Supporting Information

Mononuclear Divalent Ytterbium Hydrido Complex Supported by a Super-Bulky Scorpionate Ligand

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General remarks

All reactions were carried out under a dry and oxygen-free nitrogen atmosphere using Schlenk techniques and a Vigor glovebox. The nitrogen in the glovebox was constantly circulated through a copper/molecular sieves (4 Å) catalyst unit. The oxygen and moisture concentrations in the glovebox atmosphere were monitored using an O_2(GE)/H_2O (Xentaur) analyzer to ensure that both were always below 0.1 ppm. Toluene, hexane and Et_2O were purified by use of a Vigor VSPS-5 solvent purification system, and dried over fresh Na chips in the glovebox. Tetrahydrofuran (THF), isooctane (ISO), pentane, cyclohexane-d_{12} and benzene-d_6 were distilled from Na/K alloy/benzophenone, degassed by the freeze-pump-thaw method (three times), and dried over fresh Na chips in the glovebox. K(*p*-$CH_2C_6H_4$-Me)[1] and $YbI_2(THF)_2$[2] were prepared according to literature procedures. The substrates 1,1-diphenylethylene, cyclohexylallene, 1,1-dimethylallene, 1,3,5,7-cyclooctatetraene were dried over CaH_2 for 8 h and distilled before usage. Other commercially available reagents were used without purification.

Samples for NMR spectroscopic measurements were prepared in the glovebox by use of J. Young valve NMR tubes. ^{1}H, ^{2}H and ^{13}C NMR spectra were recorded on a Bruker AV400 or AV500 spectrometer and referenced to the resonances of the solvent used. ^{171}Yb NMR spectra were recorded on a Bruker AV600 spectrometer and referenced externally to $[(C_5Me_5)_2Yb(THF)_2]$.[3] The elemental analyses were performed on Elementar Vario EL cube (WO_3 was used as pro-oxidant) at National Analytical Research Centre of Changchun Institute of Applied Chemistry (CIAC).

Synthesis of [(Tp^{Ad,iPr})Yb(*p*-$CH_2C_6H_4$-Me)(THF)] (1)

To a solution of K(Tp^{Ad,iPr}) (1.05 g, 1.35 mmol) in THF (30 mL) was added $YbI_2(THF)_2$ (768 mg, 1.35 mmol) and stirred at 80 ^oC for 18 h. After cooling to room temperature, the reaction solution had a gradual color change from yellow-brown to dark-red when K(*p*-$CH_2C_6H_4$-Me) (195 mg, 1.35 mmol) was added and stirred at room temperature for 6 h. The resulting suspension was stripped off all the volatiles and extracted with benzene (20 mL). The filtrate was evaporated to dryness and wished with cold hexane (5 mL) to give complex **1** (1.26 g, 1.15 mmol, 85% yield) as red-orange powder. Single crystals of complex **1** • (4 x Benzene) suitable for X-ray analysis were grown from hexane/benzene solution at -30 ^oC. ^1H NMR (500 MHz, C_6D_6, 25 ^oC): δ = 1.16 (d, $^3J_{HH}$ = 7 Hz, 18H, CH(CH_3)$_2$), 1.76, 1.86 (dd, $^3J_{HH}$ = 62, 12 Hz, 18H, AdCH_2), 2.08 (br, 18H, AdCH_2), 2.14 (br, 9H, AdC*H*), 2.24 (s, 2H, Yb-CH_2), 2.39 (s, 3H, CH_3), 2.96 (br, 4H, THF), 3.57 (sept, $^3J_{HH}$ = 7 Hz, 3H, C*H*(CH_3)$_2$), 5.95 (s, 3H, 4-pz-*H*), 7.06 (br, 4H, C_6H_4) ppm. ^{13}C {^1H} NMR (125 MHz, C_6D_6, 25 ^oC): δ = 20.71 (s, *C*H_3), 23.12 (s, CH(*C*H_3)$_2$), 25.12 (s, THF), 26.70 (s, *C*H(CH_3)$_2$), 28.68 (s, Ad-γ), 34.45 (s, Ad-α), 36.65 (s, Ad-δ), 43.44 (s, Ad-β), 49.11 (s, Yb-*C*H_2), 68.25 (s, THF), 97.58 (s, pz-4*C*), 120.63 (s, Ar-C_{para}), 121.60 (s, C_{ortho}), 128.88 (s, Ar-C_{meta}), 156.57 (s, pz-3*C*), 157.41 (s, Ar-C_{ipso}), 163.31 (s, pz-5*C*) ppm. Anal. calcd. for (**1**) $C_{60}H_{87}B_1N_6O_1Yb_1$ (1092.20): C, 65.98; H, 8.03; N, 7.69; found: C, 66.34; H, 8.35; N, 7.72.

Synthesis of [(Tp^{Ad,iPr})Yb(H)(THF)] (2)

A solution of [(Tp^{Ad,iPr})Yb(*p*-$CH_2C_6H_4$-Me)(THF)] (680 mg, 0.62 mmol) in hexane (20 mL) was added into a glass tube in a medium-pressure autoclave. The autoclave was transferred outside of the glovebox and pressurized with H_2 to 20 atm. The mixture was stirred at room temperature for 24 h. Pressure was released and the autoclave was quickly returned to the glovebox. After filtration, the volatile was stripped off to give complex **2** (486 mg, 0.49 mmol, 79% yield) as red-brown powder. Single crystals of complex **2** • (2 x THF) suitable for X-ray analysis were grown from hexane/THF solution at -30 ^oC. ^1H NMR (500 MHz, C_6D_6, 25 ^oC): δ = 1.19 (d, $^3J_{HH}$ = 7 Hz, 18H, CH(CH_3)$_2$), 1.40 (m, 32H, THF), 1.74, 1.93, (dd, $^3J_{HH}$ = 102, 12 Hz, 18H, AdCH_2), 2.16 (br, 9H, AdC*H*), 2.19 (br, 18H, AdCH_2), 3.54 (m, 32H, THF), 3.63 (sept, $^3J_{HH}$ = 7 Hz, 3H, C*H*(CH_3)$_2$), 5.97 (s, 3H, 4-pz-*H*), 10.64 (s, $^1J_{YbH}$ = 830 Hz, 1H, Yb-*H*) ppm. ^{13}C {^1H} NMR (125 MHz, C_6D_6, 25 ^oC): δ = 23.23 (s, CH(*C*H_3)$_2$), 25.41 (s, THF), 26.65 (s, *C*H(CH_3)$_2$), 28.92 (s, Ad-γ), 34.68 (s, Ad-α), 36.72 (s,

Ad-δ), 43.52 (br, Ad-β), 67.53 (s, THF), 97.11 (s, pz-4*C*), 156.06 (s, pz-3*C*), 163.26 (s, pz-5*C*) ppm. ^{171}Yb NMR (105 MHz, C_6D_6, 25 ^{o}C): δ = 974.31 (d, $^{1}J_{YbH}$ = 833 Hz, *Yb*-H) ppm. Anal. calcd. for (**2**) $C_{52}H_{79}B_1N_6O_1Yb_1$ (988.06): C, 63.21; H, 8.06; N, 8.51; found: C, 65.55; H, 8.47; N, 8.22.

Synthesis of [(Tp^{Ad,iPr})Yb(μ-H)]$_2$ (3)

[(Tp^{Ad,iPr})Yb(H)(THF)] (500 mg, 0.51 mmol) underwent repeated cycles (three times) of dissolution in benzene and removal of the solvent under vacuum to give complex **3** (454 mg, 0.25 mmol, 98 % yield) as red-brown powder. ^{1}H NMR (500 MHz, C_6D_6, 25 ^{o}C): δ = 1.20 (d, $^{3}J_{HH}$ = 7 Hz, 36H, CH(C*H*$_3$)$_2$),1.74, 1.80 (dd, $^{3}J_{HH}$ = 40, 12 Hz, 36H, AdC*H*$_2$), 2.06 (br, 18H, AdC*H*), 2.16 (br, 36H, AdC*H*$_2$), 3.49 (sept, $^{3}J_{HH}$ = 7 Hz, 6H, C*H*(CH$_3$)$_2$), 5.98 (s, 6H, 4-pz-*H*), 10.32 (s, $^{1}J_{YbH}$ = 378 Hz, 2H, Yb-*H*) ppm. ^{13}C {^{1}H} NMR (125 MHz, C_6D_6, 25 ^{o}C): δ = 23.05 (s, CH(*C*H$_3$)$_2$), 26.70 (s, *C*H(CH$_3$)$_2$), 28.81 (s, Ad-γ), 34.69 (s, Ad-α), 36.85 (s, Ad-δ), 43.12 (br, Ad-β), 97.70 (s, pz-4*C*), 157.06 (s, pz-3*C*), 163.68 (s, pz-5*C*) ppm. ^{171}Yb NMR (105 MHz, C_6D_6, 25 ^{o}C): δ = 730.13 (t, $^{1}J_{YbH}$ = 374 Hz, *Yb*-H) ppm. Anal. calcd. for (**3**) $C_{96}H_{142}B_2N_{12}Yb_2$ (1832.00): C, 62.94; H, 7.81; N, 9.17; found: C, 63.25; H, 8.14; N, 8.67.

Single crystals of complex **3** suitable for X-ray analysis were grown form hexane solution at -30 ^{o}C. Attempts to solve the crystal structure were failed, due to the poor quality of the crystal data.

Syntheses of [(Tp^{Ad,iPr})Yb(D)(THF)] (2-D) and [(Tp^{Ad,iPr})Yb(μ-D)]$_2$ (3-D)

The syntheses of complexes **2-D** and **3-D** were analogous to those of complexes **2** and **3** except for the use of deuteride gas D_2 (15 atm, 3 days).

^{2}H NMR (61 MHz, C_6H_6, 25 ^{o}C) for [(Tp^{Ad,iPr})Yb(D)(THF)] : δ = 10.57 (s, Yb-*D*) ppm.

^{2}H NMR (61 MHz, C_6H_6, 25 ^{o}C) for [(Tp^{Ad,iPr})Yb(μ-D)]$_2$: δ = 10.36 (t, $^{1}J_{YbD}$ = 61 MHz, Yb-*D*) ppm.

Synthesis of [(Tp^{Ad,iPr})Yb{CPh$_2$(Me)}] (4)

A solution of 1,1-diphenylethylene (11 mg, 0.061 mmol) and [(Tp^{Ad,iPr})Yb(H)(THF)] (**2**) (60 mg, 0.061 mmol) in hexane (10 mL)/THF (1 mL) was stirred for 2 h at room temperature and then filtered. The resulting dark-red solution was slowly volatilized at room temperature for 2 days to give complex **4** (35 mg, 0.032 mmol, 52% yield) as dark-red crystals. Single crystals of complex **4** suitable for X-ray analysis were grown from hexane/benzene solution

at room temperature. ^{1}H NMR (500 MHz, C_6D_6, 25 ^{o}C): δ = 1.13 (d, $^{3}J_{HH}$ = 7 Hz, 18H, CH(CH_3)$_2$), 1.68 (dd, $^{3}J_{HH}$ = 14, 14 Hz, 18H, AdCH_2), 1.97 (br, 27H, AdCH_2 + AdCH), 2.08 (s, 3H, CH_3), 3.37 (sept, $^{3}J_{HH}$ = 7 Hz, 3H, CH(CH$_3$)$_2$), 5.96 (s, 3H, 4-pz-H), 6.12 (t, $^{3}J_{HH}$ = 7 Hz, 2H, Ar-H_{para}), 6.92 (t, $^{3}J_{HH}$ = 7 Hz, 4H, Ar-H_{ortho}), 7.04 (d, $^{3}J_{HH}$ = 7 Hz, 4H, Ar-H_{meta}) ppm. ^{13}C {^{1}H} NMR (125 MHz, C_6D_6, 25 ^{o}C): δ = 20.87 (s, CH$_3$), 22.98 (s, CH(CH$_3$)$_2$), 26.59 (s, CH(CH$_3$)$_2$), 28.52 (s, Ad-γ), 34.63 (s, Ad-α), 36.60 (s, Ad-δ), 42.86 (s, Ad-β), 82.87 (s, CPh$_2$), 98.79 (s, pz-4C), 109.81 (s, Ar-C_{para}), 118.23 (s, Ar-C_{ortho}), 130.11 (s, Ar-C_{meta}),143.44 (s, Ar-C_{ipso}), 159.55 (s, pz-3C), 164.83 (s, pz-5C) ppm. Anal. calcd. for (**4**) $C_{62}H_{83}B_1N_6Yb_1$ (1096.19): C, 67.93; H, 7.63; N, 7.67; found: C, 68.15; H, 7.96; N, 7.23.

Synthesis of [(Tp^{Ad,iPr})Yb(η^3-CH$_2$CHCHCy)] (5)

To a stirring solution of [(Tp^{Ad,iPr})Yb(H)(THF)] (**2**) (80 mg, 0.081 mmol) in hexane (10 mL)/THF (1 mL) was added cyclohexylallene (10 mg, 0.081 mmol). After 30 minutes, the solution was filtered. The volatile of filtrate was stripped off to give complex **5** (57 mg, 0.055 mmol, 68% yield) as red-brown powder. Single crystals of complex **5** • (1 x Pentane) suitable for X-ray analysis were grown from a concentrated pentane solution at −30 °C as red-brown crystals. ^{1}H NMR (500 MHz, C_6D_6, 25 ^{o}C): δ = 1.18 (d, $^{3}J_{HH}$ = 7 Hz, 18H, CH(CH_3)$_2$), 1.28 (m, 5H, Cy), 1.52 (m, 1H, Cy), 1.67 (m, 2H, Cy), 1.77 (m, 1H, Cy), 1.82, 173 (dd, $^{3}J_{HH}$ = 54, 14 Hz, 18H, AdCH_2), 2.08 (br, 9H + 1H, AdCH + CH$_2$CHCHCy), 2.14 (m, 1H, CHCy), 2.17 (br, 18H, AdCH_2), 2.22 (d, $^{3}J_{HH}$ = 3 Hz, 2H, Yb-CH_2), 2.35 (m, 1H, Cy$_{tert\text{-}C}H$), 3.59 (sept, $^{3}J_{HH}$ = 7 Hz, 3H, CH(CH$_3$)$_2$), 5.98 (s, 3H, 4-pz-H) ppm. ^{2}H NMR (61 MHz, C_6H_6, 25 ^{o}C) for [(Tp^{Ad,iPr})Yb(η^3-CH$_2$CDCHCy)]: δ = 2.08 (s, CH$_2$CDCH) ppm. ^{13}C {^{1}H} NMR (125 MHz, C_6D_6, 25 ^{o}C): δ = 23.17 (s, CH(CH$_3$)$_2$), 26.44 (s, Cy), 26.49 (s, Cy), 26.62 (s, CH(CH$_3$)$_2$), 28.91 (s, Ad-γ), 31.00 (s, YbCH$_2$), 34.45 (s, Ad-α), 35.62 (s, Cy), 36.12 (s, Cy$_{tert\text{-}C}$), 36.66 (s, Ad-δ), 43.17 (s, Ad-β), 97.30 (s, pz-4C), 108.31 (s, YbCH$_2$$C$H), 114.85 (s, Cy$C$H), 156.83 (s, pz-3$C$), 163.40 (s, pz-5$C$) ppm. Anal. calcd. for (**5**) $C_{57}H_{85}B_1N_6Yb_1$ (1038.15): C, 65.94; H, 8.25; N, 8.09; found: C, 66.36; H, 8.70; N, 7.64.

Synthesis of [(Tp^{Ad,iPr})Yb(η^1-CH=C=CMe$_2$)(THF)] (6)

To a stirring solution of [(Tp^{Ad,iPr})Yb(H)(THF)] (**2**) (80 mg, 0.081 mmol) in hexane (10 mL)/THF (1 mL) was added 1,1-dimethylallene (6 mg, 0.081 mmol). An immediate gas evolution was observed. After 30 minutes, the solution was filtered. The filtrate was concentrated to 2 mL and kept at -30 ^{o}C to give complex **6** (72 mg, 0.068 mmol, 84% yield)

as red-orange crystals. Single crystals of complex **6** • (1 x THF) suitable for X-ray analysis were grown from a concentrated hexane/THF solution at −30 °C. ^{1}H NMR (400 MHz, C_6D_6, 25 ^{o}C): δ = 1.18 (d, $^{3}J_{HH}$ = 7 Hz, 18H, CH(CH_3)$_2$), 1.29 (m, 4 H, THF), 1.77, 1.87 (dd, $^{3}J_{HH}$ = 55, 12 Hz, 18H, AdCH_2), 2.08 (d, $^{3}J_{HH}$ = 4 Hz, 6 H, C(CH_3)$_2$), 2.11 (br, 18 H, AdCH_2), 2.16 (br, 9 H, AdC*H*), 3.35 (m, 4 H, THF), 3.61 (sept, $^{3}J_{HH}$ = 7 Hz, 3H, C*H*(CH$_3$)$_2$), 5.60 (sept, $^{3}J_{HH}$ = 4 Hz, 1 H, Yb-C*H*), 5.96 (s, 3H, 4-pz-*H*) ppm. ^{13}C {^{1}H} NMR (100 MHz, C_6D_6, 25 ^{o}C): δ = 22.17 (s, C(*C*H$_3$)$_2$), 23.23 (s, CH(*C*H$_3$)$_2$), 25.29 (s, THF), 26.67 (s, *C*H(CH$_3$)$_2$), 28.72 (s, Ad-γ), 34.47 (s, Ad-α), 36.70 (s, Ad-δ), 43.53 (s, Ad-β), 64.17 (s, Yb-*C*H), 68.43 (s, THF), 97.31 (s, pz-4*C*), 111.33 (s, *C*(CH$_3$)$_2$), 156.23 (s, pz-3*C*), 163.15 (s, pz-5*C*), 202.17 (s, Yb-CH*C*) ppm. Anal. calcd. for (**6**) $C_{57}H_{85}B_1N_6O_1Yb_1$ (1054.15): C, 64.94; H, 8.13; N, 7.97; found: C, 65.38; H, 7.91; N, 7.64.

Synthesis of [(Tp^{Ad,iPr})Yb(μ-η^8,η^8-COT)Yb(Tp^{Ad,iPr})] (7)

To a stirring solution of [(Tp^{Ad,iPr})Yb(H)(THF)] (**2**) (85 mg, 0.086 mmol) in hexane (10 mL)/THF (1 mL) was added 1,3,5,7-cyclooctatetraene (5 mg, 0.43 mmol). After 10 minutes, a pale-brown precipitate was formed. The precipitate was collected and washed with cold hexane (2 x 1 mL) to give complex **7** (62 mg, 0.032 mmol, 75 % yield) as pale-brown powder. Single crystals of complex **7** • (3 x Toluene) suitable for X-ray analysis were grown from a concentrated toluene/hexane solution at −30 °C as pale-brown crystals. ^{1}H NMR (400 MHz, C_6D_6, 25 ^{o}C): δ = 1.18 (d, $^{3}J_{HH}$ = 7 Hz, 36 H, CH(CH_3)$_2$), 1.93, 2.00 (dd, $^{3}J_{HH}$ = 54, 12 Hz, 36 H, AdCH_2), 2.19 (br, 54 H, AdC*H* + AdCH_2), 3.10 (sept, $^{3}J_{HH}$ = 7 Hz, 6 H, C*H*(CH$_3$)$_2$), 6.02 (s, 6 H, 4-pz-*H*), 6.49 (s, 8 H, COT) ppm. ^{13}C {^{1}H} NMR (100 MHz, C_6D_6, 25 ^{o}C): δ = 23.29 (s, CH(*C*H$_3$)$_2$), 26.30 (s, *C*H(CH$_3$)$_2$), 29.01 (s, Ad-γ), 34.26 (s, Ad-α), 37.09 (s, Ad-δ), 42.51 (s, Ad-β), 89.84 (s, COT), 99.31 (s, pz-4*C*), 158.88 (s, pz-3*C*), 164.44 (s, pz-5*C*) ppm. Anal. calcd. for (**7**) $C_{104}H_{148}B_2N_{12}Yb_2$ (1932.04): C, 64.58; H, 7.71; N, 8.69; found: C, 65.02; H, 7.25; N, 8.31.

NMR spectroscopy

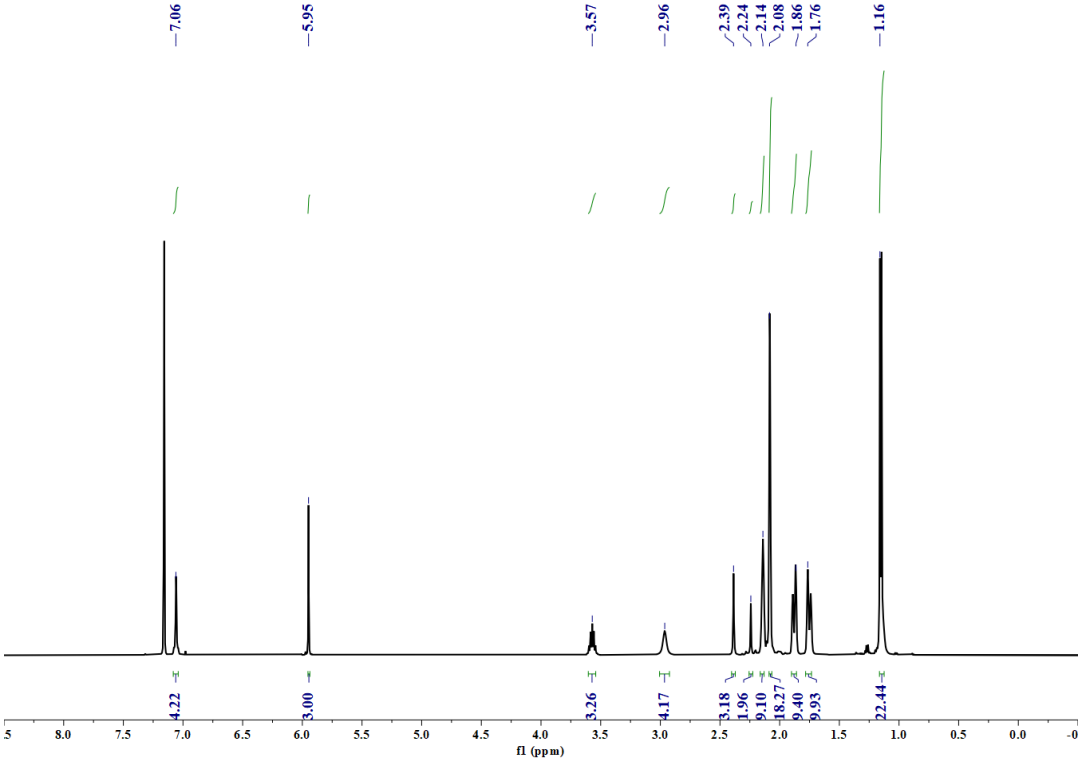

Figure S1. ^{1}H NMR spectrum (500 MHz) of [(Tp^{Ad,iPr})Yb(*p*-$CH_2C_6H_4$-Me)(THF)] (**1**) in C_6D_6 at 25 ^{o}C.

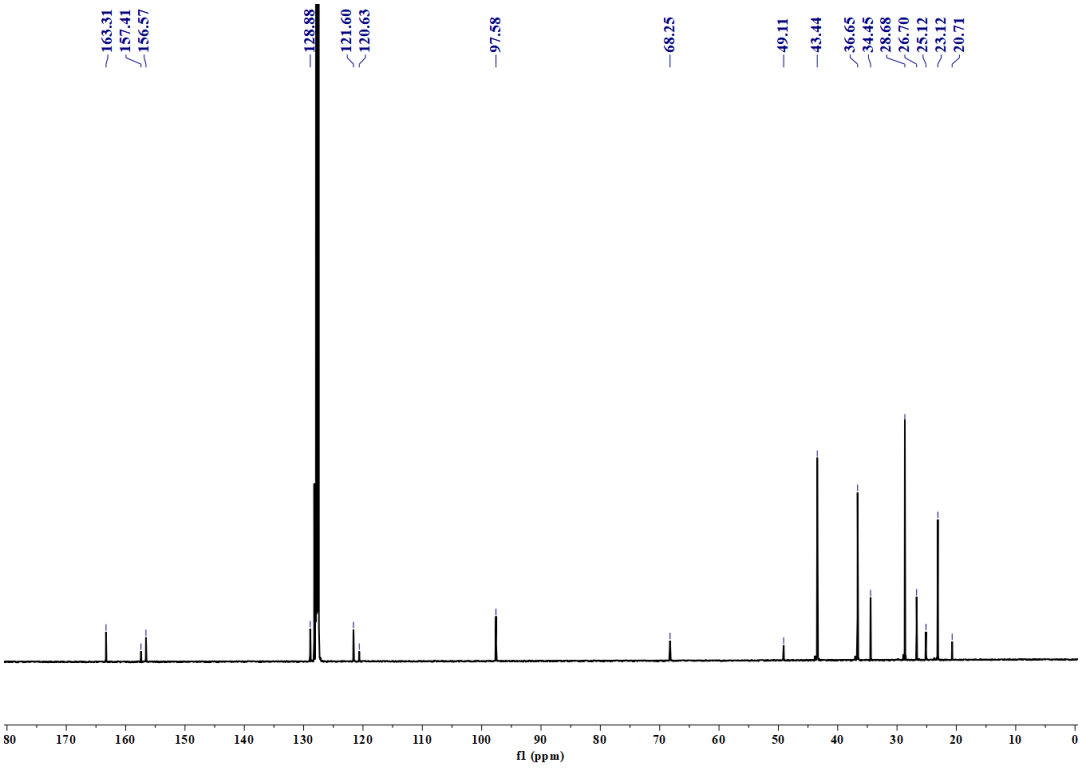

Figure S2. ^{13}C {^{1}H} NMR spectrum (125 MHz) of [(Tp^{Ad,iPr})Yb(*p*-$CH_2C_6H_4$-Me)(THF)] (**1**) in C_6D_6 at 25 ^{o}C.

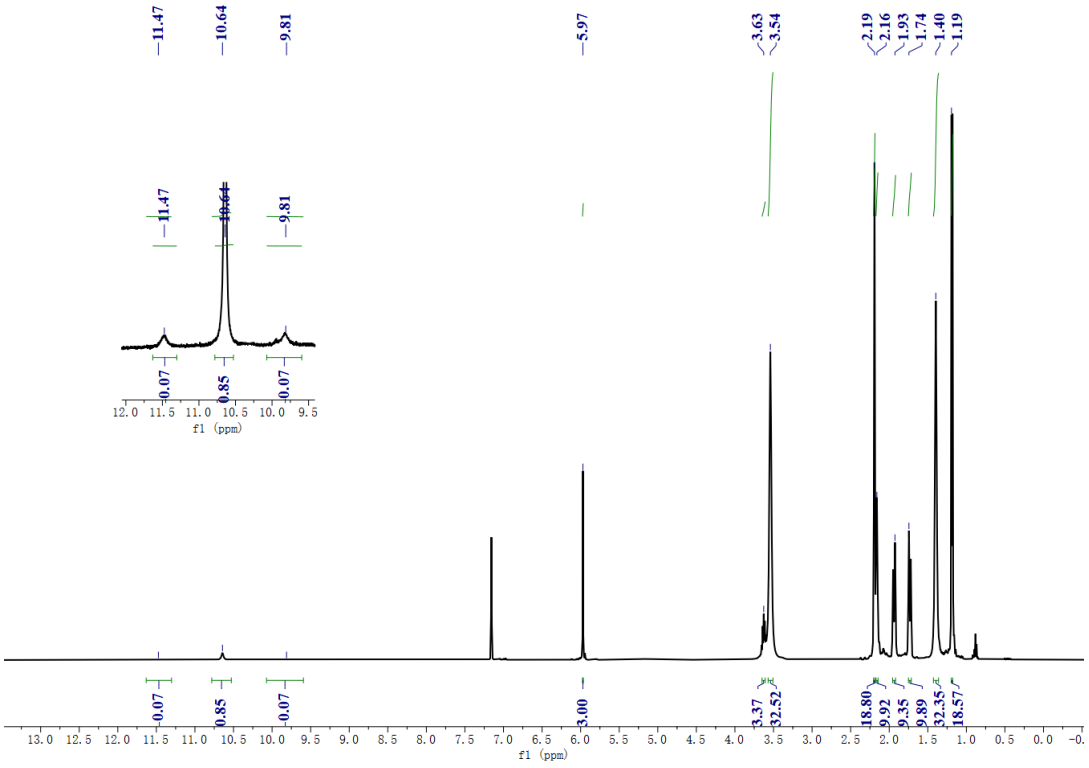

Figure S3. ^{1}H NMR spectrum (500 MHz) of [(Tp^{Ad,iPr})Yb(H)(THF)] (**2**) with seven equivalents THF in C_6D_6 at 25 ^{o}C.

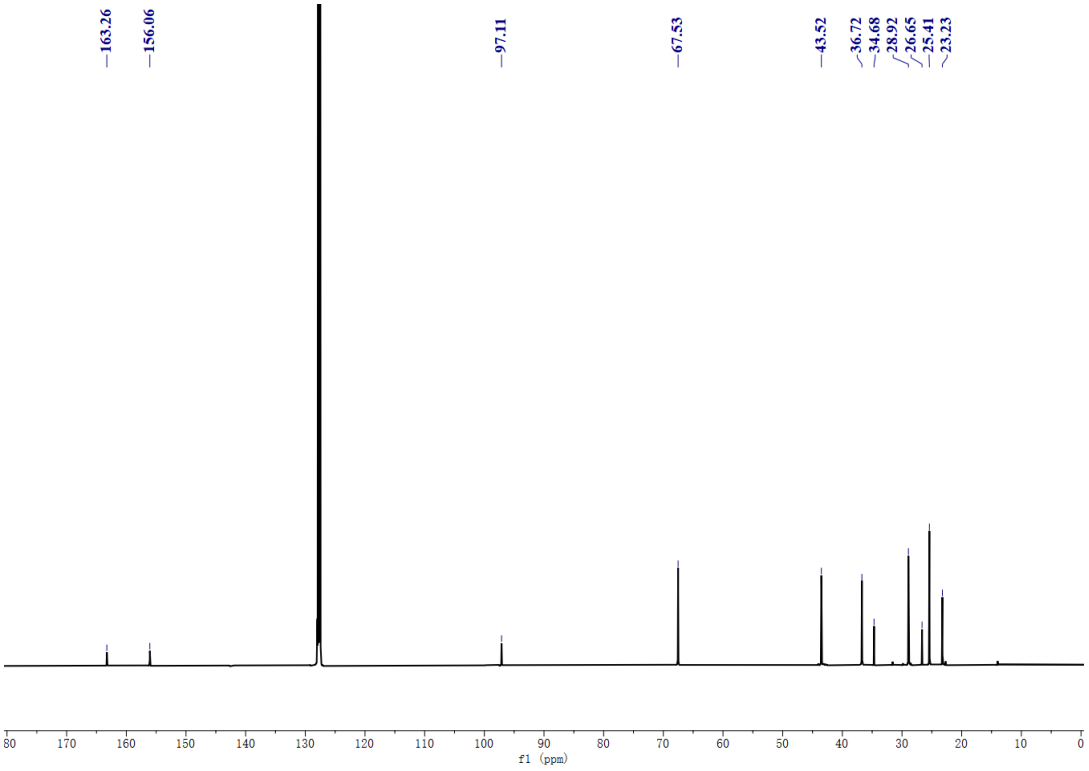

Figure S4. ^{13}C {^{1}H} NMR spectrum (125 MHz) of [(Tp^{Ad,iPr})Yb(H)(THF)] (**2**) with seven equivalents THF in C_6D_6 at 25 ^{o}C.

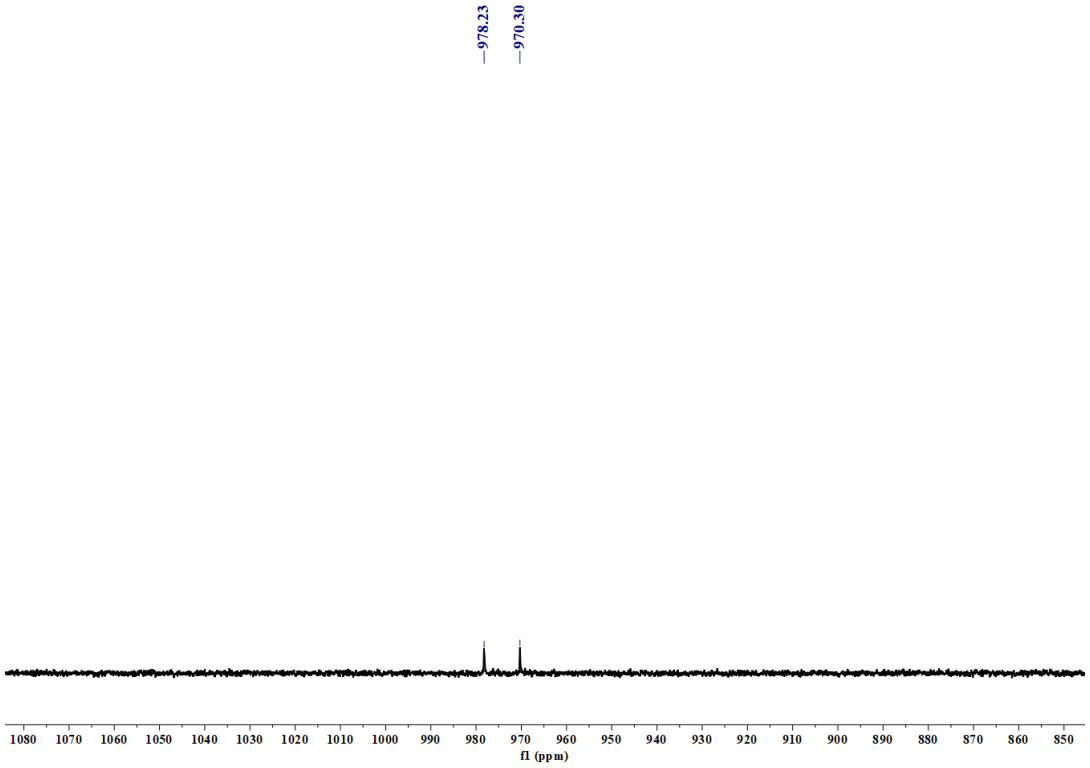

Figure S5. ^{171}Yb NMR spectrum (105 MHz) of [(Tp^{Ad,iPr})Yb(H)(THF)] (**2**) with seven equivalents THF in C_6D_6 at 25 ^{o}C.

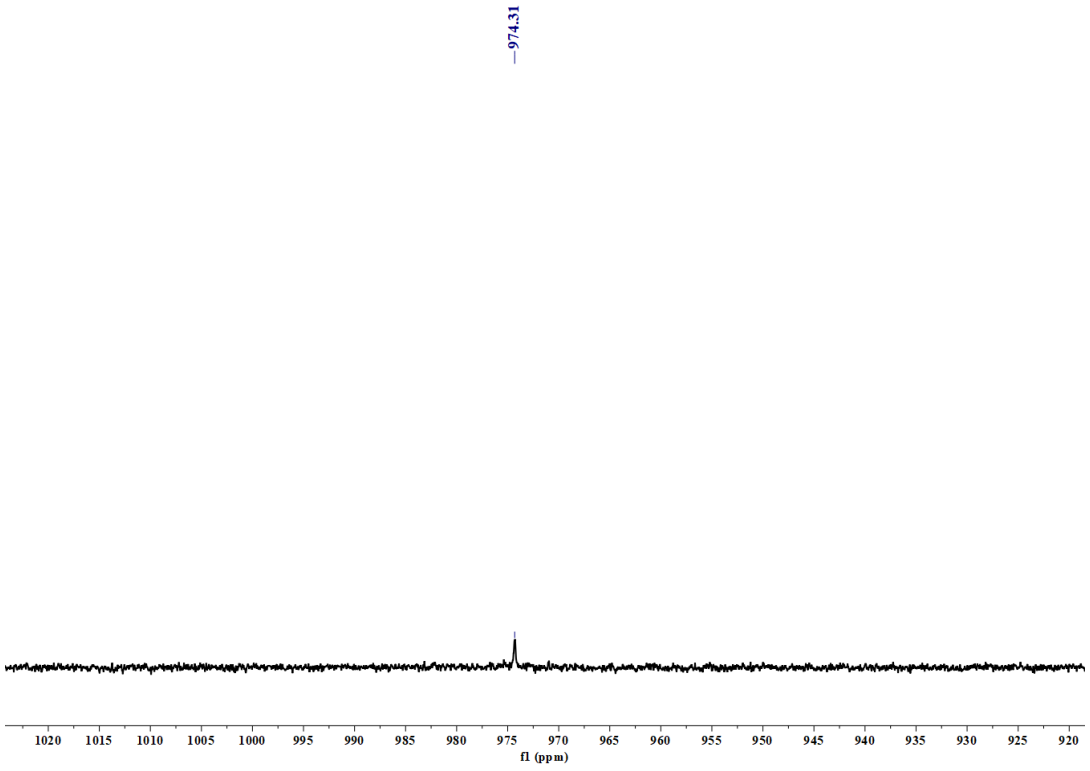

Figure S6. ^{171}Yb {^{1}H} NMR spectrum (105 MHz) of [(Tp^{Ad,iPr})Yb(H)(THF)] (**2**) with seven equivalents THF in C_6D_6 at 25 ^{o}C.

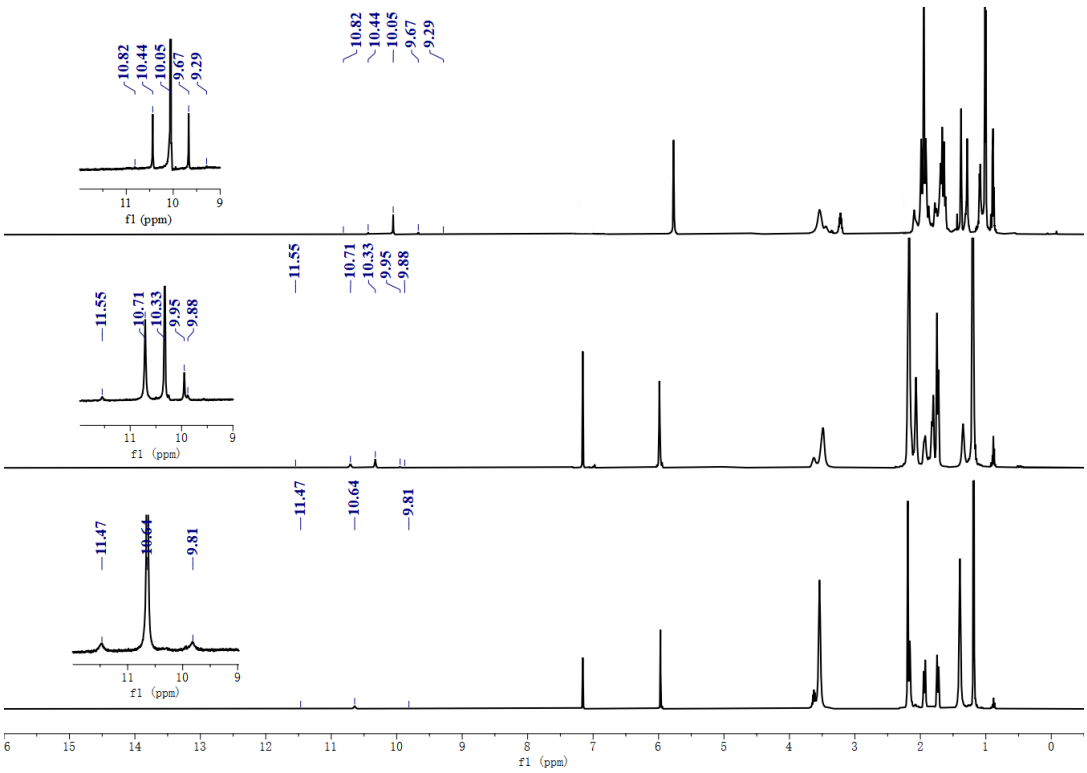

Figure S7. Stacked ^{1}H NMR spectrum (500 MHz) of [(Tp^{Ad,iPr})Yb(H)(THF)] (**2**) in d_{12}-cyclohexane (**top**) and in C_6D_6 (**middle**) and [(Tp^{Ad,iPr})Yb(H)(THF)] (**2**) with seven equivalents THF in C_6D_6 (**bottom**) at 25 ºC.

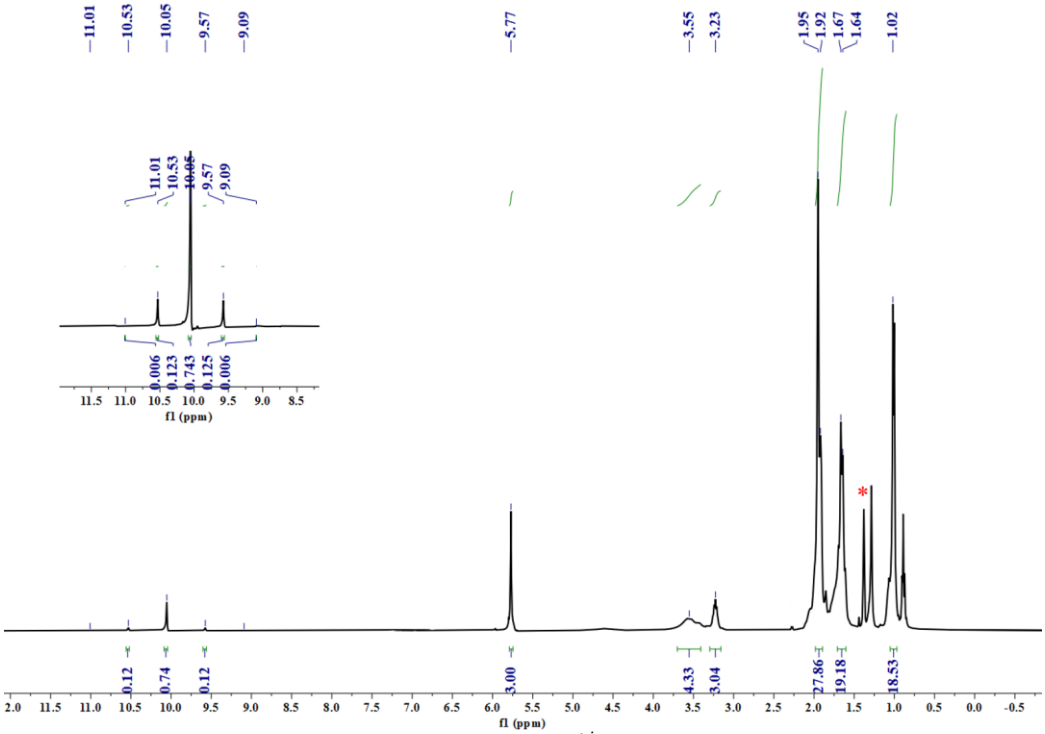

Figure S8. ^{1}H NMR spectrum (400 MHz) of [(Tp^{Ad,iPr})Yb(H)(THF)] (**2**) in d_{12}-cyclohexane at 25 ºC. (* =1.38 ppm, d_{12}-cyclohexane)

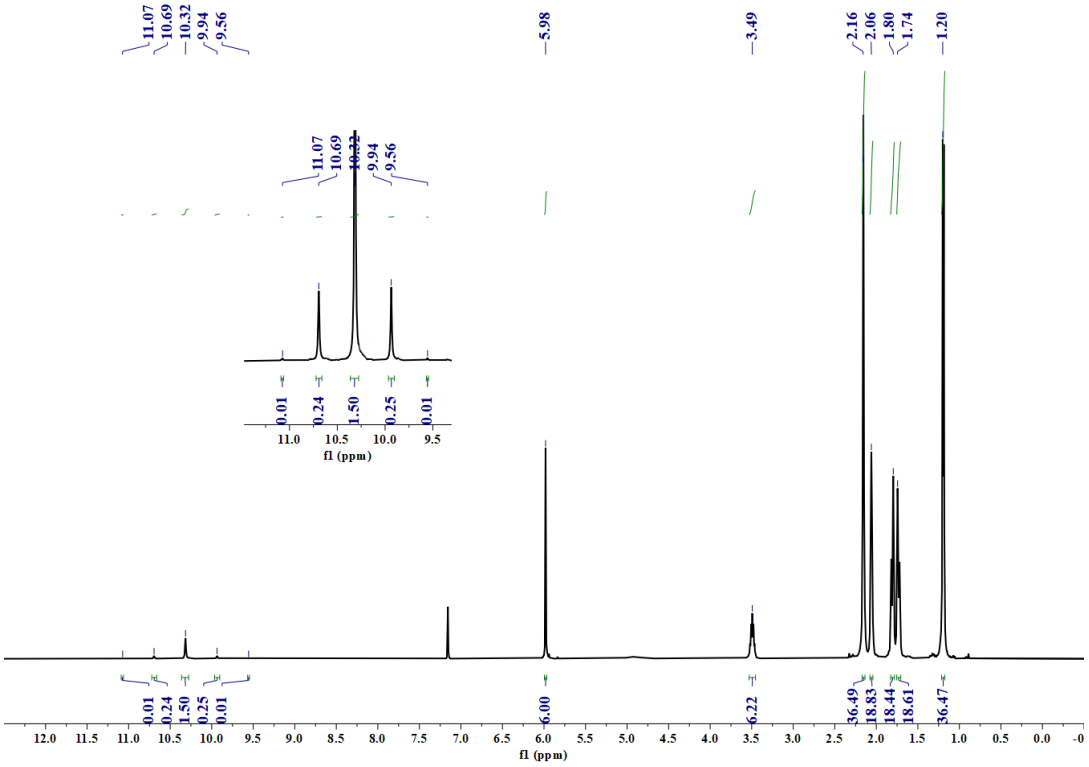

Figure S9. ^{1}H NMR spectrum (500 MHz) of [(Tp^{Ad,iPr})Yb(μ-H)]$_2$ (**3**) in C_6D_6 at 25 ^{o}C.

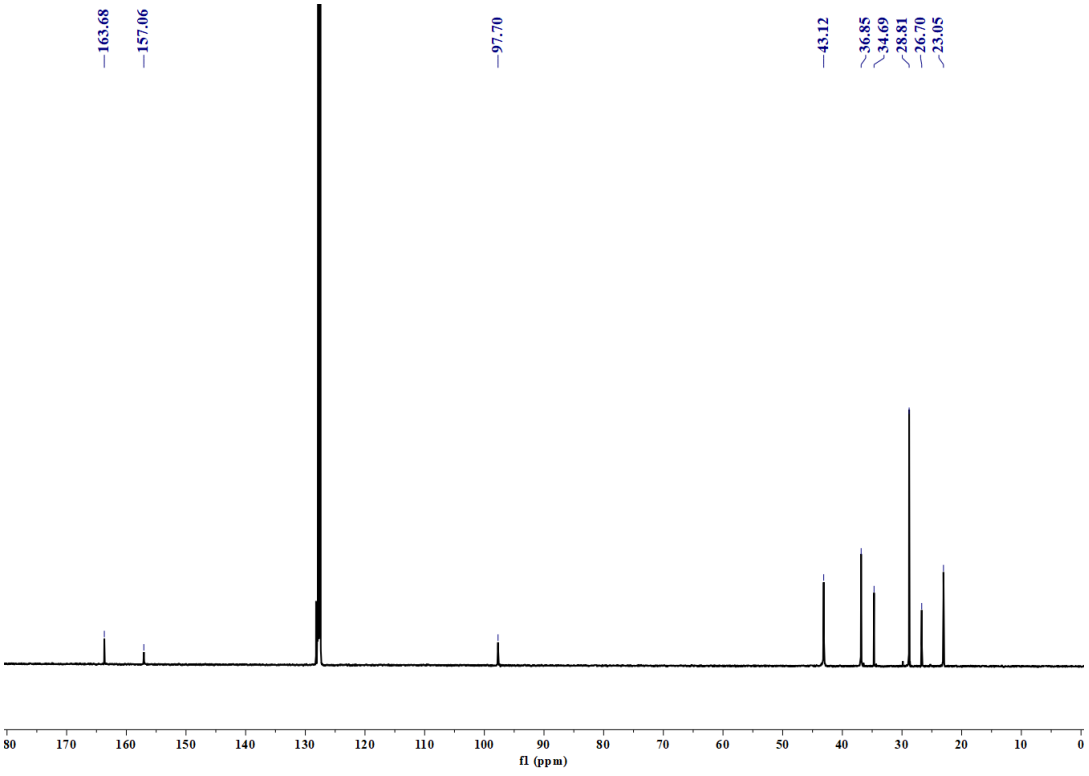

Figure S10. ^{13}C {^{1}H} NMR spectrum (125 MHz) of [(Tp^{Ad,iPr})Yb(μ-H)]$_2$ (**3**) in C_6D_6 at 25 ^{o}C.

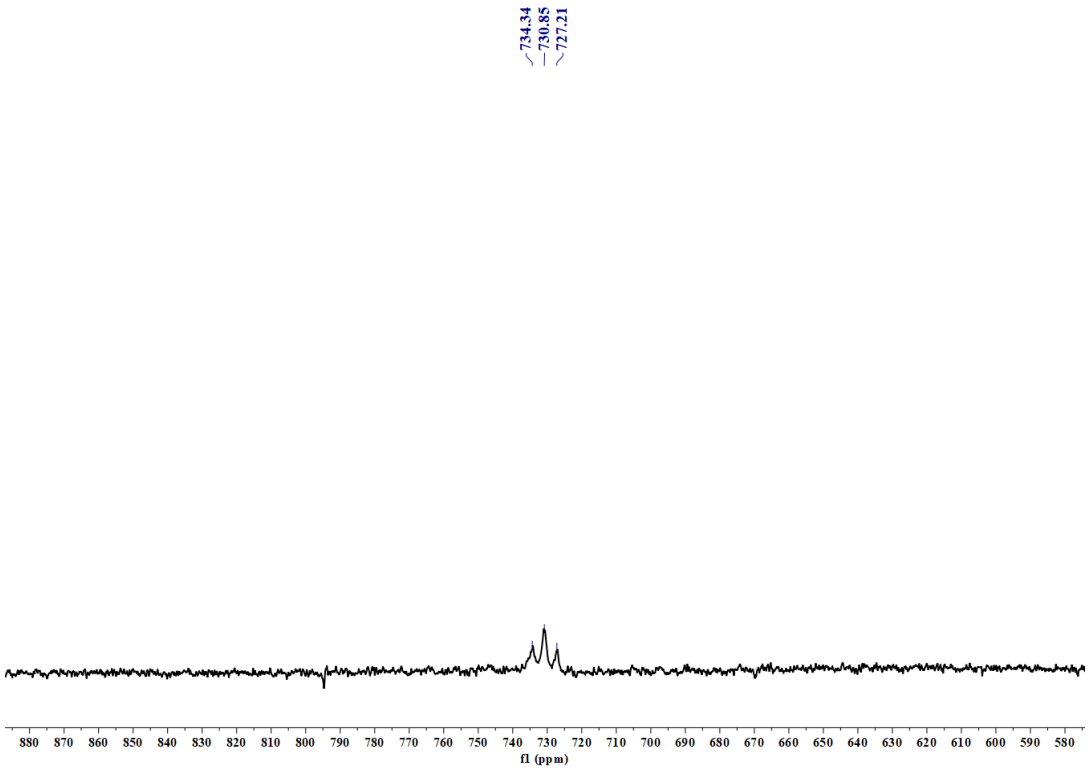

Figure S11. ^{171}Yb NMR spectrum (105 MHz) of [(Tp^{Ad,iPr})Yb(μ-H)]$_2$ (**3**) in C_6D_6 at 25 ^{o}C.

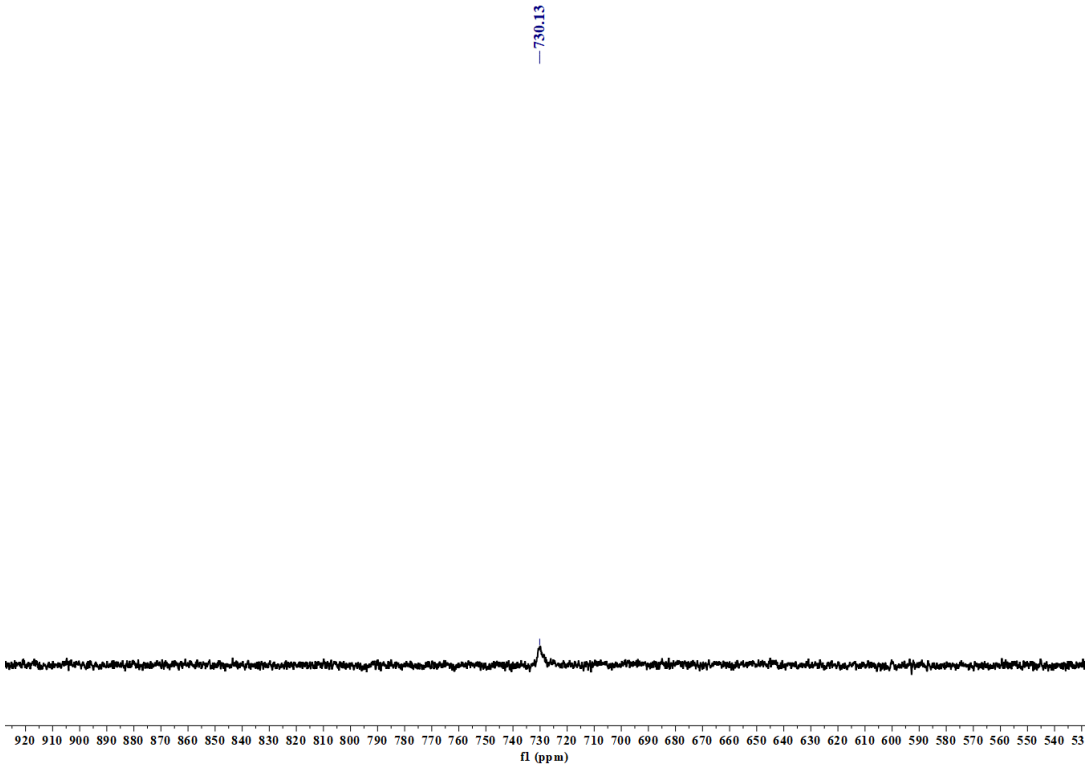

Figure S12. ^{171}Yb {^{1}H} NMR spectrum (105 MHz) of [(Tp^{Ad,iPr})Yb(μ-H)]$_2$ (**3**) in C_6D_6 at 25 ^{o}C.

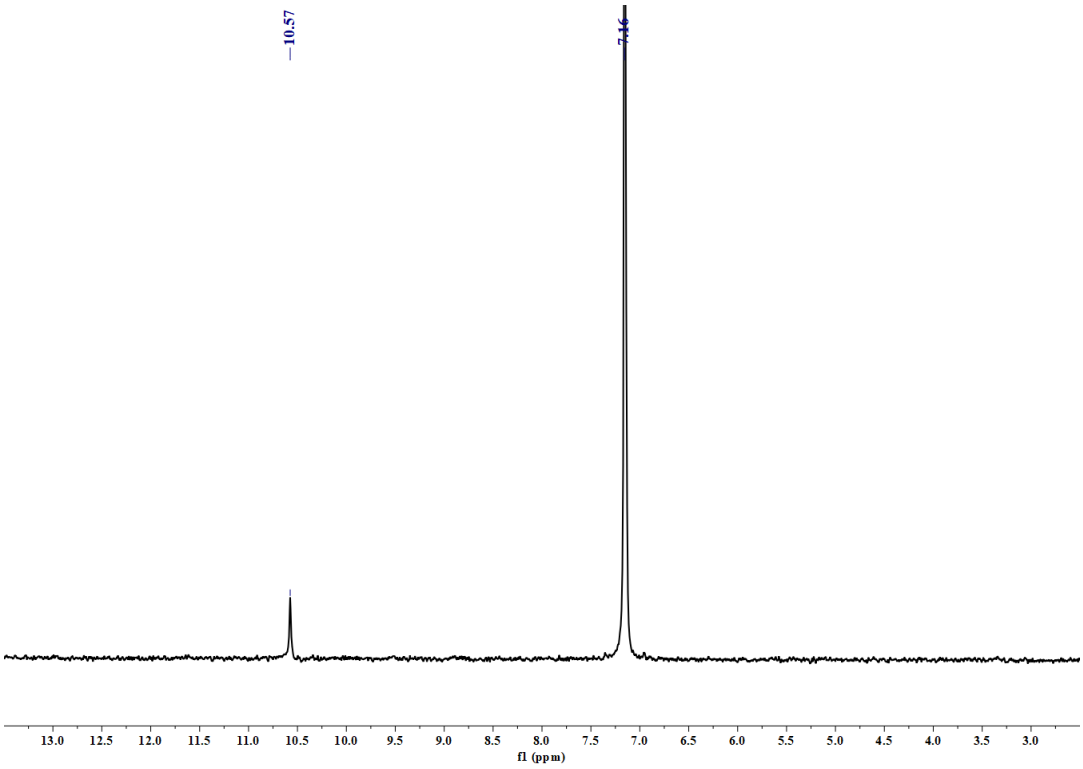

Figure S13. ^{2}H NMR spectrum (61 MHz) of [(Tp^{Ad,iPr})Yb(D)(THF)] (**2-D**) with seven equivalents THF in C_6H_6 at 25 ^{o}C. (Drops of C_6D_6 were added as internal standard)

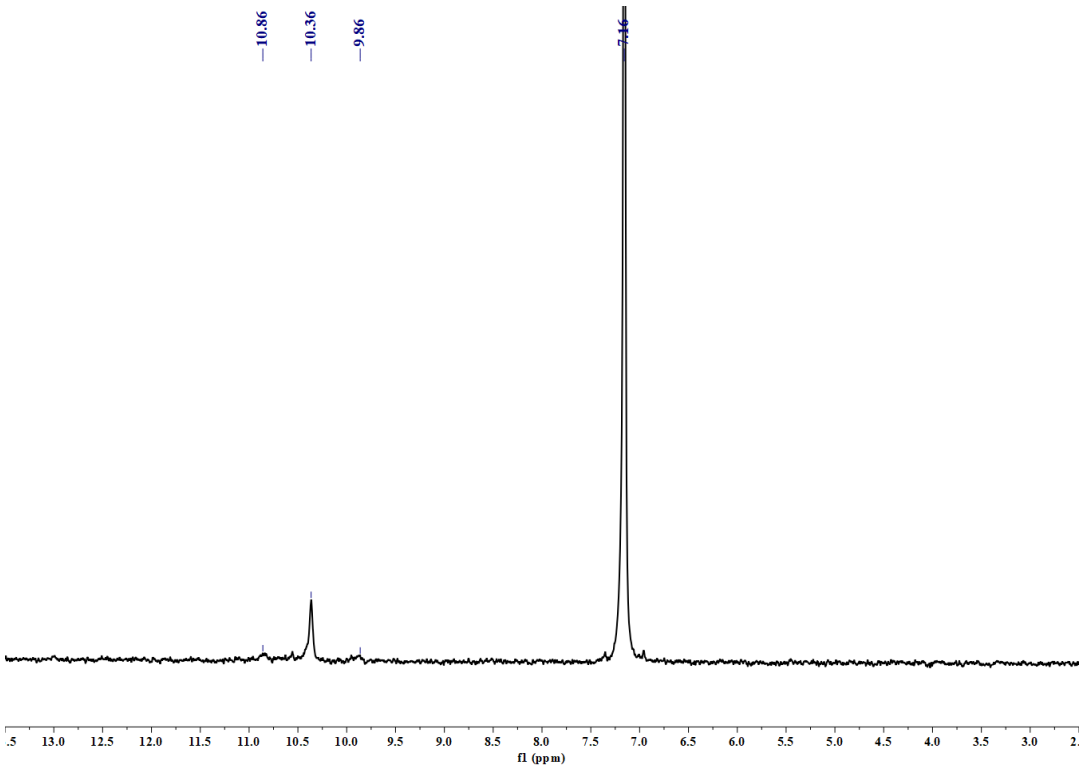

Figure S14. ^{2}H NMR spectrum (61 MHz) of [(Tp^{Ad,iPr})Yb(μ-D)]$_2$ (**3-D**) in C_6H_6 at 25 ^{o}C. (Drops of C_6D_6 were added as internal standard)

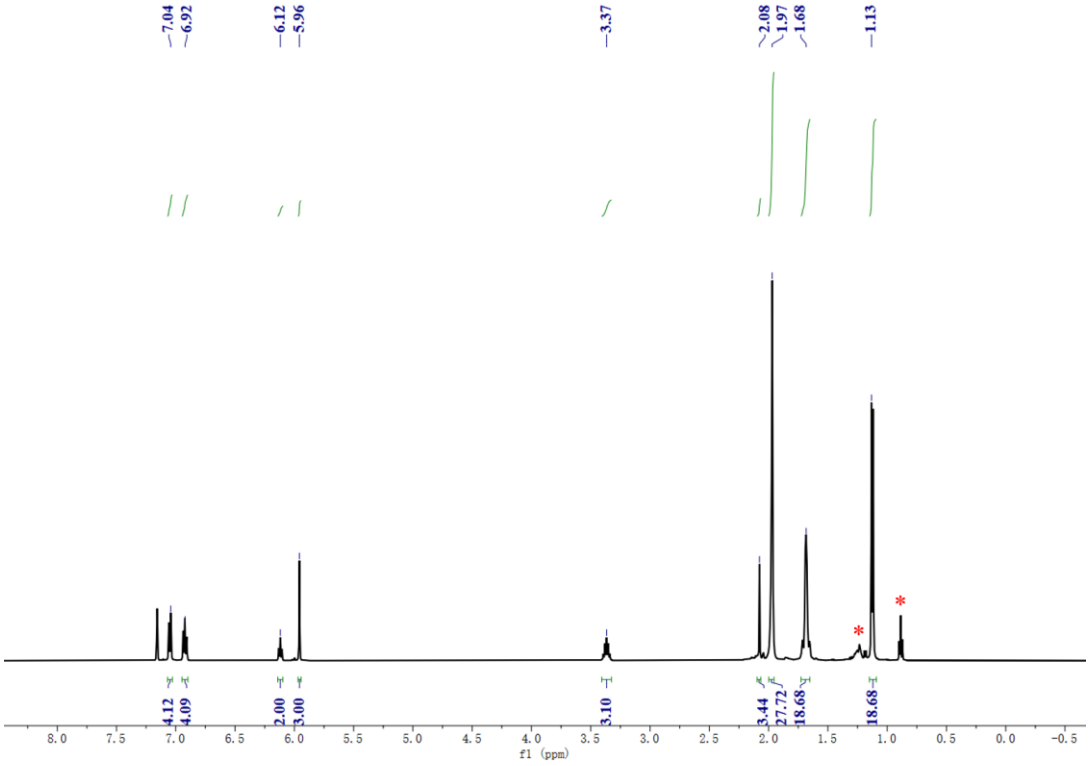

Figure S15. ^{1}H NMR spectrum (500 MHz) of [(Tp^{Ad,iPr})Yb{CPh$_2$(Me)}] (**4**) in C_6D_6 at 25 ^{o}C.

(* = residual hexane)

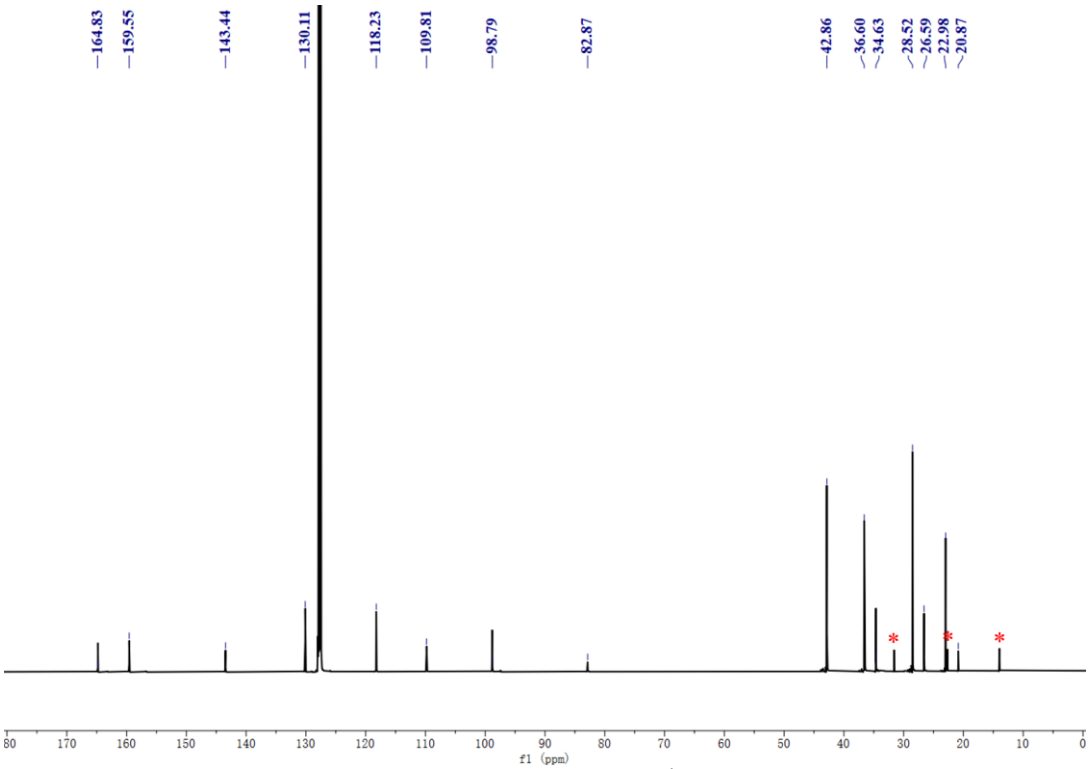

Figure S16. ^{13}C {^{1}H} NMR spectrum (125 MHz) of [(Tp^{Ad,iPr})Yb{CPh$_2$(Me)}] (**4**) in C_6D_6 at 25 ^{o}C.

(* = residual hexane)

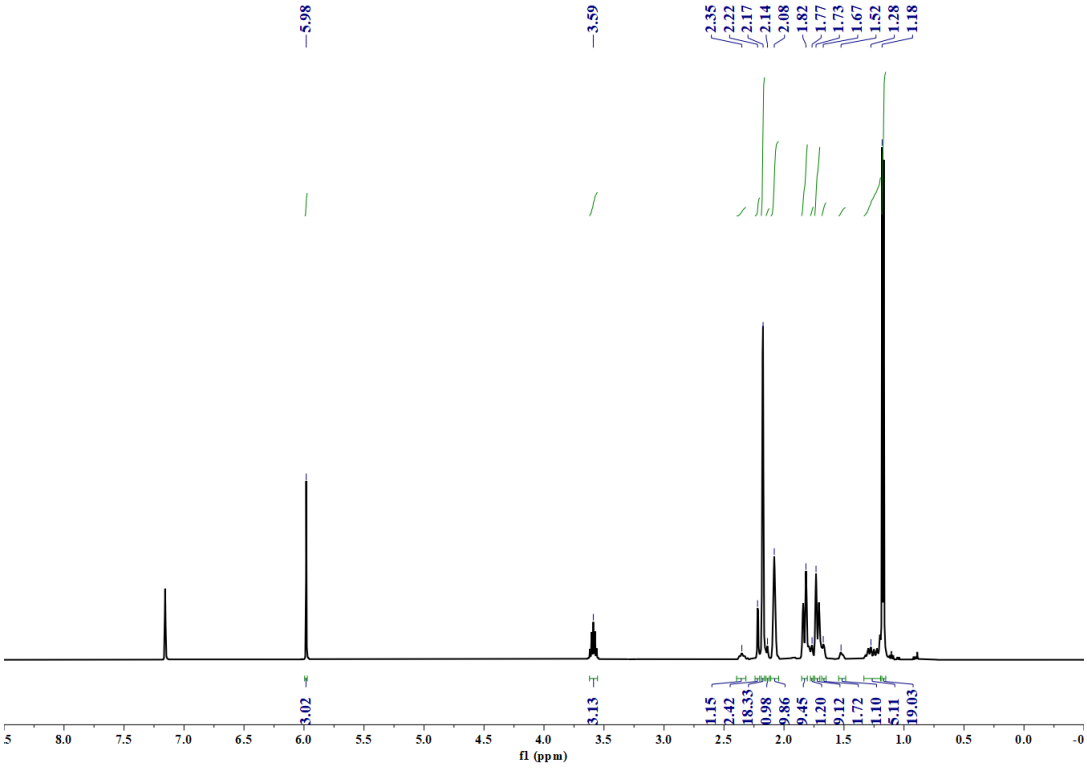

Figure S17. ^{1}H NMR spectrum (500 MHz) of [(Tp^{Ad,iPr})Yb(η^3-CH$_2$CHCHCy)] (**5**) in C_6D_6 at 25 ^{o}C.

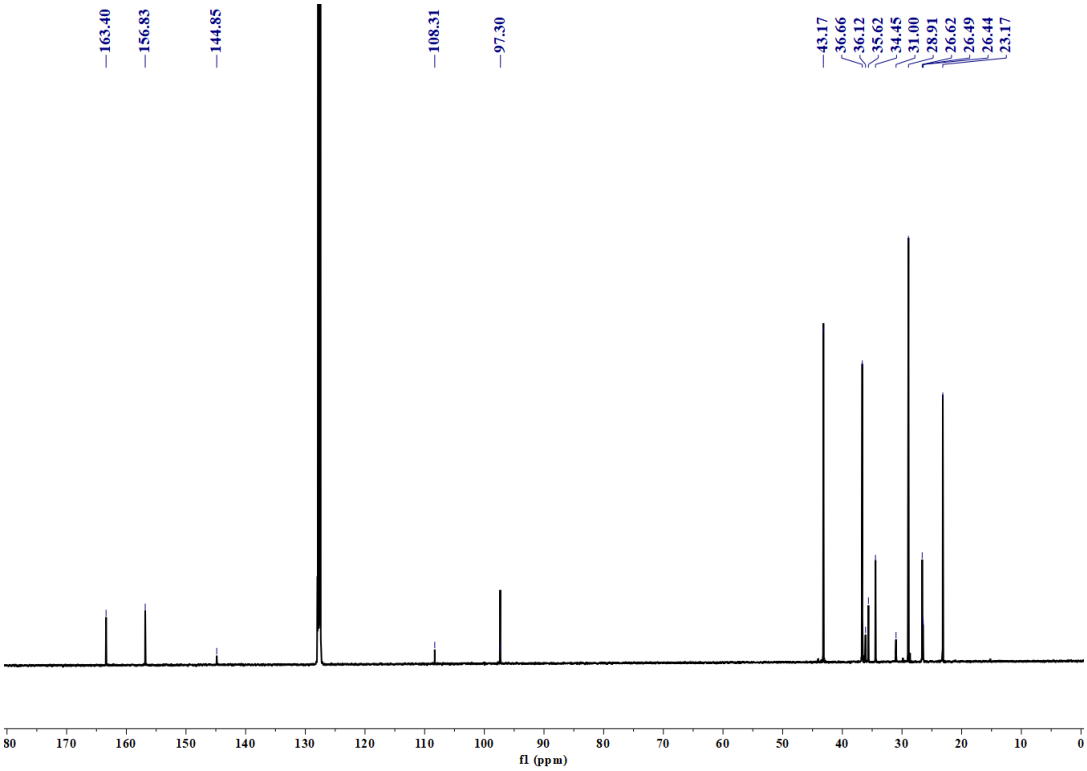

Figure S18. ^{13}C{^{1}H} NMR spectrum (125 MHz) of [(Tp^{Ad,iPr})Yb(η^3-CH$_2$CHCHCy)] (**5**) in C_6D_6 at 25 ^{o}C.

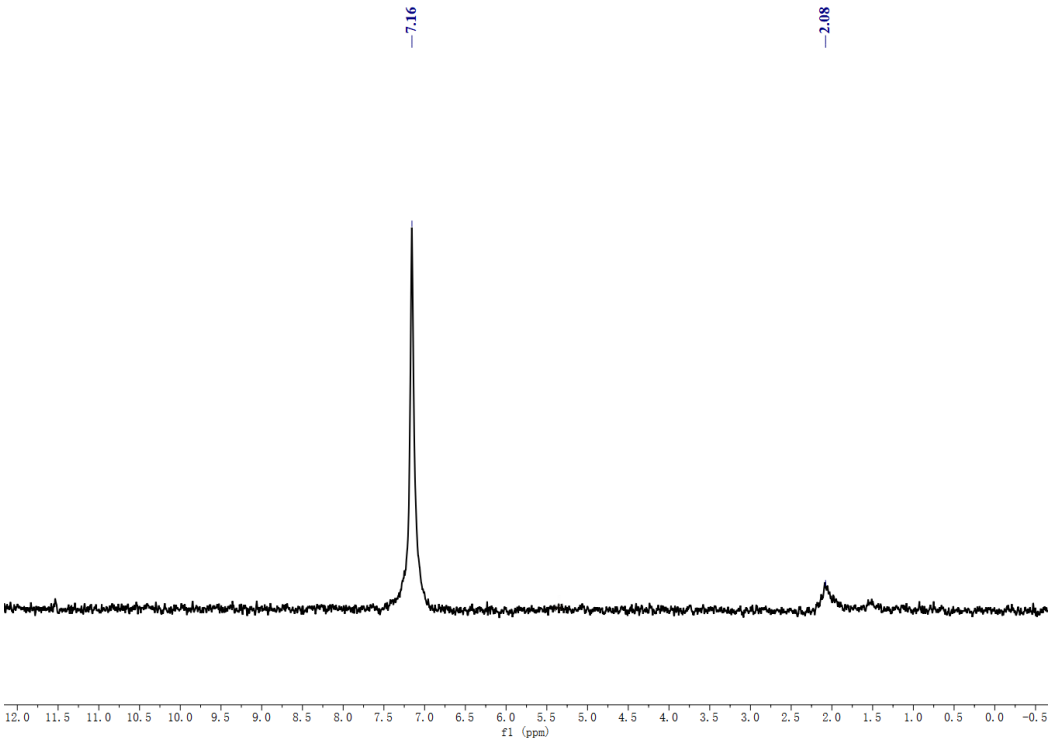

Figure S19. ^{2}H NMR spectrum (61 MHz) of [(Tp^{Ad,iPr})Yb(η^3-CH$_2$CDCHCy)] (**5-D**) in C_6H_6 at 25 ^{o}C. (Drops of C_6D_6 were added as internal standard)

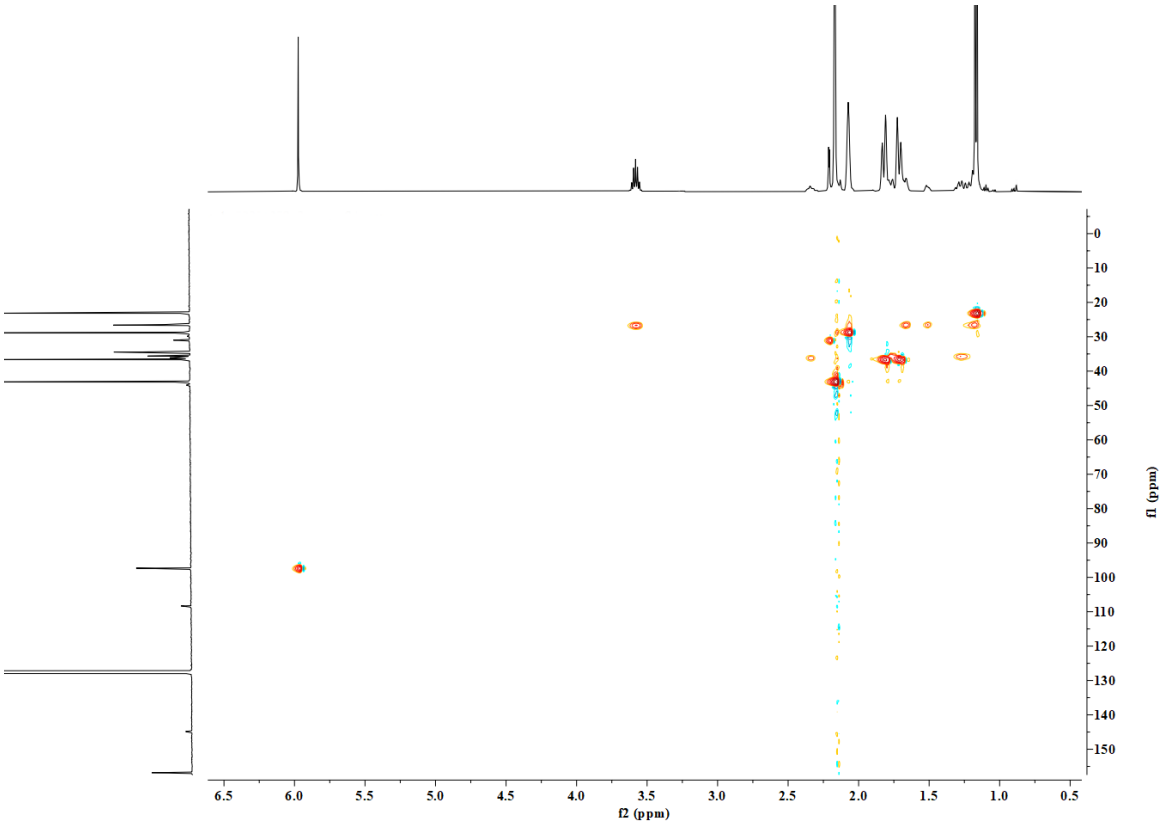

Figure S20. ^{1}H-^{13}C HSQC NMR spectrum (500 MHz) of [(Tp^{Ad,iPr})Yb(η^3-CH$_2$CHCHCy)] (**5**) in C_6D_6 at 25 ^{o}C.

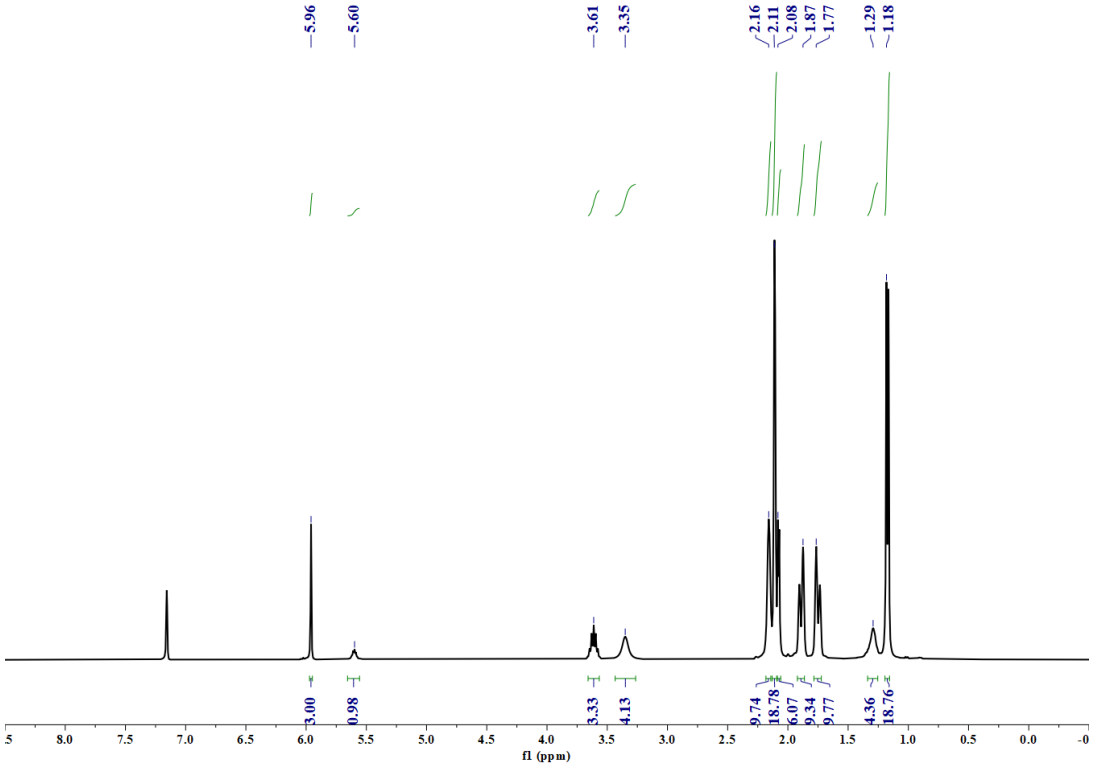

Figure S21. ^{1}H NMR spectrum (500 MHz) of [(Tp^{Ad,iPr})Yb(η^{1}-CH=C=CMe$_2$)(THF)] (**6**) in C_6D_6 at 25 ^{o}C.

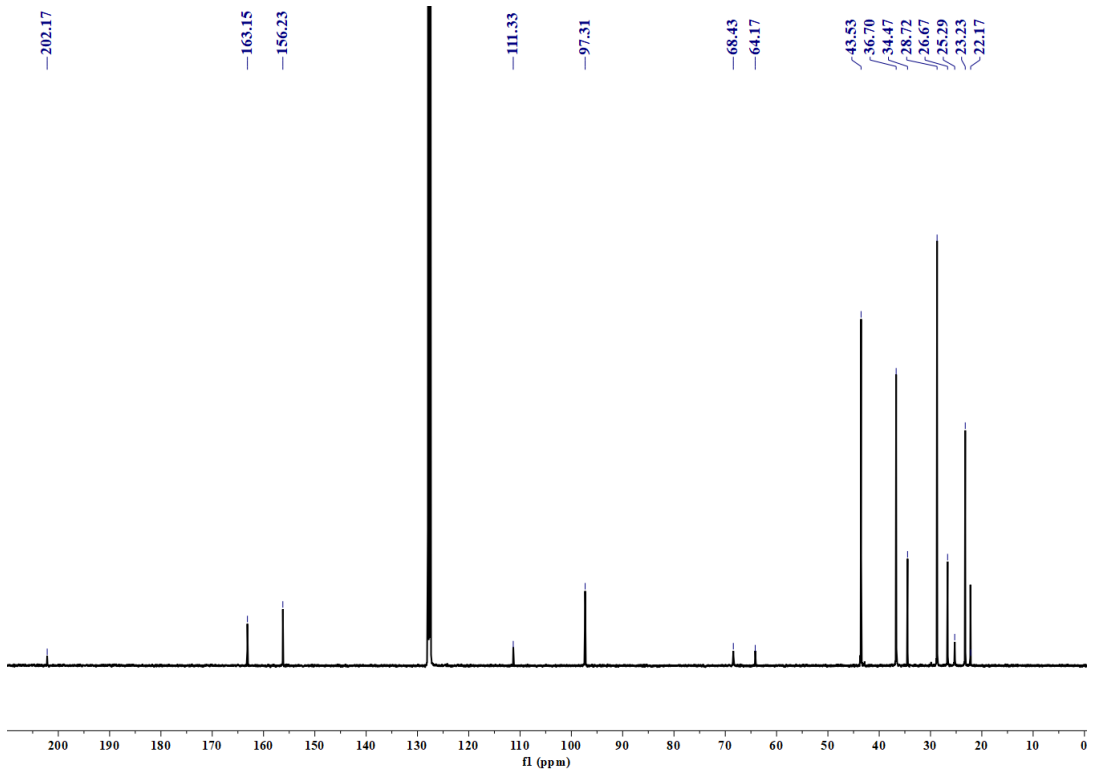

Figure S22. ^{13}C {^{1}H} NMR spectrum (125 MHz) of [(Tp^{Ad,iPr})Yb(η^{1}-CH=C=CMe$_2$)(THF)] (**6**) in C_6D_6 at 25 ^{o}C.

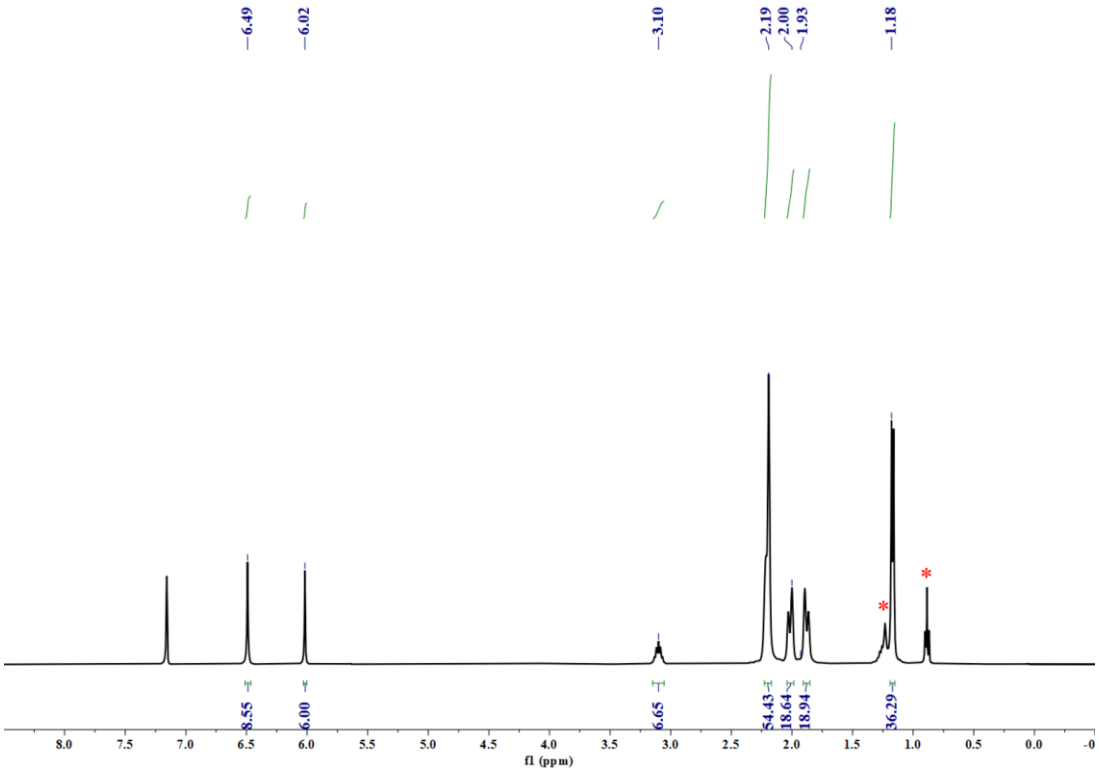

Figure S23. ^{1}H NMR spectrum (400 MHz) of [(Tp^{Ad,iPr})Yb(μ-η^8,η^8-COT)Yb(Tp^{Ad,iPr})] (**7**) in C_6D_6 at 25 ^{o}C. (* = residual hexane)

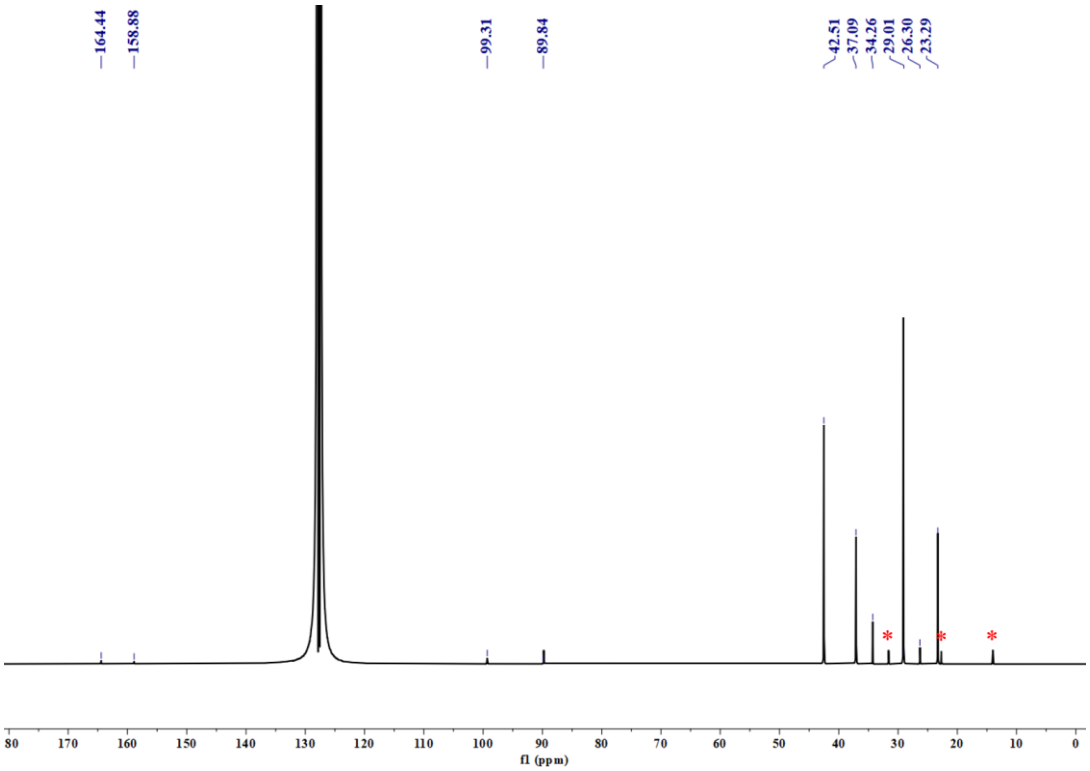

Figure S24. ^{13}C{^{1}H} NMR spectrum (100 MHz) of [(Tp^{Ad,iPr})Yb(μ-η^8,η^8-COT)Yb(Tp^{Ad,iPr})] (**7**) in C_6D_6 at 25 ^{o}C. (* = residual hexane)

X-ray Crystallographic Studies

Single crystals suitable for X-ray analysis were obtained as described in the preparation. The crystals were manipulated in the glovebox under a microscope in the glovebox. Data collection was performed at - 80 ^{o}C on D8 Venture diffractrometer with a CCD area detector, using graphite monochromated Mo K_{α} radiation (λ = 0.71073 Å). The determination of the crystal class and unit cell parameters was carried out by the SMART program packages[4]. The raw frame data were processed using SAINT[5] and absorption corrections using SADABS[6] to yield the reflection data file. The structures were solved by using SHELXS-2018,[7] SUPERFLIP[8-9] or Sir 97[10] in the WinGX program package.[11] Refinements were performed on F^2 anisotropically for all the non-hydrogen atoms by the full-matrix least-squares method using SHELXL-2018 program.[7]

Refinement of **1**: The SQUEEZE[12] routine of the program PLATON[13] was implemented to remove the contributions of four disordered benzenes to the observed structure factors. The THF ligand was disordered. C9~C12 and C9'~C12' disordered over two sites with occupancies 0.594:0.406.

Refinement of **2**: The SQUEEZE[12] routine of the program PLATON[13] was implemented to remove the contributions of two disordered THF to the observed structure factors. The terminal hydride (H1) was located by difference Fourier syntheses, and refined. One of the three adamantyl groups in the $Tp^{Ad,iPr}$ ligand was highly disordered. C18~C26 and C18'~C26' disordered over two sites with occupancies 0.573:0.427.

Refinement of **5**: The SQUEEZE[12] routine of the program PLATON[13] was implemented to remove the contributions of disordered pentane to the observed structure factors.

Refinement of **6**: The SQUEEZE[12] routine of the program PLATON[13] was implemented to remove the contributions of one disordered THF to the observed structure factors. The THF ligand was disordered. C6~C9 and C6'~C9' disordered over two sites with occupancies 0.383:0.617.

Refinement of **7**: The SQUEEZE[12] routine of the program PLATON[13] was implemented to remove the contributions of three disordered toluene to the observed structure factors. The hydrogen atoms (H1~H8) in the COT ligand were located by difference Fourier syntheses, and refined.

Other hydrogen atoms were placed at the calculated positions and were included in the structure calculation without further refinement of the parameters. The residual electron

densities were of no chemical significance. Crystal data and analysis results are listed in Table **S1-6**.

CCDC number 2080811 (**1**), 2080812 (**2**), 2080813 (**4**), 2080814 (**5**), 2080815 (**6**), 2080816 (**7**) contain the supplementary crystallographic data for this paper. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+44)1223-336-033; E-mail: deposit@ccdc.cam.ac.uk).

Table S1. Crystal data and structure refinement for complex **1**

CCDC number	2080811
Empirical formula	$C_{60}H_{87}B_1N_6O_1Yb_1$ • (4 x Benzene)
Formula weight	1092.20
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
a	11.9333(7) Å
b	24.8328(18) Å
c	25.1180(18) Å
α	90 °
β	90 °
γ	90 °
Volume	7443.4(9) $Å^3$
Z, Calculated density	4, 0.975 Mg/m^3
Absorption coefficient	1.290 mm^{-1}
F(000)	2288
Crystal size	0.190 x 0.180 x 0.150 mm
Theta range for data collection	1.889 to 24.999 °
Limiting indices	-14<=h<=14, -29<=k<=29, -29<=l<=29
Reflections collected / unique	276570 / 13052 [R(int) = 0.0841]
Completeness to theta	(24.999 °) 99.7 %
Absorption correction	Empirical
Max. and min. transmission	0.824 and 0.783
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	13052 / 0 / 645
Goodness-of-fit on F^2	1.125
Final R indices [I>2sigma(I)]	R1 = 0.0260, wR2 = 0.0628
R indices (all data)	R1 = 0.0309, wR2 = 0.0657
Largest diff. peak and hole	0.549 and -0.397 e. $Å^{-3}$

Table S2. Crystal data and structure refinement for complex **2**

CCDC number	2080812
Empirical formula	$C_{52}H_{79}B_1N_6O_1Yb_1 \bullet$ (2 x THF)
Formula weight	988.06
Temperature	193(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
a	11.6146(8) Å
b	15.7831(14) Å
c	16.3212(13) Å
α	87.388(2) °
β	89.036(2) °
γ	87.359(2) °
Volume	2985.3(4) $Å^3$
Z, Calculated density	2, 1.099 Mg/m^3
Absorption coefficient	1.601 mm^{-1}
F(000)	1032
Crystal size	0.160 x 0.130 x 0.110 mm
Theta range for data collection	2.133 to 25.000 ^{o}
Limiting indices	-13<=h<=13, -18<=k<=18, -19<=l<=19
Reflections collected / unique	82165 / 10469 [R(int) = 0.1107]
Completeness to theta	(25.000) 99.4 %
Absorption correction	Empirical
Max. and min. transmission	0.839 and 0.779
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10469 / 42 / 543
Goodness-of-fit on F^2	1.013
Final R indices [I>2sigma(I)]	R1 = 0.0449, wR2 = 0.0931
R indices (all data)	R1 = 0.0714, wR2 = 0.1054
Largest diff. peak and hole	1.456 and -1.190 e. $Å^{-3}$

Table S3. Crystal data and structure refinement for complex **4**

CCDC number	2080813
Empirical formula	$C_{62}H_{83}B_1N_6Yb_1$
Formula weight	1096.19
Temperature	193(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
a	11.7532(6) Å
b	15.0679(8) Å
c	15.7942(8) Å
α	96.7430(10) °
β	95.1850(10) °
γ	101.8520(10) °
Volume	2699.6(2) $Å^3$
Z, Calculated density	2, 1.349 Mg/m^3
Absorption coefficient	1.777 mm^{-1}
F(000)	1144
Crystal size	0.220 x 0.180 x 0.150 mm
Theta range for data collection	1.783 to 25.000 ^{o}
Limiting indices	-13<=h<=13, -16<=k<=17, -18<=l<=13
Reflections collected / unique	13828 / 9268 [R(int) = 0.0268]
Completeness to theta	(25.000) 97.4 %
Absorption correction	Empirical
Max. and min. transmission	0.766 and 0.688
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9268 / 0 / 647
Goodness-of-fit on F^2	1.017
Final R indices [I>2sigma(I)]	R1 = 0.0367, wR2 = 0.0820
R indices (all data)	R1 = 0.0446, wR2 = 0.0859
Largest diff. peak and hole	1.095 and -0.555 e. $Å^{-3}$

Table S4. Crystal data and structure refinement for complex **5**

CCDC number	2080814
Empirical formula	$C_{57}H_{85}B_1N_6Yb_1 \bullet$ (Pentane)
Formula weight	1038.15
Temperature	193(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
a	11.7224(4) Å
b	15.3253(6) Å
c	16.0077(6) Å
α	89.6000(10) °
β	89.7400(10) °
γ	72.9830(10) °
Volume	2749.79(18) $Å^3$
Z, Calculated density	2, 1.254 Mg/m^3
Absorption coefficient	1.741 mm^{-1}
F(000)	1088
Crystal size	0.170 x 0.160 x 0.140 mm
Theta range for data collection	2.311 to 25.000 °
Limiting indices	-13<=h<=13, -18<=k<=18, -19<=l<=19
Reflections collected / unique	50299 / 9580 [R(int) = 0.0354]
Completeness to theta	(25.000) 99.0 %
Absorption correction	Empirical
Max. and min. transmission	0.784 and 0.751
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9580 / 12 / 549
Goodness-of-fit on F^2	1.076
Final R indices [I>2sigma(I)]	R1 = 0.0458, wR2 = 0.1190
R indices (all data)	R1 = 0.0500, wR2 = 0.1225
Largest diff. peak and hole	2.010 and -1.159 e. $Å^{-3}$

Table S5. Crystal data and structure refinement for complex **6**

CCDC number	2080815
Empirical formula	$C_{57}H_{85}B_1N_6O_1Yb_1 \bullet (THF)$
Formula weight	1054.15
Temperature	193(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/n
a	13.6830(8) Å
b	28.2930(13) Å
c	15.3100(8) Å
α	90 °
β	98.479(2) °
γ	90 °
Volume	5862.2(5) $Å^3$
Z, Calculated density	4, 1.194 Mg/m^3
Absorption coefficient	1.635 mm^{-1}
F(000)	2208
Crystal size	0.200 x 0.180 x 0.140 mm
Theta range for data collection	1.999 to 24.999 °
Limiting indices	-16<=h<=16, -33<=k<=33, -18<=l<=18
Reflections collected / unique	155241 / 10236 [R(int) = 0.0573]
Completeness to theta	(24.999) 99.0 %
Absorption correction	Empirical
Max. and min. transmission	0.795 and 0.728
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10236 / 11 / 604
Goodness-of-fit on F^2	1.114
Final R indices [I>2sigma(I)]	R1 = 0.0386, wR2 = 0.0903
R indices (all data)	R1 = 0.0443, wR2 = 0.0939
Largest diff. peak and hole	1.218 and -1.152 e. $Å^{-3}$

Table S6. Crystal data and structure refinement for complex **7**

CCDC number	2080816
Empirical formula	$C_{104}H_{148}B_2N_{12}Yb_2$ • (3 x Toluene)
Formula weight	1934.04
Temperature	193(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
a	14.2540(10) Å
b	15.4656(11) Å
c	27.2256(17) Å
α	99.787(2) °
β	103.653(2) °
γ	100.350(2) °
Volume	5593.9(7) $Å^3$
Z, Calculated density	2, 1.148 Mg/m^3
Absorption coefficient	1.707 mm^{-1}
F(000)	2012
Crystal size	0.190 x 0.140 x 0.120 mm
Theta range for data collection	1.914 to 25.000 °
Limiting indices	-16<=h<=16, -18<=k<=18, -32<=l<=32
Reflections collected / unique	167363 / 19650 [R(int) = 0.0383]
Completeness to theta	(25.000) 99.7 %
Absorption correction	Empirical
Max. and min. transmission	0.815 and 0.751
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	19650 / 0 / 1121
Goodness-of-fit on F^2	1.024
Final R indices [I>2sigma(I)]	R1 = 0.0191, wR2 = 0.0434
R indices (all data)	R1 = 0.0243, wR2 = 0.0460
Largest diff. peak and hole	0.432 and -0.326 e. $Å^{-3}$

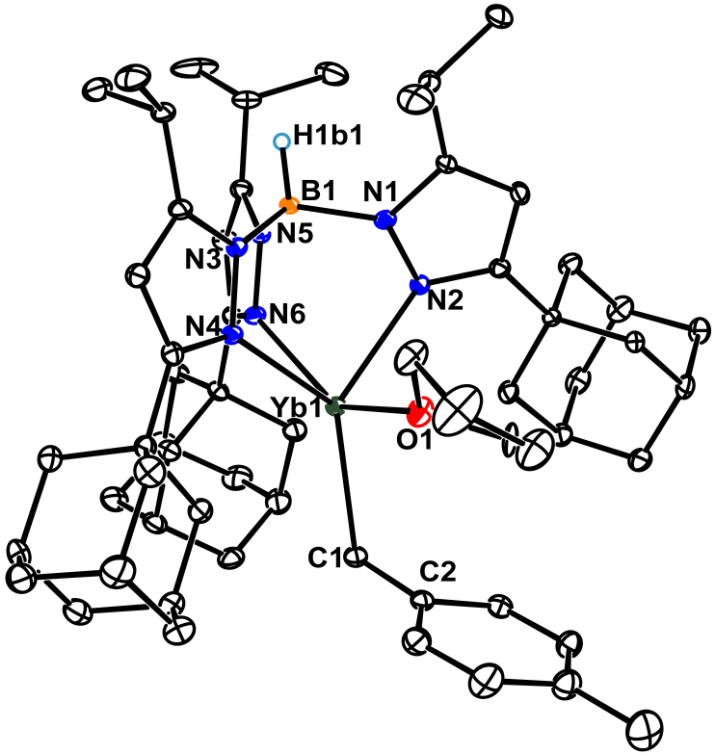

Figure S25. ORTEP drawing of [(Tp^{Ad,iPr})Yb(*p*-$CH_2C_6H_4$-Me)(THF)] (**1**) with thermal ellipsoids drawn at the 20% probability level. Except H1b1, all the hydrogen atoms are omitted for clarity. Selected interatomic distances [Å] and angles [deg]: Yb1–C1 2.562(4), Yb1–O1 2.431(4), Yb1–N2 2.435(4), Yb1–N4 2.458(4), Yb1–N6 2.512(4), Yb1–C1–C2 114.6(3).

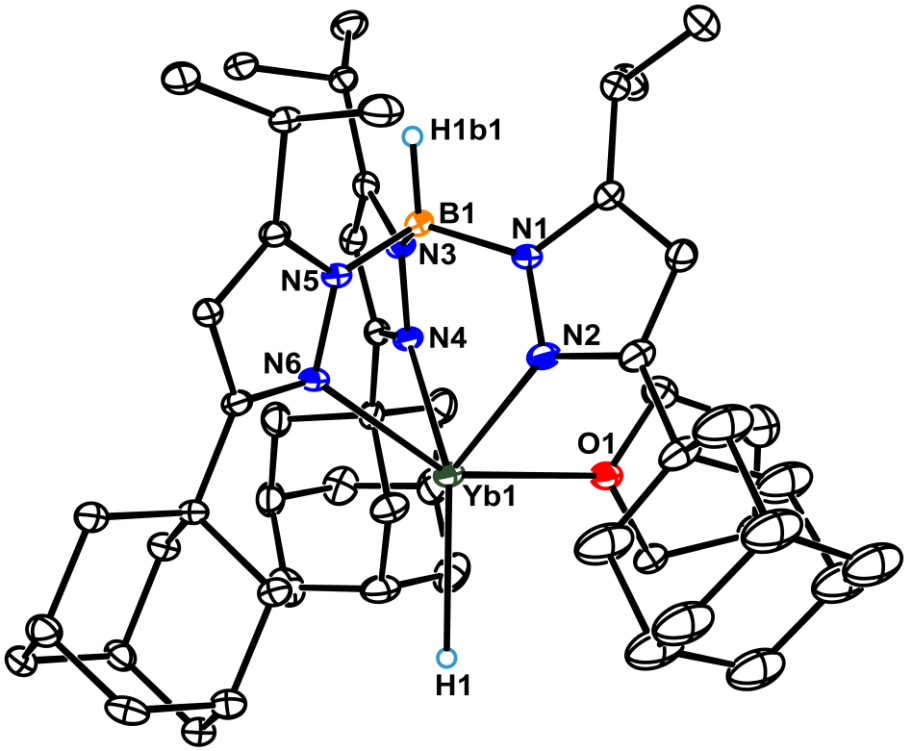

Figure S26. ORTEP drawing of [(Tp^{Ad,iPr})Yb(H)(THF)] (**2**) with thermal ellipsoids drawn at the 20% probability level. All the hydrogen atoms in pyrazolyls and THF are omitted for clarity. Selected interatomic distances [Å]: Yb1–H1 2.49(4), Yb1–O1 2.448(3), Yb1–N2 2.461(4), Yb1–N4 2.458(4), Yb1–N6 2.480(4).

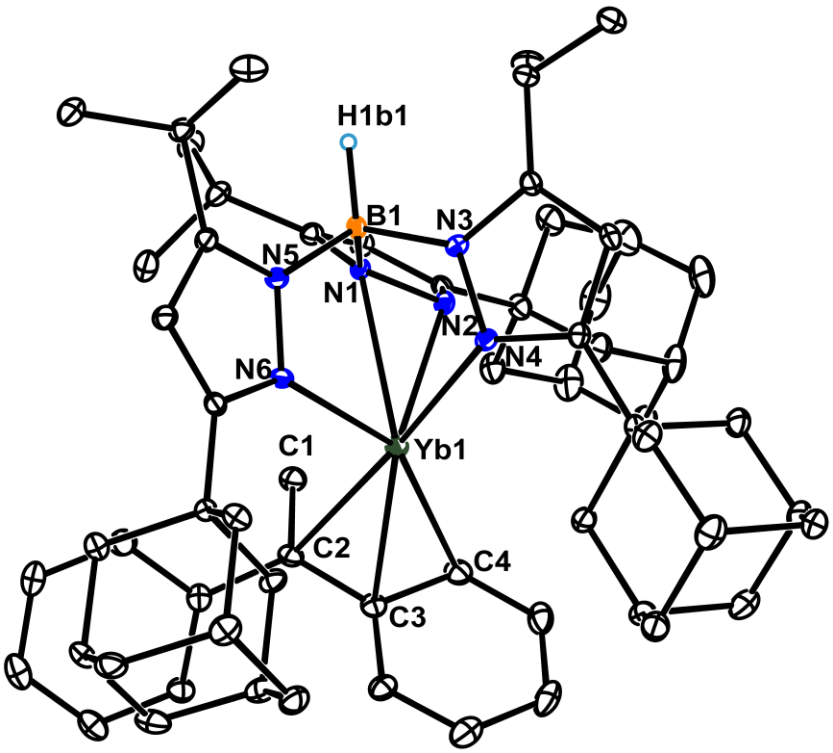

Figure S27. ORTEP drawing of [(Tp^{Ad,iPr})Yb{CPh$_2$(Me)}] (**4**) with thermal ellipsoids drawn at the 20% probability level. Except H1b1, All the other hydrogen atoms are omitted for clarity. Selected interatomic distances [Å]: Yb1–C2 2.715(4), Yb1–C3 2.698(4), Yb1–C4 2.787(4), Yb1–N1 2.723(3), Yb1–N2 2.551(3), Yb1–N4 2.457(3), Yb1–N6 2.452(3), C1–C2 1.516(6), C2–C3 1.426(6), C3–C4 1.430(6).

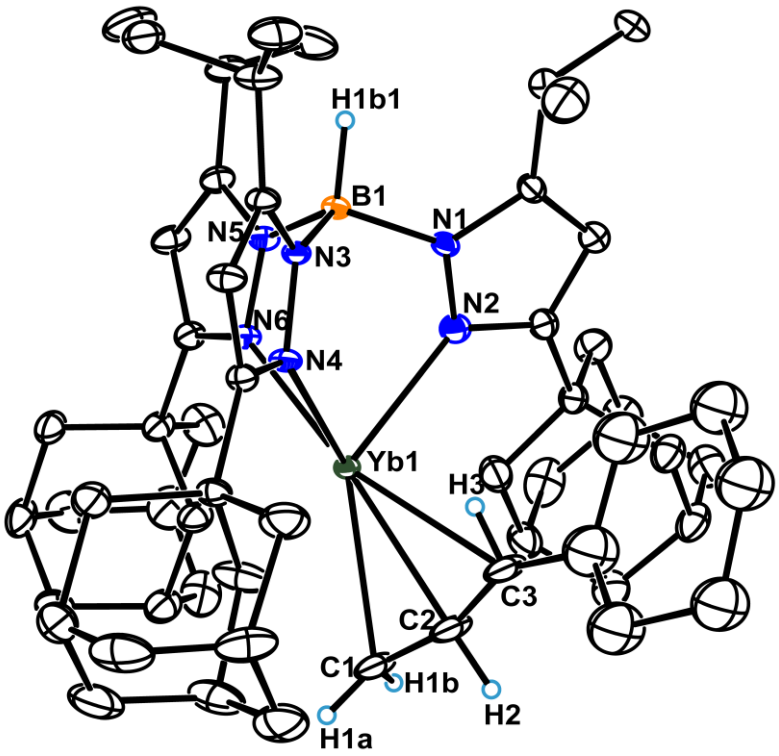

Figure S28. ORTEP drawing of [(Tp^{Ad,iPr})Yb(η^3-CH$_2$CHCHCy)] (**5**) with thermal ellipsoids drawn at the 20% probability level. All the hydrogen atoms in pyrazolyls and cyclohexane are omitted for clarity. Selected interatomic distances [Å] and angles [deg]: C1–C2 1.365(11), C2–C3 1.234(10), Yb1–C1 2.692(6), Yb1–C2 2.525(6), Yb1–C3 2.621(7), Yb1–N2 2.467(5), Yb1–N4 2.453(4), Yb1–N6 2.463(4), C1–C2–C3 162.3(7).

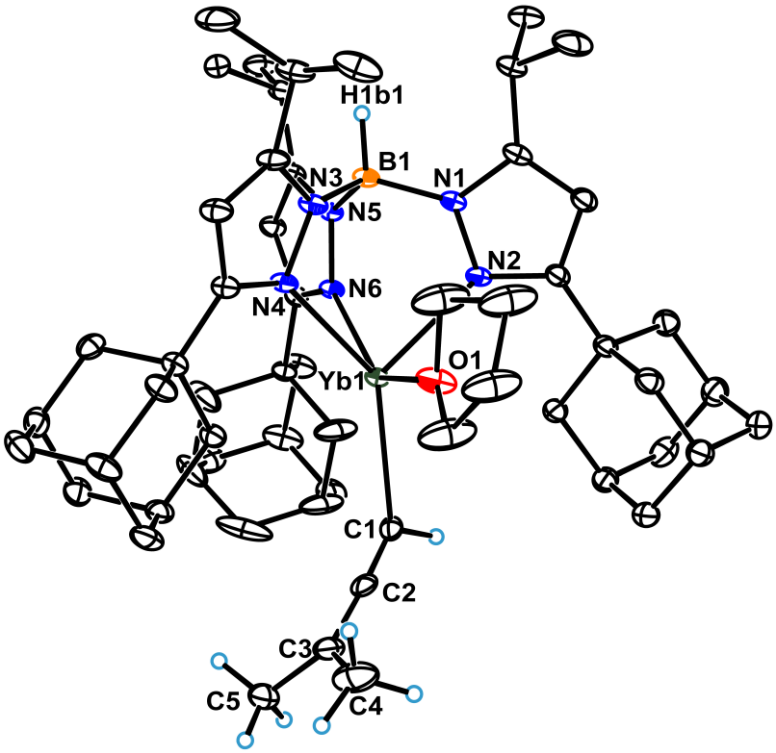

Figure S29. ORTEP drawing of [(Tp^{Ad,iPr})Yb(η^1-CH=C=CMe$_2$)(THF)] (**6**) with thermal ellipsoids drawn at the 20% probability level. All the hydrogen atoms in pyrazolyls and THF are omitted for clarity. Selected interatomic distances [Å] and angles [deg]: C1–C2 1.206(7), C2–C3 1.367(8), C3–C4 1.497(9), C3–C5 1.493(9), Yb1–C1 2.573(5), Yb1–O1 2.462(3), Yb1–N2 2.458(3), Yb1–N4 2.453(4), Yb1–N6 2.471(3), Yb1–C1–C2 134.8(4), C1–C2–C3 176.4(5).

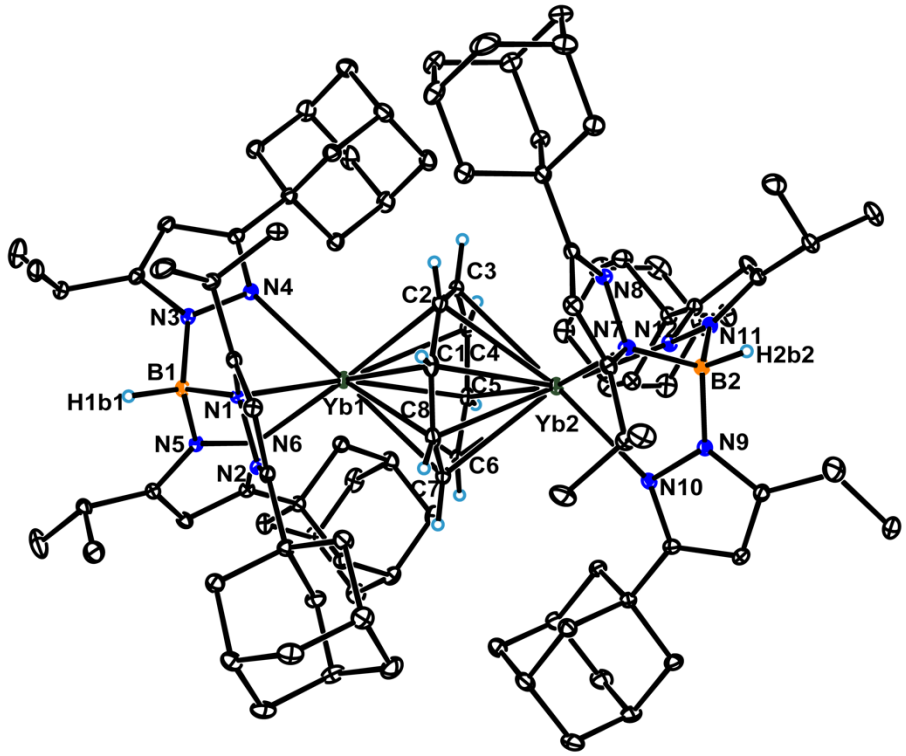

Figure S30. ORTEP drawing of [(Tp^{Ad,iPr})Yb(μ-η^8,η^8-COT)Yb(Tp^{Ad,iPr})] (**7**) with thermal ellipsoids drawn at the 20% probability level. All the hydrogen atoms in pyrazolyls are omitted for clarity. Selected interatomic distances [Å]: Yb1–C1 2.790(2), Yb1–C2 2.784(2), Yb1–C3 2.823(2), Yb1–C4 2.826(2), Yb1–C5 2.794(2), Yb1–C6 2.757(2), Yb1–C7 2.760(2), Yb1–C8 2.784(2), Yb1–N1 2.626(2), Yb1–N2 2.990(2), Yb1–N4 2.568(2), Yb1–N6 2.511(2), Yb2–C1 2.789(2), Yb2–C2 2.805(2), Yb2–C3 2.790(2), Yb2–C4 2.785(2), Yb2–C5 2.793(2), Yb2–C6 2.795(2), Yb2–C7 2.777(2), Yb2–C8 2.763(2), Yb2–N7 2.626(2), Yb2–N8 2.924(2), Yb2–N10 2.589(2), Yb2–N12 2.510(2), C1–C2 1.408(3), C2–C3 1.406(3), C3–C4 1.410(3), C4–C5 1.407(3), C5–C6 1.405(3), C6–C7 1.412(3), C7–C8 1.405(3), C8–C1 1.401(3).

Computational investigation

Computational details:

The optimization of reactants, transition states, IRC and products were carried out by employing DFT hybrid functional (B3PW91)[14] along with small core pseudopotential Stuggart basis set[15] for ytterbium atom and People basis set[16-18] (6-31G**) for the rest of the atoms. Frequency calculations were performed to locate saddle points for transition state structures, minima for rest of the structures and for obtaining thermal corrections over the energies. All the calculations were performed using Gaussian 09 suite of programs.[19]

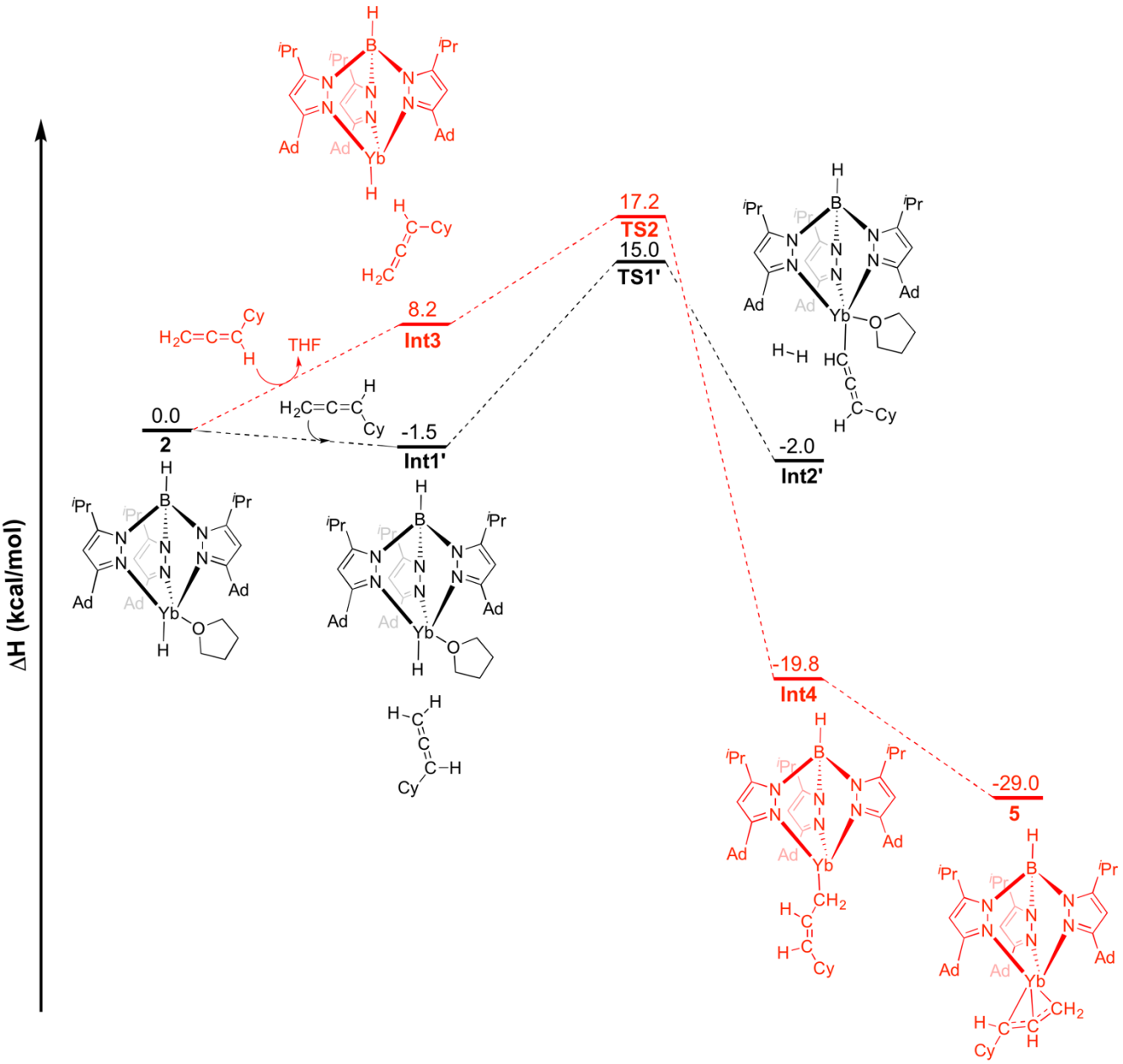

Figure S31. Different enthalpy profiles computed for the reaction of **2** with cyclohexylallene at room temperature

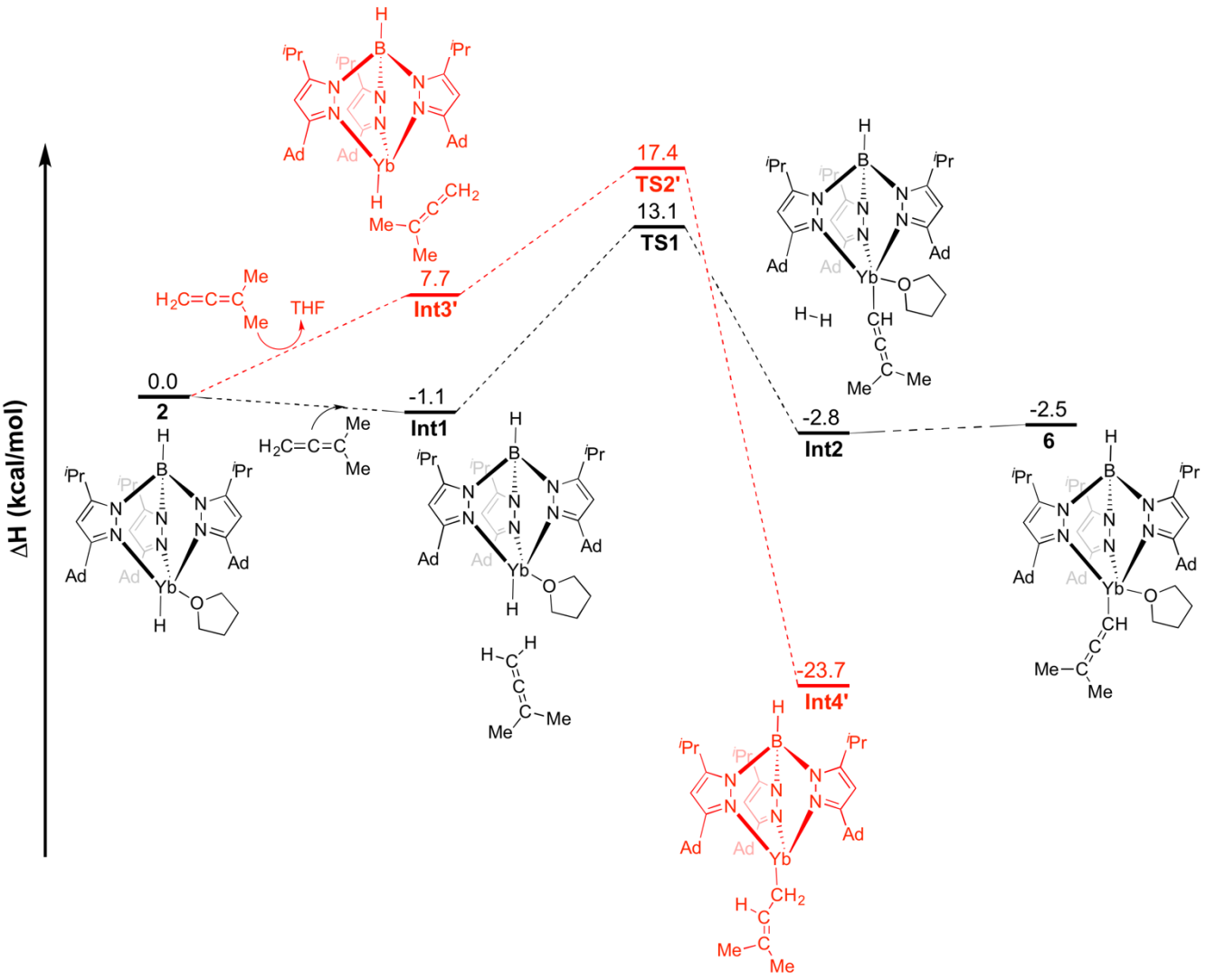

Figure S32. Different enthalpy profiles computed for the reaction of **2** with 1,1-dimethyllallene at room temperature

Optimized geometry of 2

C	7.413781000	1.399405000	0.209286000
H	6.851644000	2.337568000	0.138288000
H	6.866656000	0.712623000	0.861311000
C	7.737491000	0.815924000	-1.163751000
H	6.959542000	1.033751000	-1.900409000
H	7.850077000	-0.272330000	-1.103202000
C	9.083900000	1.469789000	-1.487227000
H	9.664063000	0.920933000	-2.233943000
H	8.937078000	2.491758000	-1.853881000
C	9.759597000	1.482532000	-0.123020000
H	10.249245000	0.524424000	0.092967000
H	10.493588000	2.277495000	0.024841000
C	2.600724000	4.437716000	2.215382000
H	1.569770000	4.128793000	2.415474000
H	2.760557000	5.414592000	2.681441000
H	2.701486000	4.558645000	1.131038000
C	3.337881000	2.025655000	2.087465000
H	2.306578000	1.694442000	2.252015000
H	3.502743000	2.090900000	1.006108000
H	4.011539000	1.262473000	2.486817000
C	3.580521000	3.390855000	2.751688000
H	3.395106000	3.275579000	3.826703000
C	5.010306000	3.828192000	2.579656000
C	5.534726000	4.743035000	1.677323000
H	4.980504000	5.341148000	0.969190000
C	6.922646000	4.752966000	1.907566000
C	7.955227000	5.654386000	1.276092000
C	7.658472000	7.119812000	1.691108000
H	7.690482000	7.196512000	2.785486000
H	6.639382000	7.388386000	1.383995000
C	7.896096000	5.569684000	-0.266818000
H	8.104162000	4.537677000	-0.578593000
H	6.882769000	5.809508000	-0.614678000
C	9.386466000	5.308689000	1.729079000
H	9.638856000	4.279867000	1.434933000
H	9.453408000	5.363059000	2.823223000
C	10.327761000	6.162329000	-0.434960000
H	10.578917000	5.141903000	-0.754768000
H	11.065244000	6.831090000	-0.898506000
C	10.405348000	6.269048000	1.095701000
H	11.410263000	5.991371000	1.435826000
C	10.088914000	7.710304000	1.522951000
H	10.824153000	8.402155000	1.090559000
H	10.163677000	7.805296000	2.614241000
C	8.673533000	8.081384000	1.055883000
H	8.438304000	9.108117000	1.365506000
C	8.592019000	7.971961000	-0.474507000
H	9.299930000	8.669415000	-0.941863000
H	7.588815000	8.255544000	-0.820811000
C	8.911925000	6.531318000	-0.903111000
H	8.849555000	6.449630000	-1.996414000
C	3.161293000	-1.047769000	5.274325000
H	2.200085000	-0.876748000	5.770053000
H	2.978986000	-1.146779000	4.200033000
H	3.551302000	-2.003743000	5.640203000
C	4.372559000	0.221505000	7.091636000
H	3.430923000	0.389831000	7.626023000
H	4.824051000	-0.698152000	7.479253000
H	5.052257000	1.046785000	7.320721000
C	4.125660000	0.103160000	5.578972000
H	3.654791000	1.032452000	5.241520000
C	5.428890000	-0.056880000	4.840750000
C	6.089529000	-1.235876000	4.533256000
H	5.745396000	-2.239761000	4.732857000
C	7.294448000	-0.851951000	3.923666000
C	8.394762000	-1.767478000	3.447037000
C	8.836699000	-2.694058000	4.608252000
H	7.972840000	-3.260085000	4.979151000

H	9.194519000	-2.079400000	5.444232000
C	7.886839000	-2.658315000	2.285927000
H	7.564886000	-2.019799000	1.452052000
H	7.001592000	-3.219205000	2.612480000
C	9.630435000	-0.992427000	2.957482000
H	10.028394000	-0.362234000	3.766000000
H	9.347889000	-0.331629000	2.127457000
C	10.733885000	-1.954436000	2.490447000
H	11.593454000	-1.363815000	2.151444000
C	10.203871000	-2.822773000	1.339183000
H	9.923209000	-2.190798000	0.485042000
H	10.990369000	-3.502947000	0.985883000
C	8.986480000	-3.625864000	1.821947000
H	8.599842000	-4.243151000	1.000206000
C	9.402819000	-4.528421000	2.993900000
H	8.544901000	-5.123572000	3.335070000
H	10.173973000	-5.238599000	2.666815000
C	9.936529000	-3.660963000	4.144334000
H	10.227983000	-4.302952000	4.985815000
C	11.152946000	-2.858304000	3.659443000
H	11.557037000	-2.249674000	4.478817000
H	11.953973000	-3.539084000	3.341711000
C	4.942276000	5.497786000	6.388000000
H	3.930523000	5.822372000	6.656293000
H	5.631225000	6.323036000	6.598395000
H	4.968349000	5.307170000	5.311612000
C	5.248301000	4.517334000	8.694503000
H	4.225064000	4.795201000	8.967424000
H	5.530939000	3.636870000	9.279459000
H	5.902386000	5.344493000	8.991243000
C	5.340057000	4.247880000	7.189903000
H	4.622035000	3.455576000	6.947614000
C	6.713674000	3.771191000	6.796319000
C	7.921488000	3.999714000	7.439489000
H	8.063568000	4.517449000	8.375123000
C	8.906224000	3.407245000	6.631867000
C	10.400854000	3.366596000	6.856661000
C	11.131758000	4.307242000	5.865636000
H	10.935137000	3.983698000	4.834177000
H	10.741157000	5.328060000	5.976953000
C	10.954710000	1.935532000	6.663098000
H	10.437615000	1.247397000	7.345234000
H	10.750595000	1.596747000	5.639137000
C	10.737349000	3.827167000	8.291758000
H	10.364435000	4.848353000	8.448049000
H	10.221729000	3.182197000	9.016211000
C	12.252977000	3.793052000	8.537611000
H	12.455870000	4.122082000	9.565568000
C	12.951365000	4.735359000	7.545245000
H	12.604129000	5.766780000	7.697211000
H	14.035508000	4.733417000	7.722572000
C	12.648515000	4.277312000	6.111385000
H	13.138285000	4.949631000	5.394862000
C	13.162194000	2.843949000	5.904085000
H	12.946751000	2.519835000	4.878066000
H	14.251310000	2.809833000	6.045778000
C	12.471485000	1.904862000	6.905631000
H	12.835446000	0.879288000	6.759171000
C	12.773049000	2.361395000	8.340574000
H	12.296628000	1.684595000	9.063314000
H	13.854271000	2.323316000	8.530838000
B	5.988444000	2.496925000	4.628172000
N	6.051916000	3.324971000	3.301395000
N	7.222890000	3.884386000	2.878818000
N	6.213241000	0.972166000	4.412777000
N	7.355540000	0.484229000	3.846509000
N	6.987419000	3.065419000	5.664928000
N	8.329118000	2.849737000	5.558353000
O	8.689566000	1.686194000	0.823661000
Yb	9.035414000	2.228256000	3.250885000

H	4.883896000	2.630861000	5.070364000
H	11.130403000	2.241024000	2.937045000

Optimized geometry of 2 without THF

C	2.710605000	4.740713000	2.508065000
H	1.663724000	4.565792000	2.775981000
H	2.995722000	5.731338000	2.874879000
H	2.769885000	4.754049000	1.414230000
C	3.184745000	2.260470000	2.569017000
H	2.133576000	2.056745000	2.801162000
H	3.307343000	2.215925000	1.481385000
H	3.794674000	1.465257000	3.006311000
C	3.597863000	3.642520000	3.100893000
H	3.449523000	3.640839000	4.187011000
C	5.056442000	3.903493000	2.832614000
C	5.624397000	4.620997000	1.788867000
H	5.098599000	5.161835000	1.016390000
C	7.013024000	4.500084000	1.954587000
C	8.106193000	5.109344000	1.113994000
C	8.088082000	6.651655000	1.268944000
H	8.234174000	6.910470000	2.325781000
H	7.100191000	7.034882000	0.982764000
C	7.892572000	4.767599000	-0.380550000
H	7.896649000	3.677023000	-0.509209000
H	6.903869000	5.119391000	-0.701631000
C	9.500696000	4.602478000	1.526998000
H	9.559093000	3.509179000	1.403966000
H	9.690619000	4.838839000	2.584561000
C	10.362179000	4.888472000	-0.808262000
H	10.415909000	3.800468000	-0.947509000
H	11.150965000	5.328587000	-1.432487000
C	10.599842000	5.244276000	0.667033000
H	11.570988000	4.855728000	0.994850000
C	10.556177000	6.770029000	0.840489000
H	11.348973000	7.237996000	0.242099000
H	10.747902000	7.037083000	1.888270000
C	9.180807000	7.296025000	0.402509000
H	9.143636000	8.385766000	0.529807000
C	8.941282000	6.939181000	-1.072862000
H	9.705127000	7.412363000	-1.704089000
H	7.968675000	7.328698000	-1.402824000
C	8.986127000	5.412896000	-1.245795000
H	8.809291000	5.155154000	-2.298125000
C	3.536359000	-1.237021000	5.691011000
H	2.626876000	-1.157879000	6.295127000
H	3.241590000	-1.343231000	4.642664000
H	4.050334000	-2.155953000	5.993504000
C	4.830210000	0.120361000	7.383357000
H	3.943599000	0.183019000	8.023953000
H	5.414299000	-0.751993000	7.695968000
H	5.442639000	1.009970000	7.554034000
C	4.422154000	-0.006704000	5.906459000
H	3.834322000	0.880691000	5.644105000
C	5.637615000	-0.036101000	5.018310000
C	6.286710000	-1.140274000	4.483931000
H	5.986940000	-2.173226000	4.578399000
C	7.396685000	-0.632873000	3.790084000
C	8.414721000	-1.402817000	2.986409000
C	9.170034000	-2.412394000	3.885850000
H	8.449430000	-3.082424000	4.372474000
H	9.688893000	-1.869481000	4.686745000
C	7.688881000	-2.195313000	1.868946000
H	7.142397000	-1.494122000	1.224604000
H	6.940351000	-2.860260000	2.318389000
C	9.454402000	-0.478638000	2.324088000
H	10.033223000	0.073007000	3.082977000
H	8.943252000	0.255924000	1.684015000
C	10.455761000	-1.290277000	1.487193000
H	11.177588000	-0.599405000	1.035353000
C	9.708515000	-2.063885000	0.391218000

H	9.195237000	-1.365659000	-0.283758000
H	10.421314000	-2.633214000	-0.220093000
C	8.691264000	-3.013162000	1.041759000
H	8.148437000	-3.564809000	0.263055000
C	9.424908000	-4.002618000	1.960623000
H	8.707212000	-4.700032000	2.413669000
H	10.131544000	-4.606978000	1.376380000
C	10.174256000	-3.227610000	3.055787000
H	10.695718000	-3.932724000	3.716087000
C	11.191947000	-2.278937000	2.404381000
H	11.749737000	-1.730643000	3.174435000
H	11.926443000	-2.853784000	1.824821000
C	4.732358000	5.543017000	6.651101000
H	3.689756000	5.821168000	6.841081000
H	5.368722000	6.379858000	6.958769000
H	4.861655000	5.404714000	5.574106000
C	4.884620000	4.468984000	8.931971000
H	3.834230000	4.703303000	9.132557000
H	5.148808000	3.571964000	9.499993000
H	5.484248000	5.301622000	9.315563000
C	5.103676000	4.270185000	7.429524000
H	4.435570000	3.467515000	7.096316000
C	6.518480000	3.853513000	7.125742000
C	7.669672000	4.117899000	7.857177000
H	7.725287000	4.626497000	8.806902000
C	8.729980000	3.577187000	7.115450000
C	10.207553000	3.581407000	7.432908000
C	10.972756000	4.528108000	6.473851000
H	10.848687000	4.189362000	5.435087000
H	10.549991000	5.539441000	6.543452000
C	10.808512000	2.162073000	7.294396000
H	10.269032000	1.470187000	7.954704000
H	10.677277000	1.798223000	6.266339000
C	10.444533000	4.069817000	8.878231000
H	10.035099000	5.082081000	8.996742000
H	9.903660000	3.419794000	9.579172000
C	11.943341000	4.078619000	9.214075000
H	12.075560000	4.426752000	10.247013000
C	12.675589000	5.025597000	8.251088000
H	12.294020000	6.049535000	8.366108000
H	13.746677000	5.054500000	8.492157000
C	12.472555000	4.540200000	6.808523000
H	12.986590000	5.215969000	6.112851000
C	13.033530000	3.117917000	6.653878000
H	12.891206000	2.772494000	5.621920000
H	14.112295000	3.114762000	6.861109000
C	12.308193000	2.174706000	7.626552000
H	12.705314000	1.157261000	7.517024000
C	12.510482000	2.658300000	9.069752000
H	12.009199000	1.978759000	9.772641000
H	13.578701000	2.651368000	9.324856000
B	5.993482000	2.567288000	4.895060000
N	6.075388000	3.393679000	3.578500000
N	7.272682000	3.756206000	3.036514000
N	6.339625000	1.069489000	4.644957000
N	7.421914000	0.701193000	3.900329000
N	6.895204000	3.179225000	6.006164000
N	8.248881000	3.015230000	5.996420000
Yb	9.156479000	2.412598000	3.826900000
H	4.861602000	2.616408000	5.280509000
H	11.237963000	2.270370000	3.523670000

Optimized geometry of 3

C	9.160745000	10.543020000	19.542699000
H	8.453151000	11.369746000	19.663086000
H	10.154143000	10.981981000	19.398343000
H	8.897129000	9.996746000	18.632061000
C	9.490392000	10.418239000	22.046526000
H	8.796428000	11.253562000	22.190506000
H	9.447801000	9.779638000	22.932372000

H	10.502642000	10.829317000	21.968738000
C	9.128903000	9.634103000	20.775121000
H	8.103805000	9.262610000	20.894437000
C	10.019866000	8.435027000	20.600776000
C	11.182328000	8.301026000	19.862153000
H	11.650410000	9.062163000	19.255961000
C	11.590475000	6.960903000	20.021397000
C	12.702353000	6.273559000	19.262543000
C	12.544301000	6.634719000	17.760204000
H	12.581882000	7.723771000	17.633046000
H	11.555104000	6.309328000	17.412844000
C	12.642974000	4.740461000	19.399432000
H	11.655002000	4.383390000	19.083441000
H	12.757233000	4.458933000	20.454173000
C	14.096734000	6.755130000	19.723913000
H	14.232415000	6.501909000	20.782750000
H	14.154962000	7.848442000	19.642318000
C	15.202539000	6.100527000	18.880833000
H	16.179615000	6.456887000	19.233085000
C	15.121549000	4.573998000	19.030546000
H	15.917336000	4.097364000	18.441315000
H	15.281634000	4.285001000	20.076709000
C	13.745917000	4.087136000	18.550410000
H	13.682388000	2.998566000	18.661888000
C	13.563049000	4.457101000	17.071590000
H	14.335767000	3.969895000	16.461320000
H	12.592067000	4.095310000	16.707255000
C	13.647327000	5.981285000	16.917724000
H	13.505676000	6.258414000	15.864575000
C	15.017883000	6.477305000	17.403104000
H	15.091253000	7.566196000	17.276513000
H	15.818080000	6.031020000	16.797374000
C	8.025885000	5.019453000	18.466806000
H	7.609482000	5.404695000	17.529539000
H	8.812461000	5.699863000	18.802319000
H	8.488759000	4.048338000	18.259824000
C	5.812941000	3.939391000	19.031119000
H	5.373829000	4.330478000	18.107912000
H	6.204598000	2.940205000	18.810369000
H	5.012855000	3.834835000	19.770393000
C	6.920825000	4.872781000	19.524814000
H	6.480928000	5.865497000	19.683434000
C	7.489400000	4.411706000	20.839669000
C	7.402226000	3.164389000	21.440537000
H	6.860414000	2.307403000	21.070346000
C	8.134473000	3.263895000	22.636384000
C	8.186575000	2.266851000	23.764798000
C	9.302380000	2.585204000	24.777054000
H	9.166016000	3.603960000	25.164635000
H	10.281610000	2.544888000	24.276582000
C	8.382870000	0.824853000	23.248603000
H	9.337787000	0.751970000	22.713281000
H	7.594476000	0.577685000	22.526169000
C	6.824680000	2.333151000	24.510564000
H	6.014591000	2.119693000	23.801522000
H	6.666551000	3.355939000	24.875561000
C	6.790251000	1.334606000	25.675042000
H	5.818400000	1.404363000	26.181138000
C	6.990631000	-0.088238000	25.131361000
H	6.178639000	-0.344232000	24.437394000
H	6.950705000	-0.816840000	25.952186000
C	8.347188000	-0.175413000	24.415345000
H	8.493149000	-1.190165000	24.022955000
C	9.467397000	0.159895000	25.410841000
H	9.461445000	-0.557612000	26.242410000
H	10.445183000	0.072596000	24.921586000
C	9.269100000	1.585697000	25.943262000
H	10.075407000	1.833936000	26.642903000
C	7.915079000	1.674425000	26.663689000
H	7.767266000	2.683718000	27.070231000

H	7.896432000	0.980356000	27.514504000
C	4.769283000	9.151799000	23.133019000
H	5.327220000	10.092748000	23.110739000
H	3.896572000	9.255880000	22.480159000
H	4.398369000	9.003135000	24.152995000
C	4.832710000	6.660943000	22.722271000
H	3.936220000	6.735558000	22.096613000
H	5.428464000	5.814493000	22.369873000
H	4.513920000	6.442436000	23.747310000
C	5.633708000	7.972516000	22.676743000
H	5.921479000	8.149787000	21.633945000
C	6.893343000	7.862518000	23.494604000
C	7.100577000	8.243813000	24.809711000
H	6.390595000	8.738916000	25.452684000
C	8.422438000	7.880377000	25.115053000
C	9.122248000	8.101018000	26.436753000
C	10.527382000	8.707305000	26.235611000
H	11.136173000	8.022580000	25.632519000
H	10.435472000	9.649249000	25.678920000
C	9.270993000	6.772168000	27.215466000
H	8.280073000	6.320112000	27.357630000
H	9.872888000	6.070561000	26.623585000
C	8.296377000	9.075473000	27.308542000
H	7.296413000	8.657455000	27.483458000
H	8.159618000	10.022996000	26.770523000
C	8.980660000	9.326691000	28.658775000
H	8.368997000	10.024736000	29.245646000
C	10.373908000	9.927938000	28.426013000
H	10.867208000	10.123996000	29.387697000
H	10.286757000	10.892894000	27.908282000
C	11.211802000	8.951529000	27.589019000
H	12.208404000	9.377610000	27.415656000
C	11.346485000	7.615830000	28.335886000
H	11.955798000	6.921324000	27.743785000
H	11.858903000	7.771179000	29.295392000
C	9.950024000	7.019329000	28.571615000
H	10.040014000	6.065462000	29.104248000
C	9.111730000	7.994471000	29.410279000
H	9.585910000	8.155002000	30.387976000
H	8.116485000	7.571030000	29.603086000
C	19.785195000	3.312218000	21.667467000
H	20.741648000	3.839665000	21.593776000
H	19.983940000	2.289940000	22.003285000
H	19.360874000	3.261227000	20.658633000
C	18.587652000	5.486289000	22.147365000
H	19.529588000	6.040703000	22.072230000
H	18.116911000	5.481133000	21.158119000
H	17.925853000	6.019964000	22.834359000
C	18.846359000	4.048482000	22.626457000
H	19.338714000	4.109580000	23.605442000
C	17.554179000	3.305044000	22.820420000
C	16.922442000	2.400144000	21.984614000
H	17.283753000	2.039735000	21.032943000
C	15.735688000	2.026316000	22.648225000
C	14.776226000	0.940875000	22.227032000
C	15.576299000	-0.382879000	22.095614000
H	16.395791000	-0.248666000	21.378172000
H	16.037805000	-0.623810000	23.062057000
C	13.643672000	0.723679000	23.247516000
H	13.060045000	1.649974000	23.339537000
H	14.072671000	0.506531000	24.233738000
C	14.143409000	1.260808000	20.855175000
H	14.935417000	1.430392000	20.114175000
H	13.571315000	2.192361000	20.938482000
C	13.231231000	0.112994000	20.396870000
H	12.793783000	0.367320000	19.422363000
C	14.049277000	-1.181501000	20.274217000
H	13.407481000	-2.003104000	19.928300000
H	14.842170000	-1.058321000	19.523885000
C	14.663647000	-1.529282000	21.638799000

H	15.256725000	-2.449606000	21.553905000
C	13.545296000	-1.725464000	22.671507000
H	13.974873000	-1.994244000	23.645969000
H	12.890736000	-2.554570000	22.370038000
C	12.732477000	-0.427820000	22.792167000
H	11.937588000	-0.570347000	23.534536000
C	12.111887000	-0.085311000	21.429208000
H	11.511072000	0.830147000	21.506536000
H	11.436901000	-0.889780000	21.106575000
C	18.444098000	0.571246000	25.693617000
H	19.447882000	0.172476000	25.509334000
H	17.768201000	-0.274501000	25.860576000
H	18.112058000	1.093743000	24.792839000
C	18.975984000	0.764914000	28.153939000
H	19.995855000	0.408695000	27.977108000
H	18.989281000	1.413918000	29.034857000
H	18.359558000	-0.110445000	28.386548000
C	18.452326000	1.500938000	26.917692000
H	19.140569000	2.327104000	26.701712000
C	17.087922000	2.088813000	27.162976000
C	16.144661000	1.718287000	28.106144000
H	16.259926000	0.961077000	28.865818000
C	15.032232000	2.547683000	27.884471000
C	13.811889000	2.617614000	28.769170000
C	14.168548000	3.469787000	30.017258000
H	15.045675000	3.033459000	30.512086000
H	14.455037000	4.478303000	29.692642000
C	13.414414000	1.202793000	29.254227000
H	13.161756000	0.576405000	28.388541000
H	14.267048000	0.725896000	29.752113000
C	12.591865000	3.253267000	28.080300000
H	12.837181000	4.265246000	27.732035000
H	12.319632000	2.660998000	27.194822000
C	11.401652000	3.320055000	29.053693000
H	10.546770000	3.776006000	28.538743000
C	11.027214000	1.906773000	29.525569000
H	10.167934000	1.954871000	30.207947000
H	10.722514000	1.284521000	28.674464000
C	12.231320000	1.269690000	30.230922000
H	11.975321000	0.252162000	30.554218000
C	12.618676000	2.117403000	31.451786000
H	13.468256000	1.659784000	31.976567000
H	11.784527000	2.153914000	32.165236000
C	12.983807000	3.535768000	30.990499000
H	13.263318000	4.147384000	31.858422000
C	11.783153000	4.170890000	30.275614000
H	10.928859000	4.246414000	30.961886000
H	12.035183000	5.191520000	29.962472000
C	19.956612000	6.884640000	27.313899000
H	20.370930000	7.118051000	26.328452000
H	19.598991000	7.818989000	27.760253000
H	20.768333000	6.510867000	27.946456000
C	18.264614000	5.528987000	28.614761000
H	19.055457000	5.161258000	29.277986000
H	17.834922000	6.429613000	29.066906000
H	17.480229000	4.769548000	28.562125000
C	18.834779000	5.845679000	27.221974000
H	19.262457000	4.921299000	26.817276000
C	17.742591000	6.291504000	26.288453000
C	17.286705000	7.575179000	26.041375000
H	17.689524000	8.492099000	26.444728000
C	16.224182000	7.438819000	25.133757000
C	15.522583000	8.586135000	24.449956000
C	16.571062000	9.321231000	23.569325000
H	16.971610000	8.619502000	22.826248000
H	17.415891000	9.636006000	24.194557000
C	14.360876000	8.141840000	23.545472000
H	13.600251000	7.623768000	24.149366000
H	14.731456000	7.424976000	22.801873000
C	14.979291000	9.593927000	25.490239000

H	15.791197000	9.920189000	26.152502000
H	14.235258000	9.093838000	26.123218000
C	14.356004000	10.811256000	24.790237000
H	13.974957000	11.506360000	25.549920000
C	15.418918000	11.514984000	23.932993000
H	16.244678000	11.868221000	24.565625000
H	14.986225000	12.400781000	23.448800000
C	15.947685000	10.537363000	22.872949000
H	16.713039000	11.032935000	22.260991000
C	14.793022000	10.065202000	21.979217000
H	15.172750000	9.383184000	21.207667000
H	14.341302000	10.920006000	21.457816000
C	13.735260000	9.358619000	22.840540000
H	12.911649000	9.020181000	22.199531000
C	13.203065000	10.346042000	23.889765000
H	12.421147000	9.871979000	24.493408000
H	12.742400000	11.210431000	23.392714000
B	8.357794000	6.742254000	21.653347000
B	17.228167000	3.928592000	25.331915000
N	9.767937000	7.226213000	21.178726000
N	10.743425000	6.321215000	20.842320000
N	8.242372000	5.199759000	21.654487000
N	8.658714000	4.490696000	22.745128000
N	8.051620000	7.307151000	23.054883000
N	8.995964000	7.302902000	24.043183000
N	16.766336000	3.453128000	23.924349000
N	15.636933000	2.683489000	23.808107000
N	16.544355000	3.094666000	26.430526000
N	15.274370000	3.374064000	26.853241000
N	16.977798000	5.444156000	25.552157000
N	16.023503000	6.138057000	24.856782000
Yb	10.843276000	5.553159000	23.319661000
Yb	14.095061000	4.477947000	24.784121000
H	18.413370000	3.740527000	25.408898000
H	7.540680000	7.167757000	20.880088000
H	12.192347000	5.693275000	25.165903000
H	12.639148000	4.192801000	23.075887000

Optimized geometry of Int1

C	-0.740146000	3.232782000	-4.344003000
C	-1.111115000	4.459994000	-4.085471000
C	-1.474034000	5.698103000	-3.835106000
C	-2.907062000	6.063167000	-3.528643000
H	-2.986710000	6.555947000	-2.550349000
H	-3.293939000	6.773709000	-4.270985000
H	-3.555853000	5.184634000	-3.526156000
C	-0.479497000	6.834676000	-3.860271000
H	-0.453221000	7.354129000	-2.893093000
H	0.528602000	6.482289000	-4.088608000
H	-0.762280000	7.582081000	-4.613265000
C	-1.307937000	2.482997000	1.970004000
H	-0.453943000	2.474088000	2.657326000
H	-1.960962000	1.640206000	2.213384000
C	-2.020738000	3.831852000	1.957523000
H	-2.000694000	4.320571000	2.935361000
H	-3.068654000	3.710909000	1.660989000
C	-1.249102000	4.595024000	0.877601000
H	-0.308808000	4.986056000	1.282112000
H	-1.809733000	5.431446000	0.452276000
C	-0.977868000	3.502016000	-0.147019000
H	-1.822271000	3.370057000	-0.833720000
H	-0.077379000	3.648316000	-0.746869000
C	-2.053246000	-5.063226000	2.741247000
H	-1.944262000	-5.837438000	3.508895000
H	-2.852321000	-5.371363000	2.058335000
H	-1.125111000	-5.014542000	2.165269000
C	-3.681376000	-3.792815000	4.195996000
H	-3.576801000	-4.535286000	4.993931000
H	-3.934102000	-2.831922000	4.654188000

H	-4.526678000	-4.101983000	3.571727000
C	-2.386627000	-3.705986000	3.381420000
H	-1.574506000	-3.450464000	4.070183000
C	-2.465651000	-2.629716000	2.330505000
C	-3.578364000	-2.233474000	1.605440000
H	-4.586511000	-2.604018000	1.716300000
C	-3.120511000	-1.263709000	0.699612000
C	-3.942310000	-0.544923000	-0.341805000
C	-5.005899000	0.348350000	0.344737000
H	-4.502287000	1.087186000	0.982837000
H	-5.629918000	-0.265778000	1.006814000
C	-4.680553000	-1.579008000	-1.229100000
H	-3.942419000	-2.226427000	-1.719853000
H	-5.302774000	-2.228838000	-0.600757000
C	-3.082222000	0.343803000	-1.257175000
H	-2.325948000	-0.264533000	-1.774493000
H	-2.553879000	1.093729000	-0.653876000
C	-3.949904000	1.055623000	-2.307224000
H	-3.302229000	1.677410000	-2.936464000
C	-4.993174000	1.933397000	-1.598826000
H	-5.608768000	2.460015000	-2.340301000
H	-4.493502000	2.704211000	-0.995797000
C	-5.879479000	1.055972000	-0.702221000
H	-6.622390000	1.680630000	-0.188691000
C	-6.595965000	0.005472000	-1.565042000
H	-7.240309000	0.500728000	-2.303641000
H	-7.249046000	-0.616510000	-0.937879000
C	-5.553613000	-0.871246000	-2.276551000
H	-6.063397000	-1.627245000	-2.887976000
C	-4.667976000	0.008490000	-3.171368000
H	-5.278334000	0.505888000	-3.936887000
H	-3.932138000	-0.609747000	-3.702050000
C	-0.975588000	-0.474223000	5.423331000
H	-1.402616000	-0.959189000	6.308078000
H	-1.026443000	0.609801000	5.575161000
H	-1.598908000	-0.724189000	4.560367000
C	1.329025000	-0.605974000	6.446908000
H	0.926784000	-1.123488000	7.323637000
H	2.368167000	-0.920828000	6.312293000
H	1.325603000	0.466805000	6.669887000
C	0.480644000	-0.919806000	5.211948000
H	0.478790000	-2.007927000	5.072227000
C	1.059458000	-0.300771000	3.968142000
C	1.923479000	0.779980000	3.858233000
H	2.370835000	1.333192000	4.670637000
C	2.117976000	0.974064000	2.478548000
C	3.060603000	1.940713000	1.804299000
C	2.866436000	1.970909000	0.276297000
H	3.005094000	0.962475000	-0.135285000
H	1.843014000	2.290089000	0.035144000
C	4.519919000	1.499987000	2.095118000
H	4.682033000	1.464858000	3.180285000
H	4.668118000	0.479717000	1.718820000
C	2.872689000	3.374558000	2.351023000
H	3.006663000	3.378583000	3.440598000
H	1.843723000	3.704967000	2.156085000
C	3.872741000	4.340690000	1.696583000
H	3.716490000	5.349259000	2.101665000
C	5.306514000	3.878813000	2.001312000
H	6.028790000	4.575569000	1.555436000
H	5.483580000	3.885965000	3.085442000
C	5.519542000	2.464712000	1.440013000
H	6.540953000	2.129207000	1.662519000
C	5.297546000	2.477241000	-0.079950000
H	5.467910000	1.475225000	-0.495222000
H	6.019041000	3.150171000	-0.562342000
C	3.863268000	2.936931000	-0.382414000
H	3.691804000	2.936096000	-1.465545000
C	3.652259000	4.352181000	0.176290000
H	4.348278000	5.054527000	-0.301372000

H	2.637676000	4.702628000	-0.057006000
C	3.125388000	-3.810239000	3.241743000
H	3.346669000	-4.334226000	4.178453000
H	4.051293000	-3.748895000	2.659597000
H	2.814677000	-2.790066000	3.483367000
C	2.471318000	-5.996877000	2.162252000
H	2.646243000	-6.532670000	3.100867000
H	1.709623000	-6.540554000	1.595249000
H	3.404660000	-6.026685000	1.589488000
C	2.039938000	-4.555713000	2.448191000
H	1.139394000	-4.593689000	3.072328000
C	1.699427000	-3.818279000	1.179637000
C	2.155300000	-4.063204000	-0.107560000
H	2.794195000	-4.874439000	-0.419555000
C	1.601767000	-3.052903000	-0.910980000
C	1.779980000	-2.838115000	-2.396900000
C	2.693406000	-1.616689000	-2.670820000
H	3.661049000	-1.766478000	-2.172790000
H	2.236944000	-0.711188000	-2.247725000
C	0.420500000	-2.591190000	-3.091781000
H	-0.053340000	-1.695731000	-2.668908000
H	-0.249591000	-3.439107000	-2.896721000
C	2.435158000	-4.079690000	-3.040623000
H	1.812484000	-4.964517000	-2.851193000
H	3.410529000	-4.266577000	-2.571638000
C	2.624752000	-3.878967000	-4.551428000
H	3.088160000	-4.779448000	-4.976179000
C	3.535216000	-2.665359000	-4.793508000
H	3.693394000	-2.521278000	-5.870948000
H	4.523258000	-2.840335000	-4.345648000
C	2.887346000	-1.414768000	-4.182055000
H	3.534927000	-0.543297000	-4.344616000
C	1.518845000	-1.166965000	-4.835345000
H	1.058399000	-0.271779000	-4.398925000
H	1.642036000	-0.989796000	-5.912670000
C	0.613464000	-2.386616000	-4.602146000
H	-0.366048000	-2.211441000	-5.066304000
C	1.259690000	-3.638414000	-5.213091000
H	0.610194000	-4.512340000	-5.065858000
H	1.383190000	-3.510297000	-6.297041000
B	0.093306000	-2.060852000	2.267059000
N	-1.404028000	-1.908036000	1.872994000
N	-1.806518000	-1.067713000	0.874940000
N	0.762354000	-0.715104000	2.703646000
N	1.402211000	0.075572000	1.793895000
N	0.904992000	-2.714541000	1.121968000
N	0.851497000	-2.239360000	-0.154580000
O	-0.809869000	2.293298000	0.627619000
Yb	0.047959000	0.118838000	-0.283352000
H	0.135448000	-2.793799000	3.212742000
H	-0.754498000	2.856051000	-5.366868000
H	0.273319000	1.022727000	-2.196262000
H	-0.398341000	2.537742000	-3.567993000

Optimized geometry of TS1

C	5.420541000	20.031786000	7.397345000
C	5.196766000	21.262067000	7.013156000
C	5.077667000	22.522158000	6.632798000
C	3.900619000	23.388484000	7.008787000
H	4.218186000	24.274156000	7.577239000
H	3.390366000	23.762294000	6.110113000
H	3.164595000	22.843966000	7.605076000
C	6.115202000	23.162574000	5.739566000
H	6.545696000	24.056086000	6.212920000
H	6.931609000	22.473089000	5.513115000
H	5.670236000	23.491586000	4.790041000
C	4.184631000	20.459034000	12.295056000

H	5.082501000	20.438807000	12.922950000
H	3.646286000	19.516184000	12.415368000
C	3.336593000	21.697918000	12.557400000
H	3.359180000	21.999142000	13.608159000
H	2.291928000	21.519474000	12.278327000
C	3.971300000	22.723470000	11.615591000
H	4.889460000	23.129211000	12.054234000
H	3.311325000	23.560783000	11.373144000
C	4.292497000	21.870301000	10.396196000
H	3.427413000	21.786251000	9.727512000
H	5.144258000	22.220064000	9.808993000
C	3.936939000	13.255661000	12.640672000
H	4.082720000	12.472109000	13.392568000
H	3.194330000	12.899931000	11.918243000
H	4.879139000	13.399986000	12.105086000
C	2.152826000	14.336917000	14.063943000
H	2.295548000	13.585410000	14.847285000
H	1.798657000	15.258673000	14.535259000
H	1.361494000	13.970402000	13.401052000
C	3.462382000	14.560204000	13.301027000
H	4.224098000	14.865710000	14.026282000
C	3.325013000	15.655057000	12.275467000
C	2.197481000	16.000719000	11.548844000
H	1.212340000	15.568883000	11.641906000
C	2.604762000	17.015895000	10.668634000
C	1.735316000	17.707664000	9.647548000
C	0.664175000	18.572183000	10.359064000
H	1.163409000	19.327518000	10.980578000
H	0.076753000	17.941974000	11.039116000
C	1.003742000	16.650607000	8.782176000
H	1.746466000	16.021437000	8.274463000
H	0.415724000	15.985652000	9.426946000
C	2.543885000	18.617008000	8.708824000
H	3.301609000	18.018161000	8.182893000
H	3.066547000	19.383729000	9.294859000
C	1.630542000	19.298875000	7.678744000
H	2.245482000	19.938928000	7.035166000
C	0.581058000	20.149326000	8.411160000
H	-0.067521000	20.655441000	7.683823000
H	1.073912000	20.936245000	8.998472000
C	-0.256446000	19.250581000	9.333229000
H	-1.003174000	19.856113000	9.863675000
C	-0.964715000	18.177543000	8.491777000
H	-1.641881000	18.651688000	7.768882000
H	-1.583061000	17.538837000	9.136935000
C	0.083653000	17.328579000	7.755885000
H	-0.419820000	16.556096000	7.160084000
C	0.920205000	18.229781000	6.835534000
H	0.276596000	18.707398000	6.084842000
H	1.658039000	17.629257000	6.286901000
C	4.607355000	17.777956000	15.446233000
H	4.191734000	17.235153000	16.302403000
H	4.490085000	18.850372000	15.638597000
H	4.016360000	17.525986000	14.561358000
C	6.892710000	17.738528000	16.516466000
H	6.501018000	17.165647000	17.363054000
H	7.950637000	17.487361000	16.395405000
H	6.824007000	18.800024000	16.779148000
C	6.090888000	17.425591000	15.250475000
H	6.154675000	16.345090000	15.071266000
C	6.661796000	18.123767000	14.045012000
C	7.494858000	19.232806000	14.001657000
H	7.910269000	19.757532000	14.847718000
C	7.714921000	19.499763000	12.638790000
C	8.653743000	20.527028000	12.041688000
C	7.912800000	21.559720000	11.162228000
H	7.401348000	21.040050000	10.343203000
H	7.151054000	22.072538000	11.765015000
C	9.713702000	19.813477000	11.165090000
H	10.247502000	19.073311000	11.776167000

H	9.206572000	19.269522000	10.359993000
C	9.390022000	21.294193000	13.161983000
H	9.928119000	20.582921000	13.802717000
H	8.660267000	21.813277000	13.799108000
C	10.379123000	22.310982000	12.571801000
H	10.884586000	22.835275000	13.393707000
C	11.417435000	21.575931000	11.710398000
H	12.140482000	22.293277000	11.298910000
H	11.985794000	20.867487000	12.328426000
C	10.700241000	20.831861000	10.574750000
H	11.436338000	20.299369000	9.958362000
C	9.931814000	21.837898000	9.704087000
H	9.423523000	21.312359000	8.886456000
H	10.628191000	22.557623000	9.252310000
C	8.899780000	22.577821000	10.569505000
H	8.344666000	23.292727000	9.947918000
C	9.616298000	23.323221000	11.704222000
H	10.311585000	24.065892000	11.290219000
H	8.888886000	23.873315000	12.317465000
C	9.026802000	14.951635000	13.227470000
H	9.307537000	14.462975000	14.167327000
H	9.935493000	15.091214000	12.631977000
H	8.625657000	15.941594000	13.460739000
C	8.567419000	12.697697000	12.186984000
H	8.802665000	12.195031000	13.130678000
H	7.853426000	12.076351000	11.637850000
H	9.492952000	12.746840000	11.602897000
C	8.006648000	14.096396000	12.458445000
H	7.120278000	13.984110000	13.094157000
C	7.583968000	14.779012000	11.184155000
C	8.026825000	14.542854000	9.893274000
H	8.721453000	13.778985000	9.577687000
C	7.377895000	15.492492000	9.085921000
C	7.489821000	15.616676000	7.587229000
C	8.958919000	15.891878000	7.180754000
H	9.605088000	15.096020000	7.573194000
H	9.289995000	16.830186000	7.643531000
C	6.620111000	16.755478000	7.029403000
H	6.960050000	17.706035000	7.464331000
H	5.570557000	16.591944000	7.314875000
C	7.040516000	14.289068000	6.925950000
H	6.001135000	14.076718000	7.209468000
H	7.648475000	13.460561000	7.311188000
C	7.172709000	14.372116000	5.397943000
H	6.849995000	13.419946000	4.956385000
C	8.638744000	14.644050000	5.025726000
H	8.749329000	14.684801000	3.933689000
H	9.276009000	13.822552000	5.380517000
C	9.090283000	15.972680000	5.652097000
H	10.139028000	16.166306000	5.391187000
C	8.207098000	17.112891000	5.123712000
H	8.529877000	18.071292000	5.549883000
H	8.306634000	17.194633000	4.032915000
C	6.742695000	16.838810000	5.499551000
H	6.111890000	17.658866000	5.133301000
C	6.289481000	15.512979000	4.870855000
H	5.236194000	15.317707000	5.114498000
H	6.358749000	15.571355000	3.776254000
B	5.835435000	16.390540000	12.265829000
N	4.343559000	16.449910000	11.843039000
N	3.904597000	17.286240000	10.858110000
N	6.401983000	17.763046000	12.757412000
N	7.031510000	18.615770000	11.894615000
N	6.706258000	15.819143000	11.124586000
N	6.589724000	16.267770000	9.841283000
O	4.601087000	20.559206000	10.912555000
Yb	5.750946000	18.649891000	9.749088000
H	5.907230000	15.636232000	13.192493000
H	5.046446000	19.239716000	6.736201000
H	7.472526000	19.496131000	8.609013000

H	6.584357000	19.796803000	8.068597000

Optimized geometry of Int2

C	-0.636530000	1.484727000	-2.590809000
C	-0.292224000	2.682265000	-2.983796000
C	0.079057000	3.906076000	-3.344210000
C	-0.827979000	5.104299000	-3.183875000
H	-0.361934000	5.898435000	-2.580205000
H	-1.061319000	5.559092000	-4.158543000
H	-1.777770000	4.833131000	-2.714205000
C	1.392951000	4.168847000	-4.042066000
H	1.996915000	4.918542000	-3.508742000
H	1.987793000	3.255971000	-4.132778000
H	1.235364000	4.566165000	-5.056399000
C	-1.598499000	2.369381000	2.234365000
H	-0.669145000	2.331608000	2.814100000
H	-2.183623000	1.471167000	2.449204000
C	-2.362596000	3.670667000	2.459739000
H	-2.242304000	4.049993000	3.478079000
H	-3.433391000	3.526412000	2.277037000
C	-1.761852000	4.588449000	1.391752000
H	-0.796122000	4.984659000	1.724650000
H	-2.404751000	5.434407000	1.134237000
C	-1.574230000	3.629403000	0.225138000
H	-2.497107000	3.519762000	-0.358099000
H	-0.768518000	3.890036000	-0.464548000
C	-1.995768000	-5.012407000	2.681940000
H	-1.782876000	-5.797640000	3.415817000
H	-2.850507000	-5.334518000	2.077385000
H	-1.134034000	-4.919698000	2.015317000
C	-3.506763000	-3.829784000	4.324461000
H	-3.296368000	-4.584245000	5.089518000
H	-3.742923000	-2.888120000	4.829045000
H	-4.400806000	-4.155999000	3.782167000
C	-2.305788000	-3.680859000	3.384894000
H	-1.436351000	-3.411411000	3.993607000
C	-2.527374000	-2.587880000	2.372155000
C	-3.722459000	-2.214026000	1.778118000
H	-4.701812000	-2.616986000	1.988795000
C	-3.392504000	-1.220151000	0.843658000
C	-4.340047000	-0.524211000	-0.101689000
C	-5.360551000	0.334774000	0.685626000
H	-4.822320000	1.091061000	1.272815000
H	-5.898802000	-0.297745000	1.403393000
C	-5.126519000	-1.583152000	-0.915608000
H	-4.418348000	-2.207949000	-1.475173000
H	-5.664875000	-2.251105000	-0.231381000
C	-3.602290000	0.389158000	-1.093858000
H	-2.881180000	-0.200768000	-1.676498000
H	-3.041922000	1.157889000	-0.545671000
C	-4.586805000	1.070476000	-2.055745000
H	-4.018172000	1.711092000	-2.740093000
C	-5.584363000	1.916401000	-1.249941000
H	-6.284759000	2.421737000	-1.928077000
H	-5.053815000	2.703920000	-0.697205000
C	-6.352217000	1.012192000	-0.273387000
H	-7.062043000	1.614009000	0.309381000
C	-7.114387000	-0.061879000	-1.065240000
H	-7.841644000	0.411686000	-1.738091000
H	-7.684507000	-0.703285000	-0.379499000
C	-6.117670000	-0.906404000	-1.874040000
H	-6.659076000	-1.679501000	-2.434749000
C	-5.350548000	-0.000374000	-2.848970000
H	-6.046944000	0.475645000	-3.552047000
H	-4.649947000	-0.596595000	-3.448326000
C	-0.846664000	-0.494360000	5.377143000
H	-1.173698000	-1.031347000	6.274349000
H	-0.910985000	0.579598000	5.584950000
H	-1.543721000	-0.724526000	4.566614000

C	1.548122000	-0.600111000	6.169886000
H	1.246098000	-1.168413000	7.055368000
H	2.577518000	-0.876035000	5.922499000
H	1.537432000	0.461007000	6.442695000
C	0.593550000	-0.885170000	5.007462000
H	0.607166000	-1.965615000	4.818144000
C	1.034349000	-0.195035000	3.744531000
C	1.847474000	0.920671000	3.605556000
H	2.346895000	1.457879000	4.398129000
C	1.912687000	1.175729000	2.223304000
C	2.759387000	2.205208000	1.517262000
C	2.477040000	2.257817000	0.003740000
H	2.637910000	1.265072000	-0.437162000
H	1.429221000	2.539116000	-0.174905000
C	4.253854000	1.836510000	1.716798000
H	4.477076000	1.785651000	2.790391000
H	4.433946000	0.834057000	1.307617000
C	2.528113000	3.615070000	2.108558000
H	2.722310000	3.602147000	3.189042000
H	1.473916000	3.892922000	1.977771000
C	3.438422000	4.646318000	1.423587000
H	3.252444000	5.636486000	1.860279000
C	4.908921000	4.255245000	1.639576000
H	5.568089000	4.998874000	1.172232000
H	5.145278000	4.248750000	2.712439000
C	5.164828000	2.866645000	1.033698000
H	6.212874000	2.581307000	1.193891000
C	4.858423000	2.897321000	-0.470845000
H	5.058135000	1.913982000	-0.917036000
H	5.515307000	3.617209000	-0.977073000
C	3.388071000	3.286619000	-0.684060000
H	3.156317000	3.301790000	-1.754423000
C	3.134552000	4.676645000	-0.081811000
H	3.766655000	5.424040000	-0.579462000
H	2.092328000	4.975262000	-0.255358000
C	3.143811000	-3.578603000	2.743431000
H	3.453971000	-4.125752000	3.640823000
H	4.019891000	-3.463080000	2.096084000
H	2.817596000	-2.579513000	3.045109000
C	2.486072000	-5.750347000	1.637137000
H	2.747946000	-6.310695000	2.540504000
H	1.703714000	-6.302303000	1.107489000
H	3.375262000	-5.726663000	0.997765000
C	2.027553000	-4.336635000	2.006708000
H	1.179212000	-4.430237000	2.694345000
C	1.567140000	-3.570332000	0.793960000
C	1.942248000	-3.755338000	-0.527262000
H	2.589638000	-4.529510000	-0.907398000
C	1.295535000	-2.745595000	-1.258027000
C	1.380870000	-2.497912000	-2.748234000
C	2.256682000	-1.256654000	-3.054258000
H	3.250578000	-1.393599000	-2.607413000
H	1.809691000	-0.365521000	-2.592866000
C	-0.016786000	-2.269917000	-3.367579000
H	-0.491071000	-1.398999000	-2.898933000
H	-0.656044000	-3.137434000	-3.156283000
C	2.023119000	-3.718562000	-3.445693000
H	1.428908000	-4.617285000	-3.232665000
H	3.026424000	-3.891621000	-3.034674000
C	2.127699000	-3.497474000	-4.960931000
H	2.581637000	-4.385263000	-5.421004000
C	3.007665000	-2.267662000	-5.231060000
H	3.110251000	-2.105250000	-6.312457000
H	4.018908000	-2.434486000	-4.835106000
C	2.372208000	-1.035366000	-4.571435000
H	2.996696000	-0.151691000	-4.756242000
C	0.971070000	-0.806519000	-5.157805000
H	0.523326000	0.088431000	-4.710864000
H	1.040856000	-0.631142000	-6.240024000
C	0.093616000	-2.038498000	-4.883773000

H	-0.911393000	-1.872843000	-5.293653000
C	0.725267000	-3.272058000	-5.545178000
H	0.099314000	-4.158684000	-5.374426000
H	0.787093000	-3.128189000	-6.632284000
B	-0.009878000	-1.925151000	2.061262000
N	-1.542048000	-1.829115000	1.814664000
N	-2.072539000	-0.988356000	0.879328000
N	0.640052000	-0.569641000	2.493844000
N	1.170537000	0.279282000	1.565699000
N	0.726803000	-2.500053000	0.827390000
N	0.565548000	-1.985569000	-0.427184000
O	-1.253650000	2.357054000	0.830424000
Yb	-0.385852000	0.346240000	-0.373461000
H	0.147922000	-2.689542000	2.968139000
H	-1.188939000	0.931616000	-3.370135000
H	12.094864000	1.499538000	1.262188000
H	11.377012000	1.507109000	1.069019000

Optimized geometry of 6

C	5.621628000	19.626830000	7.242783000
C	6.020324000	20.789081000	6.798692000
C	6.444645000	21.979450000	6.388264000
C	5.561828000	23.205688000	6.421238000
H	6.012981000	24.024888000	7.002331000
H	5.397446000	23.604282000	5.408657000
H	4.579626000	22.985816000	6.849232000
C	7.804285000	22.168590000	5.757406000
H	8.392312000	22.940224000	6.277117000
H	8.381746000	21.240189000	5.764116000
H	7.718437000	22.500452000	4.711440000
C	4.453275000	20.842035000	11.946310000
H	5.345012000	20.792088000	12.581260000
H	3.809667000	19.988670000	12.177237000
C	3.746037000	22.190506000	12.052755000
H	3.839705000	22.628718000	13.050022000
H	2.678482000	22.085459000	11.829076000
C	4.437569000	23.008974000	10.959190000
H	5.405495000	23.382251000	11.311599000
H	3.847748000	23.864072000	10.618365000
C	4.631232000	21.968017000	9.866767000
H	3.727541000	21.854237000	9.254815000
H	5.472837000	22.149627000	9.194851000
C	3.881492000	13.409946000	12.655140000
H	4.041817000	12.640099000	13.418105000
H	3.061200000	13.081582000	12.007736000
H	4.782505000	13.479453000	12.039594000
C	2.287346000	14.643474000	14.177322000
H	2.444707000	13.906094000	14.971225000
H	2.030455000	15.598935000	14.644459000
H	1.424163000	14.311300000	13.590463000
C	3.543472000	14.760068000	13.308006000
H	4.377896000	15.036118000	13.961276000
C	3.393307000	15.831293000	12.259644000
C	2.237538000	16.208793000	11.594845000
H	1.241957000	15.826215000	11.762939000
C	2.631607000	17.177227000	10.658713000
C	1.739561000	17.875154000	9.662255000
C	0.705510000	18.762778000	10.399120000
H	1.234957000	19.515944000	10.998216000
H	0.128361000	18.149109000	11.102798000
C	0.965249000	16.820862000	8.831157000
H	1.682373000	16.176177000	8.306631000
H	0.388158000	16.171463000	9.501505000
C	2.532950000	18.761877000	8.689296000
H	3.263982000	18.152187000	8.140538000
H	3.088231000	19.524864000	9.250333000
C	1.598575000	19.450114000	7.682845000
H	2.204933000	20.071019000	7.012731000
C	0.586700000	20.324378000	8.439520000

H	-0.076770000	20.834686000	7.728738000
H	1.110278000	21.108263000	9.004057000
C	-0.235545000	19.446543000	9.395303000
H	-0.955895000	20.068314000	9.943160000
C	-0.986483000	18.376936000	8.586870000
H	-1.678221000	18.855256000	7.880747000
H	-1.594588000	17.754673000	9.257422000
C	0.024733000	17.504253000	7.827232000
H	-0.509136000	16.734587000	7.254727000
C	0.845811000	18.384165000	6.872722000
H	0.185969000	18.864544000	6.138063000
H	1.557697000	17.768301000	6.307561000
C	4.911807000	18.040335000	15.256074000
H	4.518818000	17.550535000	16.153812000
H	4.845856000	19.123641000	15.407187000
H	4.268540000	17.776489000	14.412093000
C	7.245998000	17.953420000	16.214574000
H	6.877180000	17.432775000	17.104027000
H	8.286245000	17.655793000	16.052324000
H	7.230286000	19.026897000	16.433543000
C	6.369127000	17.619853000	15.004896000
H	6.382556000	16.531206000	14.869501000
C	6.903360000	18.242671000	13.743067000
C	7.750543000	19.333049000	13.605548000
H	8.212540000	19.895564000	14.403179000
C	7.907325000	19.522283000	12.220059000
C	8.824995000	20.494631000	11.521654000
C	8.596231000	20.523728000	9.998492000
H	8.729354000	19.514898000	9.585559000
H	7.567430000	20.843324000	9.780354000
C	10.292933000	20.061494000	11.780690000
H	10.477426000	20.026413000	12.862272000
H	10.438508000	19.042160000	11.400661000
C	8.641825000	21.927115000	12.073402000
H	8.800630000	21.931015000	13.159660000
H	7.606896000	22.251786000	11.902248000
C	9.621906000	22.898530000	11.397263000
H	9.468754000	23.906197000	11.805714000
C	11.064389000	22.444523000	11.671355000
H	11.772983000	23.145093000	11.209864000
H	11.264982000	22.452810000	12.751437000
C	11.273491000	21.031501000	11.105680000
H	12.301058000	20.701380000	11.307087000
C	11.018237000	21.041386000	9.591253000
H	11.185541000	20.039763000	9.173409000
H	11.724952000	21.717731000	9.092154000
C	9.575659000	21.493634000	9.319501000
H	9.380341000	21.493828000	8.241758000
C	9.368677000	22.907649000	9.882273000
H	10.050886000	23.613072000	9.389576000
H	8.347763000	23.250870000	9.668508000
C	9.017564000	14.807156000	13.013767000
H	9.270970000	14.300995000	13.952101000
H	9.929786000	14.884524000	12.412282000
H	8.685777000	15.822119000	13.249010000
C	8.400015000	12.590376000	11.976001000
H	8.604636000	12.071846000	12.918273000
H	7.642933000	12.019854000	11.429563000
H	9.324022000	12.576496000	11.387743000
C	7.936418000	14.023672000	12.251724000
H	7.049820000	13.969678000	12.893960000
C	7.552881000	14.734619000	10.979939000
C	7.995455000	14.480747000	9.691518000
H	8.650935000	13.681233000	9.384934000
C	7.403440000	15.460817000	8.878591000
C	7.572048000	15.630759000	7.384464000
C	8.470303000	16.851593000	7.062258000
H	9.437298000	16.736098000	7.570077000
H	8.003123000	17.767440000	7.449225000
C	6.211793000	15.829735000	6.677945000

H	5.717657000	16.725088000	7.074114000
H	5.557096000	14.976191000	6.898790000
C	8.244780000	14.373000000	6.788721000
H	7.634340000	13.488622000	7.015434000
H	9.222876000	14.218997000	7.263228000
C	8.433842000	14.512849000	5.272128000
H	8.907149000	13.600530000	4.885427000
C	9.334512000	15.723988000	4.986678000
H	9.497771000	15.828590000	3.905600000
H	10.321321000	15.575402000	5.446423000
C	8.670710000	16.991227000	5.544129000
H	9.309455000	17.862107000	5.347699000
C	7.305533000	17.192531000	4.869514000
H	6.839712000	18.111709000	5.242318000
H	7.436237000	17.309047000	3.785003000
C	6.406928000	15.979779000	5.159984000
H	5.426981000	16.126175000	4.686936000
C	7.066869000	14.710953000	4.600624000
H	6.427557000	13.836340000	4.783447000
H	7.188796000	14.796588000	3.512446000
B	5.931283000	16.455325000	12.077952000
N	4.418295000	16.562849000	11.739051000
N	3.951777000	17.389904000	10.757934000
N	6.578618000	17.818845000	12.488171000
N	7.185586000	18.612436000	11.557844000
N	6.727434000	15.814784000	10.915772000
N	6.640784000	16.269467000	9.630967000
O	4.877305000	20.729180000	10.568468000
Yb	5.735684000	18.620919000	9.534091000
H	6.023778000	15.730105000	13.025211000
H	5.100270000	19.038884000	6.467695000

Optimized geometry of Int3

C	5.320843000	3.322490000	-2.267805000
H	6.125919000	2.767103000	-2.745630000
H	4.908574000	4.163421000	-2.822625000
C	4.875144000	2.998949000	-1.078780000
H	1.939307000	0.613478000	0.518549000
C	4.419127000	2.668672000	0.102433000
H	3.591242000	1.949147000	0.164432000
C	4.947959000	3.183972000	1.422968000
H	4.099633000	3.665288000	1.938414000
C	5.400833000	2.011103000	2.311808000
H	6.213295000	1.477679000	1.797930000
H	4.577400000	1.295837000	2.423080000
C	5.889790000	2.495865000	3.678993000
H	5.046256000	2.938486000	4.228760000
H	6.238075000	1.645679000	4.278560000
C	7.001036000	3.539327000	3.538409000
H	7.311025000	3.903879000	4.525666000
H	7.885208000	3.064711000	3.088752000
C	6.555736000	4.707102000	2.654148000
H	7.376006000	5.424488000	2.527760000
H	5.743718000	5.250772000	3.159039000
C	6.065076000	4.222141000	1.287646000
H	5.717102000	5.066996000	0.681422000
H	6.901028000	3.771556000	0.734171000
C	-6.595437000	0.618717000	2.012698000
H	-7.509500000	0.042297000	2.187966000
H	-6.428642000	1.243468000	2.896891000
H	-6.767733000	1.280290000	1.158440000
C	-5.414482000	-0.324654000	1.766131000
H	-5.666216000	-0.960834000	0.910064000
C	-5.182632000	-1.238583000	2.980795000
H	-6.079573000	-1.829381000	3.197047000
H	-4.349211000	-1.925563000	2.809423000
H	-4.945821000	-0.642830000	3.868958000
C	-4.158351000	0.433992000	1.429906000
C	-3.793523000	1.708629000	1.838324000

H	-4.389202000	2.394184000	2.422203000
C	-2.506075000	1.923226000	1.322372000
C	-1.675910000	3.178896000	1.417205000
C	-2.482069000	4.364909000	0.827466000
H	-2.734984000	4.145569000	-0.218175000
H	-3.432422000	4.468945000	1.366608000
C	-1.339999000	3.505457000	2.892770000
H	-2.268496000	3.591896000	3.472233000
H	-0.769868000	2.674443000	3.328616000
C	-0.355098000	3.060853000	0.635541000
H	0.276959000	2.254217000	1.040911000
H	-0.569779000	2.825862000	-0.417654000
C	0.452529000	4.365740000	0.720455000
H	1.385374000	4.239770000	0.158424000
C	0.773661000	4.663034000	2.193320000
H	1.367201000	5.583669000	2.270166000
H	1.381918000	3.852117000	2.614345000
C	-0.534284000	4.811165000	2.984458000
H	-0.308285000	5.019130000	4.038461000
C	-1.359004000	5.966407000	2.395403000
H	-2.289415000	6.096829000	2.964693000
H	-0.799554000	6.907768000	2.477961000
C	-1.677847000	5.669758000	0.921919000
H	-2.274375000	6.489571000	0.500600000
C	-0.369048000	5.521359000	0.131690000
H	0.207263000	6.455065000	0.175550000
H	-0.587510000	5.330589000	-0.927746000
C	-4.051309000	-4.977187000	-0.624262000
H	-3.829414000	-4.259552000	-1.419059000
H	-3.345708000	-5.809444000	-0.721052000
H	-5.062144000	-5.368370000	-0.784320000
C	-4.263236000	-5.343781000	1.865545000
H	-5.286779000	-5.712918000	1.743900000
H	-3.596450000	-6.211735000	1.823159000
H	-4.176142000	-4.899636000	2.861537000
C	-3.933279000	-4.329992000	0.765222000
H	-4.670009000	-3.522140000	0.823716000
C	-2.563484000	-3.732574000	0.956095000
C	-1.434415000	-4.353749000	1.468297000
H	-1.377746000	-5.356881000	1.861525000
C	-0.391834000	-3.423306000	1.346500000
C	1.061611000	-3.627776000	1.707684000
C	1.993078000	-2.709495000	0.891975000
H	1.804356000	-1.646718000	1.113155000
H	1.819768000	-2.867154000	-0.182539000
C	1.314692000	-3.357764000	3.213190000
H	0.659152000	-4.000884000	3.815020000
H	1.045738000	-2.319533000	3.447842000
C	1.451115000	-5.096423000	1.410787000
H	1.264174000	-5.316112000	0.351520000
H	0.813860000	-5.773025000	1.993591000
C	2.921703000	-5.359693000	1.761140000
H	3.159900000	-6.408615000	1.541136000
C	3.142338000	-5.082419000	3.256489000
H	2.520770000	-5.757469000	3.860437000
H	4.187461000	-5.281639000	3.528294000
C	2.789430000	-3.618893000	3.563895000
H	2.942905000	-3.418763000	4.632373000
C	3.689300000	-2.695108000	2.729100000
H	4.743115000	-2.859866000	2.990568000
H	3.465085000	-1.643267000	2.947486000
C	3.467133000	-2.975483000	1.234529000
H	4.092840000	-2.301019000	0.637888000
C	3.819265000	-4.436547000	0.925155000
H	4.876756000	-4.626891000	1.151769000
H	3.679793000	-4.642672000	-0.144805000
C	-5.269694000	-2.120302000	-4.096454000
H	-4.706923000	-3.035458000	-4.304004000
H	-6.334910000	-2.371910000	-4.074677000
H	-5.114105000	-1.430497000	-4.933125000

C	-5.643095000	-0.200649000	-2.496288000
H	-6.719173000	-0.406260000	-2.487226000
H	-5.368379000	0.241894000	-1.534834000
H	-5.445264000	0.543459000	-3.275345000
C	-4.848139000	-1.488223000	-2.766620000
H	-5.084383000	-2.199865000	-1.967666000
C	-3.367066000	-1.217798000	-2.728196000
C	-2.521161000	-0.938573000	-3.792718000
H	-2.784856000	-0.924692000	-4.839632000
C	-1.263652000	-0.683907000	-3.223573000
C	0.027899000	-0.342671000	-3.922833000
C	1.136465000	0.040792000	-2.922925000
H	1.327153000	-0.799163000	-2.236478000
H	0.823487000	0.914144000	-2.328722000
C	-0.181089000	0.846902000	-4.890768000
H	-0.965737000	0.595882000	-5.615741000
H	-0.540113000	1.717847000	-4.326615000
C	0.524401000	-1.558671000	-4.745576000
H	-0.249811000	-1.851084000	-5.466577000
H	0.671253000	-2.415068000	-4.074395000
C	1.831809000	-1.219140000	-5.477938000
H	2.158812000	-2.095668000	-6.052407000
C	2.911117000	-0.838523000	-4.452560000
H	3.107661000	-1.682030000	-3.776988000
H	3.856552000	-0.613289000	-4.963136000
C	2.445156000	0.384607000	-3.649210000
H	3.201440000	0.659099000	-2.905667000
C	2.203952000	1.565384000	-4.599931000
H	3.138577000	1.829758000	-5.111148000
H	1.894366000	2.450600000	-4.029201000
C	1.125148000	1.185556000	-5.625346000
H	0.945635000	2.028572000	-6.305172000
C	1.592362000	-0.037192000	-6.430181000
H	2.515902000	0.200822000	-6.974312000
H	0.838309000	-0.305543000	-7.182459000
B	-3.079441000	-1.396874000	-0.119779000
N	-3.124336000	-0.073042000	0.702319000
N	-2.107396000	0.835760000	0.648797000
N	-2.197128000	-2.481811000	0.564435000
N	-0.867004000	-2.289337000	0.808766000
N	-2.627642000	-1.136072000	-1.586530000
N	-1.341389000	-0.806461000	-1.893855000
Yb	0.026505000	-0.158052000	0.019343000
H	-4.194581000	-1.823818000	-0.160911000

Optimized geometry of TS2

C	7.641455000	5.415132000	11.589369000
H	8.082783000	4.527094000	11.138310000
H	7.292182000	6.195375000	10.913464000
C	7.693850000	5.623654000	12.909162000
H	5.843961000	4.873669000	13.898910000
C	8.139105000	6.019775000	14.084157000
H	7.519911000	5.845448000	14.957927000
C	9.467944000	6.712666000	14.314346000
H	9.225215000	7.690000000	14.766547000
C	10.301187000	5.936939000	15.352295000
H	10.522219000	4.938688000	14.949213000
H	9.711217000	5.780856000	16.263980000
C	11.609911000	6.659730000	15.680912000
H	11.380666000	7.612600000	16.179732000
H	12.196050000	6.068977000	16.395402000
C	12.428518000	6.936627000	14.417792000
H	13.339875000	7.493320000	14.667943000
H	12.755925000	5.980928000	13.983645000
C	11.602974000	7.702556000	13.381228000
H	12.187028000	7.854201000	12.465346000
H	11.373927000	8.704750000	13.771760000
C	10.294619000	6.977864000	13.053217000
H	9.704873000	7.557925000	12.334557000

H	10.516841000	6.019466000	12.564235000
C	-1.356301000	4.529368000	14.294500000
H	-2.188492000	3.868291000	14.557071000
H	-1.126694000	5.133252000	15.179269000
H	-1.693571000	5.204481000	13.502168000
C	-0.144029000	3.704415000	13.854253000
H	-0.449844000	3.084335000	13.002648000
C	0.313700000	2.762230000	14.980071000
H	-0.504591000	2.100367000	15.285202000
H	1.158695000	2.143836000	14.665170000
H	0.630680000	3.338063000	15.856262000
C	0.991068000	4.582405000	13.401005000
C	1.270557000	5.892750000	13.760236000
H	0.675728000	6.527749000	14.399527000
C	2.474928000	6.217331000	13.114551000
C	3.192610000	7.543696000	13.126603000
C	2.264775000	8.634023000	12.534186000
H	1.989968000	8.358900000	11.507285000
H	1.331731000	8.675124000	13.110857000
C	3.562566000	7.945530000	14.575215000
H	2.655777000	7.972684000	15.193381000
H	4.220315000	7.176028000	14.998342000
C	4.491737000	7.503816000	12.300441000
H	5.171291000	6.767757000	12.760649000
H	4.265253000	7.198476000	11.268099000
C	5.182746000	8.877040000	12.305892000
H	6.101051000	8.820512000	11.706547000
C	5.537214000	9.255512000	13.752530000
H	6.050487000	10.226597000	13.772607000
H	6.227754000	8.513275000	14.171626000
C	4.252791000	9.318780000	14.591953000
H	4.502534000	9.582482000	15.628081000
C	3.310151000	10.379012000	14.002013000
H	2.395242000	10.450495000	14.605776000
H	3.788420000	11.367545000	14.030129000
C	2.958019000	10.004400000	12.553746000
H	2.279598000	10.757454000	12.131453000
C	4.241562000	9.935836000	11.712893000
H	4.737849000	10.915550000	11.698359000
H	3.996115000	9.686103000	10.671593000
C	1.306519000	-0.607819000	10.821969000
H	1.464364000	0.238465000	10.147773000
H	2.075424000	-1.356733000	10.602921000
H	0.328691000	-1.049279000	10.599217000
C	1.132786000	-1.363094000	13.225694000
H	0.139922000	-1.785788000	13.040344000
H	1.863961000	-2.161623000	13.058752000
H	1.187674000	-1.069045000	14.278094000
C	1.383339000	-0.173132000	12.294482000
H	0.589099000	0.561162000	12.469400000
C	2.703332000	0.490270000	12.587296000
C	3.854606000	-0.085512000	13.103267000
H	3.972039000	-1.106933000	13.431384000
C	4.821230000	0.932167000	13.112608000
C	6.240855000	0.837884000	13.613811000
C	7.118961000	1.990899000	13.091177000
H	6.717796000	2.952644000	13.457230000
H	7.115272000	1.983773000	11.988983000
C	6.251687000	0.897819000	15.163276000
H	5.625576000	0.089335000	15.562844000
H	5.802792000	1.844663000	15.487578000
C	6.877537000	-0.502381000	13.174579000
H	6.871784000	-0.569150000	12.078373000
H	6.273911000	-1.340189000	13.545710000
C	8.311339000	-0.626036000	13.711088000
H	8.733833000	-1.585897000	13.385896000
C	8.290611000	-0.564915000	15.246540000
H	7.701942000	-1.400844000	15.648425000
H	9.309695000	-0.673533000	15.641560000
C	7.686939000	0.773899000	15.697692000

H	7.666821000	0.819910000	16.794442000
C	8.538428000	1.927821000	15.147844000
H	9.562238000	1.862104000	15.540314000
H	8.126160000	2.891566000	15.471157000
C	8.559016000	1.863045000	13.612437000
H	9.154357000	2.697571000	13.220909000
C	9.164086000	0.526667000	13.160841000
H	10.197931000	0.438863000	13.521463000
H	9.202864000	0.476860000	12.063915000
C	-0.337021000	2.624080000	7.796783000
H	0.148355000	1.703237000	7.459459000
H	-1.415090000	2.441843000	7.851195000
H	-0.173539000	3.392892000	7.033540000
C	-0.500400000	4.369598000	9.613352000
H	-1.586907000	4.232389000	9.650751000
H	-0.159289000	4.683079000	10.603693000
H	-0.284792000	5.182999000	8.911906000
C	0.192041000	3.073459000	9.161578000
H	-0.053922000	2.292533000	9.890571000
C	1.688793000	3.240273000	9.146676000
C	2.514842000	3.496882000	8.063959000
H	2.219840000	3.565110000	7.027617000
C	3.807586000	3.629253000	8.596626000
C	5.077988000	3.844527000	7.813250000
C	6.298111000	4.037828000	8.726819000
H	6.406881000	3.163821000	9.384852000
H	6.134910000	4.921945000	9.359644000
C	4.950763000	5.092850000	6.907131000
H	4.082833000	4.981449000	6.245401000
H	4.759652000	5.976900000	7.530133000
C	5.340944000	2.612590000	6.910140000
H	4.477828000	2.452488000	6.251973000
H	5.428672000	1.716715000	7.538525000
C	6.615159000	2.811516000	6.076077000
H	6.776576000	1.926401000	5.447216000
C	7.813670000	3.001145000	7.017320000
H	7.947717000	2.108237000	7.642732000
H	8.737506000	3.125629000	6.437021000
C	7.579284000	4.236316000	7.900773000
H	8.431371000	4.371664000	8.579356000
C	7.425877000	5.479929000	7.011891000
H	8.342644000	5.640623000	6.429293000
H	7.282846000	6.374541000	7.633079000
C	6.225525000	5.290967000	6.072988000
H	6.108130000	6.180896000	5.441143000
C	6.457063000	4.055817000	5.188304000
H	7.354603000	4.196788000	4.571493000
H	5.612826000	3.922285000	4.498796000
B	2.054484000	2.874759000	11.709742000
N	1.989217000	4.166520000	12.573374000
N	2.902417000	5.165404000	12.406598000
N	2.988915000	1.792884000	12.314966000
N	4.285509000	2.063510000	12.634847000
N	2.475526000	3.219375000	10.257804000
N	3.774410000	3.470598000	9.926350000
Yb	5.139039000	4.270011000	11.996863000
H	0.951038000	2.411489000	11.671847000

Optimized geometry of Int4

C	2.753285000	0.249203000	0.225130000
H	3.065013000	-0.810745000	0.260710000
H	3.179658000	0.673136000	-0.688337000
C	3.187382000	0.926493000	1.453027000
H	2.989254000	0.335289000	2.355453000
C	3.743078000	2.129743000	1.744844000
H	3.899777000	2.325191000	2.808506000
C	4.273491000	3.255135000	0.887609000
H	3.743802000	4.180345000	1.185323000
C	5.762639000	3.506689000	1.209809000

H	6.333412000	2.609653000	0.929905000
H	5.889308000	3.626007000	2.293475000
C	6.321419000	4.728115000	0.475707000
H	5.813506000	5.632544000	0.842115000
H	7.387048000	4.857068000	0.704212000
C	6.110279000	4.614369000	-1.035551000
H	6.466029000	5.519724000	-1.543537000
H	6.715747000	3.781414000	-1.421607000
C	4.638567000	4.357381000	-1.367700000
H	4.509567000	4.237030000	-2.451033000
H	4.045969000	5.239105000	-1.081304000
C	4.099286000	3.126511000	-0.630953000
H	3.042521000	2.971787000	-0.878349000
H	4.637585000	2.234994000	-0.979414000
C	-6.241373000	0.241442000	2.297588000
H	-7.135908000	-0.382950000	2.387946000
H	-6.020890000	0.641911000	3.293143000
H	-6.477194000	1.082387000	1.638535000
C	-5.071871000	-0.587338000	1.759086000
H	-5.373748000	-1.007063000	0.792045000
C	-4.756378000	-1.761198000	2.700670000
H	-5.642624000	-2.390526000	2.837648000
H	-3.949329000	-2.385963000	2.308890000
H	-4.447816000	-1.391372000	3.684509000
C	-3.851140000	0.263420000	1.529254000
C	-3.500752000	1.455615000	2.144515000
H	-4.081230000	1.999669000	2.874181000
C	-2.253757000	1.813995000	1.606783000
C	-1.465369000	3.063110000	1.909721000
C	-2.373338000	4.295183000	1.656918000
H	-2.693505000	4.299155000	0.606667000
H	-3.283486000	4.211257000	2.263864000
C	-1.030668000	3.076887000	3.396202000
H	-1.913705000	2.967732000	4.039216000
H	-0.384584000	2.211301000	3.594546000
C	-0.203622000	3.207571000	1.035530000
H	0.496292000	2.377963000	1.223640000
H	-0.483330000	3.181868000	-0.026533000
C	0.531722000	4.518170000	1.363860000
H	1.421321000	4.590638000	0.727731000
C	0.957059000	4.501678000	2.839779000
H	1.504900000	5.422013000	3.082453000
H	1.641860000	3.662364000	3.013981000
C	-0.289134000	4.380132000	3.728917000
H	0.009410000	4.362239000	4.785208000
C	-1.218450000	5.577441000	3.474882000
H	-2.107545000	5.510753000	4.116832000
H	-0.706277000	6.513246000	3.734891000
C	-1.637240000	5.597617000	1.996431000
H	-2.308407000	6.447062000	1.813496000
C	-0.392069000	5.717335000	1.106824000
H	0.141033000	6.653037000	1.321536000
H	-0.685993000	5.752946000	0.048913000
C	-3.064664000	-4.449965000	-2.047416000
H	-2.808333000	-3.477814000	-2.476802000
H	-2.212596000	-5.121030000	-2.201070000
H	-3.919347000	-4.855398000	-2.600033000
C	-3.806092000	-5.699186000	0.018850000
H	-4.686750000	-6.079480000	-0.508258000
H	-3.006821000	-6.438294000	-0.104250000
H	-4.047393000	-5.635218000	1.084162000
C	-3.397821000	-4.337717000	-0.550536000
H	-4.254182000	-3.659786000	-0.449448000
C	-2.247656000	-3.740015000	0.214597000
C	-1.293607000	-4.383635000	0.988713000
H	-1.247271000	-5.439746000	1.207342000
C	-0.425777000	-3.378078000	1.445465000
C	0.746534000	-3.545836000	2.381250000
C	1.314512000	-2.195796000	2.858313000
H	0.519968000	-1.606169000	3.334214000

H	1.686348000	-1.619993000	1.998347000
C	0.281030000	-4.339227000	3.629448000
H	-0.131746000	-5.307264000	3.318947000
H	-0.532045000	-3.792049000	4.124098000
C	1.884115000	-4.343056000	1.697068000
H	2.228576000	-3.798066000	0.808027000
H	1.496158000	-5.308318000	1.346548000
C	3.052301000	-4.560261000	2.672125000
H	3.844655000	-5.123856000	2.162761000
C	2.559245000	-5.349892000	3.895385000
H	2.183064000	-6.334135000	3.584695000
H	3.392161000	-5.531019000	4.587605000
C	1.447601000	-4.559859000	4.602390000
H	1.087173000	-5.126426000	5.470950000
C	1.992170000	-3.199402000	5.060193000
H	2.817053000	-3.340198000	5.771118000
H	1.209015000	-2.636527000	5.585769000
C	2.481682000	-2.412309000	3.835628000
H	2.866251000	-1.435143000	4.152823000
C	3.596809000	-3.198781000	3.130190000
H	4.444657000	-3.341799000	3.813122000
H	3.972345000	-2.628137000	2.271127000
C	-5.007394000	-0.566851000	-4.307549000
H	-4.678043000	-1.516484000	-4.739881000
H	-6.101895000	-0.557236000	-4.298818000
H	-4.678669000	0.240621000	-4.970967000
C	-4.936572000	0.966450000	-2.301642000
H	-6.030614000	1.023700000	-2.307312000
H	-4.590926000	1.099443000	-1.273132000
H	-4.550559000	1.801492000	-2.896390000
C	-4.466589000	-0.375088000	-2.888141000
H	-4.876438000	-1.175680000	-2.260125000
C	-2.965962000	-0.485567000	-2.848485000
C	-2.054783000	-0.294045000	-3.876657000
H	-2.285268000	-0.067759000	-4.906560000
C	-0.784799000	-0.480773000	-3.306779000
C	0.547391000	-0.434169000	-4.016102000
C	1.685728000	-1.026254000	-3.163179000
H	1.436539000	-2.056409000	-2.877310000
H	1.808132000	-0.450141000	-2.234689000
C	0.918310000	1.024125000	-4.384881000
H	0.114440000	1.465790000	-4.988315000
H	0.993740000	1.625375000	-3.468703000
C	0.449495000	-1.253953000	-5.327132000
H	-0.354473000	-0.852447000	-5.956505000
H	0.177387000	-2.290044000	-5.087140000
C	1.776916000	-1.213786000	-6.097770000
H	1.674078000	-1.800925000	-7.019683000
C	2.890298000	-1.809464000	-5.224326000
H	2.663669000	-2.857592000	-4.986821000
H	3.843979000	-1.804177000	-5.768627000
C	3.016362000	-0.988387000	-3.932651000
H	3.804819000	-1.411781000	-3.298231000
C	3.362517000	0.467329000	-4.281919000
H	4.321351000	0.508375000	-4.815560000
H	3.482401000	1.057185000	-3.364319000
C	2.247918000	1.063482000	-5.154699000
H	2.488451000	2.105752000	-5.401105000
C	2.118443000	0.243171000	-6.447180000
H	3.057589000	0.284985000	-7.014635000
H	1.337245000	0.670061000	-7.090767000
B	-2.791738000	-1.235547000	-0.342108000
N	-2.849008000	-0.056813000	0.666290000
N	-1.862531000	0.888484000	0.720876000
N	-1.947736000	-2.413005000	0.222481000
N	-0.821690000	-2.190644000	0.965445000
N	-2.254258000	-0.772361000	-1.725322000
N	-0.915392000	-0.755936000	-2.000701000
Yb	0.258296000	-0.172325000	0.071529000
H	-3.911132000	-1.634949000	-0.502201000

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C	7.505465000	5.647157000	11.487928000
H	8.399254000	5.429408000	10.909010000
H	6.975955000	6.538717000	11.135592000
C	7.574071000	5.443818000	12.893738000
H	8.417423000	4.840560000	13.240224000
C	6.616043000	5.749808000	13.841335000
H	5.810323000	6.428876000	13.539169000
C	6.734061000	5.592579000	15.341755000
H	6.735954000	6.606279000	15.784873000
C	5.517869000	4.865457000	15.947076000
H	5.480542000	3.846713000	15.531525000
H	4.592840000	5.361791000	15.626919000
C	5.582865000	4.791017000	17.474859000
H	5.521397000	5.807882000	17.889590000
H	4.717260000	4.243229000	17.868067000
C	6.884631000	4.136113000	17.941671000
H	6.942903000	4.132424000	19.037285000
H	6.889921000	3.082355000	17.626293000
C	8.103456000	4.844727000	17.346003000
H	9.026699000	4.337087000	17.652497000
H	8.161357000	5.864136000	17.754241000
C	8.027895000	4.922482000	15.818062000
H	8.897450000	5.464855000	15.427186000
H	8.082476000	3.905071000	15.403356000
C	-0.322232000	4.106917000	15.132023000
H	-0.925102000	3.323007000	15.601391000
H	-0.021563000	4.804570000	15.921437000
H	-0.957252000	4.648603000	14.424535000
C	0.897927000	3.493630000	14.439978000
H	0.537608000	2.769120000	13.698712000
C	1.775440000	2.733385000	15.448486000
H	1.193105000	1.951721000	15.948730000
H	2.631230000	2.262653000	14.957990000
H	2.156907000	3.415278000	16.215921000
C	1.698337000	4.531004000	13.702235000
C	1.785711000	5.895083000	13.929531000
H	1.247089000	6.460556000	14.675429000
C	2.692314000	6.387743000	12.971572000
C	3.022392000	7.836668000	12.698155000
C	1.718724000	8.550826000	12.247510000
H	1.330212000	8.056100000	11.347986000
H	0.952573000	8.441490000	13.025716000
C	3.539571000	8.546288000	13.971924000
H	2.802452000	8.441479000	14.778734000
H	4.459567000	8.060118000	14.319345000
C	4.063507000	8.004535000	11.574951000
H	5.004201000	7.518536000	11.861540000
H	3.706785000	7.504532000	10.666011000
C	4.329809000	9.493047000	11.299770000
H	5.081219000	9.579095000	10.504411000
C	4.853071000	10.166090000	12.578057000
H	5.067791000	11.225776000	12.385407000
H	5.796518000	9.699851000	12.890842000
C	3.803139000	10.034175000	13.691903000
H	4.175032000	10.510574000	14.608297000
C	2.498230000	10.713689000	13.248807000
H	1.745510000	10.643237000	14.045768000
H	2.672094000	11.782843000	13.067683000
C	1.978949000	10.038861000	11.970223000
H	1.040221000	10.513984000	11.656145000
C	3.027206000	10.175297000	10.856327000
H	3.211099000	11.235666000	10.637250000
H	2.656252000	9.716420000	9.930074000
C	1.433900000	-0.433572000	10.665784000
H	1.582199000	0.438508000	10.023015000
H	2.139973000	-1.207422000	10.345658000
H	0.418439000	-0.812510000	10.505712000

C	1.420058000	-1.307148000	13.036745000
H	0.394081000	-1.670279000	12.917514000
H	2.090720000	-2.130646000	12.768448000
H	1.579385000	-1.072436000	14.093372000
C	1.654388000	-0.082869000	12.146121000
H	0.917959000	0.679344000	12.422830000
C	3.027462000	0.498458000	12.357035000
C	4.200157000	-0.172027000	12.666149000
H	4.309323000	-1.229859000	12.852968000
C	5.208394000	0.805010000	12.682069000
C	6.680005000	0.567899000	12.908095000
C	7.512810000	1.853640000	12.771111000
H	7.167188000	2.602346000	13.496913000
H	7.382204000	2.276851000	11.763011000
C	6.916963000	-0.019722000	14.321636000
H	6.324716000	-0.935836000	14.442015000
H	6.556033000	0.691750000	15.075837000
C	7.198057000	-0.455030000	11.864260000
H	7.030709000	-0.057460000	10.854606000
H	6.617102000	-1.382907000	11.937689000
C	8.688764000	-0.750202000	12.084868000
H	9.026573000	-1.474552000	11.332260000
C	8.889227000	-1.334385000	13.491783000
H	8.332979000	-2.276233000	13.592063000
H	9.949037000	-1.570898000	13.655430000
C	8.407390000	-0.320513000	14.540913000
H	8.545831000	-0.736192000	15.547452000
C	9.213350000	0.979057000	14.402557000
H	10.280444000	0.783861000	14.573015000
H	8.896404000	1.702122000	15.165026000
C	9.005987000	1.562988000	12.996525000
H	9.570177000	2.498694000	12.897365000
C	9.493271000	0.551125000	11.948364000
H	10.564009000	0.351351000	12.087527000
H	9.374227000	0.965297000	10.938232000
C	-0.244213000	3.097058000	7.974567000
H	0.160292000	2.183302000	7.528686000
H	-1.324763000	2.969019000	8.094267000
H	-0.088370000	3.917857000	7.265824000
C	-0.178948000	4.686017000	9.935901000
H	-1.266396000	4.601091000	10.039818000
H	0.244412000	4.892037000	10.922445000
H	0.034637000	5.545926000	9.291777000
C	0.404855000	3.400551000	9.327563000
H	0.166111000	2.573831000	10.007588000
C	1.904041000	3.487893000	9.213988000
C	2.674800000	3.750417000	8.091815000
H	2.315988000	3.890825000	7.083522000
C	4.008121000	3.772970000	8.537552000
C	5.246254000	3.991580000	7.700942000
C	6.535603000	3.605702000	8.451664000
H	6.474306000	2.557138000	8.771654000
H	6.653939000	4.219992000	9.357696000
C	5.353574000	5.477978000	7.276392000
H	4.440267000	5.773591000	6.743576000
H	5.416197000	6.108209000	8.173359000
C	5.159896000	3.128072000	6.417591000
H	4.250143000	3.382357000	5.859276000
H	5.074193000	2.069921000	6.697310000
C	6.390610000	3.348542000	5.525813000
H	6.297974000	2.725951000	4.626201000
C	7.658363000	2.956797000	6.299016000
H	7.620355000	1.893510000	6.571835000
H	8.545784000	3.093400000	5.666382000
C	7.769319000	3.824068000	7.560965000
H	8.668651000	3.545174000	8.125015000
C	7.853253000	5.305355000	7.160302000
H	8.743323000	5.478210000	6.540442000
H	7.958972000	5.931360000	8.055559000
C	6.586166000	5.698021000	6.385397000

H	6.639804000	6.757152000	6.101185000
C	6.469982000	4.829427000	5.123438000
H	7.336130000	4.997113000	4.469359000
H	5.577139000	5.112850000	4.549633000
B	2.427929000	2.971375000	11.726658000
N	2.519813000	4.237684000	12.653328000
N	3.145539000	5.379225000	12.216767000
N	3.340006000	1.815230000	12.213001000
N	4.677140000	2.005761000	12.417398000
N	2.757463000	3.356558000	10.266026000
N	4.045102000	3.546943000	9.856369000
Yb	5.366359000	4.307227000	11.834163000
H	1.294562000	2.580113000	11.760007000

Optimized geometry of Int1'

C	1.304582000	3.159422000	-3.642546000
C	0.622612000	4.275165000	-3.626850000
C	-0.056264000	5.397555000	-3.610868000
C	-1.630379000	2.236763000	1.834822000
H	-0.878488000	2.389923000	2.617816000
H	-2.220102000	1.350330000	2.084120000
C	-2.468753000	3.487981000	1.592759000
H	-2.633194000	4.060589000	2.509548000
H	-3.448219000	3.221508000	1.179864000
C	-1.637320000	4.235472000	0.546996000
H	-0.806357000	4.765454000	1.025731000
H	-2.214455000	4.961683000	-0.031090000
C	-1.117545000	3.094556000	-0.316959000
H	-1.842481000	2.809806000	-1.089244000
H	-0.162518000	3.291264000	-0.807542000
C	-1.972564000	-5.100653000	3.480878000
H	-1.917085000	-5.749302000	4.362198000
H	-2.671584000	-5.552945000	2.769088000
H	-0.987132000	-5.075750000	3.007687000
C	-3.816376000	-3.741409000	4.546015000
H	-3.771493000	-4.356216000	5.450966000
H	-4.164263000	-2.743113000	4.827929000
H	-4.568486000	-4.186972000	3.885993000
C	-2.441012000	-3.689934000	3.872560000
H	-1.727340000	-3.288233000	4.599362000
C	-2.447687000	-2.781552000	2.670928000
C	-3.479156000	-2.580563000	1.766968000
H	-4.467946000	-3.012625000	1.809197000
C	-2.967039000	-1.714801000	0.787683000
C	-3.675552000	-1.238768000	-0.456324000
C	-4.933226000	-0.416410000	-0.081239000
H	-4.632819000	0.457693000	0.512356000
H	-5.590767000	-1.019798000	0.557780000
C	-4.130363000	-2.465168000	-1.288493000
H	-3.251037000	-3.064492000	-1.557456000
H	-4.775511000	-3.107815000	-0.676062000
C	-2.773638000	-0.366707000	-1.346938000
H	-1.881843000	-0.933174000	-1.653293000
H	-2.435000000	0.513068000	-0.783956000
C	-3.521503000	0.087818000	-2.609879000
H	-2.845977000	0.705442000	-3.213746000
C	-4.761538000	0.900874000	-2.208124000
H	-5.293939000	1.244695000	-3.104937000
H	-4.462034000	1.800086000	-1.652065000
C	-5.686444000	0.030553000	-1.343777000
H	-6.571657000	0.609397000	-1.048869000
C	-6.121581000	-1.205710000	-2.146394000
H	-6.679597000	-0.896722000	-3.040338000
H	-6.800096000	-1.826198000	-1.545352000
C	-4.881347000	-2.017261000	-2.551341000
H	-5.190305000	-2.904791000	-3.118807000
C	-3.958158000	-1.145149000	-3.415118000
H	-4.478854000	-0.832973000	-4.330212000
H	-3.077268000	-1.720044000	-3.729223000
C	-1.473958000	-0.165000000	5.613190000

H	-1.971508000	-0.576323000	6.498395000
H	-1.605443000	0.922766000	5.627225000
H	-1.977397000	-0.554806000	4.724134000
C	0.701581000	-0.011826000	6.886099000
H	0.232825000	-0.452863000	7.771580000
H	1.766081000	-0.263993000	6.902476000
H	0.609350000	1.076373000	6.974707000
C	0.020497000	-0.526075000	5.615179000
H	0.098721000	-1.620238000	5.610440000
C	0.701051000	-0.014555000	4.373991000
C	1.494525000	1.113968000	4.222745000
H	1.799820000	1.797259000	5.001355000
C	1.844059000	1.155179000	2.860548000
C	2.785693000	2.117607000	2.178852000
C	2.873568000	1.871786000	0.660495000
H	3.181844000	0.835729000	0.469169000
H	1.887602000	2.015146000	0.195269000
C	4.204560000	1.935963000	2.780068000
H	4.166896000	2.100949000	3.864668000
H	4.528953000	0.898421000	2.628320000
C	2.346992000	3.582235000	2.411669000
H	2.273476000	3.782022000	3.488794000
H	1.343522000	3.727857000	1.990697000
C	3.342169000	4.556517000	1.761780000
H	3.006704000	5.586584000	1.941488000
C	4.735124000	4.353096000	2.378214000
H	5.448958000	5.060659000	1.935782000
H	4.706159000	4.561173000	3.456534000
C	5.199426000	2.909340000	2.131194000
H	6.191456000	2.759207000	2.577046000
C	5.263392000	2.640614000	0.620266000
H	5.613706000	1.616783000	0.433512000
H	5.986029000	3.317578000	0.145265000
C	3.869620000	2.843178000	0.007510000
H	3.901362000	2.643825000	-1.070112000
C	3.409747000	4.288450000	0.250769000
H	4.106308000	4.990701000	-0.226216000
H	2.428191000	4.452535000	-0.212762000
C	3.052969000	-3.452614000	4.328291000
H	3.189763000	-3.850639000	5.340121000
H	4.036748000	-3.393870000	3.850109000
H	2.659597000	-2.435562000	4.408988000
C	2.652684000	-5.787517000	3.454526000
H	2.743300000	-6.199997000	4.464630000
H	1.994726000	-6.442693000	2.875618000
H	3.647878000	-5.818697000	2.997712000
C	2.112420000	-4.355934000	3.514106000
H	1.147391000	-4.384127000	4.033574000
C	1.885616000	-3.792691000	2.135632000
C	2.503318000	-4.152086000	0.946417000
H	3.217968000	-4.948227000	0.808243000
C	1.994572000	-3.280527000	-0.030282000
C	2.327410000	-3.228836000	-1.504181000
C	3.162739000	-1.967764000	-1.838855000
H	4.076670000	-1.964075000	-1.229337000
H	2.590053000	-1.064573000	-1.586665000
C	1.040081000	-3.199176000	-2.361479000
H	0.447891000	-2.310710000	-2.106369000
H	0.425003000	-4.078521000	-2.127997000
C	3.150690000	-4.470601000	-1.910339000
H	2.584163000	-5.381509000	-1.674000000
H	4.077438000	-4.506611000	-1.322002000
C	3.494569000	-4.435343000	-3.406810000
H	4.075604000	-5.331768000	-3.661342000
C	4.323514000	-3.177933000	-3.710033000
H	4.590737000	-3.150097000	-4.775160000
H	5.265258000	-3.202148000	-3.144443000
C	3.509796000	-1.930878000	-3.335588000
H	4.097927000	-1.027258000	-3.542388000
C	2.208633000	-1.895249000	-4.152754000

H	1.629753000	-1.001915000	-3.886560000
H	2.438752000	-1.837899000	-5.225555000
C	1.386143000	-3.159243000	-3.857574000
H	0.454983000	-3.136228000	-4.439062000
C	2.198530000	-4.407809000	-4.230886000
H	1.610317000	-5.315801000	-4.038972000
H	2.433714000	-4.399566000	-5.303816000
B	0.065551000	-2.038201000	2.815273000
N	-1.381651000	-2.049083000	2.241387000
N	-1.702499000	-1.391167000	1.089213000
N	0.590941000	-0.602456000	3.148581000
N	1.282370000	0.123329000	2.222300000
N	1.045106000	-2.758954000	1.856466000
N	1.117617000	-2.438287000	0.533547000
O	-0.942195000	1.982932000	0.590204000
Yb	0.188592000	-0.181507000	0.021947000
H	0.040878000	-2.649240000	3.844401000
H	2.231728000	3.088846000	-4.210610000
H	0.591745000	0.528740000	-1.944348000
H	0.987211000	2.263177000	-3.095194000
H	0.176161000	6.130092000	-2.834142000
C	-1.150975000	5.791411000	-4.578602000
C	-2.455670000	6.114501000	-3.827268000
C	-3.565170000	6.564518000	-4.781123000
C	-3.810433000	5.526494000	-5.878973000
C	-2.516894000	5.196790000	-6.628330000
C	-1.407753000	4.750682000	-5.672204000
H	-0.826376000	6.724222000	-5.071497000
H	-2.269044000	6.884898000	-3.067585000
H	-2.778047000	5.212508000	-3.287241000
H	-4.489293000	6.756693000	-4.222052000
H	-3.277677000	7.519743000	-5.243952000
H	-4.576969000	5.883955000	-6.577385000
H	-4.207205000	4.607749000	-5.423330000
H	-2.700065000	4.418822000	-7.379339000
H	-2.183825000	6.087625000	-7.180605000
H	-0.480593000	4.554044000	-6.222549000
H	-1.687824000	3.800247000	-5.197016000

Optimized geometry of TS1'

C	5.154374000	20.222336000	8.065252000
C	5.161801000	21.273401000	7.286139000
C	5.325032000	22.324454000	6.505918000
C	2.949618000	21.101730000	12.580445000
H	3.709248000	21.300002000	13.345201000
H	2.508925000	20.119270000	12.763707000
C	1.933572000	22.232807000	12.483044000
H	1.714201000	22.676848000	13.457715000
H	0.991625000	21.871966000	12.054662000
C	2.624202000	23.197275000	11.516330000
H	3.384974000	23.785109000	12.041403000
H	1.936271000	23.891894000	11.026867000
C	3.276218000	22.238883000	10.528260000
H	2.583665000	21.952855000	9.727597000
H	4.192038000	22.618667000	10.070002000
C	3.401660000	14.054377000	14.036941000
H	3.489850000	13.411426000	14.919756000
H	2.837718000	13.508029000	13.273155000
H	4.404465000	14.238161000	13.641884000
C	1.294798000	15.095919000	14.962069000
H	1.370019000	14.487258000	15.869059000
H	0.773664000	16.023961000	15.215822000
H	0.673235000	14.543162000	14.249269000
C	2.690206000	15.369866000	14.392265000
H	3.277113000	15.869233000	15.170512000
C	2.629344000	16.280758000	13.193935000
C	1.622567000	16.372594000	12.246802000
H	0.685835000	15.835635000	12.246143000
C	2.078260000	17.295430000	11.291740000

C	1.350468000	17.709171000	10.036534000
C	0.060010000	18.487366000	10.395716000
H	0.326023000	19.385288000	10.969441000
H	-0.570246000	17.870731000	11.049299000
C	0.944922000	16.448439000	9.231402000
H	1.846982000	15.878106000	8.974002000
H	0.325938000	15.793114000	9.856763000
C	2.213986000	18.597096000	9.126590000
H	3.125644000	18.048642000	8.847166000
H	2.514394000	19.502639000	9.669498000
C	1.449618000	18.992272000	7.853854000
H	2.096802000	19.628446000	7.238532000
C	0.177849000	19.763056000	8.240448000
H	-0.367674000	20.065196000	7.336712000
H	0.441973000	20.685697000	8.774894000
C	-0.711163000	18.876341000	9.125114000
H	-1.618565000	19.425910000	9.408235000
C	-1.096936000	17.606758000	8.350101000
H	-1.667701000	17.873413000	7.450651000
H	-1.749012000	16.972162000	8.965391000
C	0.174832000	16.837309000	7.960515000
H	-0.098622000	15.925666000	7.413507000
C	1.061512000	17.726306000	7.075869000
H	0.528244000	17.997911000	6.155211000
H	1.963173000	17.178043000	6.771809000
C	3.109905000	18.954016000	16.168218000
H	2.610753000	18.482080000	17.021745000
H	2.852512000	20.019171000	16.174560000
H	2.708894000	18.514206000	15.250832000
C	5.169248000	19.345110000	17.574144000
H	4.699825000	18.843959000	18.426672000
H	6.252529000	19.216751000	17.657570000
H	4.946844000	20.414557000	17.659558000
C	4.633132000	18.768308000	16.261276000
H	4.837262000	17.690435000	16.260023000
C	5.327443000	19.367324000	15.067317000
C	6.027285000	20.562708000	14.984551000
H	6.226420000	21.247296000	15.794041000
C	6.452575000	20.672035000	13.648866000
C	7.363933000	21.727692000	13.058603000
C	6.695511000	22.507015000	11.903245000
H	6.421036000	21.808063000	11.103698000
H	5.775263000	22.982895000	12.268339000
C	8.650139000	21.058325000	12.511245000
H	9.136288000	20.496422000	13.320020000
H	8.376074000	20.338995000	11.730993000
C	7.773385000	22.744075000	14.147138000
H	8.255992000	22.216017000	14.980280000
H	6.877899000	23.235480000	14.552777000
C	8.733396000	23.800116000	13.579553000
H	9.004166000	24.502697000	14.378899000
C	9.998208000	23.108964000	13.047411000
H	10.699748000	23.857899000	12.655527000
H	10.512934000	22.584980000	13.864336000
C	9.608434000	22.115747000	11.942905000
H	10.507700000	21.613959000	11.562354000
C	8.914457000	22.867247000	10.796548000
H	8.640592000	22.164958000	9.999770000
H	9.597636000	23.609611000	10.361678000
C	7.654335000	23.564171000	11.332884000
H	7.152781000	24.095590000	10.513389000
C	8.042962000	24.558302000	12.436192000
H	8.714526000	25.328229000	12.033037000
H	7.150593000	25.077829000	12.812477000
C	8.125532000	16.445804000	15.128245000
H	8.289141000	16.126952000	16.163856000
H	9.103739000	16.622287000	14.668076000
H	7.587092000	17.397252000	15.142163000
C	8.095730000	14.033025000	14.385810000
H	8.215241000	13.695478000	15.420382000

H	7.558100000	13.256534000	13.833175000
H	9.098192000	14.123942000	13.953418000
C	7.351236000	15.370511000	14.348617000
H	6.384645000	15.229615000	14.846976000
C	7.086806000	15.816247000	12.934483000
C	7.768282000	15.467745000	11.780098000
H	8.583766000	14.764999000	11.698170000
C	7.171573000	16.207225000	10.744720000
C	7.528053000	16.145754000	9.280548000
C	8.988812000	16.613902000	9.065166000
H	9.665229000	16.001337000	9.675347000
H	9.088438000	17.648889000	9.415857000
C	6.613372000	17.033380000	8.419956000
H	6.735521000	18.077687000	8.739206000
H	5.564564000	16.737263000	8.567808000
C	7.403266000	14.684679000	8.780255000
H	6.372904000	14.336173000	8.931110000
H	8.048600000	14.031676000	9.381483000
C	7.790892000	14.583834000	7.297391000
H	7.695944000	13.539738000	6.970878000
C	9.243255000	15.052443000	7.115543000
H	9.538404000	14.964865000	6.061185000
H	9.921608000	14.408123000	7.691351000
C	9.375241000	16.510804000	7.581590000
H	10.413234000	16.845947000	7.456510000
C	8.440855000	17.399902000	6.747346000
H	8.536715000	18.448006000	7.057750000
H	8.719024000	17.350309000	5.685928000
C	6.989851000	16.930018000	6.933421000
H	6.319852000	17.573448000	6.349102000
C	6.855868000	15.473802000	6.464754000
H	5.816790000	15.133733000	6.572924000
H	7.108198000	15.396096000	5.398622000
B	5.016199000	17.317720000	13.468418000
N	3.623855000	17.129081000	12.809889000
N	3.287807000	17.754140000	11.644609000
N	5.339312000	18.805494000	13.826695000
N	6.012409000	19.611928000	12.952402000
N	6.127899000	16.716579000	12.579639000
N	6.188282000	16.968932000	11.240093000
O	3.604102000	21.059011000	11.290480000
Yb	5.149733000	19.190971000	10.652994000
H	5.002851000	16.709089000	14.499070000
H	4.806056000	19.288310000	7.606721000
H	6.962027000	20.043096000	9.697612000
H	6.160934000	20.194062000	8.969429000
H	6.278525000	22.388482000	5.975782000
C	4.361573000	23.458415000	6.235500000
C	4.839696000	24.773304000	6.881812000
C	3.907487000	25.943816000	6.558207000
C	2.463259000	25.633332000	6.958861000
C	1.979826000	24.328251000	6.320926000
C	2.915987000	23.160093000	6.642162000
H	4.363616000	23.624263000	5.144568000
H	5.863272000	24.996540000	6.556199000
H	4.888221000	24.627056000	7.970511000
H	4.255577000	26.856066000	7.058427000
H	3.945398000	26.148450000	5.478337000
H	1.801336000	26.462757000	6.680717000
H	2.405723000	25.543220000	8.053744000
H	0.959164000	24.097428000	6.651099000
H	1.928592000	24.459686000	5.230304000
H	2.575385000	22.244937000	6.143685000
H	2.887236000	22.953205000	7.720111000

Optimized geometry of Int2'

C	0.202921000	1.118461000	-2.447019000
C	0.417698000	2.350517000	-2.813729000
C	0.654956000	3.619354000	-3.136403000

C	-2.061894000	1.945852000	1.919033000
H	-1.271159000	2.070969000	2.667097000
H	-2.567907000	0.993105000	2.095630000
C	-3.005956000	3.144586000	1.880098000
H	-3.129799000	3.604704000	2.864189000
H	-3.996925000	2.845507000	1.520278000
C	-2.326266000	4.060069000	0.858916000
H	-1.495979000	4.604333000	1.322424000
H	-3.004393000	4.791847000	0.411796000
C	-1.806464000	3.055856000	-0.158684000
H	-2.591071000	2.771921000	-0.872064000
H	-0.930816000	3.377474000	-0.727446000
C	-1.839263000	-5.095934000	3.272303000
H	-1.755305000	-5.724906000	4.165530000
H	-2.479162000	-5.614429000	2.550141000
H	-0.846412000	-4.997127000	2.824952000
C	-3.816244000	-3.877495000	4.266224000
H	-3.745514000	-4.472661000	5.182534000
H	-4.252577000	-2.907248000	4.521827000
H	-4.511045000	-4.393678000	3.594956000
C	-2.431941000	-3.722847000	3.627855000
H	-1.773748000	-3.253607000	4.366419000
C	-2.480216000	-2.836240000	2.410838000
C	-3.503704000	-2.729020000	1.482315000
H	-4.458623000	-3.232233000	1.512961000
C	-3.036505000	-1.845031000	0.497081000
C	-3.758100000	-1.430632000	-0.760949000
C	-5.049225000	-0.650461000	-0.409554000
H	-4.785261000	0.246780000	0.166145000
H	-5.686073000	-1.265949000	0.238896000
C	-4.159077000	-2.690870000	-1.569078000
H	-3.255572000	-3.261478000	-1.820945000
H	-4.782603000	-3.345885000	-0.947436000
C	-2.887485000	-0.541124000	-1.663728000
H	-1.970260000	-1.080243000	-1.943838000
H	-2.593550000	0.367339000	-1.122222000
C	-3.641300000	-0.144255000	-2.941575000
H	-2.985341000	0.490501000	-3.548311000
C	-4.915160000	0.627141000	-2.563918000
H	-5.454645000	0.929775000	-3.471102000
H	-4.653908000	1.549580000	-2.027926000
C	-5.810782000	-0.259469000	-1.685552000
H	-6.719570000	0.290552000	-1.407835000
C	-6.192661000	-1.528267000	-2.463836000
H	-6.756627000	-1.260255000	-3.367137000
H	-6.849931000	-2.162605000	-1.853677000
C	-4.919184000	-2.299040000	-2.845287000
H	-5.190019000	-3.209757000	-3.395254000
C	-4.024660000	-1.409974000	-3.722476000
H	-4.550864000	-1.137995000	-4.647086000
H	-3.120969000	-1.958590000	-4.019781000
C	-1.706701000	-0.177890000	5.418619000
H	-2.168178000	-0.632494000	6.302142000
H	-1.925740000	0.895557000	5.438947000
H	-2.178936000	-0.602566000	4.528396000
C	0.450098000	0.145021000	6.689945000
H	0.017402000	-0.334379000	7.573783000
H	1.531112000	-0.022669000	6.706179000
H	0.272390000	1.222281000	6.781622000
C	-0.188254000	-0.417443000	5.417321000
H	-0.023015000	-1.501960000	5.409103000
C	0.450156000	0.150674000	4.177973000
C	1.176118000	1.324859000	4.037185000
H	1.445450000	2.015572000	4.822397000
C	1.515901000	1.403192000	2.673652000
C	2.402984000	2.422226000	2.002506000
C	2.489108000	2.207958000	0.479720000
H	2.842443000	1.189195000	0.269304000
H	1.496716000	2.321477000	0.020790000
C	3.833440000	2.295457000	2.590899000

H	3.795975000	2.439468000	3.678499000
H	4.204116000	1.276643000	2.418692000
C	1.898643000	3.860312000	2.264658000
H	1.826320000	4.037890000	3.345812000
H	0.885928000	3.967283000	1.854766000
C	2.842990000	4.889670000	1.623714000
H	2.461250000	5.899740000	1.822687000
C	4.248491000	4.740874000	2.227533000
H	4.925487000	5.487928000	1.792237000
H	4.218554000	4.929300000	3.309501000
C	4.777577000	3.324681000	1.952989000
H	5.778444000	3.213033000	2.390449000
C	4.843237000	3.083546000	0.437587000
H	5.239576000	2.079972000	0.232363000
H	5.530617000	3.800516000	-0.030892000
C	3.437506000	3.232557000	-0.162540000
H	3.469410000	3.050414000	-1.243103000
C	2.911331000	4.649980000	0.107932000
H	3.571484000	5.392286000	-0.360426000
H	1.920722000	4.770595000	-0.348536000
C	3.006627000	-3.023928000	4.232697000
H	3.137493000	-3.395163000	5.255375000
H	3.999477000	-2.896506000	3.787779000
H	2.534234000	-2.039017000	4.281657000
C	2.822718000	-5.394149000	3.382983000
H	2.909686000	-5.785492000	4.401751000
H	2.240081000	-6.107063000	2.791739000
H	3.833196000	-5.351342000	2.962042000
C	2.168419000	-4.009688000	3.402596000
H	1.191671000	-4.108644000	3.889814000
C	1.946159000	-3.483776000	2.008486000
C	2.645827000	-3.795931000	0.855445000
H	3.439509000	-4.521225000	0.757351000
C	2.101786000	-2.984002000	-0.153967000
C	2.504740000	-2.989673000	-1.607351000
C	4.023716000	-2.718251000	-1.741126000
H	4.584510000	-3.458978000	-1.157031000
H	4.255916000	-1.735171000	-1.310708000
C	1.755024000	-1.932629000	-2.432174000
H	1.964781000	-0.927949000	-2.039350000
H	0.671191000	-2.099363000	-2.352714000
C	2.206010000	-4.384085000	-2.216287000
H	1.132406000	-4.595329000	-2.125140000
H	2.729698000	-5.156377000	-1.638657000
C	2.640067000	-4.439113000	-3.688479000
H	2.418546000	-5.435933000	-4.092003000
C	4.148867000	-4.164766000	-3.787529000
H	4.474735000	-4.221371000	-4.834765000
H	4.708883000	-4.932986000	-3.237091000
C	4.456930000	-2.772661000	-3.214116000
H	5.535341000	-2.577219000	-3.279044000
C	3.688292000	-1.709445000	-4.012477000
H	3.914214000	-0.706485000	-3.627593000
H	4.001754000	-1.725559000	-5.064761000
C	2.180785000	-1.984863000	-3.908224000
H	1.628492000	-1.218585000	-4.465641000
C	1.871629000	-3.374332000	-4.485160000
H	0.792352000	-3.572972000	-4.437559000
H	2.156969000	-3.413547000	-5.544890000
B	-0.038938000	-1.896757000	2.600091000
N	-1.462181000	-2.034216000	1.988213000
N	-1.804982000	-1.424770000	0.816353000
N	0.366028000	-0.426244000	2.944640000
N	1.010794000	0.349416000	2.025133000
N	1.026573000	-2.534323000	1.677747000
N	1.127394000	-2.216990000	0.352938000
O	-1.439252000	1.893023000	0.615060000
Yb	-0.035308000	-0.004486000	-0.196667000
H	-0.044102000	-2.504859000	3.630567000
H	0.335956000	0.409712000	-3.280408000

H	2.313303000	2.444202000	-6.173171000
H	1.958469000	2.580275000	-5.531327000
H	1.675064000	3.995296000	-3.026467000
C	-0.320728000	4.598468000	-3.760139000
C	-0.470805000	5.884630000	-2.926413000
C	-1.394266000	6.903629000	-3.599802000
C	-2.764407000	6.293549000	-3.906025000
C	-2.627896000	5.012166000	-4.732927000
C	-1.698015000	3.999177000	-4.059442000
H	0.106684000	4.910909000	-4.730310000
H	0.517801000	6.325640000	-2.744733000
H	-0.876149000	5.619373000	-1.938694000
H	-1.504602000	7.795768000	-2.970183000
H	-0.933508000	7.242165000	-4.539294000
H	-3.400405000	7.020272000	-4.427036000
H	-3.272692000	6.058468000	-2.958918000
H	-3.615031000	4.564931000	-4.906214000
H	-2.226350000	5.267399000	-5.724455000
H	-1.581706000	3.106311000	-4.684478000
H	-2.150639000	3.654035000	-3.119571000

Optimized geometry of Int3'

C	6.517808000	-0.155937000	-0.918804000
H	6.589762000	-1.077783000	-0.343608000
H	6.511193000	-0.256078000	-2.003013000
C	6.444343000	1.013448000	-0.335695000
H	1.817912000	1.568699000	0.337958000
C	6.395048000	2.186536000	0.249918000
C	-6.649741000	0.440906000	1.547458000
H	-7.542471000	-0.191985000	1.579317000
H	-6.602080000	0.986395000	2.496133000
H	-6.777932000	1.171811000	0.743424000
C	-5.400094000	-0.418547000	1.334807000
H	-5.534365000	-0.980394000	0.403473000
C	-5.235428000	-1.434702000	2.476610000
H	-6.118113000	-2.079622000	2.549800000
H	-4.356971000	-2.067541000	2.323095000
H	-5.111149000	-0.918598000	3.434767000
C	-4.162903000	0.428497000	1.193765000
C	-3.915721000	1.682787000	1.737496000
H	-4.605039000	2.282037000	2.311523000
C	-2.600052000	2.006505000	1.377272000
C	-1.808726000	3.251333000	1.707173000
C	-2.712639000	4.291218000	2.403522000
H	-3.559736000	4.539398000	1.749908000
H	-3.131286000	3.858760000	3.322257000
C	-0.633635000	2.920507000	2.660591000
H	-1.023637000	2.444755000	3.570409000
H	0.051312000	2.206423000	2.180623000
C	-1.228039000	3.895574000	0.425310000
H	-0.562638000	3.183844000	-0.081881000
H	-2.045076000	4.126556000	-0.271170000
C	-0.433313000	5.163833000	0.771051000
H	-0.031137000	5.595241000	-0.154836000
C	0.724071000	4.796678000	1.712590000
H	1.318469000	5.691074000	1.943888000
H	1.388490000	4.072183000	1.224794000
C	0.158875000	4.190707000	3.006902000
H	0.984135000	3.922750000	3.679047000
C	-0.766690000	5.204553000	3.694165000
H	-1.162988000	4.786119000	4.629585000
H	-0.204361000	6.109177000	3.961768000
C	-1.921364000	5.562041000	2.746136000
H	-2.593093000	6.278847000	3.236647000
C	-1.359227000	6.179070000	1.456816000
H	-0.805798000	7.098957000	1.688585000
H	-2.180499000	6.461177000	0.783717000
C	-3.051841000	-4.799359000	-1.206005000
H	-2.883348000	-3.944611000	-1.866743000

H	-2.185834000	-5.464417000	-1.293162000
H	-3.934472000	-5.342175000	-1.561988000
C	-3.513658000	-5.555722000	1.159443000
H	-4.420693000	-6.076087000	0.835580000
H	-2.691012000	-6.278104000	1.119650000
H	-3.647993000	-5.252607000	2.202154000
C	-3.243531000	-4.351937000	0.252265000
H	-4.124556000	-3.700800000	0.289078000
C	-2.057008000	-3.554940000	0.726405000
C	-0.961172000	-3.996164000	1.455282000
H	-0.806885000	-4.988588000	1.851629000
C	-0.109690000	-2.886572000	1.572510000
C	1.210267000	-2.796621000	2.295777000
C	1.895882000	-1.438850000	2.062012000
H	1.241737000	-0.621972000	2.401941000
H	2.096676000	-1.295362000	0.988211000
C	0.986304000	-2.968658000	3.819704000
H	0.494165000	-3.931345000	4.008906000
H	0.301525000	-2.187389000	4.174590000
C	2.170384000	-3.911538000	1.815064000
H	2.336301000	-3.808779000	0.734421000
H	1.703622000	-4.892652000	1.970705000
C	3.506032000	-3.836290000	2.571532000
H	4.166437000	-4.636669000	2.213139000
C	3.253353000	-4.010934000	4.077122000
H	2.804617000	-4.993939000	4.274656000
H	4.205442000	-3.979683000	4.623416000
C	2.322444000	-2.894532000	4.575538000
H	2.134688000	-3.021634000	5.649638000
C	2.977136000	-1.528654000	4.321018000
H	3.924273000	-1.454347000	4.871338000
H	2.329179000	-0.723055000	4.691253000
C	3.230993000	-1.354848000	2.816147000
H	3.682179000	-0.375850000	2.619585000
C	4.162316000	-2.470799000	2.319232000
H	5.127332000	-2.413583000	2.839580000
H	4.368642000	-2.338643000	1.248986000
C	-4.731576000	-1.915412000	-4.414358000
H	-4.143077000	-2.818597000	-4.601668000
H	-5.792077000	-2.182667000	-4.462397000
H	-4.535884000	-1.208882000	-5.228365000
C	-5.236110000	-0.031244000	-2.808870000
H	-6.306896000	-0.254766000	-2.870674000
H	-5.030420000	0.400165000	-1.825359000
H	-5.003535000	0.729264000	-3.562117000
C	-4.403245000	-1.300810000	-3.050682000
H	-4.674515000	-2.030694000	-2.279433000
C	-2.933090000	-1.005461000	-2.915029000
C	-2.021757000	-0.704883000	-3.917859000
H	-2.212597000	-0.690744000	-4.980429000
C	-0.810140000	-0.432869000	-3.263942000
C	0.520950000	-0.090842000	-3.883629000
C	1.580665000	0.259172000	-2.822360000
H	1.713568000	-0.592200000	-2.136289000
H	1.267332000	1.131478000	-2.227799000
C	0.377300000	1.117300000	-4.840463000
H	-0.374236000	0.892536000	-5.608185000
H	0.006134000	1.984803000	-4.278959000
C	1.039822000	-1.301638000	-4.701076000
H	0.297704000	-1.573104000	-5.462873000
H	1.142221000	-2.169384000	-4.036137000
C	2.385884000	-0.972055000	-5.363906000
H	2.726769000	-1.844323000	-5.936847000
C	3.418307000	-0.626391000	-4.280109000
H	3.568852000	-1.485358000	-3.612429000
H	4.390537000	-0.406427000	-4.740777000
C	2.930448000	0.588481000	-3.477593000
H	3.652141000	0.832041000	-2.689747000
C	2.756369000	1.790010000	-4.418837000
H	3.718843000	2.046891000	-4.880713000

H	2.431400000	2.670376000	-3.849088000
C	1.724007000	1.445651000	-5.502788000
H	1.592926000	2.303317000	-6.175337000
C	2.211234000	0.229426000	-6.305681000
H	3.163916000	0.462100000	-6.799693000
H	1.491103000	-0.013286000	-7.098867000
B	-2.801165000	-1.249925000	-0.299018000
N	-3.036134000	0.041517000	0.537196000
N	-2.077767000	1.005056000	0.653032000
N	-1.852310000	-2.239629000	0.438209000
N	-0.657045000	-1.833742000	0.952726000
N	-2.274291000	-0.918301000	-1.726207000
N	-0.976219000	-0.560379000	-1.941580000
Yb	0.161773000	0.284715000	0.045668000
H	-3.858311000	-1.795390000	-0.425330000
C	7.661296000	2.947309000	0.566904000
H	7.734891000	3.138671000	1.645097000
H	8.554226000	2.403509000	0.250724000
H	7.656441000	3.925583000	0.069515000
C	5.093656000	2.844338000	0.637926000
H	4.215774000	2.236320000	0.402483000
H	5.084474000	3.056678000	1.714987000
H	4.991129000	3.810453000	0.126605000

Optimized geometry of TS2'

C	7.656745000	5.435352000	11.780196000
H	8.045819000	4.522578000	11.328045000
H	7.312261000	6.216105000	11.101680000
C	7.750226000	5.654618000	13.092141000
H	5.683603000	4.842426000	14.069670000
C	8.262293000	6.049615000	14.242786000
C	-1.400483000	4.612858000	14.288908000
H	-2.229989000	3.957815000	14.574198000
H	-1.181165000	5.255898000	15.148312000
H	-1.736609000	5.250672000	13.465773000
C	-0.179237000	3.778508000	13.893550000
H	-0.473935000	3.120494000	13.066787000
C	0.276140000	2.888561000	15.062130000
H	-0.538770000	2.231958000	15.387104000
H	1.130130000	2.266203000	14.781008000
H	0.579596000	3.503367000	15.916294000
C	0.953834000	4.643642000	13.411977000
C	1.223875000	5.970290000	13.716923000
H	0.619463000	6.629390000	14.321894000
C	2.432875000	6.271258000	13.068747000
C	3.137593000	7.601962000	12.989021000
C	2.262365000	8.588424000	12.174036000
H	2.085109000	8.172588000	11.173483000
H	1.280168000	8.687141000	12.654054000
C	3.365036000	8.198167000	14.397944000
H	2.403139000	8.294412000	14.918159000
H	3.980953000	7.506198000	14.985256000
C	4.508527000	7.479632000	12.296385000
H	5.145199000	6.808439000	12.896895000
H	4.373569000	7.050579000	11.291336000
C	5.188911000	8.852708000	12.185041000
H	6.160377000	8.735088000	11.687025000
C	5.402395000	9.424343000	13.594882000
H	5.906341000	10.398500000	13.534378000
H	6.054979000	8.757087000	14.171717000
C	4.043582000	9.573761000	14.295476000
H	4.192508000	9.976757000	15.305768000
C	3.155245000	10.530012000	13.484082000
H	2.186996000	10.663762000	13.985228000
H	3.623398000	11.521984000	13.425503000
C	2.943201000	9.961151000	12.072601000
H	2.303493000	10.639331000	11.492553000
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H	4.790644000	10.784440000	11.272321000

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C	1.188741000	-0.664604000	11.104295000
H	1.350191000	0.125803000	10.366073000
H	1.930370000	-1.449326000	10.919302000
H	0.193191000	-1.092223000	10.940819000
C	1.070822000	-1.240141000	13.560492000
H	0.063605000	-1.650516000	13.434021000
H	1.778393000	-2.066453000	13.431762000
H	1.164060000	-0.872312000	14.586571000
C	1.320643000	-0.126805000	12.538342000
H	0.550444000	0.638490000	12.682524000
C	2.665311000	0.519974000	12.742888000
C	3.830700000	-0.065354000	13.213400000
H	3.948564000	-1.080246000	13.562219000
C	4.815331000	0.932554000	13.141660000
C	6.268487000	0.800385000	13.521417000
C	7.096203000	2.027773000	13.097884000
H	6.705885000	2.930454000	13.600227000
H	7.017252000	2.155573000	12.004790000
C	6.404740000	0.638625000	15.056355000
H	5.815205000	-0.226635000	15.385996000
H	5.981226000	1.522535000	15.549270000
C	6.872526000	-0.453067000	12.841481000
H	6.776345000	-0.357664000	11.751547000
H	6.300274000	-1.343564000	13.130480000
C	8.345628000	-0.630746000	13.236633000
H	8.745640000	-1.525850000	12.742383000
C	8.448021000	-0.792408000	14.761305000
H	7.896170000	-1.686063000	15.083000000
H	9.495746000	-0.941632000	15.055176000
C	7.878905000	0.457745000	15.450135000
H	7.948309000	0.342783000	16.539759000
C	8.678426000	1.692548000	15.009289000
H	9.731451000	1.587403000	15.303625000
H	8.291908000	2.591133000	15.505951000
C	8.573760000	1.852160000	13.484702000
H	9.132505000	2.743308000	13.172213000
C	9.146084000	0.604341000	12.796839000
H	10.205803000	0.481611000	13.058349000
H	9.097971000	0.715948000	11.704855000
C	-0.249310000	2.428158000	7.818915000
H	0.284465000	1.522479000	7.515207000
H	-1.319429000	2.199477000	7.851296000
H	-0.100245000	3.186166000	7.042023000
C	-0.531551000	4.206680000	9.588920000
H	-1.611843000	4.023899000	9.606105000
H	-0.226052000	4.557083000	10.578521000
H	-0.334211000	5.012038000	8.872949000
C	0.225698000	2.931213000	9.184856000
H	-0.005943000	2.157855000	9.926256000
C	1.714006000	3.162149000	9.201444000
C	2.552214000	3.442374000	8.133612000
H	2.277674000	3.484385000	7.090226000
C	3.824099000	3.643738000	8.694489000
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H	6.414536000	3.418000000	9.599427000
H	5.998335000	5.146881000	9.488762000
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C	6.800200000	2.940615000	6.333468000
H	7.061497000	2.044675000	5.755496000
C	7.934831000	3.270795000	7.314974000
H	8.110334000	2.422225000	7.990008000
H	8.872078000	3.443221000	6.769581000
C	7.560993000	4.522272000	8.123674000

H	8.366216000	4.759003000	8.830812000
C	7.348969000	5.708009000	7.170744000
H	8.276069000	5.918906000	6.621645000
H	7.104076000	6.613593000	7.742165000
C	6.213451000	5.377672000	6.190204000
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C	6.586588000	4.126556000	5.379978000
H	7.498607000	4.312159000	4.797038000
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N	3.766994000	3.498545000	10.024286000
Yb	5.123984000	4.294014000	12.105064000
H	0.929291000	2.420072000	11.744205000
C	9.652825000	6.656041000	14.191248000
H	10.339510000	6.082081000	14.825872000
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H	6.647413000	5.522970000	15.529401000
H	8.275634000	5.385542000	16.277571000
H	7.567002000	6.980463000	16.040566000

Optimized geometry of Int4'

C	2.898373000	0.954783000	-0.091345000
H	3.362385000	-0.038748000	-0.251944000
H	3.121979000	1.540485000	-0.995196000
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H	3.433525000	0.934780000	2.010496000
C	4.044621000	2.780567000	1.321738000
C	-5.872765000	0.370177000	2.538986000
H	-6.715814000	-0.293960000	2.754400000
H	-5.617319000	0.886783000	3.470684000
H	-6.206075000	1.120481000	1.815697000
C	-4.685935000	-0.438635000	2.007966000
H	-5.019545000	-0.978223000	1.113214000
C	-4.231250000	-1.481925000	3.041673000
H	-5.060913000	-2.147106000	3.305231000
H	-3.408451000	-2.092822000	2.660865000
H	-3.887789000	-0.989155000	3.957723000
C	-3.543079000	0.454474000	1.604962000
C	-3.249763000	1.737124000	2.044655000
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C	-2.060834000	2.104212000	1.393034000
C	-1.346210000	3.430520000	1.465908000
C	-2.354127000	4.559871000	1.128097000
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H	-3.202055000	4.514065000	1.823173000
C	-0.797692000	3.682546000	2.891681000
H	-1.618949000	3.621019000	3.617877000
H	-0.081701000	2.892032000	3.152774000
C	-0.172505000	3.516695000	0.470641000
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H	-0.534896000	3.320095000	-0.547431000
C	0.497157000	4.898352000	0.543022000
H	1.325665000	4.926898000	-0.174256000
C	1.039783000	5.116520000	1.963147000
H	1.545352000	6.089269000	2.027419000
H	1.787023000	4.346778000	2.191528000
C	-0.118560000	5.059063000	2.969783000
H	0.266457000	5.210788000	3.986473000
C	-1.141223000	6.155688000	2.634265000
H	-1.967379000	6.140346000	3.358313000
H	-0.669588000	7.144447000	2.709590000
C	-1.680963000	5.936506000	1.212379000

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C	-0.734057000	-4.125254000	1.289870000
H	-0.616666000	-5.153649000	1.596360000
C	0.151974000	-3.060804000	1.519340000
C	1.465055000	-3.128666000	2.259042000
C	2.105152000	-1.743384000	2.462791000
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H	2.314526000	-1.273834000	1.490301000
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C	3.791455000	-4.143206000	2.246098000
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C	3.532390000	-4.776573000	3.622000000
H	3.112466000	-5.784523000	3.502038000
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C	2.562753000	-3.891131000	4.419970000
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C	4.404151000	-2.747603000	2.433028000
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H	-6.049059000	-1.326602000	-3.974534000
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H	-4.743255000	1.335668000	-2.912495000
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H	-4.666347000	-1.571507000	-1.957264000
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H	1.813372000	0.243216000	-2.417618000
C	0.588869000	1.110520000	-4.719594000
H	-0.300858000	1.275410000	-5.341099000
H	0.560799000	1.864261000	-3.921251000
C	0.563475000	-1.345268000	-5.239904000
H	-0.323169000	-1.224833000	-5.874980000
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C	1.836087000	-1.181899000	-6.084286000
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C	3.059722000	-0.345235000	-4.064569000
H	3.931243000	-0.489445000	-3.414548000
C	3.096827000	1.066576000	-4.669292000
H	4.015032000	1.200060000	-5.256468000
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C	1.863800000	1.273371000	-5.561692000
H	1.883100000	2.283027000	-5.992069000
C	1.869470000	0.230018000	-6.689749000
H	2.766629000	0.352783000	-7.310806000
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B	-2.498834000	-1.176665000	-0.166943000
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Yb	0.504062000	0.135784000	-0.042095000
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C	4.287658000	3.787087000	0.231260000
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H	4.007044000	3.406147000	-0.754439000
H	3.734438000	4.723398000	0.397365000
C	4.544954000	3.188911000	2.682524000
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H	5.625363000	3.400446000	2.668821000
H	4.064245000	4.109071000	3.049650000

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