341
C	9.80632	4.45724	4.38740
H	10.62570	4.80747	3.77607
C	8.58049	5.09494	4.61622
C	8.05304	6.36831	4.03939
H	7.44630	6.16841	3.14854
H	8.87130	7.02978	3.74398

H	7.42684	6.89879	4.76352
C	-1.10718	9.12276	5.86025
H	-0.48337	9.50413	5.04542
H	-2.04504	8.75520	5.44547
C	-1.26724	10.14922	6.97032
H	-2.16282	9.94036	7.56505
H	-1.34990	11.16657	6.57829
C	-0.00146	9.92074	7.79649
H	0.85557	10.41410	7.32486
H	-0.07736	10.28305	8.82508
C	0.15540	8.40609	7.73241
H	1.19803	8.08347	7.75640
H	-0.38961	7.90494	8.54032
C	-3.69791	3.36089	6.27287
H	-4.28306	4.19496	6.66871
H	-4.32920	2.46364	6.29779
H	-3.45879	3.57375	5.22961
C	-2.91037	2.71349	9.07229
H	-2.20963	2.29828	9.80254
H	-3.74104	2.00327	8.97900
H	-3.31863	3.64306	9.48226
C	-1.59688	1.25320	6.74575
H	-2.29764	0.49358	7.11276
H	-0.59725	0.99047	7.10059
H	-1.59623	1.19736	5.65385
C	-0.50109	4.86799	10.25833
H	-0.80622	5.90936	10.10532
H	0.26485	4.86040	11.04319
H	-1.36882	4.31944	10.63257
C	0.84993	2.37755	9.07858
H	0.04483	1.67642	9.31507
H	1.50847	2.43321	9.95376
H	1.42822	1.96053	8.24724
C	1.83151	5.14756	8.45428
H	1.60794	6.21631	8.47157
H	2.40195	4.93739	9.37042
C	8.89630	5.50090	8.56756
H	8.42238	4.85388	9.31077
H	9.85576	5.83563	8.98112
H	9.11175	4.90539	7.67680
C	9.03238	8.13972	7.12679
H	9.39038	7.58272	6.25555
H	9.91108	8.42069	7.71966
H	8.55856	9.05872	6.77321
C	7.69284	7.92368	9.87740
H	7.25325	8.92327	9.81322
H	8.68508	8.03014	10.33169
H	7.07867	7.32653	10.55981
C	5.85675	9.75571	7.10272
H	6.57705	10.07461	7.86153
H	5.03770	10.48532	7.09918
H	6.34781	9.80513	6.12505
C	4.19767	8.12476	9.07724
H	3.68456	7.18422	9.29802
H	3.44759	8.92456	9.04764
H	4.87889	8.34014	9.90547
C	3.80607	7.82111	6.04289
H	4.01269	8.56040	5.25624
H	2.82167	8.07380	6.45514
C	2.06297	5.39827	5.52777

159

CO insertion final product

Y	-3.12696	0.74583	-0.19634
Y	3.36381	-0.64482	0.25739
B	-5.39357	1.71939	-2.73959
H	-6.17192	1.99418	-3.60613
B	5.50737	-3.23533	1.16296
H	6.28700	-4.07742	1.50288
P	0.57422	-0.82796	1.16485
P	1.28030	0.08843	-1.55222
Si	-4.46248	-2.53852	0.51206
Si	-2.37206	-1.53376	2.37482
Si	5.46878	2.19190	0.90062
Si	2.78107	2.67134	-0.39245
O	-0.96353	0.96530	-0.15838
O	-3.27083	2.57959	1.46495
N	-4.41124	2.89494	-2.55955
N	-3.37537	2.81498	-1.68108
N	-6.19172	1.48529	-1.43187
N	-5.57571	1.18806	-0.25504
N	-4.60892	0.45766	-3.16925
N	-3.57655	-0.03743	-2.42657
N	4.26158	-3.91057	0.55962
N	3.27497	-3.17941	-0.03519
N	5.12686	-2.41126	2.42451
N	4.16602	-1.44443	2.40554
N	6.18364	-2.37024	0.06308
N	5.48870	-1.41170	-0.60934
N	-3.33622	-1.22357	0.92585
N	3.98670	1.52778	0.20886
C	-5.33287	4.45101	-4.31080
H	-5.32285	3.75752	-5.15762
H	-5.08067	5.44500	-4.68734
H	-6.35726	4.48448	-3.92708
C	-4.35198	4.05661	-3.25599
C	-3.23852	4.75095	-2.80925
H	-2.88963	5.71232	-3.15881
C	-2.65322	3.93580	-1.82905
C	-1.42461	4.20547	-1.02660
H	-0.98429	3.27555	-0.66090
H	-1.63780	4.85332	-0.16705
H	-0.67861	4.72212	-1.63699
C	-8.50999	1.87196	-2.33543
H	-9.52100	1.87007	-1.92167
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160

CS_2 coordination TS

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C	7.09966	12.62299	-0.00723
O	6.22111	13.31958	-0.92194
C	6.56531	14.73452	-0.90884
C	7.78699	14.87546	0.00108
Y	4.09041	12.34297	-1.96839
N	5.00705	10.79925	-3.34297
Si	4.89175	10.59316	-5.10216
C	3.97887	9.00499	-5.64014
N	1.96255	12.81068	-3.07173
C	1.04946	12.00767	-3.64657
C	-0.02702	12.77707	-4.10457
C	0.28308	14.08939	-3.78745
N	1.48887	14.08718	-3.16921
C	1.22326	10.53544	-3.77700
B	2.31492	15.30833	-2.72880
N	3.67372	15.34131	-3.47638
N	4.58425	14.33212	-3.38086
C	5.62924	14.67130	-4.15452
C	5.38859	15.91526	-4.75115
C	4.13789	16.31126	-4.30052
C	-0.52200	15.31802	-4.05615
C	3.39073	17.56008	-4.63537
C	6.83572	13.80502	-4.30642
N	2.54728	15.32525	-1.20399
N	3.29898	14.37492	-0.57903
C	3.41663	14.76251	0.70440
C	2.71970	15.96113	0.90434
C	2.18119	16.29282	-0.32842
C	4.23188	14.02866	1.71595
C	1.33888	17.47502	-0.67982
P	4.37301	10.56760	0.32004
Y	3.09467	8.60183	2.01023
N	3.78963	6.51730	0.58011
N	4.57023	5.57763	1.18975
C	4.76721	4.51778	0.36626
C	4.09610	4.78045	-0.81474
C	3.49306	6.03320	-0.63929
B	5.03469	5.70522	2.65307
N	5.90434	6.96292	2.87601
N	5.38874	8.22593	2.88189
C	6.39300	9.05300	3.22667
C	7.56675	8.31537	3.41813
C	7.22127	6.99240	3.18999
C	6.21192	10.51684	3.44204
C	8.09980	5.78681	3.25994
C	5.56948	3.30806	0.71901
C	2.62092	6.73073	-1.62921
P	2.29503	10.22121	-0.39926
C	1.40188	11.49137	0.67625
Si	0.94992	11.20180	2.52167
C	0.79092	12.98139	3.19430
C	5.41784	9.35082	-0.69164
Si	6.01712	9.62816	-2.49655
C	7.85188	10.17244	-2.49807
C	6.07150	7.86156	-3.20347
C	-0.82630	10.53282	2.67320
N	2.12845	10.15984	3.32206
Si	2.43495	10.46927	5.03454
C	3.34286	12.11783	5.35585
N	2.82686	6.62768	3.52248

N	3.82273	5.70221	3.61032
C	3.52079	4.77774	4.55421
C	2.28766	5.11518	5.08901
C	1.88521	6.27503	4.41398
C	4.40173	3.62825	4.91920
C	0.61657	7.03787	4.61101
C	0.84931	10.54971	6.09420
C	3.51055	9.12067	5.83364
C	6.59267	10.46840	-5.96301
C	3.97705	12.03133	-5.93966
H	5.70784	4.75025	2.91000
H	3.93927	3.06418	5.73256
H	5.38775	3.96201	5.25672
H	4.55615	2.94407	4.07915
H	1.75284	4.59198	5.86892
H	0.37467	7.09757	5.67659
H	-0.22356	6.54198	4.11197
H	0.69425	8.05350	4.21638
H	6.59827	3.55989	0.99356
H	5.60427	2.63661	-0.14222
H	5.13281	2.75632	1.55745
H	4.04780	4.14889	-1.69039
H	1.58831	6.37129	-1.55800
H	2.96816	6.52614	-2.64591
H	2.59932	7.81282	-1.48012
H	7.75713	5.07136	4.01348
H	9.11461	6.09530	3.52204
H	8.14472	5.25847	2.30255
H	8.53900	8.69310	3.70123
H	7.11646	11.05841	3.14870
H	6.03071	10.72962	4.50132
H	5.36961	10.89991	2.86139
H	2.98402	8.16628	5.91373
H	3.76784	9.44725	6.84859
H	4.44355	8.93601	5.29426
H	4.19327	12.24976	4.68137
H	3.72111	12.13612	6.38508
H	2.67830	12.97708	5.23244
H	0.18991	11.37362	5.80398
H	1.12373	10.70441	7.14476
H	0.27157	9.62268	6.03379
H	0.42489	13.02101	4.22453
H	0.05979	13.50653	2.56729
H	1.72881	13.53815	3.14017
H	-0.93239	9.49342	2.35647
H	-1.51865	11.14305	2.08196
H	-1.14028	10.59486	3.72135
H	1.95939	12.43470	0.64016
H	0.46233	11.69292	0.14601
H	1.70612	16.29552	-3.02229
H	3.99195	18.16949	-5.31400
H	2.43752	17.34561	-5.12786
H	3.17361	18.15847	-3.74538
H	6.03350	16.45337	-5.43136
H	7.10504	13.71392	-5.36286
H	7.70466	14.22984	-3.78985
H	6.65347	12.80298	-3.91218
H	0.36269	17.17702	-1.07429
H	1.17045	18.07651	0.21637
H	1.81495	18.11299	-1.43074
H	2.61454	16.51065	1.82890

H 5.25019 14.43267 1.75999
H 3.80121 14.14564 2.71291
H 4.30111 12.96138 1.49038
H -0.00429 16.00986 -4.72779
H -1.46600 15.03408 -4.52680
H -0.75369 15.86379 -3.13663
H -0.91519 12.42303 -4.60791
H 0.57513 10.00159 -3.07581
H 0.96733 10.21867 -4.79329
H 2.24789 10.23350 -3.55790
H 4.50838 12.98159 -5.84768
H 3.88541 11.79932 -7.00752
H 2.96973 12.17444 -5.54026
H 3.67747 9.10495 -6.68972
H 4.62267 8.12487 -5.56541
H 3.07887 8.81371 -5.05157
H 7.12626 9.55514 -5.68157
H 6.44157 10.43409 -7.04875
H 7.24512 11.31774 -5.74438
H 6.55633 7.80022 -4.18236
H 6.65239 7.24284 -2.50850
H 5.07485 7.42089 -3.28150
H 7.97730 11.24827 -2.34706
H 8.43240 9.64163 -1.73400
H 8.29331 9.93380 -3.47173
H 4.92150 8.37386 -0.69647
H 6.31319 9.19427 -0.07366
H 7.23852 11.60866 -0.37819
H 6.62606 12.57346 0.97946
H 8.96677 13.26960 -0.87740
H 8.98364 13.25451 0.89718
H 7.49043 15.17329 1.01250
H 8.48770 15.62643 -0.37385
H 5.69692 15.29936 -0.56471
H 6.78368 15.02954 -1.93528
C 0.25381 8.38470 0.13072
S 0.63564 7.31009 1.26612
S -0.74775 9.00090 -0.92839
160
CS_2 coordination product
C 4.95494 1.94240 -1.01956
C 3.65170 1.24792 -1.38557
O 2.66813 2.30782 -1.51022
C 3.20733 3.54313 -0.96573
C 4.45551 3.13324 -0.19925
Y 0.36352 1.87726 -2.32041
N 0.92030 0.39178 -3.90195
Si 1.10851 0.66100 -5.64842
C 0.24335 -0.62565 -6.75774
N -1.71825 2.73259 -3.24049
C -2.69905 2.12992 -3.93795
C -3.70219 3.06218 -4.23026
C -3.28257 4.26025 -3.67626
N -2.08365 4.03949 -3.08538
C -2.67729 0.68805 -4.30183
B -1.17488 5.06914 -2.40089
N 0.18078 5.17658 -3.14340
N 1.01510 4.11092 -3.30803
C 2.08813 4.56268 -3.98197
C 1.94409 5.92986 -4.24415
C 0.72063 6.28739 -3.69901

C	-3.97793	5.58156	-3.69985
C	0.07174	7.63245	-3.69513
C	3.21950	3.68631	-4.40496
N	-0.92455	4.73811	-0.91268
N	-0.16530	3.67127	-0.52874
C	0.02564	3.79473	0.79770
C	-0.62716	4.94098	1.26848
C	-1.22128	5.51620	0.15646
C	0.83016	2.82643	1.59667
C	-2.04928	6.75743	0.09220
P	0.54437	-0.37119	-0.18296
Y	-0.15314	-2.14156	2.06782
N	1.05858	-4.42998	1.29297
N	1.85043	-4.99587	2.25478
C	2.51073	-6.07351	1.75893
C	2.12978	-6.21880	0.43948
C	1.21388	-5.18391	0.19184
B	1.78458	-4.57345	3.73104
N	2.42116	-3.17338	3.92222
N	2.05841	-2.09716	3.16751
C	2.91209	-1.10296	3.46764
C	3.82924	-1.54318	4.42768
C	3.48817	-2.86146	4.69433
C	2.82376	0.24838	2.84582
C	4.14248	-3.80677	5.64698
C	3.46354	-6.91459	2.54367
C	0.47524	-4.98083	-1.08868
P	-1.51119	-0.09721	-0.88763
C	-2.25688	0.90688	0.47554
Si	-2.65275	0.33092	2.27199
C	-3.09327	2.03671	3.01807
C	1.32494	-1.45810	-1.50540
Si	1.01960	-1.30079	-3.38995
C	2.51949	-2.22380	-4.12672
C	-0.51263	-2.33606	-3.80992
C	-4.29241	-0.62340	2.24206
N	-1.34444	-0.53808	3.09843
Si	-1.19955	-0.20343	4.83731
C	-0.47737	1.52184	5.21030
N	-0.67790	-3.92555	3.64370
N	0.32176	-4.64266	4.23105
C	-0.19930	-5.49141	5.14938
C	-1.57630	-5.31599	5.15032
C	-1.83589	-4.33270	4.18874
C	0.60970	-6.43279	5.97929
C	-3.15342	-3.78916	3.75123
C	-2.85210	-0.36670	5.77583
C	-0.03223	-1.38656	5.75823
C	2.93814	0.60475	-6.19616
C	0.34985	2.30779	-6.21529
H	2.42581	-5.34586	4.38161
H	-0.04450	-6.93622	6.69481
H	1.39229	-5.91492	6.54127
H	1.09538	-7.20031	5.36837
H	-2.29626	-5.83753	5.76463
H	-3.91455	-3.97339	4.51376
H	-3.48417	-4.25959	2.81881
H	-3.09397	-2.71374	3.56901
H	4.28031	-6.32146	2.96700
H	3.90170	-7.66987	1.88686
H	2.97158	-7.43393	3.37230

H	2.45731	-6.98095	-0.25343
H	-0.04716	-5.90372	-1.36371
H	1.16257	-4.74486	-1.90847
H	-0.27399	-4.19297	-1.00771
H	3.43451	-4.18812	6.38859
H	4.94286	-3.28766	6.17934
H	4.57809	-4.66996	5.13475
H	4.63630	-0.97908	4.87304
H	3.81491	0.58110	2.51983
H	2.44881	0.98823	3.56065
H	2.15674	0.24078	1.98015
H	-0.36707	-2.42601	5.72920
H	-0.03063	-1.06727	6.80799
H	1.00010	-1.34035	5.40241
H	0.50964	1.62815	4.74788
H	-0.34910	1.63600	6.29335
H	-1.10618	2.34245	4.85850
H	-3.63854	0.29893	5.41059
H	-2.68970	-0.13791	6.83585
H	-3.22688	-1.39364	5.71438
H	-3.40755	1.99798	4.06420
H	-3.93372	2.43968	2.43996
H	-2.26808	2.74996	2.93100
H	-4.21036	-1.58352	1.72654
H	-5.05330	-0.02911	1.72400
H	-4.64752	-0.80366	3.26238
H	-1.64799	1.81458	0.54995
H	-3.22394	1.23962	0.07365
H	-1.71178	6.13624	-2.45649
H	0.71351	8.34399	-4.21983
H	-0.90019	7.61874	-4.19699
H	-0.08815	8.00673	-2.67936
H	2.63420	6.57390	-4.77047
H	3.18206	3.49709	-5.48220
H	4.18117	4.16572	-4.19335
H	3.18954	2.72290	-3.89542
H	-3.04144	6.56162	-0.32523
H	-2.18104	7.15570	1.10080
H	-1.58310	7.53472	-0.52102
H	-0.66423	5.30326	2.28588
H	1.46114	3.36192	2.31358
H	0.19362	2.14222	2.16787
H	1.45752	2.21063	0.95195
H	-3.39784	6.34063	-4.23410
H	-4.93934	5.47328	-4.20692
H	-4.16884	5.96242	-2.69205
H	-4.61854	2.88287	-4.77387
H	-3.22258	0.09205	-3.55914
H	-3.15606	0.53896	-5.27450
H	-1.65615	0.30536	-4.34480
H	0.74969	3.19238	-5.71737
H	0.53235	2.41221	-7.29169
H	-0.73355	2.30510	-6.06125
H	-0.83681	-0.65803	-6.58767
H	0.40499	-0.33031	-7.80182
H	0.63942	-1.63850	-6.64203
H	3.27050	-0.43119	-6.31290
H	3.05939	1.10103	-7.16635
H	3.61066	1.08707	-5.48278
H	-0.69051	-2.38312	-4.88702
H	-0.36843	-3.36164	-3.45357

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H 3.45349 -1.67514 -3.96522
H 2.61674 -3.20112 -3.63920
H 2.41587 -2.40486 -5.20087
H 1.12503 -2.50819 -1.27312
H 2.40536 -1.33596 -1.35641
H 3.68205 0.70573 -2.33419
H 3.31393 0.57055 -0.59395
H 5.47658 2.28807 -1.91882
H 5.62947 1.28334 -0.46678
H 4.19983 2.81806 0.81805
H 5.18042 3.94887 -0.13187
H 2.43125 4.00876 -0.35826
H 3.44584 4.20994 -1.79914
C -2.58097 -1.63447 -0.73589
S -2.09648 -2.94150 0.26806
S -4.01056 -1.56857 -1.56957
160
CS_2 coordination TS less favorable (THF side)
N 3.77204 5.56534 3.53640
N 2.85566 6.56551 3.37151
C 1.72245 6.16924 3.97303
C 1.91702 4.90913 4.55163
C 3.22504 4.55451 4.25377
Y 3.68933 8.65037 2.40612
N 2.39637 9.96364 3.63289
Si 2.50535 10.14837 5.38391
C 3.51094 8.72141 6.14155
C 0.47341 6.98429 3.93105
C 3.95269 3.30584 4.62821
B 5.13516 5.57237 2.79275
N 4.86363 5.75070 1.28242
N 4.11878 6.79314 0.80385
C 3.83152 6.51389 -0.47644
C 4.41705 5.29390 -0.83695
C 5.05993 4.83468 0.30168
C 2.95476 7.39476 -1.29600
C 5.84517 3.57692 0.47670
P 3.56865 10.79624 0.42894
C 2.71464 12.03325 1.56822
Si 1.46448 11.09387 2.64012
C 0.37063 12.35021 3.55690
P 5.68882 11.47198 0.19424
C 6.29111 9.94706 -0.71320
Si 6.38510 10.02230 -2.61655
C 8.08140 10.73226 -3.11019
Y 4.24776 12.64379 -1.99148
N 1.81925 12.56185 -2.57518
C 0.94752 11.54677 -2.69492
C -0.29446 12.03350 -3.11964
C -0.13346 13.40292 -3.25519
N 1.14686 13.69643 -2.92471
C 1.30715 10.13425 -2.40100
C -1.14532 14.41186 -3.68952
B 1.81155 15.08311 -2.92075
N 2.98634 15.13569 -3.92822
N 4.06891 14.31990 -3.81802
C 4.91290 14.64705 -4.80908
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C	2.12826	16.99137	-5.40089
N	3.24993	14.73873	-0.84927
C	3.48147	15.37320	0.31200
C	2.65004	16.49853	0.41251
C	1.90777	16.52103	-0.75669
N	2.28963	15.45398	-1.50141
C	4.52549	14.94193	1.28576
C	0.86611	17.50829	-1.17067
N	5.04591	10.95393	-3.30338
Si	4.54653	10.47972	-4.93535
C	3.31049	11.68237	-5.73315
C	3.66956	8.78618	-5.03791
C	5.99940	10.34884	-6.17073
C	0.27170	10.10819	1.52790
N	5.73811	7.98578	3.37695
N	6.08047	6.66381	3.35350
C	7.29229	6.50081	3.93260
C	7.73882	7.75040	4.34486
C	6.73722	8.65311	3.98271
C	7.98718	5.18629	4.06642
C	6.66653	10.12014	4.23053
O	6.22620	14.38527	-1.78617
C	6.10284	15.82845	-1.90482
C	7.49604	16.40197	-1.65233
C	8.15599	15.31424	-0.80510
C	7.59089	14.06015	-1.44596
C	3.35967	11.77507	5.87925
C	0.82733	10.10348	6.28181
C	6.49271	8.18344	-3.12243
C	7.90777	12.07223	1.77782
S	7.51834	13.36015	2.63828
S	8.94196	10.96996	1.27093
H	5.66478	4.51408	2.96330
H	3.30481	2.68022	5.24617
H	4.86063	3.52049	5.20004
H	4.24662	2.72426	3.74901
H	1.19844	4.32579	5.10941
H	-0.11504	6.83439	4.84028
H	-0.15408	6.68884	3.08159
H	0.70658	8.04780	3.83232
H	6.85445	3.77660	0.84850
H	5.93446	3.06942	-0.48634
H	5.36538	2.88736	1.17859
H	4.38039	4.80956	-1.80200
H	3.04416	8.43907	-0.98602
H	1.90393	7.09702	-1.19326
H	3.21220	7.32855	-2.35507
H	7.40544	4.47398	4.65890
H	8.94866	5.33533	4.56230
H	8.17659	4.72702	3.09157
H	8.67488	7.97537	4.83469
H	6.14389	10.64709	3.42582
H	7.66909	10.54673	4.29189
H	6.15291	10.33302	5.17460
H	2.99400	7.76322	6.02849
H	3.62953	8.91125	7.21498
H	4.51334	8.61094	5.71734
H	2.74859	12.64589	5.62198
H	4.32345	11.88869	5.37356
H	3.53673	11.80484	6.96077
H	0.20462	10.97112	6.04827

H	0.99735	10.10036	7.36506
H	0.26080	9.20111	6.03267
H	-0.46462	11.86603	4.07144
H	-0.05118	13.03400	2.81073
H	0.92143	12.95459	4.28286
H	0.77465	9.31509	0.96103
H	-0.20839	10.77078	0.79882
H	-0.51430	9.64006	2.13080
H	3.43751	12.47285	2.26406
H	2.25219	12.84538	0.99787
H	0.99730	15.89037	-3.26383
H	2.48892	17.51301	-6.29050
H	1.16403	16.53497	-5.64422
H	1.94988	17.73754	-4.62046
H	4.78985	16.16165	-6.44176
H	7.04447	14.59441	-4.56630
H	6.26015	13.00646	-4.50119
H	6.45452	13.84689	-6.05196
H	-0.10453	17.03195	-1.33962
H	0.74244	18.25480	-0.38253
H	1.13786	18.03204	-2.09230
H	2.59856	17.20555	1.22848
H	5.05338	14.04559	0.95635
H	5.27035	15.73378	1.42312
H	4.09125	14.73893	2.26921
H	-0.83548	14.93836	-4.59742
H	-2.09064	13.90583	-3.89904
H	-1.32996	15.16711	-2.91931
H	-1.19111	11.46152	-3.31109
H	1.10964	9.89361	-1.35257
H	0.71750	9.45773	-3.02703
H	2.36741	9.95302	-2.58089
H	3.76317	12.63945	-6.00147
H	2.94116	11.21497	-6.65413
H	2.44856	11.88510	-5.09163
H	2.72438	8.78503	-4.48833
H	3.43619	8.57780	-6.08933
H	4.28617	7.96440	-4.66701
H	6.71466	9.56426	-5.90472
H	5.60287	10.10673	-7.16419
H	6.55186	11.28911	-6.25643
H	6.62497	8.02243	-4.19615
H	7.36871	7.75942	-2.61588
H	5.62001	7.61404	-2.79070
H	8.21701	11.76201	-2.77451
H	8.88405	10.12989	-2.66933
H	8.20342	10.71523	-4.19813
H	5.68085	9.07644	-0.43800
H	7.30720	9.74373	-0.33826
H	8.13717	13.81274	-2.36624
H	7.56776	13.18732	-0.79169
H	9.24863	15.34009	-0.83457
H	7.83888	15.37759	0.24069
H	7.45073	17.37548	-1.15590
H	8.04153	16.53187	-2.59431
H	5.38227	16.16214	-1.15536
H	5.70991	16.06908	-2.89462

160

CS_2 coordination product less favorable (THF side)

N	-0.12189	-5.50089	3.99633
N	-1.05078	-4.50276	4.05331

C	-2.06425	-4.94367	4.81433
C	-1.77671	-6.23674	5.26989
C	-0.54051	-6.56066	4.72981
Y	-0.44813	-2.41988	2.91595
N	-1.66162	-1.01720	4.12535
Si	-1.34533	-0.69704	5.83172
C	-0.20757	-2.04843	6.54178
C	-3.29558	-4.13269	5.04457
C	0.23724	-7.82499	4.89008
B	1.10352	-5.42491	3.04674
N	0.58558	-5.22937	1.59650
N	-0.35793	-4.28836	1.27465
C	-0.80340	-4.58577	0.04326
C	-0.11903	-5.70524	-0.44703
C	0.75013	-6.08961	0.56096
C	-1.92685	-3.85682	-0.61586
C	1.71766	-7.22677	0.56085
P	-1.02631	-0.59036	0.77160
C	-1.72445	0.80617	1.79040
Si	-2.75133	0.00214	3.17407
C	-3.67005	1.37926	4.11045
P	0.70781	0.21227	-0.32889
C	1.11848	-1.23718	-1.39524
Si	1.75985	-0.84094	-3.14506
C	3.61735	-0.46090	-3.12180
Y	0.13801	2.17173	-2.50240
N	-2.12408	1.97246	-3.28513
C	-2.92016	0.89940	-3.43605
C	-4.06908	1.27406	-4.14187
C	-3.93003	2.63033	-4.40435
N	-2.74968	3.03165	-3.87577
C	-2.56413	-0.43923	-2.88461
C	-4.87302	3.53366	-5.12809
B	-2.21131	4.47505	-3.73019
N	-0.86178	4.67979	-4.46840
N	0.25564	3.97425	-4.14238
C	1.25296	4.42344	-4.92267
C	0.77176	5.44067	-5.75342
C	-0.57513	5.57619	-5.44120
C	2.63047	3.84755	-4.87728
C	-1.56989	6.51463	-6.04083
N	-1.21328	4.11156	-1.41825
C	-1.35107	4.64087	-0.19042
C	-2.28529	5.68666	-0.22402
C	-2.71330	5.76673	-1.53683
N	-2.05475	4.81114	-2.23801
C	-0.59910	4.16729	1.00492
C	-3.71283	6.70545	-2.12891
N	0.81716	0.50305	-3.84297
Si	0.48982	0.34123	-5.58675
C	-0.37003	1.82948	-6.39741
C	-0.69361	-1.08656	-6.03313
C	2.09843	0.10693	-6.58553
C	-4.11406	-1.07898	2.39559
N	1.73375	-3.00777	3.59020
N	2.09566	-4.32216	3.48787
C	3.38018	-4.46580	3.89163
C	3.85302	-3.21518	4.26400
C	2.79395	-2.32622	4.05902
C	4.11181	-5.76717	3.91074
C	2.76120	-0.85322	4.27320

O	2.06226	3.42527	-1.73498
C	2.03760	4.85019	-1.42539
C	3.48048	5.22826	-1.12329
C	4.04355	3.92938	-0.54484
C	3.37686	2.88009	-1.41448
C	-0.48034	0.97076	6.12026
C	-2.90169	-0.72057	6.92866
C	1.61334	-2.53700	-4.00878
C	2.17287	0.44988	0.81876
S	1.95133	1.77374	1.85400
S	3.49480	-0.58181	0.73887
H	1.68397	-6.46913	3.09778
H	-0.29378	-8.49354	5.57143
H	1.23286	-7.64011	5.30429
H	0.36830	-8.34713	3.93719
H	-2.38916	-6.86009	5.90562
H	-3.62094	-4.20752	6.08640
H	-4.11927	-4.49384	4.41756
H	-3.12090	-3.08003	4.80719
H	2.73896	-6.88910	0.76108
H	1.70843	-7.70854	-0.41945
H	1.46661	-7.98229	1.31199
H	-0.24436	-6.17781	-1.41068
H	-1.92532	-2.79060	-0.36869
H	-2.89062	-4.27778	-0.30313
H	-1.86145	-3.96328	-1.70205
H	3.63944	-6.49288	4.57974
H	5.13380	-5.60094	4.25810
H	4.16190	-6.21996	2.91615
H	4.84422	-2.97803	4.62184
H	1.74784	-0.44882	4.20617
H	3.35236	-0.34137	3.50573
H	3.16380	-0.59469	5.25736
H	-0.67740	-3.03642	6.50942
H	-0.00504	-1.81050	7.59284
H	0.76092	-2.12019	6.03724
H	-1.13367	1.81397	5.87663
H	0.42114	1.06542	5.50734
H	-0.18869	1.07119	7.17238
H	-3.55230	0.13865	6.74481
H	-2.60173	-0.68612	7.98281
H	-3.49110	-1.63072	6.78103
H	-4.38666	0.97710	4.83256
H	-4.23499	1.96660	3.37695
H	-2.99673	2.06356	4.63370
H	-3.71098	-1.90687	1.80099
H	-4.74013	-0.47904	1.72502
H	-4.75825	-1.50284	3.17403
H	-0.91573	1.37265	2.26959
H	-2.32687	1.49083	1.18039
H	-3.00906	5.22204	-4.21674
H	-1.08696	7.09811	-6.82790
H	-2.41619	5.98200	-6.48421
H	-1.97224	7.21294	-5.30056
H	1.32277	5.99384	-6.50057
H	3.26832	4.37783	-4.16246
H	2.60934	2.79067	-4.59679
H	3.10264	3.92798	-5.86014
H	-4.57490	6.17589	-2.54637
H	-4.07721	7.38121	-1.35181
H	-3.28162	7.31326	-2.93032

H	-2.60876	6.30065	0.60446
H	0.06720	3.32447	0.80383
H	0.00682	4.97746	1.42785
H	-1.29054	3.84881	1.79085
H	-4.39172	4.02995	-5.97596
H	-5.71231	2.94871	-5.51076
H	-5.27487	4.31412	-4.47435
H	-4.89795	0.64083	-4.42369
H	-2.53987	-0.43382	-1.78708
H	-3.29290	-1.18594	-3.20912
H	-1.57239	-0.74755	-3.22968
H	0.27587	2.70254	-6.50863
H	-0.66516	1.50426	-7.40286
H	-1.27780	2.13511	-5.87079
H	-1.70224	-0.87012	-5.66627
H	-0.75345	-1.15437	-7.12624
H	-0.39261	-2.06448	-5.65545
H	2.65544	-0.79062	-6.30326
H	1.86289	0.03048	-7.65354
H	2.76386	0.96670	-6.45333
H	1.91552	-2.54756	-5.05927
H	2.27938	-3.21997	-3.46735
H	0.60093	-2.94556	-3.93650
H	3.86412	0.38144	-2.47381
H	4.16943	-1.32678	-2.74190
H	3.97184	-0.23796	-4.13398
H	0.20413	-1.82892	-1.51836
H	1.85960	-1.84620	-0.85910
H	3.91341	2.72679	-2.35785
H	3.23674	1.92666	-0.90469
H	5.13360	3.86789	-0.59660
H	3.73456	3.79037	0.49617
H	3.53836	6.07139	-0.42954
H	4.01305	5.50803	-2.03971
H	1.39538	4.98978	-0.55408
H	1.60106	5.36990	-2.28044

163

Coordination of the second CS_2 adduct

C	0.93602	4.62638	-4.69643
N	-0.09316	3.93940	-4.17573
N	-1.22579	4.41077	-4.76411
C	-0.92094	5.39157	-5.64696
C	0.45689	5.55793	-5.62618
Y	-0.18778	2.13226	-2.47693
N	-2.13040	3.72668	-1.92078
N	-2.93510	4.18513	-2.91629
C	-3.95932	4.90948	-2.40380
C	-3.80549	4.92607	-1.02628
C	-2.65307	4.17193	-0.76791
B	-2.63071	3.87535	-4.39386
N	-2.75033	2.35872	-4.65486
N	-2.01730	1.43980	-3.96358
C	-2.41351	0.22523	-4.37999
C	-3.40732	0.36646	-5.35599
C	-3.59936	1.73133	-5.50487
C	-1.86297	-1.04240	-3.81918
C	-4.54695	2.43666	-6.41835
C	-2.05004	3.86308	0.56061
C	-5.03237	5.54409	-3.22604
C	-1.92729	6.12250	-6.47371
C	2.35342	4.37756	-4.30141

O	0.97496	4.19867	-1.34321
C	2.24391	4.21203	-0.64170
C	2.22362	5.48393	0.18602
C	1.51944	6.45124	-0.76576
C	0.46905	5.56118	-1.42621
N	1.28970	0.88825	-3.73060
Si	2.56491	0.01249	-2.86944
C	4.09302	1.09918	-2.53271
P	-0.01682	0.02438	1.20940
C	-0.16726	1.29747	2.55184
Si	-0.86574	0.86146	4.28992
C	0.01371	2.16516	5.37028
P	1.31849	0.91034	-0.23515
C	1.87286	-0.58533	-1.20342
Si	1.38422	0.70946	-5.49845
C	0.90725	-1.03241	-6.11999
C	3.13636	1.08269	-6.17232
C	0.25906	1.83354	-6.53707
Y	-0.63825	-2.26351	2.97351
N	-0.50533	-0.82091	4.68012
Si	-0.18949	-1.21559	6.37902
C	1.49159	-0.56614	6.99213
C	3.22996	-1.59353	-3.65957
N	1.35465	-3.49846	3.50044
N	1.25460	-4.82768	3.78652
C	2.43300	-5.27646	4.28071
C	3.31581	-4.20305	4.30852
C	2.60201	-3.10925	3.80699
B	0.00220	-5.65313	3.38361
N	-1.27132	-5.25492	4.18340
N	-1.85122	-4.02928	4.04693
C	-3.00874	-4.04797	4.72573
C	-3.17611	-5.30486	5.31595
C	-2.05768	-6.04589	4.95073
C	2.67902	-6.68717	4.70320
C	3.06220	-1.70744	3.57327
C	-1.73116	-7.45850	5.30722
C	-3.91132	-2.85849	4.76788
N	-0.59294	-4.24354	1.36325
N	-0.26980	-5.46488	1.88062
C	-0.29057	-6.41016	0.91003
C	-0.63917	-5.77981	-0.27346
C	-0.82310	-4.42974	0.05407
C	-1.24116	-3.33174	-0.86420
C	0.02204	-7.85262	1.13731
C	-2.71346	1.27731	4.38743
C	-1.53926	-0.53723	7.54148
C	-0.13136	-3.08358	6.71329
S	-2.76778	-1.07068	1.53795
C	-1.75878	-0.08604	0.55602
S	-2.24648	0.61761	-0.87964
C	10.60526	-1.08636	-2.45258
S	11.64005	-0.07585	-1.86942
S	9.57070	-2.09578	-3.03555
H	0.23087	-6.80611	3.60637
H	-2.49855	-7.84898	5.97927
H	-0.76483	-7.53804	5.81375
H	-1.69432	-8.10372	4.42407
H	-4.00112	-5.63769	5.92929
H	-4.62239	-2.94806	5.59268
H	-4.48534	-2.76200	3.83952

H	-3.34309	-1.93302	4.90641
H	1.03506	-7.99574	1.52642
H	-0.05365	-8.39220	0.19053
H	-0.67117	-8.31687	1.84582
H	-0.74568	-6.23656	-1.24698
H	-2.28029	-3.03628	-0.68589
H	-1.14957	-3.66016	-1.90219
H	-0.62560	-2.43759	-0.73832
H	1.97564	-7.00796	5.47739
H	3.68971	-6.77327	5.10820
H	2.58826	-7.38602	3.86597
H	4.34222	-4.21822	4.64584
H	3.26393	-1.52796	2.51148
H	3.98286	-1.50915	4.12732
H	2.30496	-0.98616	3.89687
H	-1.10256	-3.56743	6.58157
H	0.17209	-3.22085	7.75842
H	0.60094	-3.60028	6.08685
H	1.57064	0.52263	6.95475
H	2.30778	-0.98736	6.39663
H	1.64674	-0.87793	8.03183
H	-1.61233	0.55426	7.52368
H	-1.32518	-0.83722	8.57401
H	-2.52129	-0.94254	7.27501
H	-0.28668	2.13552	6.42165
H	-0.24609	3.15917	4.98582
H	1.10263	2.06606	5.32175
H	-3.30041	0.66585	3.69708
H	-2.88564	2.33145	4.14079
H	-3.08483	1.10801	5.40388
H	0.88047	1.57079	2.73570
H	-0.66026	2.19588	2.16794
H	-3.43531	4.43862	-5.07777
H	-1.41324	6.84064	-7.11680
H	-2.49919	5.44385	-7.11336
H	-2.64345	6.67333	-5.85613
H	1.03650	6.24915	-6.22148
H	3.01771	4.55782	-5.15131
H	2.66915	5.04744	-3.49431
H	2.49262	3.34496	-3.97039
H	-5.61136	4.80030	-3.78243
H	-5.72034	6.08232	-2.56988
H	-4.62970	6.25651	-3.95256
H	-4.44732	5.41321	-0.30604
H	-0.98291	3.64449	0.46968
H	-2.17319	4.70897	1.24431
H	-2.53472	2.99179	1.01297
H	-4.02564	3.10173	-7.11361
H	-5.09763	1.69867	-7.00611
H	-5.27400	3.04097	-5.86723
H	-3.92237	-0.42319	-5.88397
H	-2.39508	-1.31808	-2.90299
H	-1.98015	-1.85587	-4.54021
H	-0.80062	-0.94010	-3.58188
H	0.57714	2.87822	-6.54421
H	0.31739	1.45916	-7.56703
H	-0.78689	1.79041	-6.22783
H	1.18476	-1.11782	-7.17766
H	1.38805	-1.85059	-5.58116
H	-0.17614	-1.17193	-6.05749
H	3.92018	0.43947	-5.76266

H 3.13801 0.95118 -7.26105
H 3.41792 2.12088 -5.96835
H 3.63452 -1.48086 -4.66823
H 4.03935 -1.96126 -3.01701
H 2.45759 -2.36869 -3.68590
H 3.83670 1.97389 -1.92706
H 4.85330 0.52998 -1.98508
H 4.54126 1.45016 -3.46804
H 1.04654 -1.26166 -1.45148
H 2.63191 -1.16173 -0.66071
H 3.05647 4.23814 -1.38009
H 2.31302 3.28433 -0.07094
H 3.22728 5.80851 0.47398
H 1.63512 5.33652 1.09864
H 1.06597 7.30943 -0.26192
H 2.22897 6.83539 -1.50735
H -0.48394 5.59433 -0.89417
H 0.28837 5.80243 -2.47520
163
Coordination of the second CS_2 TS
C 4.88984 15.43750 -4.86923
N 3.91076 14.74764 -4.26193
N 2.72963 15.23033 -4.73411
C 2.95418 16.22107 -5.62942
C 4.32884 16.38235 -5.73724
Y 3.98550 12.93293 -2.58767
N 2.09921 14.49242 -1.82659
N 1.21032 14.98207 -2.73177
C 0.25226 15.71068 -2.10966
C 0.53613 15.69523 -0.75275
C 1.69496 14.91918 -0.62017
B 1.36616 14.69199 -4.23625
N 1.22388 13.17872 -4.50271
N 2.03217 12.25476 -3.90828
C 1.60173 11.04304 -4.30162
C 0.50956 11.19315 -5.16442
C 0.29409 12.55863 -5.26904
C 2.21440 9.76769 -3.82874
C -0.74990 13.27054 -6.06476
C 2.41336 14.56788 0.63848
C -0.88107 16.38064 -2.81418
C 1.87732 16.96449 -6.34894
C 6.33670 15.17351 -4.61674
O 5.24466 14.91479 -1.55560
C 6.58086 14.89646 -0.98240
C 6.70088 16.19209 -0.20160
C 5.90027 17.15513 -1.07709
C 4.74120 16.28225 -1.54350
N 5.29973 11.69094 -3.98469
Si 6.62060 10.76642 -3.24919
C 8.19260 11.81460 -3.03754
P 4.43899 10.63799 1.11813
C 4.38333 11.92260 2.44674
Si 3.64061 11.56563 4.18639
C 4.57327 12.84753 5.24325
P 5.68023 11.56037 -0.43261
C 6.05569 10.13786 -1.54049
Si 5.24543 11.53591 -5.75937
C 4.68392 9.81037 -6.35501
C 6.94643 11.88597 -6.56053
C 4.05569 12.68580 -6.69036

Y	3.75503	8.37933	2.98405
N	3.89739	9.87728	4.63358
Si	4.09482	9.52578	6.36381
C	5.77179	10.09858	7.05685
C	7.17755	9.15610	-4.11002
N	5.55801	6.96562	3.69622
N	5.31906	5.64901	3.95861
C	6.41796	5.08990	4.51846
C	7.39153	6.07687	4.61592
C	6.81423	7.23600	4.08653
B	4.00877	4.95494	3.50621
N	2.75297	5.51481	4.23488
N	2.30718	6.78747	4.03032
C	1.13348	6.91422	4.67041
C	0.82167	5.70745	5.30443
C	1.86823	4.84209	5.00703
C	6.50718	3.65881	4.93433
C	7.41567	8.58894	3.90120
C	2.04036	3.42176	5.43339
C	0.35110	8.18540	4.63629
N	3.70874	6.36741	1.42353
N	3.83017	5.13074	1.98736
C	3.72037	4.16780	1.04036
C	3.52310	4.80274	-0.17554
C	3.51853	6.17441	0.10945
C	3.30944	7.29842	-0.84681
C	3.80991	2.70376	1.32006
C	1.81821	12.09344	4.21957
C	2.72911	10.33300	7.42014
C	4.01250	7.67221	6.76558
S	1.67851	9.60001	1.48670
C	2.67669	10.59052	0.51002
S	2.12926	11.37220	-0.86364
C	8.02700	11.55339	0.99282
S	8.01804	12.89324	1.86850
S	8.72402	10.20186	0.51559
H	4.09571	3.78974	3.76277
H	1.21692	3.13931	6.09303
H	2.97747	3.27191	5.97747
H	2.04158	2.73650	4.58022
H	-0.05054	5.48698	5.90290
H	-0.34624	8.22617	5.47666
H	-0.23182	8.26679	3.71215
H	1.00829	9.05847	4.69356
H	4.76941	2.43060	1.77010
H	3.70682	2.14964	0.38439
H	3.02013	2.36766	1.99929
H	3.40125	4.33399	-1.14150
H	2.27446	7.65501	-0.82162
H	3.53678	6.97540	-1.86579
H	3.95369	8.14747	-0.60762
H	5.73462	3.39807	5.66384
H	7.48132	3.47462	5.39252
H	6.39869	2.97974	4.08308
H	8.38928	5.96490	5.01508
H	7.81720	8.70993	2.88927
H	8.23891	8.74454	4.60261
H	6.67411	9.37703	4.06765
H	3.02979	7.23651	6.56748
H	4.21501	7.56144	7.83804
H	4.76632	7.09092	6.22772

H	5.93641	11.17252	6.94558
H	6.59879	9.57704	6.56527
H	5.82116	9.86101	8.12617
H	2.72419	11.42507	7.35398
H	2.87534	10.06841	8.47393
H	1.73828	9.97391	7.12246
H	4.24946	12.86629	6.28789
H	4.38184	13.84302	4.82459
H	5.65471	12.68245	5.21947
H	1.20966	11.49871	3.53305
H	1.72357	13.14749	3.93344
H	1.40884	11.98452	5.22916
H	5.44548	12.13085	2.63589
H	3.95472	12.85015	2.05521
H	0.49984	15.26428	-4.83144
H	2.33101	17.69292	-7.02487
H	1.24906	16.29522	-6.94415
H	1.22089	17.50512	-5.66013
H	4.85217	17.07873	-6.37700
H	6.91292	15.33237	-5.53261
H	6.74331	15.84886	-3.85650
H	6.49557	14.14299	-4.28795
H	-1.52085	15.65985	-3.33281
H	-1.49681	16.91275	-2.08539
H	-0.53381	17.10505	-3.55732
H	-0.02633	16.17636	0.03471
H	3.46331	14.33330	0.44469
H	2.37086	15.39766	1.35096
H	1.95654	13.69339	1.11307
H	-0.31063	13.95212	-6.79947
H	-1.35411	12.53742	-6.60398
H	-1.41953	13.85827	-5.42929
H	-0.05363	10.40804	-5.64813
H	1.79209	9.47551	-2.86157
H	2.01449	8.96630	-4.54486
H	3.29713	9.87005	-3.71595
H	4.36694	13.73223	-6.69482
H	4.04683	12.33507	-7.73039
H	3.03271	12.62619	-6.31319
H	4.95980	9.69294	-7.40988
H	5.11909	8.97751	-5.80047
H	3.59428	9.73114	-6.29388
H	7.74130	11.21442	-6.22481
H	6.85983	11.77549	-7.64817
H	7.27227	12.91189	-6.36014
H	7.49872	9.27417	-5.14757
H	8.03216	8.77112	-3.54063
H	6.39466	8.39171	-4.08002
H	8.01506	12.69552	-2.41323
H	8.98401	11.22790	-2.55922
H	8.56020	12.15812	-4.01015
H	5.18740	9.49255	-1.71418
H	6.85690	9.52572	-1.09582
H	7.30919	14.85861	-1.80181
H	6.67532	13.99429	-0.37809
H	7.74250	16.49110	-0.05997
H	6.23976	16.08595	0.78645
H	5.54932	18.04312	-0.54397
H	6.50521	17.49126	-1.92691
H	3.90127	16.32430	-0.84616
H	4.37677	16.52286	-2.54281

163

Coordination of the second CS_2 product

C	2.70745	-2.76547	4.03496
N	1.51620	-3.25683	3.65219
N	1.49136	-4.58362	3.97453
C	2.66153	-4.92799	4.56321
C	3.45852	-3.79132	4.61855
Y	-0.50582	-2.20805	2.97002
N	-0.61334	-0.67235	4.58003
Si	-0.36818	-0.98300	6.31595
C	-1.85017	-0.39629	7.36087
B	0.32388	-5.50684	3.54496
N	-1.01896	-5.16478	4.25859
N	-1.67071	-3.98818	4.03845
C	-2.86315	-4.05933	4.65067
C	-2.98083	-5.30045	5.28333
C	-1.79545	-5.97655	5.01360
C	-3.84300	-2.93388	4.58350
C	-1.39770	-7.34777	5.44989
C	2.98103	-6.30393	5.04645
C	3.08399	-1.34055	3.80375
N	-0.31421	-4.25956	1.42459
C	-0.51234	-4.55351	0.12871
C	-0.19714	-5.89745	-0.10905
C	0.19359	-6.41515	1.11491
N	0.11224	-5.41245	2.02227
C	-1.02855	-3.57339	-0.87004
C	0.63914	-7.80382	1.43565
S	-2.49275	-1.13231	1.23367
C	-1.42792	-0.15855	0.30710
P	0.13232	0.15408	1.24872
C	-0.38021	1.47459	2.41134
Si	-1.08335	0.97372	4.13977
C	-0.37858	2.36037	5.23530
S	-1.75865	0.39657	-1.23364
Y	0.13983	2.25091	-2.79759
N	1.50780	0.78759	-3.86413
Si	2.34913	-0.52561	-3.01410
C	1.84371	-0.58307	-1.16682
P	1.45626	1.00229	-0.33197
C	2.98098	1.50113	0.65508
S	2.74598	2.96123	1.47479
N	-0.34654	4.23585	-4.32807
C	0.38062	5.14611	-5.00384
C	-0.44430	6.18851	-5.43935
C	-1.71980	5.86239	-5.00652
N	-1.63578	4.68316	-4.34830
C	1.83402	4.99106	-5.29534
C	-2.98565	6.63173	-5.19536
B	-2.79954	3.89055	-3.72142
N	-2.66422	3.90650	-2.18093
N	-1.44296	3.88688	-1.56019
C	-1.65864	4.26848	-0.28917
C	-3.02613	4.49100	-0.08119
C	-3.63518	4.25383	-1.30190
C	-5.08289	4.34277	-1.65340
C	-0.56559	4.53176	0.69007
N	-1.87809	1.54863	-4.02823
N	-2.85168	2.46428	-4.29442
C	-3.82030	1.91135	-5.06073
C	-3.46613	0.59073	-5.28962

C	-2.25277	0.39876	-4.62092
C	-1.48032	-0.86955	-4.50810
C	-5.02442	2.64412	-5.55355
O	2.04675	3.70152	-2.32390
C	3.44210	3.26699	-2.32281
C	4.24426	4.41452	-1.71696
C	3.34205	5.63128	-1.93887
C	1.96213	5.03066	-1.74085
S	4.35046	0.54507	0.59898
C	-2.96445	1.22956	4.11252
Si	1.88411	0.89276	-5.60365
C	3.53088	1.78457	-5.96304
C	0.50537	1.75837	-6.58267
C	2.07985	-0.78004	-6.49785
C	1.89108	-2.30081	-3.54412
C	4.24089	-0.43535	-3.13300
C	-0.16741	-2.82494	6.72994
C	1.20402	-0.17218	7.01300
H	0.61470	-6.62972	3.83556
H	-2.17594	-7.76290	6.09400
H	-0.45994	-7.33987	6.01300
H	-1.26586	-8.02346	4.59932
H	-3.81617	-5.66547	5.86341
H	-4.55805	-2.99824	5.40726
H	-4.41129	-2.95808	3.64669
H	-3.33880	-1.96398	4.64666
H	1.64404	-7.81983	1.86872
H	0.65796	-8.39787	0.51918
H	-0.03257	-8.29887	2.14408
H	-0.24674	-6.42310	-1.05187
H	-0.45915	-2.64178	-0.86223
H	-2.07302	-3.31115	-0.67458
H	-0.95981	-3.99912	-1.87367
H	2.25643	-6.65351	5.78797
H	3.96858	-6.30341	5.51281
H	2.99285	-7.03092	4.22865
H	4.45658	-3.71957	5.02595
H	3.44274	-1.17595	2.78105
H	3.88702	-1.04134	4.48132
H	2.23240	-0.67394	3.97293
H	-1.07394	-3.40837	6.55125
H	0.06269	-2.88603	7.80076
H	0.66152	-3.29088	6.19038
H	1.20583	0.91660	6.93171
H	2.09504	-0.55112	6.50306
H	1.29713	-0.42930	8.07497
H	-2.02272	0.68206	7.29838
H	-1.67557	-0.64133	8.41512
H	-2.77101	-0.90177	7.05103
H	-0.70776	2.30818	6.27668
H	-0.72464	3.31887	4.82981
H	0.71514	2.37239	5.21581
H	-3.45508	0.57824	3.38405
H	-3.20147	2.26706	3.84943
H	-3.39165	1.03112	5.10117
H	0.54556	2.04006	2.59923
H	-1.07691	2.15300	1.91032
H	-3.82356	4.43736	-4.01407
H	-2.77025	7.55224	-5.74276
H	-3.72828	6.06429	-5.76428
H	-3.44235	6.90377	-4.23896

H	-0.15164	7.06121	-6.00552
H	1.98490	4.51703	-6.27118
H	2.32301	5.96893	-5.32668
H	2.32659	4.37929	-4.54139
H	-5.45333	3.39943	-2.06673
H	-5.66251	4.56729	-0.75522
H	-5.27956	5.12772	-2.39095
H	-3.50652	4.80021	0.83615
H	0.26990	3.82958	0.62483
H	-0.16333	5.54131	0.54210
H	-0.95325	4.49358	1.71104
H	-4.75296	3.47584	-6.21142
H	-5.65625	1.95808	-6.12229
H	-5.62076	3.05461	-4.73356
H	-4.01935	-0.14112	-5.86049
H	-1.80880	-1.43796	-3.63008
H	-1.64175	-1.49217	-5.39257
H	-0.41277	-0.66869	-4.40004
H	0.18669	2.71843	-6.17267
H	0.86335	1.92580	-7.60576
H	-0.38017	1.11787	-6.64090
H	2.15806	-0.56865	-7.57132
H	2.98593	-1.31890	-6.20684
H	1.22175	-1.44252	-6.35247
H	4.36917	1.26542	-5.48914
H	3.71082	1.78515	-7.04495
H	3.54702	2.82337	-5.62660
H	2.29513	-2.58975	-4.51589
H	2.30987	-2.98435	-2.79509
H	0.80858	-2.45787	-3.56260
H	4.64017	0.53470	-2.82854
H	4.67487	-1.18825	-2.46659
H	4.58469	-0.64987	-4.15059
H	0.94349	-1.20696	-1.13202
H	2.64254	-1.08304	-0.60137
H	3.71395	3.05334	-3.35968
H	3.52472	2.35012	-1.73756
H	5.22486	4.51486	-2.18975
H	4.39015	4.23973	-0.64672
H	3.53763	6.43889	-1.22825
H	3.45433	6.03035	-2.95235
H	1.73911	4.91799	-0.67714
H	1.14930	5.55494	-2.24770

163

CS insertion into the P-P bond TS

C	2.30525	-3.14663	5.27527
N	1.29796	-3.73478	4.61177
N	1.26177	-5.04372	4.99174
C	2.23676	-5.27993	5.90222
C	2.92067	-4.08810	6.10835
Y	-0.48471	-2.87119	3.23638
N	-1.07375	-1.15384	4.56262
Si	-1.37278	-1.27491	6.30404
C	-3.09950	-0.63415	6.79763
B	0.34309	-6.07282	4.27656
N	-1.16819	-5.81214	4.53499
N	-1.80888	-4.70732	4.05530
C	-3.11470	-4.84329	4.33559
C	-3.31927	-6.05156	5.00973
C	-2.06559	-6.64114	5.11840
C	-4.12051	-3.81207	3.94085

C	-1.71354	-7.94717	5.75068
C	2.48384	-6.60989	6.53393
C	2.65913	-1.71392	5.04609
N	0.45087	-4.89927	2.03218
C	0.79414	-5.19333	0.76907
C	1.19171	-6.53452	0.68640
C	1.07355	-7.04209	1.97085
N	0.62706	-6.03754	2.76327
C	0.75079	-4.18788	-0.33199
C	1.36638	-8.42416	2.45460
S	-2.29369	-2.38459	1.11032
C	-1.49542	-1.09312	0.31581
P	0.18804	-0.81387	1.29001
C	-0.32032	0.67453	2.25053
Si	-1.45120	0.38532	3.78725
C	-1.06538	1.93525	4.82993
S	-2.04471	-0.17221	-0.92061
Y	0.26445	2.52764	-3.32413
N	1.33012	0.95584	-4.55096
Si	2.08542	-0.43249	-3.73953
C	1.20015	-0.76816	-2.08698
P	0.88238	0.75746	-1.06064
C	2.41631	0.79836	-0.03993
S	3.60394	1.95703	0.02082
N	-0.55234	4.58913	-4.55972
C	-0.01272	5.46976	-5.42337
C	-0.92166	6.50212	-5.67719
C	-2.04947	6.20016	-4.92782
N	-1.80352	5.04437	-4.26755
C	1.34207	5.29525	-6.02550
C	-3.32216	6.97431	-4.82436
B	-2.75993	4.29071	-3.30791
N	-2.19800	4.31443	-1.87338
N	-0.91909	3.93064	-1.58447
C	-0.71104	4.22483	-0.29022
C	-1.86945	4.78888	0.26028
C	-2.79406	4.82889	-0.76982
C	-4.20248	5.32300	-0.72781
C	0.58765	3.99556	0.40438
N	-2.01797	1.91907	-3.89136
N	-3.00970	2.85566	-3.81173
C	-4.18038	2.33027	-4.24253
C	-3.94068	1.01546	-4.60909
C	-2.58126	0.79255	-4.37203
C	-1.83475	-0.48211	-4.57064
C	-5.47117	3.07899	-4.29500
O	2.13204	4.02364	-3.04635
C	3.52347	3.59453	-3.18864
C	4.35553	4.72341	-2.60208
C	3.47974	5.95323	-2.84793
C	2.08615	5.40494	-2.58971
S	2.41888	-0.55044	1.08790
C	-3.26407	0.54646	3.25541
Si	1.45592	1.12532	-6.30717
C	3.06840	1.99286	-6.84074
C	-0.03821	2.09663	-6.97914
C	1.42222	-0.46616	-7.35312
C	1.95217	-2.10989	-4.63773
C	3.93895	-0.18588	-3.40234
C	-1.29513	-3.06255	6.94307
C	-0.09658	-0.33375	7.35836

H	0.60456	-7.15967	4.70253
H	-2.61312	-8.39619	6.17760
H	-0.98120	-7.82683	6.55454
H	-1.29400	-8.65177	5.02612
H	-4.25569	-6.44957	5.37351
H	-5.03490	-3.93166	4.52722
H	-4.38518	-3.89797	2.88145
H	-3.74084	-2.79856	4.10313
H	2.14139	-8.43279	3.22740
H	1.71787	-9.03305	1.61852
H	0.47852	-8.90820	2.87376
H	1.52497	-7.06522	-0.19399
H	1.43679	-3.35732	-0.13628
H	-0.25291	-3.76978	-0.45172
H	1.04577	-4.65244	-1.27591
H	1.59339	-6.98929	7.04389
H	3.28376	-6.51857	7.27204
H	2.78614	-7.36082	5.79740
H	3.75833	-3.92913	6.77215
H	3.31848	-1.60444	4.17780
H	3.18084	-1.30160	5.91342
H	1.76315	-1.11080	4.86745
H	-2.10806	-3.68890	6.56614
H	-1.38315	-3.02414	8.03572
H	-0.34490	-3.54985	6.70707
H	-0.05192	0.73292	7.12594
H	0.90506	-0.75304	7.22244
H	-0.35553	-0.43584	8.41903
H	-3.22657	0.43679	6.61230
H	-3.26359	-0.80497	7.86817
H	-3.88661	-1.16424	6.25108
H	-1.66941	2.00583	5.73953
H	-1.28327	2.82313	4.22403
H	-0.00962	1.97892	5.11587
H	-3.55543	-0.25390	2.57018
H	-3.42551	1.50349	2.74641
H	-3.92450	0.51201	4.12811
H	0.60256	1.11845	2.64130
H	-0.79234	1.39822	1.57705
H	-3.80784	4.86668	-3.30851
H	-3.25564	7.86479	-5.45363
H	-4.18507	6.38899	-5.15544
H	-3.51917	7.29867	-3.79812
H	-0.78193	7.35522	-6.32574
H	1.27854	4.81786	-7.00916
H	1.82807	6.26580	-6.16189
H	1.98093	4.67506	-5.39564
H	-4.91485	4.53454	-0.98964
H	-4.43560	5.66303	0.28372
H	-4.36906	6.15912	-1.41394
H	-2.01638	5.12335	1.27731
H	1.35003	3.58413	-0.25863
H	0.96655	4.93303	0.82783
H	0.47323	3.29244	1.23382
H	-5.41548	3.94365	-4.96356
H	-6.25659	2.41616	-4.66483
H	-5.77287	3.44344	-3.30867
H	-4.66152	0.30496	-4.98692
H	-1.96235	-1.13573	-3.70044
H	-2.21991	-1.01199	-5.44671
H	-0.76707	-0.29561	-4.70661

H -0.29092 3.01533 -6.44482
H 0.14882 2.36066 -8.02703
H -0.92615 1.45579 -6.95462
H 1.28315 -0.16239 -8.39811
H 2.35219 -1.03756 -7.30084
H 0.59605 -1.13265 -7.09044
H 3.93739 1.41475 -6.50797
H 3.11699 2.06390 -7.93381
H 3.16781 3.00473 -6.43802
H 2.63619 -2.20921 -5.48391
H 2.22120 -2.88412 -3.90877
H 0.93863 -2.32553 -4.98805
H 4.12069 0.56075 -2.62461
H 4.37713 -1.12925 -3.05640
H 4.47344 0.11795 -4.30902
H 0.22340 -1.22480 -2.28832
H 1.78439 -1.49534 -1.51174
H 3.71395 3.44009 -4.25486
H 3.63784 2.65709 -2.64461
H 5.33990 4.79118 -3.07260
H 4.49588 4.55834 -1.52904
H 3.71591 6.79033 -2.18542
H 3.57581 6.29995 -3.88273
H 1.84623 5.40368 -1.52330
H 1.28764 5.90742 -3.13701
163
CS insertion into the P-P bond porduct
C 2.66909 -3.26906 5.91683
N 1.73457 -4.15728 5.54444
N 2.10574 -5.37702 6.02890
C 3.26725 -5.25779 6.71585
C 3.65291 -3.92360 6.66669
Y -0.43324 -3.92981 4.53247
N -1.16085 -2.18800 5.74546
Si -1.13465 -2.15385 7.51731
C -2.85586 -1.81707 8.26275
B 1.37115 -6.67701 5.59836
N -0.08718 -6.75592 6.14003
N -1.06184 -5.90524 5.71061
C -2.22714 -6.32173 6.23015
C -2.00077 -7.45780 7.01307
C -0.63493 -7.70674 6.93263
C -3.50999 -5.61334 5.93883
C 0.14172 -8.80507 7.58063
C 3.96390 -6.39760 7.38276
C 2.59618 -1.83741 5.49704
N 0.75647 -5.80927 3.29028
C 0.93141 -6.17776 2.01142
C 1.65029 -7.37991 1.95954
C 1.90465 -7.72565 3.27668
N 1.35802 -6.76428 4.06048
C 0.41409 -5.38756 0.85613
C 2.63759 -8.91745 3.79875
S -2.52504 -3.92722 2.64812
C -1.91481 -2.73462 1.54491
P -0.43572 -1.96741 2.37975
C -1.15097 -0.51060 3.21241
Si -1.96874 -0.84328 4.93044
C -1.76703 0.85204 5.77478
S -2.51958 -2.32809 0.07544
Y 0.15549 2.62749 -3.12859

N	0.90447	0.91415	-4.38249
Si	1.28655	-0.65356	-3.63103
C	0.12434	-0.97086	-2.14651
P	0.01071	0.56762	-1.15152
C	0.67512	0.36656	0.44419
S	1.04233	1.64902	1.47909
N	0.84241	4.68036	-4.23754
C	2.03365	5.14035	-4.65470
C	1.85591	6.36040	-5.31436
C	0.49006	6.61217	-5.28002
N	-0.09883	5.58340	-4.62679
C	3.30760	4.39058	-4.43667
C	-0.24832	7.77872	-5.84850
B	-1.60061	5.40048	-4.29072
N	-1.83187	5.34195	-2.76491
N	-1.43929	4.26446	-2.01556
C	-2.02148	4.39579	-0.81196
C	-2.76973	5.58100	-0.77716
C	-2.63508	6.15243	-2.03135
C	-3.24208	7.41812	-2.54130
C	-1.91223	3.37392	0.26771
N	-1.82910	2.87435	-4.49073
N	-2.18924	4.11555	-4.92967
C	-3.25793	4.01527	-5.75810
C	-3.59844	2.67301	-5.84627
C	-2.68778	1.99326	-5.02801
C	-2.64661	0.54075	-4.68703
C	-3.91087	5.18105	-6.42402
O	1.88583	3.49577	-1.67986
C	3.05190	2.76976	-1.19273
C	3.73188	3.69085	-0.17826
C	3.14966	5.07318	-0.49096
C	1.73816	4.72881	-0.93120
S	1.06559	-1.33114	1.01660
C	-3.82913	-1.11057	4.69372
Si	1.16369	1.00819	-6.13774
C	2.93844	0.49840	-6.61183
C	0.94174	2.75372	-6.86133
C	-0.05139	-0.02678	-7.17824
C	1.05037	-2.18905	-4.73410
C	3.07487	-0.71837	-2.99483
C	-0.57438	-3.80905	8.26586
C	0.06816	-0.86919	8.24290
H	1.97505	-7.60855	6.04419
H	-0.52820	-9.40665	8.19891
H	0.93787	-8.41625	8.22243
H	0.60729	-9.46578	6.84305
H	-2.73077	-8.02924	7.56806
H	-4.25343	-5.83696	6.70781
H	-3.92247	-5.92158	4.97183
H	-3.37173	-4.52743	5.90734
H	3.51412	-8.63391	4.38976
H	2.98062	-9.52688	2.95954
H	2.00265	-9.54489	4.43237
H	1.94649	-7.92604	1.07538
H	-0.67376	-5.28364	0.89742
H	0.67647	-5.88442	-0.08095
H	0.84212	-4.38006	0.82838
H	3.31538	-6.90665	8.10191
H	4.83797	-6.02377	7.92058
H	4.30493	-7.14556	6.66021

H	4.53565	-3.48849	7.11275
H	2.94207	-1.71229	4.46477
H	3.22620	-1.21560	6.13763
H	1.56967	-1.46179	5.55502
H	-1.28851	-4.61892	8.09510
H	-0.48839	-3.66516	9.34981
H	0.40602	-4.12930	7.90051
H	-0.15621	0.15243	7.92775
H	1.10057	-1.09399	7.95731
H	0.01431	-0.90219	9.33775
H	-3.25220	-0.83154	7.99926
H	-2.80249	-1.86830	9.35667
H	-3.57988	-2.56795	7.92885
H	-2.22527	0.89980	6.76705
H	-2.25667	1.60846	5.15000
H	-0.71326	1.13263	5.86693
H	-4.03308	-2.02262	4.12643
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H	-1.83684	0.00971	2.53440
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H	0.45953	8.45222	-6.33676
H	-0.98829	7.46801	-6.59194
H	-0.77725	8.34428	-5.07556
H	2.61624	6.97576	-5.77375
H	3.99036	4.55757	-5.27437
H	3.81707	4.71692	-3.52462
H	3.13208	3.31417	-4.35747
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H	-3.34709	5.96273	0.05273
H	-0.87743	3.14255	0.54524
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H	-2.37272	2.42982	-0.04160
H	-3.19449	5.77628	-6.99783
H	-4.67988	4.82191	-7.11156
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H	-4.40672	2.24581	-6.42219
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H	-3.12541	-0.05345	-5.46906
H	-1.61426	0.19871	-4.57296
H	1.75047	3.44196	-6.60762
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H	3.66998	1.12745	-6.09277
H	1.65415	-2.18746	-5.64567
H	1.34604	-3.06436	-4.14350
H	0.00185	-2.32569	-5.01573
H	3.24240	0.01650	-2.20275
H	3.29889	-1.70875	-2.58298
H	3.78574	-0.51800	-3.80309
H	-0.87747	-1.25697	-2.48663
H	0.50247	-1.79914	-1.53837
H	3.67989	2.55802	-2.06360

H 2.70606 1.83725 -0.74112
H 4.82149 3.65837 -0.26304
H 3.45431 3.38171 0.83313
H 3.15618 5.74168 0.37423
H 3.69831 5.56330 -1.30278
H 1.08617 4.53670 -0.07288
H 1.27241 5.45830 -1.59632
163
C-S activation TS
C 2.54504 -4.18265 5.50502
N 1.36935 -4.55379 4.97799
N 1.13927 -5.84553 5.34344
C 2.16309 -6.28880 6.11183
C 3.07745 -5.24977 6.23875
Y -0.34339 -3.33018 3.80077
N -0.50897 -1.55513 5.17844
Si -0.64319 -1.65492 6.93650
C -2.18543 -0.75977 7.61384
B -0.02515 -6.66376 4.71731
N -1.42652 -6.13608 5.13904
N -1.90037 -4.92782 4.72236
C -3.17386 -4.82810 5.13243
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C 0.38592 -7.17123 1.05944
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C 0.35209 -9.10864 2.78225
S -2.16118 -2.43654 1.82919
C -1.01013 -1.54134 0.91298
P 0.61656 -1.45374 1.86014
C 0.34401 0.12098 2.79874
Si -0.67724 0.03501 4.42553
C 0.05558 1.47860 5.43735
S -1.30887 -0.88711 -0.58637
Y 0.17064 2.93350 -3.72473
N 1.40640 1.50075 -4.92520
Si 2.52260 0.36790 -4.12107
C 1.70679 -0.27326 -2.52077
P 0.94824 1.08340 -1.53851
C 2.09601 1.70387 -0.50250
S 2.86247 2.48872 0.62443
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C 1.91243 5.53574 -5.93915
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N -2.58916 4.70961 -2.92450
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N	-2.91898	3.12013	-4.85085
C	-4.00230	2.49135	-5.36670
C	-3.75022	1.12724	-5.34236
C	-2.47640	0.98190	-4.78293
C	-1.75096	-0.27892	-4.45565
C	-5.22368	3.19716	-5.85504
O	1.59740	4.65587	-2.74491
C	3.03100	4.55117	-2.50241
C	3.38324	5.75022	-1.63694
C	2.37651	6.80083	-2.10694
C	1.12227	5.96912	-2.32572
S	2.29534	-1.32890	0.73401
C	-2.48151	0.51373	4.07745
Si	1.33999	1.40993	-6.70265
C	3.03742	1.80013	-7.47234
C	0.10354	2.64162	-7.46055
C	0.75159	-0.25860	-7.40325
C	2.96103	-1.22455	-5.06523
C	4.18881	1.17075	-3.69083
C	-0.79038	-3.44528	7.55995
C	0.86571	-0.94645	7.85955
H	0.06969	-7.79327	5.10149
H	-3.14708	-8.44326	6.92309
H	-1.41331	-8.17286	7.14917
H	-2.00074	-8.91074	5.65799
H	-4.47890	-6.21558	6.28806
H	-4.85337	-3.56567	5.51724
H	-4.40605	-3.66860	3.80799
H	-3.42755	-2.70254	4.91637
H	1.18510	-9.28886	3.46932
H	0.49215	-9.74984	1.90877
H	-0.56543	-9.42543	3.28853
H	0.53615	-7.73016	0.14676
H	-0.68153	-4.28051	-0.02834
H	0.54948	-5.25281	-0.84929
H	1.03351	-3.98199	0.28132
H	1.36517	-7.89656	7.30394
H	3.12845	-7.74645	7.31632
H	2.30311	-8.42964	5.90784
H	4.00848	-5.27085	6.78686
H	3.62393	-2.80495	4.26308
H	3.85390	-2.56306	6.00193
H	2.33829	-2.06557	5.22663
H	-1.72510	-3.92604	7.25844
H	-0.76949	-3.41793	8.65640
H	0.04219	-4.07368	7.23098
H	1.03071	0.11319	7.64996
H	1.77815	-1.49040	7.59538
H	0.71697	-1.05582	8.94051
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H	-0.45700	1.64414	6.38982
H	-0.04048	2.39884	4.84824
H	1.12010	1.32656	5.64216
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H	-2.52823	1.50178	3.60431

H -3.05557 0.55916 5.00884
H 1.35870 0.41470 3.09527
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H 2.22458 4.51615 -5.69823
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H 0.45775 6.34641 -3.10412
163
C-S activation product
N 0.95540 -4.53363 5.87112
N 0.65886 -3.47257 5.06776
C 1.16938 -2.37198 5.64123
C 1.79372 -2.72588 6.84228
C 1.64188 -4.10284 6.95638
Y -0.83784 -3.82215 3.22054
N -2.32763 -2.19716 3.65344
Si -3.07870 -1.97346 5.24463
C -2.56501 -3.31956 6.48444

C	1.06946	-1.03414	4.98437
C	2.12483	-4.99869	8.04855
B	0.69655	-5.99635	5.41209
N	-0.81976	-6.33325	5.30663
N	-1.62220	-5.75263	4.36974
C	-2.82336	-6.34918	4.43298
C	-2.79826	-7.32592	5.43293
C	-1.51384	-7.29060	5.96497
C	-3.93777	-5.96466	3.51568
C	-0.94658	-8.12941	7.06194
P	-0.25341	-2.14170	0.89206
C	-1.55486	-0.86374	1.04016
Si	-2.95653	-1.21312	2.32610
C	-3.47898	0.55435	2.80476
C	-1.00295	-3.38962	-0.26816
S	-1.84787	-4.54922	0.69770
S	-0.87063	-3.35491	-1.90498
S	1.43988	-1.22618	0.02341
P	0.70934	-0.21005	-1.76232
C	1.73552	-0.78981	-3.15687
Si	2.22471	0.61234	-4.39302
C	3.10542	-0.34636	-5.79120
Y	0.44546	3.34219	-3.26649
N	0.40323	4.87043	-5.24001
C	1.22371	5.00831	-6.29580
C	0.62914	5.85087	-7.24365
C	-0.59803	6.21511	-6.70765
N	-0.70760	5.61405	-5.49748
C	2.55978	4.34402	-6.36513
C	-1.64552	7.09142	-7.31203
B	-1.85662	5.75799	-4.47300
N	-1.33170	6.33914	-3.14634
N	-0.49379	5.63149	-2.33761
C	-0.32848	6.37129	-1.22782
C	-1.05541	7.56608	-1.33443
C	-1.68756	7.51084	-2.56506
C	0.49177	5.95403	-0.05100
C	-2.59658	8.51975	-3.18668
O	2.51334	4.76333	-2.80127
C	2.60049	6.16106	-3.19814
C	3.98788	6.61332	-2.77463
C	4.19185	5.81757	-1.48560
C	3.57457	4.47406	-1.84835
N	-1.96539	3.36860	-3.56992
N	-2.57948	4.41960	-4.18653
C	-3.89834	4.15703	-4.34241
C	-4.14269	2.89961	-3.80886
C	-2.90975	2.44208	-3.33382
C	-4.87438	5.08955	-4.98052
C	-2.61732	1.14411	-2.66140
N	0.96004	1.71509	-4.87082
Si	0.05976	1.27140	-6.32412
C	-1.49631	2.30631	-6.65850
C	-0.57775	-0.52727	-6.23803
C	1.04866	1.45751	-7.94815
C	0.82622	1.49220	-1.70480
S	0.55884	2.65114	-0.53666
C	3.67205	1.48255	-3.50881
N	1.05326	-5.49213	2.94543
C	1.83439	-5.93170	1.94539
C	2.66620	-6.95850	2.41211

C	2.35071	-7.12315	3.75078
N	1.37820	-6.22770	4.05086
C	1.78051	-5.38305	0.55833
C	2.93612	-8.08714	4.72964
C	-4.44059	-1.98050	1.43352
C	-2.60422	-0.33631	6.09185
C	-4.98121	-2.04904	5.17106
H	1.17651	-6.72982	6.22611
H	-1.72636	-8.78280	7.45928
H	-0.56447	-7.51790	7.88455
H	-0.12363	-8.75897	6.70997
H	-3.60534	-7.97803	5.73432
H	-4.90404	-6.21245	3.96202
H	-3.86343	-6.49488	2.55983
H	-3.92871	-4.89147	3.29946
H	3.40259	-7.57851	5.57913
H	3.70340	-8.68479	4.23238
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H	1.89950	-4.29518	0.54043
H	1.30575	-5.56553	8.50100
H	2.59267	-4.39727	8.83105
H	2.86461	-5.71995	7.68775
H	2.29647	-2.07085	7.53918
H	1.87171	-0.89633	4.25046
H	1.15460	-0.23351	5.72322
H	0.11220	-0.92049	4.46543
H	-2.93551	-4.31294	6.21790
H	-3.00187	-3.05238	7.45444
H	-1.48120	-3.37826	6.62057
H	-2.89651	0.54399	5.51506
H	-1.52555	-0.28316	6.26910
H	-3.10183	-0.27819	7.06723
H	-5.41741	-1.24699	4.56793
H	-5.39234	-1.95986	6.18341
H	-5.32244	-3.00345	4.75627
H	-4.33223	0.57813	3.48906
H	-3.77641	1.08669	1.89335
H	-2.65611	1.11308	3.26115
H	-4.19748	-2.95642	1.00583
H	-4.76929	-1.32423	0.61944
H	-5.28080	-2.10298	2.12487
H	-1.03235	0.03033	1.40345
H	-1.96531	-0.62748	0.05152
H	-2.65853	6.51777	-4.93250
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H	-1.85978	7.96658	-6.69118
H	1.03348	6.14903	-8.20058
H	2.91149	4.30962	-7.39919
H	3.31439	4.88172	-5.77878
H	2.48676	3.32211	-5.98166
H	-3.59845	8.11620	-3.36334
H	-2.69301	9.37905	-2.51880
H	-2.21518	8.88027	-4.14714
H	-1.11824	8.36155	-0.60521
H	1.36872	5.37841	-0.34649
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H	-0.08820	5.32690	0.63476

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H -5.85418 4.60869 -5.02643
H -4.98107 6.02079 -4.41564
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H -1.84057 0.57984 -3.18445
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H 3.67084 0.33641 -6.43448
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163
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C -1.37260 -4.47644 4.45906
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S 2.15176 -0.70633 2.25865
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C	-4.94839	-5.35337	4.09570
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S	-0.77144	-2.29429	-0.23161
C	-0.67575	-2.32061	1.41184
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Y	3.08104	3.56118	-1.60440
N	2.21042	5.27507	-3.05977
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B	3.96667	4.58787	-4.79286
N	5.23729	4.42220	-3.91822
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C	7.32685	4.21657	-3.21146
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C	6.75826	3.02104	-0.95845
C	6.94361	5.36017	-5.50901
C	2.87393	7.24809	-6.06924
C	0.13075	6.03856	-1.93123
C	-0.71638	-1.04598	3.84769
Si	-2.50773	-0.59103	3.26865
C	-2.28376	0.76930	1.96629
C	-3.10683	0.26504	4.87215
P	1.52634	1.32985	1.91278
C	3.14549	2.13697	2.30770
Si	3.55568	4.00690	2.00563
C	5.24713	3.99886	2.89329
S	0.64964	2.66936	-0.58273
N	3.64070	4.61575	0.33996
Si	4.02335	6.35666	0.24082
C	2.47910	7.46821	0.35567
N	2.70602	2.56282	-3.94613
C	2.10859	1.47744	-4.46271
C	2.32119	1.43514	-5.84963
C	3.07310	2.55692	-6.15184
N	3.28896	3.22249	-4.98996
C	1.33194	0.49282	-3.65308
C	3.58065	3.00727	-7.48218
C	5.22119	7.03462	1.56185
C	4.88403	6.82370	-1.38817
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H	3.16508	3.97663	-7.77565
H	3.29795	2.27657	-8.24347
H	4.67129	3.10022	-7.49354
H	1.96582	0.68512	-6.54189
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H	0.80891	0.97825	-2.82604
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H	-0.42082	-3.95842	4.29581
H	-6.19620	-2.61590	0.81954
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H	-6.96305	-1.87962	4.77885
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163
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C	6.46988	2.62984	-0.46330
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C	-0.22801	5.02513	-2.15936
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Si	-2.86186	-0.65053	4.28119
C	-3.04510	1.10340	3.58930
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P	1.30195	1.75084	2.67651
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Si	3.27661	4.35679	2.02707
C	4.97243	4.63395	2.86673
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Si	3.65061	6.13478	-0.31421
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C	1.26840	-0.68408	-2.59537
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C	-5.72847	-3.04268	5.23010
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163
C - C coupling product
C -0.70715 -5.35911 3.02468
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C	0.12023	-5.56638	4.28335
Y	-2.49462	-2.68842	1.55652
N	-3.86141	-1.69482	3.05018
Si	-5.52571	-2.24504	3.34480
C	-6.82094	-0.85449	3.49587
N	-3.71409	-2.35845	-0.53283
C	-4.61169	-1.44792	-0.95351
C	-4.98750	-1.73798	-2.26967
C	-4.26783	-2.86654	-2.62997
N	-3.50573	-3.22112	-1.56814
C	-5.08247	-0.31020	-0.11153
B	-2.54010	-4.41720	-1.45831
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C	-3.71849	-6.06560	1.59073
C	-4.13166	-6.01969	3.02422
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S	1.82349	0.37243	0.15361
Y	2.29483	2.80836	-1.10145
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C	2.04216	5.46070	-4.78209
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C	1.01753	5.55240	-2.81131
B	3.11010	3.09498	-4.52882
N	4.36170	2.68074	-3.72002
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C	5.47434	1.79425	-2.07182
C	6.36594	1.94074	-3.14155
C	5.62676	2.50921	-4.17132
C	5.73679	1.26726	-0.69997
C	6.08671	2.88908	-5.54015
C	2.53252	5.71336	-6.16965
C	0.11769	5.88467	-1.66508
C	-1.51690	0.03976	4.05055
Si	-3.41971	-0.20289	3.89495
C	-4.09112	1.38886	3.11541
C	-3.93361	-0.19319	5.73175
P	1.29436	1.83418	2.91102
C	3.05050	2.16613	2.56449
Si	3.66313	3.90515	1.98039
C	5.41844	3.81347	2.73965
S	0.07559	2.91508	0.49321
N	3.60973	4.13797	0.23859

Si	4.37259	5.63484	-0.33963
C	3.16953	7.11339	-0.40741
N	1.41837	1.68071	-3.30956
C	0.47867	0.77447	-3.61313
C	0.54096	0.46128	-4.98053
C	1.56356	1.23886	-5.49685
N	2.07053	1.96606	-4.47191
C	-0.48244	0.24416	-2.60833
C	2.06388	1.31336	-6.90212
C	5.83072	6.30519	0.69947
C	5.13938	5.46874	-2.06654
C	2.67647	5.20394	2.95113
C	-6.18319	-3.29698	1.90278
C	-5.67619	-3.24888	4.95831
H	-2.55746	-4.99814	-2.50324
H	3.44793	3.27634	-5.66314
H	-4.97426	-3.09324	-4.61695
H	-4.64643	-4.63162	-3.80757
H	-3.30792	-3.64475	-4.39775
H	-5.69044	-1.19324	-2.88336
H	-4.85135	-0.47057	0.94314
H	-6.16408	-0.18138	-0.21795
H	-4.60746	0.62661	-0.42255
H	0.89156	-4.60801	-3.85350
H	-0.72045	-3.90086	-4.00468
H	-0.54388	-5.59076	-3.52428
H	2.14552	-3.91294	-1.60489
H	1.90416	-2.12884	1.08972
H	2.39979	-3.82069	1.23995
H	0.98400	-3.22044	2.12806
H	-3.82908	-7.05913	-2.56931
H	-3.48270	-8.50581	-1.61140
H	-2.16261	-7.45474	-2.14430
H	-4.10371	-8.16883	0.96821
H	-3.65202	-5.19220	3.54856
H	-3.86654	-6.95294	3.53036
H	-5.21502	-5.89273	3.11915
H	5.56485	2.32753	-6.32123
H	7.15596	2.68477	-5.63263
H	5.92787	3.95337	-5.73908
H	7.41260	1.67268	-3.16613
H	6.71799	0.78817	-0.65503
H	4.98128	0.53332	-0.40064
H	5.71254	2.08202	0.03126
H	1.93709	2.31144	-7.33380
H	1.50901	0.60578	-7.52303
H	3.12690	1.06053	-6.97117
H	-0.08742	-0.23114	-5.52292
H	-0.01982	-0.51480	-1.96981
H	-1.34755	-0.19872	-3.11025
H	-0.83537	1.03910	-1.94774
H	2.18936	6.69588	-6.50216
H	2.15790	4.96719	-6.87772
H	3.62475	5.69769	-6.22332
H	0.66167	7.13262	-4.34307
H	-0.82827	5.33750	-1.74589
H	-0.11140	6.95331	-1.65446
H	0.56722	5.62818	-0.70217
H	-0.12673	-5.22847	2.11105
H	-1.42491	-6.17070	2.87202
H	1.05696	-5.00113	4.23035

H 0.36532 -6.61969 4.44275
H -1.58727 -5.69687 5.62062
H -0.26578 -4.71742 6.28246
H -2.36777 -3.47132 4.99174
H -0.69782 -2.90308 4.74568
H -6.43329 -2.65364 1.05374
H -7.10816 -3.79021 2.22508
H -5.50373 -4.06797 1.53451
H -4.96235 -4.07547 5.01172
H -6.68396 -3.67127 5.04788
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H -1.23021 -0.38477 5.02212
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H 3.53232 2.07761 3.54784
H 6.03115 3.06417 2.22589
H 5.33053 3.50247 3.78762
H 5.96208 4.75821 2.72406
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H 6.65454 5.59125 0.78684
H 5.54451 6.63398 1.70286
H 5.89676 4.67888 -2.09457
H 5.63083 6.41869 -2.31009
H 4.40196 5.26576 -2.84469
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163
Final C - S activation TS
C -3.66160 29.23954 1.42391
N -2.81604 28.34829 1.97342
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C -3.61156 27.46622 0.08616
C -4.18520 28.71859 0.23495
Y -1.50668 28.33168 4.07344
P 0.60025 30.23420 5.16965
C -0.54849 31.21832 6.22858
Si -2.44066 31.13247 5.97219
C -3.07232 31.50097 7.73449
B -1.90869 26.03428 1.42408
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N -2.39922 25.99706 3.92902
C -2.84747 25.11506 4.84018
C -3.07488 23.87742 4.22781
C -2.74887 24.05594 2.89154
C -3.09119 25.47154 6.26879
C -2.80589 23.05351 1.78624
C -3.82852 26.47708 -1.01117
C -3.95811 30.56979 2.02848

S	-0.64186	30.75065	2.55891
C	0.58629	31.18053	3.57892
C	1.72662	32.08841	3.28860
P	1.96590	33.29071	4.66010
S	1.07834	34.34934	2.97346
Y	3.40628	34.46936	1.39898
N	4.67921	35.70041	2.81279
Si	5.65419	37.13149	2.40600
C	7.16732	37.42629	3.53250
N	2.38295	33.67810	-0.85877
C	1.33057	32.94178	-1.24350
C	1.35090	32.77004	-2.63664
C	2.46707	33.45472	-3.08222
N	3.06929	33.99704	-1.99480
C	0.31656	32.41524	-0.29240
B	4.20817	35.02589	-1.96251
N	5.42738	34.43617	-1.21241
N	5.31412	33.91642	0.04166
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C	7.38561	33.53394	-0.70835
C	6.67478	34.21698	-1.68845
C	2.97101	33.60856	-4.47943
C	6.73586	32.72898	1.68732
C	7.14691	34.65862	-3.03416
N	3.06195	36.32166	-0.08551
N	3.64475	36.33024	-1.31883
C	3.35682	37.49746	-1.94594
C	2.56330	38.25339	-1.09311
C	2.39239	37.47446	0.05785
C	3.83867	37.84996	-3.31435
C	1.56605	37.75937	1.26958
S	2.86787	31.65381	2.09014
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Si	4.54927	35.29452	4.52045
C	3.48972	36.51521	5.51410
C	6.17738	35.02865	5.47550
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N	-0.41593	26.40876	1.48175
C	0.56584	25.98510	0.64904
C	1.76647	26.47064	1.13930
C	1.44288	27.19848	2.29129
C	0.33798	25.15052	-0.56838
C	2.39257	27.92155	3.18216
O	-0.34459	27.06993	5.85464
C	-0.12320	27.57324	7.20206
C	0.45042	26.39835	7.97620
C	1.28421	25.70427	6.89718
C	0.38882	25.82667	5.67278
N	-2.93705	29.55401	5.33176
Si	-4.63627	29.14375	5.65606
C	-5.30885	27.82832	4.46074
C	-4.90740	28.50530	7.43304
C	-5.85380	30.59758	5.44718
S	2.44528	30.29543	5.99730
C	-2.93348	32.62318	4.90421
C	6.41143	37.04844	0.67090
C	4.67933	38.76516	2.51173
H	-2.06363	25.25669	0.52861
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H	-4.24197	25.53555	-0.63669

H	-2.90050	26.24107	-1.54050
H	-4.89319	29.19238	-0.42987
H	-3.71691	30.58241	3.09277
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H	-0.32217	25.64856	-1.28526
H	-0.10953	24.18095	-0.32914
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H	2.04117	27.99326	4.21320
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H	2.95260	34.65112	-4.81290
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H	0.60041	28.39430	7.14809
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H 7.75621 38.22885 3.07195
H 7.81403 36.54863 3.62025
H 6.90143 37.76037 4.53971
H 7.06091 36.17511 0.55563
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H 5.66122 37.02769 -0.12105
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163
Final product
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N -2.37578 -5.55972 -0.94250
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C -3.31974 -4.96954 -2.85305
Y -2.46854 -3.08180 1.32375
P -1.23286 -0.28278 2.12980
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Si -4.35753 -0.08911 1.37216
C -5.69269 0.76520 2.43621
B -1.64024 -6.33259 0.17041
N -2.54853 -6.48492 1.41419
N -3.05735 -5.40729 2.06976
C -3.78163 -5.88238 3.09718
C -3.73353 -7.28157 3.10248
C -2.94153 -7.63131 2.01824
C -4.51928 -4.99566 4.04440
C -2.56391 -8.99854 1.55145
C -2.30741 -7.34815 -2.71516
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P 1.20125 1.67797 1.54604
S 0.95058 3.65970 1.22543
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N 4.36293 3.21625 -0.18734
Si 5.92745 3.79592 -0.79235
C 7.00474 2.39975 -1.51261
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C -0.57955 5.25813 -4.35119
N 0.58346 5.03466 -3.69224
C -1.55973 3.03286 -1.58810
B 1.98679 5.56433 -4.02891
N 2.92386 4.37386 -4.38132
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C	3.54417	4.12346	-5.55857
C	-0.69927	6.10657	-5.57433
C	4.10504	1.04691	-3.60342
C	3.57700	5.07680	-6.70726
N	2.60351	5.89234	-1.58026
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C	2.82218	7.72362	-2.82225
C	3.11093	8.07098	-1.50867
C	2.95884	6.89662	-0.76300
C	2.82606	8.59937	-4.03169
C	3.12944	6.70097	0.70666
S	1.41975	0.88013	-1.28534
C	2.94791	1.22760	1.75988
Si	4.40615	2.45334	1.38979
C	4.39344	3.66103	2.85690
C	5.86473	1.25563	1.66473
N	-0.30167	-4.38982	1.10678
N	-0.31999	-5.63483	0.55384
C	0.94359	-6.09926	0.39802
C	1.80647	-5.12325	0.87239
C	0.98790	-4.06979	1.29864
C	1.28513	-7.42931	-0.18879
C	1.41650	-2.75548	1.85794
O	-1.86290	-3.23939	3.76517
C	-2.24492	-2.28998	4.79211
C	-1.80624	-2.90485	6.11438
C	-0.58673	-3.72548	5.69131
C	-1.03611	-4.28192	4.35035
N	-4.38950	-1.85690	1.46624
Si	-6.03352	-2.52969	1.35830
C	-6.05758	-4.34192	0.78704
C	-6.98972	-2.44089	3.00867
C	-7.15972	-1.66673	0.08080
S	0.16963	0.96071	3.26088
C	-4.48424	0.62834	-0.37548
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H	1.92345	6.27651	-4.98871
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H	-2.76325	-8.14792	-2.12357
H	-1.22616	-7.51640	-2.71786
H	-3.68915	-4.98262	-3.86836
H	-4.30658	-2.10605	-1.21882
H	-4.89070	-2.66183	-2.80375
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H	1.49913	-2.00648	1.06354
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H	0.70049	-2.37437	2.59236
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H	-3.01819	-9.74382	2.20836
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H	-4.22030	-7.95411	3.79445
H	-4.47356	-3.95202	3.73080
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H	4.01483	6.03876	-6.42447
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H	-1.30681	1.98560	-1.78364
H	-2.64713	3.13619	-1.61674
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H	3.15499	9.60258	-3.75108
H	1.83046	8.68201	-4.47863
H	3.50303	8.22482	-4.80521
H	3.39310	9.04805	-1.14337
H	2.16433	6.71478	1.22526
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H	0.28756	-3.07709	5.56826
H	-0.32932	-4.51703	6.40003
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H	-6.38699	-2.75537	3.86507
H	-7.86968	-3.09329	2.96037
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H	-6.70958	0.62177	2.06085
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H	-5.38558	0.29424	-0.89554
H	-2.61360	1.69269	1.69996
H	-2.99677	0.84249	3.20349
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H	5.23855	4.35358	2.81016
H	4.46650	3.10724	3.80071
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H	7.99643	2.79265	-1.76688
H	6.56073	2.00706	-2.43213
H	7.14048	1.56535	-0.82020
H	5.24898	4.68083	-3.06374
H	6.79628	5.32638	-2.50722
H	5.28529	5.99261	-1.86963

H	6.44303	5.55005	0.94082
H	7.89918	5.03867	0.07961
H	7.25194	4.03781	1.38108

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