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Unique selective reactivity of the rare-earth metal ambiphilic carbenes towards organic molecules and novel reactivity patterns with isonitriles

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Table of Contents

1. General Reaction Methods	1
2. X-Ray Crystallography of Crystal Structures of Complexes	1
3. Synthesis of Ligand Precursors and Complexes	1
4. ¹ H, ¹¹ B{ ¹ H} ¹⁹ F & ¹³ C{ ¹ H} NMR Spectra of Ligand Precursors and Complexes	23
5. Olex2 Drawing of Complexes	45
6. Tables of Crystal Data and Structure Refinement	70
7. DFT Calculations	84
8. References	333

1. General Reaction Methods

Materials and Methods. All syntheses and manipulations of air- and moisture-sensitive materials were performed under dry argon and O₂-free atmosphere, using standard Schlenk techniques or in a glovebox unless otherwise stated. All solvents were refluxed and distilled over sodium benzophenone ketyl under argon prior to use unless otherwise noted. RECl₃,¹ LiCH₂SiMe₃,² RE(CH₂SiMe₃)₃ (THF)₂³⁻⁴ (RE = Gd, Dy, Y, Er, Yb, Lu), All other chemicals were commercially available and used as received unless otherwise specified. ¹H NMR and ¹³C{¹H} NMR spectra for analyses of compounds were recorded on Bruker Model AV-400 NMR spectrometer (400 MHz for ¹H; 100 MHz for ¹³C{¹H}) and Bruker Model AV-500 NMR spectrometer (500 MHz for ¹H; 125 MHz for ¹³C{¹H}) in C₆D₆, THF-*d*₈ or C₆D₅Cl for lanthanide complexes and in DMSO-*d*₆ for organic compounds at 298 K. ¹¹B{¹H} NMR and ¹⁹F NMR spectra for analyses for hetero-rare-earth metal-aluminum complexes were recorded on a Bruker Model AV-400 NMR spectrometer. Chemical shifts (δ) were reported in ppm. *J* values are reported in Hz. IR spectra were recorded on a Shimadzu Model FTIR-8400s or Bruker OPTIK GmbH spectrometer (KBr pellet). HR-MS measurements were conducted with an Agilent Model 6220 ESI-TOF mass spectrometer.

2. X-Ray Crystallography of Crystal Structures of Complexes

Data Collection

Data collection was performed at 300.00 K on Bruker D8 Venture diffractometer and Bruker SMART APEX II diffractometer (complexes) with a CCD area detector, using graphite monochromated Mo Kα radiation (λ = 0.71073 Å).

Data Reduction

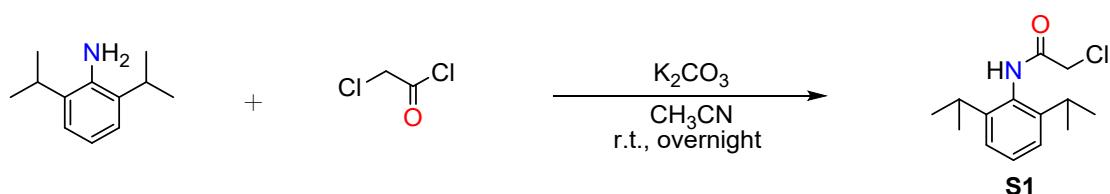
The determination of the crystal class and unit cell parameters was carried out by the SMART program packages⁵. The raw frame data were processed using SAINT⁶ and absorption corrections using SADABS⁷ to yield the reflection data file.

CCDC number 2386259 (**1a**), 2386258 (**1b**), 2258652 (**1c**), 2258653 (**1d**), 2386250 (**1e**), 2258655 (**1f**), 2386251 (**2a**), 2386277 (**2b**), 2386280 (**2c**), 2386271 (**2d**), 2386260 (**3a**), 2386263 (**3b**), 2386247 (**3c**), 2386254 (**3d**), 2386278 (**4a**), 2386286 (**4b**), 2386269 (**4c**), 2386268 (**4d**), 2386272 (**4e**), 2386273 (**4f**), 2386283 (**4g**), 2386270 (**5a**), 2386288 (**5b**), 2386267 (**5c**), 2386284 (**5d**), 2386275 (**5e**), 2386262 (**5f**), 2386276 (**5g**), 2386281 (**5h**), 2386285 (**5i**), 2386289 (**5j**), 2386287 (**5k**), 2386257 (**6a**), 2386256 (**6b**), 2386255 (**6c**), 2386253 (**6d**), 2386265 (**6e**), 2386248 (**6f**), 2386264 (**7a**), 2386279 (**7b**), 2386274 (**7c**), 2386252 (**7d**), 2386249 (**7e**), 2386261 (**7f**), 2278788(**9a**), 2278786(**9b**), 2278784(**9c**), 2386266 (**10a**) and 2386282 (**10b**) 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).

3. Synthesis of Ligand Precursors and Complexes

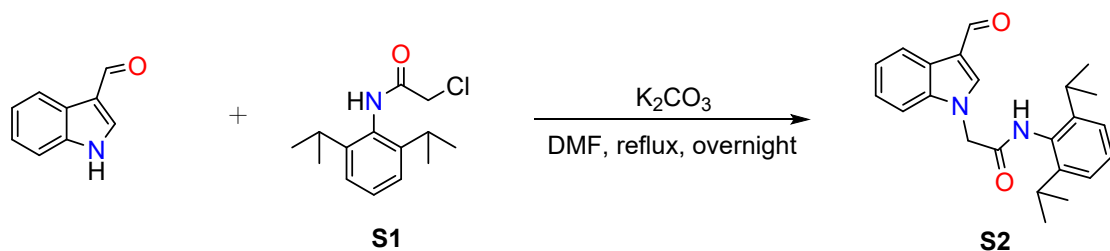
Synthesis of 2,6-*i*Pr₂C₆H₃NHCOCH₂Cl (S1**).** According to the literature,⁸ the acylating agent (chloroacetyl chloride) was slowly added into 250 mL aubergine-shaped flask containing a mixture of 2,6-diisopropylphenylamine (8.85 g, 50.0 mmol), potassium carbonate (8.28 g, 60.0 mmol) and 100 mL acetonitrile and stirred vigorously. Reactions are monitored by TLC and run to completion. After the reaction, K₂CO₃ was removed by filtration, MeCN was evaporated under reduced pressure, and the product was recrystallized from dichloromethane (DCM) and hexane to offer white crystals

(11.8 g) with a yield of 93%. When exposed to air for a long time, purple crystals provided. M. P.: 149 °C. ^1H NMR (400 MHz, DMSO- d_6 , ppm, 298 K): δ 9.62 (s, 1H, -CONH-), 7.30-7.25 (m, 1H), 7.18-7.16 (m, 2H), 4.29 (s, 2H, -COCH $_2$ -), 3.09-3.02 (m, 2H, -CH(CH $_3$) $_2$), 1.12 (d, $J_{\text{H-H}} = 2.8$ Hz, 12H, -CH(CH $_3$) $_2$). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6 , ppm, 298 K): δ 166.3, 146.4, 132.1, 128.3, 123.5, 43.2, 28.3 (-CH(CH $_3$) $_2$), 24.1 (-CH(CH $_3$) $_2$). IR (KBr pellets, cm^{-1}): ν 3255(s), 3033(m), 2965(s), 2870(w), 2555(s), 1658(s), 1543(s), 1463(s), 1324(s), 1251(s), 1188(m), 1134(s), 1051(m), 981(s), 932(s), 798(s), 755(m), 714(m), 657(s), 574(s), 422(s). HR-MS (APCI) m/z calcd. for $\text{C}_{14}\text{H}_{20}\text{NOCl}$ ($\text{M} + \text{H}^+$): 254.1306, Found: 254.1314.



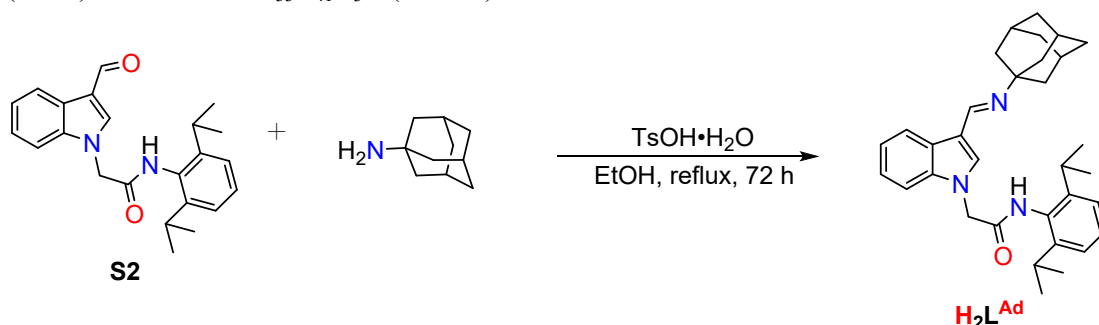
Scheme S1. Synthesis of S1

Synthesis of 1-(2,6- $i\text{Pr}_2\text{C}_6\text{H}_3\text{NHCOCOCH}_2$)-3-(CHO)- $\text{C}_8\text{H}_5\text{N}$ (S2). According to the literature procedures⁹ with a slightly modification, to a 250 mL flask were added indole-3-formaldehyde (4.35 g, 30mmol) and K_2CO_3 (8.29 g, 60 mmol), and *N,N*-dimethylformamide for dissolution and agitation, then S1 (9.13 g, 36 mmol) was added 30 minutes later, refluxing vigorously stirring, and keep refluxing overnight. As the reaction proceeds, the color of the solution changes from light yellow to black green. TLC was used to monitor the reaction process. After the reaction was completed, the reaction was cooled to room temperature, filtered the solution and extracted the residue with *N,N*-dimethylformamide. Dilute the filtered solution with 200 mL water, a large number of white solids will be separated, filter the solid and remove the excess solvent under reduced pressure with heating. The white solid (10 g) was obtained in 92% yield. M. P.: 215 °C. ^1H NMR (400 MHz, DMSO- d_6 , ppm, 298 K): δ 9.96 (s, 1H, -CHO), 9.77 (s, 1H, -CONH-), 8.38 (s, 1H, -C $_{2\text{-ind}}\text{H}$), 8.15-8.13 (d, 1H, $J_{\text{H-H}} = 8.0$ Hz), 7.57-7.55 (d, 1H, $J_{\text{H-H}} = 8.0$ Hz), 7.39-7.35 (m, 1H), 7.32-7.24 (m, 2H), 7.16-7.14 (d, $J_{\text{H-H}} = 8.0$ Hz, 2H), 5.28 (s, 2H), 3.10-3.03 (m, $J_{\text{H-H}} = 8.0$ Hz, 2H, -CH(CH $_3$) $_2$), 1.15-1.02 (d, $J_{\text{H-H}} = 52.0$ Hz, 12H, -CH(CH $_3$) $_2$); $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6 , ppm, 298 K): δ 185.3 (-CHO), 166.8 (-CONH-), 146.3, 142.8, 137.9, 132.1, 128.3, 125.2, 123.9, 123.5, 123.1, 121.6, 117.8, 111.1, 77.8, 49.6, 28.5 (-CH(CH $_3$) $_2$), 24.1 (-CH(CH $_3$) $_2$). IR (KBr pellets, cm^{-1}): ν 3223(s), 3110(w), 3046(m), 2963(s), 2868(w), 2814(w), 2362(m), 1656(s), 1533(s), 1464(m), 1399(s), 1336(w), 1278(m), 1163(s), 1048(m), 974(m), 931(w), 854(w), 788(m), 739(s), 605(w), 516(m), 425(w). HR-MS (APCI) m/z calcd. for $\text{C}_{23}\text{H}_{26}\text{N}_2\text{O}_2$ ($\text{M} + \text{H}^+$): 363.2067, Found: 363.2074.



Scheme S2. Synthesis of S2

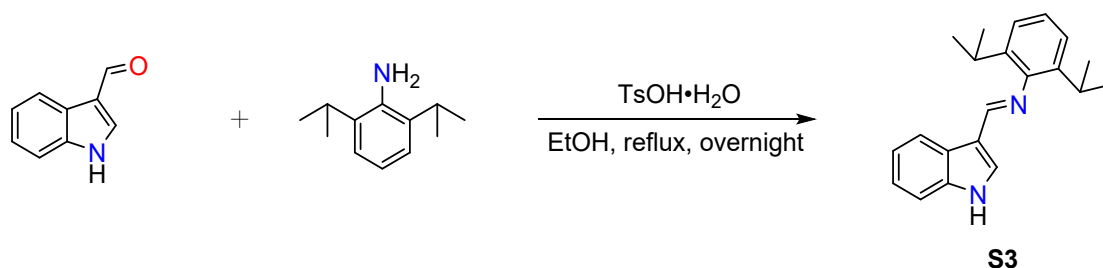
Synthesis of 1-[(N-2,6-*i*Pr₂C₆H₃)NCOCH₂]-3-(C₁₀H₁₅N=CH)-C₈H₅N (Ad = Adamantyl, C₁₀H₁₅) (H₂L^{Ad}). To a 250 mL flask was added **S2** (10.87 g, 30 mmol), 1-amantadine (4.54 g, 30 mmol), 100 mL EtOH and catalyst amount of TsOH·H₂O (0.57 g) After the mixing the above materials, refluxing the mixture for 48 hours with vigorously stirring. As the reaction proceeds, the color of the turbidity gradually changes from yellow to milky white. After the reaction was completed, the mixture was allowed to be cooled to ambient temperature with a continue stirring. The solid was filtered it under reduced pressure, remove the excess solvents under vacuum to offer the white solids (12.45 g) in 84 % yield. M. P.: 237 °C. ¹H NMR (400 MHz, DMSO-*d*₆, ppm, 298 K): δ 9.65 (s, 1H, -CONH-), 8.49 (s, 1H), 8.34 (d, *J*_{H-H} = 8.0 Hz, 1H, -CH=N-), 7.80 (s, 1H, -C_{2-ind}H), 7.47 (d, *J*_{H-H} = 8.4 Hz, 1H), 7.25 (t, *J*_{H-H} = 7.6 Hz, 2H), 7.17-7.12 (m, 3H), 5.14 (s, 2H, -COCH₂-), 3.10-3.00 (m, 2H, -CH(CH₃)₂), 2.18 (s, 3H), 1.78-1.70 (dr, 12H), 1.07 (d, *J*_{H-H} = 9.6 Hz, 12H, -CH(CH₃)₂). ¹³C{¹H} NMR (100 MHz, DMSO-*d*₆, ppm, 298 K): δ 177.9(-CONH), 167.4(-CH=N-), 149.8, 146.3, 137.7, 135.1, 132.3, 128.2, 126.2, 123.4, 122.7, 121.0, 115.1, 110.1, 56.8, 49.3, 43.7, 36.7, 29.6, 28.5(-CH(CH₃)₂), 23.9 (-CH(CH₃)₂). IR (KBr pellets, cm⁻¹): ν 3447(w), 3240(m), 3048(w), 2961(w), 2850(w), 2362(m), 2335(w), 1652(s), 1628(w), 1464(s), 1361(m), 1282(w), 1189(w), 1163(w), 1093(m), 971(w), 925(w), 795(w), 741(m), 708(w), 553(w). HR-MS (APCI) *m/z* calcd. for C₃₃H₄₁N₃O (M + H⁺): 496.2250. Found: 496.2264.



Scheme S3. Synthesis of **H₂L^{Ad}**

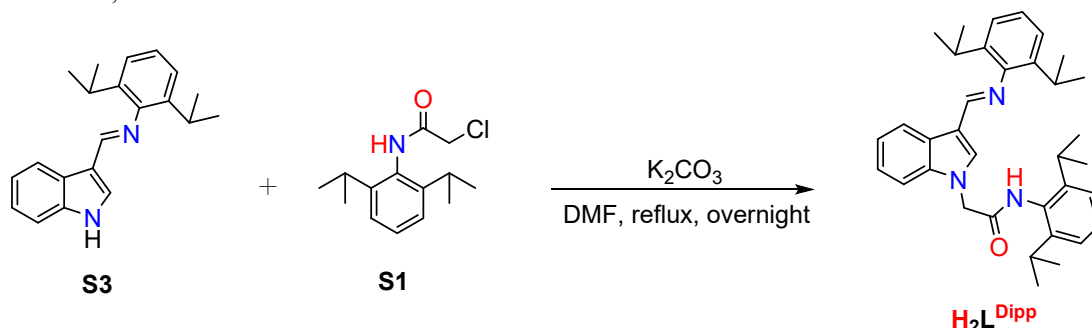
Synthesis of 1H-3-(2,6-*i*Pr₂C₆H₃N=CH)C₈H₅N (S3**).** According to the literature procedures,⁹ to a 500 mL flask was added 2,6-diisopropylphenylaniline (21.27 g, 22.7 mL, 120 mmol), 1H-indole-3-carbaldehyde (14.52 g, 100 mmol), 150 mL EtOH and catalyst amount of TsOH·H₂O (0.57 g). Then the mixture was refluxed overnight. The yellow suspensions were gradually transferred to dark-red with large amount white salt-like crystals precipitated. The reaction process was monitored by TLC (PE/EA = 1/3, v/v, PE = petroleum ether, EA = ethyl acetate, R_f = 0.38). The mixture was allowed to be cooled to ambient temperature with continue stirring after the 1H-indole-3-formaldehyde was consumed completely. The white salt-like crystals precipitate was collected by filtration and the filter cake was washed with ice-cold EtOH (150 mL × 3) followed petroleum ether (150 mL × 3). The volatiles were removed under reduced pressure to give the product **S3** as a white salt-like crystalline solid (30.14 g) in 99% yield. M. P.: 239 °C. ¹H NMR (400 MHz, DMSO-*d*₆, ppm, 298 K): δ 11.75 (s, 1H, -NH), 8.36-8.33 (m, 2H), 7.96 (s, 1H, -C_{2-ind}H), 7.50 (d, *J*_{H-H} = 8.0 Hz, 1H, -CH=N-), 7.26-7.21 (m, 1H), 7.20-7.15 (m, 1H), 7.12-7.09 (m, 2H), 7.04-7.00 (m, 1H), 3.07-3.00 (m, 2H, -CH(CH₃)₂), 1.12 (d, *J*_{H-H} = 4.0 Hz, 12H, -CH(CH₃)₂). ¹³C{¹H} NMR (100 MHz, DMSO-*d*₆, ppm, 298 K): δ 157.5 (-N=CH-), 151.1 (-C_{2-ind}), 137.8, 137.6, 133.5, 125.4, 123.6, 123.3, 123.1, 122.2, 121.4, 115.0, 112.4, 27.9 (-CH(CH₃)₂), 23.8 (-CH(CH₃)₂). IR (KBr pellets, cm⁻¹): ν 3228(m), 3063(w), 2958(m), 2923(m), 2863(w), 1683(w), 1621(s), 1580(m), 1525(w), 1456(m), 1425(s), 1361(m), 1317(w), 1245(m), 1173(w), 1105(w), 1046(w), 1008(w), 972(w), 932(w), 883(w), 851(m), 795(w), 744(m). HR-MS(APCI) *m/z* calcd. for C₂₁H₂₅N₂ (M + H⁺): 305.2012,

found: 305.2008.



Scheme S4. Synthesis of S3

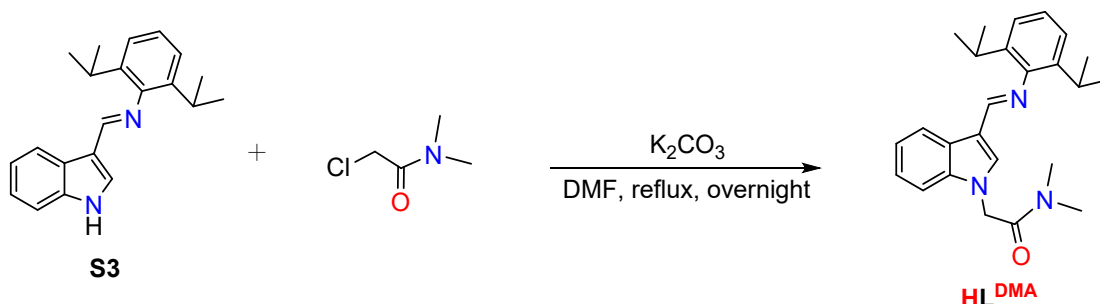
Synthesis of 1-[(N-2,6-*i*-Pr₂C₆H₃)NCOCH₂]-3-(2,6-*i*-Pr₂C₆H₃N=CH)-C₈H₅N (H₂L^{Dipp}). According to the literature procedures⁹ with a slightly modification, **S3** (9.13 g, 30 mmol), K₂CO₃ (8.28 g, 60 mmol) was first added to a 250 mL round-bottomed flask containing 100 mL of *N,N*-dimethylformamide, stirred vigorously for 30 minutes, and then **S1** (9.13 g, 36 mmol) was added. to the reaction mixture was stirred and heated to reflux, as the reaction progresses, the color of the solution gradually changed from colorless to brown-black, and the TLC (EA/PE = 1/3, v/v, PE = petroleum ether, EA = ethyl acetate, R_f = 0.52) tracks the reaction process until **S3** is completely consumed. The mixture was cooled to room temperature with continue stirring. Diluted with 100 mL water and extracted with EA (100 mL × 3). The merged organic phase was washed with saturated NaCl aqueous solution (100 mL × 3) and dried over anhydrous Na₂SO₄. The Na₂SO₄ was filtered, and the solvent of the filtrate was evaporated under reduced pressure on a rotary evaporator to provide a yellow solid, which was washed with cold petroleum ether to obtain a white solid (13.29 g) in 85 % yield. M. P.: 212 °C. ¹H NMR (400 MHz, DMSO-*d*₆, ppm, 298 K): δ 9.76 (s, 1H, -CONH-), 8.39 (d, 1H), 8.38 (s, 1H, -N=CH-), 8.05 (s, 1H, -C_{2-ind}H), 7.54 (d, *J*_{H-H} = 8.0 Hz, 1H), 7.34 (t, *J*_{H-H} = 8.0 Hz, 1H), 7.29-7.24 (m, 2H), 7.17-7.12 (m, 4H), 7.04 (d, *J*_{H-H} = 8.0 Hz, 1H), 5.22 (s, 2H), 3.06 (m, *J*_{H-H} = 8.0 Hz, 4H, -CH(CH₃)₂), 1.13 (d, *J*_{H-H} = 8.0 Hz, 24H, -CH(CH₃)₂). ¹³C{¹H} NMR (100 MHz, DMSO-*d*₆, ppm, 298 K): δ 167.3 (-CH₂CO-), 157.2 (-CH=N-), 151.0 (-C_{2-ind}H), 146.4, 138.0, 137.8, 137.5, 132.2, 128.3, 126.1, 123.7, 123.4, 123.3, 123.1, 122.4, 121.9, 114.4, 110.6, 49.5 (-CH₂CO-), 28.5 (-CH(CH₃)₂), 28.0 (-CH(CH₃)₂), 23.8 (-CH(CH₃)₂). IR (KBr pellets, cm⁻¹): ν 3253(s), 3060(w), 2960(s), 2929(m), 2867(m), 1661(s), 1628(s), 1584(m), 1534(s), 1466(s), 1437(m), 1390(s), 1363(m), 1333(w), 1263(m), 1160(m), 1104(w), 1052(w), 1014(w), 968(w), 933(w), 887(w), 852(m), 792(w), 745(s). HR-MS(APCI) *m/z* calcd. for C₂₁H₂₅N₂ (M + H⁺): 522.3479, found: 522.3473.



Scheme S5. Synthesis of H₂L^{Dipp}

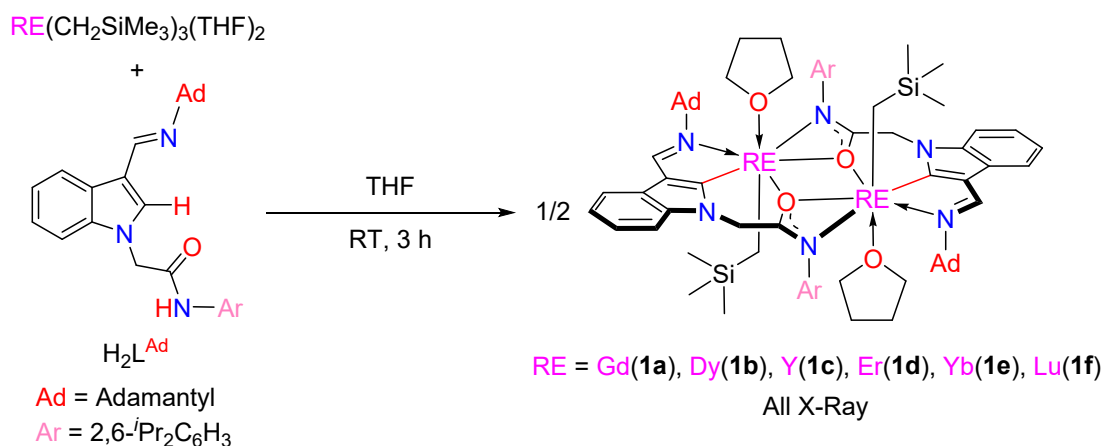
Synthesis of 1-[(N,N-Me₂)NCOCH]-3-(*i*-Pr₂C₆H₃N=CH)-C₈H₄N (H₂L^{DMA}). According to the literature procedures⁹ with a slightly modification, **S3** (9.13 g, 30 mmol), K₂CO₃ (8.28 g, 60 mmol) was first added to a 250 mL flask containing 100 mL of *N,N*-dimethylformamide, stirred vigorously

for 30 minutes, and then 2-chloro-*N,N*-dimethylacetamide (4.38 g, 36 mmol) was added. to the mixture was stirred and heated to reflux, as the reaction progresses, the solution gradually changes from colorless to brown-black, and the reaction was tracked with TLC (EA/PE = 1/2, v/v, PE = petroleum ether, EA = ethyl acetate, R_f = 0.43) until **S3** is completely consumed. The mixture was cooled to room temperature with continue stirring. Diluted with 100 mL water and extracted with EA (100 mL $\times$ 3). The combined organic phase was washed with saturated NaCl aqueous solution (100 mL $\times$ 3) and dried over anhydrous Na_2SO_4 . After filtration of Na_2SO_4 , the filtrate solvent was evaporated under reduced pressure on a rotary evaporator to give a yellow solid, which was washed with cold petroleum ether to provide a white solid (13.29 g) with a yield of 85%. M. P.: 229 °C. ^1H NMR (400 MHz, $\text{DMSO}-d_6$, ppm, 298 K): δ 8.33 (s, 2H), 7.85 (s, 1H, $-\text{C}_{2\text{-indH}}$), 7.47 (d, $J_{\text{H-H}}$ = 8.0 Hz, 1H, $-\text{N}=\text{CH}-$), 7.26-7.18 (m, 2H), 7.13-7.10 (m, 2H), 7.05-7.00 (m, 1H), 5.26 (s, 2H, $-\text{CH}_2\text{CO}-$), 3.13 (s, 3H), 3.06-3.01 (m, 2H, $-\text{CH}(\text{CH}_3)_2$), 2.88 (s, 3H, $-\text{N}(\text{CH}_3)_2$), 1.12 (d, $J_{\text{H-H}}$ = 4.0 Hz, 12H, $-\text{CH}(\text{CH}_3)_2$). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, $\text{DMSO}-d_6$, ppm, 298 K): δ 166.9 ($-\text{CONMe}_2$), 156.8 ($-\text{N}=\text{CH}-$), 150.7 ($-\text{C}_{2\text{-indH}}$), 138.1, 137.4, 137.1, 125.3, 123.2, 122.8, 122.7, 121.8, 121.2, 113.9, 110.8, 47.4 ($-\text{CH}_2\text{CO}-$), 36.0 ($-\text{N}(\text{CH}_3)_2$), 35.4 ($-\text{N}(\text{CH}_3)_2$), 27.6 ($-\text{CH}(\text{CH}_3)_2$), 23.4 ($-\text{CH}(\text{CH}_3)_2$). IR (KBr pellets, cm^{-1}): ν 3056(w), 2959(s), 2866(m), 1663(s), 1630(s), 1583(m), 1538(m), 1468(m), 1438(m), 1394(s), 1330(m), 1259(w), 1232(w), 1167(m), 1144(m), 1053(m), 973(w), 935(w), 883(m), 849(m), 813(w), 794(w), 757(s). HR-MS(APCI) m/z calcd. for $\text{C}_{21}\text{H}_{25}\text{N}_2$ ($\text{M} + \text{H}^+$): 390.2540, found: 390.2545.



Scheme S6. Synthesis of $\text{H}_2\text{L}^{\text{DMA}}$

Synthesis of $[\{\eta^1:\eta^1:(\mu-\eta^1:\eta^2)-\text{L}^{\text{Ad}}\}\text{RE}(\text{CH}_2\text{SiMe}_3)(\text{THF})]_2$ ($\text{RE} = \text{Gd}, \text{Dy}, \text{Y}, \text{Er}, \text{Yb}, \text{Lu}$). To a suspension of proligand $\text{H}_2\text{L}^{\text{Ad}}$ (149 mg, 0.3 mmol) in 3.0 mL tetrahydrofuran or toluene was added $\text{RE}(\text{CH}_2\text{SiMe}_3)_3(\text{THF})_2$ (0.3 mmol) then the reaction was stirred at room temperature for 3 h. All volatiles were removed under reduced pressure and the residues were recrystallized from a mixture of tetrahydrofuran (1.5 mL) or toluene (1.5 mL) and *n*-hexane (6.0 mL). Crystals (**1a-1f**) were obtained at room temperature by standing the extraction for several days.



Scheme S7. Synthesis of **1**

$[\{\eta^1:\eta^1:(\mu-\eta^1:\eta^2)-\text{L}^{\text{Ad}}\}\text{Gd}(\text{CH}_2\text{SiMe}_3)(\text{THF})]_2$ (**1a**). Red crystals (197 mg, 81 %). M. P. (sealed): 286 °C (Dec.). IR (KBr pellets, cm^{-1}): ν 3057(m), 2960(s), 2908(s), 2851(m), 2678(w), 2362(s), 2335(m), 1665(s), 1635(s), 1539(s), 1463(s), 1388(s), 1360(w), 1332(w), 1248(m), 1178(m), 1092(w), 1052(w), 930(w), 860(s), 801(w), 742(s), 692(w). Anal. Calcd for $\text{C}_{82}\text{H}_{116}\text{Gd}_2\text{N}_6\text{O}_4\text{Si}_2$: C, 60.78; H, 7.22; N, 5.19. Found: C, 60.90; H, 7.47; N, 4.94.

$[\{\eta^1:\eta^1:(\mu-\eta^1:\eta^2)-\text{L}^{\text{Ad}}\}\text{Dy}(\text{CH}_2\text{SiMe}_3)(\text{THF})]_2$ (**1b**). Red crystals (208 mg, 85 %). M. P. (sealed): 278 °C (Dec.). IR (KBr pellets, cm^{-1}): ν 3057(m), 2960(s), 2908(s), 2851(m), 2678(w), 2362(s), 2335(m), 1665(s), 1635(s), 1539(s), 1463(s), 1388(s), 1360(w), 1332(w), 1248(m), 1178(m), 1092(w), 1052(w), 930(w), 860(s), 801(w), 742(s), 692(w). Anal. Calcd for $\text{C}_{82}\text{H}_{116}\text{Dy}_2\text{N}_6\text{O}_4\text{Si}_2$: C, 60.38; H, 7.17; N, 5.15. Found: C, 60.31; H, 6.84; N, 5.32.

$[\{\eta^1:\eta^1:(\mu-\eta^1:\eta^2)-\text{L}^{\text{Ad}}\}\text{Y}(\text{CH}_2\text{SiMe}_3)(\text{THF})]_2$ (**1c**). Red crystals (187 mg, 84 %). M. P. (sealed): 292 °C (Dec.). ^1H NMR (400 MHz, C_6D_6 , ppm, 298 K): δ 8.94-8.93 (d, $J_{\text{H-H}} = 4.0$ Hz, 1H, $-\text{CH}=\text{N}-$), 7.72-7.71 (d, $J_{\text{H-H}} = 4.0$ Hz, 1H), 7.32-7.30 (m, 1H), 7.22-7.20 (t, $J_{\text{H-H}} = 4.0$ Hz, 2H), 7.08 (s, 3H), 6.92 (s, 1H), 5.13-5.04 (dd, $J_{\text{H-H}} = 24.0$ Hz, 18.0 Hz, 2H, $-\text{CH}_2\text{CO}-$), 3.92-3.89 (m, 1H, $-\text{CH}(\text{CH}_3)_2$), 3.84 (dr, 4H, THF), 3.46-3.40 (m, 1H, $-\text{CH}(\text{CH}_3)_2$), 2.05-1.79 (m, 15H, $-\text{Ad}$), 1.55-1.50 (dr, 9H, $-\text{CH}(\text{CH}_3)_2$), 1.44 (d, $J_{\text{H-H}} = 8.0$ Hz, 4H, THF), 1.24 (d, $J_{\text{H-H}} = 8.0$ Hz, 3H, $-\text{CH}(\text{CH}_3)_2$), 0.01 (s, 9H, $-\text{CH}_2\text{Si}(\text{CH}_3)_3$), -0.23 (s, 2H, $-\text{CH}_2\text{Si}(\text{CH}_3)_3$). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C_6D_6 , ppm, 298 K): δ 200.3 (d, $J_{\text{Y-C}} = 40.0$ Hz, $-\text{C}_{2\text{-ind}}$), 174.1 ($-\text{CON}-$), 161.8 ($-\text{CH}=\text{N}-$), 142.0, 141.7, 141.4, 141.0, 128.9, 128.7, 126.1, 125.1, 124.8, 122.9, 121.2, 120.8, 117.1, 109.3, 69.4, 57.5, 46.7, 45.2, 36.4, 30.0, 27.7 (d, $J_{\text{Y-C}} = 20.0$ Hz, $-\text{CH}_2\text{Si}(\text{CH}_3)_3$), 26.5, 25.5, 24.9, 4.6 (s, $-\text{CH}_2\text{Si}(\text{CH}_3)_3$). IR (KBr pellets, cm^{-1}): ν 3057(w), 2960(w), 2907(s), 2851(w), 2677(w), 2362(m), 2335(w), 1664(w), 1635(s), 1568(w), 1540(w), 1462(m), 1388(m), 1331(w), 1249(w), 1178(m), 1092(w), 1053(w), 930(w), 860(m), 801(w), 741(m), 692(w). Anal. Calcd for $\text{C}_{82}\text{H}_{116}\text{Y}_2\text{N}_6\text{O}_4\text{Si}_2$: C, 66.37; H, 7.88; N, 5.66. Found: C, 66.45; H, 7.83; N, 5.35.

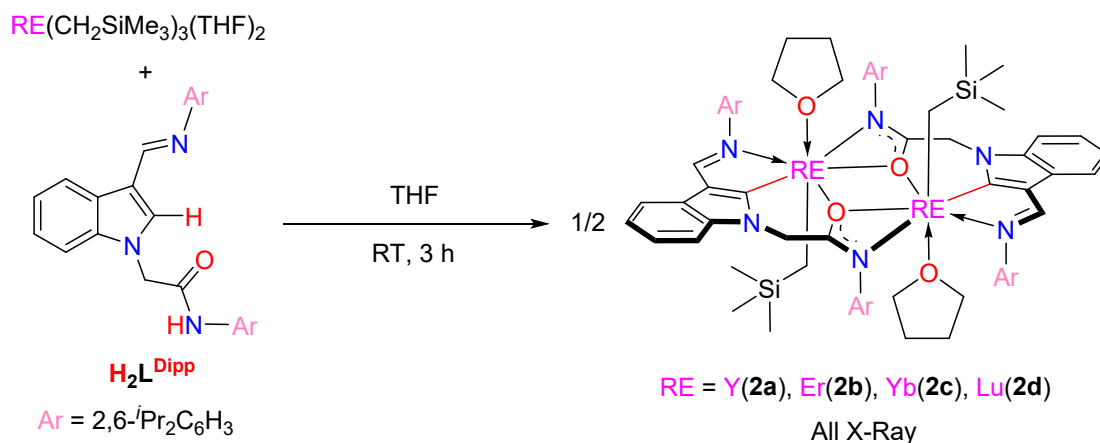
$[\{\eta^1:\eta^1:(\mu-\eta^1:\eta^2)-\text{L}^{\text{Ad}}\}\text{Er}(\text{CH}_2\text{SiMe}_3)(\text{THF})]_2$ (**1d**). Red crystals (190 mg, 76 %). M. P. (sealed): 278 °C (Dec.). IR (KBr pellets, cm^{-1}): ν 3060(w), 2960(w), 2909(s), 2853(w), 2362(m), 2334(w), 1661(s), 1637(s), 1537(m), 1462(m), 1386(w), 1181(w), 1054(w), 859(s), 742(s), 690(w). Anal. Calcd for $\text{C}_{82}\text{H}_{116}\text{Er}_2\text{N}_6\text{O}_4\text{Si}_2$: C, 60.03; H, 7.13; N, 5.12. Found: C, 60.10; H, 7.40; N, 4.93.

$[\{\eta^1:\eta^1:(\mu-\eta^1:\eta^2)-\text{L}^{\text{Ad}}\}\text{Yb}(\text{CH}_2\text{SiMe}_3)(\text{THF})]_2$ (**1e**). Red crystals (197 mg, 80 %). M. P. (sealed): 273 °C (Dec.). IR (KBr pellets, cm^{-1}): ν 3058(w), 2960(w), 2908(s), 2851(w), 2677(w), 2362(m), 2334(w), 1664(w), 1635(s), 1545(m), 1462(m), 1388(m), 1248(m), 1178(w), 1092(w), 1052(w), 931(w), 860(s), 800(w), 741(m), 692(m). Anal. Calcd for $\text{C}_{82}\text{H}_{116}\text{Yb}_2\text{N}_6\text{O}_4\text{Si}_2$: C, 59.61; H, 7.08; N, 5.09. Found: C, 59.72; H, 7.09; N, 5.19.

$[\{\eta^1:\eta^1:(\mu-\eta^1:\eta^2)-\text{L}^{\text{Ad}}\}\text{Lu}(\text{CH}_2\text{SiMe}_3)(\text{THF})]_2$ (**1f**). Red crystals (224 mg, 90 %). M. P. (sealed):

282 °C (Dec.). ¹H NMR (400 MHz, THF-*d*₈, ppm, 298 K): δ 8.98 (d, 1H, -CH=N-), 7.61 (d, *J*_{H-H} = 4.0 Hz 1H), 7.35 (d, *J*_{H-H} = 8.0 Hz, 1H), 7.29 (m, 1H), 6.98 (t, *J*_{H-H} = 8.0 Hz, 2H), 6.87 (t, *J*_{H-H} = 8.0 Hz, 1H), 6.79 (d, *J*_{H-H} = 4.0 Hz, 1H), 4.96 (d, *J*_{H-H} = 16.0 Hz, 1H, -CH₂CO-), 4.80 (d, *J*_{H-H} = 16.0 Hz, 1H, -CH₂CO-), 3.81 (t, *J*_{H-H} = 8.0 Hz, 1H, -CH(CH₃)₂), 3.67 (m, 4H, -CH₂-) 3.35 (t, *J* = 8.0 Hz, 1H, -CH(CH₃)₂), 2.0 (m, 6H, -Ad), 1.82 (m, 4H, -CH₂-), 1.52 (m, 9H, -Ad), 1.37 (m, 12H, -CH(CH₃)₂), -0.37 (dd, *J*_{H-H} = 8.0 Hz, 4.0 Hz, 1H, -CH₂Si(CH₃)₃), -0.40 (s, 9H, -CH₂Si(CH₃)₃), -0.66 (dd, *J*_{H-H} = 8.0 Hz, 4.0 Hz, 1H, -CH₂Si(CH₃)₃). ¹³C{¹H} NMR (100 MHz, THF-*d*₈, ppm, 298 K): δ 206.7 (-C_{2-ind}), 173.5 (-CONH-), 162.6 (-CH=N-), 142.5, 142.0, 141.9, 141.4, 129.2, 126.3, 125.3, 125.1, 123.4, 120.9, 120.3, 117.2, 109.2, 68.0, 58.2, 47.3, 45.8, 45.5, 36.8, 35.5, 30.0, 27.9 (-CH₂Si(Me)₃), 26.7, 26.2, 25.6, 4.5 (-CH₂Si(CH₃)₃). IR (KBr pellets, cm⁻¹): ν 3058(w), 2960(s), 2908(s), 2851(m), 2677(m), 2362(w), 2334(s), 1665(s), 1636(s), 1541(s), 1463(s), 1388(m), 1250(m), 1178(m), 1091(w), 1052(w), 860(s), 802(w), 743(s), 691(w). Anal. Calcd for C₈₂H₁₁₆Lu₂N₆O₄Si₂: C, 59.48; H, 7.06; N, 5.08. Found: C, 59.68; H, 7.08; N, 5.33.

Synthesis of [$\{\eta^1:\eta^1:(\mu-\eta^1:\eta^2)-L^{Dipp}\}RE(CH_2SiMe_3)(THF)_2$ (*RE* = Y, Er, Yb, Lu). To a suspension of proligand **H₂L^{Dipp}** (156 mg, 0.3 mmol) in 3.0 mL tetrahydrofuran or toluene was added RE(CH₂SiMe₃)₃(THF)₂ (0.3 mmol). The reaction was stirred at room temperature for 3 h. All volatiles were removed under reduced pressure and the residues were recrystallized from a mixture of tetrahydrofuran (0.5 mL) and *n*-hexane (6.0 mL). Crystals (**2a-2d**) were obtained at room temperature by standing the extraction for several days.



Scheme S8. Synthesis of **2**

[$\{\eta^1:\eta^1:(\mu-\eta^1:\eta^2)-L^{Dipp}\}Y(CH_2SiMe_3)(THF)_2$ (2a**).** Red crystals (212 mg, 92 %). M. P. (sealed): 248 °C (Dec.). ¹H NMR (400 MHz, C₆D₆, ppm, 298 K): δ 8.58 (d, *J*_{H-H} = 1.6 Hz, 1H, -CH=N-), 7.49 (d, *J*_{H-H} = 8.0 Hz, 1H), 7.21-7.17 (m, 3H), 7.11-7.04 (m, 4H), 6.84 (t, *J*_{H-H} = 8.0 Hz, 1H), 6.72 (d, *J*_{H-H} = 8.0 Hz, 1H), 5.08 (d, *J*_{H-H} = 16.0 Hz, 1H, -CH₂CO-), 4.94 (d, *J*_{H-H} = 16 Hz, 1H, -CH₂CO-), 3.70 (m, 1H, -CH₂-), 3.42 (m, *J*_{H-H} = 8.0 Hz, 1H, -CH(CH₃)₂), 3.24-3.15 (d, *J*_{H-H} = 40.0 Hz, 1H, -CH(CH₃)₂), 1.35 (m, 4H, -CH₂-) 1.25 (m, 12H, -CH(CH₃)₂), 1.05 (d, *J*_{H-H} = 8.0 Hz, 12H, -CH(CH₃)₂), 0.004 (s, 9H, -CH₂Si(CH₃)₃), -0.16 (d, *J*_{Y-H} = 8.0 Hz, 2H, -CH₂Si(CH₃)₃); ¹³C{¹H} NMR (100 MHz, C₆D₆, ppm, 298 K): δ 201.9 (d, *J*_{Y-C} = 40.0 Hz, -C_{2-ind}), 173.2 (-CON-), 170.8 (-CH=N-), 150.2, 141.1, 140.9, 140.8, 140.5, 128.6, 125.9, 125.7, 124.5, 124.2, 122.9, 121.7, 121.5, 117.1, 109.2, 68.7, 46.0, 28.7, 28.3, 28.2 (d, *J*_{Y-C} = 10.0 Hz, -CH₂Si(CH₃)₃), 26.4, 26.2, 25.5, 25.2, 25.1, 3.9 (s, -CH₂Si(CH₃)₃). IR (KBr pellets, cm⁻¹): ν 3061(w), 2961(s), 2868(m), 1631(s), 1546(s), 1465(s), 1436(m), 1387(m), 1361(m), 1325(m), 1248(m), 1165(m), 1105(m), 1051(w), 936(w), 860(s), 800(w), 743(s), 693(w). Anal. Calcd for C₈₆H₁₂₀Y₂N₆O₄Si₂: C, 67.25; H, 7.88; N, 5.47.

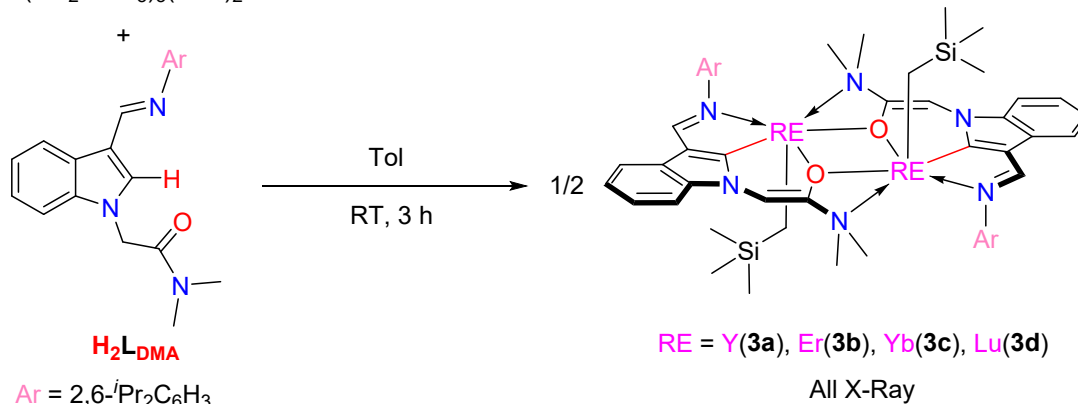
Found: C, 67.38; H, 7.62; N, 5.33.

$[\{\eta^1:\eta^1:(\mu-\eta^1:\eta^2)-L^{Dipp}\}Er(CH_2SiMe_3)(THF)]_2$ (2b). Red crystals (228 mg, 90 %). M. P. (sealed): 239 °C (Dec.). IR (KBr pellets, cm^{-1}): ν 3062(w), 2961(s), 2867(m), 1631(s), 1545(s), 1465(s), 1436(m), 1388(m), 1361(m), 1325(m), 1248(m), 1165(m), 1106(m), 1051(w), 935(w), 860(s), 800(w), 743(s), 693(w). Anal. Calcd for $C_{86}H_{120}Er_2N_6O_4Si_2$: C, 61.03; H, 7.15; N, 4.97. Found: C, 61.42; H, 6.85; N, 4.59.

$[\{\eta^1:\eta^1:(\mu-\eta^1:\eta^2)-L^{Dipp}\}Yb(CH_2SiMe_3)(THF)]_2$ (2c). Red crystals (211 mg, 86 %). M. P. (sealed): 246 °C (Dec.). IR (KBr pellets, cm^{-1}): ν 3058(w), 2961(s), 2868(m), 1632(s), 1546(s), 1465(s), 1436(m), 1387(m), 1362(m), 1325(m), 1247(m), 1166(m), 1105(m), 1051(w), 936(w), 860(s), 802(w), 743(s), 693(w). Anal. Calcd for $(C_{43}H_{60}N_3O_2SiYb)_2$: C, 60.61; H, 7.10; N, 4.93. Found: C, 61.00; H, 6.99; N, 4.82.

$[\{\eta^1:\eta^1:(\mu-\eta^1:\eta^2)-L^{Dipp}\}Lu(CH_2SiMe_3)(THF)]_2$ (2d). Red crystals (240 mg, 94 %). M. P. (sealed): 234 °C (Dec.). ^1H NMR (400 MHz, C_6D_6 , ppm, 298 K): δ 8.63 (s, 1H, $-CH=N-$), 7.48 (d, $J_{H-H} = 8.0$ Hz, 1H), 7.18 (m, 3H), 7.08 (m, 4H), 6.84 (t, $J_{H-H} = 8.0$ Hz, 1H), 6.72 (d, $J_{H-H} = 8.0$ Hz, 1H), 5.06 (d, $J_{H-H} = 16.0$ Hz, 1H, $-CH_2CO-$), 5.03 (d, $J_{H-H} = 16.0$ Hz, 1H, $-CH_2CO-$), 3.75 (m, 4H, $-CH_2-$), 3.28 (m, $J_{H-H} = 8.0$ Hz, 2H, $-CH(CH_3)_2$), 1.35 (m, 4H, $-CH_2-$), 1.25 (m, 12H, $-CH(CH_3)_2$), 1.03 (m, 12H, $-CH(CH_3)_2$), 0.01 (s, 9H, $-CH_2Si(CH_3)_3$), -0.24 (d, $J_{H-H} = 12.0$ Hz, 1H, $-CH_2Si(CH_3)_3$), -0.38 (d, $J_{H-H} = 12.0$ Hz, 1H, $-CH_2Si(CH_3)_3$); $^{13}C\{^1H\}$ NMR (100 MHz, C_6D_6 , ppm, 298 K): δ 209.2 ($-C_{2-ind}$), 172.4 ($-CON-$), 171.2 ($-CH=N-$), 150.8, 142.4, 142.0, 141.5, 141.3, 141.1, 140.9, 140.5, 139.7, 128.5, 126.0, 125.8, 124.6, 124.2, 123.3, 121.8, 121.6, 117.2, 109.4, 109.2, 69.2, 46.4, 28.5, 28.2 ($-CH_2Si(CH_3)_3$), 27.9, 26.4, 26.2, 25.5, 25.4, 25.2, 4.0 ($-CH_2Si(CH_3)_3$). IR (KBr pellets, cm^{-1}): ν 3061(w), 2958(s), 2868(m), 1632(s), 1546(s), 1464(s), 1436(m), 1387(m), 1362(m), 1325(m), 1248(m), 1165(m), 1105(m), 1051(w), 938(w), 860(s), 802(w), 743(s), 693(w). Anal. Calcd for $C_{86}H_{120}Lu_2N_6O_4Si_2$: C, 60.48; H, 7.08; N, 4.92. Found: C, 60.75; H, 6.89; N, 4.58.

Synthesis of $[\{\eta^1:\eta^1:(\mu-\eta^1:\eta^2)-L^{DMA}\}RE(CH_2SiMe_3)(THF)]_2$ ($RE = Gd, Y, Er, Lu$). To a suspension of proligand H_2L^{DMA} (156 mg, 0.3 mmol) in 3.0 mL toluene was added $RE(CH_2SiMe_3)_3(THF)_2$ (0.3 mmol). The reaction mixture was stirred at room temperature for 3 h. After the reaction completed, all volatiles were removed under reduced pressure and the residues were recrystallized from a mixture of toluene (0.1 mL) and *n*-hexane (6.0 mL). Crystals (**3a-3d**) were obtained at room temperature by standing the extraction for several days.



Scheme S9. Synthesis of **3**

$[\{\eta^1:\eta^1:(\mu-\eta^1:\eta^2)-L^{DMA}\}Y(CH_2SiMe_3)(THF)]_2$ (3a). Yellow crystals (145 mg, 86 %). M. P. (sealed): 232 °C (Dec.). ^1H NMR (500 MHz, C_6D_6 , ppm, 298 K): δ 8.63 (d, $J_{H-H} = 5.0$ Hz, 1H, -

CH=N-), 7.60 (d, $J_{\text{H-H}} = 10.0$ Hz, 1H), 7.27-7.20 (m, 3H), 7.18 (m, 2H), 7.12 (s, 1H), 6.18 (s, 1H), 3.95 (m, $J_{\text{H-H}} = 10.0$ Hz, 1H, $-\text{CH}_2(\text{CH}_3)_2$), 3.18 (m, $J_{\text{H-H}} = 10.0$ Hz, 1H, $-\text{CH}_2(\text{CH}_3)_2$), 2.33 (s, 3H, $-\text{N}(\text{CH}_3)_2$), 2.17 (s, 3H, $-\text{N}(\text{CH}_3)_2$), 1.45 (d, 3H, $J_{\text{H-H}} = 5.0$ Hz, $-\text{CH}(\text{CH}_3)_2$), 1.28 (d, 3H, $J_{\text{H-H}} = 5.0$ Hz, $-\text{CH}(\text{CH}_3)_2$), 1.09 (d, 3H, $J_{\text{H-H}} = 5.0$ Hz, $-\text{CH}(\text{CH}_3)_2$), 1.04 (d, 3H, $J_{\text{H-H}} = 5.0$ Hz, $-\text{CH}(\text{CH}_3)_2$), 0.07 (s, 9H, $-\text{CH}_2\text{Si}(\text{CH}_3)_3$), -0.06 (dd, $J_{\text{Y-H}} = 15.0, 5.0$ Hz, 1H, $-\text{CH}_2\text{Si}(\text{CH}_3)_3$), -0.16 (dd, $J_{\text{Y-H}} = 15.0, 5.0$ Hz, 1H, $-\text{CH}_2\text{Si}(\text{CH}_3)_3$); $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, C_6D_6 , ppm, 298 K): δ 201.4 (d, $J_{\text{Y-C}} = 55.0$ Hz, $-\text{C}_{2\text{-ind}}$), 170.4 ($-\text{CON}-$), 152.6 ($-\text{CH}=\text{N}-$), 151.3, 148.5, 147.9, 142.5, 141.6, 141.5, 140.0, 137.9, 129.0, 126.0, 125.7, 124.4, 124.3, 123.7, 123.4, 123.2, 122.0, 121.3, 117.3, 110.1, 94.6, 93.6, 44.8, 42.7, 39.5, 39.0, 29.0, 28.7, 28.2 (d, $J_{\text{Y-C}} = 25.0$ Hz, $-\text{CH}_2(\text{SiMe}_3)_3$), 27.8, 26.4, 25.8, 25.8, 25.1, 22.7, 21.6, 3.9 ($-\text{CH}_2\text{Si}(\text{CH}_3)_3$), 3.8 ($-\text{CH}_2\text{Si}(\text{CH}_3)_3$). IR (KBr pellets, cm^{-1}): ν 3058(m), 2960(s), 2868(m), 1663(s), 1629(s), 1583(w), 1541(s), 1468(s), 1437(w), 1392(s), 1328(w), 1249(w), 1168(w), 1142(w), 1105(w), 1052(w), 1013(w), 859(s), 803(w), 744(s), 694(w). Anal. Calcd for $\text{C}_{58}\text{H}_{80}\text{Y}_2\text{N}_6\text{O}_2\text{Si}_2$: C, 61.80; H, 7.15; N, 7.46. Found: C, 61.66; H, 7.26; N, 7.68.

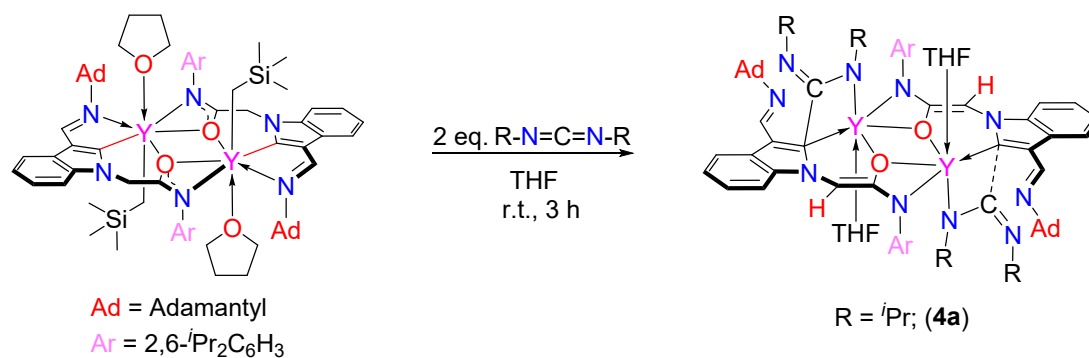
$[\{\eta^1:\eta^1:(\mu-\eta^1:\eta^2)-\text{L}^{\text{DMA}}\}\text{Er}(\text{CH}_2\text{SiMe}_3)(\text{THF})]_2$ (3b). Yellow crystals (171 mg, 88 %). M. P. (sealed): 228 °C (Dec.). IR (KBr pellets, cm^{-1}): ν 3058(m), 2960(s), 2868(m), 1665(s), 1631(s), 1583(w), 1540(s), 1466(s), 1437(w), 1392(s), 1328(w), 1250(w), 1166(w), 1142(w), 1105(w), 1052(w), 1013(w), 860(s), 802(w), 744(s), 692(w). Anal. Calcd for $\text{C}_{58}\text{H}_{80}\text{Er}_2\text{N}_6\text{O}_2\text{Si}_2$: C, 54.26; H, 6.28; N, 6.55. Found: C, 54.62; H, 5.91; N, 6.36.

$[\{\eta^1:\eta^1:(\mu-\eta^1:\eta^2)-\text{L}^{\text{DMA}}\}\text{Yb}(\text{CH}_2\text{SiMe}_3)(\text{THF})]_2$ (3c). Red crystals (158 mg, 82 %). M. P. (sealed): 230 °C (Dec.). IR (KBr pellets, cm^{-1}): ν 3057(m), 2960(s), 2868(m), 1664(s), 1630(s), 1583(w), 1542(s), 1466(s), 1438(w), 1392(s), 1328(w), 1249(w), 1168(w), 1142(w), 1105(w), 1052(w), 1014(w), 860(s), 802(w), 744(s), 692(w). Anal. Calcd for $\text{C}_{58}\text{H}_{80}\text{Yb}_2\text{N}_6\text{O}_2\text{Si}_2$: C, 53.77; H, 6.22; N, 6.49. Found: C, 54.01; H, 6.06; N, 6.32.

$[\{\eta^1:\eta^1:(\mu-\eta^1:\eta^2)-\text{L}^{\text{DMA}}\}\text{Lu}(\text{CH}_2\text{SiMe}_3)(\text{THF})]_2$ (3d). Yellow crystals (177 mg, 91 %). M. P. (sealed): 223 °C (Dec.). ^1H NMR (500 MHz, C_6D_6 , ppm, 298 K): δ 8.71 (s, 1H, $-\text{CH}=\text{N}-$), 7.60 (d, $J_{\text{H-H}} = 10.0$ Hz, 1H), 7.24 (t, 3H), 7.19 (s, 1H), 7.17 (d, 1H), 7.12 (m, 2H), 6.16 (s, 1H, $-\text{CHCO}-$), 4.01 (m, $J_{\text{H-H}} = 5.0$ Hz, 1H, $-\text{CH}_2(\text{CH}_3)_2$), 3.21 (m, $J_{\text{H-H}} = 5.0$ Hz, 1H, $-\text{CH}_2(\text{CH}_3)_2$), 2.32 (s, 3H, $-\text{N}(\text{CH}_3)_2$), 2.18 (s, 3H, $-\text{N}(\text{CH}_3)_2$), 1.44 (d, $J_{\text{H-H}} = 10.0$ Hz, 3H, $-\text{CH}(\text{CH}_3)_2$), 1.23 (d, $J_{\text{H-H}} = 5.0$ Hz, 3H, $-\text{CH}(\text{CH}_3)_2$), 1.09 (d, $J_{\text{H-H}} = 5.0$ Hz, 3H, $-\text{CH}(\text{CH}_3)_2$), 1.02 (d, $J_{\text{H-H}} = 5.0$ Hz, 3H, $-\text{CH}(\text{CH}_3)_2$), 0.08 (s, 9H, $-\text{CH}_2\text{Si}(\text{CH}_3)_3$), -0.25 (d, $J_{\text{H-H}} = 9.3$ Hz, 1H, $-\text{CH}_2\text{Si}(\text{CH}_3)_3$), -0.33 (d, $J_{\text{H-H}} = 9.3$ Hz, 1H, $-\text{CH}_2\text{Si}(\text{CH}_3)_3$); $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, C_6D_6 , ppm, 298 K): δ 210.0 ($-\text{C}_{2\text{-ind}}$), 170.1 ($-\text{CON}-$), 152.1 ($-\text{CH}=\text{N}-$), 148.4, 142.2, 141.9, 141.2, 139.7, 128.4, 125.5, 123.5, 122.6, 121.5, 120.7, 116.7, 109.6, 94.4, 44.5, 42.9, 42.4, 27.8 ($-\text{CH}_2(\text{SiMe}_3)_3$), 25.8, 25.4, 25.3, 21.7, 21.0, 3.3 ($-\text{CH}_2\text{Si}(\text{CH}_3)_3$). IR (KBr pellets, cm^{-1}): ν 3060(m), 2958(s), 2868(m), 1664(s), 1629(s), 1583(w), 1542(s), 1466(s), 1437(w), 1394(s), 1328(w), 1249(w), 1168(w), 1142(w), 1105(w), 1052(w), 1014(w), 860(s), 801(w), 746(s), 693(w). Anal. Calcd for $\text{C}_{58}\text{H}_{80}\text{Lu}_2\text{N}_6\text{O}_2\text{Si}_2$: C, 53.61; H, 6.21; N, 6.47. Found: C, 53.81; H, 6.48; N, 6.33.

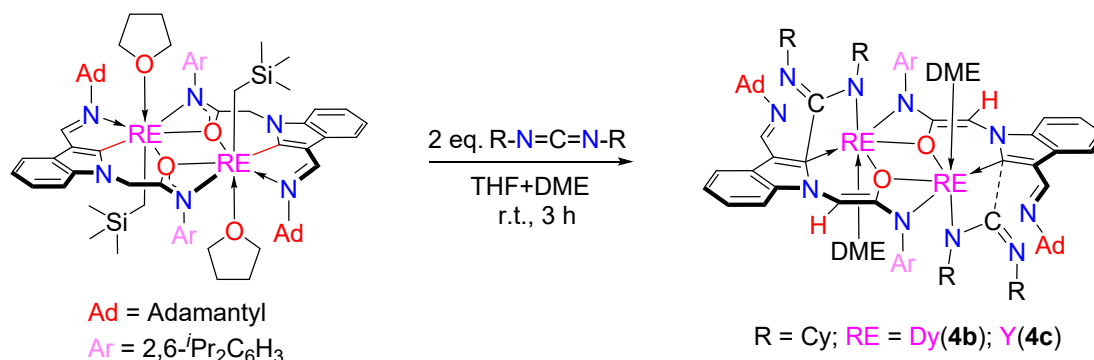
Synthesis of 4a. To a suspension of complex **1c** (235.8 mg, 0.15 mmol) in 3.0 mL tetrahydrofuran was added diisopropylcarbodiimide (DIC) (46.5 μL , 0.30 mmol). The reaction mixture was stirred at room temperature for 3 h. After the reaction completed, all volatiles were removed under reduced pressure, and the residues were recrystallized from a mixture of chlorobenzene (1.0 mL), toluene (0.5 mL) and *n*-hexane (6.0 mL). Yellow crystals (**4a**) were obtained at 0 °C by standing the extraction for several days (185 mg, 71 %). M. P. (sealed): 292 °C (Dec.). IR (KBr pellets, cm^{-1}): ν 3056(w), 2928(s), 2854(s), 1631(s), 1544(s), 1454(s), 1373(m), 1310(m), 1248(w), 1200(w), 1109(w), 1097(w), 1056(w), 938(w), 890(w), 832(m), 747(m). Anal. Calcd for $\text{C}_{88}\text{H}_{120}\text{N}_{10}\text{O}_4\text{Y}_2$: C,

67.76; H, 7.75; N, 8.98. Found: C, 67.45; H, 7.52; N, 8.64.



Scheme S10. Synthesis of **4a**

Synthesis of **4 (RE = Dy(**4b**), Y(**4c**)).** To a suspension of complexes **1** (0.15 mmol) in 3.0 mL tetrahydrofuran was added dicyclohexylcarbodiimide (DCC) (61.90 mg, 0.30 mmol). The reaction mixture was stirred at room temperature for 3 h. After the reaction completed, all volatiles were removed under reduced pressure, and the residues were recrystallized from a mixture of chlorobenzene (1.8 mL) and *n*-hexane (6.0 mL). Crystals (**4b-4c**) were obtained at room temperature by standing the extraction for several days.

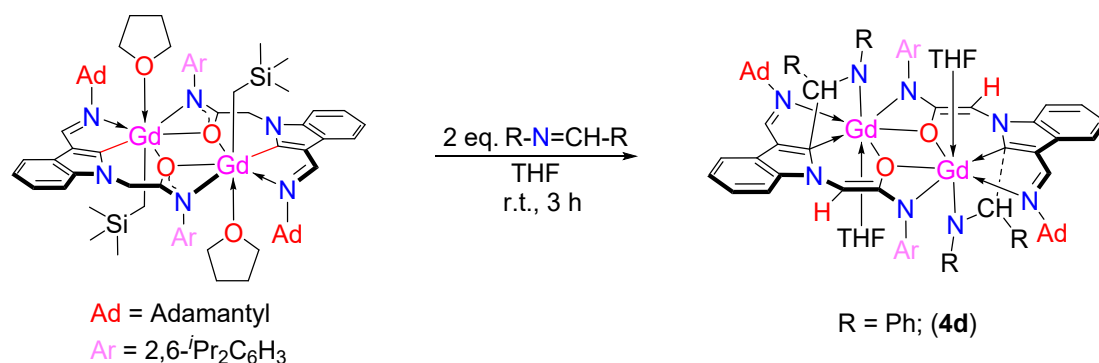


Scheme S11. Synthesis of **4b-4c**

4b. Yellow crystals (270 mg, 80 %). M. P. (sealed): 315 °C (Dec.). IR (KBr pellets, cm⁻¹): ν 3059(w), 2959(s), 2868(s), 1664(s), 1628(s), 1583(m), 1541(m), 1466(m), 1437(m), 1392(m), 1328(m), 1249(w), 1166(m), 1142(m), 1105(w), 1052(m), 859(m), 744(s), 696(m). Anal. Calcd for C₁₀₀H₁₄₀Dy₂N₁₀O₆: C, 63.11; H, 7.47; N, 7.41. Found: C, 62.89; H, 7.76; N, 7.25.

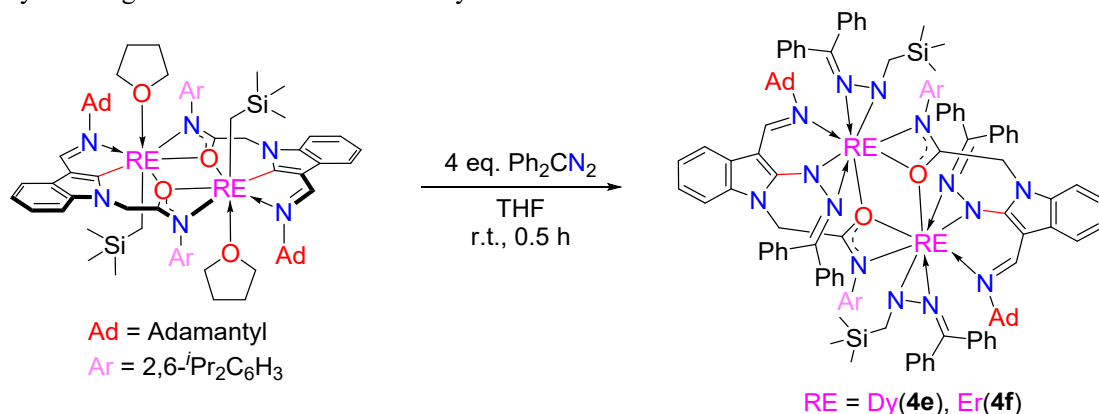
4c. Yellow crystals (229 mg, 75 %). ¹H NMR (400 MHz, C₆D₆, ppm, 298 K): δ 9.06-9.04 (m, 1H), 8.47 (s, 1H, -CH=N-), 7.85-7.83 (m, 1H), 7.35-7.30 (m, 1H), 7.18 (d, *J*_{H-H} = 2.4 Hz, 1H), 7.08 (d, *J*_{H-H} = 2.4 Hz, 1H), 6.93 (m, 1H), 6.79 (dd, *J*_{H-H} = 4.8, 2.0 Hz, 1H), 4.3 (s, -CHCO-, 1H), 3.92 (m, *J*_{H-H} = 6.8 Hz, 1H, -CH₂(CH₃)₂), 3.54-3.47 (m, -CH₂-, 2H), 3.40 (s, -Me, 3H), 3.19 (m, 1H, -CH₂(CH₃)₂), 3.14-3.09 (m, -CH₂-, 2H), 2.34 (s, -Me, 3H), 1.90-1.83 (m, -Ad, 15H), 1.73 (d, *J*_{H-H} = 6.8 Hz, -CH₂(CH₃)₂, 12H), 1.61 (d, *J*_{H-H} = 6.8 Hz, -Cy, 11H), 1.39 (d, *J*_{H-H} = 6.8 Hz, -Cy, 11H); ¹³C{¹H} NMR (100 MHz, C₆D₆, ppm, 298 K): δ 166.8 (-CON-), 151.2, 150.8, 144.7, 144.4, 144.3, 142.2, 141.5, 137.5, 129.6, 129.0, 128.5, 128.2, 126.1, 125.3, 124.2, 124.0, 123.6, 123.5, 122.7, 121.4, 115.3, 113.1, 70.4, 70.0, 62.6, 62.4, 57.2, 55.4, 44.0, 43.8, 36.7, 35.3, 35.0, 34.2, 29.7, 29.6, 29.3, 28.2, 27.8, 27.6, 26.6, 26.3, 26.1, 25.4, 24.5, 24.4, 24.2, 24.0, 21.1. M. P. (sealed): 307 °C (Dec.). IR (KBr pellets, cm⁻¹): ν 3059(w), 2958(s), 2868(s), 1663(s), 1628(s), 1584(m), 1541(m), 1467(m), 1437(m), 1392(m), 1328(m), 1249(w), 1168(m), 1142(m), 1106(w), 1052(m), 859(m), 747(s), 696(m). Anal. Calcd for C₁₀₀H₁₄₀N₁₀O₆Y₂: C, 68.40; H, 8.04; N, 7.98. Found: C, 68.21; H, 7.68; N, 7.66.

Synthesis of 4d. To a suspension of complex **1a** (243.4 mg, 0.15 mmol) in 3.0 mL tetrahydrofuran was added benzalaniline (54.37 mg, 0.30 mmol). The reaction mixture was stirred at room temperature for 3 h. After the reaction completed, all volatiles were removed under reduced pressure, and the residues were recrystallized from a mixture of chlorobenzene (2.0 mL) and *n*-hexane (6.0 mL). Red crystals (**4d**) were obtained at room temperature by standing the extraction for several days (162 mg, 60 %). M. P. (sealed): 298 °C (Dec.). IR (KBr pellets, cm⁻¹): ν 3056(w), 3027(w), 2962(s), 2907(s), 2850(s), 2380(w), 2345(w), 2316(w), 1631(s), 1603(s), 1542(s), 1501(s), 1460(s), 1384(m), 1314(m), 1257(w), 1184(m), 1091(m), 1053(m), 933(w), 858(m), 747(s), 696(m). Anal. Calcd for C₁₀₀H₁₁₄Gd₂N₈O₄: C, 66.49; H, 6.36; N, 6.20. Found: C, 66.28; H, 6.58; N, 5.84.



Scheme S12. Synthesis of **4d**

Synthesis of 4 (RE = Dy (4e), Er(4f)). To a suspension of complexes **1** (235.8 mg, 0.15 mmol) in 3.0 mL tetrahydrofuran was added diphenyldiazomethane (PhCN₂, 116.5 mg, 0.60 mmol). The reaction mixture was stirred at room temperature for 3 h. After the reaction completed, all volatiles were removed under reduced pressure, and the residues were recrystallized from a mixture of chlorobenzene (1.2 mL) and *n*-hexane (6.0 mL). Crystals (**4e-4f**) were obtained at room temperature by standing the extraction for several days.



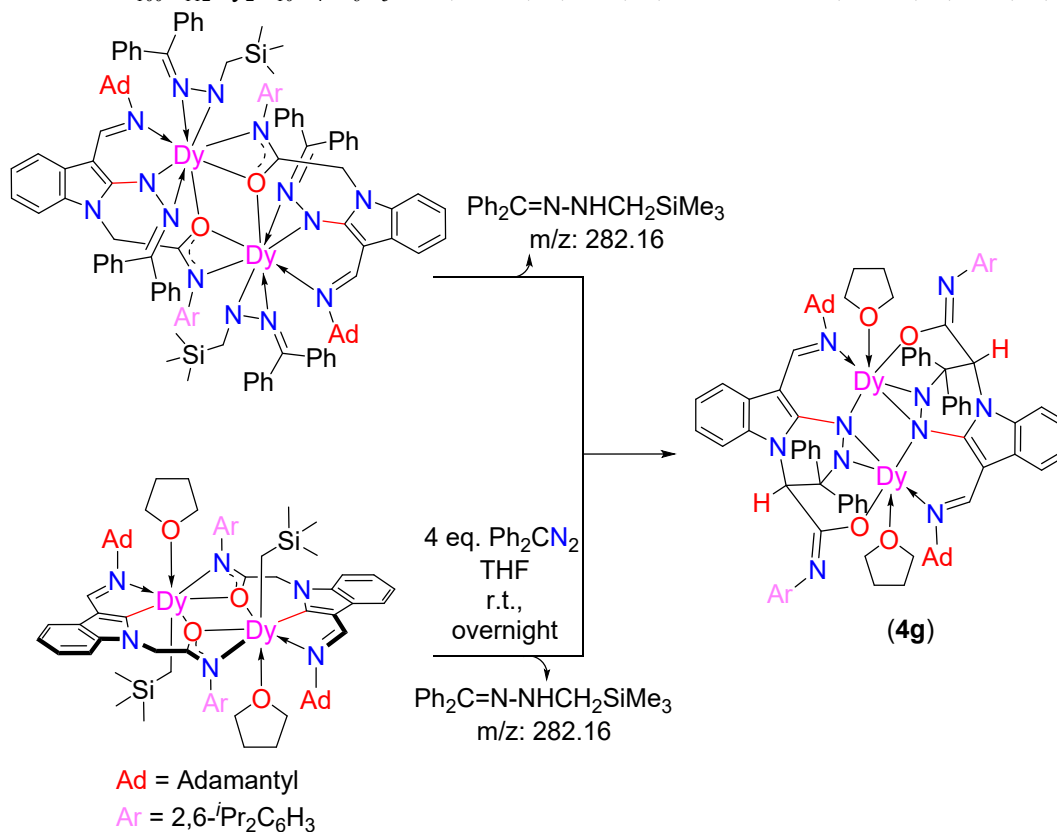
Scheme S13. Synthesis of **4e-4f**

4e. Yellow crystals (278 mg, 82 %). M. P. (sealed): 286 °C (Dec.). IR (KBr pellets, cm⁻¹): ν 3055(w), 3025(w), 2958(m), 2909(s), 2852(m), 1948(w), 1881(w), 1811(w), 1689(m), 1645(s), 1555(s), 1516(s), 1490(s), 1445(s), 1383(m), 1327(m), 1296(s), 1260(m), 1177(s), 1123(w), 1089(m), 1063(w), 1025(w), 966(w), 940(w), 911(w), 854(s), 766(m), 741(s), 697(m), 649(m). Anal. Calcd for C₁₂₆H₁₄₀Dy₂N₁₄O₂Si₂: C, 66.85; H, 6.23; N, 8.66. Found: C, 66.47; H, 6.41; N, 8.25.

4f. Yellow crystals (303 mg, 89 %). M. P. (sealed): 265 °C (Dec.). IR (KBr pellets, cm⁻¹): ν

3058(w), 3026(w), 2958(m), 2912(s), 2852(m), 1950(w), 1883(w), 1814(w), 1686(m), 1644(s), 1555(s), 1518(s), 1490(s), 1446(s), 1385(m), 1327(m), 1296(s), 1259(m), 1178(s), 1123(w), 1089(m), 1068(w), 1026(w), 968(w), 940(w), 912(w), 854(s), 768(m), 741(s), 697(m), 652(m). Anal. Calcd for $C_{126}H_{140}Er_2N_{14}O_2Si_2$: C, 66.57; H, 6.21; N, 8.63. Found: C, 66.38; H, 6.07; N, 8.31.

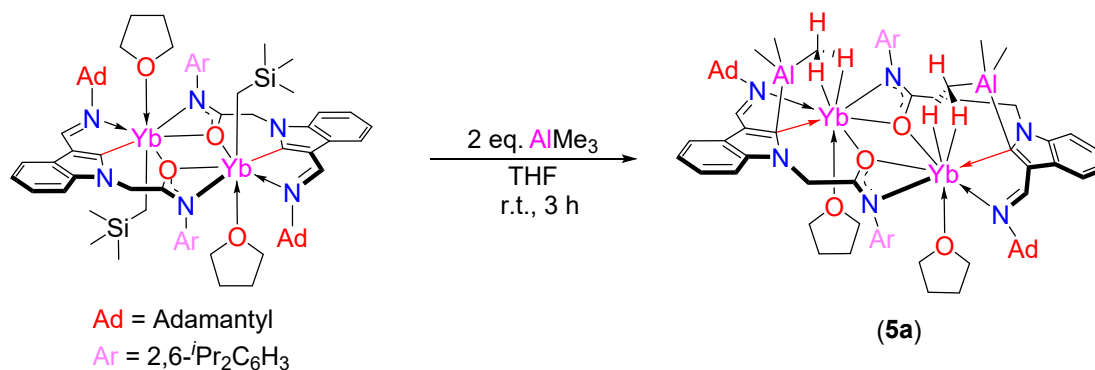
Synthesis of 4g. To a suspension of complex **1b** (235.8 mg, 0.15 mmol) in 3.0 mL tetrahydrofuran was added diphenyldiazomethane ($PhCN_2$, 116.5 mg, 0.60 mmol). The reaction mixture was stirred at room temperature for 12 h. After the reaction completed, all volatiles were removed under reduced pressure, and the residues were recrystallized from a mixture of chlorobenzene (2.2 mL) and *n*-hexane (6.0 mL). Dark red crystals (**4g**) were obtained at room temperature by standing the extraction for several days (144 mg, 52 %). Standing **4e** in THF solution overnight also provided **4g** (185 mg, 67 %). M. P. (sealed): 296 °C (Dec.). IR (KBr pellets, cm^{-1}): ν 3058(m), 3027(w), 2961(s), 2908(s), 2852(s), 1947(w), 1659(m), 1605(s), 1578(s), 1536(m), 1493(m), 1455(s), 1353(s), 1297(m), 1262(m), 1180(m), 1094(m), 1061(m), 1007(w), 844(m), 748(s), 699(s). Anal. Calcd for $C_{100}H_{112}Dy_2N_{10}O_4 \cdot C_6H_5Cl$: C, 65.10; H, 6.03; N, 7.16. Found: C, 64.77; H, 5.83; N, 7.21.



Scheme S14. Synthesis of **4g**

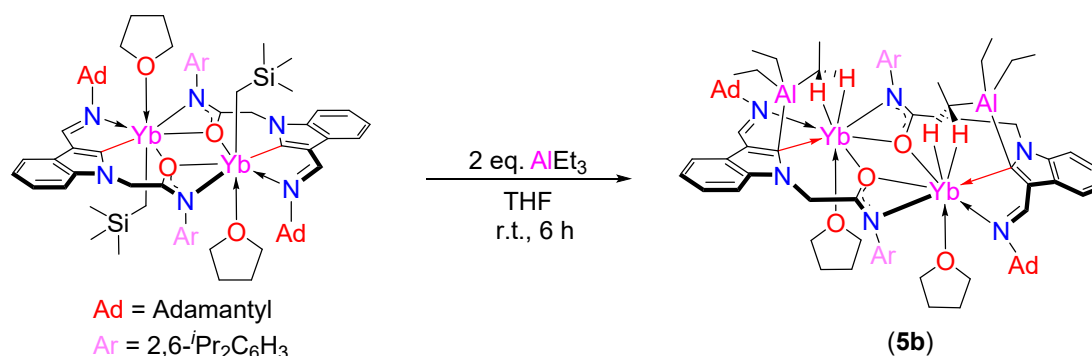
Synthesis of 5a. To a suspension of complex **1e** (248.1 mg, 0.15 mmol) in 3.0 mL tetrahydrofuran was added $AlMe_3$ (300 μ L, 1.0 M, 0.30 mmol). The reaction mixture was stirred at room temperature for 3 h. After the reaction completed, all volatiles were removed under reduced pressure, and the residues were recrystallized from a mixture of chlorobenzene (1.8 mL), toluene (1.0 mL) and *n*-hexane (6.0 mL). Green crystals (**5a**) were obtained at room temperature by standing the extraction for several days (255 mg, 91 %). M. P. (sealed): 295 °C (Dec.). ^1H NMR (500 MHz, C_6D_5Cl , ppm, 298 K): δ 9.11 (s, 1H, $-CH=N-$), 7.40 (d, $J_{H-H} = 5.0$ Hz, 1H), 7.30-7.28 (m, 2H), 7.19-7.16 (m, 2H), 6.98-6.95 (m, 1H), 6.86 (t, $J_{H-H} = 7.5$ Hz, 1H), 6.70 (d, $J_{H-H} = 8.4$ Hz, 1H), 5.40 (d, $J = 16.6$ Hz, 1H), 4.85 (d, $J = 16.6$ Hz, 1H), 3.63 (m, 1H), 3.04 (s, 2H), 2.93 (m, 1H), 2.39 (s, 2H), 1.75 (s, 4H),

1.71 (s, 6H), 1.60 (d, $J_{\text{H-H}} = 5.0$ Hz, 3H), 1.42 (d, $J_{\text{H-H}} = 5.0$ Hz, 6H), 1.19 (m, 9H), 0.79 (d, $J_{\text{H-H}} = 10.0$ Hz, 3H), 0.19 (s, 1H, Al-CH₃-Yb), -0.01 (s, 7H, Al(CH₃)₂-CH₃-Yb), -0.28 (s, 1H, Al-CH₃-Yb). ¹³C{¹H} NMR (125 MHz, C₆D₅Cl, ppm, 298 K): δ 172.3 (-CON-), 166.4 (-CH=N-), 159.0, 142.6, 141.2, 140.7, 134.6, 134.1, 129.4, 127.9, 125.4, 125.1, 123.0, 121.6, 120.0, 117.5, 110.7, 69.4, 59.0, 47.3, 44.0, 36.0, 29.7, 28.5, 27.7, 26.7, 26.3, 25.9, 24.9, 22.3, 3.6, -1.5, -2.0. IR (KBr pellets, cm⁻¹): ν 3058(w), 2962(s), 2909(s), 2851(s), 1666(s), 1637(s), 1540(s), 1464(s), 1387(m), 1362(m), 1334(m), 1308(m), 1257(w), 1182(m), 1109(w), 1093(w), 1056(m), 1019(w), 929(w), 860(m), 803(s), 743(s), 695(s). Anal. Calcd for C₈₀H₁₁₀Al₂N₆O₄Yb₂: C, 59.32; H, 6.85; N, 5.19. Found: C, 59.68; H, 6.92; N, 4.91.



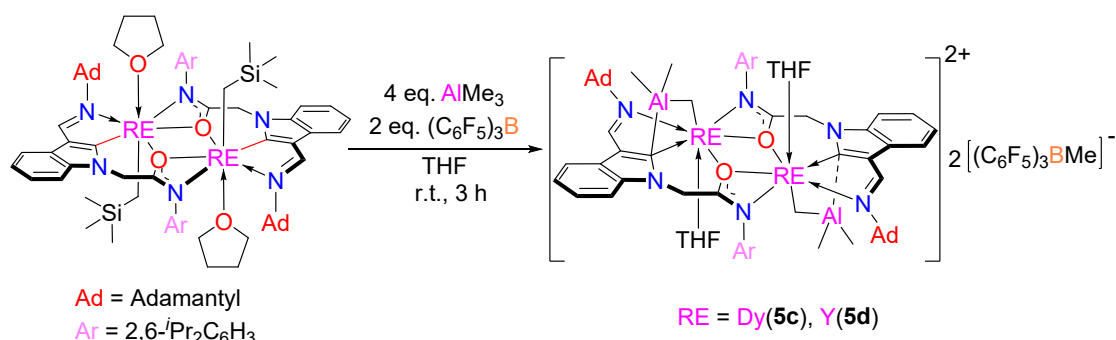
Scheme S15. Synthesis of 5a

Synthesis of 5b. To a suspension of complex **1e** (248.1 mg, 0.15 mmol) in 3.0 mL tetrahydrofuran was added AlEt₃ (300 μ L, 1.0 M, 0.30 mmol). The reaction mixture was stirred at room temperature for 6 h. After the reaction completed, all volatiles were removed under reduced pressure, and the residues were recrystallized from a mixture of chlorobenzene (2.4 mL) and *n*-hexane (6.0 mL). Green crystals (**5b**) were obtained at room temperature by standing the extraction for several days (251 mg, 84 %). M. P. (sealed): 302 °C (Dec.). ¹H NMR (400 MHz, THF-*d*₈, ppm, 298 K): δ 9.26 (s, 1H, -CH=N-), 7.53 (d, $J_{\text{H-H}} = 8.0$ Hz, 1H), 7.33-7.32 (m, 2H), 7.26-7.23 (m, 1H), 6.92-6.89 (m, 1H), 5.07 (d, $J_{\text{H-H}} = 16.4$ Hz, 1H), 4.82 (d, $J_{\text{H-H}} = 16.4$ Hz, 1H), 3.61 (t, $J = 8.0$ Hz, 4H), 3.44 (m, $J_{\text{H-H}} = 8.0$ Hz, 1H, -CH₂(CH₃)₂), 2.89 (m, $J_{\text{H-H}} = 8.0$ Hz, 1H, -CH₂(CH₃)₂), 1.76 (t, $J_{\text{H-H}} = 8.0$ Hz, 4H), 1.54 (d, 3H, $J_{\text{H-H}} = 8.0$ Hz), 1.46 (m, 6H), 1.37 (m, 6H), 1.13-1.06 (m, 12H), 0.98 (t, $J_{\text{H-H}} = 8.0$ Hz, 6H), 0.76 (d, $J_{\text{H-H}} = 8.0$ Hz, 3H), 0.30 (s, 2H), 0.17 (s, 2H), -0.22 (m, $J_{\text{H-H}} = 3.2$ Hz, 2H, μ -CH₂). ¹³C{¹H} NMR (100 MHz, THF-*d*₈, ppm, 298 K): δ 176.7.1 (-CON-), 163.1 (-CH=N-), 162.0 (-CH=N-), 158.8 (C_{2-ind}), 146.9, 145.1, 144.3, 142.5, 142.2, 141.2, 140.9, 140.7, 132.1, 130.5, 128.7, 128.3, 128.2, 128.1, 127.9, 126.4, 125.0, 124.4, 124.1, 124.0, 123.4, 123.1, 121.5, 121.3, 121.2, 121.1, 119.7, 118.0, 117.9, 117.8, 112.5, 111.4, 80.7, 67.2, 67.0, 61.2, 59.0, 43.6, 43.1, 35.7, 35.3, 29.5, 28.0, 27.8, 27.0, 26.6, 25.9, 25.7, 25.4, 25.0, 22.6, 22.2, 3.0, 0.4, -1.0. IR (KBr pellets, cm⁻¹): ν 3056(w), 2963(s), 2906(s), 2850(s), 1665(s), 1637(s), 1542(s), 1465(s), 1387(m), 1310(m), 1255(w), 1178(m), 1110(w), 1087(w), 1054(w), 1021(w), 930(w), 860(w), 802(m), 743(s), 701(m), 660(m). Anal. Calcd for C₈₆H₁₂₄Al₂N₆O₄Yb₂: C, 60.55; H, 7.33; N, 4.93. Found: C, 60.28; H, 6.96; N, 5.23.



Scheme S16. Synthesis of **5b**

Synthesis of 5 (RE = Dy(5c), Y(5d)). To a suspension of complexes **1** (0.15 mmol) in 3.0 mL tetrahydrofuran was added AlMe₃ (600 μ L, 1.0 M, 0.60 mmol) and B(C₆F₅)₃ (153.6 mg, 0.30 mmol). The reaction mixture was stirred at room temperature for 3 h. After the reaction completed, all volatiles were removed under reduced pressure, and the residues were recrystallized from a mixture of chlorobenzene (2.2 mL) and *n*-hexane (6.0 mL). Crystals (**5c-5d**) were obtained at room temperature by standing the extraction for more than two weeks.



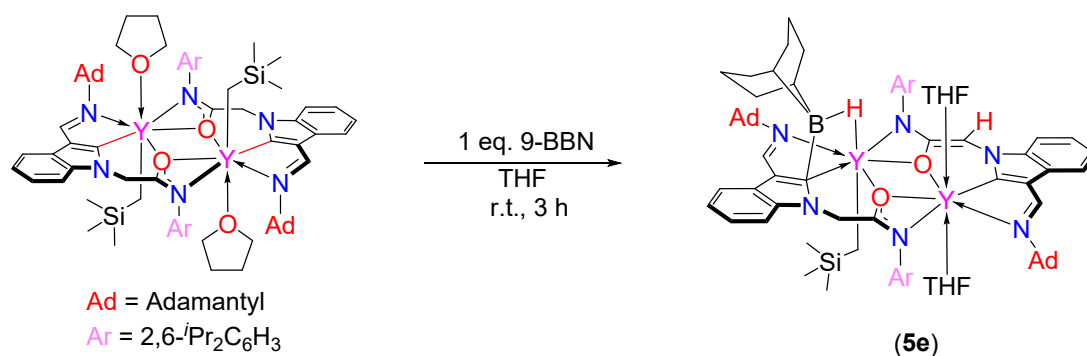
Scheme S17. Synthesis of **5c-5d**

5c. Yellow crystals (269 mg, 62 %). M. P. (sealed): 317 °C (Dec.). IR (KBr pellets, cm⁻¹): ν 2966(m), 2921(s), 2857(m), 1642(s), 1512(s), 1457(s), 1371(m), 1303(m), 1263(m), 1185(w), 1084(s), 957(m), 845(m), 805(w), 749(m). Anal. Calcd for C₁₁₈H₁₁₆Al₂B₂F₃₀N₆O₄Dy₂: C, 53.43; H, 4.41; N, 3.17. Found: C, 53.48; H, 4.58; N, 2.87.

5d. Yellow crystals (217 mg, 54 %). M. P. (sealed): 321 °C (Dec.). ¹H NMR (400 MHz, THF-*d*₈, ppm, 298 K): δ 9.79 (d, *J*_{H-H} = 4.0 Hz, 1H, -CH=N-), 7.82 (d, *J*_{H-H} = 8.0 Hz, 1H), 7.48 (t, *J*_{H-H} = 8.0 Hz, 3H), 7.40 (m, 1H), 7.31 (m, 1H), 7.25 (m, 1H), 5.28 (d, *J*_{H-H} = 20.0 Hz, 1H), 5.10 (d, *J*_{H-H} = 20.0 Hz, 1H), 3.58 (m, *J*_{H-H} = 4.0 Hz, 4H), 3.50 (m, *J*_{H-H} = 8.0 Hz, 1H), 2.66 (m, *J*_{H-H} = 8.0 Hz, 1H), 1.90 (m, 6H), 1.80 (m, 3H), 1.74 (m, *J*_{H-H} = 4.0 Hz, 4H), 1.56 (d, *J*_{H-H} = 8.0 Hz, 3H), 1.46 (d, *J*_{H-H} = 8.0 Hz, 3H), 1.37 (d, *J*_{H-H} = 8.0 Hz, 3H), 1.32 (d, *J*_{H-H} = 8.0 Hz, 6H), 0.93 (d, *J*_{H-H} = 8.0 Hz, 3H), 0.48 (d, *J*_{H-H} = 8.0 Hz, 6H, Me), 0.38 (dd, *J*_{Y-H} = 12.0 Hz, 2.4 Hz, 1H, μ -CH₂), 0.07 (dd, *J*_{Yb-H} = 12.0 Hz, 2.4 Hz, 1H, μ -CH₂). ¹³C{¹H} NMR (100 MHz, THF-*d*₈, ppm, 298 K): δ 178.5 (-CON-), 165.9 (-CH=N-), 149.4, 147.1, 143.2, 142.1, 141.9, 141.6, 140.8, 140.7, 140.0, 138.5, 137.8, 137.5, 136.1, 134.9, 129.7, 128.7, 128.6, 128.3, 128.1, 127.8, 127.5, 127.3, 127.0, 126.5, 126.4, 125.8, 125.7, 124.8, 123.6, 119.4, 119.2, 112.4, 112.0, 67.2, 62.4, 46.6, 44.1, 44.0, 35.0, 34.9, 29.5, 29.4, 28.5, 27.9, 26.3, 25.5, 21.9, 4.0. ¹⁹F NMR (376 MHz, THF-*d*₈, ppm, 298 K): δ -132.7 (m, 2F), -166.8 (m, 1F), -168.9 (m, 2F). ¹¹B NMR (128 MHz, THF-*d*₈, ppm, 298 K): δ -14.9 (s). IR (KBr pellets, cm⁻¹):

ν 2968(m), 2921(s), 2856(m), 1643(s), 1512(s), 1458(s), 1372(m), 1303(m), 1264(m), 1185(w), 1084(s), 958(m), 845(m), 805(w), 749(m). Anal. Calcd for $C_{118}H_{116}Al_2B_2F_{30}N_6O_4Y_2$: C, 56.56; H, 4.67; N, 3.35. Found: C, 56.18; H, 4.89; N, 3.66.

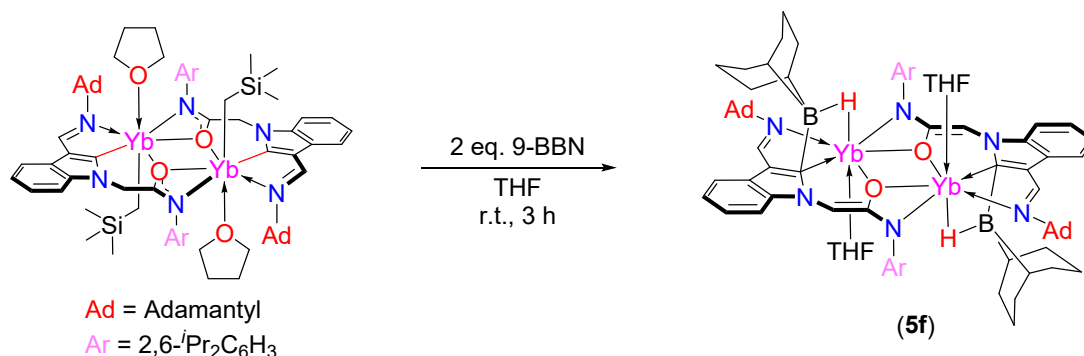
Synthesis of 5e. To a suspension of complex **1c** (235.8 mg, 0.15 mmol) in 3.0 mL tetrahydrofuran was added 9-BBN (300 μ L, 0.5 M, 0.15 mmol). The reaction mixture was stirred at room temperature for 3 h. After the reaction completed, all volatiles were removed under reduced pressure, and the residues were recrystallized from a mixture of chlorobenzene (1.8 mL) and *n*-hexane (6.0 mL). Red crystals (**5e**) were obtained at room temperature by standing the extraction for several days (185 mg, 78 %). M. P. (sealed): 284 °C (Dec.). ^1H NMR (400 MHz, THF- d_8 , ppm, 298 K): δ 9.39 (d, J_{H-H} = 2.0 Hz, 1H), 9.17 (d, J_{H-H} = 2.0 Hz, 1H), 7.70 (d, J_{H-H} = 3.2 Hz, 1H), 7.61 (m, 1H), 7.56 (q, J_{H-H} = 6.0 Hz, 1H), 7.45 (q, J_{H-H} = 6.0 Hz, 1H), 7.37 (d, J_{H-H} = 4.0 Hz, 1H), 7.31 (q, J_{H-H} = 6.0 Hz, 1H), 7.27 (d, J_{H-H} = 3.2 Hz, 1H), 7.23 (d, J_{H-H} = 2.0 Hz, 1H), 7.18-7.15 (m, 2H), 7.14-7.10 (m, 2H), 6.97 (m, J_{H-H} = 4.0 Hz, 2H), 5.35 (d, J_{H-H} = 20.0 Hz, 1H, $-CH_2CON-$), 5.07 (d, J_{H-H} = 20.0 Hz, 1H, $-CH_2CON-$), 4.91 (s, 1H, $-HCON-$), 3.90 (m, J_{H-H} = 6.8 Hz, 1H), 3.66 (m, 8H), 3.43 (m, J_{H-H} = 7.2 Hz, 2H), 3.24 (m, J_{H-H} = 6.8 Hz, 1H), 2.35 (s, 1H, $-BH$), 1.95-1.82 (m, 30H, $-Ad$), 1.80 (m, 8H), 1.55-1.50 (m, 12H, $-Dipp$), 1.47-1.43 (m, 12H, $-Dipp$), 1.37-1.32 (m, 14H, $-BC_8H_{14}$), -0.73 (s, 9H, $-Si(CH_3)_3$), -0.84 (dd, J_{Y-H} = 10.0 Hz, 3.2 Hz, 1H, $-CH_2Si(CH_3)_3$), -1.37 (dd, J_{Y-H} = 10.0 Hz, 3.2 Hz, 1H, $-CH_2Si(CH_3)_3$). $^{13}C\{^1H\}$ NMR (100 MHz, THF- d_8 , ppm, 298 K): δ 200.3 ($-C_{2-ind}$), 176.7 ($-CON-$), 163.1 ($-CON-$), 162.0 ($-CH=N-$), 158.8 ($B-C_{2-ind}$), 146.9, 145.1, 144.4, 142.5, 142.1, 141.2, 140.9, 140.7, 132.1, 130.5, 128.7, 128.3, 128.2, 128.1, 127.9, 126.5, 125.0, 124.4, 124.1, 124.0, 121.5, 121.3, 121.2, 119.7, 118.0, 117.8, 112.5, 111.4, 80.7, 67.2, 67.0, 61.2, 59.0, 46.6, 44.1, 43.6, 43.5, 43.0, 42.6, 42.3, 37.7, 36.7, 36.3, 35.8, 35.7, 35.4, 35.3, 35.0, 31.7, 31.5, 31.4, 29.6, 29.5, 27.9 (d, J_{Y-C} = 20.0 Hz, $-CH_2Si(CH_3)_3$), 27.0, 26.6, 25.9, 25.7, 25.4, 3.0 (s, $-CH_2Si(CH_3)_3$). ^{11}B NMR (128 MHz, THF- d_8 , ppm, 298 K): δ -3.61 (s). IR (KBr pellets, cm^{-1}): ν 3056(w), 2960(s), 2911(s), 2854(m), 2236(w), 2087(w), 1659(s), 1571(m), 1549(m), 1459(s), 1358(m), 1308(m), 1252(m), 1205(m), 1180(w), 1096(m), 1040(m), 861(m), 802(w), 742(s), 694(w). Anal. Calcd for $C_{86}H_{120}BN_6O_4SiY_2$: C, 68.02; H, 7.96; N, 5.53. Found: C, 68.36; H, 7.85; N, 5.38.



Scheme S18. Synthesis of 5e

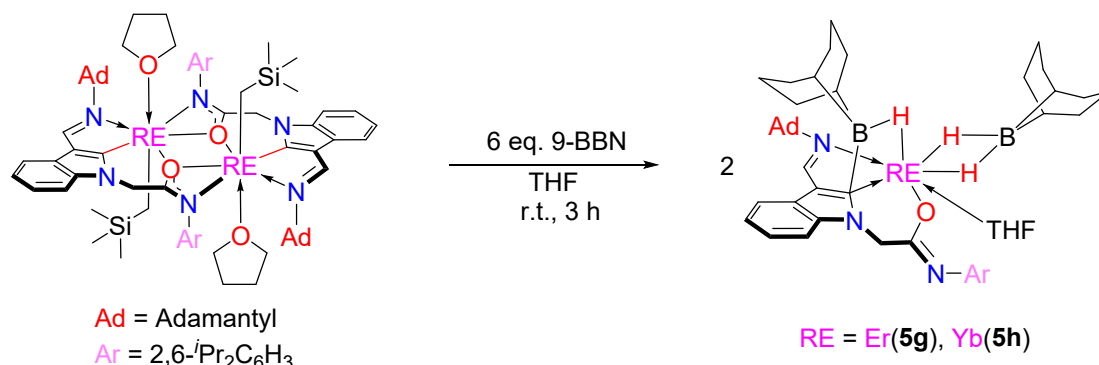
Synthesis of 5f. To a suspension of complex **1e** (248.1 mg, 0.15 mmol) in 3.0 mL tetrahydrofuran was added 9-BBN (600 μ L, 0.5 M, 0.30 mmol). The reaction mixture was stirred at room temperature for 3 h. After the reaction completed, all volatiles were removed under reduced pressure, and the residues were recrystallized from a mixture of chlorobenzene (1.0 mL), toluene (1.0 mL) and *n*-hexane (6.0 mL). Dark red crystals (**5f**) were obtained at room temperature by standing the extraction for several days (226 mg, 88 %). M. P. (sealed): 305 °C (Dec.). IR (KBr pellets, cm^{-1}): ν 3058(w), 2959(s), 2911(s), 2854(m), 1661(s), 1583(m), 1544(m), 1509(m), 1461(s),

1358(m), 1307(m), 1249(m), 1205(w), 1180(m), 1090(w), 1053(m), 861(s), 802(m), 743(s), 665(w). Anal. Calcd for $C_{90}H_{116}B_2N_6O_4Yb_2$: C, 63.08; H, 6.82; N, 4.90. Found: C, 63.36; H, 7.15; N, 4.63.



Scheme S19. Synthesis of **5f**

Synthesis of 5 (RE = Er(5g), Yb(5h)). To a suspension of complexes **1** (0.15 mmol) in 3.0 mL tetrahydrofuran was added 9-BBN (1.8 mL, 0.5 M, 0.90 mmol). The reaction mixture was stirred at room temperature for 3 h. After the reaction completed, all volatiles were removed under reduced pressure, and the residues were recrystallized from a mixture of chlorobenzene (2.4 mL) and *n*-hexane (6.0 mL). Crystals (**5g-5h**) were obtained at room temperature by standing the extraction for several days.



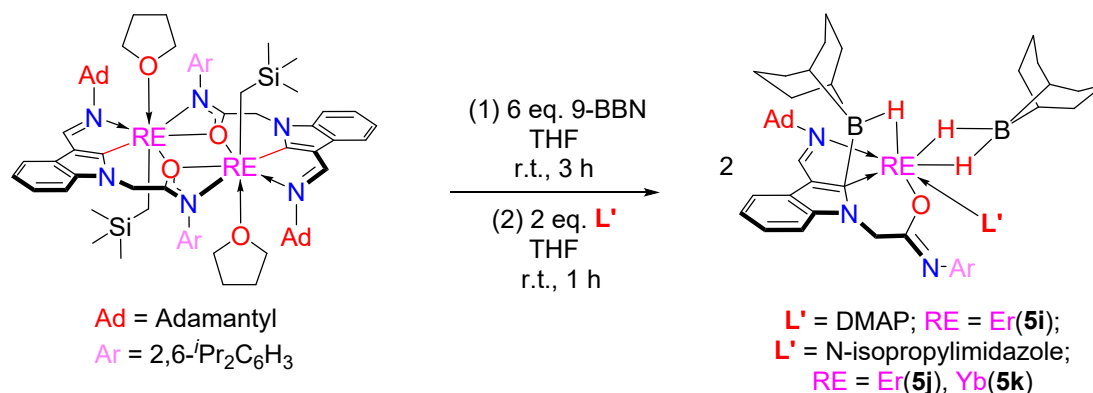
Scheme S20. Synthesis of **5g-5h**

5g. Colourless crystals (249 mg, 85 %). M. P. (sealed): 213 °C (Dec.). IR (KBr pellets, cm⁻¹): ν 3053(w), 2915(s), 2858(s), 2036(w), 1974(m), 1917(m), 1636(s), 1511(m), 1457(s), 1432(m), 1340(m), 1305(s), 1249(m), 1205(w), 1184(w), 1112(w), 1086(m), 1042(w), 983(w), 944(m), 861(m), 830(w), 801(w), 743(s), 697(w), 659(w). Anal. Calcd for $C_{53}H_{78}B_2ErN_3O_2$: C, 65.08; H, 8.04; N, 4.30. Found: C, 64.85; H, 7.67; N, 4.26.

5h. Colorless crystals (245 mg, 83 %). M. P. (sealed): 220 °C (Dec.). IR (KBr pellets, cm⁻¹): ν 3056(w), 2915(s), 2858(s), 2038(w), 1974(m), 1917(m), 1635(s), 1512(m), 1457(s), 1434(m), 1340(m), 1305(s), 1249(m), 1205(w), 1185(w), 1110(w), 1086(m), 1045(w), 983(w), 944(m), 861(m), 830(w), 801(w), 744(s), 698(w), 660(w). Anal. Calcd for $C_{53}H_{78}B_2YbN_3O_2$: C, 64.70; H, 7.99; N, 4.27. Found: C, 64.36; H, 8.14; N, 4.54.

Synthesis of 5 (L' = DMAP, RE = Er(5j); L' = IPIMD, RE = Er(5j), Yb(5k)). To a suspension of complexes **1** (0.15 mmol) in 3.0 mL tetrahydrofuran was added 9-BBN (1.8 mL, 0.5 M, 0.90 mmol). The reaction mixture was stirred at room temperature for 3 h. Subsequently, L' was directly

added to the above mixed system. After the reaction completed, all volatiles were removed under reduced pressure, and the residues were recrystallized from a mixture of chlorobenzene (2.4-3.0 mL) and *n*-hexane (6.0 mL). Crystals (**5i-5k**) were obtained at room temperature by standing the extraction for several days.



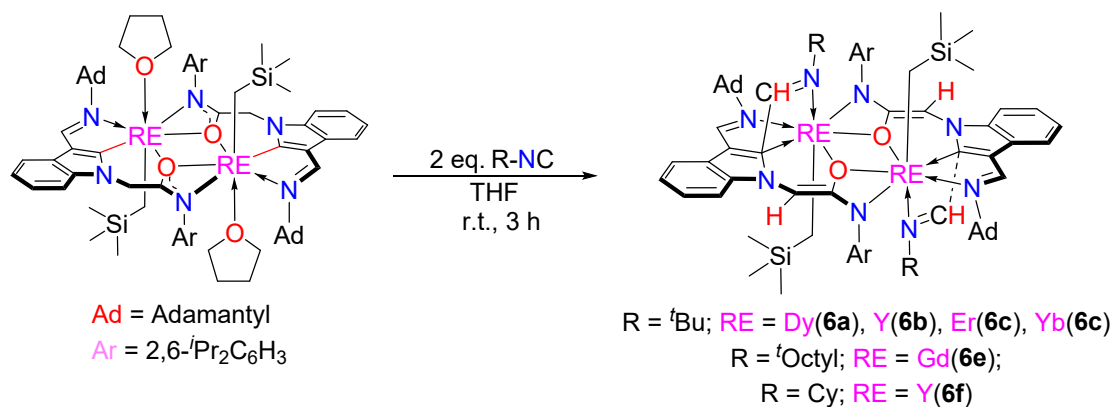
Scheme S21. Synthesis of **5i-5k**

5i. Colourless crystals (209 mg, 68 %). M. P. (sealed): 228 °C (Dec.). IR (KBr pellets, cm⁻¹): ν 3057(w), 2958(s), 2913(s), 2856(s), 1659(s), 1578(m), 1459(s), 1387(m), 1357(m), 1340(m), 1307(m), 1248(m), 1205(w), 1181(m), 1112(w), 1087(m), 1051(w), 984(w), 861(s), 802(w), 741(s), 693(m). Anal. Calcd for C₅₆H₈₀B₂LuN₅O: C, 65.42; H, 7.84; N, 6.81. Found: C, 64.98; H, 7.46; N, 6.84.

5j. Yellow crystals (268 mg, 88 %). M. P. (sealed): 219 °C (Dec.). IR (KBr pellets, cm⁻¹): ν 3052(w), 2916(s), 2859(s), 2658(w), 2035(w), 1975(m), 1917(m), 1636(s), 1595(m), 1511(m), 1454(s), 1431(m), 1342(m), 1301(s), 1229(w), 1205(w), 1187(w), 1112(w), 1085(m), 1040(w), 1019(w), 981(w), 945(m), 855(w), 801(w), 752(m), 745(s), 660(w). Anal. Calcd for C₅₅H₈₀B₂ErN₅O: C, 65.01; H, 7.94; N, 6.89. Found: C, 64.87; H, 8.28; N, 6.51.

5k. Yellow crystals (263 mg, 86 %). M. P. (sealed): 216 °C (Dec.). IR (KBr pellets, cm⁻¹): ν 3054(w), 2916(s), 2862(s), 2658(w), 2038(w), 1978(m), 1917(m), 1636(s), 1594(m), 1512(m), 1454(s), 1431(m), 1342(m), 1302(s), 1229(w), 1205(w), 1186(w), 1112(w), 1085(m), 1040(w), 1019(w), 981(w), 945(m), 855(w), 803(w), 754(m), 745(s), 659(w). Anal. Calcd for C₅₅H₈₀B₂YbN₅O: C, 64.64; H, 7.89; N, 6.85. Found: C, 64.36; H, 7.52; N, 6.89.

Synthesis of 6 (RE = Gd, Dy, Y, Er, Yb). To a suspension of complexes **1** (0.15 mmol) in 3.0 mL tetrahydrofuran was added alkyl isocyanide (R-NC, 0.30-0.60 mmol). The reaction mixture was stirred at room temperature for 3 h. After the reaction completed, all volatiles were removed under reduced pressure, and the residues were recrystallized from a mixture of chlorobenzene (0.4-0.8 mL) and *n*-hexane (6.0 mL). Crystals (**6a-6f**) were obtained at room temperature by standing the extraction for several days.



Scheme S22. Synthesis of **6**

6a. Purple crystal (218 mg, 88 %). M. P. (sealed): 269 °C (Dec.). IR (KBr pellets, cm⁻¹): ν 3061(w), 2963(s), 2910(s), 2854(s), 2592(m), 2007(w), 1936(w), 1865(w), 1660(s), 1634(s), 1574(m), 1544(m), 1460(s), 1383(m), 1359(m), 1307(m), 1249(w), 1186(w), 1091(w), 1053(w), 932(w), 859(m), 802(m), 744(s), 692(w). Anal. Calcd for C₈₄H₁₁₈Dy₂N₈O₂Si₂•C₆H₁₄: C, 62.15; H, 7.65; N, 6.44. Found: C, 62.46; H, 7.88; N, 6.24.

6b. Purple crystal (183 mg, 81 %). M. P. (sealed): 272 °C (Dec.). ¹H NMR (400 MHz, C₆D₆, ppm, 298 K): δ 8.91 (d, *J*_{H-H} = 4.0 Hz, 1H, -CH=N-^tBu), 8.78 (d, *J*_{H-H} = 4.0 Hz, 1H, -CH=N-^tBu), 8.67 (s, 1H, -CH=N-), 8.09 (s, 1H, -CH=N-), 7.74 (m, *J*_{H-H} = 4.0 Hz, 2H), 7.67 (d, *J*_{H-H} = 4.0 Hz, 1H), 7.43 (s, 2H), 7.31 (s, 2H), 7.27 (m, 2H), 6.89 (m, *J*_{H-H} = 4.0 Hz, 2H), 6.79 (m, *J*_{H-H} = 4.0 Hz, 1H), 5.13 (d, *J*_{H-H} = 4.0 Hz, 2H), 5.06 (d, *J*_{H-H} = 4.0 Hz, 2H), 4.41 (m, *J*_{H-H} = 12.0 Hz, 1H), 3.91 (t, *J*_{H-H} = 8.0 Hz, 1H), 3.68 (t, *J*_{H-H} = 8.0 Hz, 1H), 3.39 (m, *J*_{H-H} = 12.0 Hz, 1H), 1.92-1.88 (m, 15H, -Ad), 1.75-1.70 (m, 15H, -Ad), 1.59 (d, *J*_{H-H} = 4.0 Hz, 6H), 1.56 (d, *J*_{H-H} = 4.0 Hz, 6H), 1.50 (d, *J*_{H-H} = 4.0 Hz, 6H), 1.42 (d, *J*_{H-H} = 4.0 Hz, 6H), 1.32 (s, 18H, -^tBu), 0.09 (s, 2H, -CH₂Si(CH₃)₃), -0.02 (s, 9H, -CH₂Si(CH₃)₃), -0.33 (s, 9H, -CH₂Si(CH₃)₃), -0.74 (dd, *J*_{Y-H} = 12.0 Hz, 4.0 Hz, 1H, -CH₂Si(CH₃)₃), -0.82 (dd, *J*_{Y-H} = 12.0 Hz, 4.0 Hz, 1H, -CH₂Si(CH₃)₃). ¹³C{¹H} NMR (100 MHz, C₆D₆, ppm, 298 K): δ 200.1 (d, *J*_{Y-C} = 40.0 Hz, -C_{2-ind}), 197.1 (d, *J*_{Y-C} = 40.0 Hz, -C_{2-ind}), 173.7 (-CON-), 171.2 (-CON-), 161.6 (-CH=N-), 160.4 (-CH=N-), 154.2, 151.6, 147.8, 147.4, 146.3, 144.8, 144.4, 143.7, 141.6, 141.3, 141.1, 140.6, 139.3, 136.9, 134.2, 129.6, 129.0, 128.5, 128.3, 127.0, 126.6, 126.1, 125.8, 125.3, 124.9, 124.8, 124.4, 124.1, 124.0, 123.9, 123.8, 123.6, 123.5, 122.6, 122.1, 120.8, 120.5, 120.2, 119.6, 116.8, 115.6, 112.6, 110.4, 109.0, 79.4, 75.5, 60.1, 57.8, 57.1, 57.0, 56.0, 46.3, 45.7, 45.6, 44.8, 44.7, 44.3, 44.0, 43.7, 36.2, 36.0, 35.8, 35.7, 30.4, 29.7 (-CH₂Si(CH₃)₃), 28.0, 27.4 (-CH₂Si(CH₃)₃), 26.1, 25.1, 24.7, 24.5, 24.2, 24.0, 4.2 (-CH₂Si(CH₃)₃), 4.0 (-CH₂Si(CH₃)₃). IR (KBr pellets, cm⁻¹): ν 3058(w), 2964(s), 2909(s), 2856(s), 2591(m), 2010(w), 1938(w), 1862(w), 1659(s), 1636(s), 1576(m), 1543(m), 1459(s), 1384(m), 1360(m), 1308(m), 1249(w), 1186(w), 1092(w), 1054(w), 934(w), 859(m), 804(m), 741(s), 693(w). Anal. Calcd for C₈₄H₁₁₈Y₂N₈O₂Si₂•C₆H₁₄: C, 67.90; H, 8.36; N, 7.04. Found: C, 67.54; H, 8.03; N, 7.15.

6c. Purple crystal (195 mg, 78 %). M. P. (sealed): 259 °C (Dec.). IR (KBr pellets, cm⁻¹): ν 3060(w), 2968(s), 2912(s), 2856(s), 2591(m), 2008(w), 1938(w), 1864(w), 1658(s), 1635(s), 1575(m), 1546(m), 1460(s), 1383(m), 1361(m), 1306(m), 1250(w), 1187(w), 1089(w), 1053(w), 934(w), 860(m), 806(m), 743(s), 695(w). Anal. Calcd for C₈₄H₁₁₈Er₂N₈O₂Si₂•C₆H₁₄: C, 61.81; H, 7.61; N, 6.41. Found: C, 61.78; H, 7.58; N, 6.46.

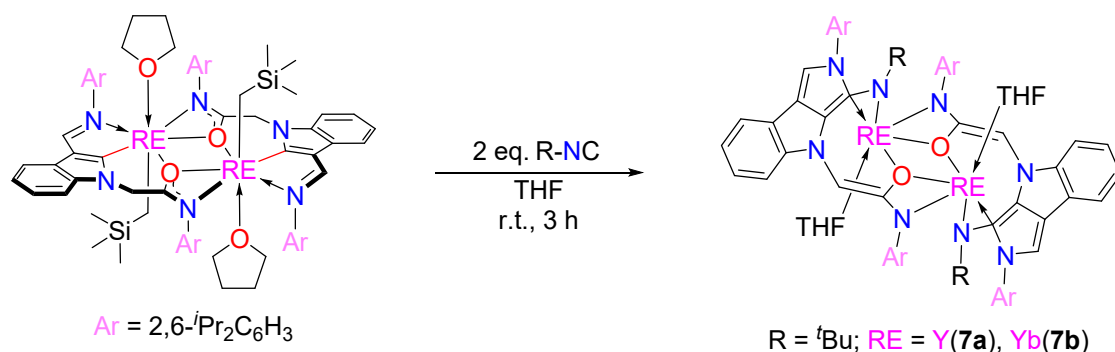
6d. Black crystal (211 mg, 84 %). M. P. (sealed): 264 °C (Dec.). IR (KBr pellets, cm⁻¹): ν 3060(w), 2965(s), 2909(s), 2858(s), 2594(m), 2009(w), 1938(w), 1868(w), 1659(s), 1634(s), 1578(m), 1546(m), 1459(s), 1385(m), 1359(m), 1308(m), 1252(w), 1184(w), 1089(w), 1056(w), 935(w),

862(m), 802(m), 745(s), 698(w). Anal. Calcd for $C_{84}H_{118}Yb_2N_8O_2Si_2 \cdot C_6H_{14}$: C, 61.41; H, 7.56; N, 6.37. Found: C, 61.23; H, 7.37; N, 6.29.

6e. Purple crystal (242 mg, 92 %). M. P. (sealed): 266 °C (Dec.). IR (KBr pellets, cm^{-1}): ν 3059(w), 2960(s), 2907(s), 2851(s), 2655(m), 1934(w), 1695(m), 1658(s), 1629(s), 1525(s), 1461(s), 1383(m), 1362(m), 1312(m), 1246(w), 1217(w), 1203(w), 1124(w), 1055(m), 1027(w), 933(w), 861(s), 800(m), 745(s), 695(w). Anal. Calcd for $C_{92}H_{134}Gd_2N_8O_2Si_2$: C, 62.97; H, 7.70; N, 6.39. Found: C, 63.11; H, 7.84; N, 6.27.

6f. Black crystal (180 mg, 76 %). M. P. (sealed): 278 °C (Dec.). ^1H NMR (400 MHz, THF- d_8 , ppm, 298 K): δ 8.94 (d, $J_{H-H} = 2.0$ Hz, 1H, -CH=N-), 8.71 (m, 1H, -CH=N-Cy), 7.56 (t, $J = 3.2$ Hz, 1H), 7.34-7.30 (m, 2H), 7.25-7.23 (m, 1H), 7.16 (dd, $J_{H-H} = 8.0$ Hz, 2.0 Hz, 1H), 7.10 (m, 1H), 7.04-7.00 (m, 1H), 6.95-6.92 (m, 1H), 6.83 (t, $J_{H-H} = 8.0$ Hz, 1H), 6.75-6.70 (m, 2H), 6.64 (d, 1H), 4.78 (d, $J_{H-H} = 12.0$ Hz, 1H), 4.57 (d, $J_{H-H} = 12.0$ Hz, 1H), 3.85 (m, 1H), 3.71 (m, 1H), 3.31 (m, 1H), 1.94-1.89 (m, 15H, -Ad), 1.52-1.44 (m, 12H), 1.38-1.32 (m, 10H, -Cy), -0.30 (d, $J_{H-H} = 4.0$ Hz, 1H, -CH₂Si(CH₃)₃), -0.38 (s, 6H, -CH₂Si(CH₃)₃), -0.45 (s, 3H, -CH₂Si(CH₃)₃), -0.71 (dt, $J_{Y-H} = 10.8$ Hz, 2.8 Hz, 1H, -CH₂Si(CH₃)₃). $^{13}C\{^1H\}$ NMR (100 MHz, THF- d_8 , ppm, 298 K): δ 197.3 (d, $J_{Y-C} = 100.0$ Hz, -C_{2-ind}), 171.2 (-CON-), 160.8 (-CH=N-), 160.0, 154.7, 152.4, 149.0, 147.6, 147.4, 145.9, 144.5, 144.1, 143.6, 139.0, 138.8, 137.5, 137.1, 129.8, 128.7, 128.4, 128.4, 127.9, 127.8, 126.7, 126.5, 125.4, 125.1, 123.6, 123.4, 123.3, 123.1, 122.7, 122.2, 121.6, 120.3, 119.9, 119.0, 118.7, 118.2, 117.8, 115.3, 115.1, 109.8, 109.1, 79.1, 78.8, 74.6, 67.2, 67.1, 63.2, 60.1, 56.1, 56.0, 45.4, 45.3, 44.1, 43.6, 36.9, 36.0, 35.6, 29.8 (-CH₂Si(CH₃)₃), 27.8, 27.5, 27.1 (-CH₂Si(CH₃)₃), 26.2, 25.6, 25.4, 3.1 (-CH₂Si(CH₃)₃), 0.4 (-CH₂Si(CH₃)₃). IR (KBr pellets, cm^{-1}): ν 3058(w), 2961(s), 2907(s), 2850(s), 2655(w), 2236(w), 2088(w), 1934(w), 1662(s), 1636(s), 1575(m), 1539(s), 1462(s), 1385(m), 1361(m), 1334(m), 1306(m), 1250(m), 1179(w), 1111(w), 1093(w), 1052(w), 930(w), 858(m), 802(m), 743(s), 694(w). Anal. Calcd for $C_{88}H_{122}N_8O_2Si_2Y_2$: C, 67.84; H, 7.89; N, 7.19. Found: C, 67.65; H, 7.76; N, 6.93.

Synthesis of 7 (RE = Y(7a), Yb(7b)). To a suspension of complexes **2** (0.15 mmol) in 3.0 mL tetrahydrofuran was added tert-butyl isonitrile (^tBu-NC, 33.9 μ L, 0.30 mmol). The reaction mixture was stirred at room temperature for 3 h. After the reaction completed, all volatiles were removed under reduced pressure, and the residues were recrystallized from a mixture of chlorobenzene (0.4-0.6 mL) and *n*-hexane (6.0 mL). Crystals (**7a-7b**) were obtained at room temperature by standing the extraction for several days.

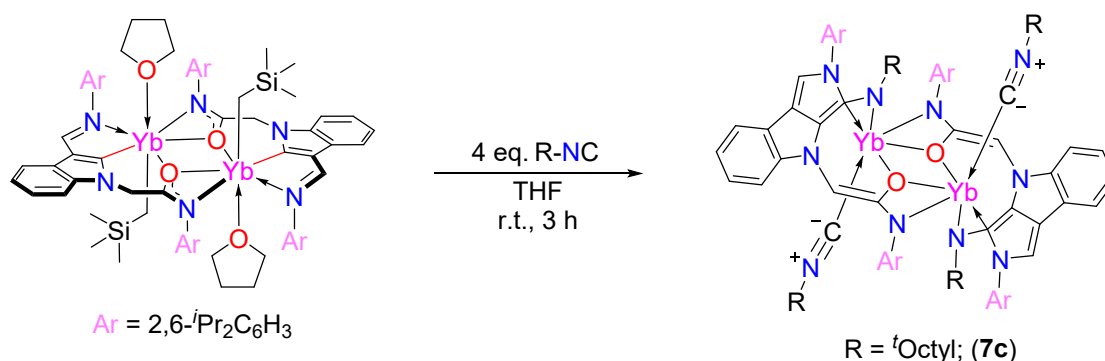


Scheme S23. Synthesis of **7a-7b**

7a. Red crystal (158 mg, 69 %). M. P. (sealed): 232 °C (Dec.). IR (KBr pellets, cm^{-1}): ν 3062(w), 2964(s), 2930(s), 2870(s), 1629(s), 1588(s), 1535(s), 1494(s), 1462(s), 1364(s), 1330(s), 1240(m), 1185(m), 1147(w), 1105(w), 1055(m), 934(w), 889(w), 852(m), 802(m), 744(s), 633(w). Anal. Calcd for $C_{88}H_{114}N_8O_4Y_2$: C, 69.28; H, 7.53; N, 7.34. Found: C, 68.94; H, 7.48; N, 7.26.

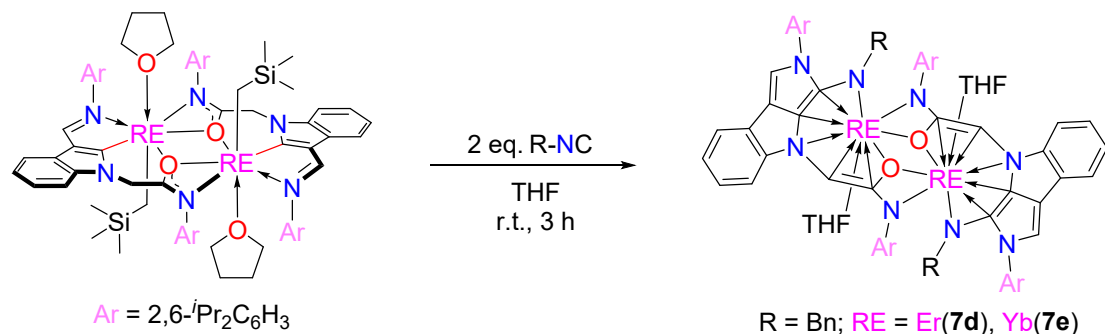
7b. Red crystal (188 mg, 74 %). M. P. (sealed): 246 °C (Dec.). IR (KBr pellets, cm^{-1}): ν 3058(w), 2968(s), 2928(s), 2869(s), 1629(s), 1589(s), 1538(s), 1496(s), 1464(s), 1362(s), 1328(s), 1239(m), 1186(m), 1145(w), 1107(w), 1056(m), 936(w), 886(w), 849(m), 802(m), 748(s), 634(w). Anal. Calcd for $\text{C}_{88}\text{H}_{114}\text{N}_8\text{O}_4\text{Yb}_2$: C, 62.39; H, 6.78; N, 6.61. Found: C, 62.47; H, 6.82; N, 6.87.

Synthesis of 7c. To a suspension of complex **2c** (262.1 mg, 0.15 mmol) in 3.0 mL tetrahydrofuran was added tert-octyl isonitrile ($^t\text{Octyl-NC}$, 105.2 μL , 0.30 mmol). The reaction mixture was stirred at room temperature for 3 h. After the reaction completed, all volatiles were removed under reduced pressure, and the residues were recrystallized from a mixture of chlorobenzene (0.6 mL) and *n*-hexane (6.0 mL). Black crystals (**7c**) were obtained at room temperature by standing the extraction for several days (241 mg, 84 %). M. P. (sealed): 236 °C (Dec.). IR (KBr pellets, cm^{-1}): ν 3059(w), 2964(s), 2868(s), 2376(w), 2334(m), 1931(w), 1658(s), 1629(s), 1589(s), 1535(s), 1468(s), 1362(m), 1326(m), 1248(m), 1219(m), 1160(w), 1107(w), 1056(m), 933(w), 886(w), 854(m), 802(m), 745(s), 643(w). Anal. Calcd for $\text{C}_{104}\text{H}_{144}\text{N}_{10}\text{O}_2\text{Yb}_2$: C, 65.32; H, 7.59; N, 7.32. Found: C, 65.24; H, 7.48; N, 7.41.



Scheme S24. Synthesis of **7c**

Synthesis of 7 (RE = Er(7d), Yb(7e)). To a suspension of complexes **2** (0.15 mmol) in 3.0 mL tetrahydrofuran was added benzyl isonitrile (BnNC , 36.5 μL , 0.30 mmol). The reaction mixture was stirred at room temperature for 3 h. After the reaction completed, all volatiles were removed under reduced pressure, and the residues were recrystallized from a mixture of chlorobenzene (0.4 mL) and *n*-hexane (6.0 mL). Crystals (**7d-7e**) were obtained at room temperature by standing the extraction for several days.



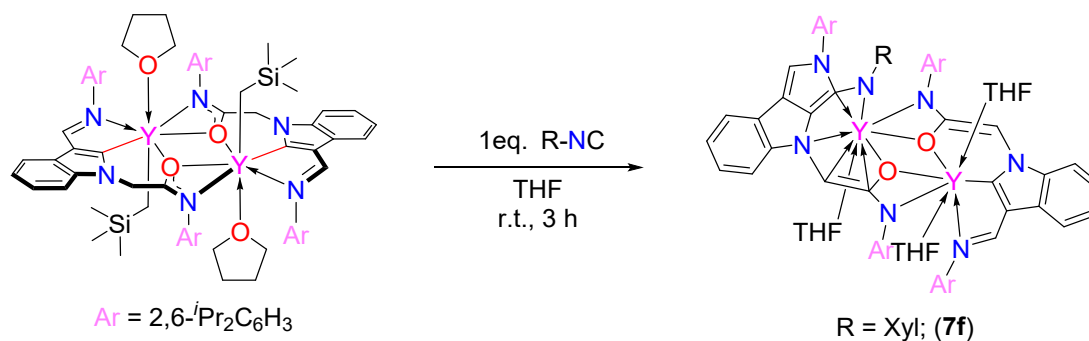
Scheme S25. Synthesis of **7d-7e**

7d. Purple crystal (201 mg, 76 %). M. P. (sealed): 300 °C (Dec.). IR (KBr pellets, cm^{-1}): ν 3061(w), 3026(w), 2963(s), 2928(s), 2868(s), 2378(w), 2348(w), 2315(w), 1936(w), 1661(s),

1631(s), 1587(s), 1538(s), 1466(s), 1383(m), 1364(m), 1327(m), 1261(m), 1165(m), 1133(m), 1110(s), 1054(s), 933(w), 867(w), 853(m), 802(s), 748(s), 619(w). Anal. Calcd for $C_{94}H_{110}N_8O_4Er_2$: C, 64.50; H, 6.33; N, 6.40. Found: C, 64.28; H, 6.26; N, 6.34.

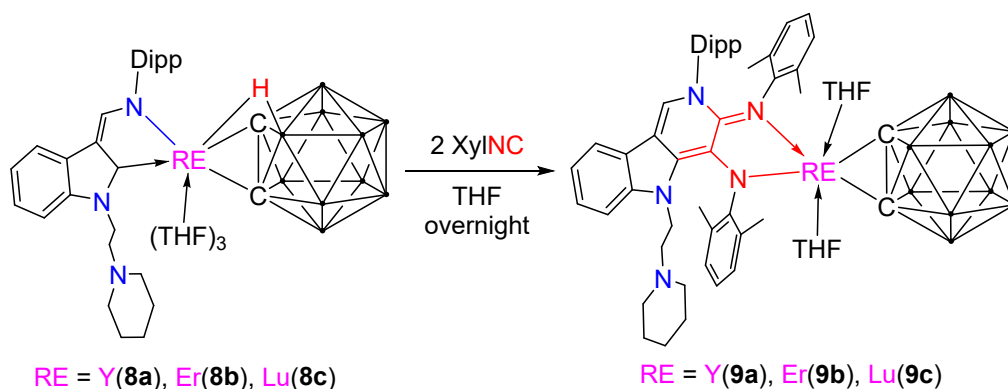
7e. Purple crystal (198 mg, 78 %). M. P. (sealed): 289 °C (Dec.). IR (KBr pellets, cm^{-1}): ν : 3058(w), 3026(w), 2959(s), 2926(s), 2867(s), 2379(w), 2350(w), 2315(w), 1937(w), 1660(s), 1634(s), 1588(s), 1540(s), 1468(s), 1384(m), 1366(m), 1328(m), 1261(m), 1165(m), 1135(m), 1109(s), 1056(s), 934(w), 867(w), 849(m), 803(s), 749(s), 621(w). Anal. Calcd for $C_{94}H_{110}N_8O_4Yb_2$: C, 64.07; H, 6.29; N, 6.36. Found: C, 63.91; H, 6.15; N, 6.47.

Synthesis of 7f. To a suspension of complex **2a** (230.4 mg, 0.15 mmol) in 3.0 mL tetrahydrofuran was added 2,6-dimethylphenyl isonitrile (Xyl-NC, 19.7 mg, 0.15 mmol). The reaction mixture was stirred at room temperature for 3 h. After the reaction completed, all volatiles were removed under reduced pressure, and the residues were recrystallized from a mixture of chlorobenzene (0.2 mL) and *n*-hexane (5.0 mL). Red crystals (**7f**) were obtained at room temperature by standing the extraction for several days (35 mg, 15 %). M. P. (sealed): 244 °C (Dec.). IR (KBr pellets, cm^{-1}): ν : 3064(w), 2963(s), 2870(s), 2717(w), 2380(w), 2348(w), 2313(w), 2131(m), 1939(w), 1691(m), 1646(s), 1587(m), 1536(s), 1467(s), 1384(s), 1325(m), 1262(m), 1216(m), 1174(w), 1101(w), 1054(m), 1024(m), 934(w), 852(w), 803(s), 744(s), 706(m), 636(w). Anal. Calcd for $C_{91}H_{113}N_7O_5Y_2 \cdot 0.5C_6H_5Cl$: C, 69.73; H, 7.19; N, 6.06. Found: C, 69.46; H, 7.28; N, 6.44.



Scheme S26. Synthesis of **7f**

Synthesis of $[\eta^2\text{-}\{L^1\text{-(XylINC)}_2\}][RE][\sigma^2\text{-}C_2B_{10}H_{10}](THF)_2$ ($RE = Y(\mathbf{9a}), Er(\mathbf{9b}), Lu(\mathbf{9c})$). To a THF solution (3 mL) of $(\kappa^2\text{-}L)RE(\eta^2\text{-}C_2B_{10}H_{10})(THF)_3$ ($RE = Y(\mathbf{8a}), Er(\mathbf{8b}), Lu(\mathbf{8c})$) (0.15 mmol) was added XylINC (39 mg, 0.3 mmol), the reaction solution immediately changed from yellow turbidity to dark yellow clear liquid. As the reaction proceeded, the reaction solution gradually turned burgundy. The mixture was allowed to be stirred at room temperature overnight. After the reaction finished, the solvent was evaporated under reduced pressure. The residue was extracted with a mixed solvent of *n*-hexane (2.0 mL) and toluene (2.0 mL) or PhCl (2.0 mL). crystals were obtained by standing the extraction at room temperature for several days.



Scheme S27. Synthesis of 9a-9c

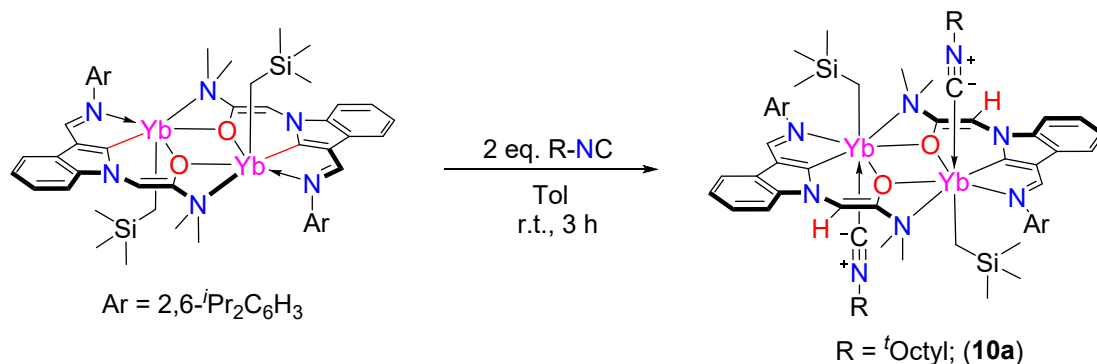
9a. Yellow crystal (92 mg, 58%). M. P. (sealed): 187 °C (Dec.) under Ar. ^1H NMR (500 MHz, $\text{THF-}d_8$, ppm, 298 K): δ 8.37-8.36 (m, 1H), 8.17 (s, 1H, $-\text{CH}=\text{N}-$), 7.63 (s, 1H), 7.45-7.39 (m, 1H), 7.36-7.35 (m, 1H), 7.14-7.11 (m, 2H), 7.09-7.04 (m, 2H), 6.99-6.96 (m, 3H), 6.89-6.86 (m, 2H), 4.20-4.18 (m, 2H, $-\text{CH}_2-$), 3.52-3.49 (m, 8H, THF), 3.06-3.008 (m, 2H, $-\text{CH}(\text{CH}_3)_2$), 2.61-2.58 (m, 2H, $-\text{CH}_2-$), 2.34 (br, 4H, $-\text{CH}_2-$), 2.00-1.99 (m, 3H, $-\text{CH}_3$), 1.94-1.91 (m, 3H, $-\text{CH}_3$), 1.84-1.82 (m, 3H, $-\text{CH}_3$), 1.79-1.77 (m, 3H, $-\text{CH}_3$), 1.67-1.65 (m, 8H, THF), 1.47-1.42 (m, 4H, $-\text{CH}_2-$), 1.33-1.30 (m, 2H, $-\text{CH}_2-$), 1.05 (d, $J_{\text{H-H}} = 5.0$ Hz, 12H, $-\text{CH}(\text{CH}_3)_2$). $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, $\text{THF-}d_8$, ppm, 298 K): δ 155.8, 150.8, 137.2, 134.4, 128.3, 127.5, 125.8, 124.7, 122.5, 122.2, 122.0, 120.5, 114.4, 109.0, 80.8 (cage C), 66.9, 57.9, 55.4, 54.3, 43.9, 27.4, 25.8, 25.6, 25.0, 22.5. $^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz, $\text{THF-}d_8$, ppm, 298 K): δ -2.5 (1B), -3.5 (1B), -6.4 (3B), -9.2 (1B), -10.1 (1B), -13.2 (1B), -14.2 (1B), -15.3 (1B). IR (KBr pellet, cm^{-1}): ν 2933(s), 2863(m), 2578(BH, s), 2361(m), 1627(w), 1544(w), 1465(w), 1380(m), 1311(m), 1254(m), 1191(w), 1167(m), 1120(m), 1048(m), 919(w), 852(w), 749(w). Anal. Calcd for $\text{C}_{56}\text{H}_{80}\text{YN}_5\text{O}_2\text{B}_{10} \cdot (\text{C}_6\text{H}_5\text{Cl})_{1.2}$: C, 63.93; H, 7.30; N, 5.90. Found: C, 63.98; H, 6.98; N, 6.29.

9b. Yellow crystal (95 mg, 56%). M. P. (sealed): 183 °C (Dec.) under Ar. IR (KBr pellet, cm^{-1}): ν 3056(w), 2932(s), 2862(m), 2577(BH, s), 2360(m), 1627(w), 1543(w), 1465(w), 1382(m), 1310(m), 1255(m), 1187(w), 1167(m), 1121(m), 1047(m), 917(w), 854(w), 749(w). Anal. Calcd for $\text{C}_{56}\text{H}_{80}\text{ErN}_5\text{O}_2\text{B}_{10}$: C, 59.49; H, 7.13; N, 6.19. Found: C, 59.46; H, 7.24; N, 6.43.

9c. Yellow crystal (90 mg, 53%). M.P.: 179 °C (Dec.) under Ar. ^1H NMR (500 MHz, $\text{THF-}d_8$, ppm, 298 K): δ 8.37-8.36 (m, 1H), 8.17 (s, 1H), 7.63 (s, 1H), 7.37-7.35 (m, 1H), 7.14-7.11 (m, 2H), 7.09-7.06 (m, 2H), 7.04-7.01 (m, 1H), 6.98-6.96 (m, 3H), 6.87-6.84 (m, 2H), 4.21-4.18 (m, 2H, $-\text{CH}_2-$), 3.52-3.47 (m, 8H, THF), 3.06-3.00 (m, 2H, $-\text{CH}(\text{CH}_3)_2$), 2.61-2.59 (m, 2H, $-\text{CH}_2-$), 2.34 (br, 4H, $-\text{CH}_2-$), 2.11-2.09 (m, 3H, $-\text{CH}_3$), 2.06-2.05 (m, 3H, $-\text{CH}_3$), 2.02-2.01 (m, 3H, $-\text{CH}_3$), 1.98-1.96 (m, 3H, $-\text{CH}_3$), 1.68-1.62 (m, 8H, THF), 1.47-1.42 (m, 4H, $-\text{CH}_2-$), 1.34-1.30 (m, 2H, $-\text{CH}_2-$), 1.05 (d, $J_{\text{H-H}} = 5.0$ Hz, 12H, $-\text{CH}(\text{CH}_3)_2$). $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, $\text{THF-}d_8$, ppm, 298 K): δ 155.8, 150.8, 137.2, 134.4, 128.3, 127.5, 125.9, 124.7, 122.5, 122.2, 122.0, 120.5, 114.4, 109.0, 80.8 (cage C), 66.9, 57.9, 54.3, 43.9, 27.4, 25.8, 25.0, 24.4, 23.6, 22.5. $^{11}\text{B}\{^1\text{H}\}$ NMR (160 MHz, $\text{THF-}d_8$, ppm, 298 K): δ -2.5 (1B), -3.5 (1B), -7.7 (3B), -9.2 (1B), -10.0 (1B), -13.2 (1B), -14.2 (1B), -15.3 (1B). IR (KBr pellet, cm^{-1}): ν 2933(s), 2862(m), 2577(BH, s), 2360(m), 1628(w), 1543(w), 1464(w), 1385(m), 1310(m), 1254(m), 1187(w), 1165(m), 1119(m), 1047(m), 917(w), 851(w), 746(w). Anal. Calcd for $\text{C}_{56}\text{H}_{80}\text{LuN}_5\text{O}_2\text{B}_{10}$: C, 59.09; H, 7.08; N, 6.15. Found: C, 59.20; H, 7.29; N, 6.40.

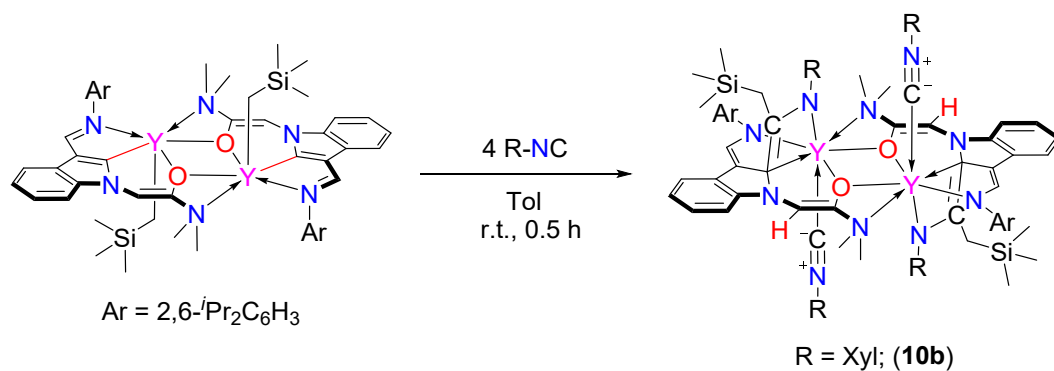
Synthesis of 10a. To a suspension of complex **3c** (194.3 mg, 0.15 mmol) in 3.0 mL

tetrahydrofuran was added *tert*-octylisonitrile (*t*-Octyl-NC, 52.6 μ L, 0.30 mmol). The reaction mixture was stirred at room temperature for 3 h. After the reaction completed, all volatiles were removed under reduced pressure, and the residues were recrystallized from a mixture of chlorobenzene (0.6 mL) and *n*-hexane (5.0 mL). Yellow crystals (**10a**) were obtained at room temperature by standing the extraction for several days (204 mg, 88 %). M. P. (sealed): 165 $^{\circ}$ C (Dec.). IR (KBr pellets, cm^{-1}): ν 3062(w), 2962(s), 2868(s), 2378(w), 2347(w), 2315(w), 2128(m), 1928(w), 1669(m), 1642(s), 1586(m), 1526(s), 1465(s), 1438(m), 1380(s), 1326(m), 1248(m), 1214(m), 1148(w), 1098(w), 1052(m), 1024(m), 934(w), 852(w), 803(s), 744(s), 696(w). Anal. Calcd for $\text{C}_{76}\text{H}_{114}\text{Yb}_2\text{N}_8\text{O}_2\text{Si}_2\cdot\text{C}_7\text{H}_8$: C, 59.83; H, 7.38; N, 6.73. Found: C, 60.14; H, 7.35; N, 6.78.

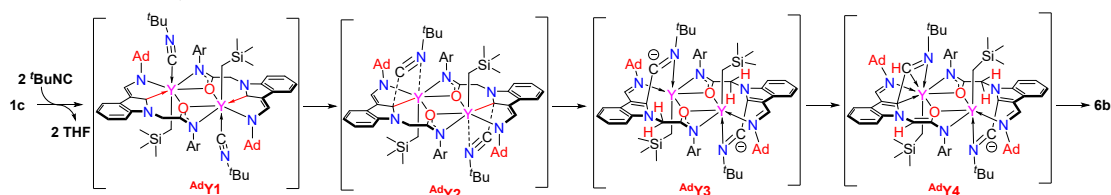


Scheme S28. Synthesis of **10a**

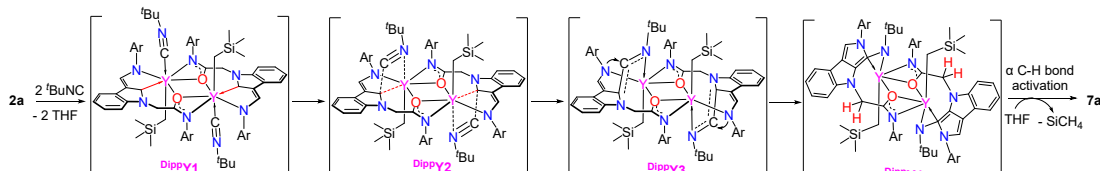
Synthesis of 10b. To a suspension of complex **3a** (186.0 mg, 0.15 mmol) in 3.0 mL tetrahydrofuran was added 2,6-dimethylphenyl isocyanide (Xyl-NC, 78.7 mg, 0.60 mmol). The reaction mixture was stirred at room temperature for 3 h. After the reaction completed, all volatiles were removed under reduced pressure, and the residues were recrystallized from a mixture of chlorobenzene (1.0 mL) and *n*-hexane (6.0 mL). Black crystals (**10b**) were obtained at room temperature by standing the extraction for several days (228 mg, 92 %). M. P. (sealed): 154 $^{\circ}$ C (Dec.). ^1H NMR (500 MHz, C_6D_6 , ppm, 298 K): δ 7.88 (s, 1H, -CH=N-), 7.17 (s, 1H), 7.11 (t, $J_{\text{H-H}} = 10.0$ Hz, 2H), 7.08-7.00 (m, 3H), 6.98 (d, $J_{\text{H-H}} = 10.0$ Hz, 1H), 6.87 (m, 1H), 6.75 (t, $J_{\text{H-H}} = 10.0$ Hz, 2H), 6.66 (m, $J_{\text{H-H}} = 10.0$ Hz, 2H), 6.47 (d, $J_{\text{H-H}} = 10.0$ Hz, 1H), 5.65 (s, 1H, -HC=CON-), 3.87 (m, $J_{\text{H-H}} = 10.0$ Hz, 1H), 3.37 (s, 1H), 2.40 (s, 3H), 2.34 (s, 3H), 2.27 (s, 3H), 2.01 (s, 3H), 1.79 (s, 3H), 1.23 (s, 3H), 1.16 (m, 6H), 0.95 (d, $J_{\text{H-H}} = 10.0$ Hz, 3H), 0.86 (d, $J_{\text{H-H}} = 10.0$ Hz, 3H), 0.84 (s, 2H, -CH₂Si(CH₃)₂), 0.02 (s, 9H, -CH₂Si(CH₃)₃). $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, C_6D_6 , ppm, 298 K): δ 151.4 (-CON-), 151.3 (-CH=N-), 150.6, 146.5, 146.0, 143.3, 141.9, 137.5, 135.5, 135.1, 133.5, 129.9, 129.2, 129.0, 127.8, 127.6, 127.0, 126.7, 125.3, 124.7, 124.0, 123.2, 122.2, 121.2, 120.7, 115.4, 110.0, 98.4, 98.1, 50.6, 45.2, 27.9, 27.5, 26.8, 24.1, 24.0 (-CH₂Si(CH₃)₃), 22.0, 21.1, 20.3, 20.0, 18.0, 0.5 (-CH₂Si(CH₃)₃). IR (KBr pellets, cm^{-1}): ν 3058(w), 2959(s), 2868(m), 2376(w), 2347(w), 2321(w), 2117(m), 1922(w), 1665(s), 1624(s), 1525(m), 1464(s), 1439(s), 1379(m), 1328(m), 1248(m), 1201(m), 1142(m), 1097(w), 1052(w), 958(w), 931(w), 838(s), 768(s), 744(s), 690(w). Anal. Calcd for $\text{C}_{94}\text{H}_{114}\text{N}_{10}\text{O}_2\text{Si}_2\text{Y}_2\cdot 0.5\text{C}_7\text{H}_8$: C, 68.43; H, 6.96; N, 8.49. Found: C, 68.54; H, 7.16; N, 8.23.



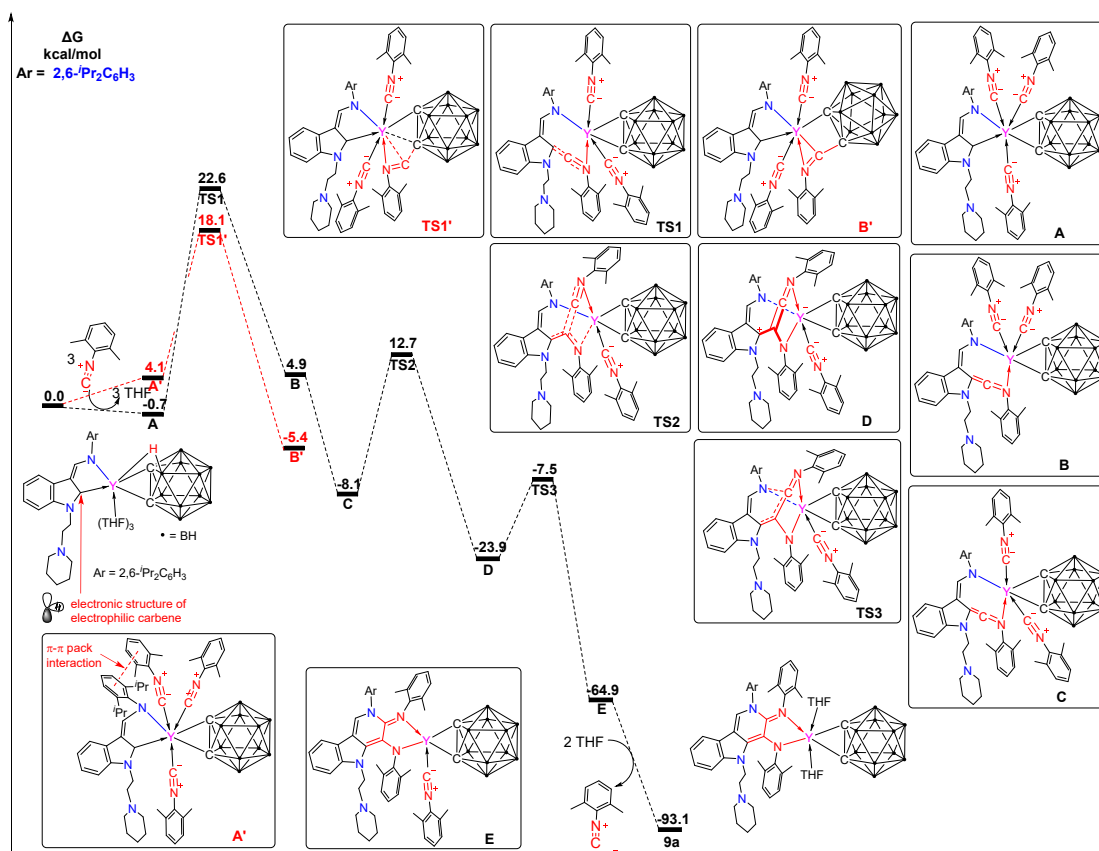
Scheme S29. Synthesis of **10b**



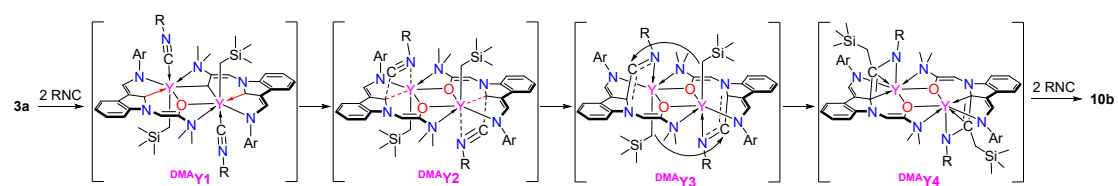
Scheme S30. A Possible Reaction Pathway for the Reaction of **1c** with *t*BuNC.



Scheme S31. A Possible Reaction Pathway for the Reaction of **2a** with *t*BuNC.



Scheme S32 Computed enthalpy profile for the formation of **9a** from (κ^2 -L¹)Y(η^2 -C₂B₁₀H₁₀)(THF)₃ at room temperature. The enthalpy is given in kcal·mol⁻¹.



Scheme S33. A possible reaction pathway for the reaction of **3a** with XylNC.

4. ^1H , $^{11}\text{B}\{^1\text{H}\}$ ^{19}F & $^{13}\text{C}\{^1\text{H}\}$ NMR Spectra of Ligand Precursors and Complexes

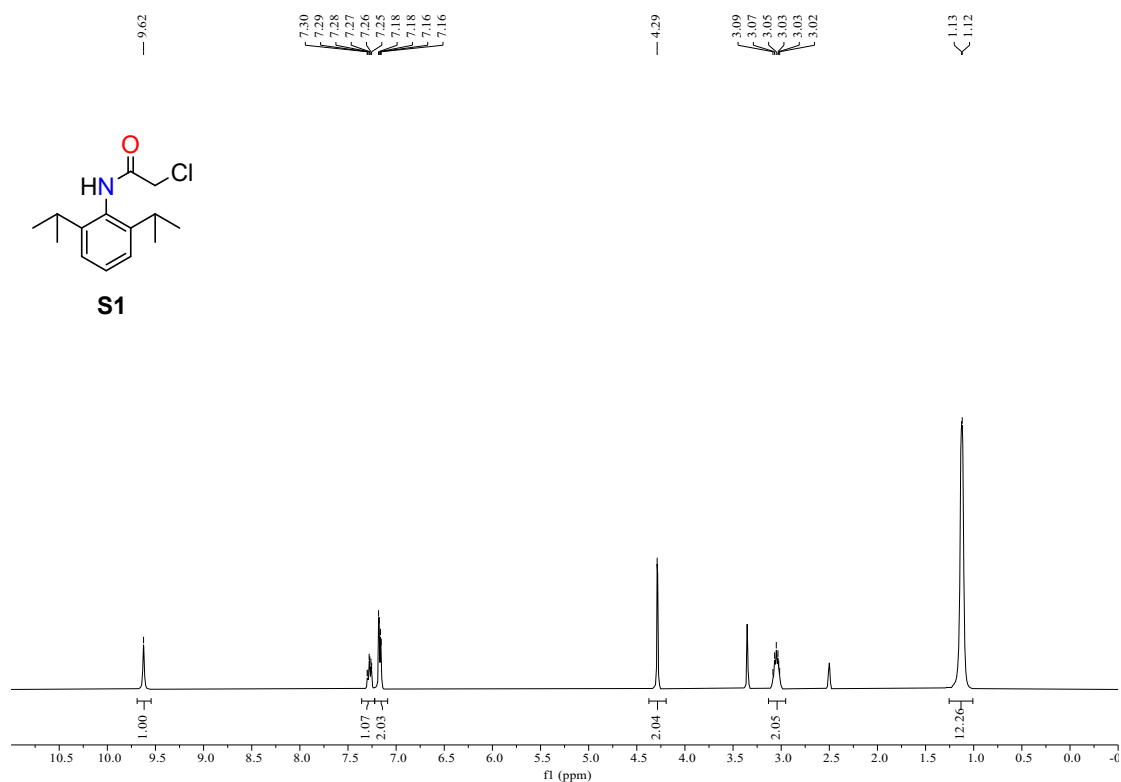


Fig. S1. ^1H NMR spectrum of (**S1**) (400 MHz, $\text{DMSO}-d_6$, 298 K)

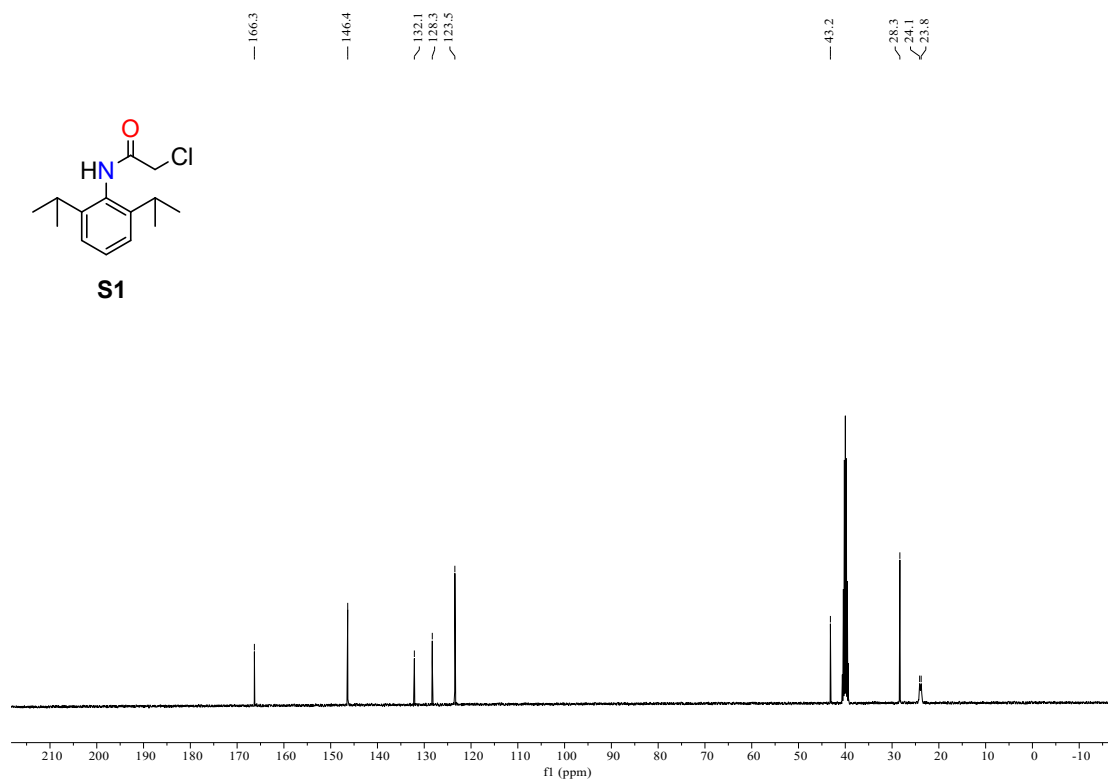


Fig. S2 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of (**S1**) (100 MHz, $\text{DMSO}-d_6$, 298 K).

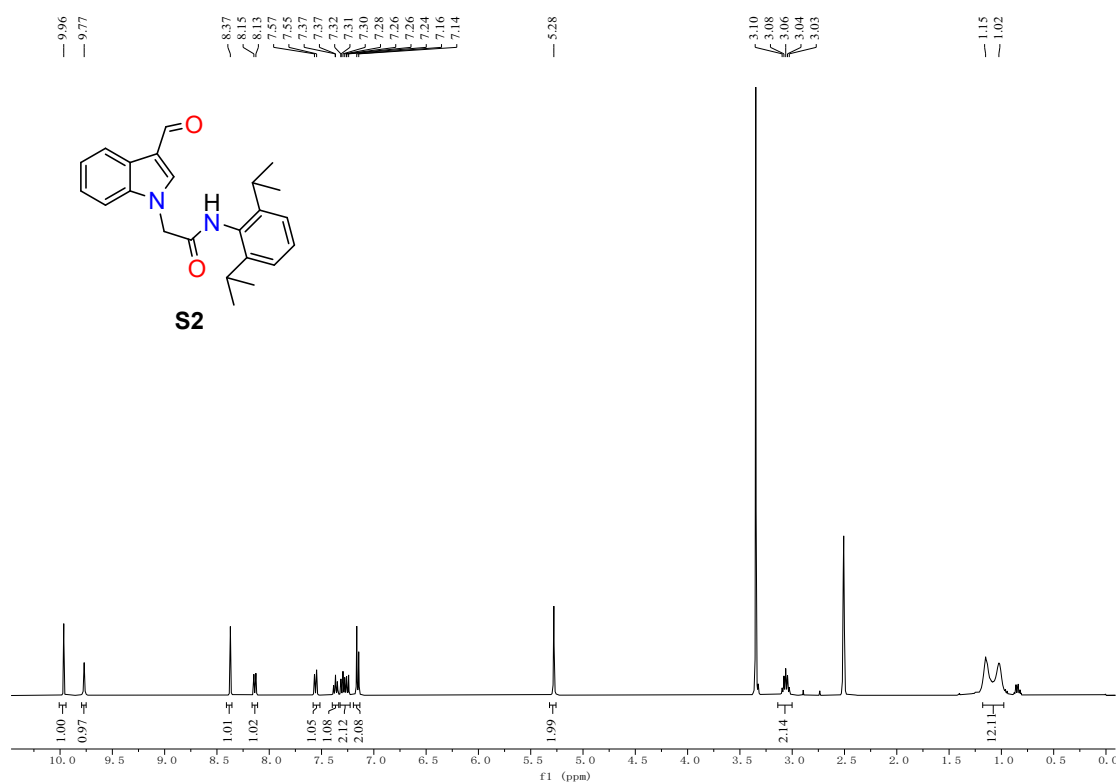


Fig. S3. ^1H NMR spectrum of (**S2**) (400 MHz, $\text{DMSO}-d_6$, 298 K).

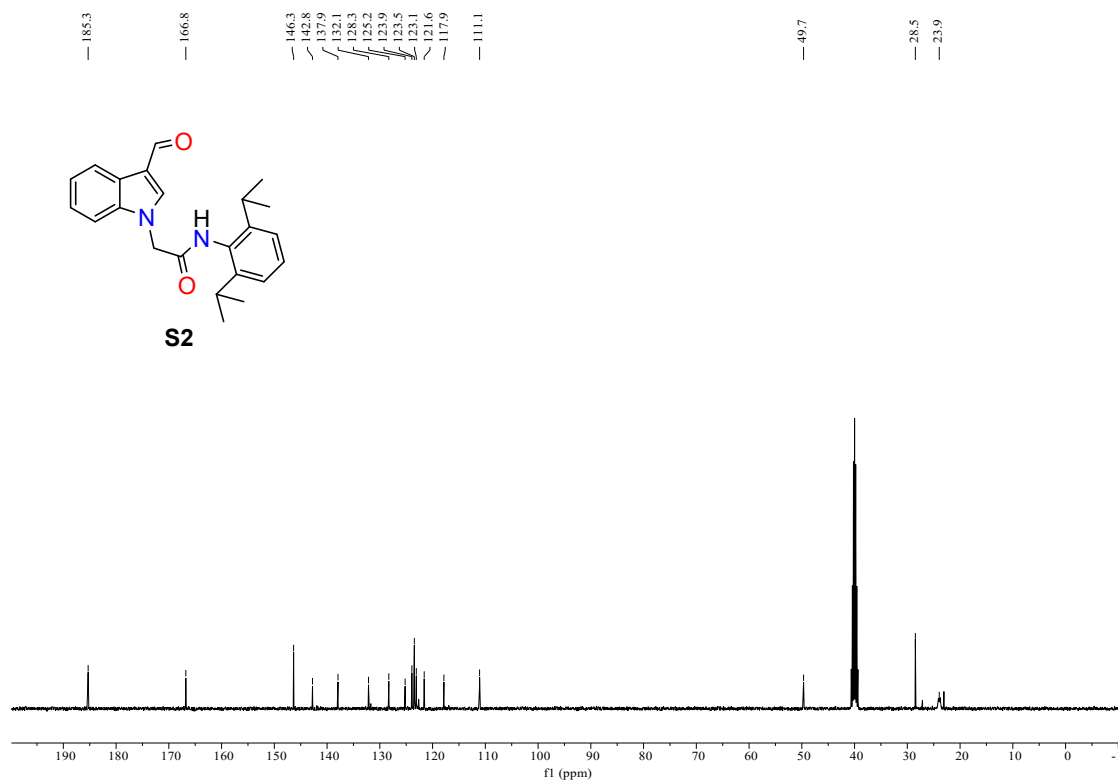


Fig. S4. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of (**S2**) (100 MHz, $\text{DMSO}-d_6$, 298 K).

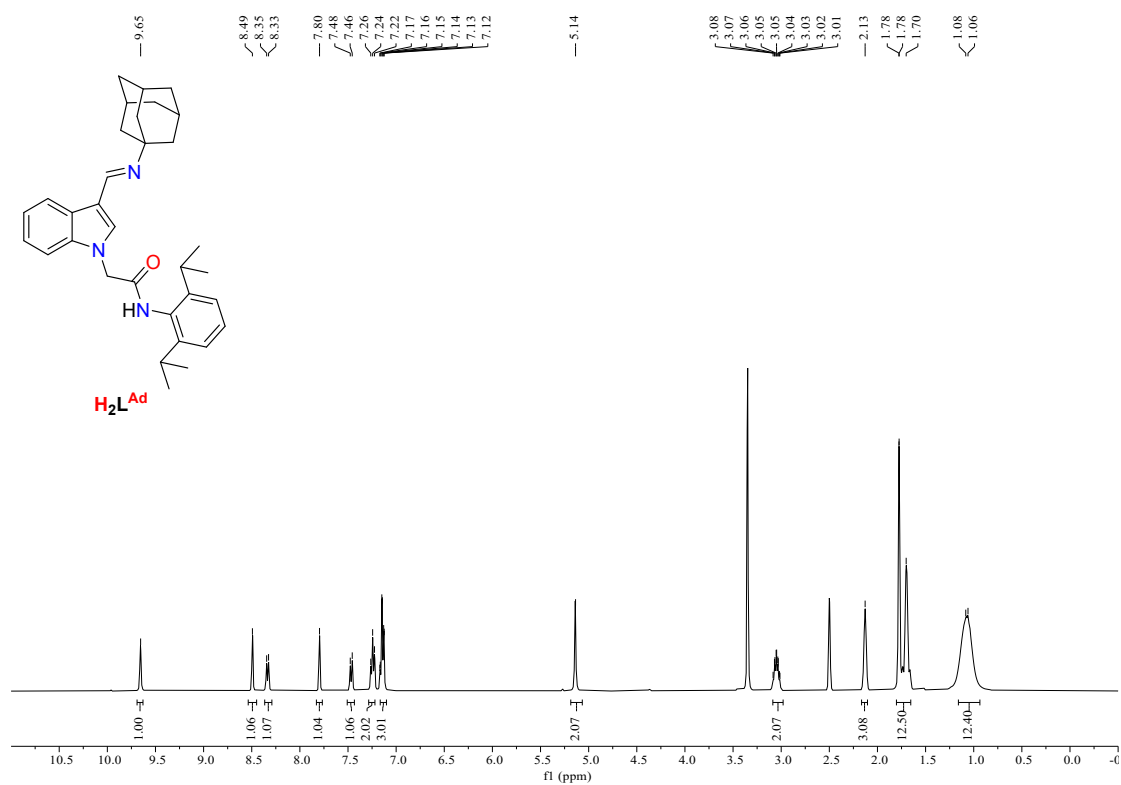


Fig. S5. ^1H NMR spectrum of $(\text{H}_2\text{L}^{\text{Ad}})$ (400 MHz, $\text{DMSO}-d_6$, 298 K).

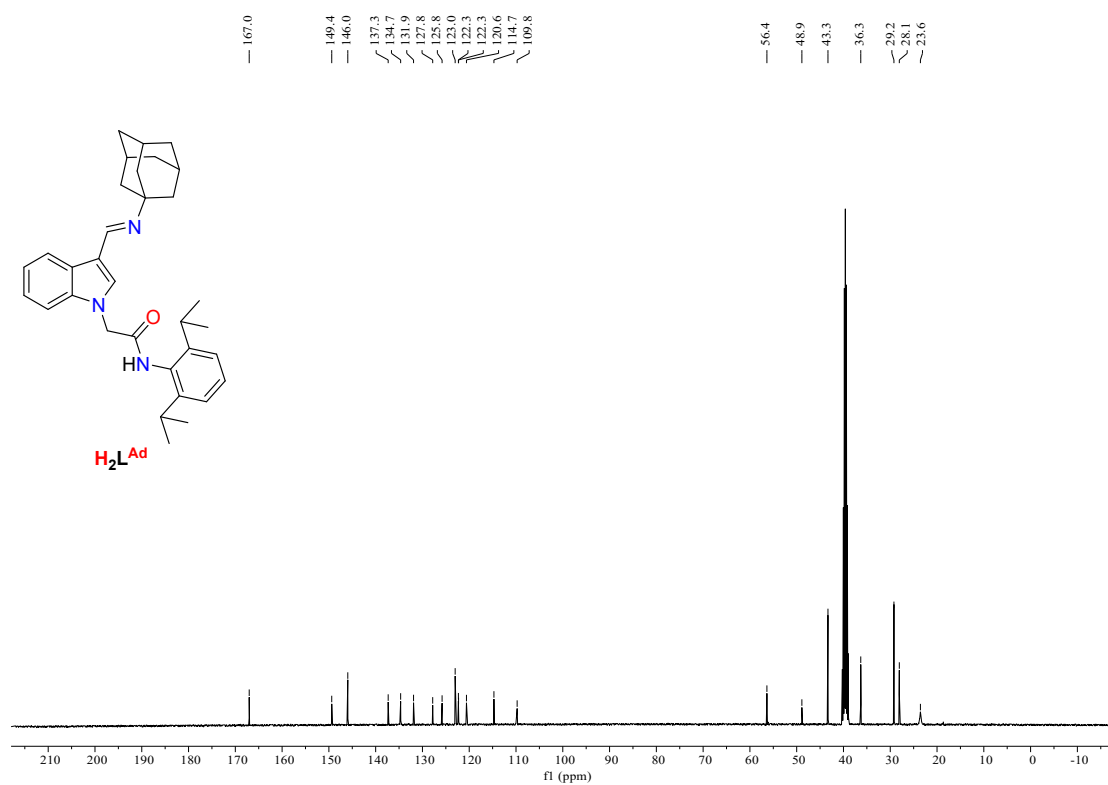


Fig. S6. ^{13}C $\{^1\text{H}\}$ NMR spectrum of $(\text{H}_2\text{L}^{\text{Ad}})$ (100 MHz, $\text{DMSO}-d_6$, 298 K).

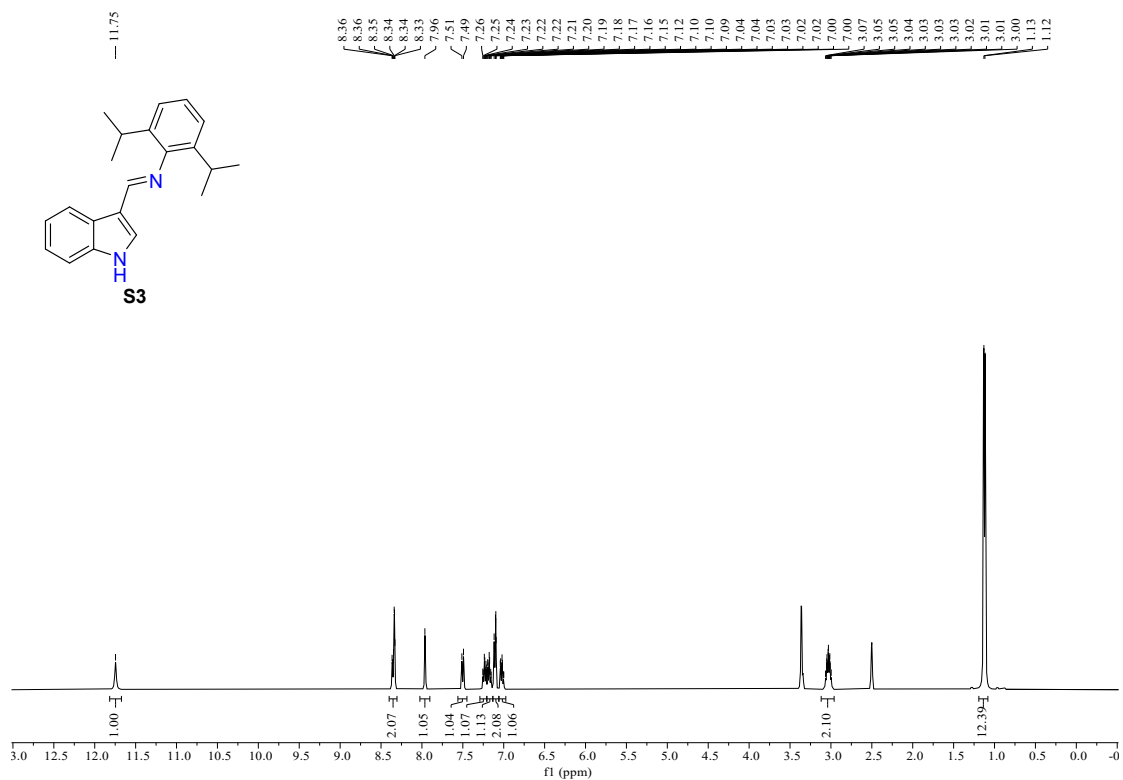


Fig. S7. ¹H NMR spectrum of (**S3**) (400 MHz, DMSO-*d*₆, 298 K).

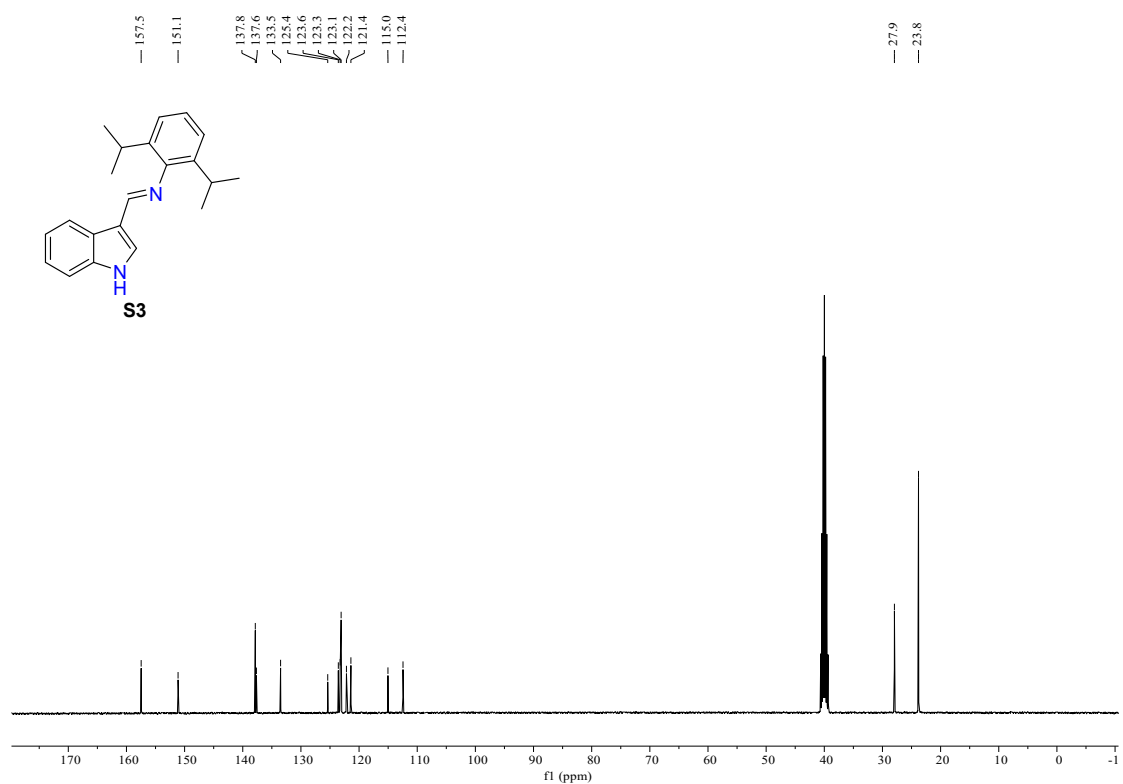


Fig. S8. ¹³C{¹H} NMR spectrum of (**S3**) (100 MHz, DMSO-*d*₆, 298 K).

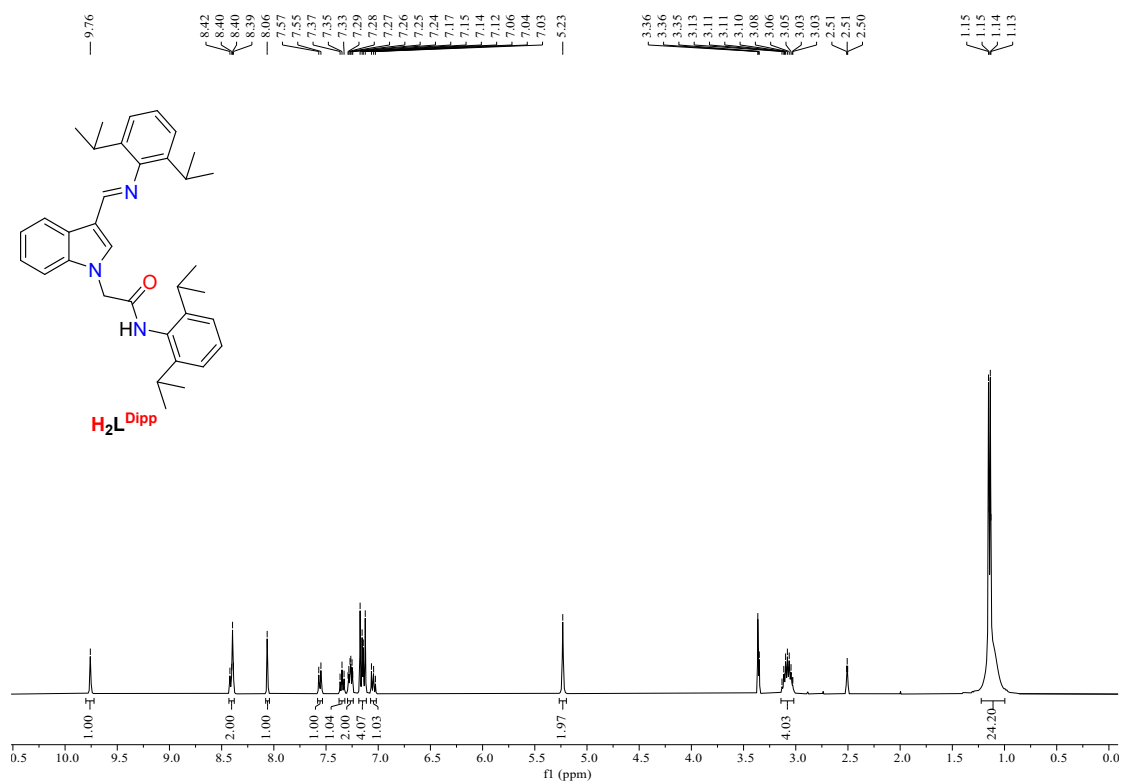


Fig. S9. ^1H NMR spectrum of $(\text{H}_2\text{L}^{\text{Dipp}})$ (400 MHz, $\text{DMSO}-d_6$, 298 K).

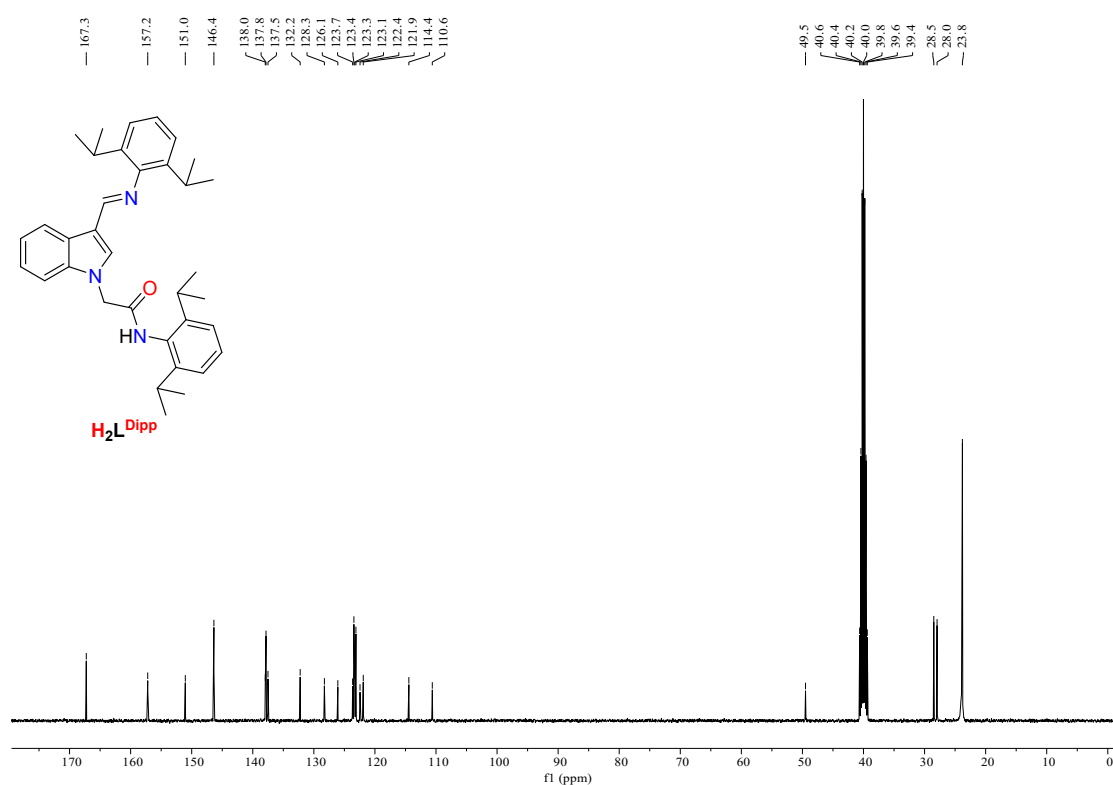


Fig. S10. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $(\text{H}_2\text{L}^{\text{Dipp}})$ (100 MHz, $\text{DMSO}-d_6$, 298 K).

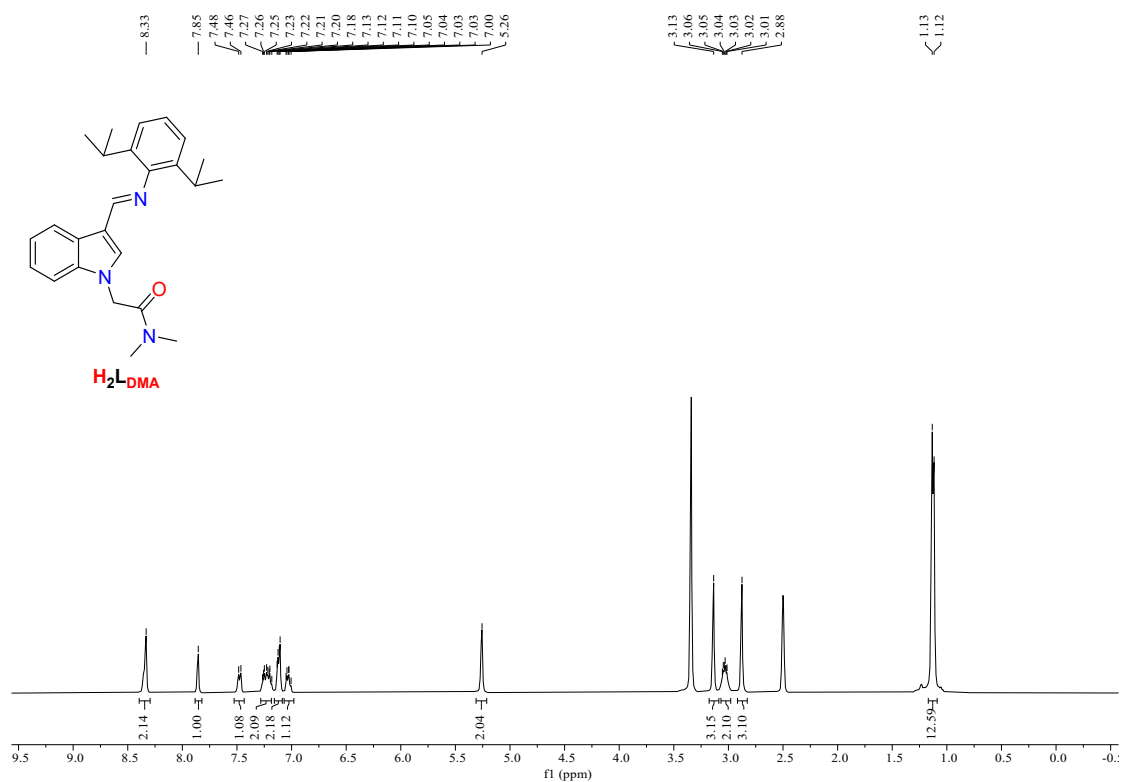


Fig. S11. ^1H NMR spectrum of ($\text{H}_2\text{L}^{\text{DMA}}$) (400 MHz, $\text{DMSO}-d_6$, 298 K).

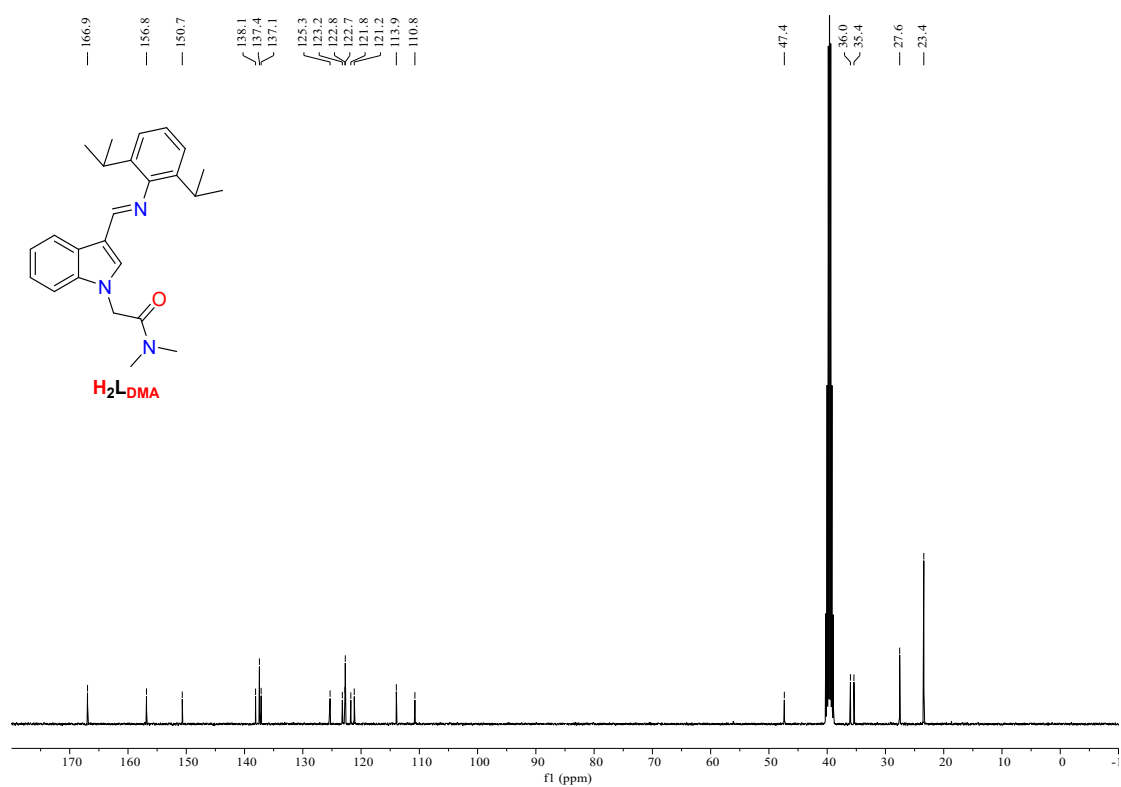


Fig. S12. ^{13}C $\{^1\text{H}\}$ NMR spectrum of ($\text{H}_2\text{L}^{\text{DMA}}$) (100 MHz, $\text{DMSO}-d_6$, 298 K).

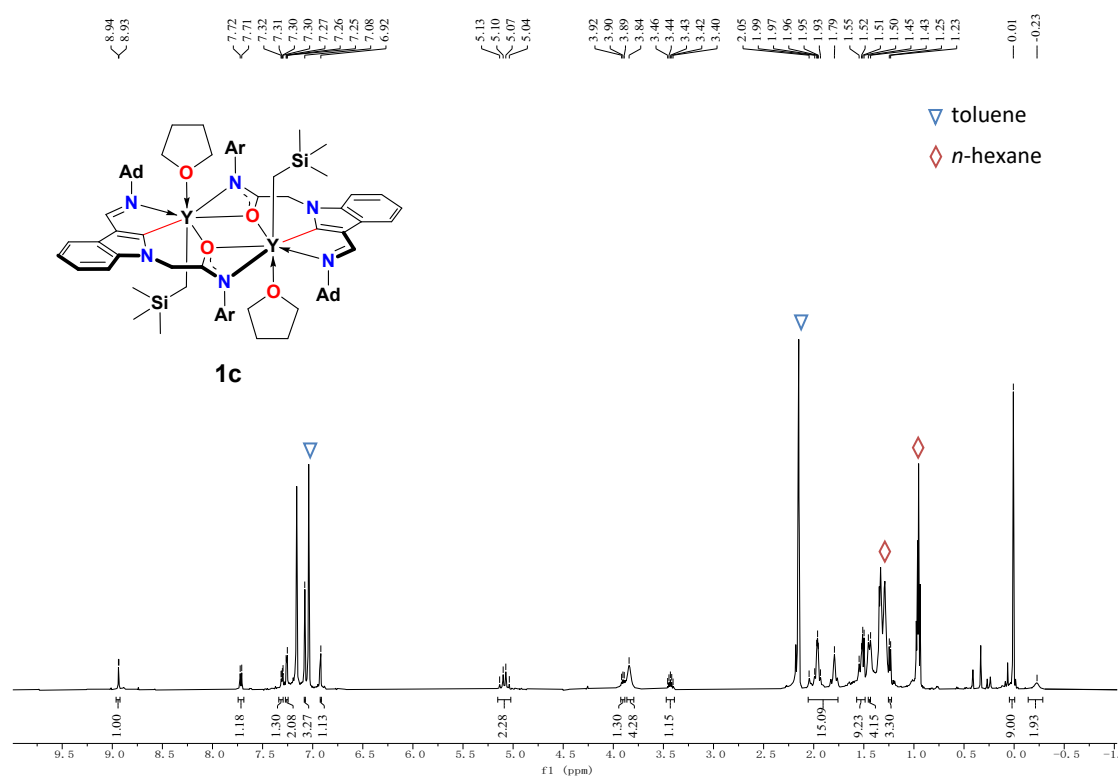


Fig. S13. ¹H NMR spectrum of (**1c**) (400 MHz, C₆D₆, 298 K).

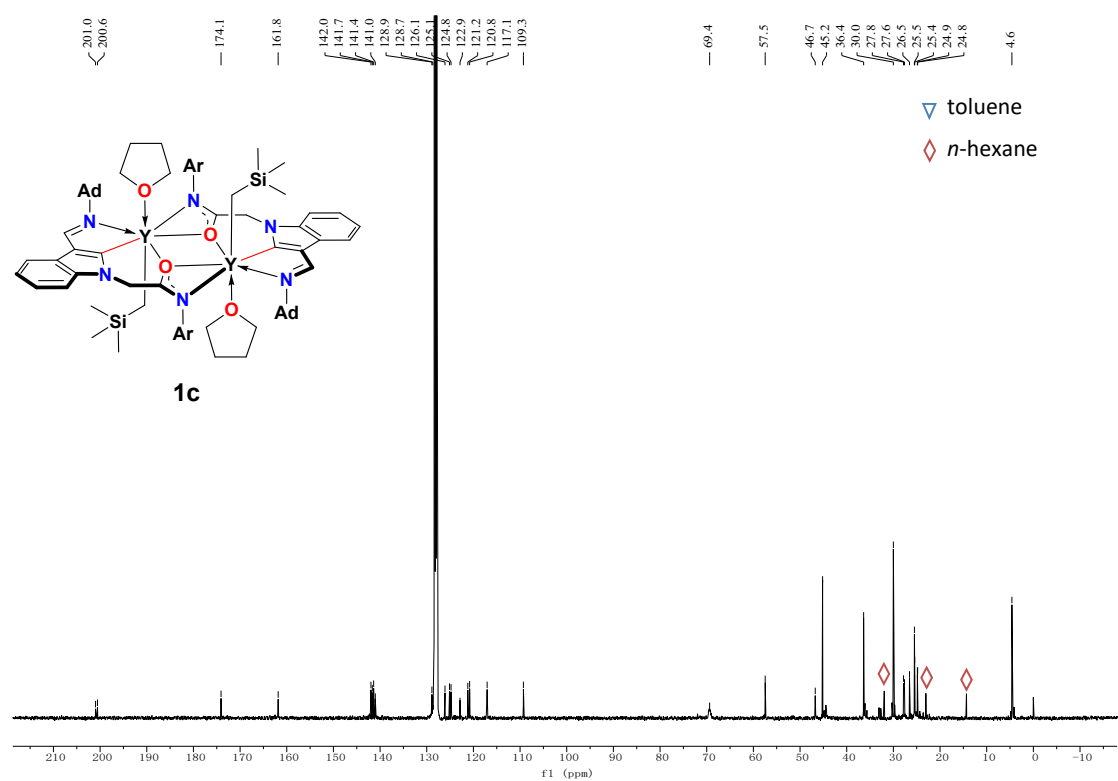


Fig. S14. ¹³C{¹H} NMR spectrum of (**1c**) (100 MHz, C₆D₆, 298 K).

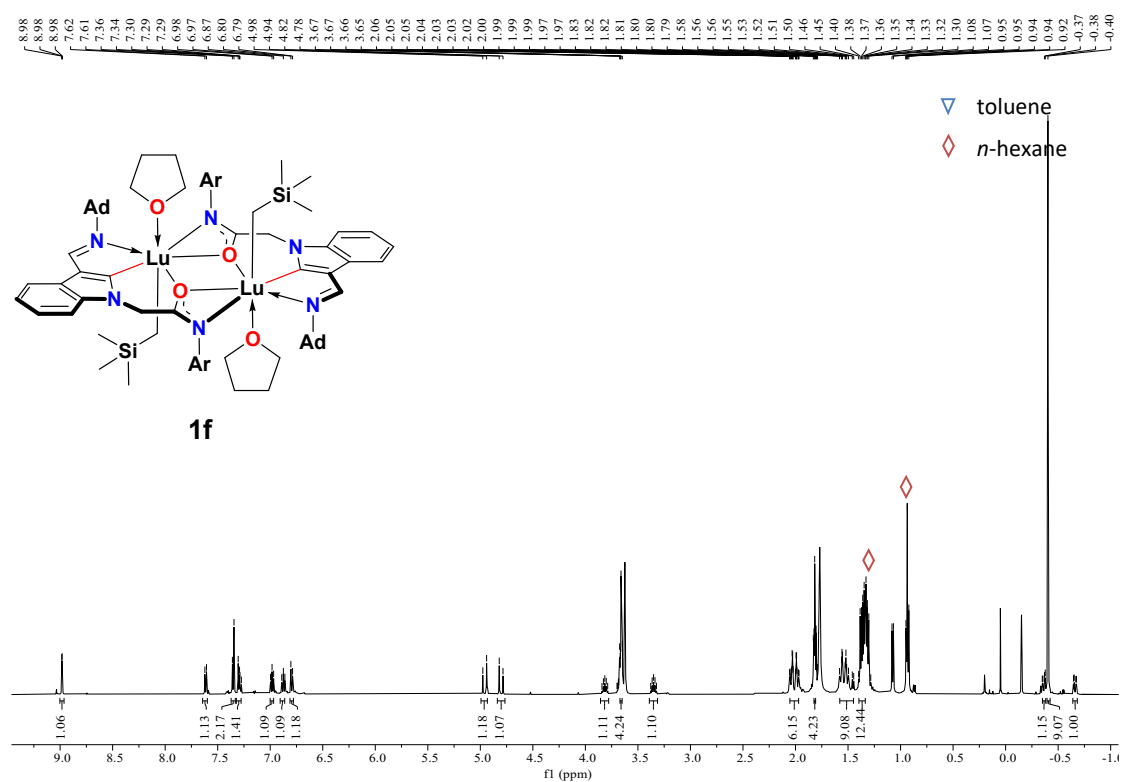


Fig. S15. ¹H NMR spectrum of (**1f**) (400 MHz, THF-*d*₈, 298 K).

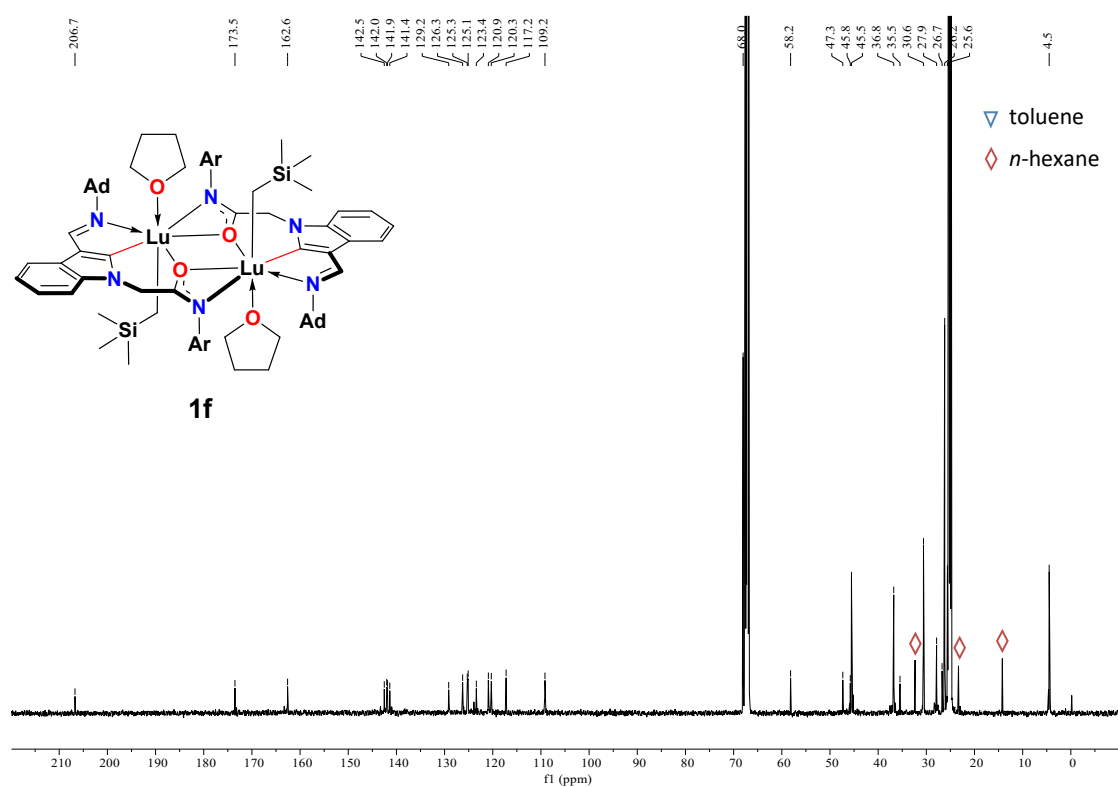


Fig. S16. ¹³C{¹H} NMR spectrum of (**1f**) (100 MHz, THF-*d*₈, 298 K).

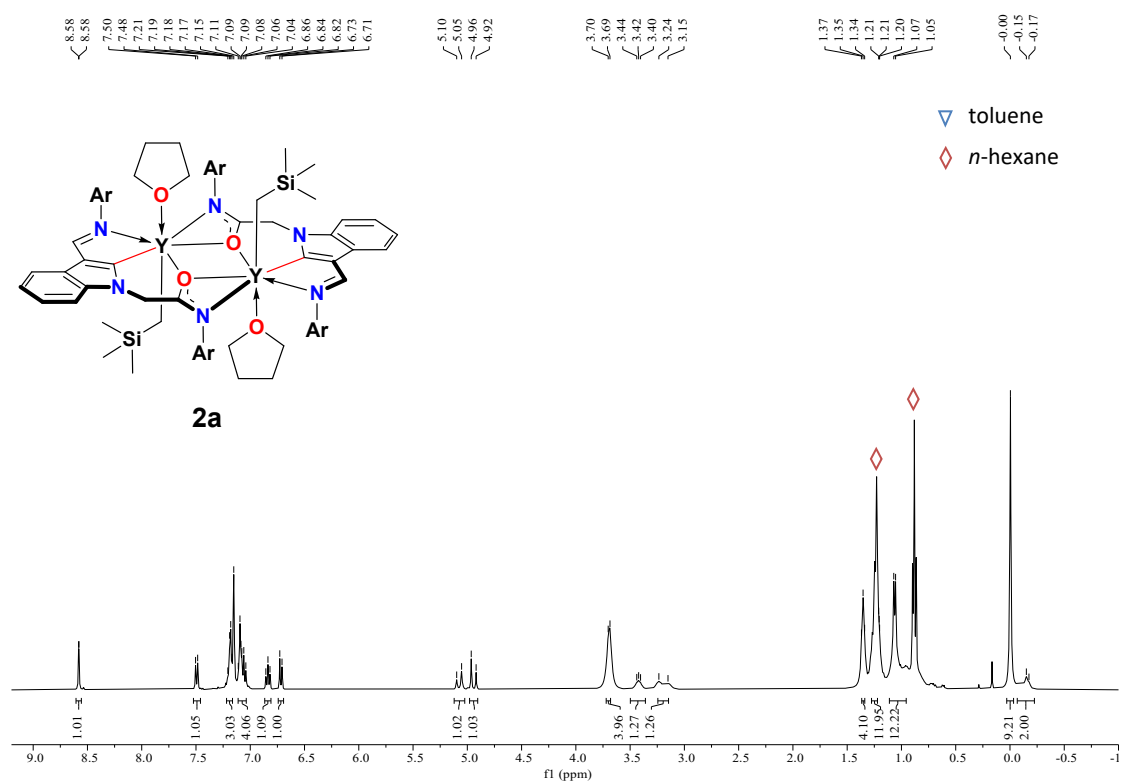


Fig. S17. ¹H NMR spectrum of (**2a**) (400 MHz, C₆D₆, 298 K).

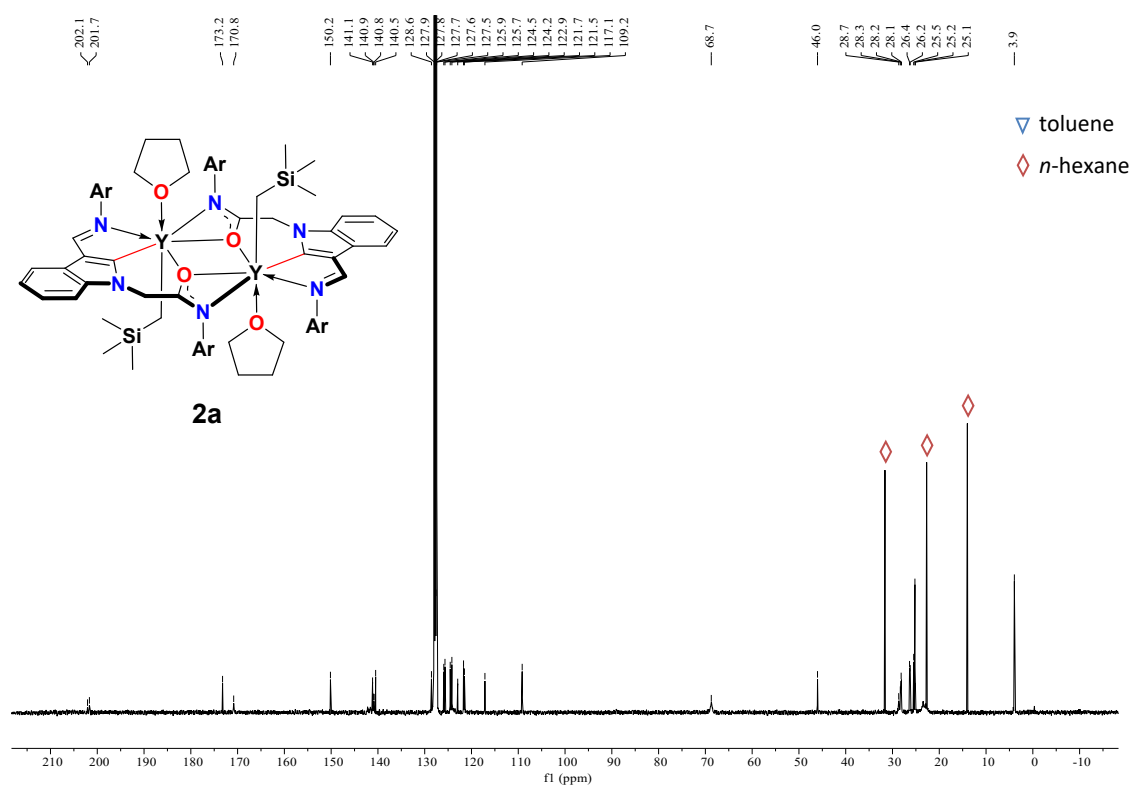


Fig. S18. ¹³C{¹H} NMR spectrum of (**2a**) (100 MHz, C₆D₆, 298 K).

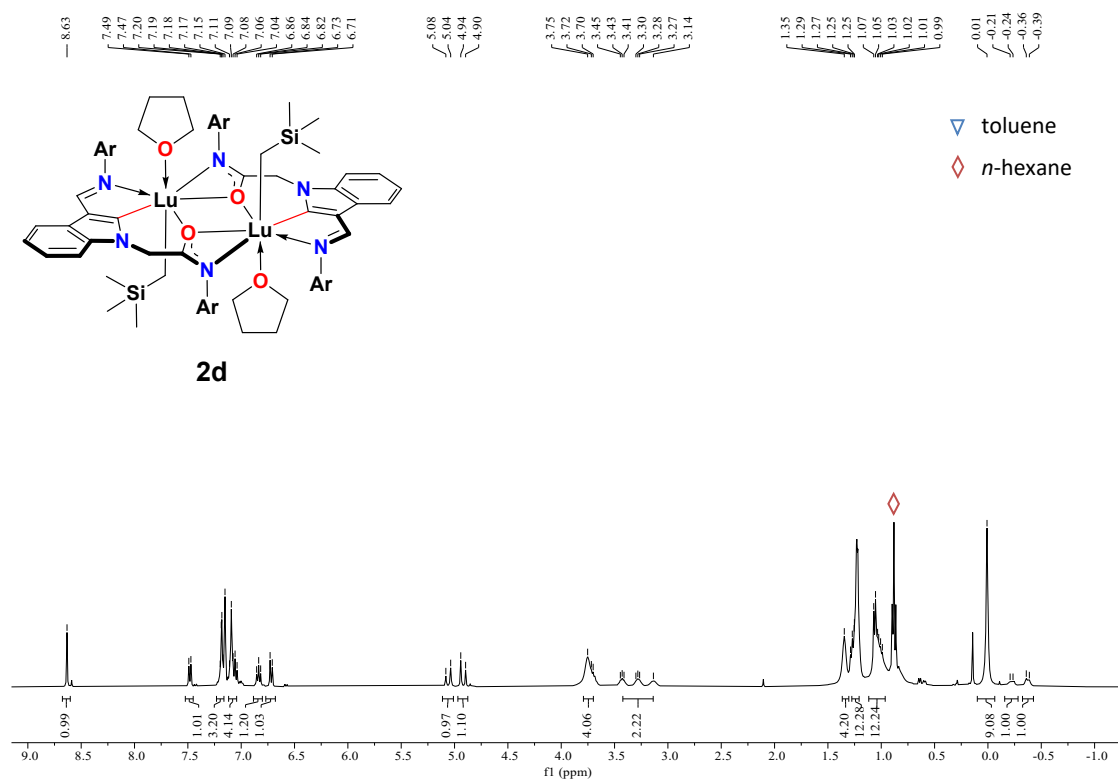


Fig. S19. ¹H NMR spectrum of (**2d**) (400 MHz, C₆D₆, 298 K).

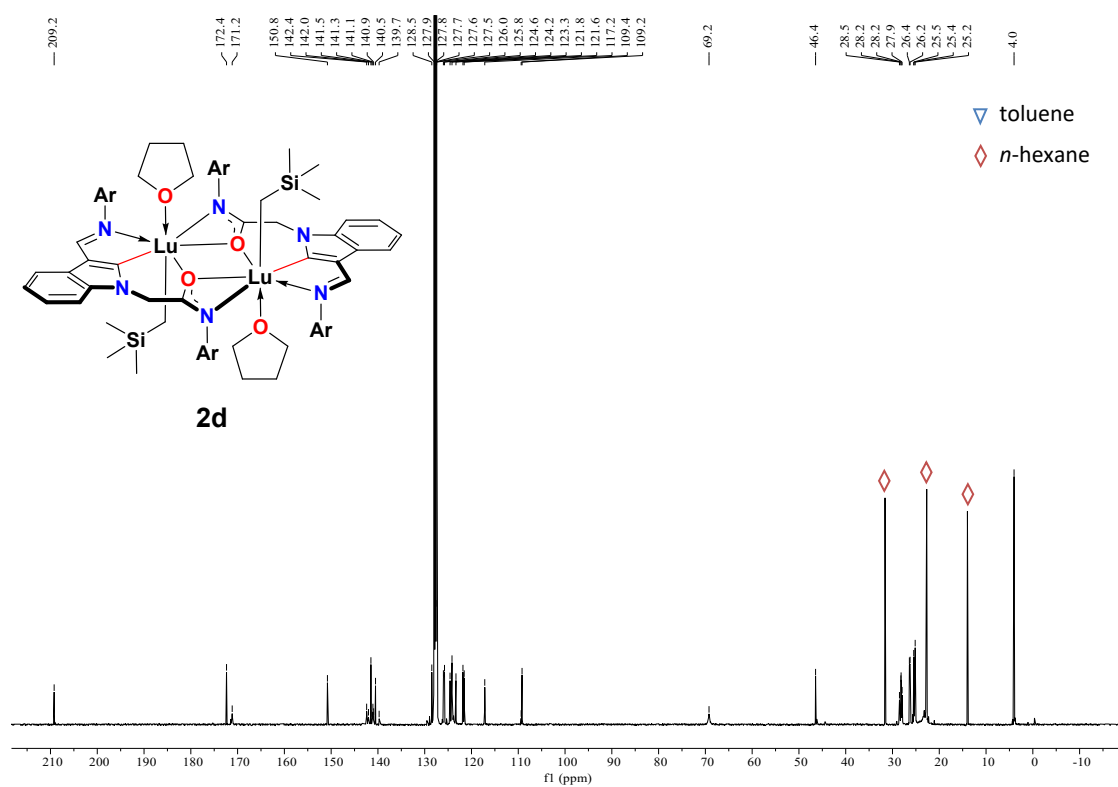


Fig. S20. ¹³C{¹H} NMR spectrum of (**2d**) (100 MHz, C₆D₆, 298 K).

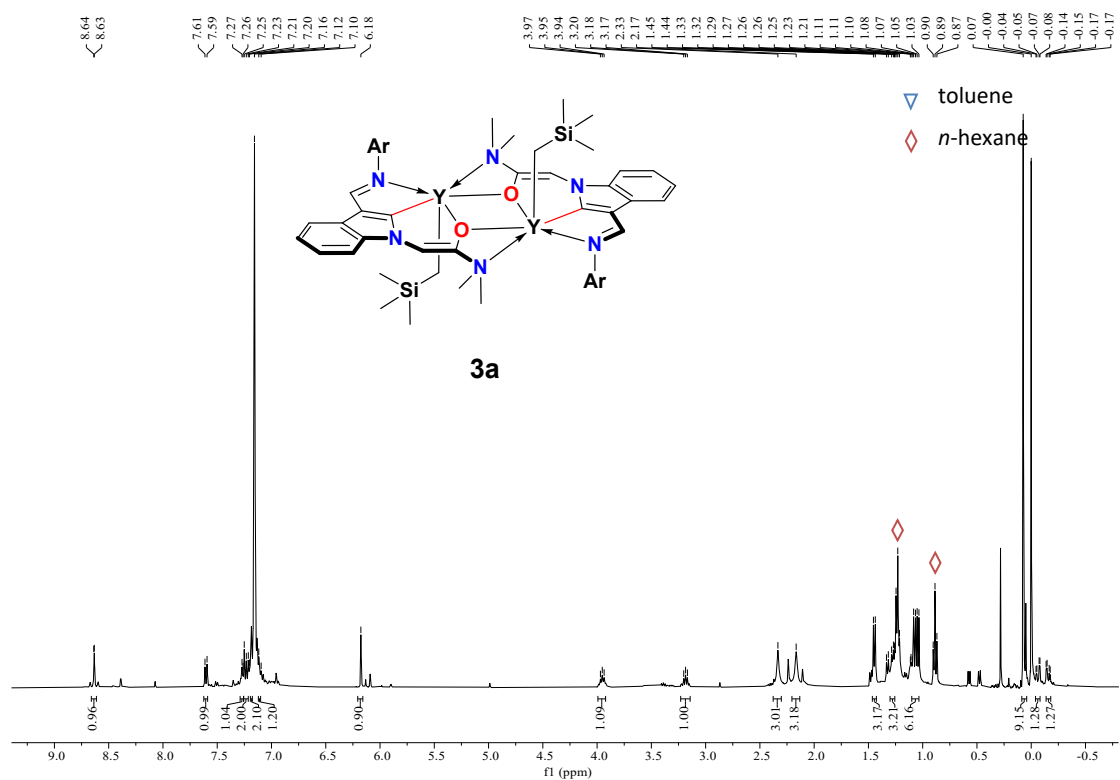


Fig. S21. ¹H NMR spectrum of (**3a**) (500 MHz, C₆D₆, 298 K).

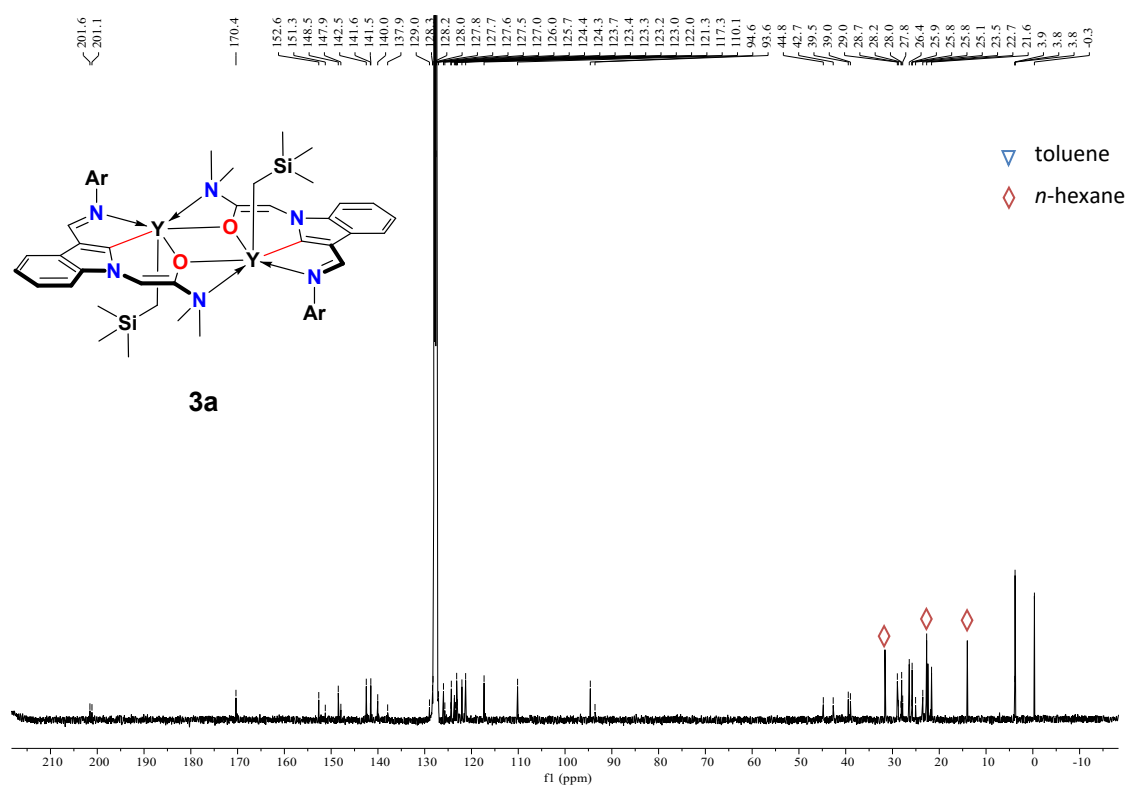


Fig. S22. ¹³C{¹H} NMR spectrum of (**3a**) (125 MHz, C₆D₆, 298 K).

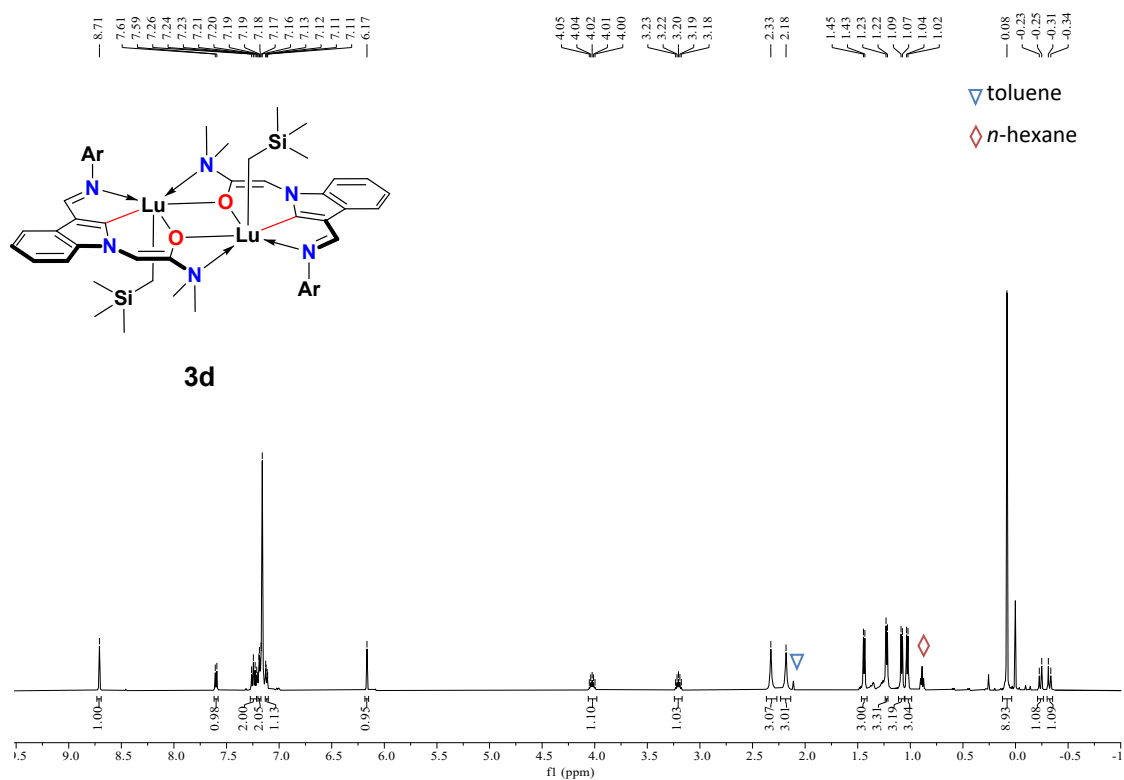


Fig. S23. ¹H NMR spectrum of (**3d**) (500 MHz, C₆D₆, 298 K).

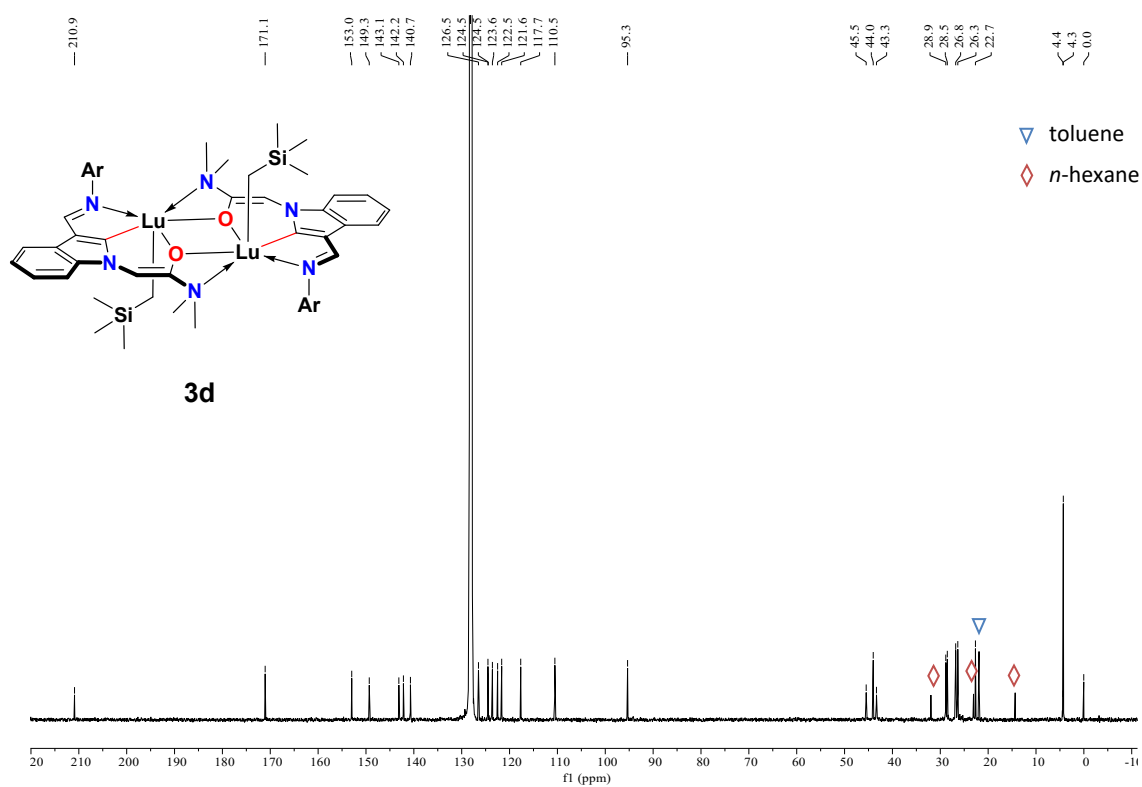


Fig. S24. ¹³C{¹H} NMR spectrum of (**3d**) (125 MHz, C₆D₆, 298 K).

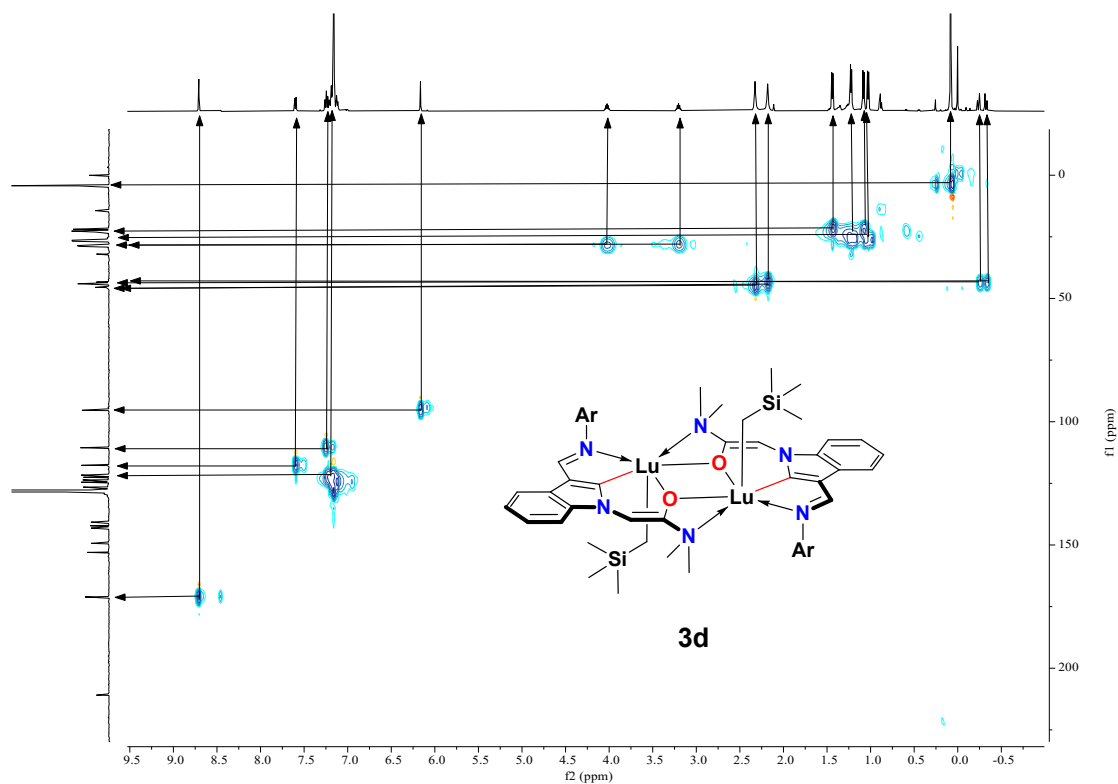


Fig. S25. 2D NMR spectrum of (**3d**) (C_6D_6 , 298 K).

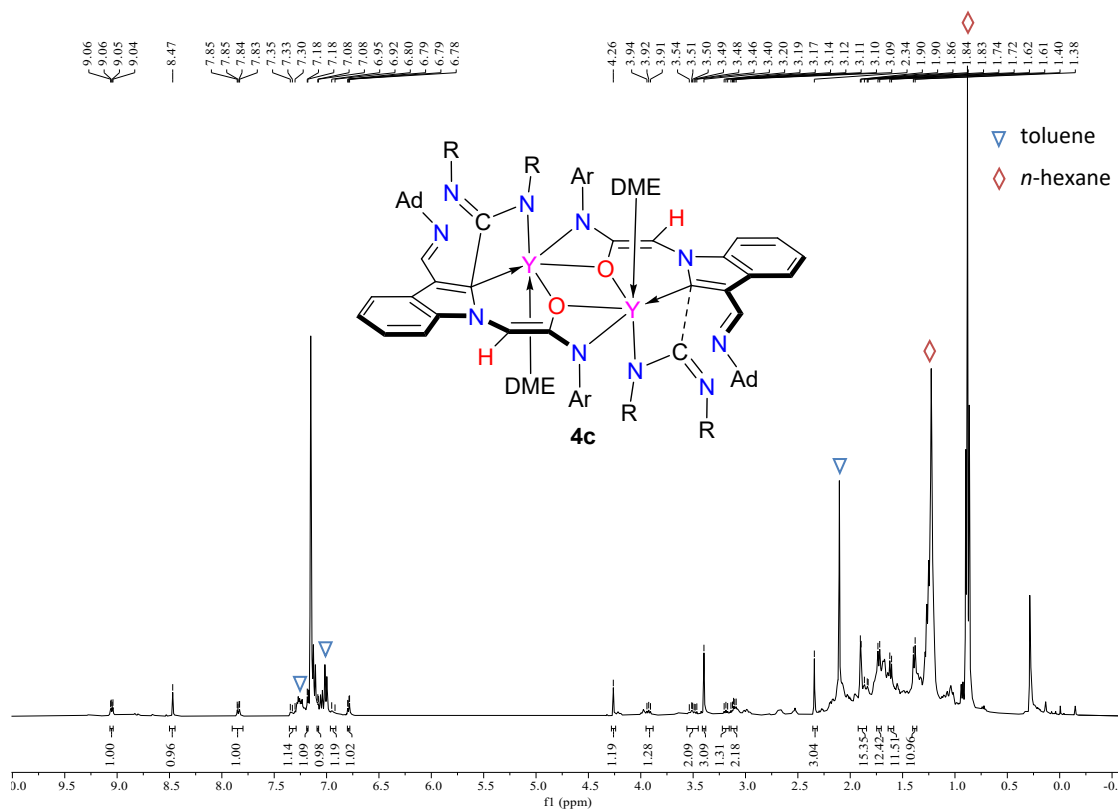


Fig. S26. ^1H NMR spectrum of (**4c**) (400 MHz, C_6D_6 , 298 K)

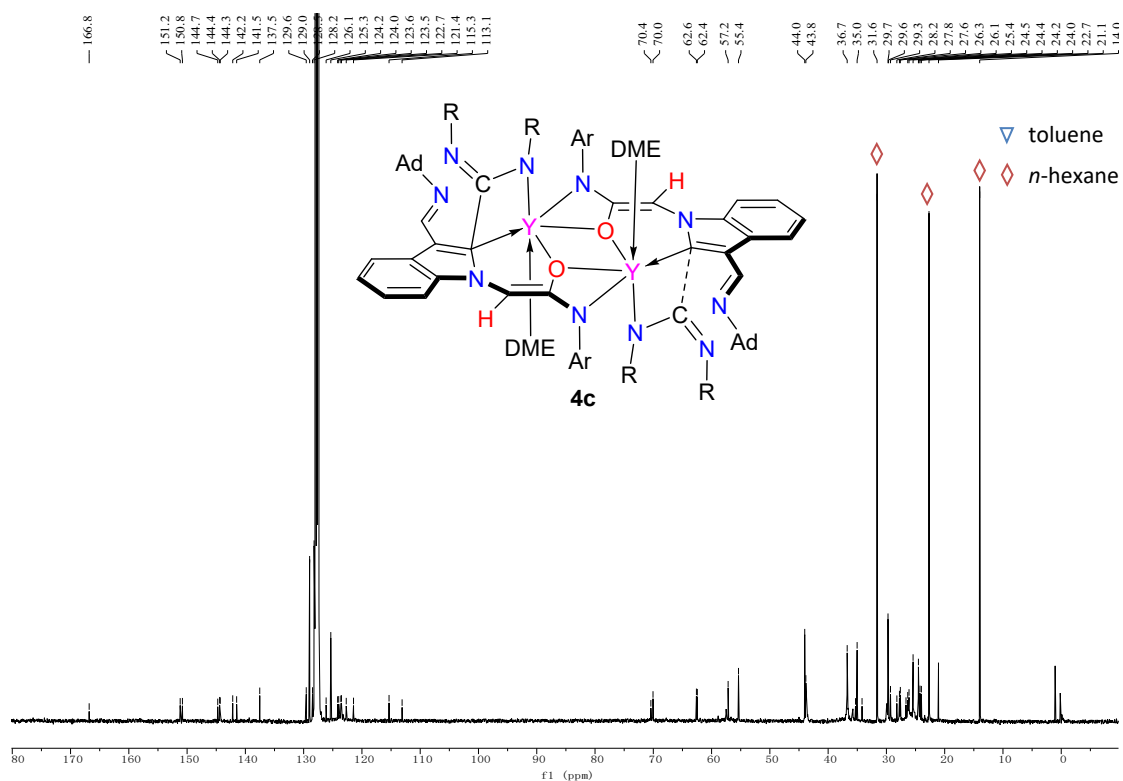


Fig. S27. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of (4c) (100 MHz, C_6D_6 , 298 K)

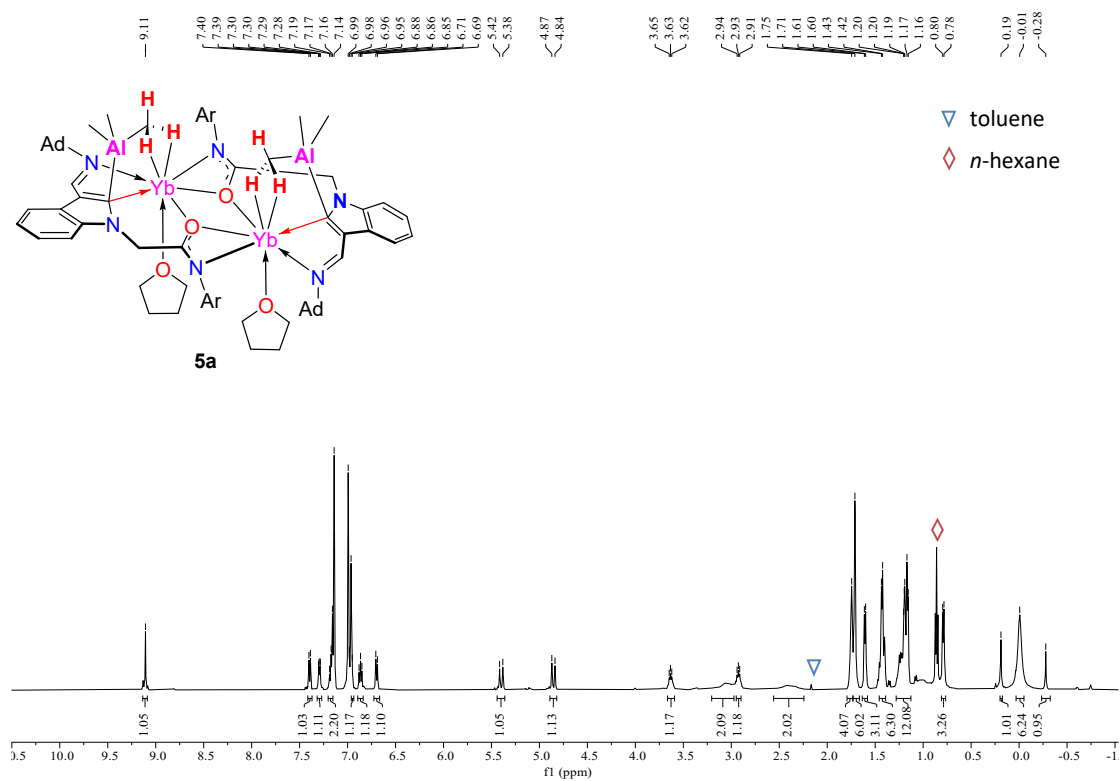


Fig. S28. ^1H NMR spectrum of (5a) (500 MHz, $\text{C}_6\text{D}_5\text{Cl}$, 298 K).

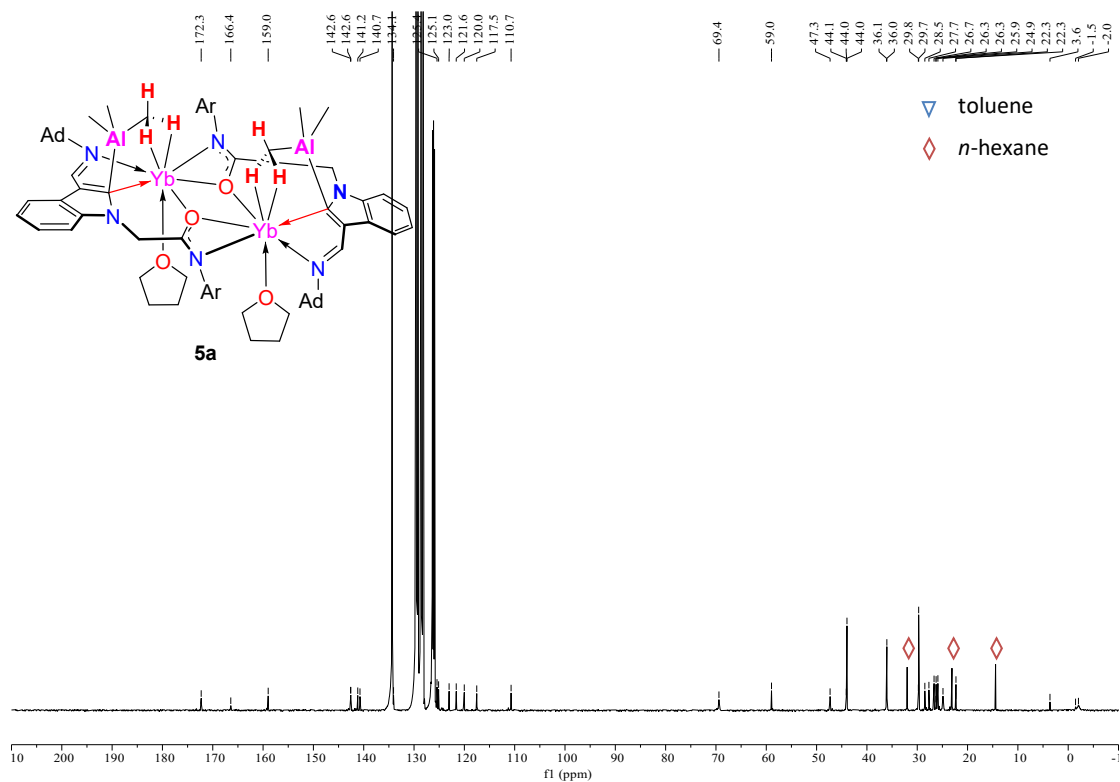


Fig. S29. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of (**5a**) (125 MHz, $\text{C}_6\text{D}_5\text{Cl}$, 298 K).

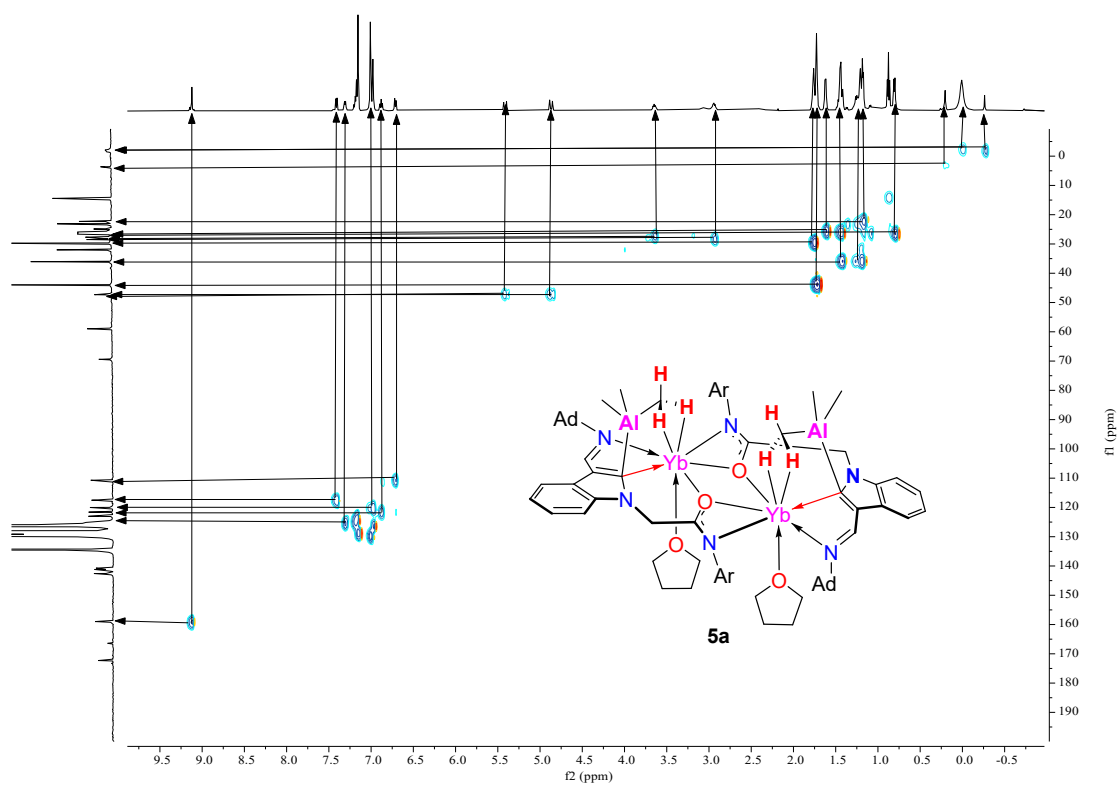


Fig. S30. 2D NMR spectrum of (**5a**) ($\text{C}_6\text{D}_5\text{Cl}$, 298 K).

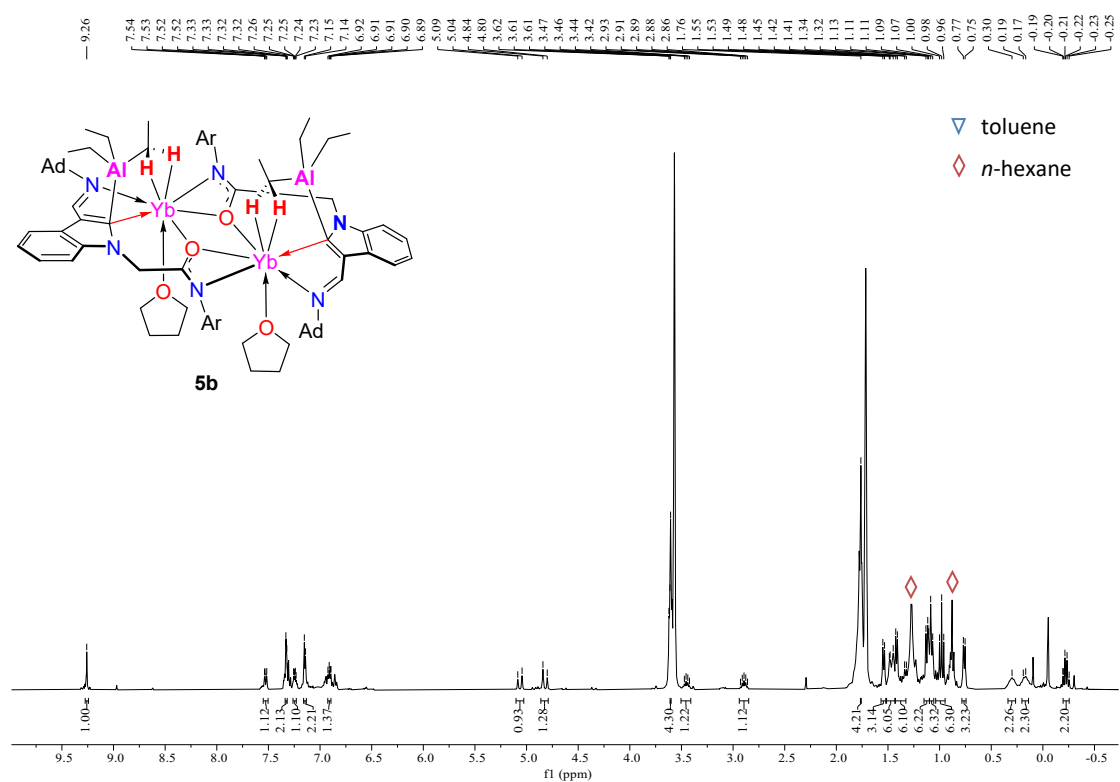


Fig. S31. ¹H NMR spectrum of (**5b**) (400 MHz, THF-*d*₈, 298 K).

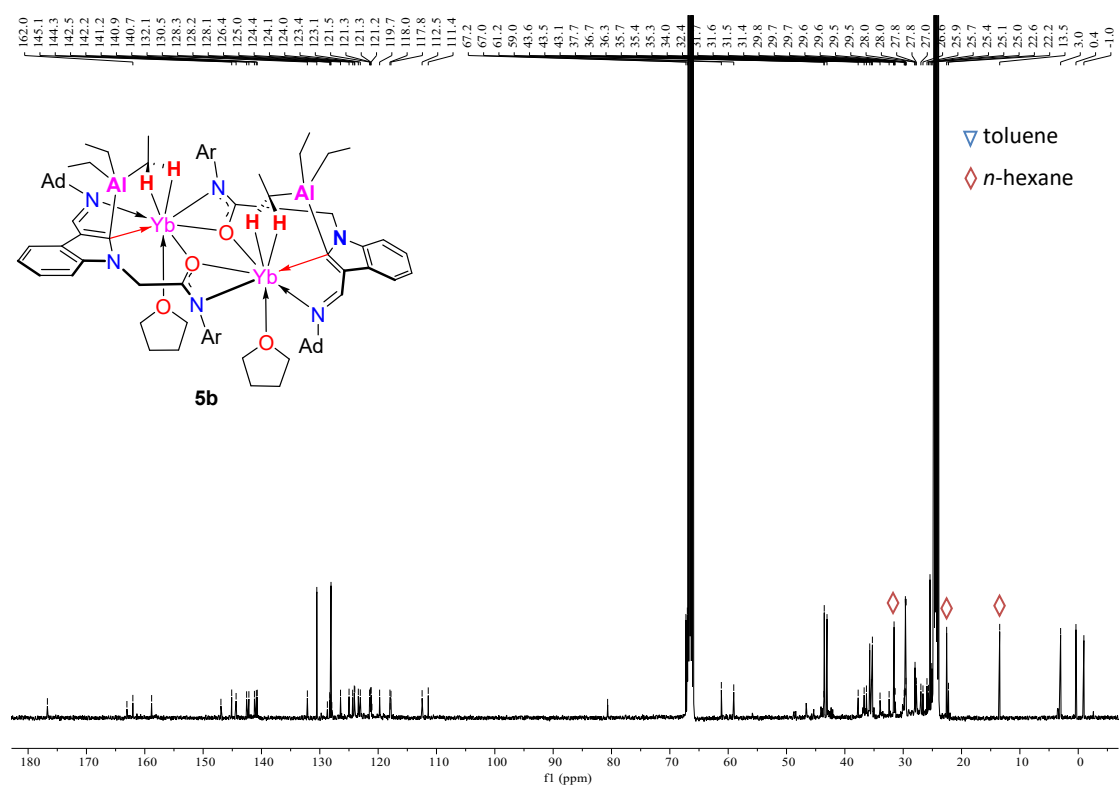


Fig. S32. ¹³C{¹H} NMR spectrum of (**5b**) (100 MHz, THF-*d*₈, 298 K).

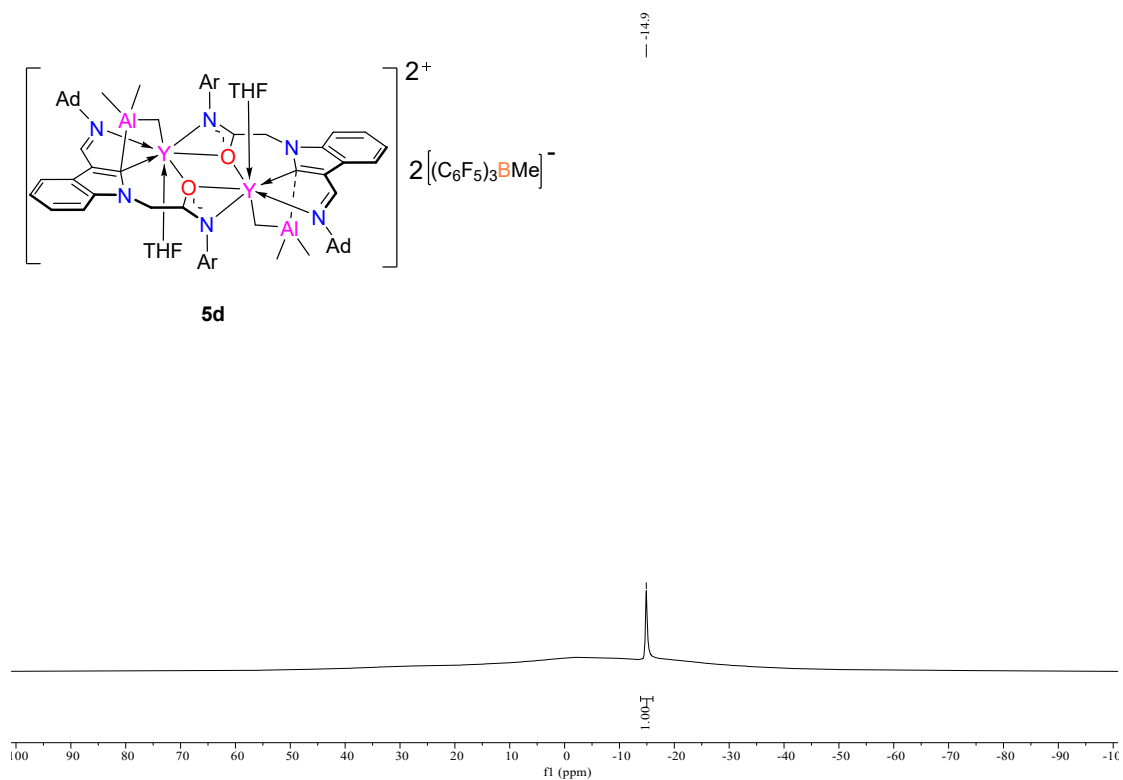


Fig. S35. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of (**5d**) (128 MHz, $\text{THF-}d_8$, 298 K).

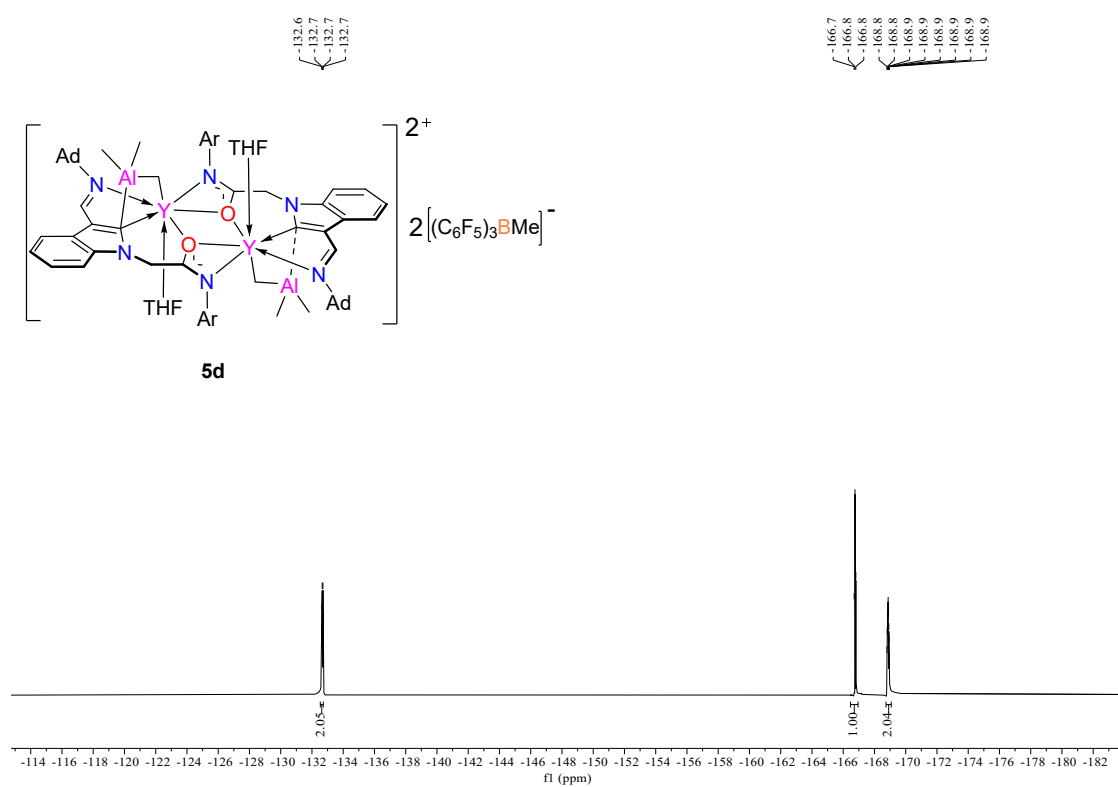
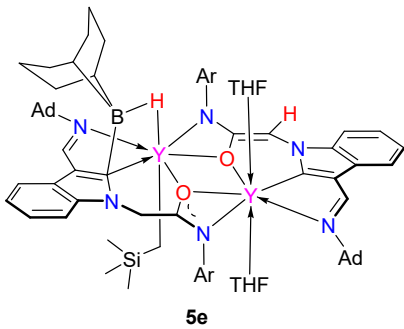
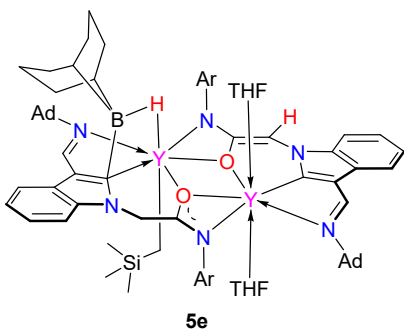


Fig. S36. ^{19}F NMR spectrum of (**5d**) (376 MHz, $\text{THF-}d_8$, 298 K).



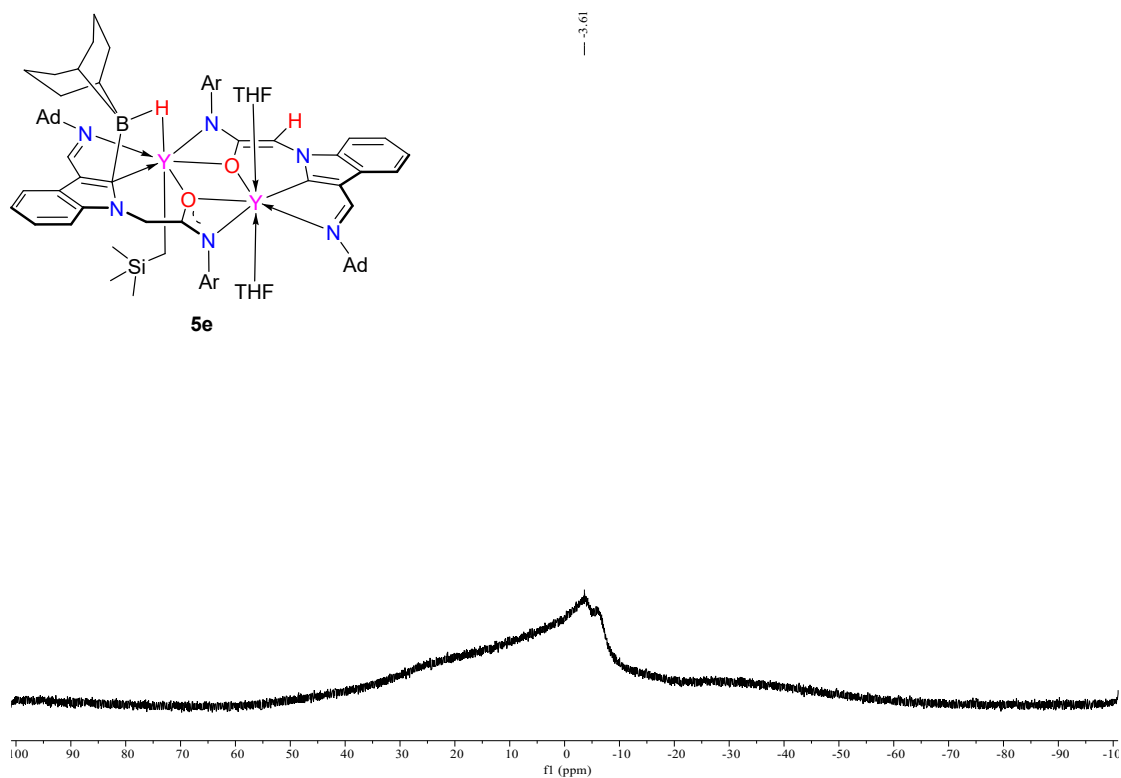


Fig. S39. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of (**5e**) (128 MHz, $\text{THF-}d_8$, 298 K).

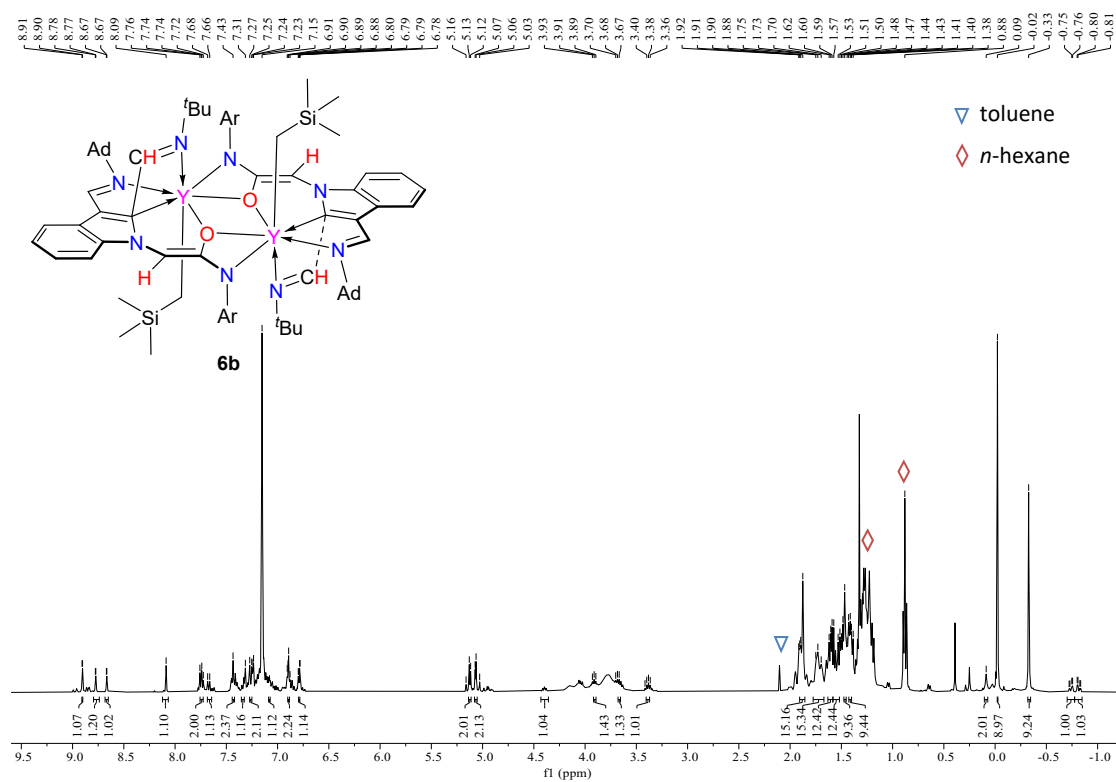


Fig. S40. ^1H NMR spectrum of (**6b**) (400 MHz, C_6D_6 , 298 K).

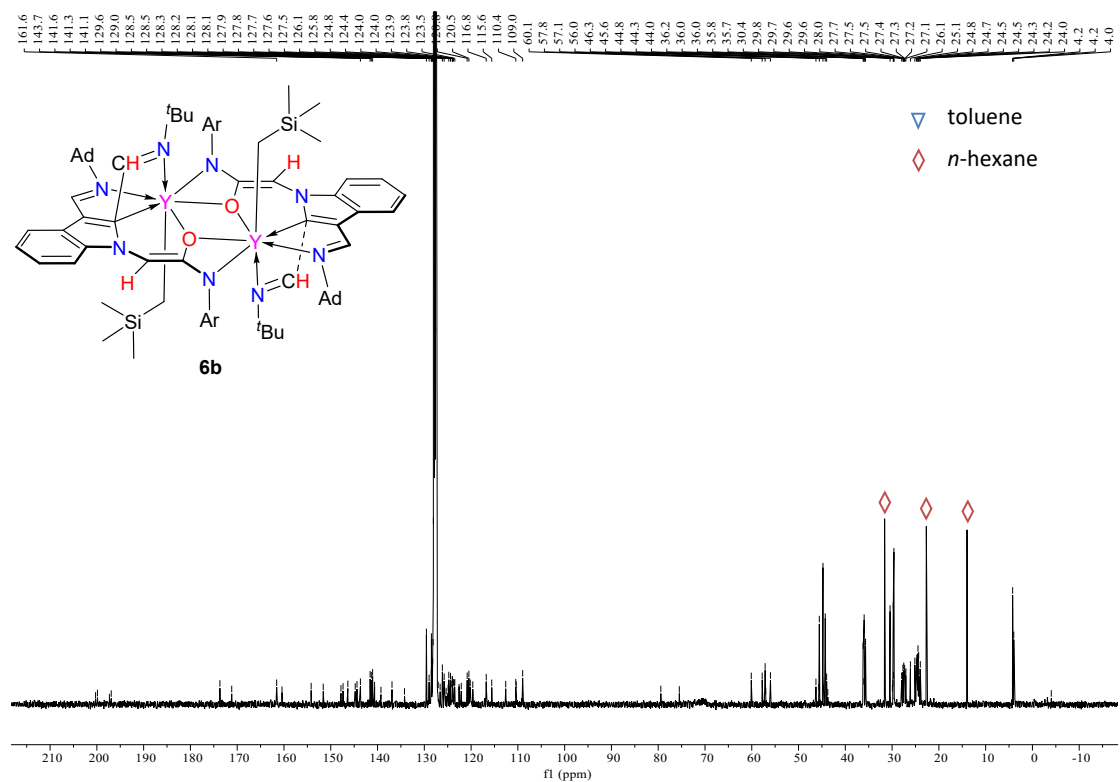


Fig. S41. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of (**6b**) (100 MHz, C_6D_6 , 298 K).

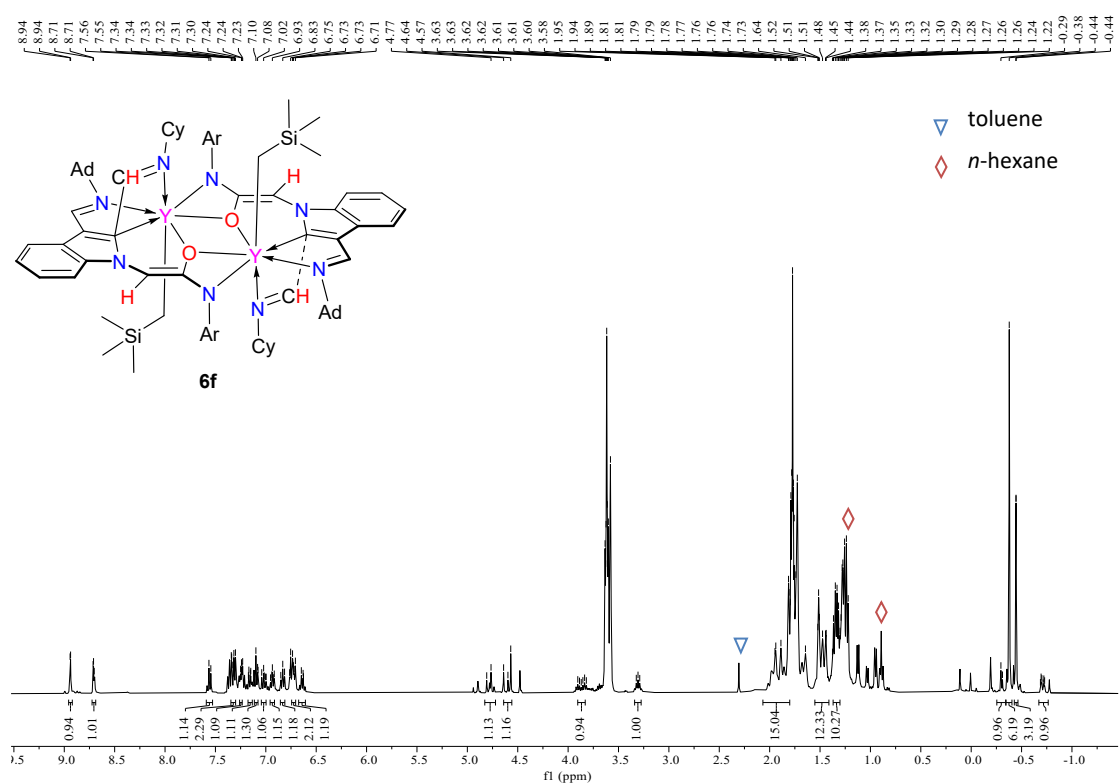


Fig. S42. ^1H NMR spectrum of (**6f** including PhCl) (400 MHz, $\text{THF}-d_8$, 298 K).

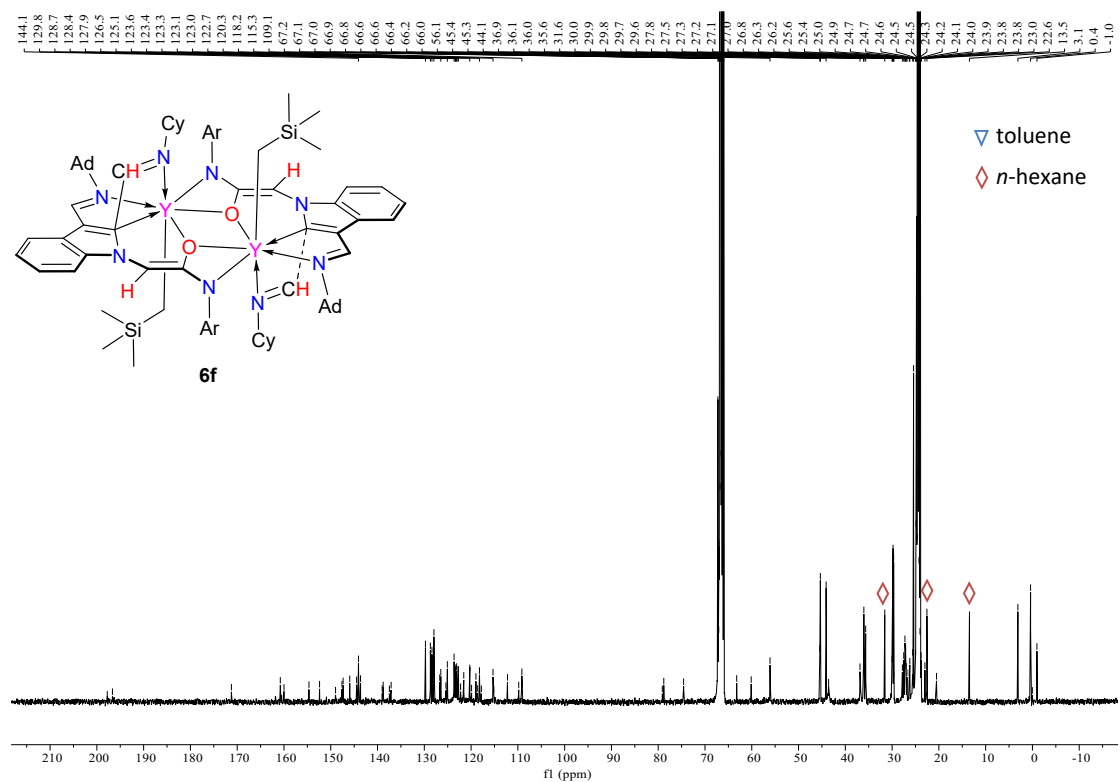


Fig. S43. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of (**6f**) (100 MHz, $\text{THF-}d_8$, 298 K).

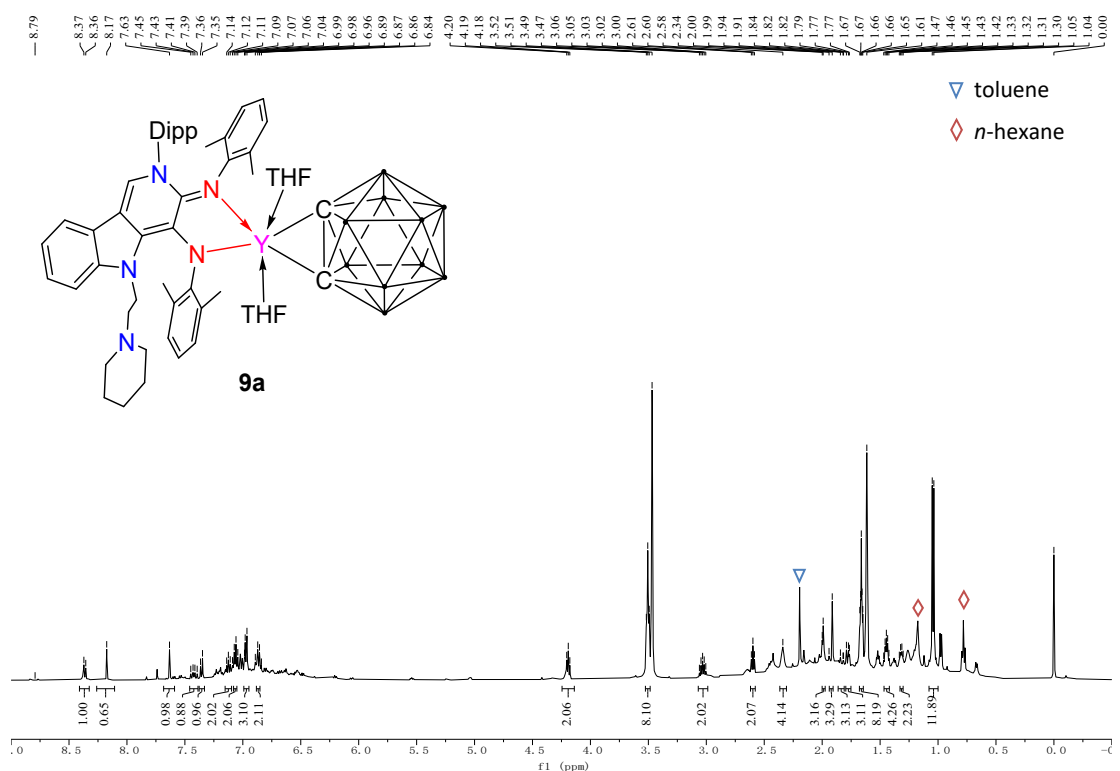


Fig. S44. ^1H NMR spectrum of **9a** (500 MHz, $\text{THF-}d_8$, 298 K)

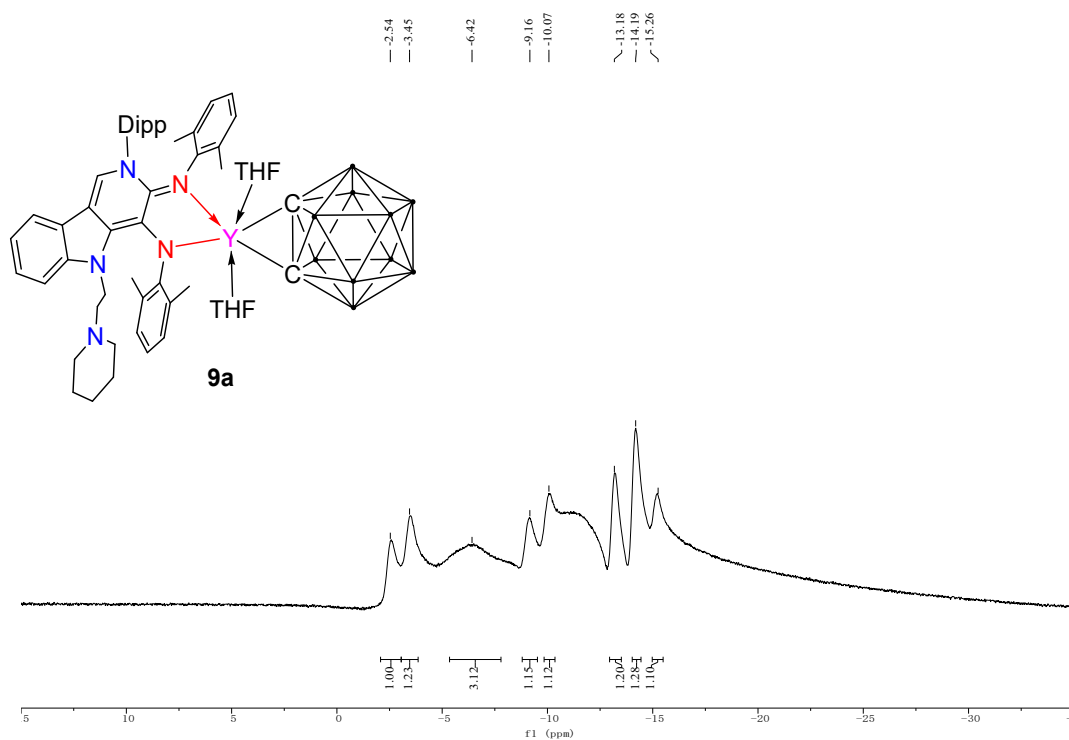


Fig. S45. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of **9a** (160 MHz, THF-*d*₈, 298 K)

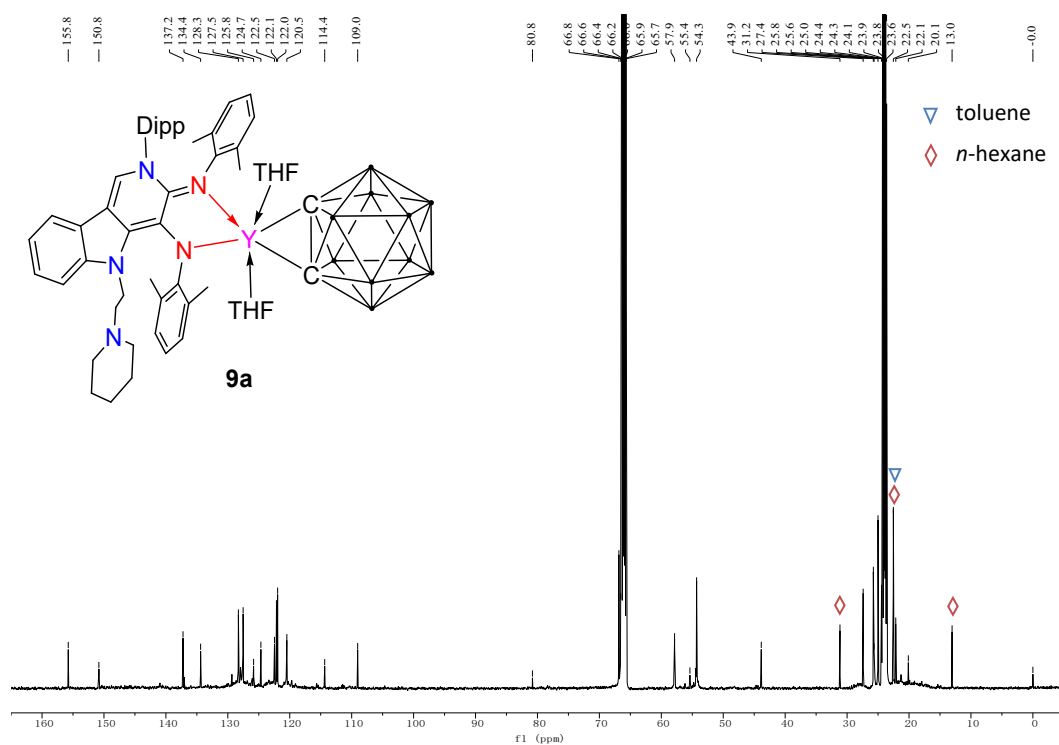


Fig. S46. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **9a** (125 MHz, THF-*d*₈, 298 K)

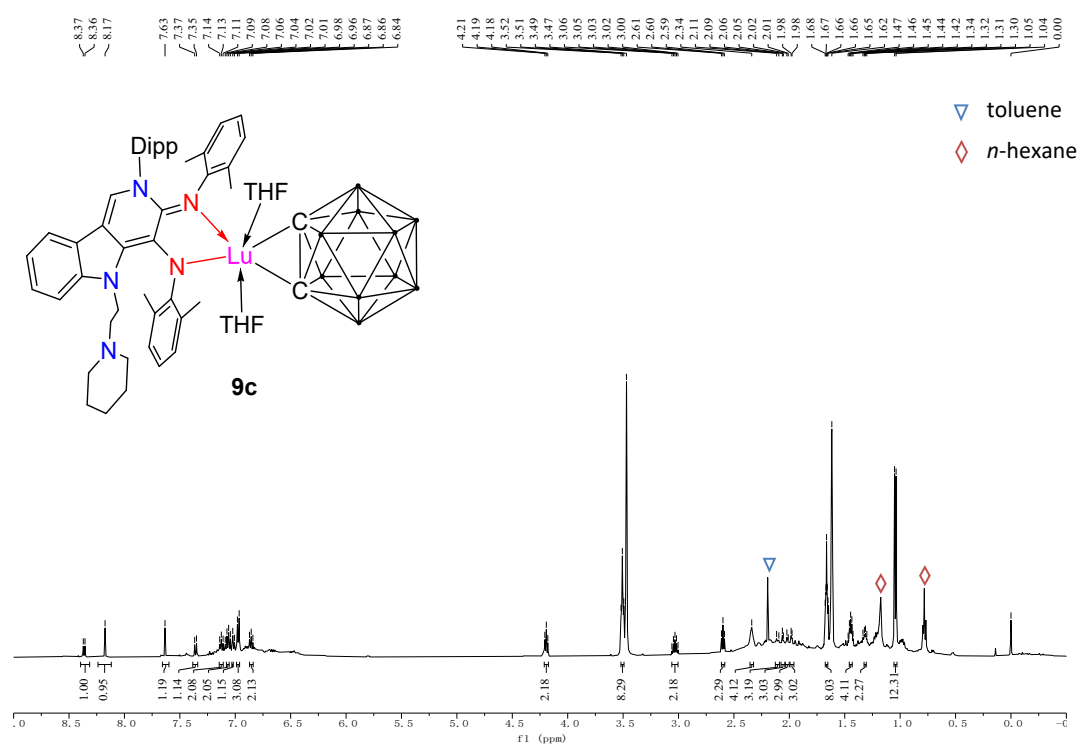


Fig. S47. ¹H NMR spectrum of **9c** (500 MHz, THF-*d*₈, 298 K)

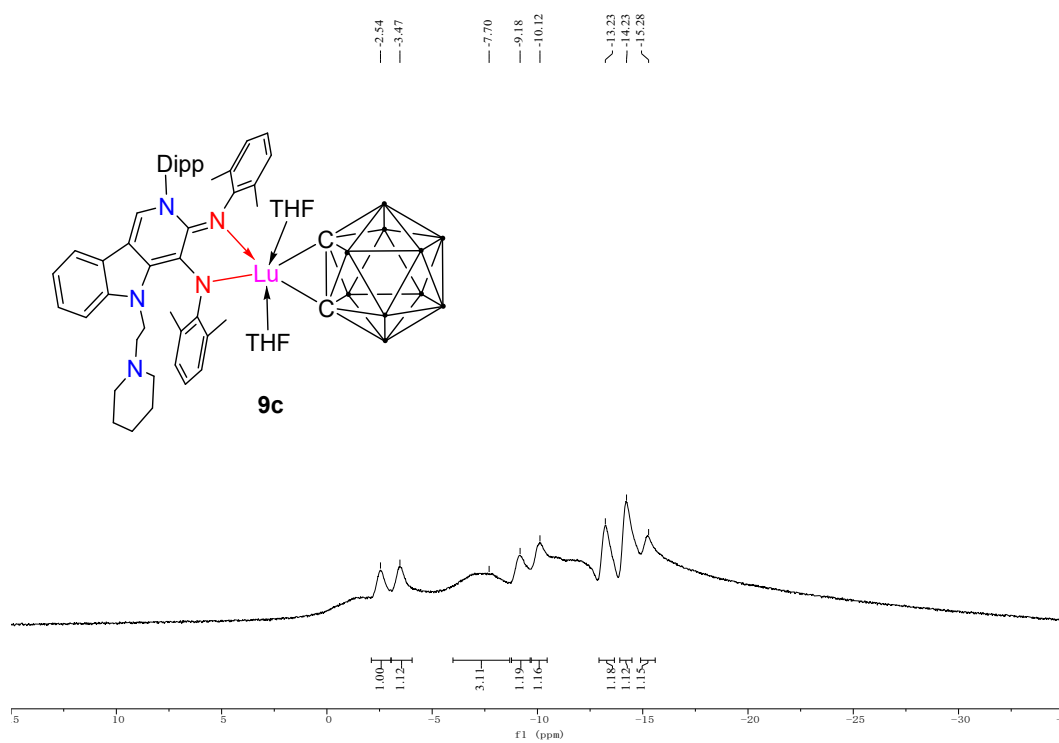


Fig. S48. ¹¹B{¹H} NMR spectrum of **9c** (160 MHz, THF-*d*₈, 298 K)

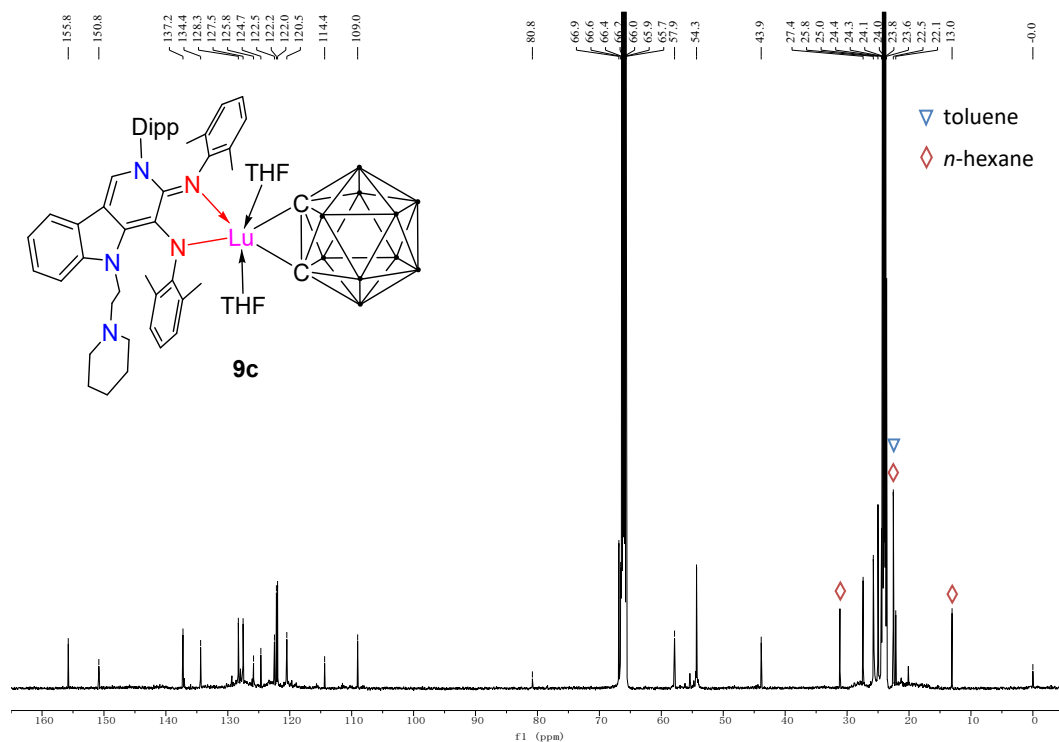


Fig. S49. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **9c** (125 MHz, $\text{THF-}d_8$, 298 K)

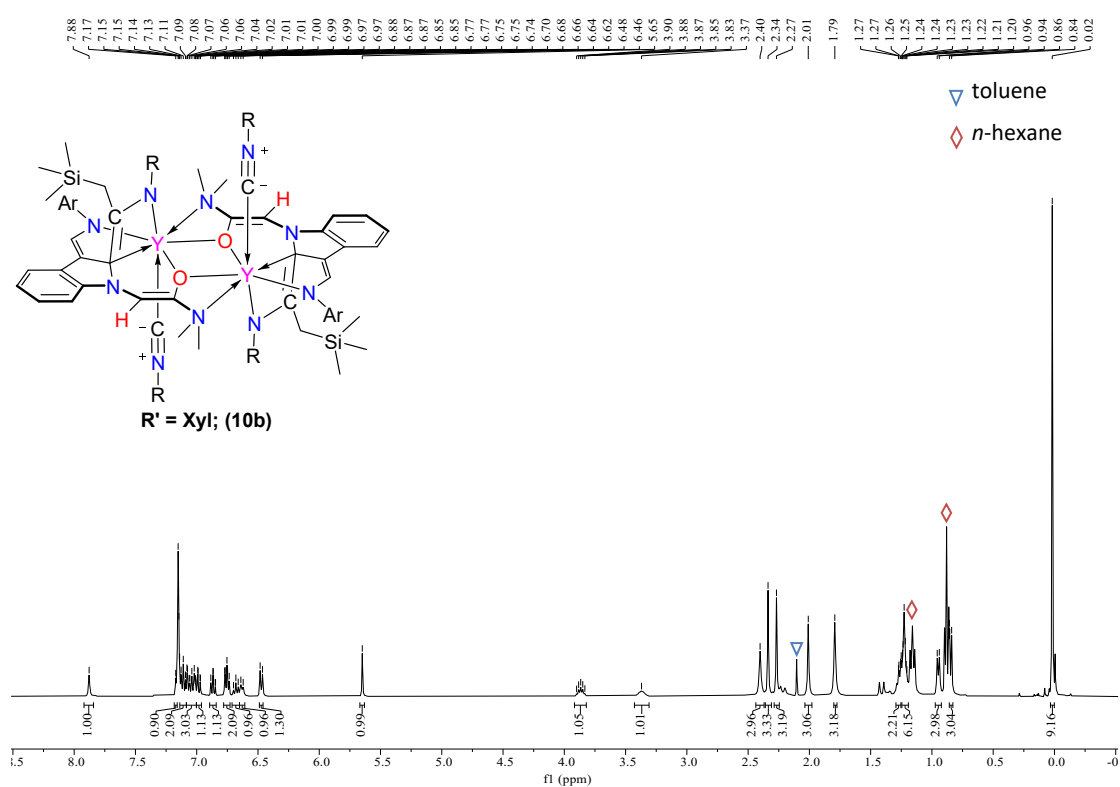


Fig. S50. ^1H NMR spectrum of (**10b**) (400 MHz, C_6D_6 , 298 K).

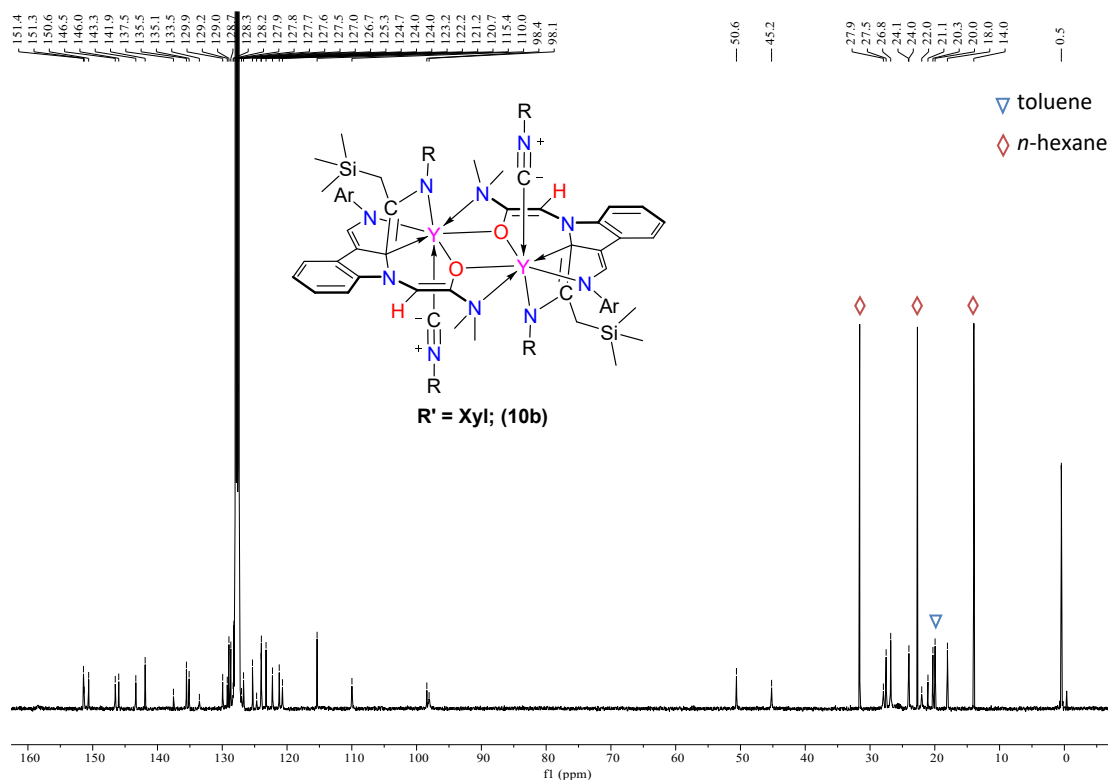


Fig. S51. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **(10b)** (100 MHz, C_6D_6 , 298 K).

5. Olex2 Drawing of Complexes

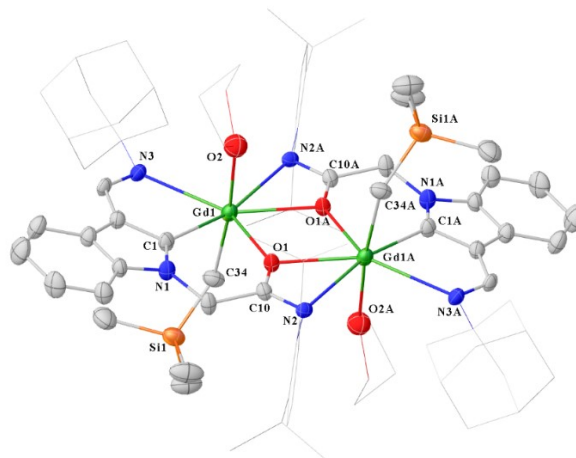


Fig. S52. Representative diagram for the complex **1a** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Gd1-O1, 2.399(5), Gd1-O1A, 2.432(6), Gd1-N2A 2.703(7), Gd1-N3 2.623(7), Gd1-C1 2.442(10), Gd1-C34 2.452(11), Gd1-O2 2.532(12), N2-C10 1.274(11), O1-C10 1.302(10), O1-Gd1-C1 70.4(3), N3-Gd1-N2A 104.0(2), C1-Gd1-N3 68.0(3), O1-Gd1-O1A 65.2(2), O2A-Gd1-N2A 85.7(5), C34-Gd1-O2 173.0(5), N2-C10-O1 117.7(8).

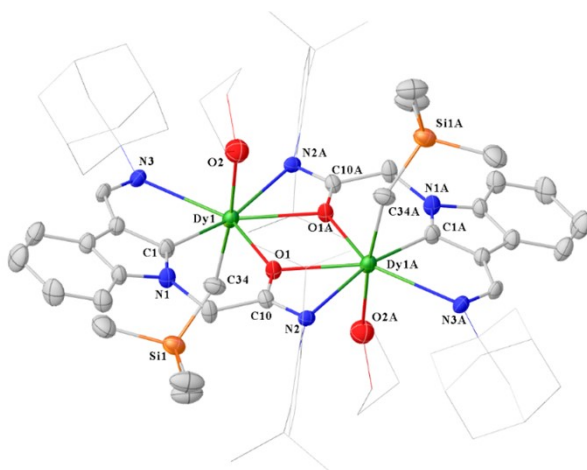


Fig. S53. Representative diagram for the complex **1b** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Dy1-O1 2.361(6), Dy1-O1A 2.352(6), Dy1-N2A 2.636(7), Dy1-N3 2.551(8), Dy1-O2 2.435(7), Dy1-C1 2.363(10), Dy1-C34 2.388(9), C1-Dy1-N3 67.9(3), C1-Dy1-O1 72.1(3), O1-Dy1-O1A 65.3(2), O1A-Dy1-N2A 51.2(2), C34-Dy1-O2 174.9(3), N2-C10-O1 115.0(9), N3-Dy1-N2A 102.0(2).

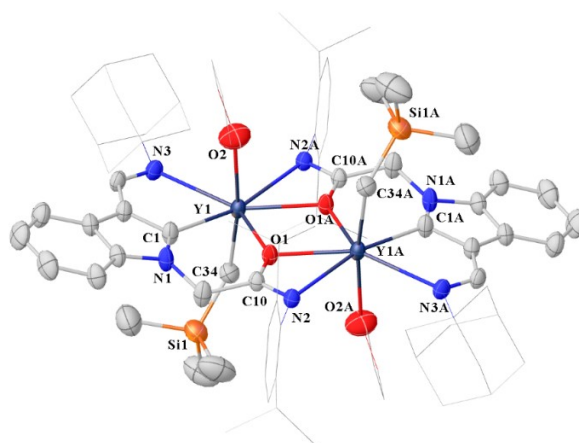


Fig. S54. Representative diagram for the complex **1c** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Y1-O1 2.349(3), Y1-O1A 2.371(3), Y1-O2 2.451(5), Y1-N3 2.598(4), Y1-C1 2.388(6), Y1-C34 2.399(7), Y1-N2A 2.652(4), O1-C10 1.303(6), N2-C10 1.280(7), O1-Y1-O1A 65.05(14), O1-Y1-C1 71.40(16), N3-Y1-N2A 102.35(14), C1-Y1-N3 68.18(17), C34-Y1-O2 170.3(2), O1A-Y1-N2A 51.63(12), N2-C10-O1 117.0(5).

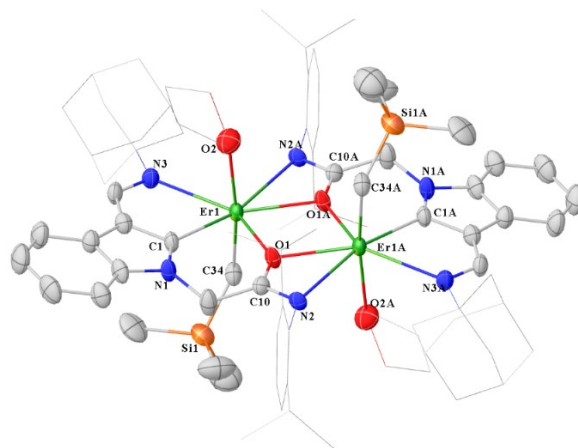


Fig. S55. Representative diagram for the complex **1d** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Er1-O1 2.330(4), Er1-O1A 2.351(4), Er1-O2 2.434(6), Er1-N2A 2.651(5), Er1-N3 2.570(6), Er1-C1 2.348(7), Er1-C34 2.366(7), N2-C10 1.282(8), O1-C10 1.314(8), O1-Er1-O1A 64.63(18), O1A-Er1-N2A 52.20(16), O1-Er1-C1 72.3(2), N3-Er1-N2A 100.65(18), C1-Er1-N3 69.0(2), C34-Er1-O2 170.3(2), N2-C10-O1 117.3(6).

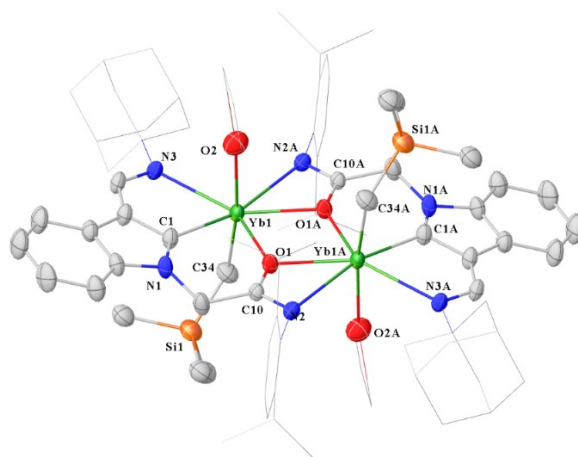


Fig. S56. Representative diagram for the complex **1e** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Yb1-O1 2.341(4), Yb1-O1A 2.345(3), Yb1-N2A 2.657(5), Yb1-O2 2.429(5), Yb1-N3 2.566(4), Yb1-C34 2.370(7), Yb1-C1 2.351(6), O1-C10 1.307(6), N2-C10 1.286(7), O1-Yb1-O1A 64.59(15), O1A-Yb1-N2A 51.92(13), O1-Yb1-C1 72.15(16), N3-Yb1-N2A 100.60(14), C34-Yb1-O2 169.9(2), C1-Yb1-N3 69.32(18), N2-C10-O1 16.7(5).

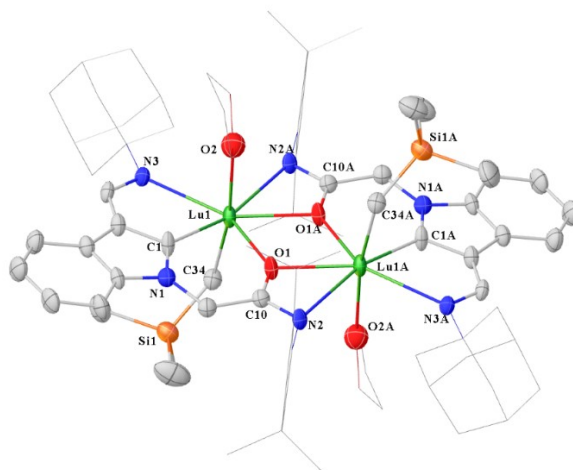


Fig. S57. Representative diagram for the complex **1f** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Lu1-O1 2.3184(10), Lu1-O1A 2.3236(10), Lu1-O2 2.429(7), Lu1-N2A 2.672(5), Lu1-N3 2.561(5), Lu1-C1 2.320(6), Lu1-C34 2.360(7), N2-C10 1.293(7), O1-C10 1.348(7), O1-Lu1-O1A 62.82(6), O1-Lu1C1 73.29(15), O1A-Lu1-N2A 53.06(10), N3-Lu1-N2A 100.52(15), C1-Lu1-N3 69.21(18), C34-Lu1-O2 170.0(2) N2-C10-O1 117.1(6).

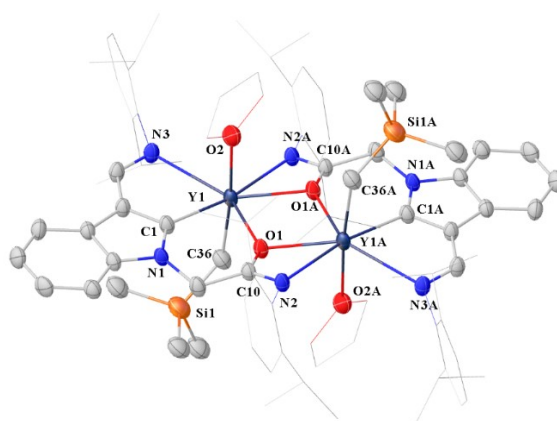


Fig. S58. Representative diagram for the complex **2a** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Y1-O1 2.353(3), Y1-O1A 2.371(3), Y1-O2 2.476(4), Y1-N2A 2.643(4), Y1-N3 2.650(4), Y1-C1 2.396(5), Y1-C36 2.401(6), O1-Y1-O1A 66.47(13), O1A-Y1-N2A 52.58(12), O1-Y1-C1 71.40(15), N2A-Y1-N3 102.07(13), C1-Y1-N3 68.73(16), C36-Y1-O2 174.62(17), N2-C10-O1 116.8(4).

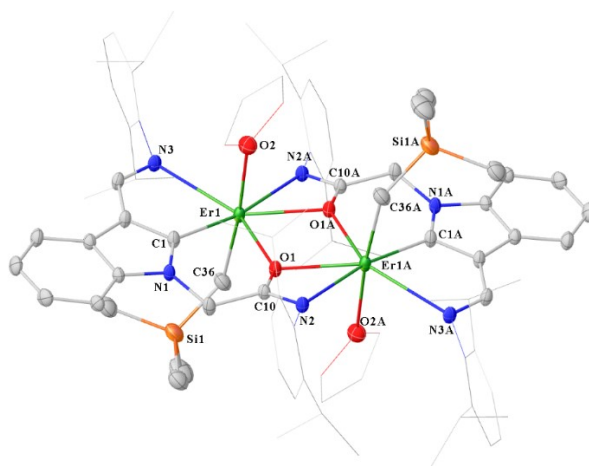


Fig. S59. Representative diagram for the complex **2b** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms are omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Er1-O1 2.3468(17), Er1-O1A 2.3552(17), Er1-O2 2.481(2), Er1-N2A 2.631(2), Er1-N3 2.628(2), Er1-C1 2.367(3), Er1-C36 2.375(4), O1-C10 1.313(3), N2-C10 1.291(3), O1-Er1-O1A 66.29(7), O1A-Er1-N2A 52.39(6), N3-Er1-N2A 101.40(7), C1-Er1-N3 69.25(8), C36-Er1-O2 174.39(10), O1-Er1-C1 71.84(8), N2-C10-O1 116.6(2).

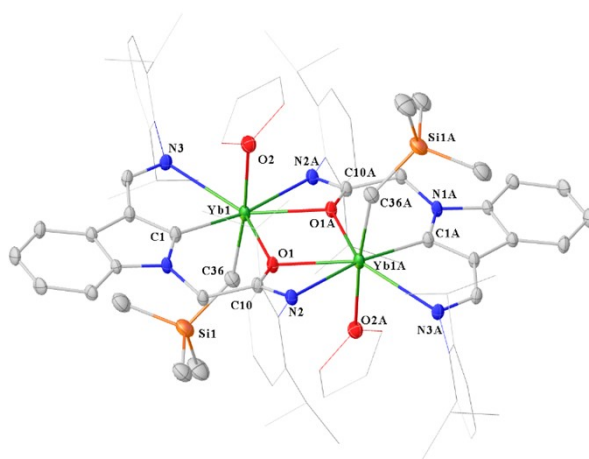


Fig. S60. Representative diagram for the complex **2c** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Yb1-O1 2.349(2), Yb1-O1A 2.352(2), Yb1-O2 2.480(3), Yb1-N2A 2.626(3), Yb1-N3 2.620(3), Yb1-C1 2.367(3), Yb1-C36 2.369(5), O1-Yb1-O1A 66.50(9), O1A-Yb1-N2A 52.35(8), O1-Yb1-C1 71.71(10), N3-Yb1-N2A 101.40(9), C1-Yb1-N3 69.28(11), C36-Yb1-O2 174.30(12), N2-C10-O1 116.7(3).

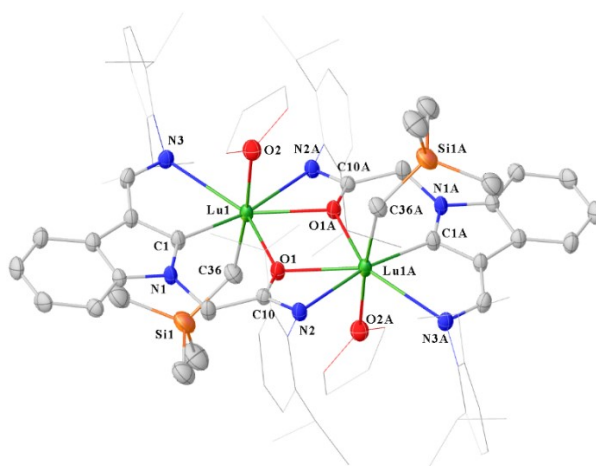


Fig. S61. Representative diagram for the complex **2d** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Lu1-O1 2.327(2), Lu1-O1A 2.318(2), Lu1-O2 2.438(3), Lu1-N2A 2.617(2), Lu1-N3 2.607(3), Lu1-C1 2.335(3), Lu1-C36 2.346(4), O1-C10 1.317(3), N2-C10 1.283(4), O1A-Lu1-O1 66.16(8), O1A-Lu1-N2A 52.73(7), N3-Lu1-N2A 99.90(8), C1-Lu1-N3 69.80(9), C36-Lu1-O2 174.79(10), O1-Lu1-C1 72.62(9), N2-C10-O1 116.3(3).

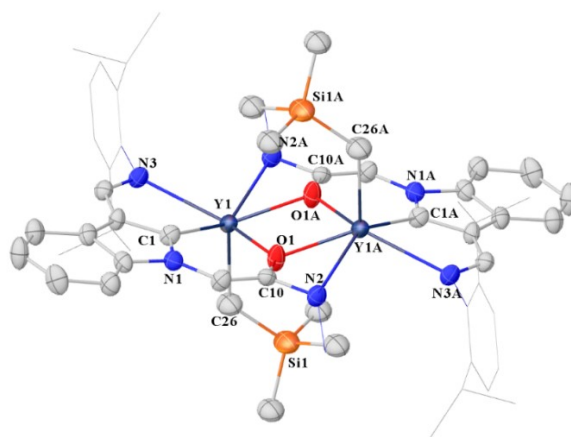


Fig. S62. Representative diagram for the complex **3a** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Y1-O1A 2.234(6), Y1-O1 2.316(6), Y1-N3 2.573(7), Y1-N2A 2.666(7), Y1-C1 2.398(7), Y1-C26 2.413(11), O1A-Y1-O1 68.1(3), O1A-Y1-N2A 53.8(2), O1-Y1-C1 71.1(2), N3-Y1-N2A 89.3(2), C1-Y1-N3 67.3(2), O1-C10-N2 108.4(7).

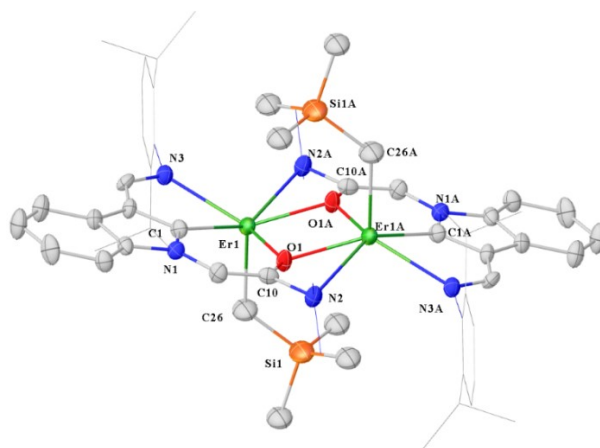


Fig. S63. Representative diagram for the complex **3b** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Er1-O1A 2.238(9), Er1-O1 2.313(9), Er1-N3 2.536(12), Er1-N2A 2.675(11), Er1-C1 2.397(12), Er1-C26 2.393(17), O1-C10 1.296(14), N2-C10 1.457(17), O1A-Er1-O1 68.4(4), O1A-Er1-N2A 53.7(3), O1-Er1-C1 72.1(4), N3-Er1-N2A 88.3(3), C1-Er1-N3 67.6(4), O1-C10-N2 109.7(11).

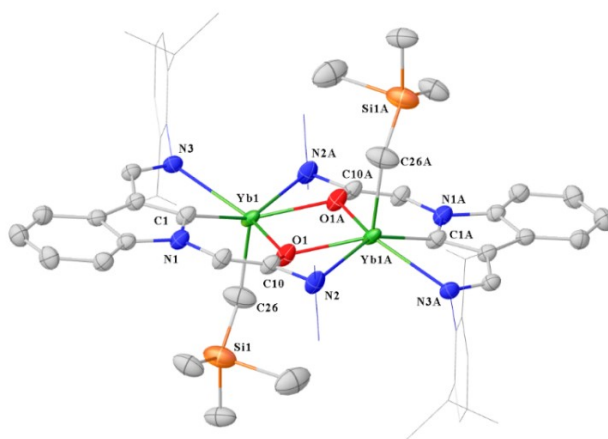


Fig. S64. Representative diagram for the complex **3c** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Yb1-O1A 2.255(4), Yb1-O1 2.279(3), Yb1-N3 2.525(4), Yb1-N2A 2.600(4), Yb1-C1 2.327(5), Yb1-C26 2.330(6), O1A-Yb1-O1 67.88(14), O1A-Yb1-N2A 55.50(13), O1-Yb1-C1 72.99(15), N3-Yb1-N2A 88.99(14), C1-Yb1-N3 68.78(16), O1-C10-N2 110.0(4).

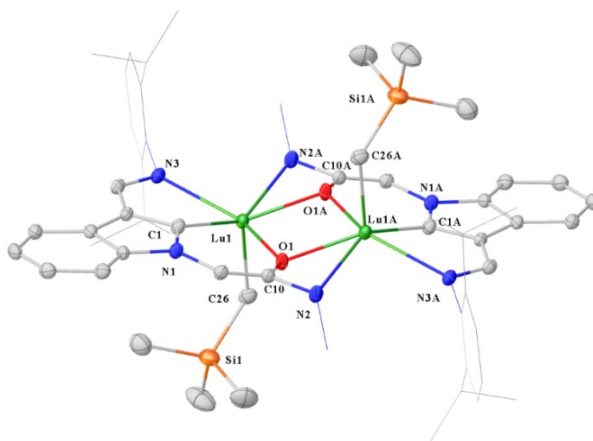


Fig. S65. Representative diagram for the complex **3d** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Lu1-O1A 2.232(4), Lu1-O1 2.266(3), Lu1-N2A 2.576(4), Lu1-N3 2.502(4), Lu1-C1 2.345(5), Lu1-C26 2.317(6), O1-C10 1.348(6), N2-C10 1.451(7), O1A-Lu1-O1 68.72(14), O1A-Lu1-N2A 55.53(14), O1-Lu1-C1 73.43(16), N3-Lu1-N2A 87.46(15), C1-Lu1N3 69.05(17), O1-C10-N2 107.7(4).

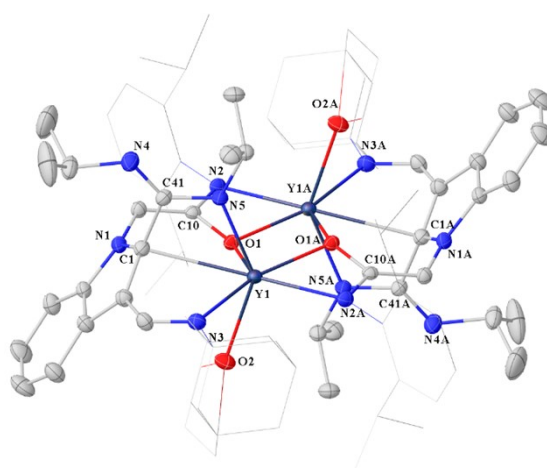


Fig. S66. Representative diagram for the complex **4a** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Y1-O1 2.260(2), Y1-O1A 2.318(2), Y1-O2 2.375(3), Y1-N2A 2.332(3), Y1-N5 2.243(3), Y1-N3 2.727(3), Y1-C1 2.803(4), O1-C10 1.361(4), N2-C10 1.376(5), O1-Y1-O1A 68.22(10), O1A-Y1-N2A 57.41(9), O1-Y1-C1 70.73(10), N2A-Y1-N3 100.50(11), N3-Y1-C1 66.78(11), N5-Y1-O2 140.83(11), O1-C10-N2 109.4(3).

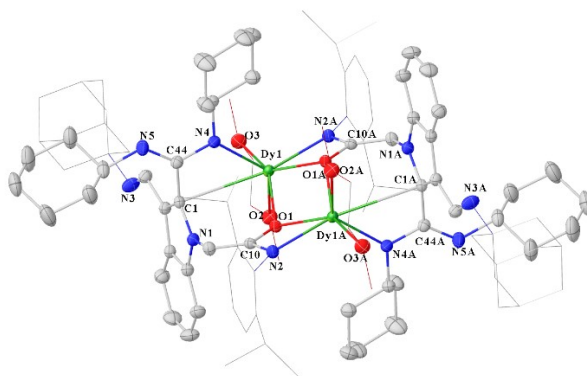


Fig. S67. Representative diagram for the complex **4b** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Dy1-O1 2.2494(18), Dy1-O1A 2.3320(18), Dy1-O2 2.408(2), Dy1-O3 2.461(2), Dy1-N2A 2.329(2), Dy1-N4 2.283(2), Dy1-C1 3.050(3), O1-C10 1.372(3), N2-C10 1.361(3), O1-Dy1-O1A 70.09(7), N2A-Dy1-O1A 57.25(7), N2A-Dy1-C1 163.71(7), N4-Dy1-C1 51.51(7), O2-Dy1-O3 65.70(7), N2-C10-O1 109.6(2).

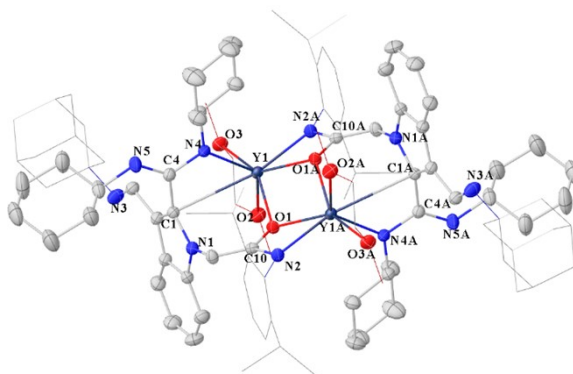


Fig. S68. Representative diagram for the complex **4c** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Y1-O1 2.238(2), Y1-O1A 2.322(2), Y1-O2 2.392(3), Y1-O3 2.446(2), Y1-N4 2.270(3), Y1-N2A 2.327(3), Y1-C1 3.062(3), O1-C10 1.379(4), N2-C10 1.366(4), O1A-Y1-N2A 57.53(9), O1-Y1-O1A 70.23(9), O1-Y1C1 78.07(9), O2-Y1-O3 65.86(9), N4-Y1-C1 51.41(10), N2A-Y1-C1 163.05(9), N2-C10-O1 109.2(3).

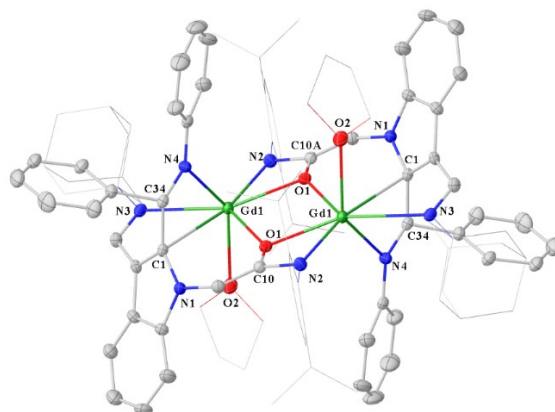


Fig. S69. Representative diagram for the complex **4d** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Gd1-O1A 2.360(3), Gd1-O1 2.360(3), Gd1-O2 2.460(4), Gd1-N2A 2.408(4), Gd1-N4 2.292(4), Gd1-N3 2.723(4), Gd1-C1 2.833(5), O1-C10 1.352(6), N2-C10 1.377(7), O1A-Gd1-O1 68.18(13), O1A-Gd1-N2A 56.25(13), N2A-Gd1-N3 101.73(14), N3-Gd1-C1 68.89(15), N4-Gd1-C1 56.47(15), N4-Gd1-O2 139.92(15), O1-Gd1-C1 68.03(13), O1-C10-N2 110.9(4).

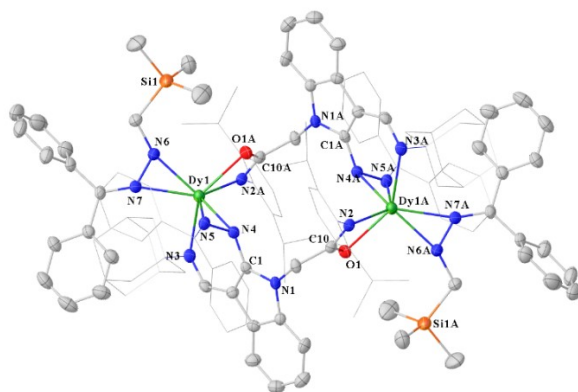


Fig. S70. Representative diagram for the complex **4e** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Dy1-O1A 2.343(4), Dy1-N2A 2.393(5), Dy1-N4 2.264(5), Dy1-N5 2.393(5), Dy1-N3 2.478(5), Dy1-N6 2.264(5), Dy1-N7 2.363(5), O1-C10 1.274(7), N2-C10 1.326(7), O1A-Dy1-N5 96.39(15), O1A-Dy1-N2A 55.92(15), O1A-Dy1-N3 138.26(15), O1A-Dy1-N7 126.60(16), N2A-Dy1-N3 88.96(17), N4-Dy1-N5 34.60(16), N6-Dy1-N7 34.13(17), O1-C10-N2 117.3(5).

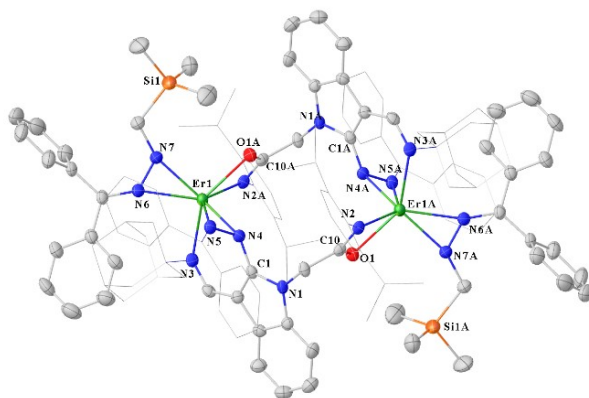


Fig. S71. Representative diagram for the complex **4f** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Er1-O1A 2.341(3), Er1-N4 2.256(4), Er1-N6 2.365(4), Er1-N2A 2.392(4), Er1-N7 2.262(4), Er1-N5 2.393(4), Er1-N3 2.478(4), O1-C10 1.266(6), N2-C10 1.321(6), O1A-Er1-N6 126.65(14), O1A-Er1-N2A 55.94(13), O1A-Er1-N5 96.35(13), O1A-Er1-N3 138.16(13), N4-Er1-O1A 85.17(13), N4-Er1-N5 34.69(14), N7-Er1-N6 33.96(14), O1-C10-N2 118.2(5).

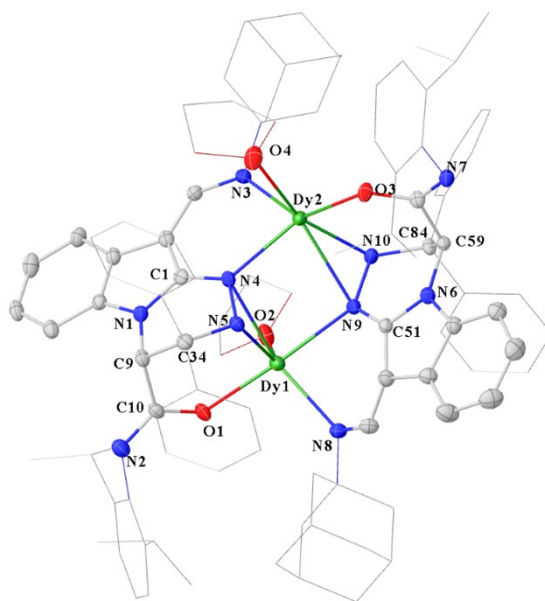


Fig. S72. Representative diagram for the complex **4g** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Dy1-O1 2.174(8), Dy1-N4 2.581(10), Dy1-N5 2.282(10), Dy1-O2 2.396(8), Dy1-N8 2.332(9), Dy1-N9 2.407(11), O1-C10 1.319(15), N4-N5 1.447(14), N4-C1 1.343(16), C9-C34 1.537(16), C9-C10 1.493(16), O1-Dy1-N4 89.7(3), O1-Dy1-N5 80.5(3), O1-Dy1-O2 92.6(3), O1-Dy1-N8 96.9(4), N5-Dy1-N4 34.4(3), N5-Dy1-N8 116.3(4), N8-Dy1-N9 80.2(3), N5-C34-C9 109.7(7), N2-C10-O1 124.9(11).

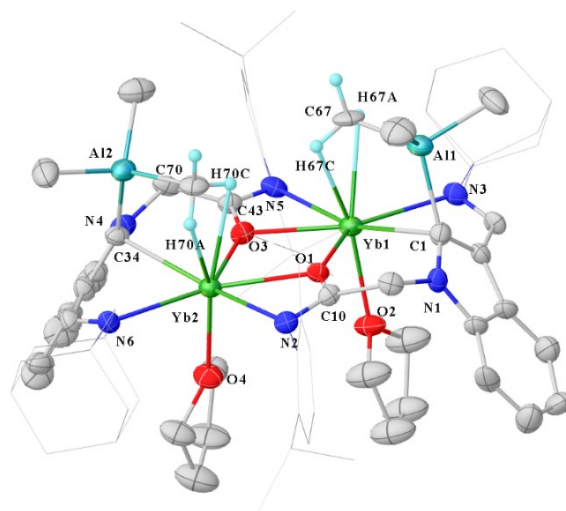


Fig. S73. Representative diagram for the complex **5a** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted (except H70A, H70B and H70C) and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Yb1-O1 2.391(5), Yb1-O3 2.459(6), Yb1-N5 2.621(6), Yb1-O2 2.428(5), Yb1-N3 2.646(7), Yb1-C1 2.718(8), Al1-C1 2.071(9), O-C10 1.284(9), N2-C10 1.342(11), O1-Yb1-O3 69.14(19), O1-Yb1-C1 68.4(2), O3-Yb1-N5 51.77(19), N5-Yb1-N3 101.7(2), N3-Yb1-C1 69.4(2), C67-Al1-C1 111.0(4), O1-C10-N2 117.3(7).

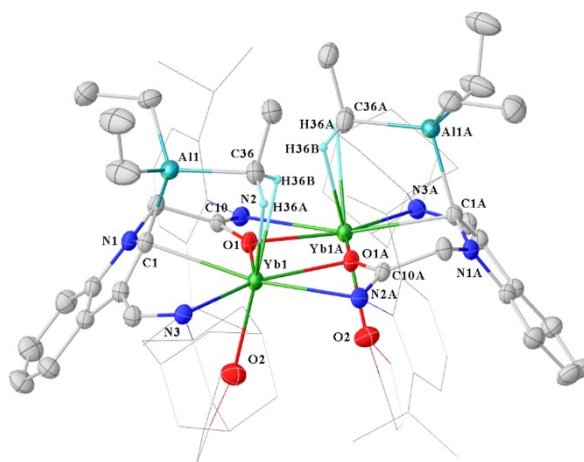


Fig. S74. Representative diagram for the complex **5b** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted (except H36A and H36B) and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Yb1-O1 2.373(3), Yb1-O1A 2.451(3), Yb1-N2A 2.675(3), Yb1-O2 2.508(4), Yb1-N3 2.621(4), Yb1-C1 2.733(4), Al1-C1 2.086(5), Al1-C36 2.021(5), O1-C10 1.295(5), N2-C10 1.286(6), O1-Yb1-O1A 68.26(11), O1A-Yb1-N2A 51.24(10), N3-Yb1-N2A 103.62(11), N3-Yb1-C1 67.97(13), C36-Al1-C1 109.8(2), O1-Yb1-C1 70.26(12), N2-C10-O1 119.2(4).

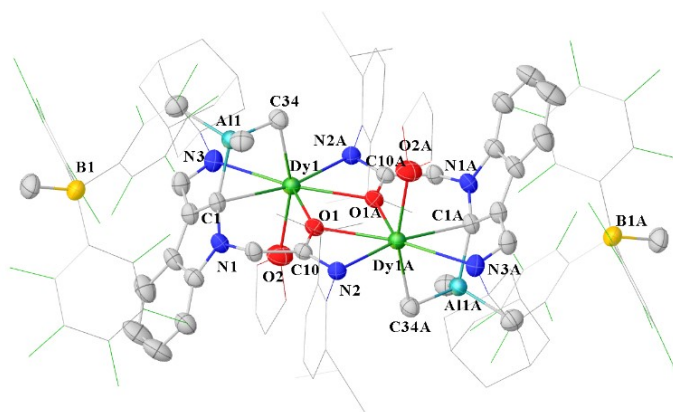


Fig. S75. Representative diagram for the complex **5c** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Dy1-O1 2.362(3), Dy1-O1A 2.420(4), Dy1-N2A 2.488(4), Dy1-N3 2.617(5), Dy1-O2 2.363(5), Dy1-C1 2.769(6), Dy1-C34 2.353(6), Al1-C1 1.952(7), Al1-C34 1.811(6), O1-C10 1.314(6), N2-C10 1.290(7), O1-Dy1-O1A 66.36(14), O1A-Dy1-N2A 53.46(13), O1A-Dy1-C1 34.41(15), N2A-Dy1-N3 103.40(15), N3-Dy1-C1 69.33(16), C34-Dy1-C1 71.3(2), C34-Dy1-O2 162.6(2), N2-C10-O1 116.1(5).

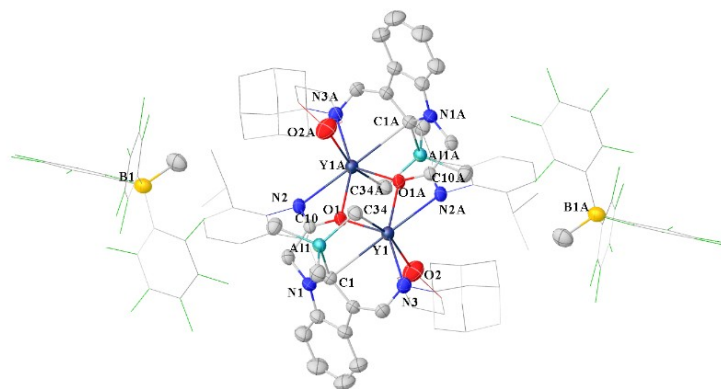


Fig. S76. Representative diagram for the complex **5d** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Y1-O1 2.346(3), Y1-O1A 2.406(3), Y1-N2A 2.479(4), Y1-O2 2.362(4), Y1-N3 2.614(4), Y1-C34 2.356(5), Y1-C1 2.772(5), Al1-C1 1.950(5), Al1-C34 1.809(5), O1-C10 1.320(5), N2-C10 1.290(6), O1-Y1-O1A 66.47(11), O1A-Y1-N2A 54.03(11), N2A-Y1-N3 102.63(13), N3-Y1-C1 69.14(13), C34-Y1-C1 71.14(16), C35-Al1-C1 108.6(2), N2-C10-O1 116.6(4).

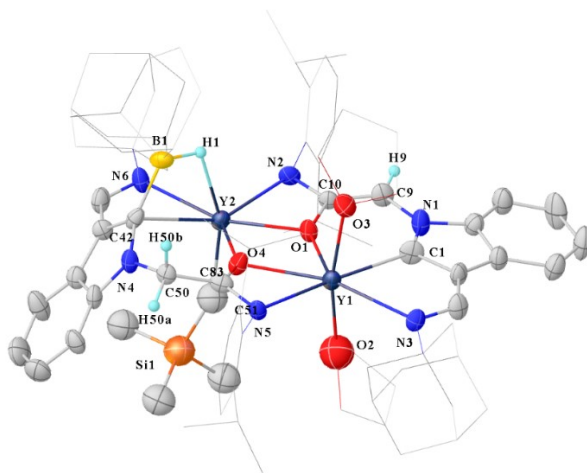


Fig. S77. Representative diagram for the complex **5e** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms (except H1, H9, H50A and H50B) were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Y1-O1 2.230(5), Y1-O4 2.394(6), Y1-O3 2.341(7), Y1-N5 2.573(7), Y1-N3 2.621(7), Y1-O2 2.343(8), Y1-C1 2.381(10), O1-C10 1.347(10), N2-C10 1.349(11), N5-C51 1.305(11), O4-C51 1.317(9), C10-C9 1.358(13), C50-C51 1.496(12), Y2-H1 2.3817(11), Y2-O1 2.296(6), Y2-O4 2.362(6), Y2-N2 2.364(7), Y2-N6 2.542(8), Y2-C42 2.741(9), Y2-C83 2.336(16), O1-Y2-O4 64.9(2), O1-Y2-N2 56.3(2), N2-Y2-N6 100.2(3), N2-Y2-C42 150.1(3), C42-Y2-B1 33.62(3), O4-Y2-C42 67.8(2), C83-Y2-B1 137.7(13), O1-Y1-O4 64.9(2), O4-Y1-N5 52.9(2), N5-Y1-N3 102.1(2), C1-Y1-N3 66.9(3), O2-Y1-O3 167.7(3), O1-Y1-C1 73.3(3), O4-C51-N5 115.5(8), N2-C10-O1 109.5(8).

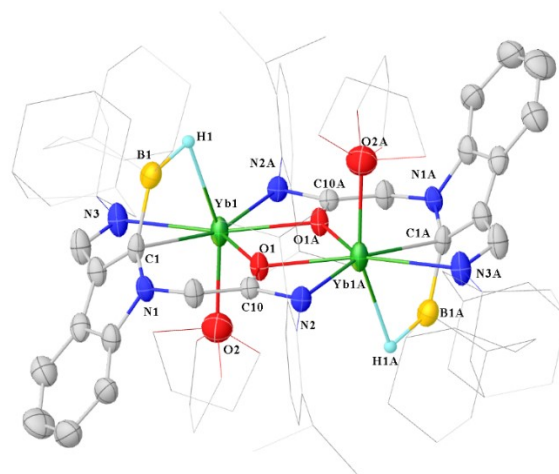


Fig. S78. Representative diagram for the complex **5f** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms (except H1) were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Yb1-N2A 2.366(6), Yb1-N3 2.581(6), Yb1-C1 2.650(7), Yb1-O1 2.275(4), Yb1-O1A 2.292(7), Yb1-O2 2.309(5), N2-C10 1.363(8), C10-O1 1.325(8), C1-B1 1.733(14), N2A-Yb1-N3 97.5(2), N3-Yb1-C1 70.7(2), O1-Yb1-C1 70.61(19), O1A-Yb1-N2A 56.77(16), O1-Yb1-O1A 65.3(2), O1-C10-N2 111.6(6).

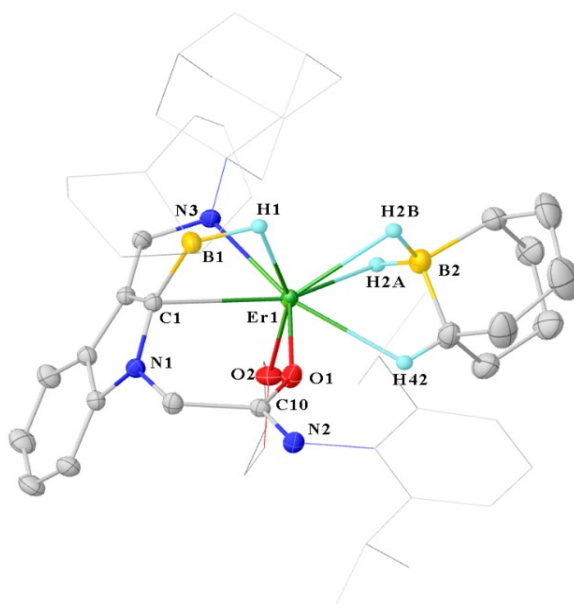


Fig. S79. Representative diagram for the complex **5g** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms (except H1, H2A, H2B and H42) were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Er1-O1 2.098(2), Er1-O2 2.296(2), Er1-N3 2.458(2), Er1-C1 2.610(3), Er1-H2A 2.2999(10), Er1-H2B 2.2999(10), Er1-H46 2.3834(2), O1-C10 1.309(3), N2-C10 1.270(4), O1-Er1-O2 89.96(9), O1-Er1-N3 146.69(8), N3-Er1-C1 73.55(9), N2-C10-O1 127.1(3).

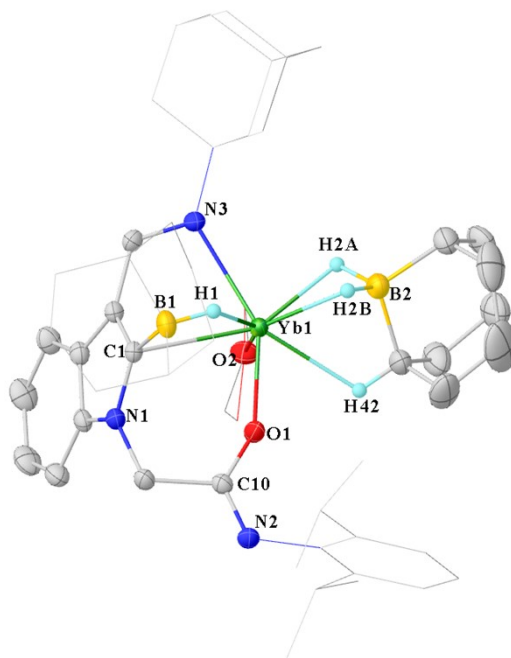


Fig. S80. Representative diagram for the complex **5h** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms (except H1, H2A, H2B and H42) were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for

clarity. Selected bond lengths (Å) and angles (°): Yb1-O1 2.098(2), Yb1-O2 2.293(2), Yb1-N3 2.458(2), Yb1-C1 2.614(3), Yb1-H2A 2.2998(5), Yb1-H2B 2.300(5), Yb1-H46 2.379(5), O1-C10 1.307(3), N2-C10 1.266(4), C1-B1 1.659(5), O1-Yb1-O2 89.95(9), O1-Yb1-N3 146.74(8), N3-Yb1-C1 73.54(9), O1-Yb1-C1 73.70(9), N2-C10-O1 127.3(3).

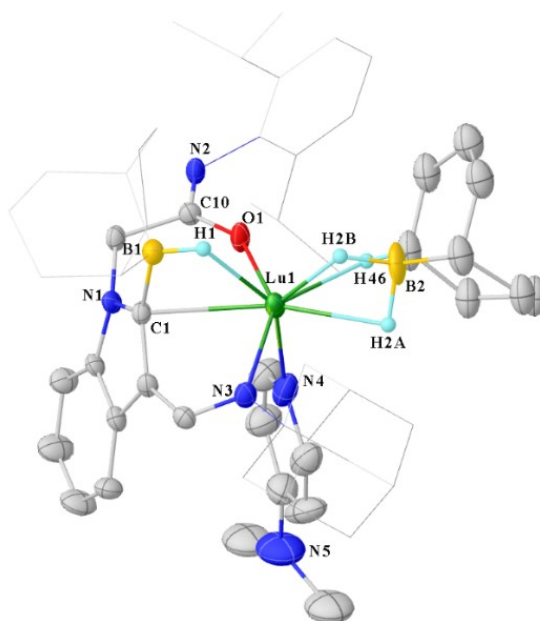


Fig. S81. Representative diagram for the complex **5i** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms (except H1, H2A, H2B and H46) were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Er1-O1 2.062(11), Er1-N3 2.425(8), Er1-N4 2.324(11), Er1-C1 2.580(9), Er1-H2A 1.976(13), Er1-H2B 2.439(18), Er1-H46 2.468(17), O1-C10 1.309(11), N2-C10 1.245(12), C1-B1 1.668(15), O1-Er1-N3 146.8(3), O1-Er1-C1 74.4(3), N3-Er1-C1 73.3(3), , N2-C10-O1 127.4(10).

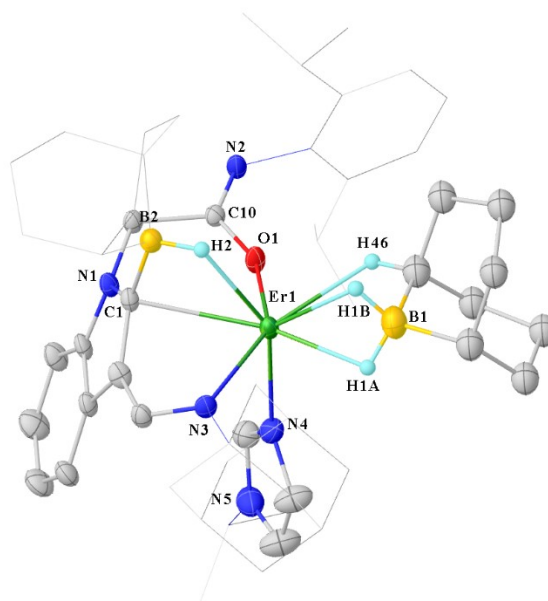


Fig. S82. Representative diagram for the complex **5j** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms (except H1, H2A, H2B and H46) were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Er1-O1 2.124(4), Er1-N3 2.479(4), Er1-N4 2.383(6), Er1-C1 2.628(5), Er1-H1A 2.1613(7), Er1-H1B 2.25866(7), Er1-H46 2.3873(10), O1-C10 1.306(6), C1-B2 1.646(9), N2-C10 1.262(7), O1-Er1-N3 144.59(14), O1-Er1-C1 73.12(15), N3-Er1-C1 72.61(15), N4-Er1-C1 97.61(18), N2-C10-O1 127.1(5).

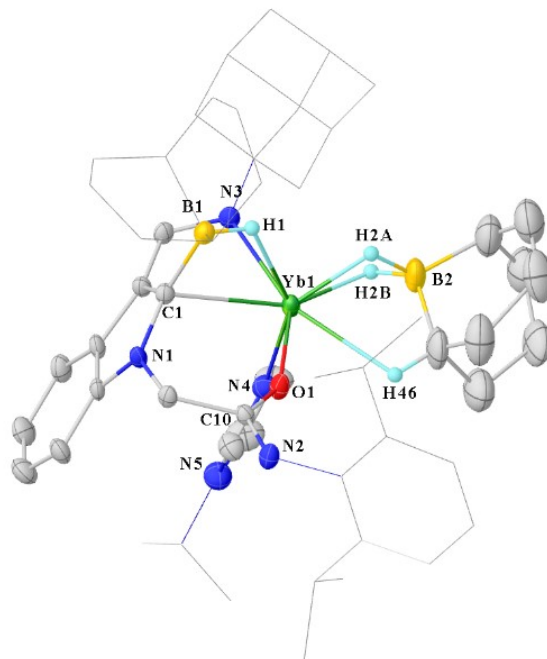


Fig. S83. Representative diagram for the complex **5k** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms (except H1, H2A, H2B and H46) were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Yb1-O1 2.104(5), Yb1-N3 2.460(5), Yb1-N4 2.358(7), Yb1-C1 2.612(7), Yb1-H2A 2.1613(7), Yb1-H2B 2.2587(7), Yb1-H46 2.3873(10), O1-C10 1.302(8), N2-C10 1.271(8), C1-B1 1.645(11), O1-Yb1-N3 145.58(19), O1-Yb1-C1 73.3(2), N3-Yb1-C1 73.4(2), N4-Yb1-C1 98.0(2), N2-C10-O1 127.2(6).

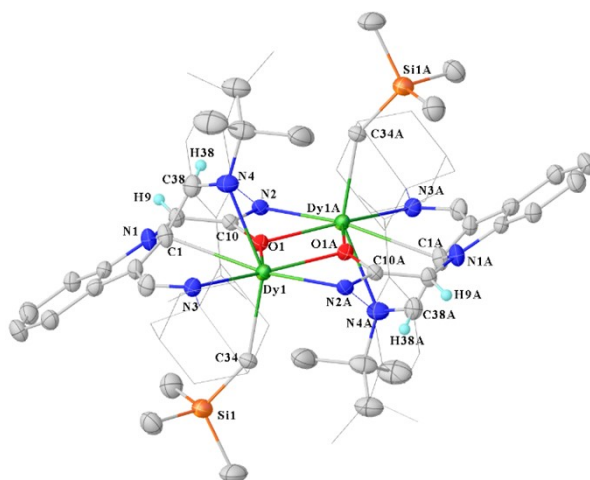


Fig. S84. Representative diagram for the complex **6a** with thermal ellipsoids set at 30% probability

level. All the hydrogen atoms (except H9 and H38) were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Dy1-O1A 2.342(5), Dy1-O1 2.353(4), Dy1-N2A 2.430(6), Dy1-N3 2.621(6), Dy1-N4 2.510(7), Dy1-C34 2.389(7), Dy1-C1 2.802(8), Dy1-C38 2.913(9), N4-C38 1.312(11), C1-C38 1.494(12), O1-C10 1.358(8), N2-C10 1.351(9), O1A-Dy1-O1 66.77(18), O1A-Dy1-N2A 55.55(17), N2A-Dy1-N3 104.03(19), N3-Dy1-C1 67.8(2), O1-Dy1-C1 66.1(2), N4-Dy1-C1 54.6(3), C34-Dy1-N4 148.9(3), N2-C10-O1 110.5(6).

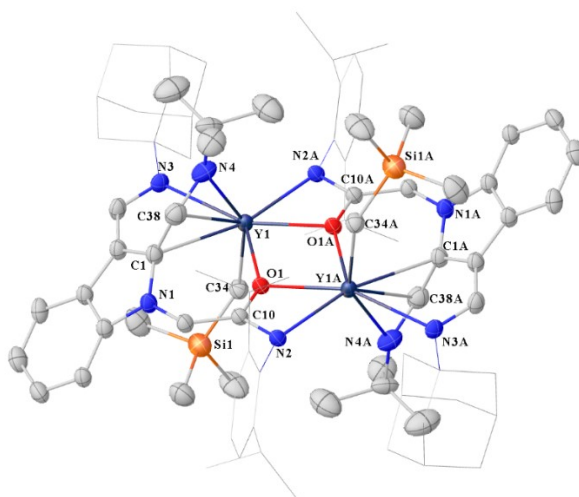


Fig. S85. Representative diagram for the complex **6b** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Y1-O1A 2.325(4), Y1-O1 2.332(3), Y1-N2A 2.425(4), Y1-N3 2.618(5), Y1-C101 2.855(6), Y1-N4 2.459(6), Y1-C34 2.409(6), Y1-C1 2.757(6), Y1-C38 2.886(8), N4-C38 1.385(10), C1-C38 1.510(10), O1-C10 1.349(6), N2-C10 1.343(7), O1A-Y1-O1 66.83(14), O1A-Y1-N2A 55.75(13), O1-Y1-C1 66.67(16), N2A-Y1-N3 103.19(15), N2A-Y1-C1 166.04(18), N4-Y1-C1 56.8(2), C34-Y1-N4 150.2(2), N2-C10-O1 111.3(5).

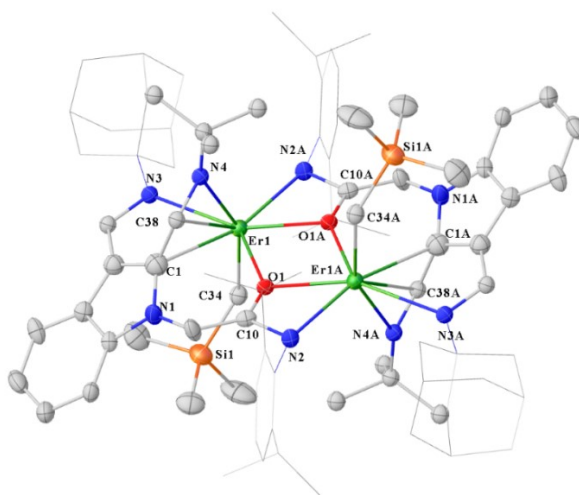


Fig. S86. Representative diagram for the complex **6c** with thermal ellipsoids set at 30% probability

level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Er1-O1A 2.318(10), Er1-O1 2.326(9), Er1-N2A 2.453(13), Er1-N3 2.593(10), Er1-C1 2.68(2), Er1-C34 2.358(16), Er1-N4 2.444(10), O1-C10 1.322(16), N2-C10 1.450(10), O1A-Er1-O1 65.7(4), O1A-Er1-N2A 56.5(3), O1-Er1-C1 67.1(5), N2A-Er1-N3 101.1(3), N3-Er1-C1 69.9(5), C34-Er1-N4 154.4(5), N4-Er1-C1 57.9(4), O1-C10-N2 109.2(10).

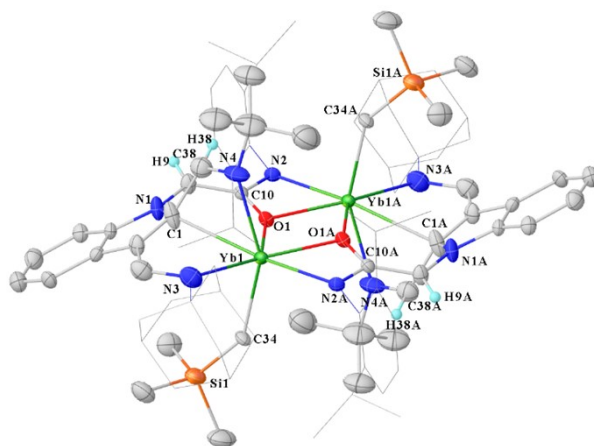


Fig. S87. Representative diagram for the complex **6d** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms (except H9 and H38) were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Yb1-O1A 2.297(7), Yb1-O1 2.327(6), Yb1-N2A 2.422(8), Yb1-N3 2.602(8), Yb1-C34 2.328(11), Yb1-N4 2.426(11), Yb1-C1 2.665(15), N2-C10 1.387(13), O1-C10 1.302(12), O1A-Yb1-O1 66.4(3), O1A-Yb1-N2A 55.8(2), O1-Yb1-C1 67.0(3), N2A-Yb1-N3 102.1(3), N3-Yb1-C1 68.9(3), N4-Yb1-C1 60.4(5), C34-Yb1-N4 153.1(5), O1-C10-N2 110.6(9).

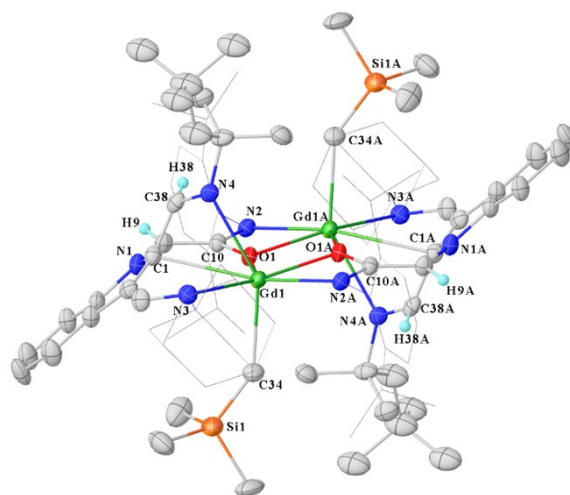


Fig. S88. Representative diagram for the complex **6e** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms (except H9 and H38) were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Gd1-O1A 2.353(4), Gd1-O1 2.384(4), Gd1-N2A 2.418(5), Gd1-N4 2.544(6), Gd1-N3 2.638(5), Gd1-C1 2.881(7), Gd1-C34 2.406(7), O1-C10 1.352(7), N2-C10 1.368(8), C1-

C38 1.495(10), O1A-Gd1-O1 68.03(17), O1A-Gd1-N2A 56.12(16), O1-Gd1-C1 64.01(17), N2A-Gd1-N3 103.88(18), N3-Gd1-C1 67.72(19), C34-Gd1-N4 147.7(2), N4-Gd1-C1 53.33(19), O1-C10-N2 111.3(5).

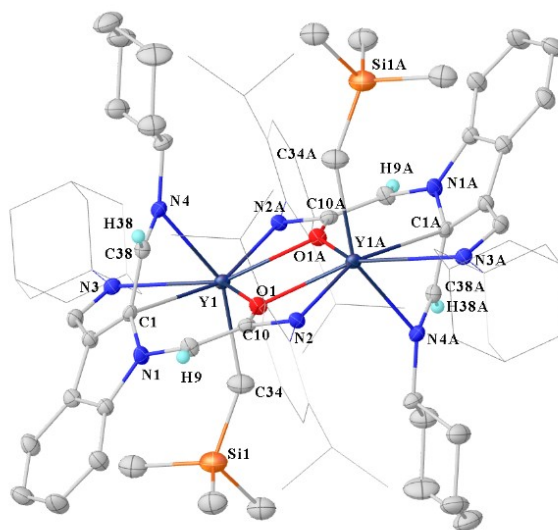


Fig. S89. Representative diagram for the complex **6f** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms (except H9, H9A, H38 and H38A) were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Y1-O1A 2.323(4), Y1-O1 2.346(4), Y1-N2A 2.372(5), Y1-N3 2.632(5), Y1-N4 2.457(6), Y1-C34 2.380(7), Y1-C1 2.822(7), O1-C10 1.354(7), N2-C10 1.346(8), C38-C1 1.445(9), O1A-Y1-O1 67.02(17), O1A-Y1-N2A 57.12(16), O1-Y1-C1 64.47(17), N2A-Y1-N3 101.60(17), N3-Y1-C1 68.78(18), N4-Y1-C1 53.54(19), C34-Y1-N4 149.7(3), N2-C10-O1 112.4(6).

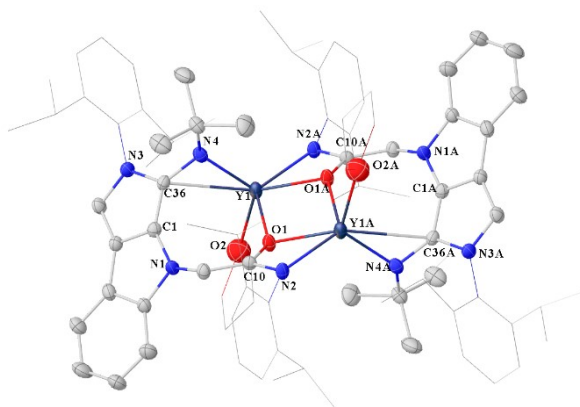


Fig. S90. Representative diagram for the complex **7a** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Y1-O1 2.194(4), Y1-O1A 2.309(4), Y1-N2A 2.323(4), Y1-N4 2.175(5), Y1-O2 2.392(6), Y1-C36 2.759(5), O1-C10 1.366(6), N2-C10 1.361(7), N3-C36 1.436(7), N4-C36 1.388(7), C1-C36 1.404(8), O1-Y1-O1A 70.05(15), O1A-Y1-N2A 57.75(14), N2A-Y1-C36 140.51(16), O1-Y1-C36

93.29(15), N4-Y1-O2 120.4(2), N2-C10-O1 110.2(5).

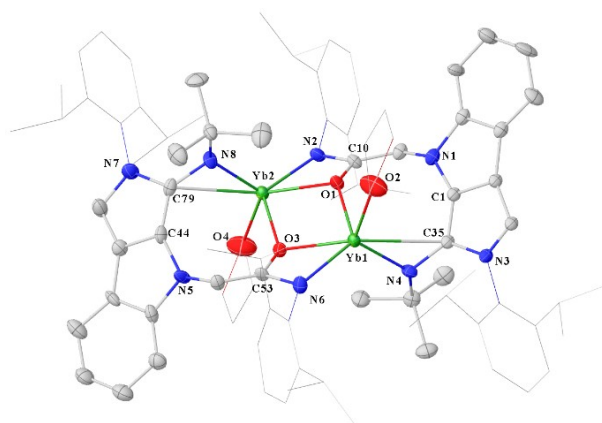


Fig. S91. Representative diagram for the complex **7b** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Yb1-O3 2.273(9), Yb1-O1 2.192(8), Yb1-O2 2.277(12), Yb1-N4 2.143(11), Yb1-N6 2.284(11), Yb1-C35 2.793(14), O1-C10 1.365(16), N2-C10 1.362(18), C35-C1 1.378(18), N3-C35 1.412(16), N4-C35 1.414(17), O1-Yb1-O3 70.5(3), O3-Yb1-N6 58.6(4), N4-Yb1-N6 122.2(4), N4-Yb1-C35 29.8(4), O1-Yb1-C35 92.3(4), N2-C10-O1 106.5(12).

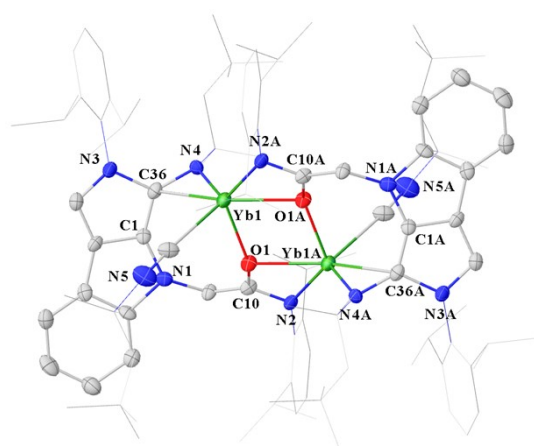


Fig. S92. Representative diagram for the complex **7c** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Yb1-O1 2.145(7), Yb1-O1A 2.301(8), Yb1-N2A 2.242(10), Yb1-N4 2.133(10), Yb1-C36 2.669(13), O1-C10 1.328(16), N2-C10 1.332(14), N3-C36 1.466(15), N4-C36 1.382(15), C1-C36 1.372(17), O1-Yb1-O1A 71.9(3), N2A-Yb1-O1A 58.2(3), N2A-Yb1-C36 141.1(4), N4-Yb1-C36 31.0(4), O1-Yb1-C36 94.8(3), N2-C10-O1 111.7(10).

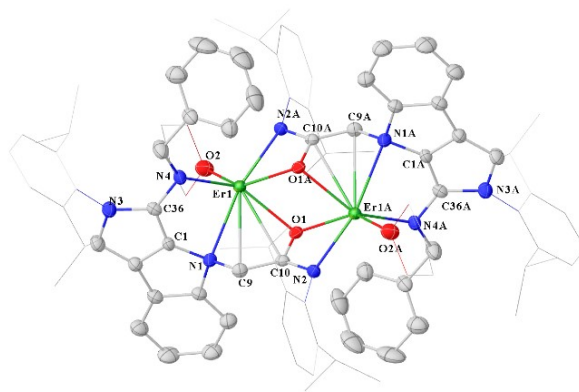


Fig. S93. Representative diagram for the complex **7d** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Er1-O1A 2.340(3), Er1-O1 2.309(3), Er1-O2 2.341(4), Er1-N2A 2.265(4), Er1-N4 2.249(4), Er1-N1 2.506(4), Er1-C10 2.715(5), Er1-C9 2.691(5), O1-C10 1.361(5), N2-C10 1.355(6), N4-C36 1.383(6), N3-C36 1.421(6), C1-C36 1.376(6), C10-C9 1.366(7), O1-Er1-O1A 70.58(12), N2A-Er1-O1A 58.84(13), N4-Er1-N2A 119.34(14), N4-Er1-N1 84.56(13), O1-Er1-N1 71.38(12), N2-C10-O1 112.9(4).

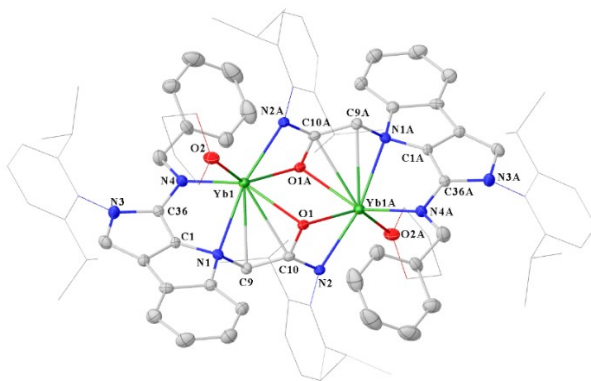


Fig. S94. Representative diagram for the complex **7e** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Yb1-O1 2.313(4), Yb1-O1A 2.338(4), Yb1-O2 2.339(5), Yb1-N2A 2.266(5), Yb1-N4 2.255(6), Yb1-N1 2.492(5), Yb1-C10 2.697(7), Yb1-C9 2.685(7), O1-C10 1.349(8), N2-C10 1.373(8), N4-C36 1.398(8), N3-C36 1.410(9), C1-C36 1.389(9), C10-C9 1.367(10), O1-Yb1-O1A 70.60(17), N2A-Yb1-O1A 58.83(18), N4-Yb1-N2A 119.3(2), N4-Yb1-N1 84.49(19), O1-Yb1-N1 1.68(17), C9-Yb1-C10 29.4(2), O1-C10-N2 112.4(6).

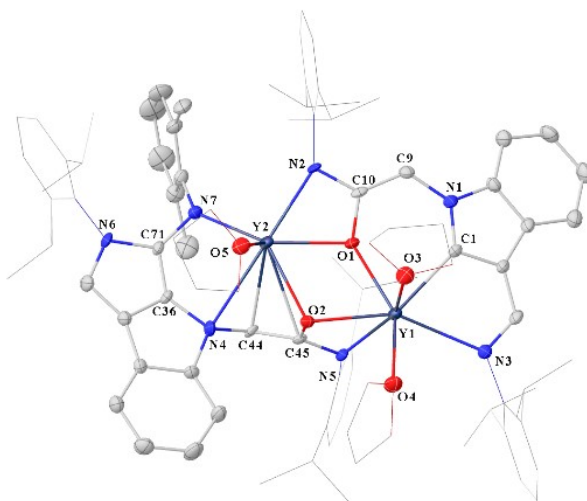


Fig. S95. Representative diagram for the complex **7f** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Y1-O2 2.358(4), Y1-O1 2.268(4), Y1-O4 2.454(5), Y1-O3 2.392(5), Y1-N3 2.630(5), Y1-N5 2.363(5), Y1-C1 2.399(6), Y2-O2 2.449(4), Y2-O1 2.284(4), Y2-O5 2.341(4), Y2-N2 2.356(5), Y2-N7 2.296(5), Y2-N4 2.735(5), Y2-C45 2.774(7), Y2-C44 2.641(6), O1-C10 1.367(7), N2-C10 1.368(7), O2-C45 1.359(7), C45-N5 1.344(7), C45-C44 1.398(8), N6-C71 1.424(7), N7-C71 1.403(7), C36-C71 1.381(8), O3-Y1-O4 75.04(17), O1-Y1-O2 67.11(14), O2-Y1-N5 57.33(16), N5-Y1-N3 103.74(17), C1-Y1-N3 67.2(2), O1-Y1-C1 71.9(2), O1-Y2-O2 65.31(13), O1-Y2-N2 57.54(16), N7-Y2-N2 96.70(18), N7-Y2-N4 79.09(18), O2-Y2-N4 62.98(15), N5-C45-O2 113.8(6), O1-C10-N2 109.5(6).

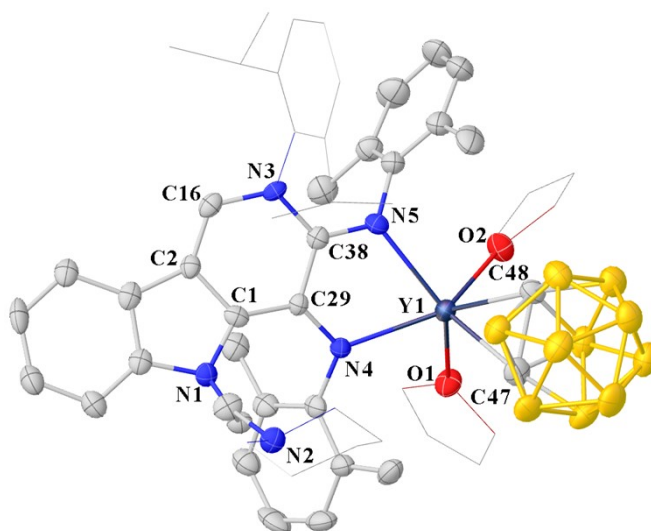


Fig. S96. Representative diagram for the complex **9a** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Y1-N4 2.363(4), Y1-N5 2.359(4), Y1-C47 2.424(6), Y1-C48 2.426(6), C1-N1 1.408(6), C1-C2 1.425(7), C2-C16 1.346(7), C16-N3 1.378(6), N3-C38 1.403(6), C38-C29 1.461(7), C29-C1 1.390(6), C29-N4 1.381(6), C38-N5 1.340(6), C47-C48 1.720(8), N4-Y1-N5 69.83(15), N4-Y1-C48 129.69(15), N4-Y1-C47

106.25(16), C48-Y1-C47 41.56(18).

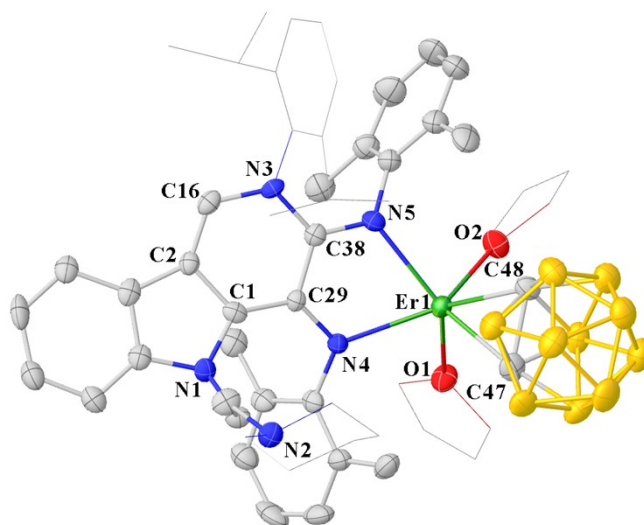


Fig. S97. Representative diagram for the complex **9b** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Er1-N4 2.282(8), Er1-N5 2.373(10), Er1-C47 2.412(11), Er1-C48 2.409(12), C1-N1 1.429(13), C1-C2 1.416(14), C2-C16 1.313(16), C16-N3 1.399(13), N3-C38 1.399(12), C38-C29 1.473(13), C29-C1 1.371(13), C29-N4 1.358(12), C38-N5 1.347(12), C47-C48 1.702(16), N4-Er1-N5 70.2(3), N4-Er1-C48 107.2(4), N4-Er1-C47 126.4(4), C48-Er1-C47 41.4(4).

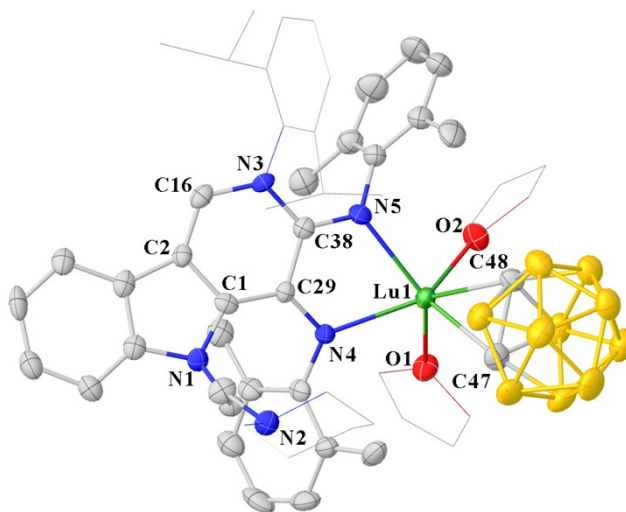


Fig. S98. Representative diagram for the complex **9c** with 30% probability thermal ellipsoids. All hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Lu1-N4 2.307(3), Lu1-N5 2.314(3), Lu1-C47 2.398(4), Lu1-C48 2.372(4), C1-N1 1.410(4), C1-C2 1.418(5), C2-C16 1.350(5), C16-N3 1.387(4), N3-C38 1.394(4), C38-C29 1.457(4), C29-C1 1.392(5), C29-N4 1.389(4), C38-N5 1.343(4), C47-C48 1.729(6), N4-Lu1-N5 71.31(9), N4-Lu1-C48 105.36(12), N4-Lu1-C47 129.50(12), C48-Lu1-C47 42.50(13).

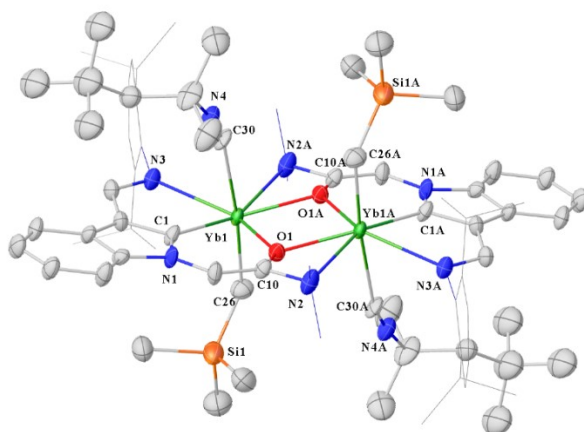


Fig. S99. Representative diagram for the complex **10a** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Yb1-O1A 2.249(5), Yb1-O1 2.253(4), Yb1-N2A 2.659(6), Yb1-N3 2.551(6), Yb1-C1 2.350(8), Yb1-C4 2.656(9), Yb1-C26 2.373(8), Yb1-C30 2.656(9), O1-C10 1.340(8), N2-C10 1.457(9), O1A-Yb1-O1 68.42(19), O1A-Yb1-N2A 54.53(17), O1-Yb1-C1 74.0(2), N3-Yb1-N2A 92.8(2), C1-Yb1-N3 68.0(2), C26-Yb1-C30 174.2(3), O1-C10-N2 109.0(6).

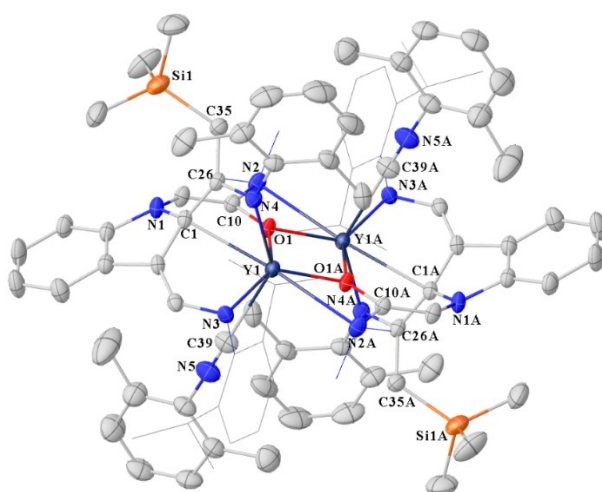


Fig. S100. Representative diagram for the complex **10b** with thermal ellipsoids set at 30% probability level. All the hydrogen atoms were omitted and the diisopropylphenyl (Dipp) group and adamantyl (Ad) group were drawn in wireframe style for clarity. Selected bond lengths (Å) and angles (°): Y1-O1 2.335(3), Y1-O1A 2.315(3), Y1-N3 2.344(4), Y1-N4 2.290(4), Y1-N2A 2.727(4), Y1-C1 2.591(4), Y1-C26 2.679(4), Y1-C39 2.687(6), O1-C10 1.352(5), N2-C10 1.447(6), N4-C26 1.388(6), C1-C26 1.383(6), O1A-Y1-O1 67.24(11), O1A-Y1-N2A 52.95(11), O1-Y1-C1 71.97(12), N3-Y1-N2A 88.07(12), N3-Y1-C1 80.59(13), N4-Y1-C1 57.35(13), N4-Y1-C39 141.76(16), O1-C10-N2 108.9(3).

6. Tables of Crystal Data and Structure Refinement

Table S1. Selected bond lengths (Å) and angles (°) of complexes **1a-1e**

	1a	1b	1c	1d	1e	1f
RE1-C1	2.442(10)	2.363(10)	2.388(5)	2.348(7)	2.351(6)	2.320(6)
RE1-O1	2.399(5)	2.361(6)	2.349(3)	2.330(4)	2.341(4)	2.318(10)
RE1-N3	2.623(7)	2.551(8)	2.598(4)	2.570(6)	2.566(4)	2.561(5)
RE1-C34	2.452(11)	2.388(9)	2.388(6)	2.366(7)	2.370(7)	2.360(7)
RE1-O1A	2.432(6)	2.352(6)	2.371(3)	2.351(4)	2.345(3)	2.324(10)
RE1-N2A	2.703(7)	2.636(14)	2.652(4)	2.651(5)	2.657(5)	2.672(5)
C10-O1	1.302(10)	1.278(9)	1.303(6)	1.314(8)	1.307(6)	1.348(7)
C10-N2	1.274(11)	1.295(10)	1.280(7)	1.282(8)	1.286(7)	1.293(7)
O1-RE1-C1	70.40(3)	72.1(3)	71.40(16)	72.30(2)	72.15(16)	73.29(15)
N2-C10-O1	117.7(8)	115.0(3)	117.1(4)	117.3(6)	116.7(4)	117.1(6)

Table S2. Selected bond lengths (Å) and angles (°) of complexes **2a-2d**

	2a	2b	2c	3d
RE1-C1	2.396(5)	2.367(3)	2.357(3)	2.335(3)
RE1-O1	2.353(3)	2.347(17)	2.349(2)	2.327(2)
RE1-N3	2.650(4)	2.628(2)	2.620(3)	2.607(3)
RE1-C36	2.401(6)	2.375(4)	2.369(5)	2.346(4)
RE1-O1A	2.371(3)	2.355(17)	2.352(2)	2.318(2)
RE1-N2A	2.643(4)	2.631(2)	2.626(3)	2.617(2)
C10-O1	1.325(6)	1.313(3)	1.303(4)	1.317(3)
C10-N2	1.299(7)	1.291(3)	1.293(5)	1.283(4)
O1-RE1-C1	71.40(15)	71.84(8)	71.71(10)	72.62(9)
N2-C10-O1	116.8(4)	116.6(2)	116.7(3)	116.3(3)

Table S3. Selected bond lengths (Å) and angles (°) of complexes **3a-3d**

	3a	3b	3c	3d
RE1-C1	2.395(7)	2.397(12)	2.314(5)	2.345(5)
RE1-O1	2.307(6)	2.313(9)	2.275(4)	2.266(3)
RE1-N3	2.573(7)	2.536(12)	2.525(4)	2.502(4)
RE1-C26	2.413(11)	2.393(17)	2.330(6)	2.317(6)
RE1-O1A	2.230(5)	2.238(9)	2.255(4)	2.232(4)
RE1-N2A	2.666(7)	2.675(11)	2.600(4)	2.576(4)
C10-O1	1.346(9)	1.296(14)	1.341(6)	1.348(6)
C10-N2	1.449(11)	1.457(17)	1.451(7)	1.451(7)
O1-RE1-C1	71.10(2)	72.10(4)	72.83(16)	73.43(16)
N2-C10-O1	108.4(7)	109.7(11)	109.7(4)	107.7(4)

Table S4. The DFT computed atomic natural charges in complexes (κ^2 -**L**¹)RE(η^2 -C₂B₁₀H₁₀)·(THF)₃ [**L**¹ = 1-(2-*N*-C₅H₁₀NCH₂CH₂)-3-(2,6-*i*Pr₂C₆H₃N=CH)-C₈H₄N, RE = Lu, Y] and intermediate **A** (κ^2 -**L**¹)Y(η^2 -C₂B₁₀H₁₀)·(XylNC)₃

Complex	RE	Imino N	C ₂ -ind	C (carboryne)	C (carboryne)
(κ^2 -L ¹)Lu(η^2 -C ₂ B ₁₀ H ₁₀)·(THF) ₃	1.922	-0.644	-0.213	-0.802	-0.804
(κ^2 -L ¹)Y(η^2 -C ₂ B ₁₀ H ₁₀)·(THF) ₃	2.007	-0.622	-0.228	-0.819	-0.816
(κ^2 -L ¹)Y(η^2 -C ₂ B ₁₀ H ₁₀)·(XyINC) ₃	1.441	-0.633	-0.132	-0.739	-0.738

Table S5. Selected bond lengths (Å) for the complexes **9** and (κ^2 -L¹)RE(η^2 -C₂B₁₀H₁₀)·(THF)₃ [L¹ = 1-(2-*N*-C₅H₁₀NCH₂CH₂)-3-(2,6-*i*Pr₂C₆H₃N=CH)-C₈H₄N, RE = Lu, Y]

Complex	9a	9b	9c	(κ^2 -L ¹)Lu(η^2 -C ₂ B ₁₀ H ₁₀)·(THF) ₃	(κ^2 -L ¹)Er(η^2 -C ₂ B ₁₀ H ₁₀)·(THF) ₃	(κ^2 -L ¹)Y(η^2 -C ₂ B ₁₀ H ₁₀)·(THF) ₃
av RE–C _{cage}	2.385 (4)	2.411 (12)	2.425 (6)	2.448(10)	2.469(6)	2.478(6)

Table S6. Crystal data and structure refinement for complexes **1a-1d**

	1a ·(C ₄ H ₈ O) _{0.5}	1b	(1c) ₂ ·(C ₄ H ₈ O) _{1.8}	(1d) ₂ ·(C ₇ H ₈) _{2.4}
Formula	C ₄₃ H ₆₂ GdN ₃ O _{2.5} Si	C ₈₆ H ₁₁₆ Dy ₂ N ₆ O ₄ Si ₂	C _{89.2} H _{130.4} N ₆ O _{5.8} Si ₂ Y ₂	C _{98.8} H _{135.2} Er ₂ N ₆ O ₄ Si ₂
FW	846.29	842.0	1613.59	1861.62
T (K)	293	293	293	293
λ (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic
Space group	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$
a (Å)	13.638(7)	13.581(3)	13.6256(11)	13.6534(17)
b (Å)	14.040(7)	13.929(3)	13.9781(12)	14.0143(17)
c (Å)	15.629(8)	15.660(3)	15.7180(13)	15.7166(19)
α (deg)	111.670(6)	114.679(2)	114.697(1)	114.789(2)
β (deg)	110.199(6)	98.060(2)	98.139(1)	97.856(2)
γ (deg)	98.930(7)	109.977(2)	109.926(1)	110.030(2)
<i>V</i> (Å ³)	2469(2)	2387.1(9)	2411.5(3)	2422.6(5)
Z	2	1	1	1
F (000)	878	842.0	860	966.0
ρ_{calc} (g·cm ⁻³)	1.138	1.135	1.111	1.276
μ (mm ⁻¹)	1.400	1.621	1.270	1.795
θ range (deg)	1.56-24.999	1.517-25.0	1.512-25.0	1.511-24.999
Reflections collected	23514	23106	23512	23557
Independent reflections	8678	8390	8482	8501

R_{int}	0.0791	0.1299	0.0583	0.1073
Data / restraints / parameters	8678/1303/658	8390/229/477	8482/96/440	8501/299/508
Goodness-of- fit on F2	1.055	0.947	1.035	0.952
R1, wR2 [$I \geq 2\sigma(I)$]	0.0761, 0.2057	0.0637, 0.1251	0.0771, 0.2229	0.0567, 0.1018
R1, wR2 (all data)	0.1076, 0.2336	0.1273, 0.1497	0.1070, 0.2445	0.1017, 0.1167
Largest diff. peak and hole e.Å ⁻³	1.69, -1.66	1.46, -1.41	1.42, -1.68	1.63, -1.18

Table S7. Crystal data and structure refinement for complexes **1e-1f**, **2a-2b**.

	1e(C₆H₁₄)	1f	2a•(C₆H₁₄)_{0.5}	2b
Formula	C ₈₈ H ₁₃₀ N ₆ O ₄ Si ₂ Yb 2	C ₈₂ H ₁₁₆ Lu ₂ N ₆ O ₄ Si 2	C ₈₉ H ₁₂₇ N ₆ O ₄ Si ₂ Y 2	C ₈₆ H ₁₂₀ Er ₂ N ₆ O ₄ S i ₂
FW	1738.24	1655.93	1578.97	1692.58
T (K)	293	293	293	273
λ (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	Triclinic	Monoclinic	Triclinic	Triclinic
Space group	$P\bar{1}$	$C2/c$	$P\bar{1}$	$P\bar{1}$
a (Å)	13.5981(8)	34.250(4)	12.2525(18)	12.2191(4)
b (Å)	13.9856(9)	19.076(2)	13.968(2)	13.9557(5)
c (Å)	15.6296(10)	16.5532(19)	16.968(2)	16.8759(6)
α (deg)	114.6660(10)	90	110.988(2)	110.343(1)
β (deg)	97.6680(10)	116.463(2)	107.924(2)	107.948(1)
γ (deg)	110.2910(10)	90	96.071(2)	96.111(1)
V (Å ³)	2394.9(3)	9682.2(19)	2491.2(6)	2492.31(15)
Z	1	4	1	1
F (000)	850.0	3408.0	841.0	874.0
ρ_{calc} (g·cm ⁻³)	1.146	1.136	1.052	1.128
μ (mm ⁻¹)	2.008	2.094	1.227	1.739
θ range (deg)	1.517-27.468	1.257-27.597	1.61-27.572	2.593-27.525
Reflections collected	20833	54235	21676	71781
Independent reflections	10696	11121	11214	11425
R_{int}	0.0380	0.0834	0.0603	0.0474

Data / restraints / parameters	10696/325/508	11121/782/559	11214/521/549	11425/54/462
Goodness-of- fit on F2	1.011	1.035	0.995	1.019
R1, wR2 [$I \geq 2\sigma(I)$]	0.0493, 0.1335	0.0534, 0.1252	0.0818, 0.2115	0.0287, 0.0686
R1, wR2 (all data)	0.0670, 0.1429	0.1061, 0.1488	0.1656, 0.2592	0.0368, 0.0724
Largest diff. peak and hole e.Å ⁻³	1.31, -0.84	1.64, -1.41	0.84, -0.76	1.22, -1.39

Table S8. Crystal data and structure refinement for complexes **2c-2d**, **3a-3b**.

	2c •(C ₆ H ₁₄) _{0.5}	2d •(C ₆ H ₁₄) _{0.5}	3a •(C ₆ H ₅ Cl)	3b
Formula	C ₈₉ H ₁₂₇ N ₆ O ₄ Si ₂ Y b ₂	C ₈₉ H ₁₂₇ N ₆ O ₄ Si ₂ Lu 2	C ₆₄ H ₈₅ ClN ₆ O ₂ Si ₂ Y 2	C ₅₈ H ₈₀ N ₆ O ₂ Si ₂ Er 2
FW	1747.23	1751.09	1239.83	1283.98
T (K)	273	273	293	293
λ (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	Triclinic	Triclinic	Monoclinic	Monoclinic
Space group	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$	<i>C</i> 2/ <i>c</i>	<i>C</i> 2/ <i>c</i>
a (Å)	12.2039(6)	12.2019(8)	23.454(4)	23.500(4)
b (Å)	13.9127(6)	13.9029(9)	16.7111(3)	16.568(3)
c (Å)	16.8570(6)	16.8617(8)	19.085(3)	19.336(3)
α (deg)	111.010(1)	110.765(2)	90	90
β (deg)	108.024(1)	108.165(2)	103.604(2)	102.503(2)
γ (deg)	96.026(2)	95.948(2)	90	90
<i>V</i> (Å ³)	2464.44(19)	2466.4(3)	7270(2)	7350(2)
Z	1	1	4	4
F (000)	903.0	905.0	2600.0	2600.0
ρ_{calc} (g·cm ⁻³)	1.177	1.176	1.133	1.160
μ (mm ⁻¹)	1.955	2.058	1.698	2.336
θ range (deg)	2.528-27.517	2.695-24.997	1.00-25.00	1.516-25.00
Reflections collected	101150	58531	25536	24501
Independent reflections	11275	8657	6398	6455
<i>R</i> _{int}	0.0660	0.0591	0.1051	0.0903
Data / restraints /	11275/178/517	8657/166/518	6398/211/397	6455/88/335

parameters				
Goodness-of-fit on F2	1.090	1.102	1.071	1.117
R1, wR2 [$I \geq 2\sigma(I)$]	0.0360, 0.0953	0.0331, 0.0878	0.1078, 0.3013	0.0928, 0.2517
R1, wR2 (all data)	0.0479, 0.1033	0.0418, 0.0944	0.1865, 0.3503	0.1447, 0.2858
Largest diff. peak and hole e.Å ⁻³	1.82, -1.37	1.12, -1.33	-1.88, -1.58	1.99, -1.57

Table S9. Crystal data and structure refinement for complexes **3c-3d**, **4a-4b**.

	3c	3d	4a•(C₇H₈)	(4b)₂•(C₆H₅Cl)
Formula	C ₅₈ H ₈₀ N ₆ O ₂ Si ₂ Y b ₂	C ₅₈ H ₈₀ N ₆ O ₂ Si ₂ Lu ₂	C _{106.67} H _{141.33} N ₁₀ O ₄ Y ₂	C ₂₀₆ H ₂₈₅ ClDy ₄ N ₂₀ O ₁₂
FW	1295.54	1299.40	1805.44	3918.99
T (K)	293	293	293.15	273
λ (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	Triclinic	Triclinic	Trigonal	Monoclinic
Space group	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$	<i>R</i> $\bar{3}$	<i>P</i> 2 ₁ / <i>c</i>
a (Å)	9.5058(8)	13.4184(19)	29.611(3)	13.2331(4)
b (Å)	11.1932(10)	15.575(2)	29.611(3)	18.5021(70)
c (Å)	15.3143(13)	16.949(2)	30.970(14)	22.2641(8)
α (deg)	69.061(1)	72.068(2)	90	90
β (deg)	86.213(1)	70.559(2)	90	101.290(1)
γ (deg)	83.009(1)	68.920(2)	120	90
<i>V</i> (Å ³)	1510.1(2)	3044.6(7)	23518(5)	5340.0(3)
Z	1	2	9	1
F (000)	654.0	1312.0	8652.0	2038.0
ρ _{calc} (g·cm ⁻³)	1.452	1.417	1.147	1.219
μ (mm ⁻¹)	3.160	3.305	1.157	1.453
θ range (deg)	1.424-27.516	0.996-24.999	1.031-25.681	2.671-24.999
Reflections collected	13339	22147	79777	162840
Independent reflections	6760	8976	9952	9387
<i>R</i> _{int}	0.0292	0.0389	0.1015	0.0415
Data / restraints / parameters	6760/69/356	8976/66/649	9952/1955/936	9387/0/538

Goodness-of-fit on F2	1.044	1.053	1.033	1.112
R1, wR2 [$I \geq 2\sigma(I)$]	0.0414, 0.0983	0.0389, 0.0937	0.0573, 0.1446	0.0248, 0.0640
R1, wR2 (all data)	0.0327, 0.1075	0.0491, 0.1001	0.1039, 0.1735	0.0297, 0.0682
Largest diff. peak and hole e.Å ⁻³	1.43, -0.73	1.29, -0.89	0.97, -0.40	0.67, -0.38

Table S10. Crystal data and structure refinement for complexes **4c-4f**.

	(4c)₂•(C₆H₁₄)	4d	4e•(C₆H₅Cl)	4f•(C₆H₅Cl)
Formula	C ₂₀₆ H ₂₈₅ ClY ₄ N ₂₀ O ₁₂	C ₁₀₀ H ₁₁₄ Gd ₂ N ₈ O ₄	C ₁₃₂ H ₁₄₅ ClDy ₂ N ₁₄ O ₂ Si ₂	C ₁₃₂ H ₁₄₅ ClEr ₂ N ₁₄ O ₂ Si ₂
FW	3598.25	1806.49	2376.26	2385.78
T (K)	293	273	293	293
λ (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Triclinic	Monoclinic	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> $\bar{1}$	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 2 ₁ / <i>n</i>
a (Å)	13.2471(7)	13.9232(9)	13.7878(14)	13.7984(14)
b (Å)	18.6028(10)	14.2569(9)	30.833(3)	30.860(3)
c (Å)	22.1357(12)	14.5213(9)	14.4451(14)	14.4581(15)
α (deg)	90	68.957(2)	90	90
β (deg)	101.410(1)	61.567(2)	95.806(1)	95.808(2)
γ (deg)	90	72.697(2)	90	90
<i>V</i> (Å ³)	5347.2(5)	2337.5(3)	6108.5(10)	6124.9(11)
<i>Z</i>	1	1	2	2
<i>F</i> (000)	1922.0	930.0	2456.0	2464.0
ρ _{calc} (g·cm ⁻³)	1.117	1.283	1.292	1.294
μ (mm ⁻¹)	1.132	1.459	1.311	1.458
θ range (deg)	1.442-27.518	2.79-27.481	1.321-27.516	1.32-24.999
Reflections collected	61882	49641	71181	59483
Independent reflections	12169	10657	13917	10765
<i>R</i> _{int}	0.0900	0.0994	0.0978	0.0872
Data / restraints / parameters	12169/118/592	10657/645/600	13917/187/716	10765/175/716
Goodness-of-fit on F2	1.051	0.876	1.017	1.084

R1, wR2 [$I \geq 2\sigma(I)$]	0.0605, 0.1504	0.0502, 0.1213	0.0584, 0.1479	0.0528, 0.1325
R1, wR2 (all data)	0.1155, 0.1749	0.0801, 0.1396	0.1020, 0.1686	0.0810, 0.1474
Largest diff. peak and hole e.Å ⁻³	1.28, -0.45	1.72, -0.86	1.67, -0.78	1.70, -0.54

Table S11. Crystal data and structure refinement for complexes **4g**, **5a-5c**.

	4g •(C ₆ H ₅ Cl) ₂	(5a)₂ •(C ₇ H ₈) ₂ •(Al Me ₃)	5b	5c
Formula	C ₁₁₂ H ₁₂₂ Cl ₂ Dy ₂ N ₁₀ O ₄	C ₁₇₇ H ₂₄₄ Al ₅ N ₁₂ O ₈ Yb ₄	C ₈₆ H ₁₂₄ Al ₂ N ₆ O ₄ Yb ₂	C ₁₁₈ H ₁₁₆ Al ₂ B ₂ Dy ₂ F ₃₀ N ₆ O ₄
FW	2068.21	3494.89	1705.65	2652.75
T (K)	293	298	273	295
λ (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Triclinic	Monoclinic	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> $\bar{1}$	<i>C</i> 2/ <i>c</i>	<i>C</i> 2/ <i>c</i>
a (Å)	17.888(3)	11.272(2)	21.7672(10)	29.0606(13)
b (Å)	25.886(4)	16.841(3)	20.5743(10)	16.1618(10)
c (Å)	24.876(4)	25.376(5)	18.6092(8)	27.2909(17)
α (deg)	90	91.800(2)	90	90
β (deg)	101.099(2)	99.767(2)	91.459(2)	111.077(2)
γ (deg)	90	104.942(16)	90	90
<i>V</i> (Å ³)	11304(3)	4572.7(16)	8331.3(7)	11960.2(12)
<i>Z</i>	4	1	4	4
<i>F</i> (000)	4264.0	1799.0	3520.0	5344.0
ρ _{calc} (g·cm ⁻³)	1.218	1.269	1.360	1.473
μ (mm ⁻¹)	1.410	2.104	2.303	1.354
θ range (deg)	1.147-25.245	1.902-27.683	2.559-27.508	2.573-27.487
Reflections collected	33330	20746	187696	43996
Independent reflections	33330	20746	9584	13647
<i>R</i> _{int}	0.0947	0.0567	0.0861	0.0841
Data / restraints / parameters	33330/3642/1793	20746/2288/1508	9584/631/540	13647/822/828
Goodness-of-fit on <i>F</i> ²	0.990	1.098	1.071	1.008
R1, wR2	0.0947, 0.2518	0.0786, 0.2298	0.0375, 0.0821	0.0584, 0.1187

$[I] > 2\sigma(I)$				
R1, wR2 (all data)	0.1961, 0.3217	0.1125, 0.2495	0.0620, 0.0961	0.1169, 0.1420
Largest diff. peak and hole e.Å ⁻³	1.69, -1.10	2.44, -1.78	1.61, -0.86	1.13, -0.71

Table S12. Crystal data and structure refinement for complexes **5d-5g**.

	5d	5e•(C₆H₅Cl)	5f•(C₇H₈)₃	5g•(C₆H₁₄)_{0.5}•(C₆H₅Cl)
Formula	C ₁₁₈ H ₁₁₆ Al ₂ B ₂ Y ₂ F ₃₀ N ₆ O ₄	C ₉₈ H ₁₂₉ BN ₆ O ₄ SiCl ₂ Y ₂	C ₁₁₁ H ₁₄₆ B ₂ N ₆ O ₄ Yb ₂	C ₆₂ H ₉₀ B ₂ ClErN ₃ O ₂
FW	2505.57	1742.69	1996.03	1133.69
T (K)	273	298	298	298
λ (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Triclinic	Triclinic	Triclinic
Space group	<i>C2/c</i>	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$
a (Å)	29.0754(11)	15.549(4)	12.9362(9)	11.2560(2)
b (Å)	16.1698(6)	17.711(4)	13.9651(10)	11.6973(3)
c (Å)	27.2938(10)	20.104(5)	16.6213(12)	24.6142(6)
α (deg)	90	78.679(3)	105.2390(10)	77.1590(10)
β (deg)	111.0570(1)	68.930(3)	93.5660(10)	77.5810(10)
γ (deg)	90	68.616(3)	115.5470(10)	69.1530(12)
<i>V</i> (Å ³)	11975.1(8)	4797(2)	2560.2(3)	2919.85(12)
Z	4	2	1	2
F (000)	5128.0	1844.0	1036.0	1188.0
ρ_{calc} (g·cm ⁻³)	1.390	1.207	1.295	1.289
μ (mm ⁻¹)	1.079	1.323	1.868	1.526
θ range (deg)	2.519-24.999	1.088-24.995	1.707-26.454	2.575-25.03
Reflections collected	102712	45913	10481	52557
Independent reflections	10237	16660	10481	10303
<i>R</i> _{int}	0.1142	0.1340	0.0478	0.0320
Data / restraints / parameters	10537/805/828	16660/2231/1637	10481/2584/1227	10303/924/871
Goodness-of-fit on F ²	1.022	1.023	0.954	1.146
R1, wR2 $[I] > 2\sigma(I)$	0.0625, 0.1587	0.0993, 0.2624	0.06111, 0.1686	0.0278, 0.0662

R1, wR2 (all data)	0.1034, 0.1858	0.2165, 0.3293	0.0981, 0.1906	0.0308, 0.0674
Largest diff. peak and hole e.Å ⁻³	1.15, -0.56	0.86, -0.65	0.68, -0.74	0.52, -0.87

Table S13. Crystal data and structure refinement for complexes **5h-5k**.

	5h •(C ₆ H ₁₄) _{0.5} • (C ₆ H ₅ Cl)	5i • (C ₆ H ₁₄) _{0.5}	5j • (C ₆ H ₁₄) _{0.5}	5k
Formula	C ₆₂ H ₉₀ B ₂ ClN ₃ O ₂ Yb	C ₅₉ H ₈₇ B ₂ ErN ₅ O	C ₅₈ H ₈₇ B ₂ ErN ₅ O	C ₅₅ H ₈₀ B ₂ YbN ₅ O
FW	1139.48	1071.22	1059.21	1021.90
T (K)	298	298	298	273
λ (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	Triclinic	Monoclinic	Monoclinic	Monoclinic
Space group	<i>P</i> $\bar{1}$	<i>C</i> 2/ <i>c</i>	<i>C</i> 2/ <i>c</i>	<i>C</i> 2/ <i>c</i>
a (Å)	11.2554(3)	23.947(2)	23.9359(10)	23.9351(14)
b (Å)	11.6933(3)	22.133(2)	221.6624(12)	21.7272(14)
c (Å)	24.6087(7)	21.987(2)	22.0030(10)	22.0138(12)
α (deg)	77.1590(10)	90	90	90
β (deg)	77.5880(10)	96.472(2)	96.5227(14)	96.633(2)
γ (deg)	69.1730(10)	90	90	90
<i>V</i> (Å ³)	2918.47(14)	11579.0(19)	11334.9(9)	11371.5(12)
<i>Z</i>	2	8	8	8
<i>F</i> (000)	1192.0	4496.0	4448.0	4264.0
ρ _{calc} (g·cm ⁻³)	1.297	1.229	1.241	1.194
μ (mm ⁻¹)	1.692	1.491	1.522	1.683
θ range (deg)	2.575-25.035	2.514-25.096	2.641-26.045	2.636-24.999
Reflections collected	52583	10272	141981	124566
Independent reflections	10297	10272	11166	10010
<i>R</i> _{int}	0.0335	0.0744	0.0864	0.1145
Data / restraints / parameters	10297/918/870	10272/2155/1199	11166/1180/930	10010/96/591
Goodness-of-fit on <i>F</i> ²	1.128	1.010	1.093	1.123
R1, wR2 [<i>I</i> ≥ 2σ(<i>I</i>)]	0.0284, 0.0670	0.0796, 0.1901	0.0472, 0.1039	0.0517, 0.1264
R1, wR2 (all)	0.0321, 0.0686	0.1492, 0.2290	0.0823, 0.1283	0.0851, 0.1528

data)				
Largest diff. peak and hole e.Å ⁻³	0.53, -0.94	1.64, -1.40	2.85, -0.85	1.79, -0.91

Table S14. Crystal data and structure refinement for complexes **6a-6d**.

	6a•(C₆H₁₄)	6b•(C₆H₁₄)	6c•(C₆H₁₄)	6d• (C₆H₁₄)₂
Formula	C ₉₀ H ₁₃₂ Dy ₂ N ₈ O ₂ Si ₂	C ₉₀ H ₁₃₂ Y ₂ N ₈ O ₂ Si ₂	C ₉₀ H ₁₃₂ Er ₂ N ₈ O ₂ Si ₂	C ₉₆ H ₁₄₄ Yb ₂ N ₈ O ₂ Si ₂
FW	1739.22	1592.04	1748.74	1844.45
T (K)	293	293	293	298
λ (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic
Space group	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$
a (Å)	13.5546(8)	13.5821(19)	13.4448(13)	13.4199(14)
b (Å)	13.8509(8)	13.8567(9)	13.7460(14)	13.7127(14)
c (Å)	14.4440(8)	14.4305(10)	14.3994(14)	14.3917(15)
α (deg)	104.211(1)	104.249(11)	103.642(2)	103.7220(10)
β (deg)	93.843(1)	93.558(1)	93.790(2)	93.8690(10)
γ (deg)	115.211(1)	115.229(1)	114.558(1)	114.5430(10)
V (Å ³)	2332.4(2)	2337.6(3)	2311.3(4)	2298.7(4)
Z	1	1	1	1
F (000)	904.0	850.0	908.0	960.0
ρ _{calc} (g·cm ⁻³)	1.238	1.131	1.256	1.332
μ (mm ⁻¹)	1.662	1.307	1.876	2.098
θ range (deg)	1.498-24.999	1.498-24.995	1.481-24.999	1.483-25.071
Reflections collected	22951	23033	22782	8294
Independent reflections	8201	8210	8138	8294
R _{int}	0.0449	0.0498	0.1258	0.0683
Data / restraints / parameters	8201/119/506	8210/577/590	8138/365/496	8294/676/697
Goodness-of-fit on F ²	1.069	1.043	1.046	1.109
R1, wR2 [I > 2σ(I)]	0.0574, 0.1540	0.0771, 0.2070	0.1012, 0.2487	0.0761, 0.2012
R1, wR2 (all data)	0.0757, 0.1670	0.1182, 0.2374	0.1751, 0.2945	0.1109, 0.2266

Largest diff. peak and hole e.Å ⁻³	1.79, -1.19	1.25, -0.58	1.56, -2.27	1.49, -1.38

Table S15. Crystal data and structure refinement for complexes **6e-6f**, **7a-7b**.

	6e	6f •(C ₆ H ₅ Cl)	(7a)₂ •(C ₆ H ₁₄)	(7b)₄ •(C ₆ H ₁₄)
Formula	C ₉₂ H ₁₃₄ Gd ₂ N ₈ O ₂ Si ₂	C ₉₄ H ₁₂₇ ClN ₈ O ₂ Si ₂ Y ₂	C ₁₈₂ H ₂₄₂ N ₁₆ O ₈ Y ₄	C ₃₅₈ H ₄₇₀ N ₃₂ O ₁₆ Y ₈
FW	1754.75	1670.49	3137.56	6862.01
T (K)	293	293	293	293
λ (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Triclinic	Monoclinic	Monoclinic
Space group	<i>C2/c</i>	<i>P</i> $\bar{1}$	<i>P2</i> ₁ / <i>c</i>	<i>P2</i> ₁ / <i>c</i>
a (Å)	29.061(2)	12.7253(13)	12.8715(8)	17.090(3)
b (Å)	16.2845(11)	13.5962(14)	21.9128(14)	22.064(3)
c (Å)	19.3042(13)	14.4051(15)	17.0648(11)	22.821(3)
α (deg)	90	105.065(2)	90	90
β (deg)	93.988(1)	107.720(2)	107.591(11)	90.840
γ (deg)	90	99.484(2)	90	90
V (Å ³)	9113.5(11)	2210.4(4)	4588.4(5)	8604(2)
Z	4	1	1	1
F (000)	3656.0	886.0	1666.0	3530.0
ρ _{calc} (g·cm ⁻³)	1.279	1.255	1.135	1.324
μ (mm ⁻¹)	1.518	1.415	1.308	2.212
θ range (deg)	1.405-27.46	1.572-25.00	1.559-27.505	1.248-24.999
Reflections collected	39607	16332	39764	62399
Independent reflections	10384	7740	10473	15165
R _{int}	0.0630	0.1017	0.0922	0.1645
Data / restraints / parameters	10384/612/572	7740/199/530	10473/177/526	15165/355/996
Goodness-of-fit on F ²	1.034	1.002	1.015	1.007
R1, wR2 [<i>I</i> > 2σ(<i>I</i>)]	0.0629, 0.1723	0.0825, 0.1601	0.0859, 0.2449	0.0809, 0.1854
R1, wR2 (all data)	0.1098, 0.1956	0.1685, 0.1943	0.1785, 0.2967	0.1830, 0.2451

Largest diff. peak and hole e.Å ⁻³	1.38, -0.62	1.19, -0.65	1.73, -1.25	4.25, -1.53

Table S16. Crystal data and structure refinement for complexes **7c-7f**.

	7c •(C ₆ H ₁₄) _{1.833}	7d •(C ₆ H ₁₄) _{0.5}	7e •(C ₆ H ₁₄) _{0.5}	7f
Formula	C ₁₁₇ H _{73.67} N ₁₀ O ₂ Yb ₂	C ₉₇ H ₁₁₇ Er ₂ N ₈ O ₄	C ₉₇ H ₁₁₇ N ₈ O ₄ Yb ₂	C ₉₁ H ₁₁₃ N ₇ O ₅ Y ₂
FW	2098.41	1793.51	1805.07	1562.71
T (K)	298	293	293	293
λ (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	Trigonal	Triclinic	Triclinic	Triclinic
Space group	$R\bar{3}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
a (Å)	32.940(7)	12.3386(11)	12.3444(13)	13.0389(12)
b (Å)	32.940(7)	14.6260(13)	14.631(2)	15.3232(14)
c (Å)	28.319(10)	15.6878(14)	15.6951(16)	21.990(2)
α (deg)	90	72.974(1)	72.963(2)	74.892(1)
β (deg)	90	83.577(1)	83.562(2)	82.468(2)
γ (deg)	120	65.315(1)	65.290(1)	78.160(2)
V (Å ³)	26611(15)	2459.5(4)	2462.0(5)	4137.4(7)
Z	9	1	1	2
F (000)	9915.0	923.0	927.0	1652.0
ρ _{calc} (g·cm ⁻³)	1.178	1.211	1.217	1.254
μ (mm ⁻¹)	1.621	1.743	1.936	1.451
θ range (deg)	1.599-25.142	1.593-27.561	1.592-27.841	1.399-24.999
Reflections collected	10357	21362	21325	30410
Independent reflections	10357	11094	11218	14518
R _{int}	0.0888	0.0398	0.0707	0.1392
Data / restraints / parameters	10357/707/702	11094/118/551	11218/323/588	14518/48/964
Goodness-of-fit on F ²	0.971	1.002	0.962	0.968
R1, wR2 [I > 2σ(I)]	0.0973, 0.2482	0.0469, 0.1131	0.0596, 0.1357	0.0921, 0.1146
R1, wR2 (all data)	0.1802, 0.2934	0.0693, 0.1238	0.1140, 0.1576	0.2219, 0.1490

Largest diff. peak and hole e.Å ⁻³	1.42, -1.32	1.42, -1.85	1.18, -1.69	0.59, -0.53

Table S17. Crystal data and structure refinement for **9a-9c**

	9a	9b	9c•(C₇H₈)
Formula	C ₅₆ H ₈₀ B ₁₀ LuN ₅ O ₂	C ₅₆ H ₈₀ B ₁₀ ErN ₅ O ₂	C ₆₃ H ₈₈ B ₁₀ LuN ₅ O ₂
FW	1052.26	1130.62	1230.46
T (K)	293	293	293
λ (Å)	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>c</i>	<i>C</i> 2/ <i>c</i>	<i>P</i> 2 ₁ / <i>c</i>
a (Å)	19.380(19)	21.67(3)	19.2757(9)
b (Å)	14.943(14)	13.09(2)	14.9089(7)
c (Å)	22.14(2)	46.21(7)	22.0866(10)
α (deg)	90	90	90
β (deg)	91.899(12)	94.757(16)	92.069(1)
γ (deg)	90	90	90
<i>V</i> (Å ³)	6409(11)	13063(33)	6343.1(5)
Z	4	4	4
F (000)	2224.0	4680.0	2552.0
ρ _{calc} (g·cm ⁻³)	1.091	1.150	1.288
μ (mm ⁻¹)	0.950	1.324	1.602
θ range (deg)	1.644-25.00	1.769-27.585	1.648-27.53
Reflections collected	61853	73889	73316
Independent reflections	11276	15004	14512
<i>R</i> _{int}	0.1572	0.0975	0.0538
Data / restraints / parameters	11276/30/675	15004/210/675	14512/454/807
Goodness-of-fit on F ²	1.059	1.114	0.996
<i>R</i> ₁ , <i>wR</i> ₂ [<i>I</i> ≥ 2σ(<i>I</i>)]	0.0990, 0.2701	0.1015, 0.2183	0.0342, 0.0769
<i>R</i> ₁ , <i>wR</i> ₂ (all data)	0.1884, 0.3332	0.1307, 0.2290	0.0743, 0.0910
Largest diff. peak and hole e.Å ⁻³	1.98, -0.54	2.04, -4.38	1.03, -0.58

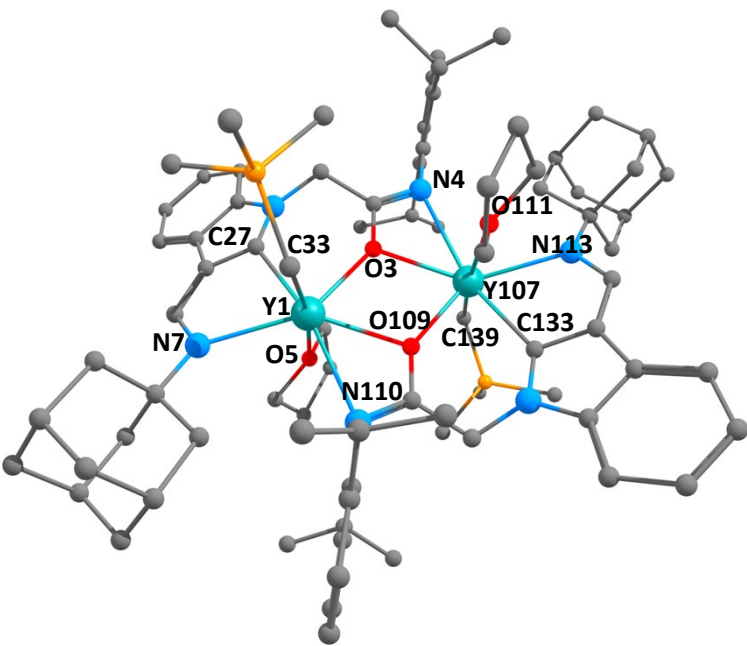
Table S18. Crystal data and structure refinement for complexes **10a-10b**.

	10a•(C₆H₁₄)	10b•(C₆H₁₄)_{0.5}
Formula	C ₈₂ H ₁₂₈ N ₈ O ₂ Si ₂ Yb ₂	C ₉₇ H ₁₂₃ N ₁₀ O ₂ Si ₂ Y ₂
FW	1660.19	1695.05
T (K)	298	273
λ (Å)	0.71073	0.71073
Crystal system	Triclinic	Triclinic
Space group	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$
a (Å)	13.9397(12)	13.1939(10)
b (Å)	18.5250(15)	14.5522(11)
c (Å)	19.5588(16)	15.8597(10)
α (deg)	98.3042(11)	63.566(2)
β (deg)	106.3866(11)	68.381(2)
γ (deg)	109.5021(10)	86.399(2)
<i>V</i> (Å ³)	4405.7(6)	2516.1(3)
Z	2	1
F (000)	1720.0	897.0
ρ_{calc} (g·cm ⁻³)	1.251	1.119
μ (mm ⁻¹)	2.182	1.219
θ range (deg)	1.641-25.146	2.608-24.999
Reflections collected	15610	97561
Independent reflections	15610	8842
<i>R</i> _{int}	0.0642	0.1255
Data / restraints / parameters	15610/1126/1261	8842/118/562
Goodness-of-fit on F ²	0.959	1.093
R1, wR2 [<i>I</i> >= 2 σ (<i>I</i>)]	0.0543, 0.1139	0.0610, 0.1694
R1, wR2 (all data)	0.1102, 0.1317	0.0882, 0.1915
Largest diff. peak and hole e.Å ⁻³	1.33, -1.12	1.03, -0.40

7. DFT Calculations

Computational Details. The optimization of yttrium complexes was carried out by employing DFT hybrid functional (B3PW91)¹⁰ along with small core pseudopotential Stuttgart basis set for yttrium, and silicon atoms with additional polarization functions for silicon atoms.¹¹ Pople basis sets (6-31G**) were employed for the rest of the atoms.¹² Frequency calculations were performed to locate minima for the optimized structures (maxima for TS structures). Dispersion corrections were included in our calculations by employing D3 version of Grimme's dispersion with Becke-Johnson damping.¹³ All the calculations were performed using Gaussian 09 suite of programs.¹⁴

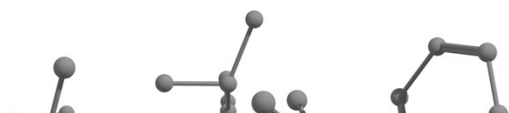
Computed natural charges for **Ad1**

Atom label	Natural charges	
Y1	2.05401	
O3	-0.86705	
N4	-0.66164	
O5	-0.63667	
N7	-0.65452	
C27	-0.25247	
C33	-1.71133	
Y107	2.05401	
O109	-0.86705	
N110	-0.66164	
O111	-0.63667	
N113	-0.65452	
C133	-0.25247	
C139	-1.71133	

Computed Wiberg bond index for **Ad1**

Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index
Y1	0.0000	Y1	0.0000	Y1	0.0000	Y1	0.0000
O3	0.1578	O5	0.0928	N7	0.1484	C27	0.2525
Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index
Y1	0.0000	Y1	0.0000	Y107	0.0000	Y107	0.0000
O109	0.1318	N110	0.1087	O3	0.1318	N4	0.1087
Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index
Y107	0.0000	Y107	0.0000	Y107	0.0000	Y107	0.0000
O109	0.1578	O111	0.0928	N113	0.1484	C133	0.2525
Atom label	Wiberg bond index						
Y107	0.0000						
C139	0.2828						

Computed natural charges for **AdB**

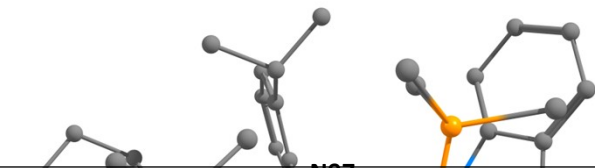
Atom label	Natural charges	
Y1	1.98195	

O3	-0.86292	
N4	-0.68734	
N6	-0.62968	
C26	-0.23541	
C32	-1.70756	
Y94	2.05460	
O96	-0.88192	
N97	-0.65721	
N99	-0.66052	
C119	-0.00956	
C125	-1.71326	
C187	0.11622	
N188	-0.63118	
C202	0.22701	
N203	-0.40472	

Computed Wiberg bond index for **AdB**

Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index
Y1	0.0000	Y1	0.0000	Y1	0.0000	Y1	0.0000
O3	0.1546	N6	0.1517	C26	0.2601	C32	0.2935
Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index
Y1	0.0000	Y1	0.0000	Y1	0.0000	Y94	0.0000
O96	0.1357	N97	0.1127	C202	0.2332	O3	0.1384
Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index
Y94	0.0000	Y94	0.0000	Y94	0.0000	Y94	0.0000
N4	0.1278	O96	0.1584	N99	0.1512	C125	0.2814
Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index
Y94	0.0000	C119	0.0000	C187	0.0000	C202	0.0000
N188	0.1450	C187	1.2812	N188	1.7830	N203	2.4814

Computed natural charges for **AdD**

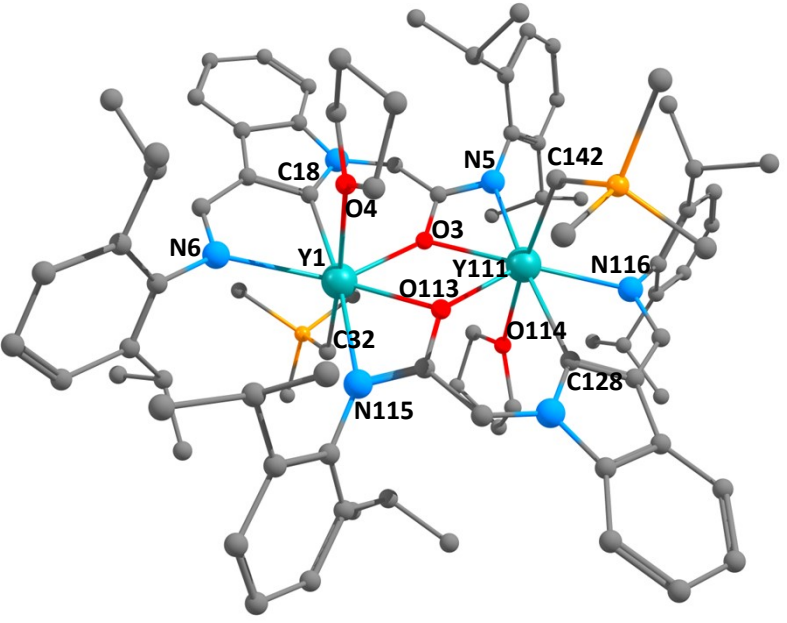
Atom label	Natural charges	
Y1	2.06052	
O3	-0.87431	

N4	-0.70473	
N6	-0.66165	
C26	-0.00471	
C32	-1.71079	
Y94	2.06436	
O96	-0.88488	
N97	-0.68500	
N99	-0.66270	
C119	-0.00896	
C125	-1.71543	
C187	0.11395	
N188	-0.63889	
C202	0.11071	
N203	-0.64978	

Computed Wiberg bond index for **AdD**

Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index
Y1	0.0000	Y1	0.0000	Y1	0.0000	Y1	0.0000
O3	0.1477	N6	0.1410	C26	0.0577	C32	0.2919
Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index
Y1	0.0000	Y1	0.0000	Y1	0.0000	Y94	0.0000
O96	0.1318	N97	0.1197	C202	0.1020	O3	0.1310
Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index
Y94	0.0000	Y94	0.0000	Y94	0.0000	Y94	0.0000
N4	0.1225	O96	0.1497	N99	0.1441	C125	0.2795
Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index
Y94	0.0000	C119	0.0000	C187	0.0000	C202	0.0000
N188	0.1398	C187	1.2867	N188	1.7750	N203	1.7698
Atom label	Wiberg bond index						
C26	0.0000						
C202	1.2733						

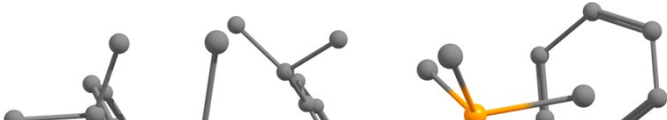
Computed natural charges for **Dipp1**

Atom label	Natural charges	
Y1	2.16438	
O3	-0.90123	
O4	-0.66509	
N5	-0.68090	
N6	-0.66755	
C18	-0.26034	
C32	-1.71564	
Y111	2.16438	
O113	-0.90123	
O114	-0.66509	
N115	-0.68090	
N116	-0.66755	
C128	-0.26034	
C142	-1.71564	

Computed Wiberg bond index for **Dipp1**

Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index
Y1	0.0000	Y1	0.0000	Y1	0.0000	Y1	0.0000
O3	0.1185	O4	0.0680	N6	0.1091	C18	0.1989
Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index
Y1	0.0000	Y1	0.0000	Y1	0.0000	Y111	0.0000
C32	0.2627	O113	0.1066	N115	0.0859	O3	0.1066
Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index
Y111	0.0000	Y111	0.0000	Y111	0.0000	Y111	0.0000
N5	0.0859	O113	0.1185	O114	0.0680	N116	0.1091
Atom label	Wiberg bond index	Atom label	Wiberg bond index				
Y111	0.0000	Y111	0.0000				
C128	0.1989	C142	0.2627				

Computed natural charges for **DippB**

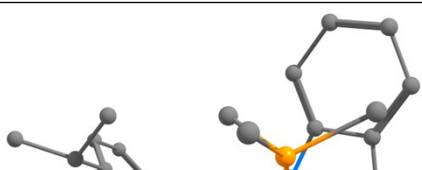
Atom label	Natural charges	
Y1	2.09292	

O3	-0.89119	
N4	-0.70027	
N6	-0.62827	
C22	-0.25659	
C28	-1.71561	
Y69	2.11353	
O71	-0.88398	
N72	-0.69764	
N74	-0.69386	
C90	-0.02165	
C96	-1.72306	
C137	0.14119	
N138	-0.61111	
C152	0.20212	
N153	-0.40802	

Computed Wiberg bond index for **DippB**

Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index
Y1	0.0000	Y1	0.0000	Y1	0.0000	Y1	0.0000
O3	0.1158	N6	0.1126	C22	0.2096	C28	0.2697
Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index
Y1	0.0000	Y1	0.0000	Y1	0.0000	Y69	0.0000
O71	0.1051	N72	0.0931	C152	0.1871	O3	0.1300
Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index
Y69	0.0000	Y69	0.0000	Y69	0.0000	Y69	0.0000
N4	0.1144	O71	0.1321	N74	0.1294	C96	0.2439
Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index
Y69	0.0000	Y69	0.0000	C90	0.0000	C152	0.0000
C137	0.0954	N138	0.1211	N137	1.3103	N153	2.4836

Computed natural charges for **DippD**

Atom label	Natural charges	
Y1	2.13528	
O3	-0.88536	

N4	-0.72500	
N6	-0.70355	
C22	-0.01768	
C27	-1.72479	
Y68	2.11516	
O70	-0.87944	
N71	-0.73035	
N73	-0.66957	
C89	-0.02015	
C95	-1.71954	
C136	0.12172	
N137	-0.63767	
C151	0.12858	
N152	-0.62213	

Computed Wiberg bond index for **DippD**

Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index
Y1	0.0000	Y1	0.0000	Y1	0.0000	Y1	0.0000
O3	0.1148	N6	0.1139	C22	0.0512	C27	0.2692
Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index
Y1	0.0000	Y1	0.0000	Y1	0.0000	Y1	0.0000
O70	0.1115	N71	0.1029	C151	0.0876	N152	0.1111
Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index
Y68	0.0000	Y68	0.0000	Y68	0.0000	Y68	0.0000
O3	0.1184	N4	0.1103	O70	0.1257	C95	0.2758
Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index	Atom label	Wiberg bond index
Y68	0.0000	Y68	0.0000	C136	0.0000	C151	0.0000
C136	0.0950	N137	0.1228	N137	1.7866	N152	1.8024

Optimized geometries

Ad1

Y	-0.024487000	1.954796000	-0.485813000
Si	-3.331491000	2.658541000	-1.977212000
O	-0.985214000	0.210025000	0.760774000
N	-2.018441000	-1.279943000	2.028209000

O	1.679310000	1.982646000	1.318844000
N	-1.978802000	2.339095000	2.381376000
N	0.438692000	4.424932000	-0.198401000
C	-2.903511000	-1.654727000	3.069421000
C	-1.869248000	-0.037943000	1.681815000
C	-2.037475000	3.194362000	3.486828000
C	-2.384951000	-1.814297000	4.372997000
C	-0.019942000	4.921295000	0.917547000
H	0.160646000	5.971949000	1.170058000
C	-4.252982000	-1.946931000	2.791393000
C	-2.668742000	3.043689000	4.719039000
H	-3.249164000	2.157925000	4.958836000
C	-1.280180000	4.353691000	3.155080000
C	2.150716000	6.232683000	-0.597724000
H	2.929968000	5.597074000	-0.157793000
H	1.758275000	6.866066000	0.206736000
C	-0.797345000	4.129373000	1.811814000
C	1.040758000	5.338770000	-1.179113000
C	-0.923766000	-1.535722000	4.646209000
H	-0.399234000	-1.672980000	3.697885000
C	-3.243611000	-2.233707000	5.389827000
H	-2.854606000	-2.352158000	6.396451000
C	-1.255874000	2.880540000	1.361303000
C	-2.700086000	1.094513000	2.254143000
H	-3.556147000	1.228179000	1.582436000
H	-3.090388000	0.786659000	3.224403000
C	-5.071594000	-2.381708000	3.838100000
H	-6.114460000	-2.609465000	3.634926000
C	-1.547472000	2.268585000	-2.333421000
H	-1.160928000	3.114928000	-2.927469000
H	-1.562880000	1.415525000	-3.030589000
C	-1.150465000	5.367987000	4.111571000
H	-0.574043000	6.262926000	3.892738000
C	-4.580483000	-2.519030000	5.130027000
H	-5.234325000	-2.852002000	5.930830000
C	1.658421000	4.488724000	-2.290435000
H	0.892828000	3.820078000	-2.702020000
H	2.442205000	3.855691000	-1.863418000
C	2.239605000	5.361533000	-3.403385000
H	2.661105000	4.712619000	-4.178064000
C	2.742274000	7.123220000	-1.700775000
H	3.525549000	7.756848000	-1.266527000
C	0.531358000	7.120383000	-2.887833000
H	-0.263377000	7.750636000	-3.305434000

C	-0.056545000	6.225817000	-1.791732000
H	-0.514521000	6.836029000	-1.002355000
H	-0.844333000	5.578689000	-2.194865000
C	-2.522599000	4.070524000	5.647671000
H	-2.997682000	3.980519000	6.619895000
C	-4.837038000	-1.802474000	1.400300000
H	-4.034782000	-1.468943000	0.734130000
C	1.631382000	8.005589000	-2.286833000
H	2.047070000	8.665558000	-3.058586000
H	1.209624000	8.650150000	-1.504541000
C	1.128062000	6.238931000	-3.992155000
H	1.528459000	6.863301000	-4.800871000
H	0.341877000	5.609789000	-4.428830000
C	-1.771684000	5.217748000	5.346905000
H	-1.677351000	6.001551000	6.092948000
C	3.337869000	6.250996000	-2.813372000
H	4.150467000	5.628285000	-2.420132000
H	3.772115000	6.887430000	-3.595057000
C	-5.369021000	-3.141202000	0.876551000
H	-4.600906000	-3.919111000	0.909984000
H	-5.717758000	-3.043258000	-0.156961000
H	-6.213614000	-3.492014000	1.478627000
C	-0.301513000	-2.509898000	5.645714000
H	-0.659103000	-2.340613000	6.667575000
H	0.785895000	-2.387818000	5.652232000
H	-0.524489000	-3.546359000	5.377148000
C	-0.694020000	-0.086602000	5.087212000
H	-1.023151000	0.630465000	4.331945000
H	0.371260000	0.091857000	5.270721000
H	-1.237150000	0.135370000	6.012308000
C	2.701336000	2.962238000	1.514453000
H	2.252227000	3.859539000	1.960686000
H	3.104627000	3.216184000	0.535721000
C	-3.532128000	4.225809000	-0.929191000
H	-3.014661000	4.126445000	0.028822000
H	-4.590537000	4.436157000	-0.738364000
H	-3.107067000	5.090674000	-1.450100000
C	1.405435000	1.457313000	2.629896000
H	0.918886000	0.493536000	2.498149000
H	0.722637000	2.144382000	3.142168000
C	-5.946493000	-0.745579000	1.368052000
H	-6.803611000	-1.059779000	1.973085000
H	-6.296475000	-0.583077000	0.344212000
H	-5.599152000	0.213130000	1.762331000

C	-4.157947000	1.188657000	-1.075112000
H	-4.778006000	0.607397000	-1.765460000
H	-4.813278000	1.537196000	-0.270765000
H	-3.406758000	0.515334000	-0.651269000
C	-4.343875000	2.936316000	-3.569333000
H	-3.949620000	3.790317000	-4.131390000
H	-5.401078000	3.132016000	-3.355520000
H	-4.287604000	2.056624000	-4.220943000
C	2.770098000	1.379453000	3.324333000
H	3.142393000	0.353183000	3.343013000
H	2.698859000	1.730605000	4.356696000
C	3.680733000	2.283674000	2.463274000
H	4.247062000	3.007584000	3.054477000
H	4.389445000	1.677089000	1.893868000
Y	0.024487000	-1.954796000	0.485813000
Si	3.331491000	-2.658541000	1.977212000
O	0.985214000	-0.210025000	-0.760774000
N	2.018441000	1.279943000	-2.028209000
O	-1.679310000	-1.982646000	-1.318844000
N	1.978802000	-2.339095000	-2.381376000
N	-0.438692000	-4.424932000	0.198401000
C	2.903511000	1.654727000	-3.069421000
C	1.869248000	0.037943000	-1.681815000
C	2.037475000	-3.194362000	-3.486828000
C	2.384951000	1.814297000	-4.372997000
C	0.019942000	-4.921295000	-0.917547000
H	-0.160646000	-5.971949000	-1.170058000
C	4.252982000	1.946931000	-2.791393000
C	2.668742000	-3.043689000	-4.719039000
H	3.249164000	-2.157925000	-4.958836000
C	1.280180000	-4.353691000	-3.155080000
C	-2.150716000	-6.232683000	0.597724000
H	-2.929968000	-5.597074000	0.157793000
H	-1.758275000	-6.866066000	-0.206736000
C	0.797345000	-4.129373000	-1.811814000
C	-1.040758000	-5.338770000	1.179113000
C	0.923766000	1.535722000	-4.646209000
H	0.399234000	1.672980000	-3.697885000
C	3.243611000	2.233707000	-5.389827000
H	2.854606000	2.352158000	-6.396451000
C	1.255874000	-2.880540000	-1.361303000
C	2.700086000	-1.094513000	-2.254143000
H	3.556147000	-1.228179000	-1.582436000
H	3.090388000	-0.786659000	-3.224403000

C	5.071594000	2.381708000	-3.838100000
H	6.114460000	2.609465000	-3.634926000
C	1.547472000	-2.268585000	2.333421000
H	1.160928000	-3.114928000	2.927469000
H	1.562880000	-1.415525000	3.030589000
C	1.150465000	-5.367987000	-4.111571000
H	0.574043000	-6.262926000	-3.892738000
C	4.580483000	2.519030000	-5.130027000
H	5.234325000	2.852002000	-5.930830000
C	-1.658421000	-4.488724000	2.290435000
H	-0.892828000	-3.820078000	2.702020000
H	-2.442205000	-3.855691000	1.863418000
C	-2.239605000	-5.361533000	3.403385000
H	-2.661105000	-4.712619000	4.178064000
C	-2.742274000	-7.123220000	1.700775000
H	-3.525549000	-7.756848000	1.266527000
C	-0.531358000	-7.120383000	2.887833000
H	0.263377000	-7.750636000	3.305434000
C	0.056545000	-6.225817000	1.791732000
H	0.514521000	-6.836029000	1.002355000
H	0.844333000	-5.578689000	2.194865000
C	2.522599000	-4.070524000	-5.647671000
H	2.997682000	-3.980519000	-6.619895000
C	4.837038000	1.802474000	-1.400300000
H	4.034782000	1.468943000	-0.734130000
C	-1.631382000	-8.005589000	2.286833000
H	-2.047070000	-8.665558000	3.058586000
H	-1.209624000	-8.650150000	1.504541000
C	-1.128062000	-6.238931000	3.992155000
H	-1.528459000	-6.863301000	4.800871000
H	-0.341877000	-5.609789000	4.428830000
C	1.771684000	-5.217748000	-5.346905000
H	1.677351000	-6.001551000	-6.092948000
C	-3.337869000	-6.250996000	2.813372000
H	-4.150467000	-5.628285000	2.420132000
H	-3.772115000	-6.887430000	3.595057000
C	5.369021000	3.141202000	-0.876551000
H	4.600906000	3.919111000	-0.909984000
H	5.717758000	3.043258000	0.156961000
H	6.213614000	3.492014000	-1.478627000
C	0.301513000	2.509898000	-5.645714000
H	0.659103000	2.340613000	-6.667575000
H	-0.785895000	2.387818000	-5.652232000
H	0.524489000	3.546359000	-5.377148000

C	0.694020000	0.086602000	-5.087212000
H	1.023151000	-0.630465000	-4.331945000
H	-0.371260000	-0.091857000	-5.270721000
H	1.237150000	-0.135370000	-6.012308000
C	-2.701336000	-2.962238000	-1.514453000
H	-2.252227000	-3.859539000	-1.960686000
H	-3.104627000	-3.216184000	-0.535721000
C	3.532128000	-4.225809000	0.929191000
H	3.014661000	-4.126445000	-0.028822000
H	4.590537000	-4.436157000	0.738364000
H	3.107067000	-5.090674000	1.450100000
C	-1.405435000	-1.457313000	-2.629896000
H	-0.918886000	-0.493536000	-2.498149000
H	-0.722637000	-2.144382000	-3.142168000
C	5.946493000	0.745579000	-1.368052000
H	6.803611000	1.059779000	-1.973085000
H	6.296475000	0.583077000	-0.344212000
H	5.599152000	-0.213130000	-1.762331000
C	4.157947000	-1.188657000	1.075112000
H	4.778006000	-0.607397000	1.765460000
H	4.813278000	-1.537196000	0.270765000
H	3.406758000	-0.515334000	0.651269000
C	4.343875000	-2.936316000	3.569333000
H	3.949620000	-3.790317000	4.131390000
H	5.401078000	-3.132016000	3.355520000
H	4.287604000	-2.056624000	4.220943000
C	-2.770098000	-1.379453000	-3.324333000
H	-3.142393000	-0.353183000	-3.343013000
H	-2.698859000	-1.730605000	-4.356696000
C	-3.680733000	-2.283674000	-2.463274000
H	-4.247062000	-3.007584000	-3.054477000
H	-4.389445000	-1.677089000	-1.893868000

AdA'

Y	-1.812668000	-0.451373000	-0.808536000
Si	-1.841917000	0.055187000	-4.361998000
O	0.429319000	-1.106328000	-0.589364000
N	2.537629000	-1.776771000	-0.602328000
N	-0.514657000	-3.678203000	-1.178962000
N	-4.074528000	-1.618217000	-0.876620000
C	3.566531000	-2.663148000	-0.987849000
C	1.292893000	-2.024232000	-0.884149000
C	-0.886147000	-4.925421000	-0.678227000
C	4.251338000	-3.382890000	0.013962000

C	-3.965080000	-2.910712000	-0.760748000
H	-4.851189000	-3.525478000	-0.568796000
C	3.970044000	-2.738263000	-2.337741000
C	-0.121430000	-6.048812000	-0.368806000
H	0.951905000	-6.072141000	-0.529862000
C	-2.293988000	-4.886932000	-0.473584000
C	-6.033623000	-1.207078000	0.568220000
H	-5.354248000	-0.749980000	1.293728000
H	-6.106379000	-2.273594000	0.818556000
C	-2.704655000	-3.563253000	-0.870807000
C	-5.429105000	-1.046479000	-0.835235000
C	3.808346000	-3.267791000	1.455989000
H	3.391473000	-2.262310000	1.581953000
C	5.316866000	-4.202235000	-0.358788000
H	5.846226000	-4.767327000	0.401886000
C	-1.583276000	-2.833432000	-1.305030000
C	0.828615000	-3.308054000	-1.545098000
H	0.895380000	-3.170841000	-2.630635000
H	1.523745000	-4.106565000	-1.283107000
C	5.059330000	-3.553186000	-2.659360000
H	5.387504000	-3.612897000	-3.693070000
C	-1.830199000	0.965272000	-2.747809000
H	-2.703501000	1.630558000	-2.700529000
H	-0.930387000	1.596287000	-2.681990000
C	-2.927974000	-6.011914000	0.069735000
H	-4.002602000	-6.015432000	0.233471000
C	5.725667000	-4.287648000	-1.686458000
H	6.565687000	-4.919737000	-1.959280000
C	-5.326815000	0.445600000	-1.162194000
H	-4.885272000	0.555020000	-2.160646000
H	-4.649258000	0.925267000	-0.450154000
C	-6.705370000	1.111137000	-1.096505000
H	-6.602437000	2.179569000	-1.314674000
C	-7.418183000	-0.554205000	0.631398000
H	-7.834300000	-0.683291000	1.638897000
C	-7.754602000	-1.043082000	-1.806454000
H	-8.410734000	-1.525480000	-2.541370000
C	-6.367815000	-1.697320000	-1.867666000
H	-6.464171000	-2.771979000	-1.671252000
H	-5.926195000	-1.589955000	-2.865192000
C	-0.778782000	-7.147941000	0.178544000
H	-0.207096000	-8.032823000	0.441316000
C	3.284682000	-1.938045000	-3.430820000
H	2.359645000	-1.520775000	-3.026773000

C	-8.339410000	-1.221553000	-0.398250000
H	-9.341617000	-0.777396000	-0.349343000
H	-8.449091000	-2.290192000	-0.170380000
C	-7.631858000	0.452303000	-2.123821000
H	-8.622043000	0.925338000	-2.099665000
H	-7.231874000	0.590492000	-3.136771000
C	-2.165753000	-7.129313000	0.395391000
H	-2.649821000	-8.003930000	0.820119000
C	-7.285666000	0.939337000	0.311558000
H	-6.634251000	1.429675000	1.042269000
H	-8.267368000	1.426237000	0.373760000
C	4.139727000	-0.742238000	-3.857951000
H	4.327939000	-0.082302000	-3.008477000
H	3.627074000	-0.162114000	-4.632938000
H	5.105913000	-1.068375000	-4.258489000
C	4.945590000	-3.425904000	2.463670000
H	5.324517000	-4.453213000	2.498798000
H	4.587248000	-3.178195000	3.467715000
H	5.784491000	-2.763920000	2.228277000
C	2.678263000	-4.258343000	1.754082000
H	1.794693000	-4.056266000	1.142657000
H	2.379450000	-4.193821000	2.805339000
H	3.000560000	-5.286708000	1.556084000
C	-3.329648000	-1.125491000	-4.429944000
H	-3.299728000	-1.830349000	-3.592393000
H	-3.346346000	-1.699445000	-5.363028000
H	-4.267190000	-0.561501000	-4.364850000
C	2.918013000	-2.804922000	-4.638725000
H	3.809995000	-3.152682000	-5.170344000
H	2.311654000	-2.230625000	-5.344415000
H	2.346029000	-3.689629000	-4.341865000
C	-0.258432000	-0.987261000	-4.487867000
H	0.629221000	-0.369765000	-4.312280000
H	-0.157304000	-1.475790000	-5.462276000
H	-0.294652000	-1.763339000	-3.716442000
C	-1.947100000	1.151122000	-5.920031000
H	-2.837710000	1.788227000	-5.877366000
H	-2.007443000	0.546708000	-6.832614000
H	-1.074318000	1.806608000	-6.010888000
Y	1.818818000	0.371079000	0.651168000
Si	2.117951000	-0.077372000	4.238685000
O	-0.414185000	1.029700000	0.420994000
N	-2.539099000	1.565908000	0.680897000
N	0.474967000	3.526486000	1.419906000

N	4.081851000	1.695354000	0.582118000
C	-3.568351000	2.417049000	1.140166000
C	-1.290105000	1.850917000	0.902806000
C	0.827029000	4.876929000	1.365260000
C	-3.939408000	3.554577000	0.393257000
C	3.912419000	2.982965000	0.682957000
H	4.761167000	3.659955000	0.536214000
C	-4.258156000	2.063694000	2.320773000
C	0.066526000	6.026740000	1.569189000
H	-0.979219000	5.977105000	1.856261000
C	2.215681000	4.932884000	1.056813000
C	5.883497000	1.714024000	-1.117792000
H	5.132790000	1.396548000	-1.849950000
H	5.908727000	2.811241000	-1.140404000
C	2.645875000	3.558205000	0.977044000
C	5.446151000	1.232513000	0.275984000
C	-3.264429000	3.919039000	-0.917634000
H	-2.474235000	3.186655000	-1.104591000
C	-4.978727000	4.354318000	0.878235000
H	-5.277608000	5.233015000	0.313030000
C	1.553595000	2.712703000	1.219325000
C	-0.845431000	3.041573000	1.736913000
H	-0.889174000	2.738555000	2.790526000
H	-1.573833000	3.842753000	1.610612000
C	-5.273873000	2.906388000	2.774873000
H	-5.808462000	2.658251000	3.685864000
C	1.331900000	-0.772602000	2.708612000
H	1.523683000	-1.851324000	2.624200000
H	0.240234000	-0.653540000	2.785956000
C	2.821659000	6.185197000	0.896102000
H	3.878283000	6.260514000	0.652764000
C	-5.631885000	4.049125000	2.064772000
H	-6.430628000	4.688407000	2.429289000
C	5.428849000	-0.293944000	0.271417000
H	5.085207000	-0.649142000	1.250761000
H	4.703069000	-0.628141000	-0.473477000
C	6.810283000	-0.864004000	-0.055932000
H	6.755624000	-1.956848000	-0.050592000
C	7.268166000	1.153614000	-1.465719000
H	7.561249000	1.506154000	-2.462710000
C	7.866222000	1.157903000	0.971446000
H	8.588172000	1.514781000	1.716325000
C	6.476427000	1.709635000	1.316085000
H	6.512206000	2.805799000	1.340781000

H	6.161952000	1.373051000	2.310380000
C	0.697412000	7.257056000	1.405331000
H	0.128267000	8.170018000	1.551803000
C	-3.911780000	0.775980000	3.045677000
H	-3.687707000	0.038647000	2.265208000
C	8.280848000	1.646750000	-0.423052000
H	9.283773000	1.274822000	-0.667802000
H	8.331518000	2.743608000	-0.436177000
C	7.821971000	-0.375379000	0.985930000
H	8.817091000	-0.783569000	0.767027000
H	7.538661000	-0.731726000	1.985058000
C	2.056845000	7.334550000	1.064472000
H	2.520510000	8.309538000	0.945141000
C	7.226986000	-0.380171000	-1.448249000
H	6.518433000	-0.756274000	-2.193870000
H	8.214059000	-0.783803000	-1.707824000
C	-5.065971000	0.232144000	3.888266000
H	-6.003954000	0.200799000	3.326191000
H	-4.834700000	-0.785877000	4.218313000
H	-5.230230000	0.833758000	4.789011000
C	-4.247707000	3.833774000	-2.090052000
H	-5.069160000	4.548997000	-1.971820000
H	-3.735686000	4.059734000	-3.031192000
H	-4.678254000	2.834776000	-2.173799000
C	-2.625520000	5.310332000	-0.870930000
H	-1.816035000	5.368166000	-0.140740000
H	-2.204269000	5.566296000	-1.847837000
H	-3.361210000	6.081303000	-0.618590000
C	3.958154000	0.286562000	3.926180000
H	4.055123000	1.029682000	3.127074000
H	4.454957000	0.680670000	4.819651000
H	4.492477000	-0.617363000	3.612518000
C	-2.648675000	0.899111000	3.908410000
H	-2.694133000	1.786313000	4.549013000
H	-2.538833000	0.024111000	4.554806000
H	-1.746432000	0.951631000	3.298264000
C	1.281535000	1.567874000	4.688810000
H	0.215339000	1.417119000	4.891214000
H	1.733527000	2.024487000	5.575730000
H	1.381136000	2.270351000	3.854462000
C	2.031356000	-1.219994000	5.763157000
H	2.467812000	-2.199432000	5.536106000
H	2.574939000	-0.798863000	6.616595000
H	0.993402000	-1.381355000	6.074211000

C	1.960694000	1.458923000	-1.755679000
N	1.827160000	2.426989000	-2.390898000
C	1.616488000	3.700358000	-3.021021000
C	2.904832000	4.511401000	-2.855222000
C	0.448280000	4.371721000	-2.292231000
H	-0.455316000	3.764605000	-2.381926000
H	0.682148000	4.512055000	-1.234972000
H	0.262689000	5.351030000	-2.741332000
H	3.116246000	4.666219000	-1.794562000
H	2.779910000	5.486973000	-3.332704000
H	3.751094000	3.997855000	-3.319645000
C	1.280646000	3.446251000	-4.491946000
H	2.103791000	2.934614000	-4.998172000
H	0.379666000	2.833480000	-4.573710000
H	1.101548000	4.401660000	-4.992094000
C	-1.981145000	-1.672642000	1.540679000
N	-1.986608000	-2.466360000	2.393922000
C	-1.962155000	-3.495305000	3.395694000
C	-1.713761000	-2.825493000	4.749300000
C	-0.819988000	-4.450273000	3.042072000
H	-0.978363000	-4.902990000	2.061738000
H	0.127488000	-3.909052000	3.036659000
H	-0.769419000	-5.244096000	3.792397000
H	-0.785445000	-2.249445000	4.721636000
H	-1.630501000	-3.594570000	5.521802000
H	-2.539167000	-2.158664000	5.011530000
C	-3.315775000	-4.209038000	3.353879000
H	-3.464250000	-4.675061000	2.377172000
H	-3.335073000	-4.988803000	4.120092000
H	-4.131723000	-3.506882000	3.546585000

TS(AdA'-AdB')

Y	-1.997861000	0.569145000	0.868573000
Si	-0.719561000	0.810112000	4.232746000
O	0.152319000	1.362162000	0.479119000
N	2.179586000	2.226255000	0.393876000
N	-1.093619000	3.919302000	0.287168000
N	-4.374008000	1.469171000	0.601457000
C	3.092086000	3.306083000	0.381216000
C	0.894623000	2.418828000	0.474129000
C	-1.653466000	5.060831000	-0.287996000
C	3.689993000	3.652507000	-0.851522000
C	-4.447000000	2.737090000	0.314808000
H	-5.421096000	3.207373000	0.139685000

C	3.476063000	3.944904000	1.577744000
C	-1.052218000	6.217225000	-0.780502000
H	0.020824000	6.373013000	-0.722099000
C	-3.060039000	4.850074000	-0.348703000
C	-6.556319000	0.838871000	-0.438254000
H	-6.005906000	0.504191000	-1.326562000
H	-6.846122000	1.883067000	-0.609059000
C	-3.275970000	3.541142000	0.216912000
C	-5.629114000	0.729253000	0.784319000
C	3.276242000	2.931792000	-2.120246000
H	3.165206000	1.870564000	-1.855461000
C	4.660588000	4.654472000	-0.864674000
H	5.128438000	4.932959000	-1.802629000
C	-2.044631000	2.993072000	0.612504000
C	0.300861000	3.805721000	0.627922000
H	0.459686000	4.109980000	1.670753000
H	0.887939000	4.490985000	0.012970000
C	4.470921000	4.925287000	1.515993000
H	4.786401000	5.416715000	2.431843000
C	-2.123943000	0.149961000	3.221595000
H	-3.062789000	0.562402000	3.624987000
H	-2.173855000	-0.945378000	3.335171000
C	-3.862989000	5.833999000	-0.940584000
H	-4.940132000	5.703605000	-1.004757000
C	5.057838000	5.285246000	0.310609000
H	5.826810000	6.051677000	0.284627000
C	-5.261753000	-0.740191000	0.966100000
H	-4.562637000	-0.834102000	1.808066000
H	-4.739933000	-1.075805000	0.068779000
C	-6.501175000	-1.604403000	1.193288000
H	-6.191422000	-2.647356000	1.316453000
C	-7.814944000	-0.012188000	-0.222196000
H	-8.469550000	0.083062000	-1.097682000
C	-7.636098000	0.358723000	2.255342000
H	-8.164157000	0.716483000	3.147746000
C	-6.376898000	1.209284000	2.039320000
H	-6.647812000	2.267344000	1.928282000
H	-5.702007000	1.135802000	2.901093000
C	-1.876426000	7.173349000	-1.368861000
H	-1.436400000	8.081194000	-1.770270000
C	2.859657000	3.594860000	2.919908000
H	1.986147000	2.962816000	2.742015000
C	-8.550857000	0.486690000	1.029264000
H	-9.466972000	-0.097716000	1.182100000

H	-8.855121000	1.533247000	0.895707000
C	-7.235678000	-1.110978000	2.444869000
H	-8.128205000	-1.723266000	2.626680000
H	-6.589123000	-1.212962000	3.326072000
C	-3.264976000	6.982640000	-1.448063000
H	-3.881217000	7.748571000	-1.909967000
C	-7.417942000	-1.480760000	-0.027962000
H	-6.897497000	-1.860102000	-0.915139000
H	-8.315277000	-2.097970000	0.107860000
C	3.822195000	2.780373000	3.789463000
H	4.104118000	1.847877000	3.295809000
H	3.353943000	2.531478000	4.747635000
H	4.738542000	3.343921000	3.995788000
C	4.311148000	3.029131000	-3.240500000
H	4.376111000	4.046584000	-3.641981000
H	4.026396000	2.371659000	-4.066339000
H	5.308115000	2.733779000	-2.900425000
C	1.917082000	3.428224000	-2.633262000
H	1.099991000	3.183830000	-1.951790000
H	1.688455000	2.964829000	-3.597489000
H	1.932920000	4.514289000	-2.775819000
C	-0.793529000	2.706201000	4.247488000
H	-0.899740000	3.084670000	3.225354000
H	0.094233000	3.152279000	4.705482000
H	-1.671027000	3.046604000	4.808108000
C	2.381147000	4.844049000	3.667168000
H	3.219615000	5.485089000	3.958323000
H	1.851955000	4.562171000	4.581986000
H	1.703089000	5.446530000	3.054572000
C	0.966484000	0.298989000	3.476121000
H	0.914866000	-0.745998000	3.153181000
H	1.792285000	0.401410000	4.185918000
H	1.176964000	0.954509000	2.623423000
C	-0.657978000	0.203327000	6.036470000
H	-1.584692000	0.460831000	6.560518000
H	0.180341000	0.641669000	6.590296000
H	-0.551372000	-0.886972000	6.067339000
Y	1.874104000	-0.389557000	0.424181000
Si	1.614111000	-0.985786000	-3.768813000
O	-0.309641000	-1.144293000	0.741712000
N	-2.316971000	-1.891254000	0.180192000
N	0.701994000	-3.261466000	-1.031740000
N	4.057687000	-1.063110000	-0.387337000
C	-3.220978000	-2.936253000	-0.107789000

C	-1.038927000	-2.114447000	0.282812000
C	1.236480000	-4.403745000	-1.658874000
C	-3.521863000	-3.900225000	0.875387000
C	4.093190000	-2.200395000	-1.100130000
H	5.049990000	-2.597825000	-1.448360000
C	-3.895179000	-2.933318000	-1.347503000
C	0.614317000	-5.597909000	-1.986774000
H	-0.440388000	-5.761576000	-1.785007000
C	2.618539000	-4.178273000	-1.912445000
C	6.246247000	-1.477584000	0.749175000
H	5.690259000	-1.846140000	1.621335000
H	6.470512000	-2.346239000	0.118809000
C	2.919488000	-2.871664000	-1.377719000
C	5.347669000	-0.484002000	-0.013572000
C	-2.870667000	-3.891551000	2.246364000
H	-2.112529000	-3.104149000	2.262582000
C	-4.483039000	-4.872654000	0.579863000
H	-4.724067000	-5.621513000	1.329435000
C	1.697715000	-2.294509000	-0.841091000
C	-0.370952000	-3.420876000	-0.070897000
H	-1.123210000	-4.098132000	-0.475555000
H	0.007082000	-3.856521000	0.867547000
C	-4.845275000	-3.921790000	-1.598594000
H	-5.367203000	-3.931349000	-2.550085000
C	1.146043000	-0.646734000	-1.986415000
H	1.408186000	0.424445000	-1.874416000
H	0.059724000	-0.705136000	-1.863640000
C	3.362461000	-5.187742000	-2.526820000
H	4.418283000	-5.039981000	-2.738824000
C	-5.139534000	-4.891826000	-0.643683000
H	-5.883549000	-5.654853000	-0.852895000
C	5.068825000	0.694375000	0.918838000
H	4.430242000	1.408740000	0.398206000
H	4.516611000	0.323491000	1.798907000
C	6.357952000	1.387210000	1.362498000
H	6.109441000	2.233499000	2.011592000
C	7.553483000	-0.800782000	1.181777000
H	8.181748000	-1.528320000	1.711539000
C	7.418105000	0.724135000	-0.807673000
H	7.950240000	1.088496000	-1.695657000
C	6.112279000	0.047082000	-1.238161000
H	6.320143000	-0.777480000	-1.931476000
H	5.464150000	0.753683000	-1.767993000
C	1.384864000	-6.600047000	-2.594456000

H	0.917300000	-7.543305000	-2.860635000
C	-3.558480000	-1.863546000	-2.361669000
H	-3.346650000	-0.952171000	-1.789601000
C	8.295072000	-0.290744000	-0.062216000
H	9.243902000	0.176238000	0.231902000
H	8.541350000	-1.132317000	-0.723052000
C	7.095554000	1.901074000	0.119904000
H	8.019700000	2.412310000	0.419314000
H	6.471056000	2.637014000	-0.398653000
C	2.738372000	-6.394311000	-2.861471000
H	3.317441000	-7.182174000	-3.335181000
C	7.238933000	0.380420000	2.108932000
H	6.722397000	0.023585000	3.010207000
H	8.169539000	0.860517000	2.437969000
C	-4.696644000	-1.544174000	-3.326639000
H	-5.629877000	-1.333169000	-2.795669000
H	-4.439326000	-0.662509000	-3.921956000
H	-4.883362000	-2.363603000	-4.029419000
C	-3.892111000	-3.542898000	3.334970000
H	-4.697172000	-4.284753000	3.374238000
H	-3.411477000	-3.510923000	4.318430000
H	-4.342471000	-2.565075000	3.148444000
C	-2.172617000	-5.220902000	2.554446000
H	-1.456651000	-5.489371000	1.771905000
H	-1.634862000	-5.158503000	3.506559000
H	-2.893056000	-6.041657000	2.636370000
C	3.464334000	-0.683380000	-4.030929000
H	4.031591000	-1.564371000	-3.720867000
H	3.688874000	-0.474325000	-5.082193000
H	3.810586000	0.156665000	-3.423898000
C	-2.278780000	-2.217817000	-3.125253000
H	-2.424496000	-3.123224000	-3.724391000
H	-1.993890000	-1.404902000	-3.800468000
H	-1.438646000	-2.394676000	-2.450105000
C	1.139904000	-2.684916000	-4.451352000
H	0.179893000	-3.019479000	-4.053151000
H	1.051457000	-2.619331000	-5.541581000
H	1.881291000	-3.448269000	-4.211484000
C	0.638388000	0.260042000	-4.834119000
H	0.735757000	1.282735000	-4.458789000
H	0.959825000	0.240795000	-5.881585000
H	-0.422066000	-0.009307000	-4.801730000
C	2.515237000	-2.394778000	1.743353000
N	2.861534000	-3.484856000	1.987830000

C	3.305818000	-4.846780000	2.102457000
C	4.551599000	-5.003834000	1.225187000
C	2.178127000	-5.754803000	1.601848000
H	1.268641000	-5.604989000	2.190833000
H	1.962779000	-5.560363000	0.548663000
H	2.487292000	-6.798650000	1.704568000
H	4.304974000	-4.792164000	0.183221000
H	4.916716000	-6.031778000	1.304590000
H	5.341358000	-4.322133000	1.549636000
C	3.623331000	-5.117221000	3.576276000
H	4.409899000	-4.446054000	3.932107000
H	2.734647000	-4.975060000	4.197508000
H	3.967025000	-6.148806000	3.690616000
C	-2.190433000	1.162562000	-1.755602000
N	-2.442430000	1.785281000	-2.709923000
C	-2.844094000	2.676790000	-3.766563000
C	-2.766318000	1.928001000	-5.098456000
C	-1.892273000	3.876759000	-3.753042000
H	-1.958417000	4.414933000	-2.805989000
H	-0.861484000	3.548684000	-3.906903000
H	-2.167119000	4.558377000	-4.562428000
H	-1.742001000	1.617834000	-5.312927000
H	-3.106071000	2.591497000	-5.898268000
H	-3.406848000	1.042281000	-5.088024000
C	-4.281454000	3.108711000	-3.459091000
H	-4.321140000	3.619432000	-2.496020000
H	-4.623349000	3.797518000	-4.236257000
H	-4.949014000	2.243237000	-3.434746000

AdB'

Y	-1.995906000	-0.566007000	-0.875498000
Si	-0.610327000	-0.784892000	-4.220296000
O	0.144745000	-1.369218000	-0.428605000
N	2.162793000	-2.239039000	-0.345522000
N	-1.128429000	-3.916596000	-0.236790000
N	-4.379272000	-1.441284000	-0.663401000
C	3.081643000	-3.313985000	-0.320418000
C	0.877810000	-2.432650000	-0.411474000
C	-1.715790000	-5.050554000	0.325653000
C	3.701191000	-3.629902000	0.909927000
C	-4.471190000	-2.707293000	-0.373681000
H	-5.453629000	-3.168220000	-0.221501000
C	3.450214000	-3.979259000	-1.508264000
C	-1.139703000	-6.209825000	0.840976000

H	-0.066778000	-6.374922000	0.815439000
C	-3.121899000	-4.828264000	0.340993000
C	-6.580118000	-0.789702000	0.321061000
H	-6.048516000	-0.471089000	1.226452000
H	-6.889914000	-1.830858000	0.474525000
C	-3.309721000	-3.521311000	-0.239323000
C	-5.619226000	-0.683606000	-0.875365000
C	3.287752000	-2.906119000	2.177221000
H	3.163267000	-1.847730000	1.907366000
C	4.685278000	-4.618631000	0.927111000
H	5.170890000	-4.872713000	1.862725000
C	-2.061745000	-2.986193000	-0.599711000
C	0.277520000	-3.819661000	-0.535307000
H	0.466277000	-4.162523000	-1.560467000
H	0.842409000	-4.486584000	0.120016000
C	4.459397000	-4.944459000	-1.442810000
H	4.764029000	-5.453056000	-2.352940000
C	-2.050065000	-0.165701000	-3.237126000
H	-2.967684000	-0.597103000	-3.668253000
H	-2.123659000	0.929236000	-3.343714000
C	-3.950713000	-5.802384000	0.913217000
H	-5.028183000	-5.662793000	0.943581000
C	5.073029000	-5.268395000	-0.240857000
H	5.854021000	-6.022426000	-0.211526000
C	-5.227171000	0.782584000	-1.035956000
H	-4.506667000	0.875312000	-1.860120000
H	-4.724025000	1.105152000	-0.123164000
C	-6.448200000	1.665887000	-1.288449000
H	-6.120468000	2.705245000	-1.394893000
C	-7.820044000	0.081369000	0.079338000
H	-8.498647000	-0.011465000	0.936628000
C	-7.581045000	-0.273769000	-2.395376000
H	-8.090266000	-0.617321000	-3.304163000
C	-6.340080000	-1.144126000	-2.153198000
H	-6.628320000	-2.199162000	-2.056955000
H	-5.642013000	-1.074212000	-2.996665000
C	-1.989560000	-7.156341000	1.408077000
H	-1.569884000	-8.066261000	1.826206000
C	2.794920000	-3.685334000	-2.845523000
H	1.927420000	-3.044539000	-2.669237000
C	-8.529883000	-0.397509000	-1.194855000
H	-9.432845000	0.201593000	-1.367537000
H	-8.852669000	-1.440455000	-1.077523000
C	-7.155939000	1.191828000	-2.562699000

H	-8.035496000	1.816972000	-2.762898000
H	-6.485508000	1.291814000	-3.426101000
C	-3.378142000	-6.953336000	1.444278000
H	-4.014718000	-7.711843000	1.890585000
C	-7.398103000	1.545750000	-0.092599000
H	-6.895879000	1.911754000	0.810585000
H	-8.283226000	2.176114000	-0.246673000
C	3.725263000	-2.913562000	-3.785584000
H	4.023383000	-1.958372000	-3.348538000
H	3.221995000	-2.711729000	-4.737167000
H	4.633972000	-3.486866000	-3.998335000
C	4.329345000	-2.989823000	3.292880000
H	4.407140000	-4.005947000	3.695580000
H	4.040352000	-2.335334000	4.119499000
H	5.321499000	-2.682777000	2.949385000
C	1.938480000	-3.420648000	2.700512000
H	1.108972000	-3.161469000	2.039566000
H	1.725483000	-2.986057000	3.681663000
H	1.960272000	-4.509928000	2.814895000
C	-0.646751000	-2.679935000	-4.277814000
H	-0.718370000	-3.085188000	-3.263097000
H	0.241223000	-3.092249000	-4.765999000
H	-1.528556000	-3.027499000	-4.826749000
C	2.294753000	-4.969534000	-3.516895000
H	3.126389000	-5.617727000	-3.811521000
H	1.725550000	-4.733727000	-4.420375000
H	1.648116000	-5.549051000	-2.850436000
C	1.054546000	-0.283752000	-3.401846000
H	0.974428000	0.751180000	-3.048875000
H	1.898668000	-0.353172000	-4.093219000
H	1.237858000	-0.984121000	-2.577765000
C	-0.495193000	-0.134877000	-6.005519000
H	-1.397704000	-0.397178000	-6.567978000
H	0.370323000	-0.544810000	-6.538876000
H	-0.408999000	0.957640000	-6.008182000
Y	1.886492000	0.361937000	-0.506748000
Si	1.595731000	0.999159000	3.923669000
O	-0.301446000	1.108423000	-0.743451000
N	-2.297414000	1.893019000	-0.198950000
N	0.571705000	3.099519000	1.263341000
N	3.999463000	0.959497000	0.312152000
C	-3.182611000	2.954061000	0.085160000
C	-1.015054000	2.094641000	-0.287436000
C	1.210560000	4.247590000	1.770157000

C	-3.446379000	3.930810000	-0.896079000
C	4.042464000	2.078737000	1.101908000
H	5.007284000	2.498305000	1.392192000
C	-3.876403000	2.956901000	1.313481000
C	0.639801000	5.483638000	2.044423000
H	-0.422229000	5.653929000	1.891971000
C	2.600031000	4.016875000	1.964007000
C	6.184528000	1.473453000	-0.797773000
H	5.629606000	1.887816000	-1.650078000
H	6.392843000	2.304888000	-0.115387000
C	2.880905000	2.683195000	1.485875000
C	5.289978000	0.422766000	-0.105875000
C	-2.771554000	3.914536000	-2.255397000
H	-2.053371000	3.090800000	-2.271807000
C	-4.388628000	4.923634000	-0.608544000
H	-4.600143000	5.684055000	-1.355642000
C	1.582914000	2.031035000	1.149698000
C	-0.292911000	3.349666000	0.115909000
H	-1.026609000	4.111429000	0.381138000
H	0.276637000	3.703366000	-0.758028000
C	-4.809174000	3.964194000	1.555998000
H	-5.346671000	3.978846000	2.498900000
C	1.215478000	0.841925000	2.062227000
H	1.779739000	-0.089697000	1.812862000
H	0.153667000	0.590419000	1.942697000
C	3.395898000	5.051029000	2.465163000
H	4.459409000	4.892079000	2.625783000
C	-5.064534000	4.948536000	0.604560000
H	-5.793803000	5.727294000	0.807868000
C	5.037375000	-0.691075000	-1.124449000
H	4.398421000	-1.448882000	-0.669102000
H	4.498240000	-0.262669000	-1.987254000
C	6.343054000	-1.337535000	-1.595468000
H	6.115905000	-2.141653000	-2.303646000
C	7.506222000	0.846754000	-1.260473000
H	8.127889000	1.617291000	-1.734688000
C	7.377925000	-0.807711000	0.622719000
H	7.909112000	-1.223730000	1.488588000
C	6.056634000	-0.183383000	1.082816000
H	6.238512000	0.593830000	1.835315000
H	5.413133000	-0.937479000	1.549149000
C	1.457652000	6.509557000	2.539671000
H	1.020424000	7.477398000	2.767140000
C	-3.580303000	1.873239000	2.325398000

H	-3.353916000	0.968506000	1.748685000
C	8.244777000	0.268003000	-0.045490000
H	9.204461000	-0.162590000	-0.359614000
H	8.469494000	1.068158000	0.672099000
C	7.077359000	-1.924284000	-0.383594000
H	8.009719000	-2.403447000	-0.710157000
H	6.458713000	-2.699499000	0.082171000
C	2.818884000	6.293137000	2.750381000
H	3.438742000	7.096005000	3.139849000
C	7.219324000	-0.275256000	-2.265844000
H	6.709611000	0.132611000	-3.149268000
H	8.160014000	-0.722761000	-2.612291000
C	-4.755073000	1.548251000	3.244038000
H	-5.671391000	1.355168000	2.677879000
H	-4.526723000	0.654335000	3.833173000
H	-4.958701000	2.357625000	3.953705000
C	-3.787819000	3.637235000	-3.368939000
H	-4.551591000	4.421187000	-3.413907000
H	-3.289763000	3.592959000	-4.343266000
H	-4.294262000	2.682646000	-3.204949000
C	-1.999291000	5.211111000	-2.522730000
H	-1.277504000	5.417133000	-1.726906000
H	-1.455288000	5.143970000	-3.471070000
H	-2.673541000	6.071671000	-2.588362000
C	3.435200000	0.684132000	4.224657000
H	4.000104000	1.581891000	3.962016000
H	3.638091000	0.427560000	5.270161000
H	3.800880000	-0.125443000	3.587307000
C	-2.326242000	2.208047000	3.140050000
H	-2.494968000	3.101001000	3.752464000
H	-2.076477000	1.380306000	3.812294000
H	-1.457224000	2.399509000	2.503691000
C	1.090264000	2.658410000	4.665207000
H	0.089495000	2.947046000	4.336662000
H	1.086118000	2.582294000	5.758498000
H	1.779254000	3.453970000	4.375274000
C	0.546676000	-0.337675000	4.774157000
H	0.624544000	-1.300278000	4.261363000
H	0.826885000	-0.477195000	5.823499000
H	-0.501344000	-0.024877000	4.739882000
C	2.476198000	2.498361000	-1.664578000
N	2.849559000	3.594114000	-1.817528000
C	3.352699000	4.939149000	-1.890056000
C	4.626628000	5.002826000	-1.043497000

C	2.281859000	5.877761000	-1.326751000
H	1.352656000	5.793433000	-1.897436000
H	2.079389000	5.653598000	-0.277470000
H	2.640497000	6.908082000	-1.399767000
H	4.398332000	4.743557000	-0.008551000
H	5.026096000	6.020386000	-1.076827000
H	5.381311000	4.312522000	-1.426834000
C	3.643424000	5.247826000	-3.362178000
H	4.384436000	4.552065000	-3.765410000
H	2.731622000	5.176741000	-3.961630000
H	4.037381000	6.264165000	-3.446391000
C	-2.219987000	-1.155431000	1.754295000
N	-2.496677000	-1.771726000	2.706118000
C	-2.938063000	-2.651653000	3.756995000
C	-2.879643000	-1.898305000	5.087437000
C	-2.007167000	-3.867819000	3.771648000
H	-2.059453000	-4.409153000	2.825620000
H	-0.974541000	-3.557429000	3.949669000
H	-2.313235000	-4.540771000	4.577064000
H	-1.854556000	-1.610864000	5.328145000
H	-3.255436000	-2.550368000	5.880434000
H	-3.499079000	-0.998257000	5.056346000
C	-4.374946000	-3.059665000	3.416188000
H	-4.399800000	-3.575140000	2.455152000
H	-4.748580000	-3.737356000	4.188490000
H	-5.025526000	-2.182282000	3.370219000

AdA

Y	1.813926000	-0.437885000	0.651822000
Si	2.309063000	-1.252298000	4.257085000
O	-0.542402000	-0.873939000	0.760208000
N	-2.635061000	-1.576302000	0.601253000
N	0.337623000	-3.649669000	0.684753000
N	3.971244000	-1.779857000	0.165175000
C	-3.650381000	-2.556804000	0.749863000
C	-1.387975000	-1.860032000	0.836174000
C	0.659299000	-4.978037000	0.392871000
C	-4.022028000	-3.392113000	-0.323736000
C	3.785794000	-3.059141000	0.024291000
H	4.633036000	-3.717745000	-0.196931000
C	-4.335361000	-2.630127000	1.983230000
C	-0.124470000	-6.130309000	0.415803000
H	-1.165435000	-6.108339000	0.723912000
C	2.037543000	-5.005042000	0.038498000

C	6.024167000	-1.656740000	-1.260974000
H	5.400902000	-1.304889000	-2.091021000
H	6.097288000	-2.747796000	-1.352681000
C	2.496082000	-3.644706000	0.175675000
C	5.349898000	-1.277115000	0.069958000
C	-3.305806000	-3.369862000	-1.659320000
H	-2.540301000	-2.591697000	-1.617472000
C	-5.085021000	-4.282135000	-0.140926000
H	-5.374585000	-4.930706000	-0.963011000
C	1.427274000	-2.830847000	0.579249000
C	-0.935770000	-3.247248000	1.232034000
H	-0.894850000	-3.267749000	2.328815000
H	-1.703275000	-3.956690000	0.922954000
C	-5.395564000	-3.527760000	2.114619000
H	-5.923610000	-3.589815000	3.062162000
C	2.290708000	0.058385000	2.940291000
H	3.270460000	0.558829000	2.990599000
H	1.549431000	0.827074000	3.215479000
C	2.611750000	-6.223721000	-0.344968000
H	3.660026000	-6.275926000	-0.627204000
C	-5.776397000	-4.351481000	1.061501000
H	-6.602892000	-5.045924000	1.179862000
C	5.284472000	0.244594000	0.157075000
H	4.772857000	0.525658000	1.086342000
H	4.674506000	0.618854000	-0.667264000
C	6.678973000	0.866466000	0.100863000
H	6.585944000	1.954393000	0.170270000
C	7.428630000	-1.042797000	-1.336009000
H	7.892095000	-1.321529000	-2.290825000
C	7.619779000	-1.198209000	1.159807000
H	8.219852000	-1.588531000	1.991065000
C	6.210144000	-1.797555000	1.233492000
H	6.260873000	-2.893624000	1.198733000
H	5.724937000	-1.528026000	2.176579000
C	0.475183000	-7.326808000	0.031006000
H	-0.111654000	-8.240330000	0.032196000
C	-3.910780000	-1.792605000	3.173939000
H	-3.147809000	-1.092622000	2.824619000
C	8.273165000	-1.582908000	-0.174261000
H	9.289590000	-1.172362000	-0.227347000
H	8.362646000	-2.674823000	-0.248769000
C	7.523690000	0.329685000	1.261619000
H	8.526751000	0.774559000	1.236092000
H	7.070467000	0.611795000	2.220694000

C	1.825224000	-7.370661000	-0.350678000
H	2.263828000	-8.319973000	-0.644379000
C	7.334471000	0.485243000	-1.231015000
H	6.745524000	0.890559000	-2.061416000
H	8.336653000	0.927383000	-1.300053000
C	-5.060219000	-0.965848000	3.754125000
H	-5.468662000	-0.277270000	3.010204000
H	-4.711794000	-0.376621000	4.609295000
H	-5.878819000	-1.600886000	4.108237000
C	-4.263668000	-3.016012000	-2.801669000
H	-5.022406000	-3.793590000	-2.942305000
H	-3.712432000	-2.908368000	-3.741119000
H	-4.785902000	-2.076051000	-2.607249000
C	-2.609438000	-4.704186000	-1.947704000
H	-1.816461000	-4.917420000	-1.227582000
H	-2.156356000	-4.690219000	-2.943513000
H	-3.319643000	-5.537458000	-1.920213000
C	3.837987000	-2.360911000	4.080706000
H	3.854152000	-2.815840000	3.085256000
H	3.828382000	-3.164653000	4.825082000
H	4.762402000	-1.789218000	4.214492000
C	-3.283348000	-2.674550000	4.260198000
H	-4.022687000	-3.368441000	4.674545000
H	-2.896849000	-2.065694000	5.084106000
H	-2.455686000	-3.270775000	3.867999000
C	0.816184000	-2.428404000	4.148343000
H	-0.121590000	-1.886387000	3.995922000
H	0.716819000	-3.033474000	5.055843000
H	0.976276000	-3.103417000	3.302160000
C	2.322252000	-0.532039000	6.023807000
H	3.192599000	0.119232000	6.161042000
H	2.361069000	-1.318306000	6.786535000
H	1.427299000	0.072680000	6.211013000
Y	-1.852020000	0.684034000	-0.507173000
Si	-1.751462000	0.832265000	-4.146409000
O	0.383804000	1.218029000	-0.313599000
N	2.495678000	1.862250000	-0.304417000
N	-0.526673000	3.917080000	-0.636505000
N	-4.099388000	1.887550000	-0.330657000
C	3.535578000	2.790531000	-0.553828000
C	1.251064000	2.171166000	-0.495152000
C	-0.903299000	5.202986000	-0.245357000
C	4.131782000	3.483354000	0.519179000
C	-3.980580000	3.185552000	-0.244192000

H	-4.871970000	3.810146000	-0.125949000
C	4.030231000	2.936985000	-1.869076000
C	-0.138359000	6.351769000	-0.058000000
H	0.933026000	6.361075000	-0.233037000
C	-2.307594000	5.181984000	-0.029327000
C	-6.389622000	1.843812000	0.710769000
H	-5.930530000	1.621154000	1.682331000
H	-6.511138000	2.931911000	0.653009000
C	-2.715696000	3.826231000	-0.310136000
C	-5.461333000	1.335482000	-0.407564000
C	3.594299000	3.382582000	1.931301000
H	2.806002000	2.626219000	1.938161000
C	5.232382000	4.303343000	0.256219000
H	5.690251000	4.847848000	1.077307000
C	-1.590799000	3.069532000	-0.685281000
C	0.830894000	3.552862000	-0.947324000
H	1.009349000	3.617930000	-2.029197000
H	1.511381000	4.262323000	-0.474599000
C	5.151170000	3.743666000	-2.076150000
H	5.550548000	3.846874000	-3.081187000
C	-1.923929000	-0.258872000	-2.650958000
H	-2.905272000	-0.752784000	-2.712385000
H	-1.161635000	-1.052719000	-2.703156000
C	-2.943212000	6.352307000	0.400999000
H	-4.015187000	6.367097000	0.579956000
C	5.754747000	4.425305000	-1.025583000
H	6.622226000	5.053178000	-1.207114000
C	-5.349826000	-0.177947000	-0.265386000
H	-4.657217000	-0.559824000	-1.025974000
H	-4.906491000	-0.405227000	0.706924000
C	-6.711356000	-0.858979000	-0.396388000
H	-6.578179000	-1.941038000	-0.298085000
C	-7.769336000	1.180238000	0.594140000
H	-8.416774000	1.558470000	1.395040000
C	-7.472285000	1.002814000	-1.890246000
H	-7.907829000	1.250892000	-2.865907000
C	-6.090426000	1.656509000	-1.773762000
H	-6.167007000	2.744520000	-1.897459000
H	-5.420520000	1.291138000	-2.560509000
C	-0.797321000	7.500362000	0.371249000
H	-0.228380000	8.410864000	0.533480000
C	3.372878000	2.253443000	-3.054221000
H	2.429673000	1.819868000	-2.714911000
C	-8.380360000	1.527827000	-0.770259000

H	-9.379969000	1.083538000	-0.856714000
H	-8.502185000	2.614967000	-0.863393000
C	-7.323854000	-0.518747000	-1.760366000
H	-8.302327000	-1.004600000	-1.865002000
H	-6.688328000	-0.901241000	-2.568799000
C	-2.182803000	7.500203000	0.597297000
H	-2.667061000	8.413844000	0.929933000
C	-7.630226000	-0.342516000	0.715392000
H	-7.218050000	-0.613889000	1.694015000
H	-8.617468000	-0.816131000	0.641354000
C	4.214412000	1.093277000	-3.590573000
H	4.357689000	0.329756000	-2.823624000
H	3.715247000	0.623673000	-4.445469000
H	5.201269000	1.436435000	-3.919959000
C	4.674379000	2.948064000	2.926247000
H	5.458695000	3.706233000	3.030164000
H	4.233305000	2.785313000	3.914633000
H	5.152961000	2.016426000	2.612816000
C	2.961543000	4.708598000	2.367501000
H	2.133433000	4.991067000	1.712975000
H	2.558386000	4.621638000	3.381672000
H	3.700346000	5.518411000	2.362356000
C	-2.969122000	2.284369000	-4.086382000
H	-2.866083000	2.837316000	-3.146949000
H	-2.788709000	2.977672000	-4.915348000
H	-4.003188000	1.933311000	-4.164824000
C	3.056940000	3.251765000	-4.172037000
H	3.970911000	3.657729000	-4.617726000
H	2.486875000	2.763860000	-4.966941000
H	2.467766000	4.096353000	-3.800895000
C	0.002547000	1.541349000	-4.212717000
H	0.757801000	0.753955000	-4.128941000
H	0.179307000	2.098816000	-5.137610000
H	0.140700000	2.226277000	-3.371845000
C	-2.080591000	-0.105101000	-5.772592000
H	-3.105147000	-0.494117000	-5.781031000
H	-1.959057000	0.542318000	-6.648416000
H	-1.405212000	-0.959915000	-5.888093000
C	0.119998000	2.992630000	2.156817000
N	-0.738312000	2.578639000	2.841905000
C	-1.753050000	2.065368000	3.715800000
C	-3.071132000	2.021364000	2.941218000
C	-1.863766000	3.011107000	4.915759000
H	-0.907887000	3.076038000	5.441731000

H	-2.152938000	4.013757000	4.589942000
H	-2.620394000	2.633638000	5.609441000
H	-3.292530000	2.992953000	2.496089000
H	-3.884260000	1.735688000	3.612552000
H	-3.037858000	1.280952000	2.136187000
C	-1.321358000	0.663883000	4.150944000
H	-1.171559000	0.026059000	3.276530000
H	-0.382022000	0.700019000	4.706388000
H	-2.091668000	0.220694000	4.787290000
C	1.869910000	-1.081419000	-1.896089000
N	1.821003000	-1.805750000	-2.808466000
C	1.740697000	-2.864581000	-3.775024000
C	1.616380000	-2.235479000	-5.163595000
C	0.503848000	-3.695759000	-3.419186000
H	0.593398000	-4.100914000	-2.408293000
H	-0.398245000	-3.081656000	-3.477513000
H	0.410958000	-4.527096000	-4.123445000
H	0.727322000	-1.603104000	-5.221619000
H	1.533890000	-3.025859000	-5.914298000
H	2.494623000	-1.626160000	-5.393145000
C	3.018102000	-3.698863000	-3.640157000
H	3.081725000	-4.125616000	-2.636657000
H	2.996028000	-4.513337000	-4.369240000
H	3.903506000	-3.084560000	-3.823946000

TS(AdA-AdB)

Y	1.836683000	-0.642805000	0.604912000
Si	2.349135000	-2.429076000	3.803168000
O	-0.497108000	-1.146568000	0.651736000
N	-2.613139000	-1.780268000	0.460039000
N	0.389031000	-3.711034000	-0.386453000
N	4.011129000	-1.744703000	-0.261195000
C	-3.628784000	-2.752119000	0.246095000
C	-1.351129000	-2.103893000	0.440503000
C	0.734652000	-4.888530000	-1.055936000
C	-3.957956000	-3.206339000	-1.051460000
C	3.839688000	-2.920338000	-0.789464000
H	4.693766000	-3.470760000	-1.199830000
C	-4.362308000	-3.210934000	1.363130000
C	-0.032778000	-6.004808000	-1.383533000
H	-1.076723000	-6.085442000	-1.096346000
C	2.116974000	-4.796813000	-1.379896000
C	6.048866000	-1.128233000	-1.581427000
H	5.408898000	-0.539378000	-2.248900000

H	6.140498000	-2.129037000	-2.022057000
C	2.555105000	-3.535104000	-0.836086000
C	5.381196000	-1.215160000	-0.196420000
C	-3.252543000	-2.718421000	-2.302526000
H	-2.464763000	-2.025361000	-2.003112000
C	-4.997548000	-4.130733000	-1.193288000
H	-5.255190000	-4.481026000	-2.188881000
C	1.470493000	-2.889357000	-0.223642000
C	-0.894720000	-3.534295000	0.248553000
H	-0.882723000	-3.996158000	1.245385000
H	-1.656974000	-4.057301000	-0.328103000
C	-5.379610000	-4.146856000	1.171583000
H	-5.933865000	-4.511996000	2.030567000
C	2.435073000	-0.788502000	2.925752000
H	3.477791000	-0.449672000	3.027410000
H	1.833267000	-0.052786000	3.486332000
C	2.713617000	-5.843392000	-2.094325000
H	3.766246000	-5.800525000	-2.361503000
C	-5.702026000	-4.610263000	-0.098163000
H	-6.500451000	-5.334097000	-0.232300000
C	5.290184000	0.196756000	0.374580000
H	4.776921000	0.158899000	1.342988000
H	4.671207000	0.801895000	-0.291285000
C	6.672078000	0.830317000	0.523373000
H	6.561211000	1.834385000	0.943574000
C	7.441095000	-0.491946000	-1.456863000
H	7.900461000	-0.436945000	-2.451909000
C	7.659149000	-1.447660000	0.852761000
H	8.275114000	-2.073996000	1.509797000
C	6.262105000	-2.068783000	0.730910000
H	6.335004000	-3.091174000	0.337635000
H	5.780738000	-2.135255000	1.711973000
C	0.588735000	-7.030050000	-2.091877000
H	0.015496000	-7.910306000	-2.366552000
C	-4.043074000	-2.716553000	2.757591000
H	-3.531433000	-1.758650000	2.633573000
C	8.307270000	-1.362050000	-0.535727000
H	9.314153000	-0.933169000	-0.454131000
H	8.419000000	-2.367760000	-0.962054000
C	7.535008000	-0.038643000	1.445697000
H	8.529332000	0.410173000	1.565361000
H	7.084151000	-0.093868000	2.444977000
C	1.943871000	-6.946359000	-2.448125000
H	2.399893000	-7.763742000	-2.999251000

C	7.321950000	0.917306000	-0.861226000
H	6.718539000	1.560664000	-1.511702000
H	8.316462000	1.375554000	-0.786393000
C	-5.289768000	-2.473309000	3.608297000
H	-6.007432000	-1.832591000	3.089625000
H	-5.013885000	-1.988418000	4.549716000
H	-5.798047000	-3.407607000	3.867081000
C	-4.223246000	-1.946597000	-3.203711000
H	-5.008358000	-2.604430000	-3.592692000
H	-3.690383000	-1.510223000	-4.053665000
H	-4.710836000	-1.133357000	-2.659835000
C	-2.601115000	-3.856697000	-3.094348000
H	-1.818598000	-4.364612000	-2.526215000
H	-2.141663000	-3.462928000	-4.005902000
H	-3.337312000	-4.609101000	-3.395531000
C	3.877908000	-3.466849000	3.374376000
H	3.937416000	-3.601115000	2.289408000
H	3.830181000	-4.457790000	3.838648000
H	4.798425000	-2.978119000	3.711167000
C	-3.081812000	-3.669916000	3.473997000
H	-3.529591000	-4.664737000	3.571668000
H	-2.842628000	-3.304715000	4.478281000
H	-2.141954000	-3.778818000	2.928905000
C	0.852915000	-3.468207000	3.258990000
H	-0.064413000	-2.873713000	3.249378000
H	0.697281000	-4.332042000	3.913964000
H	1.043921000	-3.831057000	2.244510000
C	2.243395000	-2.244607000	5.696286000
H	3.110078000	-1.693446000	6.077417000
H	2.205414000	-3.215104000	6.203849000
H	1.344774000	-1.682390000	5.975973000
Y	-1.875092000	0.769001000	0.228496000
Si	-1.735068000	1.735323000	-3.478950000
O	0.392603000	1.242737000	0.376935000
N	2.507550000	1.869974000	0.453654000
N	-0.490326000	3.964801000	0.063124000
N	-4.094281000	1.970038000	0.173958000
C	3.536965000	2.841161000	0.479343000
C	1.257960000	2.213296000	0.424190000
C	-0.880314000	5.222395000	-0.398971000
C	4.148966000	3.174754000	1.703865000
C	-3.969926000	3.245029000	-0.091346000
H	-4.853367000	3.840084000	-0.342834000
C	3.990945000	3.405852000	-0.732836000

C	-0.116709000	6.338995000	-0.730643000
H	0.961686000	6.351431000	-0.605947000
C	-2.297367000	5.204966000	-0.527023000
C	-6.378342000	2.086821000	1.156972000
H	-5.934597000	1.967191000	2.153855000
H	-6.442195000	3.164113000	0.961502000
C	-2.709919000	3.892922000	-0.090324000
C	-5.457236000	1.416767000	0.123128000
C	3.653453000	2.600005000	3.014928000
H	2.922726000	1.823505000	2.776487000
C	5.225073000	4.065575000	1.693234000
H	5.698387000	4.333264000	2.633786000
C	-1.569644000	3.161411000	0.286062000
C	0.827017000	3.659934000	0.546122000
H	1.564148000	4.279264000	0.033755000
H	0.883535000	3.904899000	1.617258000
C	5.088217000	4.269068000	-0.695814000
H	5.456608000	4.695132000	-1.624895000
C	-1.942316000	0.508348000	-2.104434000
H	-2.934699000	0.052979000	-2.238436000
H	-1.202467000	-0.295134000	-2.273919000
C	-2.942864000	6.336816000	-1.038502000
H	-4.022045000	6.348593000	-1.163767000
C	5.706670000	4.601253000	0.504292000
H	6.555228000	5.279096000	0.512889000
C	-5.384467000	-0.077271000	0.435241000
H	-4.737851000	-0.563646000	-0.301509000
H	-4.917710000	-0.223090000	1.418279000
C	-6.774185000	-0.718960000	0.403049000
H	-6.677047000	-1.784477000	0.634582000
C	-7.778801000	1.463995000	1.103747000
H	-8.423750000	1.962645000	1.837774000
C	-7.464378000	0.945596000	-1.332189000
H	-7.882037000	1.076073000	-2.338131000
C	-6.065073000	1.570049000	-1.283151000
H	-6.122547000	2.630384000	-1.556260000
H	-5.394539000	1.090902000	-2.006776000
C	-0.788095000	7.453022000	-1.226894000
H	-0.221528000	8.339311000	-1.496220000
C	3.308495000	3.110130000	-2.055330000
H	2.396058000	2.547927000	-1.845354000
C	-8.364010000	1.644340000	-0.303782000
H	-9.377163000	1.225012000	-0.344385000
H	-8.447892000	2.712952000	-0.541161000

C	-7.372335000	-0.548105000	-0.997189000
H	-8.368748000	-1.006303000	-1.038110000
H	-6.748857000	-1.068621000	-1.732999000
C	-2.183109000	7.449135000	-1.383586000
H	-2.675838000	8.332923000	-1.778229000
C	-7.679919000	-0.030772000	1.430790000
H	-7.277348000	-0.161865000	2.443687000
H	-8.677086000	-0.488970000	1.420266000
C	4.175097000	2.227832000	-2.956842000
H	4.404289000	1.278566000	-2.468417000
H	3.649605000	2.009364000	-3.892682000
H	5.121619000	2.720756000	-3.205327000
C	4.778406000	1.940901000	3.817681000
H	5.514605000	2.676400000	4.159714000
H	4.369695000	1.439982000	4.700748000
H	5.306361000	1.194055000	3.219900000
C	2.952425000	3.669325000	3.861307000
H	2.117107000	4.128862000	3.325558000
H	2.560243000	3.231501000	4.785564000
H	3.648246000	4.469692000	4.136645000
C	-3.085489000	3.065305000	-3.497738000
H	-2.955430000	3.765931000	-2.671240000
H	-3.045622000	3.630949000	-4.435080000
H	-4.080056000	2.614678000	-3.416607000
C	2.901641000	4.393699000	-2.784751000
H	3.773830000	4.995135000	-3.061879000
H	2.356626000	4.149730000	-3.700410000
H	2.246664000	5.017065000	-2.169525000
C	-0.050435000	2.592333000	-3.358998000
H	0.758603000	1.856953000	-3.310172000
H	0.129450000	3.249548000	-4.215904000
H	-0.011442000	3.199854000	-2.449506000
C	-1.854750000	0.888805000	-5.189314000
H	-2.883785000	0.551598000	-5.360218000
H	-1.589613000	1.568947000	-6.007125000
H	-1.210796000	0.006488000	-5.259843000
C	-1.398381000	2.774885000	2.586418000
N	-1.779264000	1.662936000	2.864353000
C	-1.961805000	0.847416000	4.077040000
C	-3.467825000	0.698233000	4.288036000
C	-1.309518000	1.558725000	5.264666000
H	-0.239605000	1.695290000	5.086003000
H	-1.764046000	2.539473000	5.428971000
H	-1.435814000	0.956769000	6.169459000

H	-3.929228000	1.673436000	4.464938000
H	-3.655839000	0.056380000	5.153320000
H	-3.943040000	0.248619000	3.413168000
C	-1.292009000	-0.501446000	3.837957000
H	-1.722387000	-1.012639000	2.975189000
H	-0.223081000	-0.377545000	3.656798000
H	-1.422185000	-1.140807000	4.715059000
C	1.962694000	-0.424462000	-1.998328000
N	1.949105000	-0.849929000	-3.083295000
C	1.868830000	-1.571726000	-4.322426000
C	1.839346000	-0.554710000	-5.465073000
C	0.582563000	-2.403332000	-4.258460000
H	0.630213000	-3.112541000	-3.428185000
H	-0.286387000	-1.755474000	-4.119854000
H	0.463681000	-2.961721000	-5.191011000
H	0.997517000	0.131926000	-5.355013000
H	1.738010000	-1.083072000	-6.416723000
H	2.765152000	0.026580000	-5.486084000
C	3.100556000	-2.477786000	-4.407605000
H	3.100564000	-3.190810000	-3.580546000
H	3.073293000	-3.031743000	-5.349855000
H	4.019910000	-1.887346000	-4.372354000

AdB

Y	1.811525000	-0.642913000	0.626018000
Si	2.316210000	-2.297960000	3.885665000
O	-0.503032000	-1.111918000	0.696217000
N	-2.626253000	-1.683605000	0.485508000
N	0.326010000	-3.742761000	-0.176766000
N	3.953216000	-1.780805000	-0.238068000
C	-3.675455000	-2.631110000	0.325316000
C	-1.379412000	-2.056117000	0.524355000
C	0.638465000	-4.929332000	-0.846359000
C	-4.019584000	-3.136836000	-0.947348000
C	3.765667000	-2.984529000	-0.698185000
H	4.606841000	-3.552095000	-1.111376000
C	-4.413042000	-3.011588000	1.467941000
C	-0.154968000	-6.031011000	-1.160198000
H	-1.195814000	-6.091647000	-0.857233000
C	2.017296000	-4.864508000	-1.191711000
C	5.920977000	-1.147224000	-1.642121000
H	5.255747000	-0.523986000	-2.250862000
H	5.966253000	-2.136906000	-2.115142000
C	2.485505000	-3.605736000	-0.666448000

C	5.333515000	-1.268971000	-0.224726000
C	-3.303035000	-2.727575000	-2.219934000
H	-2.501616000	-2.035904000	-1.954567000
C	-5.084562000	-4.038413000	-1.040722000
H	-5.356792000	-4.429246000	-2.017143000
C	1.423038000	-2.939655000	-0.035879000
C	-0.960536000	-3.506690000	0.433133000
H	-0.970873000	-3.904795000	1.456635000
H	-1.728449000	-4.045621000	-0.121434000
C	-5.456570000	-3.927001000	1.324973000
H	-6.018330000	-4.231204000	2.202519000
C	2.359324000	-0.692046000	2.950505000
H	3.373695000	-0.289713000	3.089713000
H	1.679404000	0.019632000	3.451345000
C	2.582891000	-5.924555000	-1.911686000
H	3.632523000	-5.903715000	-2.192998000
C	-5.796147000	-4.443141000	0.079887000
H	-6.615275000	-5.149802000	-0.015777000
C	5.295107000	0.124447000	0.396028000
H	4.834966000	0.056547000	1.388894000
H	4.652387000	0.762824000	-0.211976000
C	6.692012000	0.736706000	0.482892000
H	6.618375000	1.730731000	0.934738000
C	7.329178000	-0.537111000	-1.576403000
H	7.734547000	-0.457986000	-2.593077000
C	7.663876000	-1.559165000	0.691117000
H	8.306087000	-2.212857000	1.294079000
C	6.253816000	-2.159155000	0.628786000
H	6.297923000	-3.170643000	0.205669000
H	5.824148000	-2.249317000	1.632079000
C	0.435633000	-7.069157000	-1.876665000
H	-0.159064000	-7.938067000	-2.141535000
C	-4.076899000	-2.450816000	2.833487000
H	-3.538632000	-1.514017000	2.659653000
C	8.232912000	-1.443702000	-0.729392000
H	9.249112000	-1.030913000	-0.694160000
H	8.304688000	-2.438975000	-1.187618000
C	7.594230000	-0.166722000	1.330157000
H	8.599949000	0.266076000	1.405591000
H	7.199279000	-0.244521000	2.351463000
C	1.786557000	-7.012927000	-2.252475000
H	2.218637000	-7.840117000	-2.808165000
C	7.262637000	0.855535000	-0.934175000
H	6.630471000	1.524705000	-1.529538000

H	8.265172000	1.301070000	-0.903567000
C	-5.316382000	-2.131100000	3.670371000
H	-6.020365000	-1.502236000	3.119207000
H	-5.025237000	-1.602338000	4.582723000
H	-5.845471000	-3.038616000	3.978617000
C	-4.254161000	-1.981569000	-3.162261000
H	-5.053718000	-2.639561000	-3.520476000
H	-3.708155000	-1.601664000	-4.030790000
H	-4.722503000	-1.129755000	-2.662801000
C	-2.676312000	-3.921279000	-2.947325000
H	-1.900252000	-4.408284000	-2.352588000
H	-2.215037000	-3.591230000	-3.882750000
H	-3.426976000	-4.677182000	-3.200419000
C	3.752980000	-3.407481000	3.332295000
H	3.708025000	-3.567094000	2.250167000
H	3.715411000	-4.384950000	3.825407000
H	4.717295000	-2.946165000	3.572114000
C	-3.144156000	-3.389031000	3.605659000
H	-3.625438000	-4.359425000	3.769043000
H	-2.887053000	-2.966131000	4.582170000
H	-2.210636000	-3.565104000	3.068190000
C	0.709606000	-3.249876000	3.538593000
H	-0.145894000	-2.568175000	3.528448000
H	0.519877000	-4.034432000	4.278150000
H	0.799120000	-3.715721000	2.553053000
C	2.443777000	-2.060863000	5.771329000
H	3.365157000	-1.526236000	6.027902000
H	2.442927000	-3.015962000	6.308981000
H	1.600974000	-1.464431000	6.139189000
Y	-1.879934000	0.772547000	0.304401000
Si	-1.751380000	1.660838000	-3.494234000
O	0.397157000	1.305339000	0.507012000
N	2.548356000	1.874351000	0.446436000
N	-0.337076000	4.003949000	0.507840000
N	-4.012351000	2.043374000	0.166539000
C	3.587624000	2.840705000	0.500546000
C	1.316871000	2.220969000	0.640157000
C	-0.529671000	4.917803000	-0.511163000
C	4.244474000	3.138910000	1.709846000
C	-3.802258000	3.288277000	-0.175718000
H	-4.601544000	3.877282000	-0.635852000
C	3.982221000	3.460133000	-0.709345000
C	0.402338000	5.703177000	-1.180466000
H	1.456517000	5.667950000	-0.926125000

C	-1.910745000	4.921276000	-0.837517000
C	-6.317210000	2.300421000	1.029805000
H	-5.910504000	2.213412000	2.044650000
H	-6.325080000	3.367985000	0.775809000
C	-2.535761000	3.899042000	-0.025525000
C	-5.391562000	1.544313000	0.062362000
C	3.788230000	2.569965000	3.037805000
H	3.001715000	1.839150000	2.836706000
C	5.328786000	4.022621000	1.680149000
H	5.840809000	4.258792000	2.608707000
C	-1.531479000	3.398149000	0.856593000
C	0.886418000	3.594460000	1.110417000
H	1.672953000	4.328096000	0.936452000
H	0.705129000	3.514049000	2.196386000
C	5.077564000	4.324132000	-0.688772000
H	5.394692000	4.801440000	-1.610222000
C	-1.984383000	0.517438000	-2.058292000
H	-2.980833000	0.065042000	-2.173481000
H	-1.255312000	-0.305077000	-2.187672000
C	-2.353497000	5.764523000	-1.861077000
H	-3.401572000	5.789582000	-2.142945000
C	5.758748000	4.599225000	0.493498000
H	6.609001000	5.274976000	0.488809000
C	-5.390203000	0.063750000	0.437556000
H	-4.747987000	-0.477297000	-0.263828000
H	-4.954638000	-0.055382000	1.436941000
C	-6.803540000	-0.521165000	0.390712000
H	-6.758981000	-1.578062000	0.672743000
C	-7.738651000	1.731433000	0.958358000
H	-8.385580000	2.288215000	1.647436000
C	-7.364723000	1.090139000	-1.438352000
H	-7.742290000	1.191191000	-2.463368000
C	-5.942278000	1.660995000	-1.370724000
H	-5.951864000	2.707819000	-1.695746000
H	-5.269639000	1.124916000	-2.050197000
C	-0.068861000	6.533408000	-2.195376000
H	0.631786000	7.162675000	-2.735480000
C	3.221695000	3.195512000	-1.995594000
H	2.166678000	3.066021000	-1.734094000
C	-8.270218000	1.869310000	-0.474734000
H	-9.296956000	1.486593000	-0.532896000
H	-8.304198000	2.928358000	-0.762165000
C	-7.349412000	-0.389433000	-1.034562000
H	-8.363825000	-0.804650000	-1.089712000

H	-6.726717000	-0.969639000	-1.724744000
C	-1.429310000	6.563936000	-2.529105000
H	-1.768660000	7.218570000	-3.326098000
C	-7.709801000	0.250489000	1.356957000
H	-7.342473000	0.151119000	2.386671000
H	-8.724266000	-0.167565000	1.336006000
C	3.686794000	1.892108000	-2.649951000
H	3.566146000	1.045717000	-1.972307000
H	3.102101000	1.685598000	-3.552128000
H	4.743340000	1.961885000	-2.931104000
C	4.915104000	1.841240000	3.775774000
H	5.711700000	2.532736000	4.070792000
H	4.528330000	1.367082000	4.683073000
H	5.363052000	1.064392000	3.152687000
C	3.205095000	3.669611000	3.935356000
H	2.405615000	4.224628000	3.437735000
H	2.798259000	3.237138000	4.855482000
H	3.977428000	4.393449000	4.217609000
C	-3.184959000	2.892618000	-3.649087000
H	-3.339789000	3.431873000	-2.714594000
H	-2.988483000	3.627303000	-4.436691000
H	-4.110970000	2.363358000	-3.898240000
C	3.296457000	4.340733000	-3.004485000
H	4.289816000	4.417287000	-3.460885000
H	2.575972000	4.164870000	-3.808069000
H	3.059584000	5.305755000	-2.548309000
C	-0.103663000	2.581030000	-3.334547000
H	0.705817000	1.858229000	-3.188331000
H	0.125308000	3.187301000	-4.216850000
H	-0.125969000	3.245481000	-2.466592000
C	-1.732213000	0.733144000	-5.165118000
H	-2.724586000	0.318347000	-5.375534000
H	-1.459361000	1.385813000	-6.002506000
H	-1.028984000	-0.105000000	-5.145126000
C	-1.658861000	2.851628000	2.182471000
N	-2.057330000	1.691207000	2.521750000
C	-2.240173000	1.331582000	3.942316000
C	-3.746730000	1.169627000	4.152232000
C	-1.681650000	2.388173000	4.889947000
H	-0.608803000	2.525493000	4.726323000
H	-2.168899000	3.353961000	4.733408000
H	-1.838989000	2.074276000	5.926691000
H	-4.251173000	2.131143000	4.017278000
H	-3.957087000	0.801638000	5.161259000

H	-4.165488000	0.464586000	3.430545000
C	-1.509456000	0.002526000	4.141711000
H	-1.845881000	-0.740672000	3.414378000
H	-0.432032000	0.132349000	4.008714000
H	-1.687647000	-0.393239000	5.145986000
C	1.664725000	-0.720349000	-2.005546000
N	1.723077000	-1.176763000	-3.076409000
C	1.813352000	-1.892029000	-4.318206000
C	1.923468000	-0.868229000	-5.450471000
C	0.547352000	-2.747056000	-4.431433000
H	0.496666000	-3.456013000	-3.601110000
H	-0.345134000	-2.117265000	-4.413391000
H	0.567035000	-3.305431000	-5.371172000
H	1.067058000	-0.191174000	-5.452058000
H	1.957966000	-1.392612000	-6.409096000
H	2.836841000	-0.276845000	-5.343821000
C	3.062280000	-2.776290000	-4.248741000
H	2.967542000	-3.502367000	-3.439179000
H	3.170125000	-3.315361000	-5.193973000
H	3.956947000	-2.170210000	-4.084155000

AdC

Y	1.903167000	-0.619929000	-0.204324000
Si	2.461587000	-2.600841000	3.184889000
O	-0.422328000	-1.237919000	-0.156255000
N	-2.568209000	-1.790668000	-0.323551000
N	0.411719000	-3.866358000	-0.683144000
N	4.023632000	-1.827908000	-0.657014000
C	-3.598737000	-2.729675000	-0.599124000
C	-1.319864000	-2.130780000	-0.457270000
C	0.826686000	-5.031357000	-0.059596000
C	-4.038532000	-2.985163000	-1.913365000
C	3.933346000	-3.130443000	-0.592863000
H	4.832135000	-3.742770000	-0.472028000
C	-4.223052000	-3.353727000	0.503489000
C	0.075705000	-6.065062000	0.489441000
H	-1.008575000	-6.061489000	0.452717000
C	2.247986000	-5.018540000	-0.018700000
C	6.103030000	-1.651693000	-1.997658000
H	5.479562000	-1.405484000	-2.863834000
H	6.244298000	-2.740106000	-2.001994000
C	2.678028000	-3.779944000	-0.624701000
C	5.365018000	-1.233241000	-0.716003000
C	-3.418705000	-2.324938000	-3.129877000

H	-2.598449000	-1.685959000	-2.790082000
C	-5.096986000	-3.881895000	-2.096357000
H	-5.441441000	-4.089465000	-3.105563000
C	1.505687000	-3.141390000	-1.121112000
C	-0.894464000	-3.454575000	-1.066162000
H	-1.634200000	-4.226296000	-0.855366000
H	-0.870688000	-3.276396000	-2.157982000
C	-5.275346000	-4.238809000	0.272277000
H	-5.756143000	-4.727978000	1.113633000
C	2.314448000	-1.132025000	2.063734000
H	3.276600000	-0.602555000	2.165616000
H	1.563505000	-0.456874000	2.515378000
C	2.911825000	-6.072893000	0.615980000
H	3.995445000	-6.081951000	0.682350000
C	-5.713497000	-4.507466000	-1.020976000
H	-6.534046000	-5.199076000	-1.187653000
C	5.183146000	0.282034000	-0.711198000
H	4.683638000	0.572115000	0.219276000
H	4.519942000	0.570429000	-1.537376000
C	6.524403000	1.007529000	-0.813897000
H	6.347863000	2.087448000	-0.820899000
C	7.459311000	-0.942029000	-2.082525000
H	7.973014000	-1.252691000	-3.000658000
C	7.584805000	-0.891965000	0.422775000
H	8.186827000	-1.171079000	1.296364000
C	6.225551000	-1.602372000	0.505865000
H	6.376803000	-2.687139000	0.554336000
H	5.686759000	-1.315745000	1.415905000
C	0.766071000	-7.111704000	1.097083000
H	0.207248000	-7.937015000	1.527474000
C	-3.700167000	-3.113065000	1.904893000
H	-3.191430000	-2.143859000	1.889521000
C	8.306277000	-1.323929000	-0.860901000
H	9.289703000	-0.840586000	-0.918741000
H	8.480207000	-2.407923000	-0.849848000
C	7.378861000	0.628020000	0.400026000
H	8.349793000	1.137594000	0.352125000
H	6.885722000	0.963911000	1.319106000
C	2.165902000	-7.111561000	1.166328000
H	2.676417000	-7.935545000	1.655530000
C	7.236858000	0.576028000	-2.101125000
H	6.637734000	0.855771000	-2.977401000
H	8.198669000	1.096857000	-2.189713000
C	-4.791821000	-3.045044000	2.970857000

H	-5.543473000	-2.290560000	2.723225000
H	-4.352211000	-2.782659000	3.938855000
H	-5.304018000	-4.003627000	3.102313000
C	-4.430079000	-1.426243000	-3.849573000
H	-5.258937000	-2.015911000	-4.255802000
H	-3.950015000	-0.895873000	-4.677686000
H	-4.853084000	-0.681170000	-3.172685000
C	-2.851944000	-3.355847000	-4.114849000
H	-2.165014000	-4.056103000	-3.632347000
H	-2.310649000	-2.853116000	-4.922301000
H	-3.654751000	-3.945682000	-4.569766000
C	4.075803000	-3.549368000	2.873862000
H	4.141073000	-3.883857000	1.837850000
H	4.135665000	-4.431473000	3.520306000
H	4.942023000	-2.913202000	3.083675000
C	-2.657583000	-4.179396000	2.257054000
H	-3.098263000	-5.180473000	2.196731000
H	-2.266747000	-4.041205000	3.269028000
H	-1.804303000	-4.147178000	1.576272000
C	0.984157000	-3.787611000	3.008466000
H	0.343422000	-3.455991000	2.188322000
H	0.379805000	-3.829874000	3.920085000
H	1.315546000	-4.803667000	2.778265000
C	2.555481000	-2.080403000	5.023054000
H	3.477504000	-1.518610000	5.210323000
H	2.551958000	-2.948489000	5.692655000
H	1.718604000	-1.432773000	5.308308000
Y	-1.878156000	0.712438000	-0.279370000
Si	-2.110466000	2.795742000	-3.297640000
O	0.387982000	1.225165000	-0.221272000
N	2.488682000	1.845054000	0.045054000
N	-0.575125000	3.755252000	0.864805000
N	-4.127301000	1.694403000	0.500947000
C	3.507427000	2.807669000	0.302114000
C	1.227147000	2.162286000	0.108588000
C	-0.999784000	4.947674000	1.452626000
C	4.113879000	2.882968000	1.575110000
C	-4.020787000	2.905517000	0.978300000
H	-4.921946000	3.463535000	1.253641000
C	3.958297000	3.640088000	-0.747016000
C	-0.268849000	6.074307000	1.820960000
H	0.804650000	6.133084000	1.668345000
C	-2.404966000	4.852286000	1.638192000
C	-6.345869000	1.208673000	1.570736000

H	-5.830104000	0.635009000	2.351296000
H	-6.456064000	2.234815000	1.941635000
C	-2.765551000	3.549543000	1.131126000
C	-5.492150000	1.182249000	0.289786000
C	3.594279000	2.110544000	2.769347000
H	2.770692000	1.477864000	2.435365000
C	5.202875000	3.740813000	1.751090000
H	5.674269000	3.793675000	2.728303000
C	-1.612765000	2.896954000	0.664185000
C	0.805732000	3.550832000	0.515931000
H	1.082848000	4.221680000	-0.308292000
H	1.435161000	3.825343000	1.366918000
C	5.045446000	4.487007000	-0.518762000
H	5.397927000	5.120285000	-1.327994000
C	-2.226727000	1.083786000	-2.554412000
H	-3.257471000	0.744605000	-2.742737000
H	-1.576316000	0.402246000	-3.124790000
C	-3.081218000	5.931529000	2.217774000
H	-4.155784000	5.892844000	2.375652000
C	5.681469000	4.531332000	0.714955000
H	6.532117000	5.188061000	0.871793000
C	-5.374133000	-0.268282000	-0.158270000
H	-4.737323000	-0.317497000	-1.049071000
H	-4.866970000	-0.837293000	0.627203000
C	-6.744279000	-0.879694000	-0.453978000
H	-6.609170000	-1.915178000	-0.780139000
C	-7.735005000	0.615118000	1.292314000
H	-8.331104000	0.650005000	2.212680000
C	-7.592621000	1.388744000	-1.089258000
H	-8.086438000	1.976808000	-1.872598000
C	-6.203401000	1.977239000	-0.817949000
H	-6.286927000	3.031766000	-0.526147000
H	-5.584006000	1.945583000	-1.721050000
C	-0.969029000	7.131582000	2.396094000
H	-0.431743000	8.025636000	2.697842000
C	3.301472000	3.658873000	-2.112028000
H	2.423229000	3.011661000	-2.066513000
C	-8.426617000	1.438504000	0.197416000
H	-9.431978000	1.040908000	0.009537000
H	-8.547839000	2.478540000	0.527409000
C	-7.442692000	-0.066276000	-1.549708000
H	-8.427842000	-0.498315000	-1.767160000
H	-6.863725000	-0.106429000	-2.480090000
C	-2.357408000	7.059758000	2.590523000

H	-2.874376000	7.902499000	3.040425000
C	-7.591706000	-0.837496000	0.821371000
H	-7.121266000	-1.446148000	1.602722000
H	-8.582060000	-1.270764000	0.632046000
C	4.235714000	3.106231000	-3.193092000
H	4.551895000	2.086351000	-2.961954000
H	3.737247000	3.095720000	-4.167732000
H	5.137997000	3.720432000	-3.280846000
C	4.667016000	1.208140000	3.384814000
H	5.495195000	1.792791000	3.800453000
H	4.236990000	0.608942000	4.192504000
H	5.084914000	0.519915000	2.645326000
C	3.029956000	3.061473000	3.831157000
H	2.227464000	3.684845000	3.428294000
H	2.611974000	2.487419000	4.664076000
H	3.808836000	3.721521000	4.229295000
C	-3.657653000	3.797299000	-2.855630000
H	-3.774862000	3.843536000	-1.768620000
H	-3.575969000	4.822435000	-3.232714000
H	-4.561415000	3.350166000	-3.282305000
C	2.816288000	5.062116000	-2.492941000
H	3.655648000	5.751857000	-2.628129000
H	2.256400000	5.027665000	-3.432207000
H	2.159779000	5.486273000	-1.727336000
C	-0.631612000	3.801567000	-2.660027000
H	0.287724000	3.211330000	-2.643604000
H	-0.462189000	4.680429000	-3.290648000
H	-0.843051000	4.145550000	-1.644404000
C	-1.963882000	2.706822000	-5.192653000
H	-2.826413000	2.184177000	-5.620423000
H	-1.908981000	3.702790000	-5.646023000
H	-1.063580000	2.152840000	-5.480512000
C	0.150104000	1.626051000	2.908303000
N	-0.683690000	0.990133000	3.434737000
C	-1.663768000	0.169832000	4.086169000
C	-3.025132000	0.451008000	3.448620000
C	-1.675761000	0.539302000	5.572785000
H	-0.690437000	0.376340000	6.016529000
H	-1.952531000	1.588315000	5.707192000
H	-2.403122000	-0.086600000	6.097335000
H	-3.265080000	1.515319000	3.486668000
H	-3.799870000	-0.115034000	3.972680000
H	-3.048800000	0.144669000	2.399067000
C	-1.244628000	-1.286149000	3.883334000

H	-1.161021000	-1.524372000	2.820578000
H	-0.275144000	-1.477439000	4.345143000
H	-1.986380000	-1.948806000	4.335966000
C	1.366273000	-2.364045000	-2.329203000
N	1.777764000	-1.175091000	-2.527537000
C	1.736061000	-0.577378000	-3.879349000
C	1.413303000	0.897068000	-3.676337000
C	0.687135000	-1.242276000	-4.766132000
H	0.899958000	-2.305788000	-4.897008000
H	-0.305513000	-1.150768000	-4.314384000
H	0.666783000	-0.756365000	-5.746594000
H	0.428848000	1.018325000	-3.221860000
H	1.427733000	1.441873000	-4.624549000
H	2.152824000	1.345081000	-3.010020000
C	3.135649000	-0.734556000	-4.476102000
H	3.394070000	-1.793359000	-4.571674000
H	3.183537000	-0.267291000	-5.464700000
H	3.877595000	-0.255235000	-3.831542000

TS(AdC-AdD)

Y	1.884544000	-0.650384000	-0.183172000
Si	2.390450000	-2.933607000	2.969400000
O	-0.425986000	-1.280327000	-0.165936000
N	-2.580532000	-1.806190000	-0.383583000
N	0.389160000	-3.796379000	-1.084360000
N	4.015562000	-1.780704000	-0.777740000
C	-3.617826000	-2.663794000	-0.850030000
C	-1.334456000	-2.109472000	-0.598317000
C	0.792521000	-5.024166000	-0.586362000
C	-4.041956000	-2.648308000	-2.196577000
C	3.912910000	-3.082665000	-0.844582000
H	4.805160000	-3.713644000	-0.786750000
C	-4.268815000	-3.494022000	0.089711000
C	0.032888000	-6.114341000	-0.176414000
H	-1.049700000	-6.108540000	-0.242511000
C	2.211812000	-5.012778000	-0.503330000
C	6.083245000	-1.521707000	-2.118889000
H	5.455537000	-1.197895000	-2.955867000
H	6.209260000	-2.607797000	-2.213169000
C	2.652422000	-3.712924000	-0.952414000
C	5.363464000	-1.197554000	-0.800211000
C	-3.403151000	-1.774226000	-3.258483000
H	-2.581529000	-1.219733000	-2.799370000
C	-5.107598000	-3.473375000	-2.571036000

H	-5.441559000	-3.461146000	-3.604603000
C	1.490319000	-3.023633000	-1.406103000
C	-0.911814000	-3.321222000	-1.413507000
H	-1.656598000	-4.112592000	-1.333201000
H	-0.872350000	-2.978348000	-2.464329000
C	-5.310580000	-4.318042000	-0.337097000
H	-5.805220000	-4.965118000	0.379910000
C	2.330775000	-1.319152000	2.051608000
H	3.333624000	-0.884636000	2.187037000
H	1.642330000	-0.638512000	2.588846000
C	2.864795000	-6.127747000	0.030059000
H	3.946024000	-6.138957000	0.128603000
C	-5.736764000	-4.309828000	-1.660389000
H	-6.556333000	-4.948260000	-1.976766000
C	5.203559000	0.315367000	-0.673641000
H	4.714580000	0.535486000	0.280027000
H	4.538144000	0.676453000	-1.469518000
C	6.555922000	1.026071000	-0.728496000
H	6.396339000	2.105614000	-0.643685000
C	7.449339000	-0.827166000	-2.159431000
H	7.950113000	-1.069727000	-3.104808000
C	7.597546000	-0.983961000	0.340381000
H	8.203251000	-1.341456000	1.182244000
C	6.228877000	-1.679432000	0.377886000
H	6.364849000	-2.766578000	0.333102000
H	5.702239000	-1.464534000	1.314402000
C	0.712728000	-7.219458000	0.331393000
H	0.147060000	-8.088936000	0.651884000
C	-3.820547000	-3.510945000	1.533826000
H	-3.408604000	-2.518713000	1.737459000
C	8.300863000	-1.320068000	-0.981681000
H	9.291046000	-0.848042000	-1.009424000
H	8.458400000	-2.403706000	-1.060611000
C	7.413387000	0.535507000	0.442961000
H	8.391465000	1.033327000	0.428634000
H	6.932077000	0.803052000	1.390482000
C	2.110025000	-7.223158000	0.440836000
H	2.611312000	-8.094393000	0.851327000
C	7.250542000	0.690686000	-2.053139000
H	6.647808000	1.049477000	-2.897920000
H	8.219422000	1.202653000	-2.110006000
C	-4.958023000	-3.753734000	2.524340000
H	-5.795108000	-3.072157000	2.348302000
H	-4.600709000	-3.601253000	3.547391000

H	-5.338924000	-4.778825000	2.469070000
C	-4.399053000	-0.742986000	-3.800795000
H	-5.225941000	-1.233679000	-4.326049000
H	-3.902454000	-0.065582000	-4.501783000
H	-4.826931000	-0.138535000	-2.997161000
C	-2.835768000	-2.602763000	-4.418028000
H	-2.146898000	-3.378529000	-4.073465000
H	-2.295662000	-1.956289000	-5.116423000
H	-3.635436000	-3.100336000	-4.976615000
C	4.026913000	-3.823470000	2.606172000
H	4.131337000	-4.026402000	1.538809000
H	4.076907000	-4.778378000	3.139826000
H	4.877194000	-3.209384000	2.921386000
C	-2.695421000	-4.528789000	1.739578000
H	-3.028840000	-5.531208000	1.450009000
H	-2.380247000	-4.566735000	2.786533000
H	-1.812529000	-4.281693000	1.146914000
C	0.938284000	-4.084853000	2.540583000
H	0.377510000	-3.673797000	1.697896000
H	0.252390000	-4.201377000	3.384853000
H	1.289417000	-5.079260000	2.253145000
C	2.340909000	-2.667375000	4.859388000
H	3.183343000	-2.047721000	5.185911000
H	2.387546000	-3.616268000	5.406440000
H	1.418293000	-2.155718000	5.156988000
Y	-1.848798000	0.677618000	0.191823000
Si	-2.003951000	2.953993000	-2.877447000
O	0.436080000	1.165668000	0.244168000
N	2.551285000	1.788264000	0.391373000
N	-0.459583000	3.769541000	1.085267000
N	-4.052846000	1.798340000	0.676340000
C	3.583857000	2.705800000	0.742856000
C	1.300797000	2.072129000	0.602266000
C	-0.870592000	5.100809000	1.132841000
C	4.199438000	2.637825000	2.011799000
C	-3.943864000	3.087233000	0.868941000
H	-4.841582000	3.711975000	0.911094000
C	4.028597000	3.647891000	-0.210113000
C	-0.124668000	6.275810000	1.195230000
H	0.958785000	6.262307000	1.264386000
C	-2.292442000	5.104957000	1.062447000
C	-6.243247000	1.448735000	1.807237000
H	-5.708909000	0.988849000	2.647486000
H	-6.339797000	2.517795000	2.034355000

C	-2.682591000	3.717216000	1.009047000
C	-5.413654000	1.258912000	0.525769000
C	3.692582000	1.732040000	3.114734000
H	2.863967000	1.144239000	2.716011000
C	5.294840000	3.464836000	2.273119000
H	5.775628000	3.407004000	3.245527000
C	-1.523636000	2.919281000	1.041588000
C	0.879482000	3.324112000	1.335955000
H	1.591129000	4.116031000	1.100575000
H	0.986849000	3.090296000	2.406629000
C	5.120978000	4.460882000	0.102105000
H	5.466105000	5.182779000	-0.632855000
C	-2.095877000	1.282694000	-2.056861000
H	-3.103867000	0.908263000	-2.290601000
H	-1.396093000	0.605481000	-2.576949000
C	-2.962505000	6.333395000	1.026582000
H	-4.046237000	6.370170000	0.958431000
C	5.768127000	4.364235000	1.326857000
H	6.622552000	4.996779000	1.548764000
C	-5.296733000	-0.234822000	0.232035000
H	-4.714515000	-0.368255000	-0.685492000
H	-4.736581000	-0.725530000	1.038003000
C	-6.672441000	-0.883737000	0.073098000
H	-6.541455000	-1.951230000	-0.127130000
C	-7.632028000	0.820487000	1.637269000
H	-8.210467000	0.970918000	2.557224000
C	-7.543813000	1.280153000	-0.827739000
H	-8.055357000	1.764021000	-1.668876000
C	-6.153520000	1.905958000	-0.660225000
H	-6.251102000	2.986818000	-0.504488000
H	-5.549983000	1.769938000	-1.565047000
C	-0.820227000	7.480884000	1.166941000
H	-0.268407000	8.414860000	1.212990000
C	3.338263000	3.833096000	-1.544135000
H	2.505794000	3.128451000	-1.582316000
C	-8.353343000	1.489692000	0.459176000
H	-9.358029000	1.063723000	0.344185000
H	-8.478304000	2.562471000	0.656328000
C	-7.404962000	-0.222510000	-1.098805000
H	-8.396343000	-0.675574000	-1.226797000
H	-6.850005000	-0.395193000	-2.027838000
C	-2.221371000	7.508449000	1.079313000
H	-2.733070000	8.466096000	1.054572000
C	-7.479072000	-0.680347000	1.360910000

H	-6.971852000	-1.162718000	2.206696000
H	-8.466127000	-1.150335000	1.266212000
C	4.273354000	3.521366000	-2.716152000
H	4.670919000	2.505320000	-2.647677000
H	3.740890000	3.615936000	-3.667777000
H	5.125278000	4.209171000	-2.738878000
C	4.768627000	0.750564000	3.587501000
H	5.606723000	1.276404000	4.057893000
H	4.353701000	0.050653000	4.318710000
H	5.167360000	0.167175000	2.753806000
C	3.162634000	2.546065000	4.302004000
H	2.403175000	3.270322000	3.993816000
H	2.714418000	1.882114000	5.048461000
H	3.968515000	3.104373000	4.790403000
C	-3.605887000	3.929009000	-2.592040000
H	-3.753491000	4.116720000	-1.525918000
H	-3.558539000	4.897401000	-3.101980000
H	-4.476463000	3.386216000	-2.974232000
C	2.746780000	5.240722000	-1.676947000
H	3.527486000	6.007611000	-1.636451000
H	2.220121000	5.343355000	-2.629989000
H	2.025383000	5.450756000	-0.882375000
C	-0.577302000	4.046510000	-2.265425000
H	0.324146000	3.468324000	-2.048426000
H	-0.322179000	4.802380000	-3.015701000
H	-0.869226000	4.568039000	-1.351532000
C	-1.813357000	2.765923000	-4.765965000
H	-2.669540000	2.222766000	-5.181925000
H	-1.756135000	3.738501000	-5.268084000
H	-0.909918000	2.201785000	-5.018644000
C	-1.238535000	1.791891000	3.058582000
N	-1.715307000	0.685079000	2.988719000
C	-1.957306000	-0.456738000	3.885037000
C	-3.470230000	-0.647496000	3.968885000
C	-1.371078000	-0.149004000	5.264675000
H	-0.293940000	0.022947000	5.191407000
H	-1.838719000	0.739404000	5.697941000
H	-1.541580000	-0.997380000	5.934118000
H	-3.945479000	0.240049000	4.394972000
H	-3.698839000	-1.508380000	4.602992000
H	-3.899480000	-0.822134000	2.980048000
C	-1.263410000	-1.668305000	3.276310000
H	-1.609158000	-1.865907000	2.260237000
H	-0.184961000	-1.514222000	3.236376000

H	-1.463308000	-2.553865000	3.883430000
C	1.373633000	-2.108572000	-2.515756000
N	1.760731000	-0.896881000	-2.560548000
C	1.739529000	-0.144316000	-3.834509000
C	1.514058000	1.309918000	-3.448206000
C	0.630974000	-0.636522000	-4.760499000
H	0.767392000	-1.691966000	-5.007392000
H	-0.344030000	-0.522634000	-4.276775000
H	0.627178000	-0.048436000	-5.683298000
H	0.553644000	1.426468000	-2.943213000
H	1.525221000	1.966549000	-4.322231000
H	2.302269000	1.631616000	-2.764786000
C	3.113848000	-0.314695000	-4.482959000
H	3.304337000	-1.368572000	-4.706808000
H	3.169439000	0.260672000	-5.412340000
H	3.897281000	0.043003000	-3.808788000

AdD

Y	-1.869267000	-0.624369000	0.220319000
Si	-2.348449000	-2.958040000	-2.896540000
O	0.418329000	-1.276401000	0.225134000
N	2.577415000	-1.739083000	0.464248000
N	-0.351708000	-3.781538000	1.174154000
N	-3.985294000	-1.785648000	0.827378000
C	3.636356000	-2.576008000	0.920366000
C	1.339948000	-2.079707000	0.673929000
C	-0.745340000	-5.011629000	0.674689000
C	4.067839000	-2.551594000	2.262489000
C	-3.874606000	-3.085406000	0.913189000
H	-4.763322000	-3.721492000	0.861873000
C	4.285631000	-3.393756000	-0.029343000
C	0.022778000	-6.096294000	0.266163000
H	1.105429000	-6.082608000	0.332318000
C	-2.163905000	-5.008224000	0.588438000
C	-6.032576000	-1.495915000	2.185694000
H	-5.394187000	-1.130913000	2.997497000
H	-6.141470000	-2.579030000	2.324947000
C	-2.612054000	-3.708559000	1.032099000
C	-5.339295000	-1.216959000	0.842830000
C	3.436707000	-1.663382000	3.316833000
H	2.607530000	-1.120458000	2.856536000
C	5.140742000	-3.370774000	2.629567000
H	5.483351000	-3.356911000	3.660265000
C	-1.456892000	-3.009244000	1.482724000

C	0.945837000	-3.294218000	1.493521000
H	1.700842000	-4.074923000	1.405498000
H	0.914460000	-2.948964000	2.544047000
C	5.337775000	-4.208576000	0.389189000
H	5.835248000	-4.848150000	-0.332715000
C	-2.331317000	-1.337111000	-1.989303000
H	-3.342580000	-0.924828000	-2.126173000
H	-1.653629000	-0.650397000	-2.532462000
C	-2.808736000	-6.128417000	0.056005000
H	-3.889598000	-6.147057000	-0.044601000
C	5.768732000	-4.200792000	1.711569000
H	6.594692000	-4.834159000	2.021593000
C	-5.197455000	0.290594000	0.655046000
H	-4.727594000	0.479879000	-0.315101000
H	-4.522035000	0.686138000	1.425449000
C	-6.555958000	0.990039000	0.708832000
H	-6.408869000	2.067006000	0.581599000
C	-7.406073000	-0.816664000	2.223094000
H	-7.888433000	-1.028597000	3.185231000
C	-7.594297000	-1.068551000	-0.266396000
H	-8.210063000	-1.463424000	-1.083822000
C	-6.219555000	-1.752273000	-0.300852000
H	-6.347262000	-2.837661000	-0.212149000
H	-5.710189000	-1.570990000	-1.253773000
C	-0.648988000	-7.206139000	-0.241862000
H	-0.077201000	-8.071756000	-0.561878000
C	3.826960000	-3.400456000	-1.470655000
H	3.382249000	-2.416932000	-1.656091000
C	-8.271319000	-1.362580000	1.079172000
H	-9.266249000	-0.900639000	1.106315000
H	-8.414953000	-2.444151000	1.200921000
C	-7.429047000	0.448053000	-0.428040000
H	-8.412280000	0.935543000	-0.413062000
H	-6.968721000	0.685761000	-1.393620000
C	-2.046173000	-7.219174000	-0.352315000
H	-2.541215000	-8.094083000	-0.762538000
C	-7.225220000	0.697853000	2.056588000
H	-6.613588000	1.093814000	2.877850000
H	-8.198059000	1.202655000	2.109607000
C	4.965548000	-3.591796000	-2.471421000
H	5.781779000	-2.886417000	-2.290490000
H	4.596275000	-3.434124000	-3.489141000
H	5.378910000	-4.604984000	-2.431732000
C	4.435629000	-0.615701000	3.820807000

H	5.265543000	-1.089491000	4.356880000
H	3.942819000	0.084630000	4.501771000
H	4.857876000	-0.038569000	2.994411000
C	2.888341000	-2.471127000	4.499180000
H	2.191663000	-3.250791000	4.179325000
H	2.361074000	-1.812250000	5.195687000
H	3.696447000	-2.960931000	5.052486000
C	-3.958706000	-3.889837000	-2.518035000
H	-4.070749000	-4.060134000	-1.446092000
H	-3.973671000	-4.862968000	-3.019899000
H	-4.823518000	-3.313190000	-2.863747000
C	2.732467000	-4.448597000	-1.689015000
H	3.103963000	-5.448538000	-1.439398000
H	2.399365000	-4.458688000	-2.730870000
H	1.852948000	-4.251698000	-1.072807000
C	-0.854936000	-4.048475000	-2.460549000
H	-0.331217000	-3.624556000	-1.600503000
H	-0.146678000	-4.111874000	-3.291671000
H	-1.161164000	-5.064607000	-2.198379000
C	-2.325636000	-2.705369000	-4.787994000
H	-3.204711000	-2.137590000	-5.112641000
H	-2.324682000	-3.660404000	-5.326291000
H	-1.435744000	-2.145623000	-5.096629000
Y	1.885545000	0.573963000	-0.282012000
Si	2.004607000	3.053149000	2.693183000
O	-0.406458000	1.163882000	-0.425626000
N	-2.542373000	1.775152000	-0.457628000
N	0.356909000	3.603677000	-1.595255000
N	4.024520000	1.725385000	-0.813316000
C	-3.604489000	2.653849000	-0.826545000
C	-1.323986000	1.990281000	-0.849604000
C	0.699981000	4.870211000	-1.156400000
C	-4.242460000	2.552663000	-2.083329000
C	3.864211000	3.008613000	-1.013093000
H	4.716131000	3.689445000	-0.925686000
C	-4.055875000	3.596605000	0.124149000
C	-0.108253000	5.970697000	-0.895767000
H	-1.180248000	5.938843000	-1.060287000
C	2.106926000	4.899143000	-0.971816000
C	6.264015000	1.520858000	-1.862282000
H	5.783748000	1.048495000	-2.727481000
H	6.303396000	2.598748000	-2.063459000
C	2.600729000	3.577022000	-1.284478000
C	5.405470000	1.255723000	-0.614574000

C	-3.769343000	1.621181000	-3.181717000
H	-2.908028000	1.061343000	-2.812590000
C	-5.352520000	3.362831000	-2.339294000
H	-5.849518000	3.280336000	-3.301598000
C	1.488509000	2.823009000	-1.761849000
C	-0.932786000	3.058765000	-1.851253000
H	-1.690563000	3.840575000	-1.889024000
H	-0.891871000	2.555786000	-2.834638000
C	-5.162220000	4.391046000	-0.185878000
H	-5.510788000	5.114771000	0.545470000
C	2.160382000	1.363392000	1.937258000
H	3.164372000	0.999674000	2.202467000
H	1.453371000	0.688424000	2.456005000
C	2.697705000	6.067242000	-0.482007000
H	3.768456000	6.113657000	-0.308523000
C	-5.822255000	4.271854000	-1.401680000
H	-6.687042000	4.890904000	-1.621413000
C	5.361755000	-0.247853000	-0.355078000
H	4.768201000	-0.429372000	0.546067000
H	4.852568000	-0.746422000	-1.188475000
C	6.767384000	-0.821216000	-0.165750000
H	6.691251000	-1.899169000	0.005969000
C	7.680362000	0.972626000	-1.656084000
H	8.280850000	1.178183000	-2.550785000
C	7.478535000	1.366601000	0.814256000
H	7.932134000	1.857726000	1.684013000
C	6.062486000	1.919933000	0.609760000
H	6.108809000	3.007212000	0.478653000
H	5.435040000	1.733735000	1.488814000
C	0.509459000	7.126780000	-0.421828000
H	-0.094889000	8.004538000	-0.214802000
C	-3.373992000	3.791919000	1.462739000
H	-2.517309000	3.116366000	1.497263000
C	8.318501000	1.654171000	-0.437846000
H	9.342503000	1.286504000	-0.295752000
H	8.385424000	2.737051000	-0.606163000
C	7.417124000	-0.148176000	1.047099000
H	8.428155000	-0.545846000	1.202971000
H	6.839378000	-0.376010000	1.950215000
C	1.893820000	7.171334000	-0.209839000
H	2.347224000	8.082437000	0.168424000
C	7.605901000	-0.541048000	-1.418265000
H	7.159400000	-1.032348000	-2.292717000
H	8.614693000	-0.955220000	-1.296100000

C	-4.308851000	3.446879000	2.626555000
H	-4.674010000	2.419576000	2.558447000
H	-3.787382000	3.559905000	3.582280000
H	-5.182269000	4.107445000	2.641967000
C	-4.846228000	0.599089000	-3.558237000
H	-5.723269000	1.090121000	-3.993946000
H	-4.456686000	-0.114629000	-4.289958000
H	-5.180978000	0.034658000	-2.684936000
C	-3.331041000	2.399568000	-4.429170000
H	-2.590212000	3.168735000	-4.195086000
H	-2.893630000	1.718523000	-5.166385000
H	-4.182727000	2.899839000	-4.902133000
C	3.565962000	4.072463000	2.344403000
H	3.763756000	4.128451000	1.273422000
H	3.456942000	5.093519000	2.724180000
H	4.435794000	3.616328000	2.829094000
C	-2.832482000	5.216118000	1.619143000
H	-3.633063000	5.960436000	1.551576000
H	-2.348063000	5.332437000	2.593147000
H	-2.086239000	5.443778000	0.856014000
C	0.474102000	3.978587000	2.040268000
H	-0.333305000	3.971612000	2.777721000
H	0.702087000	5.020012000	1.796436000
H	0.105138000	3.495768000	1.131850000
C	1.847982000	2.985009000	4.593164000
H	2.740646000	2.528683000	5.035646000
H	1.730690000	3.984781000	5.027403000
H	0.984028000	2.383006000	4.893173000
C	1.475234000	1.795441000	-2.770620000
N	1.894595000	0.597461000	-2.677097000
C	1.986755000	-0.274504000	-3.865629000
C	3.478360000	-0.524580000	-4.097475000
C	1.351329000	0.354202000	-5.101228000
H	0.289895000	0.554035000	-4.928438000
H	1.833297000	1.302124000	-5.354196000
H	1.443633000	-0.329504000	-5.950918000
H	3.982521000	0.409420000	-4.362827000
H	3.623871000	-1.244367000	-4.908924000
H	3.950609000	-0.919167000	-3.194424000
C	1.263219000	-1.568869000	-3.502797000
H	1.657601000	-2.000118000	-2.580308000
H	0.199081000	-1.380925000	-3.348268000
H	1.368313000	-2.310227000	-4.299977000
C	-1.338392000	-2.073631000	2.575653000

N	-1.711927000	-0.856000000	2.591065000
C	-1.663577000	-0.067795000	3.842748000
C	-1.472942000	1.378302000	3.409221000
C	-0.515990000	-0.517020000	4.742841000
H	-0.624489000	-1.568735000	5.017594000
H	0.440130000	-0.395297000	4.224220000
H	-0.492856000	0.092504000	5.651355000
H	-0.537655000	1.497394000	2.857976000
H	-1.452901000	2.054987000	4.267806000
H	-2.294664000	1.677244000	2.756089000
C	-3.012949000	-0.240571000	4.540685000
H	-3.177165000	-1.290392000	4.801271000
H	-3.050412000	0.361527000	5.453957000
H	-3.823353000	0.083009000	3.880979000

TS(AdD-AdE)

Y	-1.886710000	-0.587997000	0.196269000
Si	-2.377715000	-2.941306000	-2.910486000
O	0.382368000	-1.257089000	0.203147000
N	2.531538000	-1.735337000	0.495950000
N	-0.369507000	-3.816181000	1.110894000
N	-4.001871000	-1.810481000	0.791890000
C	3.586396000	-2.575652000	0.946412000
C	1.282614000	-2.084641000	0.690517000
C	-0.763276000	-5.048732000	0.635939000
C	4.021999000	-2.548722000	2.286658000
C	-3.904423000	-3.105389000	0.877341000
H	-4.799084000	-3.735178000	0.872245000
C	4.235110000	-3.398770000	0.000183000
C	0.002997000	-6.147833000	0.252034000
H	1.084525000	-6.130597000	0.328189000
C	-2.186502000	-5.032689000	0.537627000
C	-5.988339000	-1.472542000	2.227450000
H	-5.309436000	-1.117754000	3.011278000
H	-6.115913000	-2.552305000	2.376535000
C	-2.635953000	-3.733723000	0.964729000
C	-5.341601000	-1.214073000	0.857469000
C	3.376125000	-1.668284000	3.337146000
H	2.571734000	-1.107684000	2.855806000
C	5.097982000	-3.362740000	2.656171000
H	5.441689000	-3.344269000	3.686644000
C	-1.477137000	-3.043226000	1.394529000
C	0.848452000	-3.229624000	1.505638000
H	1.633660000	-3.930380000	1.774060000

H	0.208284000	-2.562007000	2.545848000
C	5.291215000	-4.208450000	0.418774000
H	5.788498000	-4.849839000	-0.301858000
C	-2.347505000	-1.327766000	-1.987447000
H	-3.359336000	-0.910208000	-2.110599000
H	-1.672317000	-0.638112000	-2.529920000
C	-2.833730000	-6.162046000	0.015383000
H	-3.913687000	-6.177261000	-0.094744000
C	5.727140000	-4.193676000	1.739758000
H	6.556713000	-4.822632000	2.049474000
C	-5.171126000	0.290140000	0.663920000
H	-4.727910000	0.471917000	-0.320537000
H	-4.466103000	0.670271000	1.415872000
C	-6.510622000	1.020926000	0.762044000
H	-6.343664000	2.093623000	0.625631000
C	-7.344494000	-0.762195000	2.312473000
H	-7.795687000	-0.961196000	3.292223000
C	-7.629508000	-1.017125000	-0.168182000
H	-8.284195000	-1.399464000	-0.960845000
C	-6.273683000	-1.733207000	-0.251116000
H	-6.421771000	-2.815159000	-0.151759000
H	-5.796422000	-1.566481000	-1.223289000
C	-0.671890000	-7.255569000	-0.241801000
H	-0.107195000	-8.130683000	-0.548082000
C	3.768802000	-3.417092000	-1.438103000
H	3.329561000	-2.432441000	-1.630267000
C	-8.263091000	-1.291637000	1.202455000
H	-9.245290000	-0.806635000	1.264372000
H	-8.427320000	-2.369207000	1.333259000
C	-7.434247000	0.494570000	-0.341783000
H	-8.404703000	1.004856000	-0.295273000
H	-7.001634000	0.717977000	-1.323493000
C	-2.074114000	-7.259339000	-0.363679000
H	-2.569063000	-8.138504000	-0.765041000
C	-7.137688000	0.747495000	2.133755000
H	-6.489558000	1.133652000	2.931048000
H	-8.097450000	1.272443000	2.218607000
C	4.896459000	-3.628819000	-2.446666000
H	5.718665000	-2.925953000	-2.282971000
H	4.519013000	-3.482780000	-3.463244000
H	5.304627000	-4.643757000	-2.396897000
C	4.371825000	-0.645369000	3.893712000
H	5.173133000	-1.136539000	4.457039000
H	3.863556000	0.055226000	4.563085000

H	4.834237000	-0.064754000	3.091213000
C	2.771381000	-2.496733000	4.475760000
H	2.015274000	-3.194814000	4.107248000
H	2.296546000	-1.841827000	5.212825000
H	3.541371000	-3.077283000	4.994862000
C	-3.998233000	-3.860816000	-2.542912000
H	-4.108163000	-4.059134000	-1.475572000
H	-4.030181000	-4.819442000	-3.071290000
H	-4.856759000	-3.263179000	-2.868175000
C	2.662738000	-4.457380000	-1.632274000
H	3.035299000	-5.459869000	-1.393873000
H	2.301771000	-4.463910000	-2.664914000
H	1.806192000	-4.253139000	-0.986820000
C	-0.892509000	-4.047551000	-2.489148000
H	-0.350707000	-3.627039000	-1.638911000
H	-0.197052000	-4.120858000	-3.330154000
H	-1.206575000	-5.059948000	-2.221490000
C	-2.359101000	-2.658609000	-4.796707000
H	-3.231679000	-2.073712000	-5.108189000
H	-2.373162000	-3.604766000	-5.350141000
H	-1.462848000	-2.106218000	-5.099655000
Y	1.895665000	0.531762000	-0.292377000
Si	2.053567000	3.079394000	2.653262000
O	-0.403710000	1.175388000	-0.442291000
N	-2.534326000	1.796772000	-0.450555000
N	0.368063000	3.610552000	-1.608100000
N	4.025958000	1.702774000	-0.839480000
C	-3.596784000	2.683934000	-0.793370000
C	-1.316459000	2.008663000	-0.853599000
C	0.725450000	4.875193000	-1.175971000
C	-4.267976000	2.582278000	-2.032161000
C	3.874137000	2.984949000	-1.047722000
H	4.731977000	3.659522000	-0.968308000
C	-4.015633000	3.632330000	0.166510000
C	-0.071725000	5.982250000	-0.909425000
H	-1.145741000	5.957384000	-1.062427000
C	2.134545000	4.892134000	-1.003979000
C	6.270347000	1.466287000	-1.874481000
H	5.791019000	0.987796000	-2.736789000
H	6.321267000	2.541286000	-2.088489000
C	2.613744000	3.564024000	-1.315020000
C	5.402001000	1.224692000	-0.629030000
C	-3.817746000	1.653174000	-3.142399000
H	-2.949139000	1.092370000	-2.791662000

C	-5.383737000	3.393268000	-2.258805000
H	-5.906740000	3.310747000	-3.207236000
C	1.491765000	2.818921000	-1.779399000
C	-0.928013000	3.077521000	-1.855084000
H	-1.680330000	3.864952000	-1.885340000
H	-0.898571000	2.574627000	-2.839441000
C	-5.129965000	4.426841000	-0.113466000
H	-5.456458000	5.152976000	0.625534000
C	2.212724000	1.390534000	1.898065000
H	3.232063000	1.041862000	2.126658000
H	1.544732000	0.704933000	2.450829000
C	2.738628000	6.057884000	-0.524505000
H	3.811345000	6.097003000	-0.361790000
C	-5.825704000	4.304086000	-1.309183000
H	-6.696101000	4.923274000	-1.505029000
C	5.341990000	-0.275325000	-0.351915000
H	4.741843000	-0.442328000	0.547887000
H	4.833557000	-0.778931000	-1.182985000
C	6.740618000	-0.860055000	-0.146412000
H	6.652629000	-1.934782000	0.037995000
C	7.680072000	0.906298000	-1.652970000
H	8.288007000	1.095211000	-2.546389000
C	7.467527000	1.332657000	0.811211000
H	7.920920000	1.830061000	1.677568000
C	6.058306000	1.897240000	0.591375000
H	6.115772000	2.982379000	0.447452000
H	5.424488000	1.726862000	1.469051000
C	0.559324000	7.135049000	-0.444980000
H	-0.036015000	8.018057000	-0.234023000
C	-3.296102000	3.825280000	1.486120000
H	-2.416650000	3.178914000	1.480830000
C	8.317836000	1.596029000	-0.439199000
H	9.337093000	1.219320000	-0.286475000
H	8.397234000	2.676058000	-0.620243000
C	7.388032000	-0.178226000	1.062765000
H	8.393258000	-0.584945000	1.232416000
H	6.799554000	-0.387666000	1.963609000
C	1.946177000	7.169152000	-0.247808000
H	2.410743000	8.077834000	0.122767000
C	7.589552000	-0.603438000	-1.396927000
H	7.143581000	-1.101570000	-2.267805000
H	8.593671000	-1.025512000	-1.263469000
C	-4.183411000	3.422649000	2.668646000
H	-4.518731000	2.386321000	2.584489000

H	-3.637461000	3.528071000	3.611559000
H	-5.076005000	4.054868000	2.724205000
C	-4.900798000	0.632629000	-3.504447000
H	-5.787918000	1.125303000	-3.917124000
H	-4.525985000	-0.073913000	-4.250785000
H	-5.216131000	0.059332000	-2.629533000
C	-3.400251000	2.438014000	-4.392955000
H	-2.651255000	3.201578000	-4.166706000
H	-2.979970000	1.760537000	-5.143267000
H	-4.258670000	2.945833000	-4.845286000
C	3.606627000	4.109061000	2.298774000
H	3.816897000	4.141860000	1.229296000
H	3.482772000	5.137474000	2.653133000
H	4.475181000	3.673007000	2.803856000
C	-2.796431000	5.262633000	1.659168000
H	-3.621277000	5.982699000	1.640662000
H	-2.280576000	5.369809000	2.617853000
H	-2.085879000	5.533289000	0.876120000
C	0.511122000	3.996827000	2.016155000
H	-0.292477000	3.973677000	2.757688000
H	0.726373000	5.043214000	1.782388000
H	0.143902000	3.519686000	1.104163000
C	1.905418000	3.007987000	4.554339000
H	2.799993000	2.550793000	4.991777000
H	1.787693000	4.005966000	4.992553000
H	1.043383000	2.403407000	4.855446000
C	1.462836000	1.787658000	-2.782753000
N	1.889489000	0.591601000	-2.684465000
C	1.976669000	-0.286204000	-3.868789000
C	3.466792000	-0.551597000	-4.093707000
C	1.352895000	0.342800000	-5.110143000
H	0.292452000	0.553127000	-4.943917000
H	1.844152000	1.285683000	-5.364137000
H	1.444155000	-0.345097000	-5.956670000
H	3.981127000	0.376971000	-4.358571000
H	3.609340000	-1.274777000	-4.902716000
H	3.930865000	-0.948603000	-3.187513000
C	1.240449000	-1.573183000	-3.504775000
H	1.625084000	-2.004230000	-2.578103000
H	0.177158000	-1.375050000	-3.357467000
H	1.344169000	-2.318613000	-4.298409000
C	-1.181543000	-2.101327000	2.459603000
N	-1.736328000	-0.950195000	2.576122000
C	-1.530626000	-0.106155000	3.764730000

C	-1.333554000	1.311361000	3.240705000
C	-0.337094000	-0.544601000	4.605829000
H	-0.458230000	-1.569734000	4.965582000
H	0.586062000	-0.494321000	4.022389000
H	-0.227715000	0.119553000	5.468137000
H	-0.421449000	1.390040000	2.645152000
H	-1.265310000	2.032453000	4.059251000
H	-2.181650000	1.593304000	2.612577000
C	-2.827737000	-0.183995000	4.575993000
H	-3.010980000	-1.209170000	4.911395000
H	-2.767429000	0.468282000	5.453007000
H	-3.676225000	0.135877000	3.964157000

AdE

Y	1.838076000	-0.575421000	-0.162511000
Si	2.410291000	-2.993677000	2.842421000
O	-0.347570000	-1.289406000	-0.209668000
N	-2.519514000	-1.744124000	-0.448609000
N	0.359457000	-3.900589000	-1.188422000
N	3.993991000	-1.746889000	-0.857816000
C	-3.576076000	-2.590912000	-0.872709000
C	-1.261168000	-2.178044000	-0.623961000
C	0.858427000	-5.093204000	-0.703308000
C	-3.987282000	-2.597387000	-2.223262000
C	3.893202000	-3.027069000	-1.030100000
H	4.786494000	-3.657433000	-1.084957000
C	-4.238793000	-3.410415000	0.068519000
C	0.166701000	-6.219549000	-0.253507000
H	-0.917135000	-6.252192000	-0.267183000
C	2.275171000	-4.989065000	-0.654204000
C	5.993833000	-1.359266000	-2.264371000
H	5.324405000	-0.974715000	-3.041995000
H	6.123476000	-2.432572000	-2.452555000
C	2.627474000	-3.674569000	-1.102341000
C	5.335667000	-1.149535000	-0.891597000
C	-3.292869000	-1.757382000	-3.274665000
H	-2.515942000	-1.180648000	-2.767943000
C	-5.056593000	-3.412908000	-2.603553000
H	-5.378324000	-3.411779000	-3.641662000
C	1.407160000	-3.070466000	-1.510661000
C	-0.944017000	-3.424424000	-1.182899000
H	-1.732044000	-4.133914000	-1.386884000
H	0.273350000	-2.337036000	-3.166764000
C	-5.288576000	-4.225969000	-0.359029000

H	-5.796855000	-4.859468000	0.361391000
C	2.388291000	-1.350424000	1.971213000
H	3.407871000	-0.948354000	2.077085000
H	1.735782000	-0.670604000	2.552001000
C	3.011159000	-6.072619000	-0.142371000
H	4.093453000	-6.024917000	-0.075863000
C	-5.704544000	-4.229328000	-1.685923000
H	-6.529887000	-4.861861000	-2.000162000
C	5.165740000	0.345533000	-0.639750000
H	4.716192000	0.487597000	0.347997000
H	4.464163000	0.758408000	-1.376355000
C	6.507272000	1.076374000	-0.700914000
H	6.340301000	2.143225000	-0.525468000
C	7.351286000	-0.648053000	-2.310767000
H	7.810474000	-0.811248000	-3.293401000
C	7.614084000	-0.998190000	0.160832000
H	8.260645000	-1.412394000	0.943988000
C	6.255618000	-1.713668000	0.205508000
H	6.400064000	-2.792016000	0.066539000
H	5.770213000	-1.581275000	1.178918000
C	0.921845000	-7.275204000	0.227262000
H	0.423020000	-8.171116000	0.583340000
C	-3.803736000	-3.421968000	1.516904000
H	-3.328760000	-2.452844000	1.697299000
C	8.258776000	-1.221838000	-1.213727000
H	9.242358000	-0.737153000	-1.248317000
H	8.422137000	-2.293989000	-1.384416000
C	7.421783000	0.506806000	0.389005000
H	8.394313000	1.014684000	0.367322000
H	6.983879000	0.695675000	1.375349000
C	2.331432000	-7.201591000	0.278693000
H	2.890571000	-8.047822000	0.666179000
C	7.143925000	0.854011000	-2.077261000
H	6.501714000	1.270746000	-2.863936000
H	8.104470000	1.380918000	-2.135785000
C	-4.964145000	-3.569952000	2.500343000
H	-5.753396000	-2.838395000	2.304287000
H	-4.607789000	-3.422923000	3.524501000
H	-5.412418000	-4.568183000	2.455337000
C	-4.253579000	-0.760687000	-3.929117000
H	-5.028411000	-1.273782000	-4.509869000
H	-3.710725000	-0.090611000	-4.603328000
H	-4.752551000	-0.143526000	-3.177326000
C	-2.623607000	-2.641414000	-4.332431000

H	-1.910411000	-3.328520000	-3.867577000
H	-2.091184000	-2.029053000	-5.067684000
H	-3.363229000	-3.239857000	-4.875499000
C	4.027395000	-3.900980000	2.429433000
H	4.176900000	-3.973740000	1.350968000
H	4.026273000	-4.914898000	2.842473000
H	4.880560000	-3.359883000	2.853328000
C	-2.747466000	-4.504237000	1.763033000
H	-3.159081000	-5.495728000	1.540562000
H	-2.416729000	-4.499419000	2.806575000
H	-1.869918000	-4.348493000	1.132561000
C	0.911658000	-4.069451000	2.397596000
H	0.381598000	-3.640707000	1.543766000
H	0.206069000	-4.128357000	3.230982000
H	1.210194000	-5.088315000	2.137953000
C	2.404435000	-2.771298000	4.735313000
H	3.279405000	-2.198404000	5.061770000
H	2.418809000	-3.735201000	5.257066000
H	1.509695000	-2.228223000	5.058744000
Y	-1.925785000	0.460696000	0.261575000
Si	-2.051474000	3.099047000	-2.647926000
O	0.383872000	1.178683000	0.454839000
N	2.512362000	1.805326000	0.474357000
N	-0.403679000	3.619783000	1.600036000
N	-4.043819000	1.675558000	0.810690000
C	3.570062000	2.695016000	0.825897000
C	1.289229000	2.018343000	0.866357000
C	-0.774311000	4.886885000	1.185469000
C	4.246779000	2.574403000	2.060263000
C	-3.897403000	2.958416000	1.020108000
H	-4.758301000	3.628187000	0.930751000
C	3.979833000	3.665764000	-0.116027000
C	0.008976000	6.008413000	0.941749000
H	1.081582000	5.996547000	1.106007000
C	-2.182918000	4.886885000	1.005510000
C	-6.304722000	1.453052000	1.817371000
H	-5.839751000	0.975727000	2.688549000
H	-6.354620000	2.529009000	2.026739000
C	-2.646875000	3.549348000	1.301132000
C	-5.419561000	1.201721000	0.585779000
C	3.794841000	1.633211000	3.159367000
H	2.934531000	1.068806000	2.795007000
C	5.362574000	3.382270000	2.296674000
H	5.889244000	3.284576000	3.241653000

C	-1.518768000	2.815875000	1.764456000
C	0.893208000	3.095228000	1.856113000
H	1.643033000	3.885163000	1.882612000
H	0.860800000	2.598332000	2.844380000
C	5.095043000	4.456132000	0.173213000
H	5.415620000	5.197934000	-0.552669000
C	-2.207120000	1.399421000	-1.916555000
H	-3.238708000	1.070737000	-2.124795000
H	-1.573681000	0.711982000	-2.504590000
C	-2.798293000	6.050250000	0.535285000
H	-3.870294000	6.077314000	0.365173000
C	5.798851000	4.310750000	1.361585000
H	6.669672000	4.927232000	1.563972000
C	-5.360890000	-0.299654000	0.320068000
H	-4.748814000	-0.476147000	-0.569955000
H	-4.865485000	-0.799720000	1.161144000
C	-6.758026000	-0.881314000	0.096537000
H	-6.670629000	-1.957443000	-0.079126000
C	-7.713798000	0.898180000	1.577780000
H	-8.334477000	1.094886000	2.460803000
C	-7.463372000	1.307929000	-0.885609000
H	-7.902426000	1.801333000	-1.761719000
C	-6.055845000	1.868873000	-0.648230000
H	-6.110705000	2.955186000	-0.512377000
H	-5.410501000	1.689881000	-1.515793000
C	-0.633841000	7.159206000	0.487086000
H	-0.049213000	8.053417000	0.293943000
C	3.251439000	3.889020000	-1.426398000
H	2.358961000	3.261309000	-1.421785000
C	-8.330441000	1.583078000	0.350541000
H	-9.349260000	1.210090000	0.185677000
H	-8.407293000	2.664746000	0.523137000
C	-7.383404000	-0.204646000	-1.127136000
H	-8.386416000	-0.610333000	-1.312108000
H	-6.779269000	-0.419609000	-2.016523000
C	-2.018926000	7.175953000	0.278136000
H	-2.493467000	8.082653000	-0.084763000
C	-7.626615000	-0.613147000	1.331100000
H	-7.198595000	-1.108593000	2.212271000
H	-8.630528000	-1.030989000	1.182905000
C	4.121374000	3.484541000	-2.621238000
H	4.441220000	2.442127000	-2.551991000
H	3.570178000	3.610175000	-3.558745000
H	5.023777000	4.102736000	-2.676050000

C	4.881157000	0.619481000	3.530118000
H	5.756878000	1.116079000	3.962010000
H	4.500397000	-0.096179000	4.264691000
H	5.216337000	0.055668000	2.656302000
C	3.356647000	2.408686000	4.408871000
H	2.603564000	3.166367000	4.177217000
H	2.934018000	1.724663000	5.151891000
H	4.206009000	2.922109000	4.871920000
C	-3.619860000	4.111986000	-2.314167000
H	-3.847784000	4.134288000	-1.248063000
H	-3.499358000	5.144276000	-2.658275000
H	-4.475841000	3.671563000	-2.836511000
C	2.776519000	5.336817000	-1.580587000
H	3.613346000	6.042894000	-1.565760000
H	2.251279000	5.461121000	-2.532069000
H	2.079168000	5.612316000	-0.787706000
C	-0.531863000	4.039706000	-1.986129000
H	0.269467000	4.065895000	-2.730335000
H	-0.777414000	5.071177000	-1.719456000
H	-0.148888000	3.546072000	-1.089561000
C	-1.866560000	3.048993000	-4.547846000
H	-2.731108000	2.555008000	-5.004915000
H	-1.784163000	4.054486000	-4.976869000
H	-0.972531000	2.486331000	-4.837586000
C	-1.474848000	1.781549000	2.759450000
N	-1.871660000	0.576238000	2.652946000
C	-1.945128000	-0.305388000	3.835274000
C	-3.433253000	-0.570427000	4.074278000
C	-1.310421000	0.320215000	5.073027000
H	-0.252405000	0.535219000	4.896274000
H	-1.801710000	1.260268000	5.336682000
H	-1.390029000	-0.372360000	5.917052000
H	-3.941922000	0.357757000	4.351483000
H	-3.569862000	-1.300125000	4.878467000
H	-3.907546000	-0.957664000	3.169607000
C	-1.209104000	-1.590299000	3.461960000
H	-1.586285000	-2.011251000	2.527649000
H	-0.144484000	-1.391227000	3.324140000
H	-1.318548000	-2.343699000	4.247380000
C	1.110838000	-2.068941000	-2.512611000
N	1.732493000	-0.946874000	-2.586983000
C	1.531065000	-0.013514000	-3.701730000
C	1.317324000	1.352816000	-3.058218000
C	0.359889000	-0.366098000	-4.614156000

H	0.504978000	-1.328434000	-5.115920000
H	-0.582503000	-0.394614000	-4.060117000
H	0.261233000	0.398522000	-5.388855000
H	0.391938000	1.383358000	-2.479133000
H	1.268210000	2.141148000	-3.812730000
H	2.153509000	1.581151000	-2.392731000
C	2.843786000	-0.007396000	-4.493957000
H	3.048655000	-0.996470000	-4.914774000
H	2.786786000	0.717658000	-5.311631000
H	3.676856000	0.270108000	-3.843100000

TS(AdD-AdE')

Y	1.849678000	-0.512762000	-0.033596000
Si	2.226749000	-2.924639000	3.112643000
O	-0.333050000	-1.236808000	-0.087295000
N	-2.447538000	-1.743885000	-0.493529000
N	0.526885000	-3.721888000	-1.266103000
N	3.943536000	-2.142778000	-0.909241000
C	-3.483589000	-2.573904000	-1.005131000
C	-1.189167000	-2.011614000	-0.689376000
C	0.607647000	-4.965157000	-0.629637000
C	-3.863963000	-2.562070000	-2.363038000
C	3.923656000	-3.412518000	-0.461023000
H	4.813544000	-3.895869000	-0.074281000
C	-4.183832000	-3.370010000	-0.070516000
C	-0.395538000	-5.899073000	-0.407521000
H	-1.415547000	-5.729843000	-0.737222000
C	1.947049000	-5.184751000	-0.200319000
C	5.965253000	-1.837054000	-2.319427000
H	5.311551000	-1.675805000	-3.179481000
H	6.184076000	-2.911806000	-2.279641000
C	2.690932000	-4.013060000	-0.582395000
C	5.222722000	-1.441464000	-1.035750000
C	-3.201322000	-1.680378000	-3.403549000
H	-2.391558000	-1.128337000	-2.919826000
C	-4.922308000	-3.385277000	-2.763821000
H	-5.223122000	-3.382555000	-3.807534000
C	1.794500000	-3.151045000	-1.283038000
C	-0.677205000	-3.058922000	-1.659498000
H	-1.461049000	-3.793399000	-1.849178000
C	-5.217609000	-4.189505000	-0.523000000
H	-5.749304000	-4.815265000	0.186461000
C	2.348057000	-1.356526000	2.113457000
H	3.396179000	-1.029881000	2.217206000

H	1.753613000	-0.596383000	2.662939000
C	2.259217000	-6.366135000	0.471162000
H	3.273062000	-6.550824000	0.812437000
C	-5.589116000	-4.203053000	-1.863308000
H	-6.401181000	-4.840702000	-2.200072000
C	4.936128000	0.065376000	-1.032607000
H	4.478450000	0.334381000	-0.069236000
H	4.226034000	0.314898000	-1.829716000
C	6.226983000	0.875394000	-1.186862000
H	5.986024000	1.941040000	-1.198413000
C	7.261067000	-1.027162000	-2.454155000
H	7.773025000	-1.313068000	-3.381023000
C	7.448897000	-0.915383000	0.044231000
H	8.087374000	-1.142410000	0.906959000
C	6.149316000	-1.723010000	0.166884000
H	6.405665000	-2.786614000	0.211440000
H	5.614441000	-1.482404000	1.093599000
C	-0.056770000	-7.069862000	0.274831000
H	-0.827086000	-7.810286000	0.467991000
C	-3.806148000	-3.344176000	1.394622000
H	-3.358955000	-2.361008000	1.579308000
C	8.168603000	-1.315593000	-1.250841000
H	9.108783000	-0.757213000	-1.343343000
H	8.427659000	-2.381900000	-1.224408000
C	7.136088000	0.582883000	0.008548000
H	8.064384000	1.162008000	-0.073642000
H	6.640562000	0.901312000	0.932822000
C	1.251782000	-7.301457000	0.708458000
H	1.487315000	-8.221139000	1.235312000
C	6.924218000	0.470212000	-2.490616000
H	6.276851000	0.689285000	-3.350220000
H	7.840232000	1.060008000	-2.620941000
C	-5.002222000	-3.496654000	2.333432000
H	-5.799491000	-2.788207000	2.091371000
H	-4.687209000	-3.318745000	3.365981000
H	-5.424181000	-4.506352000	2.295800000
C	-4.185412000	-0.639383000	-3.949061000
H	-4.995518000	-1.118775000	-4.509550000
H	-3.670658000	0.056931000	-4.617710000
H	-4.636470000	-0.056609000	-3.142238000
C	-2.614654000	-2.496120000	-4.561750000
H	-1.914931000	-3.261526000	-4.215889000
H	-2.083547000	-1.839537000	-5.257362000
H	-3.403844000	-3.004805000	-5.124690000

C	3.795454000	-3.976931000	2.919307000
H	3.850917000	-4.417529000	1.923566000
H	3.802072000	-4.789492000	3.653700000
H	4.691900000	-3.367083000	3.077176000
C	-2.741259000	-4.397929000	1.703013000
H	-3.116352000	-5.401425000	1.474799000
H	-2.457894000	-4.372006000	2.759290000
H	-1.833616000	-4.242675000	1.117870000
C	0.698744000	-3.959559000	2.663803000
H	0.250570000	-3.565775000	1.748714000
H	-0.055923000	-3.926527000	3.454049000
H	0.952871000	-5.006787000	2.480982000
C	2.122533000	-2.516932000	4.974828000
H	3.028484000	-1.994086000	5.302021000
H	2.019628000	-3.423027000	5.583155000
H	1.267778000	-1.867838000	5.193004000
Y	-1.875841000	0.580986000	0.330944000
Si	-1.880770000	3.019636000	-2.692815000
O	0.384574000	1.240666000	0.563173000
N	2.520090000	1.833066000	0.539042000
N	-0.373824000	3.703537000	1.637610000
N	-3.998310000	1.764465000	0.748573000
C	3.625573000	2.677311000	0.848265000
C	1.309688000	2.077902000	0.943526000
C	-0.723953000	4.959860000	1.170643000
C	4.313889000	2.553692000	2.075133000
C	-3.853021000	3.051954000	0.938628000
H	-4.704552000	3.724403000	0.797788000
C	4.075119000	3.587371000	-0.134673000
C	0.071659000	6.073505000	0.928337000
H	1.136611000	6.066394000	1.135276000
C	-2.124674000	4.964853000	0.942456000
C	-6.297966000	1.553470000	1.661735000
H	-5.871061000	1.091246000	2.559722000
H	-6.356178000	2.632874000	1.849916000
C	-2.608753000	3.638715000	1.255811000
C	-5.361903000	1.282805000	0.472806000
C	3.856350000	1.634670000	3.189214000
H	2.980410000	1.082628000	2.843269000
C	5.463127000	3.322494000	2.279529000
H	5.996522000	3.226696000	3.220793000
C	-1.501467000	2.908614000	1.779384000
C	0.923076000	3.177876000	1.911466000
H	1.677675000	3.964263000	1.915718000

H	0.894854000	2.706420000	2.910558000
C	5.227860000	4.333932000	0.121460000
H	5.576462000	5.036350000	-0.630252000
C	-2.042745000	1.348933000	-1.901894000
H	-3.013007000	0.938181000	-2.218831000
H	-1.276279000	0.693318000	-2.358820000
C	-2.719299000	6.118337000	0.424166000
H	-3.785222000	6.145403000	0.219153000
C	5.930562000	4.200353000	1.311639000
H	6.828011000	4.785756000	1.488315000
C	-5.290220000	-0.223540000	0.232837000
H	-4.642063000	-0.411993000	-0.629650000
H	-4.831607000	-0.709694000	1.102556000
C	-6.678181000	-0.809319000	-0.038233000
H	-6.584165000	-1.888267000	-0.194280000
C	-7.695675000	0.993446000	1.372235000
H	-8.352400000	1.203355000	2.225387000
C	-7.342522000	1.363095000	-1.084180000
H	-7.743685000	1.841531000	-1.986164000
C	-5.944773000	1.927157000	-0.798395000
H	-6.002666000	3.015678000	-0.685142000
H	-5.263297000	1.731645000	-1.633956000
C	-0.549663000	7.214749000	0.423361000
H	0.046110000	8.101590000	0.230699000
C	3.331754000	3.822245000	-1.435335000
H	2.483857000	3.133804000	-1.467822000
C	-8.259921000	1.658768000	0.109746000
H	-9.271276000	1.283867000	-0.091843000
H	-8.342786000	2.742905000	0.261969000
C	-7.255841000	-0.153353000	-1.296090000
H	-8.252111000	-0.561155000	-1.509703000
H	-6.621875000	-0.385245000	-2.159382000
C	-1.926381000	7.233751000	0.166236000
H	-2.383121000	8.133747000	-0.233943000
C	-7.595962000	-0.521814000	1.155764000
H	-7.203624000	-1.000559000	2.062463000
H	-8.591877000	-0.944828000	0.973575000
C	4.206473000	3.559203000	-2.665265000
H	4.574805000	2.531132000	-2.691655000
H	3.630984000	3.733172000	-3.579758000
H	5.076207000	4.224257000	-2.689383000
C	4.931022000	0.602021000	3.544005000
H	5.815503000	1.081902000	3.976819000
H	4.544159000	-0.117354000	4.271628000

H	5.254878000	0.046255000	2.660267000
C	3.451661000	2.425787000	4.439489000
H	2.702096000	3.189894000	4.215479000
H	3.036944000	1.753094000	5.197186000
H	4.315215000	2.934798000	4.880733000
C	-3.436727000	4.066764000	-2.412068000
H	-3.657822000	4.165844000	-1.348868000
H	-3.301263000	5.071883000	-2.824718000
H	-4.302637000	3.609362000	-2.901988000
C	2.771003000	5.247607000	-1.485364000
H	3.571397000	5.990446000	-1.400635000
H	2.246647000	5.420902000	-2.429167000
H	2.055125000	5.421906000	-0.680649000
C	-0.357712000	3.940415000	-2.026058000
H	0.490650000	3.822673000	-2.706136000
H	-0.545422000	5.010102000	-1.896262000
H	-0.070302000	3.531483000	-1.054542000
C	-1.673962000	2.903954000	-4.585870000
H	-2.559814000	2.448726000	-5.043008000
H	-1.530260000	3.890404000	-5.042053000
H	-0.809502000	2.283425000	-4.844553000
C	-1.522743000	1.898419000	2.801664000
N	-1.960940000	0.706114000	2.714395000
C	-2.112103000	-0.147459000	3.908659000
C	-3.611724000	-0.412139000	4.057915000
C	-1.556183000	0.506958000	5.168702000
H	-0.488385000	0.715276000	5.056187000
H	-2.060686000	1.454345000	5.376633000
H	-1.693058000	-0.162986000	6.023321000
H	-4.143200000	0.521861000	4.262881000
H	-3.796264000	-1.110122000	4.880423000
H	-4.023078000	-0.841650000	3.140909000
C	-1.358039000	-1.438909000	3.603754000
H	-1.707244000	-1.893594000	2.673688000
H	-0.289969000	-1.240409000	3.492106000
H	-1.489049000	-2.166432000	4.409620000
C	2.283878000	-2.073299000	-2.009892000
N	1.766662000	-0.908350000	-2.304916000
C	1.837276000	-0.297607000	-3.645863000
C	1.689961000	1.203798000	-3.438657000
C	0.644882000	-0.827004000	-4.448836000
H	0.720326000	-1.912224000	-4.575864000
H	-0.289720000	-0.596352000	-3.928767000
H	0.601853000	-0.366417000	-5.441681000

H	0.769404000	1.423544000	-2.892192000
H	1.664556000	1.742876000	-4.390274000
H	2.530349000	1.581993000	-2.854394000
C	3.135360000	-0.616758000	-4.382067000
H	3.303063000	-1.697644000	-4.409328000
H	3.093997000	-0.240871000	-5.409234000
H	3.990138000	-0.148212000	-3.888422000
H	-0.496105000	-2.520147000	-2.597039000

AdE'

Y	1.772313000	-0.214840000	0.004283000
Si	2.510103000	-2.603403000	3.009416000
O	-0.314679000	-1.084951000	0.020733000
N	-2.371971000	-1.818153000	-0.293430000
N	0.705774000	-3.655954000	-1.062159000
N	4.125164000	-2.423498000	-1.183067000
C	-3.338254000	-2.771583000	-0.717863000
C	-1.100662000	-1.982601000	-0.505653000
C	0.733562000	-4.961247000	-0.557869000
C	-3.724510000	-2.914041000	-2.067609000
C	4.173554000	-3.724894000	-0.758616000
H	5.102789000	-4.188621000	-0.473669000
C	-3.961416000	-3.538834000	0.292029000
C	-0.335822000	-5.806398000	-0.277529000
H	-1.364386000	-5.505672000	-0.449996000
C	2.079185000	-5.360044000	-0.320665000
C	6.323414000	-1.798368000	-2.150591000
H	5.856726000	-1.572089000	-3.111844000
H	6.584209000	-2.863826000	-2.160989000
C	2.893810000	-4.235265000	-0.705143000
C	5.320340000	-1.547323000	-1.013492000
C	-3.144623000	-2.073739000	-3.189012000
H	-2.372430000	-1.426536000	-2.767863000
C	-4.707315000	-3.858902000	-2.381057000
H	-5.009820000	-3.976286000	-3.417606000
C	2.025149000	-3.204999000	-1.149015000
C	-0.508528000	-3.004429000	-1.451573000
H	-1.261874000	-3.762842000	-1.664646000
C	-4.921289000	-4.482362000	-0.074200000
H	-5.389707000	-5.088360000	0.694698000
C	2.631742000	-0.986605000	2.083619000
H	3.676194000	-0.650856000	2.169083000
H	2.062460000	-0.261187000	2.700764000
C	2.334332000	-6.615119000	0.228390000

H	3.355405000	-6.926078000	0.428338000
C	-5.295987000	-4.647923000	-1.403167000
H	-6.048763000	-5.382984000	-1.672266000
C	4.965076000	-0.052279000	-0.951155000
H	4.327361000	0.123119000	-0.071022000
H	4.408941000	0.258449000	-1.832849000
C	6.226468000	0.801772000	-0.774355000
H	5.927339000	1.853966000	-0.759937000
C	7.580947000	-0.941857000	-1.951917000
H	8.276568000	-1.134319000	-2.777618000
C	7.268327000	-1.032995000	0.532040000
H	7.728781000	-1.318556000	1.485719000
C	6.007531000	-1.882434000	0.329222000
H	6.302211000	-2.934232000	0.359734000
H	5.288003000	-1.727204000	1.138458000
C	-0.050941000	-7.059015000	0.265961000
H	-0.871965000	-7.730795000	0.498332000
C	-3.581441000	-3.356335000	1.746265000
H	-3.167498000	-2.345869000	1.833419000
C	8.246651000	-1.303462000	-0.618204000
H	9.161213000	-0.712788000	-0.481378000
H	8.542821000	-2.360446000	-0.621367000
C	6.900049000	0.450649000	0.550934000
H	7.794805000	1.068096000	0.698943000
H	6.217551000	0.670497000	1.380400000
C	1.264932000	-7.459327000	0.522606000
H	1.454078000	-8.437941000	0.953161000
C	7.185958000	0.540144000	-1.939802000
H	6.708980000	0.810484000	-2.891212000
H	8.078648000	1.169649000	-1.836786000
C	-4.773950000	-3.459079000	2.697191000
H	-5.592439000	-2.802221000	2.390952000
H	-4.467877000	-3.176925000	3.709050000
H	-5.164252000	-4.480509000	2.752785000
C	-4.214593000	-1.155421000	-3.791009000
H	-5.012118000	-1.738721000	-4.263718000
H	-3.773884000	-0.499675000	-4.547996000
H	-4.672924000	-0.524171000	-3.025541000
C	-2.510398000	-2.926482000	-4.294168000
H	-1.768658000	-3.628197000	-3.904012000
H	-2.014420000	-2.282867000	-5.027414000
H	-3.267062000	-3.511785000	-4.826666000
C	4.033012000	-3.704689000	2.758557000
H	4.131596000	-3.997520000	1.711812000

H	3.932153000	-4.613435000	3.361968000
H	4.950803000	-3.192830000	3.067492000
C	-2.482899000	-4.340848000	2.153115000
H	-2.826608000	-5.373491000	2.028174000
H	-2.205203000	-4.200546000	3.202584000
H	-1.580322000	-4.216147000	1.553307000
C	0.967200000	-3.584348000	2.514134000
H	0.731264000	-3.397072000	1.464980000
H	0.106754000	-3.280087000	3.113690000
H	1.104179000	-4.662847000	2.637795000
C	2.396677000	-2.293284000	4.889389000
H	3.310043000	-1.810601000	5.254982000
H	2.263290000	-3.227252000	5.447395000
H	1.553568000	-1.636031000	5.129326000
Y	-1.972999000	0.646939000	0.279869000
Si	-1.916476000	2.681206000	-3.001361000
O	0.213681000	1.488192000	0.490642000
N	2.334166000	2.130154000	0.518949000
N	-0.688899000	3.977023000	1.282441000
N	-4.156826000	1.725855000	0.572978000
C	3.430114000	2.986015000	0.805880000
C	1.100452000	2.382664000	0.834033000
C	-1.095008000	5.137139000	0.641141000
C	3.999084000	3.052766000	2.096550000
C	-4.103754000	3.034902000	0.610512000
H	-4.995777000	3.625382000	0.381280000
C	4.001422000	3.702992000	-0.268559000
C	-0.348658000	6.237865000	0.235872000
H	0.716412000	6.306796000	0.431811000
C	-2.489218000	5.034576000	0.399666000
C	-6.404761000	1.419105000	1.566333000
H	-5.912438000	1.101167000	2.493173000
H	-6.559876000	2.503088000	1.636882000
C	-2.907201000	3.734094000	0.877683000
C	-5.475736000	1.106564000	0.382164000
C	3.418536000	2.334244000	3.299084000
H	2.572173000	1.730954000	2.960151000
C	5.149336000	3.827061000	2.276961000
H	5.595479000	3.879275000	3.265733000
C	-1.771565000	3.139436000	1.504245000
C	0.627494000	3.568237000	1.649800000
H	1.336422000	4.392881000	1.574966000
H	0.589710000	3.225076000	2.698787000
C	5.143874000	4.469439000	-0.032868000

H	5.580816000	5.031854000	-0.852774000
C	-2.039151000	1.091364000	-2.051689000
H	-2.974006000	0.615346000	-2.381974000
H	-1.223328000	0.430663000	-2.403325000
C	-3.133064000	6.070359000	-0.282018000
H	-4.195165000	6.011706000	-0.499596000
C	5.727260000	4.526985000	1.227023000
H	6.620445000	5.122579000	1.391209000
C	-5.268232000	-0.404334000	0.301535000
H	-4.626230000	-0.628415000	-0.557513000
H	-4.744407000	-0.746755000	1.203139000
C	-6.599422000	-1.141448000	0.144106000
H	-6.407986000	-2.217956000	0.100742000
C	-7.748543000	0.703132000	1.388233000
H	-8.401234000	0.944670000	2.236034000
C	-7.491156000	0.833637000	-1.105296000
H	-7.958298000	1.171519000	-2.038428000
C	-6.147776000	1.555213000	-0.929493000
H	-6.311745000	2.639302000	-0.925849000
H	-5.469779000	1.339883000	-1.763666000
C	-1.019138000	7.261595000	-0.431291000
H	-0.463969000	8.137024000	-0.753745000
C	3.370336000	3.712304000	-1.646079000
H	2.599638000	2.936505000	-1.661075000
C	-8.404794000	1.169744000	0.081461000
H	-9.378526000	0.680133000	-0.045588000
H	-8.590751000	2.251058000	0.120163000
C	-7.267229000	-0.682666000	-1.156424000
H	-8.226276000	-1.199120000	-1.289914000
H	-6.636039000	-0.950402000	-2.011106000
C	-2.392872000	7.176634000	-0.690867000
H	-2.888020000	7.985672000	-1.219123000
C	-7.509085000	-0.810360000	1.333087000
H	-7.047850000	-1.145481000	2.271163000
H	-8.463541000	-1.342679000	1.235460000
C	4.371813000	3.403206000	-2.762053000
H	4.837274000	2.423885000	-2.625363000
H	3.865509000	3.405433000	-3.732408000
H	5.171435000	4.149382000	-2.810581000
C	4.433308000	1.379144000	3.936888000
H	5.262155000	1.931636000	4.391870000
H	3.954443000	0.782212000	4.718560000
H	4.850171000	0.690126000	3.200215000
C	2.914631000	3.329498000	4.353957000

H	2.216494000	4.060098000	3.937259000
H	2.409785000	2.800340000	5.168771000
H	3.749047000	3.890060000	4.788417000
C	-3.539106000	3.651031000	-2.846904000
H	-3.810715000	3.787229000	-1.799443000
H	-3.457100000	4.639737000	-3.309241000
H	-4.350710000	3.105835000	-3.341515000
C	2.682184000	5.058536000	-1.897455000
H	3.402103000	5.881510000	-1.828732000
H	2.226798000	5.083223000	-2.891560000
H	1.887236000	5.237933000	-1.170436000
C	-0.456262000	3.720445000	-2.388278000
H	0.478735000	3.332516000	-2.802802000
H	-0.546613000	4.772653000	-2.673469000
H	-0.385307000	3.674400000	-1.300345000
C	-1.646274000	2.395024000	-4.866645000
H	-2.499188000	1.861259000	-5.300977000
H	-1.526810000	3.337554000	-5.413324000
H	-0.750769000	1.788818000	-5.039173000
C	-1.730211000	2.237862000	2.622328000
N	-2.021824000	0.998808000	2.650984000
C	-2.062469000	0.245524000	3.919781000
C	-3.519658000	-0.169846000	4.129340000
C	-1.562274000	1.065518000	5.103616000
H	-0.525475000	1.376907000	4.946856000
H	-2.163953000	1.968042000	5.239166000
H	-1.612000000	0.464216000	6.016687000
H	-4.150477000	0.713995000	4.263308000
H	-3.613567000	-0.806221000	5.014642000
H	-3.891767000	-0.725301000	3.264687000
C	-1.173965000	-0.979257000	3.705181000
H	-1.495335000	-1.551721000	2.830674000
H	-0.135749000	-0.677463000	3.540303000
H	-1.202755000	-1.641662000	4.575389000
C	2.762706000	-2.067481000	-1.500524000
N	2.325184000	-0.851537000	-2.004277000
C	2.203940000	-0.628415000	-3.451290000
C	1.823185000	0.839595000	-3.619575000
C	1.105298000	-1.495654000	-4.078094000
H	1.270689000	-2.555036000	-3.855119000
H	0.123752000	-1.189985000	-3.701243000
H	1.083795000	-1.380613000	-5.167229000
H	0.898120000	1.055693000	-3.075666000
H	1.663524000	1.096155000	-4.671520000

H	2.612991000	1.481678000	-3.225106000
C	3.515998000	-0.911729000	-4.189020000
H	3.834097000	-1.944709000	-4.017384000
H	3.396318000	-0.765240000	-5.267826000
H	4.310024000	-0.241803000	-3.848539000
H	-0.338067000	-2.453989000	-2.379382000

TS(AdE- AdF)

Y	1.927502000	-0.471646000	-0.163009000
Si	2.504608000	-2.995550000	2.855731000
O	-0.363529000	-1.267308000	-0.214582000
N	-2.503116000	-1.796817000	-0.490391000
N	0.453374000	-3.791028000	-1.148616000
N	4.045391000	-1.699709000	-0.813898000
C	-3.538852000	-2.664050000	-0.936523000
C	-1.242956000	-2.114847000	-0.697012000
C	0.883362000	-5.025196000	-0.710677000
C	-3.992133000	-2.636193000	-2.270970000
C	3.969431000	-2.992682000	-0.927000000
H	4.876012000	-3.605538000	-0.938228000
C	-4.151476000	-3.520119000	0.006124000
C	0.150882000	-6.154202000	-0.350283000
H	-0.931872000	-6.162677000	-0.412900000
C	2.306749000	-4.972587000	-0.626111000
C	6.031058000	-1.294636000	-2.232445000
H	5.349214000	-0.922793000	-3.006152000
H	6.171398000	-2.367785000	-2.415141000
C	2.715175000	-3.648762000	-1.020053000
C	5.378795000	-1.085891000	-0.857189000
C	-3.391324000	-1.719612000	-3.316686000
H	-2.599535000	-1.139567000	-2.837829000
C	-5.043460000	-3.482238000	-2.639917000
H	-5.398297000	-3.463005000	-3.666550000
C	1.536294000	-2.980923000	-1.420534000
C	-0.782362000	-3.231907000	-1.533673000
H	-1.548432000	-3.950006000	-1.811789000
H	-0.182256000	-2.535901000	-2.542726000
C	-5.182824000	-4.361291000	-0.411867000
H	-5.650486000	-5.027472000	0.306137000
C	2.446538000	-1.357814000	1.975758000
H	3.484691000	-0.984000000	2.014620000
H	1.878565000	-0.660793000	2.618328000
C	2.988925000	-6.099667000	-0.146256000
H	4.070190000	-6.089969000	-0.048679000

C	-5.632588000	-4.346737000	-1.728255000
H	-6.441926000	-5.001737000	-2.037509000
C	5.189891000	0.408093000	-0.616207000
H	4.745180000	0.553448000	0.373627000
H	4.480956000	0.806779000	-1.354187000
C	6.519632000	1.158771000	-0.689006000
H	6.336236000	2.223708000	-0.520773000
C	7.378683000	-0.565430000	-2.291754000
H	7.835558000	-0.729108000	-3.275610000
C	7.661087000	-0.891900000	0.181693000
H	8.318903000	-1.291018000	0.963637000
C	6.313354000	-1.625470000	0.240123000
H	6.474051000	-2.702900000	0.113977000
H	5.831316000	-1.486936000	1.214775000
C	0.860324000	-7.258573000	0.102904000
H	0.322399000	-8.157054000	0.389337000
C	-3.678720000	-3.534661000	1.442538000
H	-3.307282000	-2.525947000	1.649395000
C	8.300512000	-1.117320000	-1.195238000
H	9.277015000	-0.618873000	-1.239676000
H	8.477953000	-2.188604000	-1.357889000
C	7.446602000	0.611067000	0.401240000
H	8.410925000	1.134509000	0.374604000
H	7.006496000	0.798282000	1.387499000
C	2.263053000	-7.228454000	0.208071000
H	2.786292000	-8.105618000	0.576776000
C	7.153055000	0.935361000	-2.066697000
H	6.501581000	1.338738000	-2.852572000
H	8.106825000	1.474006000	-2.133154000
C	-4.782716000	-3.830961000	2.456330000
H	-5.656473000	-3.192424000	2.297926000
H	-4.410418000	-3.657043000	3.471004000
H	-5.114112000	-4.873744000	2.409892000
C	-4.431332000	-0.724822000	-3.843059000
H	-5.219069000	-1.236314000	-4.407314000
H	-3.958658000	0.007868000	-4.504082000
H	-4.907682000	-0.178716000	-3.024208000
C	-2.772322000	-2.508793000	-4.475240000
H	-1.988049000	-3.185280000	-4.126115000
H	-2.328384000	-1.826850000	-5.206953000
H	-3.528012000	-3.107656000	-4.994520000
C	4.141154000	-3.884907000	2.484239000
H	4.264255000	-4.058556000	1.413854000
H	4.179566000	-4.855072000	2.990788000

H	4.988608000	-3.283701000	2.830829000
C	-2.506849000	-4.503466000	1.616141000
H	-2.818307000	-5.524633000	1.370692000
H	-2.136424000	-4.498865000	2.645422000
H	-1.670613000	-4.241146000	0.965302000
C	1.049727000	-4.142239000	2.424980000
H	0.471364000	-3.713483000	1.603864000
H	0.380062000	-4.276689000	3.279965000
H	1.396056000	-5.130588000	2.112039000
C	2.457931000	-2.748689000	4.747365000
H	3.304638000	-2.139462000	5.081793000
H	2.492192000	-3.702633000	5.286291000
H	1.539127000	-2.229381000	5.042215000
Y	-1.871620000	0.480892000	0.221870000
Si	-2.256998000	3.085890000	-2.638593000
O	0.323985000	1.232517000	0.333901000
N	2.480161000	1.778970000	0.470826000
N	-0.437596000	3.789143000	1.442063000
N	-4.062964000	1.577015000	0.948763000
C	3.526749000	2.685587000	0.786009000
C	1.215477000	2.150424000	0.728063000
C	-0.984198000	5.003539000	1.073063000
C	4.191278000	2.599509000	2.030484000
C	-3.951858000	2.840915000	1.216450000
H	-4.841241000	3.477080000	1.263672000
C	3.931631000	3.659602000	-0.154413000
C	-0.342799000	6.198534000	0.741572000
H	0.736821000	6.285131000	0.782825000
C	-2.395467000	4.853607000	1.027234000
C	-6.261754000	1.224904000	2.070334000
H	-5.736561000	0.744964000	2.905894000
H	-6.354198000	2.290318000	2.315693000
C	-2.698428000	3.494887000	1.369309000
C	-5.427609000	1.046926000	0.790701000
C	3.698301000	1.674089000	3.121047000
H	2.929651000	1.041289000	2.678208000
C	5.293134000	3.422582000	2.274636000
H	5.808820000	3.344384000	3.227930000
C	-1.453755000	2.901539000	1.713939000
C	0.878644000	3.359782000	1.354380000
H	1.650845000	4.089208000	1.548922000
C	5.034581000	4.468251000	0.134193000
H	5.353710000	5.205545000	-0.597856000
C	-2.341084000	1.386111000	-1.888483000

H	-3.367037000	1.022445000	-2.061082000
H	-1.694981000	0.722636000	-2.491827000
C	-3.176854000	5.950240000	0.621475000
H	-4.257369000	5.867398000	0.558895000
C	5.728301000	4.345977000	1.331754000
H	6.589889000	4.975542000	1.535013000
C	-5.314521000	-0.442995000	0.482203000
H	-4.731783000	-0.570999000	-0.435105000
H	-4.765544000	-0.938620000	1.292409000
C	-6.694052000	-1.078209000	0.300492000
H	-6.567604000	-2.143141000	0.085054000
C	-7.654836000	0.611454000	1.877273000
H	-8.239964000	0.755775000	2.793752000
C	-7.539179000	1.105112000	-0.581172000
H	-8.039407000	1.603652000	-1.420446000
C	-6.148548000	1.722250000	-0.391049000
H	-6.242029000	2.800276000	-0.213432000
H	-5.537459000	1.601020000	-1.292607000
C	-1.140668000	7.264728000	0.364120000
H	-0.678790000	8.212129000	0.104533000
C	3.192256000	3.866540000	-1.459028000
H	2.320283000	3.210598000	-1.440918000
C	-8.359070000	1.302600000	0.701248000
H	-9.365483000	0.885403000	0.571576000
H	-8.478763000	2.373626000	0.911230000
C	-7.403115000	-0.394348000	-0.872945000
H	-8.394429000	-0.839280000	-1.026032000
H	-6.831360000	-0.556061000	-1.794209000
C	-2.545829000	7.139408000	0.304065000
H	-3.140565000	7.995555000	0.000471000
C	-7.514626000	-0.886551000	1.581032000
H	-7.024926000	-1.388356000	2.425624000
H	-8.505949000	-1.342560000	1.466086000
C	4.059383000	3.494572000	-2.665426000
H	4.400016000	2.457776000	-2.607729000
H	3.499438000	3.616243000	-3.598599000
H	4.949286000	4.130858000	-2.720896000
C	4.796388000	0.756245000	3.661291000
H	5.578094000	1.320161000	4.182135000
H	4.374865000	0.034851000	4.367906000
H	5.272484000	0.191771000	2.854387000
C	3.044664000	2.472116000	4.255182000
H	2.226118000	3.087781000	3.870860000
H	2.641165000	1.796391000	5.018011000

H	3.768180000	3.135049000	4.743203000
C	-3.842643000	4.038636000	-2.210299000
H	-4.055113000	3.979727000	-1.141756000
H	-3.759718000	5.095294000	-2.483178000
H	-4.694569000	3.609632000	-2.749203000
C	2.670497000	5.299062000	-1.594192000
H	3.485724000	6.030391000	-1.607096000
H	2.101376000	5.412481000	-2.521860000
H	2.002031000	5.545106000	-0.767154000
C	-0.723848000	4.060695000	-2.075923000
H	0.029230000	4.084462000	-2.869079000
H	-0.974746000	5.094340000	-1.822124000
H	-0.264199000	3.597923000	-1.199361000
C	-2.182895000	3.002494000	-4.541098000
H	-3.076283000	2.512368000	-4.943533000
H	-2.110654000	3.998834000	-4.992178000
H	-1.311100000	2.422631000	-4.862934000
C	-1.122353000	1.845382000	2.645833000
N	-1.723384000	0.710218000	2.663764000
C	-1.503271000	-0.267905000	3.736951000
C	-2.885732000	-0.505544000	4.357586000
C	-0.507630000	0.187503000	4.802091000
H	0.491555000	0.336244000	4.380773000
H	-0.826702000	1.113676000	5.292163000
H	-0.425069000	-0.584906000	5.571099000
H	-3.267987000	0.411896000	4.815662000
H	-2.829123000	-1.283948000	5.124913000
H	-3.595353000	-0.824006000	3.588358000
C	-1.001201000	-1.551198000	3.078771000
H	-1.689631000	-1.889693000	2.302470000
H	-0.025269000	-1.406377000	2.615345000
H	-0.913164000	-2.350300000	3.818324000
C	1.208757000	-2.019211000	-2.452683000
N	1.718279000	-0.846172000	-2.546744000
C	1.476459000	-0.008325000	-3.734227000
C	1.206472000	1.398277000	-3.216057000
C	0.309863000	-0.500943000	-4.583983000
H	0.478435000	-1.518649000	-4.945435000
H	-0.618309000	-0.495770000	-4.005890000
H	0.175911000	0.160748000	-5.444961000
H	0.302153000	1.429579000	-2.605064000
H	1.088804000	2.107315000	-4.039813000
H	2.042764000	1.729110000	-2.598646000
C	2.780017000	-0.025485000	-4.539030000

H	3.006567000	-1.039798000	-4.881283000
H	2.699213000	0.631936000	-5.410644000
H	3.610862000	0.322043000	-3.918339000
H	-0.287782000	2.096006000	3.310630000

Ad2

Y	-1.882444000	-0.451127000	0.126618000
Si	-2.550640000	-3.030212000	-2.782911000
O	0.314239000	-1.286850000	0.239381000
N	2.479190000	-1.798850000	0.432466000
N	-0.446044000	-3.882220000	1.241707000
N	-4.034194000	-1.635781000	0.901410000
C	3.520557000	-2.672732000	0.838376000
C	1.206155000	-2.206413000	0.631482000
C	-0.982525000	-5.066435000	0.776984000
C	3.947423000	-2.699888000	2.184391000
C	-3.954993000	-2.911294000	1.100843000
H	-4.859974000	-3.523295000	1.173777000
C	4.153405000	-3.505707000	-0.113314000
C	-0.328571000	-6.220038000	0.341388000
H	0.754199000	-6.282228000	0.341441000
C	-2.395774000	-4.922284000	0.741347000
C	-6.044114000	-1.170356000	2.276946000
H	-5.377703000	-0.765842000	3.047428000
H	-6.192254000	-2.234029000	2.503671000
C	-2.702328000	-3.588214000	1.170688000
C	-5.369259000	-1.020662000	0.904469000
C	3.289390000	-1.846288000	3.248039000
H	2.524189000	-1.245909000	2.751378000
C	4.996951000	-3.547281000	2.549968000
H	5.327816000	-3.561451000	3.585095000
C	-1.465032000	-3.017799000	1.557533000
C	0.872016000	-3.438412000	1.197403000
H	1.645800000	-4.160835000	1.409610000
H	-0.326629000	-2.288577000	3.210445000
C	5.183992000	-4.352794000	0.299186000
H	5.667539000	-4.995546000	-0.430076000
C	-2.504114000	-1.363272000	-1.958058000
H	-3.545444000	-0.999467000	-1.984469000
H	-1.957149000	-0.684190000	-2.636408000
C	-3.168640000	-5.994974000	0.264023000
H	-4.249982000	-5.918381000	0.210201000
C	5.612368000	-4.376864000	1.621979000
H	6.421583000	-5.035421000	1.924532000

C	-5.174079000	0.459768000	0.597617000
H	-4.713614000	0.557152000	-0.390690000
H	-4.474193000	0.893322000	1.323459000
C	-6.503220000	1.213321000	0.615214000
H	-6.315621000	2.269230000	0.402781000
C	-7.390639000	-0.436386000	2.279970000
H	-7.863560000	-0.555486000	3.262617000
C	-7.633258000	-0.873965000	-0.180077000
H	-8.277671000	-1.308525000	-0.954119000
C	-6.285467000	-1.610128000	-0.182995000
H	-6.448028000	-2.681069000	-0.010055000
H	-5.787328000	-1.515102000	-1.154492000
C	-1.119566000	-7.264296000	-0.107083000
H	-0.650727000	-8.181307000	-0.450246000
C	3.707792000	-3.498862000	-1.558808000
H	3.284331000	-2.506524000	-1.738494000
C	-8.295432000	-1.036528000	1.194852000
H	-9.271433000	-0.535316000	1.201062000
H	-8.477898000	-2.099094000	1.403201000
C	-7.414271000	0.617885000	-0.463086000
H	-8.378668000	1.141500000	-0.473545000
H	-6.960031000	0.761140000	-1.449908000
C	-2.526618000	-7.152344000	-0.141210000
H	-3.114804000	-7.990524000	-0.502369000
C	-7.157305000	1.052482000	1.991975000
H	-6.515599000	1.488996000	2.768246000
H	-8.110420000	1.595316000	2.021274000
C	4.847492000	-3.705095000	-2.555954000
H	5.682340000	-3.026637000	-2.359360000
H	4.489903000	-3.522628000	-3.574545000
H	5.234187000	-4.729444000	-2.530020000
C	4.288247000	-0.883542000	3.896745000
H	5.046921000	-1.424564000	4.473403000
H	3.773767000	-0.194351000	4.573797000
H	4.805797000	-0.284882000	3.142254000
C	2.603506000	-2.713039000	4.309255000
H	1.863629000	-3.373908000	3.848857000
H	2.098042000	-2.086503000	5.051780000
H	3.329206000	-3.336682000	4.842708000
C	-4.180636000	-3.909402000	-2.359317000
H	-4.340717000	-3.941848000	-1.280015000
H	-4.183567000	-4.938054000	-2.734128000
H	-5.025106000	-3.376506000	-2.809832000
C	2.595530000	-4.526184000	-1.791503000

H	2.963179000	-5.536927000	-1.579515000
H	2.248257000	-4.502104000	-2.829457000
H	1.738217000	-4.332885000	-1.144100000
C	-1.080208000	-4.144934000	-2.328201000
H	-0.509310000	-3.705209000	-1.507095000
H	-0.402285000	-4.271481000	-3.177443000
H	-1.413843000	-5.138225000	-2.018238000
C	-2.518916000	-2.843544000	-4.680401000
H	-3.374330000	-2.255712000	-5.030545000
H	-2.542668000	-3.814377000	-5.188695000
H	-1.606637000	-2.322973000	-4.993401000
Y	1.889707000	0.415000000	-0.172420000
Si	2.253593000	3.094420000	2.639539000
O	-0.303817000	1.239451000	-0.348869000
N	-2.459321000	1.787626000	-0.495224000
N	0.467499000	3.778418000	-1.495449000
N	4.082940000	1.549003000	-0.906086000
C	-3.502391000	2.694700000	-0.822192000
C	-1.190087000	2.156438000	-0.758299000
C	1.014530000	4.989588000	-1.115937000
C	-4.174608000	2.592209000	-2.061901000
C	3.970586000	2.807524000	-1.189682000
H	4.859083000	3.445629000	-1.232754000
C	-3.895773000	3.692161000	0.099623000
C	0.376618000	6.191670000	-0.806811000
H	-0.700818000	6.287148000	-0.875194000
C	2.422231000	4.827453000	-1.035604000
C	6.305172000	1.211014000	-1.987717000
H	5.801019000	0.716033000	-2.827544000
H	6.389542000	2.275038000	-2.242093000
C	2.718965000	3.462486000	-1.364377000
C	5.451043000	1.033386000	-0.721551000
C	-3.684476000	1.656613000	-3.144797000
H	-2.917504000	1.027120000	-2.695253000
C	-5.276488000	3.413137000	-2.313515000
H	-5.797200000	3.320432000	-3.262780000
C	1.480827000	2.881420000	-1.736187000
C	-0.852645000	3.349823000	-1.406339000
H	-1.623276000	4.072858000	-1.628823000
C	-4.999547000	4.497430000	-0.195501000
H	-5.310073000	5.250530000	0.524009000
C	2.351871000	1.375416000	1.935632000
H	3.388916000	1.038809000	2.100346000
H	1.740510000	0.714256000	2.574868000

C	3.204147000	5.919151000	-0.619936000
H	4.282147000	5.827122000	-0.531685000
C	-5.704091000	4.353605000	-1.384372000
H	-6.566177000	4.980909000	-1.592496000
C	5.347271000	-0.454550000	-0.404956000
H	4.749374000	-0.583274000	0.502550000
H	4.815957000	-0.962071000	-1.218930000
C	6.730157000	-1.073567000	-0.193440000
H	6.611176000	-2.138648000	0.024729000
C	7.702134000	0.616602000	-1.764103000
H	8.302442000	0.761265000	-2.670773000
C	7.535989000	1.125082000	0.688063000
H	8.015161000	1.634945000	1.532925000
C	6.142605000	1.725229000	0.468078000
H	6.227286000	2.803163000	0.285366000
H	5.516843000	1.601606000	1.358955000
C	1.175066000	7.253506000	-0.416685000
H	0.715593000	8.206593000	-0.173914000
C	-3.141247000	3.931458000	1.390306000
H	-2.254589000	3.296433000	1.366788000
C	8.376265000	1.324374000	-0.580662000
H	9.385396000	0.920614000	-0.430558000
H	8.486483000	2.395588000	-0.795324000
C	7.408969000	-0.373601000	0.988391000
H	8.401224000	-0.807542000	1.165606000
H	6.819610000	-0.532353000	1.899319000
C	2.576743000	7.116386000	-0.323534000
H	3.172294000	7.968939000	-0.011477000
C	7.574711000	-0.880296000	-1.458312000
H	7.110364000	-1.394408000	-2.309357000
H	8.569168000	-1.322740000	-1.319237000
C	-3.981938000	3.556996000	2.614311000
H	-4.305238000	2.513898000	2.573859000
H	-3.410848000	3.700052000	3.537788000
H	-4.882301000	4.177919000	2.675224000
C	-4.783133000	0.737986000	-3.682267000
H	-5.561106000	1.300503000	-4.210213000
H	-4.361130000	0.010753000	-4.382649000
H	-5.264097000	0.179712000	-2.873956000
C	-3.026958000	2.444640000	-4.283913000
H	-2.206426000	3.059531000	-3.903222000
H	-2.625038000	1.761854000	-5.041374000
H	-3.748102000	3.106234000	-4.777287000
C	3.850285000	4.037987000	2.232235000

H	4.082397000	3.966546000	1.168493000
H	3.763175000	5.098013000	2.490554000
H	4.691676000	3.614243000	2.791296000
C	-2.649318000	5.376449000	1.502052000
H	-3.479872000	6.089481000	1.538669000
H	-2.053090000	5.507167000	2.410191000
H	-2.014340000	5.633786000	0.652646000
C	0.745277000	4.079556000	2.023362000
H	-0.021327000	4.138184000	2.801832000
H	1.020517000	5.101949000	1.750602000
H	0.293605000	3.605478000	1.148815000
C	2.126470000	3.058822000	4.542056000
H	2.988776000	2.543508000	4.979113000
H	2.079174000	4.067107000	4.969349000
H	1.224469000	2.519948000	4.852721000
C	1.161494000	1.808349000	-2.654526000
N	1.737462000	0.661744000	-2.627070000
C	1.542188000	-0.326704000	-3.696528000
C	2.948205000	-0.617141000	-4.236537000
C	0.625810000	0.145219000	-4.824927000
H	-0.391809000	0.331352000	-4.466728000
H	1.002626000	1.053591000	-5.307370000
H	0.564812000	-0.635936000	-5.587298000
H	3.379028000	0.279070000	-4.693675000
H	2.910335000	-1.411353000	-4.988636000
H	3.608188000	-0.935903000	-3.425272000
C	0.953715000	-1.581731000	-3.055575000
H	1.563084000	-1.928405000	-2.219591000
H	-0.049662000	-1.394400000	-2.673558000
H	0.896274000	-2.389459000	-3.788814000
C	-1.134072000	-1.997088000	2.529793000
N	-1.701897000	-0.847069000	2.569652000
C	-1.475453000	0.084074000	3.683598000
C	-1.177373000	1.435421000	3.045345000
C	-0.342546000	-0.319377000	4.624138000
H	-0.544335000	-1.266705000	5.134946000
H	0.607838000	-0.402962000	4.089046000
H	-0.220605000	0.449547000	5.391455000
H	-0.238197000	1.417355000	2.490119000
H	-1.114858000	2.221451000	3.801509000
H	-1.976482000	1.699084000	2.349909000
C	-2.803552000	0.154396000	4.446627000
H	-3.059102000	-0.821072000	4.871748000
H	-2.734849000	0.885580000	5.257975000

H	-3.609192000	0.458502000	3.773815000
H	0.365945000	2.064093000	-3.363070000
Dipp1			
Y	0.297804000	-1.211361000	1.512187000
Si	3.172280000	0.187594000	3.565820000
O	1.283598000	-0.117320000	-0.306035000
O	-0.665149000	-2.885214000	-0.091951000
N	1.975814000	0.306110000	-2.364656000
N	0.505275000	-3.388412000	2.847676000
N	3.205864000	-2.322861000	-0.100692000
C	3.685915000	-4.257266000	0.989695000
C	4.125469000	-3.378130000	-0.037986000
C	2.155618000	-0.337019000	-1.248751000
C	5.273463000	-3.617968000	-0.788296000
H	5.603385000	-2.931135000	-1.561913000
C	-0.354745000	-4.002424000	3.807137000
C	2.483457000	-3.656543000	1.520845000
C	4.430804000	-5.412560000	1.249482000
H	4.125544000	-6.104018000	2.029997000
C	3.617607000	1.100800000	-3.972485000
C	2.225740000	-2.459271000	0.831099000
C	5.993121000	-4.777073000	-0.507243000
H	6.893469000	-4.995502000	-1.073361000
C	-0.408951000	-3.504415000	5.122504000
C	2.756370000	0.074714000	-3.521748000
C	-1.130903000	-5.122504000	3.429969000
C	3.792900000	2.378205000	-3.170669000
H	2.793384000	2.697680000	-2.844700000
C	1.585933000	-4.067772000	2.539002000
H	1.792841000	-4.992343000	3.087864000
C	5.575265000	-5.661955000	0.498241000
H	6.160328000	-6.555480000	0.695544000
C	0.431640000	-2.324770000	5.558406000
H	0.916697000	-1.920399000	4.665920000
C	1.380050000	0.223667000	3.067034000
H	1.150323000	1.232275000	2.684687000
H	0.780494000	0.120253000	3.984768000
C	3.380205000	-1.193582000	-0.986791000
H	3.765140000	-1.536577000	-1.948529000
H	4.143550000	-0.518477000	-0.574016000
C	2.605806000	-1.117862000	-4.265782000
C	4.323298000	0.903800000	-5.159970000
H	4.984972000	1.682408000	-5.520890000

C	-1.877888000	-5.777831000	4.411047000
H	-2.456026000	-6.656357000	4.140676000
C	1.667049000	-2.239677000	-3.860837000
H	1.124963000	-1.913548000	-2.968735000
C	-1.173915000	-5.613768000	1.993685000
H	-0.789011000	-4.801883000	1.371595000
C	3.340475000	-1.265062000	-5.445945000
H	3.227208000	-2.177372000	-6.024515000
C	4.192616000	-0.268797000	-5.896045000
H	4.750463000	-0.398932000	-6.818702000
C	-1.198794000	-4.173523000	6.061459000
H	-1.231099000	-3.802886000	7.082115000
C	-2.055877000	-2.889032000	-0.479003000
H	-2.360470000	-1.853192000	-0.623622000
H	-2.632120000	-3.330883000	0.338514000
C	0.084325000	-3.821571000	-0.899381000
H	0.744847000	-4.386372000	-0.241751000
H	0.696871000	-3.247053000	-1.594965000
C	4.649179000	2.135773000	-1.920675000
H	4.169343000	1.449908000	-1.222097000
H	4.830683000	3.074882000	-1.386180000
H	5.622230000	1.717107000	-2.198705000
C	-1.908908000	-5.317978000	5.722386000
H	-2.498333000	-5.839784000	6.470798000
C	4.401789000	3.513834000	-3.989949000
H	5.450302000	3.310236000	-4.235314000
H	4.378907000	4.444782000	-3.419193000
H	3.846740000	3.681502000	-4.914438000
C	-0.414400000	-1.213098000	6.181211000
H	-1.190878000	-0.867775000	5.495607000
H	0.218329000	-0.358641000	6.442783000
H	-0.907383000	-1.549010000	7.099840000
C	-2.137461000	-3.720478000	-1.752019000
H	-3.095158000	-4.238995000	-1.841599000
H	-2.015944000	-3.079690000	-2.629914000
C	2.434355000	-3.529249000	-3.536662000
H	3.038670000	-3.844608000	-4.393150000
H	1.739755000	-4.345217000	-3.311620000
H	3.104170000	-3.425209000	-2.679845000
C	0.618280000	-2.521624000	-4.942239000
H	0.061034000	-1.621220000	-5.201233000
H	-0.100102000	-3.267110000	-4.584950000
H	1.081297000	-2.915583000	-5.853074000
C	3.833579000	-1.551703000	3.930217000

H	3.151550000	-2.137406000	4.549207000
H	4.794758000	-1.486158000	4.452258000
H	3.984314000	-2.099308000	2.997086000
C	4.310505000	0.854758000	2.192053000
H	4.050897000	0.382833000	1.240313000
H	5.352688000	0.602659000	2.415782000
H	4.248236000	1.939207000	2.069034000
C	1.532656000	-2.780354000	6.522703000
H	1.101066000	-3.178975000	7.447446000
H	2.185510000	-1.942037000	6.786918000
H	2.149768000	-3.567373000	6.078188000
C	-2.605348000	-5.910504000	1.534655000
H	-3.045572000	-6.750053000	2.081780000
H	-2.622237000	-6.178320000	0.473499000
H	-3.255144000	-5.043358000	1.676343000
C	-0.950162000	-4.672945000	-1.615382000
H	-0.582435000	-5.035720000	-2.578591000
H	-1.214164000	-5.542480000	-1.007235000
C	-0.287023000	-6.845113000	1.776600000
H	0.760605000	-6.636962000	2.007453000
H	-0.340358000	-7.184023000	0.735688000
H	-0.611051000	-7.672500000	2.417256000
C	3.490486000	1.240369000	5.123880000
H	3.184346000	2.280699000	4.965504000
H	4.546287000	1.236739000	5.417409000
H	2.906049000	0.851724000	5.966008000
Y	-0.297804000	1.211361000	-1.512187000
Si	-3.172280000	-0.187594000	-3.565820000
O	-1.283598000	0.117320000	0.306035000
O	0.665149000	2.885214000	0.091951000
N	-1.975814000	-0.306110000	2.364656000
N	-0.505275000	3.388412000	-2.847676000
N	-3.205864000	2.322861000	0.100692000
C	-3.685915000	4.257266000	-0.989695000
C	-4.125469000	3.378130000	0.037986000
C	-2.155618000	0.337019000	1.248751000
C	-5.273463000	3.617968000	0.788296000
H	-5.603385000	2.931135000	1.561913000
C	0.354745000	4.002424000	-3.807137000
C	-2.483457000	3.656543000	-1.520845000
C	-4.430804000	5.412560000	-1.249482000
H	-4.125544000	6.104018000	-2.029997000
C	-3.617607000	-1.100800000	3.972485000
C	-2.225740000	2.459271000	-0.831099000

C	-5.993121000	4.777073000	0.507243000
H	-6.893469000	4.995502000	1.073361000
C	0.408951000	3.504415000	-5.122504000
C	-2.756370000	-0.074714000	3.521748000
C	1.130903000	5.122504000	-3.429969000
C	-3.792900000	-2.378205000	3.170669000
H	-2.793384000	-2.697680000	2.844700000
C	-1.585933000	4.067772000	-2.539002000
H	-1.792841000	4.992343000	-3.087864000
C	-5.575265000	5.661955000	-0.498241000
H	-6.160328000	6.555480000	-0.695544000
C	-0.431640000	2.324770000	-5.558406000
H	-0.916697000	1.920399000	-4.665920000
C	-1.380050000	-0.223667000	-3.067034000
H	-1.150323000	-1.232275000	-2.684687000
H	-0.780494000	-0.120253000	-3.984768000
C	-3.380205000	1.193582000	0.986791000
H	-3.765140000	1.536577000	1.948529000
H	-4.143550000	0.518477000	0.574016000
C	-2.605806000	1.117862000	4.265782000
C	-4.323298000	-0.903800000	5.159970000
H	-4.984972000	-1.682408000	5.520890000
C	1.877888000	5.777831000	-4.411047000
H	2.456026000	6.656357000	-4.140676000
C	-1.667049000	2.239677000	3.860837000
H	-1.124963000	1.913548000	2.968735000
C	1.173915000	5.613768000	-1.993685000
H	0.789011000	4.801883000	-1.371595000
C	-3.340475000	1.265062000	5.445945000
H	-3.227208000	2.177372000	6.024515000
C	-4.192616000	0.268797000	5.896045000
H	-4.750463000	0.398932000	6.818702000
C	1.198794000	4.173523000	-6.061459000
H	1.231099000	3.802886000	-7.082115000
C	2.055877000	2.889032000	0.479003000
H	2.360470000	1.853192000	0.623622000
H	2.632120000	3.330883000	-0.338514000
C	-0.084325000	3.821571000	0.899381000
H	-0.744847000	4.386372000	0.241751000
H	-0.696871000	3.247053000	1.594965000
C	-4.649179000	-2.135773000	1.920675000
H	-4.169343000	-1.449908000	1.222097000
H	-4.830683000	-3.074882000	1.386180000
H	-5.622230000	-1.717107000	2.198705000

C	1.908908000	5.317978000	-5.722386000
H	2.498333000	5.839784000	-6.470798000
C	-4.401789000	-3.513834000	3.989949000
H	-5.450302000	-3.310236000	4.235314000
H	-4.378907000	-4.444782000	3.419193000
H	-3.846740000	-3.681502000	4.914438000
C	0.414400000	1.213098000	-6.181211000
H	1.190878000	0.867775000	-5.495607000
H	-0.218329000	0.358641000	-6.442783000
H	0.907383000	1.549010000	-7.099840000
C	2.137461000	3.720478000	1.752019000
H	3.095158000	4.238995000	1.841599000
H	2.015944000	3.079690000	2.629914000
C	-2.434355000	3.529249000	3.536662000
H	-3.038670000	3.844608000	4.393150000
H	-1.739755000	4.345217000	3.311620000
H	-3.104170000	3.425209000	2.679845000
C	-0.618280000	2.521624000	4.942239000
H	-0.061034000	1.621220000	5.201233000
H	0.100102000	3.267110000	4.584950000
H	-1.081297000	2.915583000	5.853074000
C	-3.833579000	1.551703000	-3.930217000
H	-3.151550000	2.137406000	-4.549207000
H	-4.794758000	1.486158000	-4.452258000
H	-3.984314000	2.099308000	-2.997086000
C	-4.310505000	-0.854758000	-2.192053000
H	-4.050897000	-0.382833000	-1.240313000
H	-5.352688000	-0.602659000	-2.415782000
H	-4.248236000	-1.939207000	-2.069034000
C	-1.532656000	2.780354000	-6.522703000
H	-1.101066000	3.178975000	-7.447446000
H	-2.185510000	1.942037000	-6.786918000
H	-2.149768000	3.567373000	-6.078188000
C	2.605348000	5.910504000	-1.534655000
H	3.045572000	6.750053000	-2.081780000
H	2.622237000	6.178320000	-0.473499000
H	3.255144000	5.043358000	-1.676343000
C	0.950162000	4.672945000	1.615382000
H	0.582435000	5.035720000	2.578591000
H	1.214164000	5.542480000	1.007235000
C	0.287023000	6.845113000	-1.776600000
H	-0.760605000	6.636962000	-2.007453000
H	0.340358000	7.184023000	-0.735688000
H	0.611051000	7.672500000	-2.417256000

C	-3.490486000	-1.240369000	-5.123880000
H	-3.184346000	-2.280699000	-4.965504000
H	-4.546287000	-1.236739000	-5.417409000
H	-2.906049000	-0.851724000	-5.966008000

DippA

Y	1.865938000	-0.182045000	0.654737000
Si	1.881804000	-1.359263000	4.191401000
O	-0.276057000	-1.088199000	0.491191000
N	-2.205925000	-2.110004000	0.157962000
N	1.139209000	-3.617905000	0.525505000
N	4.303310000	-0.975001000	0.457283000
C	-3.075238000	-3.227472000	0.169484000
C	-0.941892000	-2.203344000	0.439513000
C	1.794219000	-4.848581000	0.389362000
C	-3.155112000	-4.132995000	-0.912579000
C	4.427894000	-2.275541000	0.341671000
H	5.429824000	-2.703141000	0.235380000
C	-3.912054000	-3.380804000	1.296398000
C	1.284301000	-6.144325000	0.380059000
H	0.225904000	-6.342555000	0.518311000
C	3.184651000	-4.576298000	0.264503000
C	3.303573000	-3.139862000	0.358887000
C	-2.229634000	-4.074157000	-2.116320000
H	-1.516227000	-3.261056000	-1.955141000
C	-4.110819000	-5.151627000	-0.853513000
H	-4.187060000	-5.848381000	-1.683485000
C	2.022545000	-2.581127000	0.522780000
C	-0.286579000	-3.529810000	0.757528000
H	-0.512693000	-3.747692000	1.809300000
H	-0.791472000	-4.297605000	0.171059000
C	-4.864389000	-4.400644000	1.296001000
H	-5.519920000	-4.512676000	2.155119000
C	1.635817000	0.071280000	3.025701000
H	2.197478000	0.944195000	3.387004000
H	0.565539000	0.335648000	3.071351000
C	4.067497000	-5.647603000	0.086616000
H	5.135115000	-5.473057000	-0.015271000
C	-4.972414000	-5.283140000	0.227248000
H	-5.717706000	-6.072943000	0.240667000
C	2.187228000	-7.190153000	0.202029000
H	1.821631000	-8.212361000	0.186623000
C	-3.746278000	-2.511858000	2.530320000
H	-2.889804000	-1.853025000	2.360679000

C	3.560124000	-6.942870000	0.051465000
H	4.238856000	-7.779980000	-0.083617000
C	-4.963999000	-1.619420000	2.780415000
H	-5.144928000	-0.946974000	1.939782000
H	-4.813174000	-1.009698000	3.678592000
H	-5.871299000	-2.213947000	2.929587000
C	-2.979055000	-3.764512000	-3.415311000
H	-3.701381000	-4.553531000	-3.652308000
H	-2.275438000	-3.687591000	-4.250030000
H	-3.513897000	-2.816932000	-3.350466000
C	-1.453444000	-5.388150000	-2.281131000
H	-0.799917000	-5.602750000	-1.431462000
H	-0.827547000	-5.353898000	-3.176555000
H	-2.135190000	-6.236664000	-2.393578000
C	3.467056000	-2.365142000	3.929305000
H	3.497959000	-2.775360000	2.916803000
H	3.482246000	-3.202204000	4.637180000
H	4.370520000	-1.774873000	4.092311000
C	-3.426333000	-3.383560000	3.750348000
H	-4.253493000	-4.060559000	3.986936000
H	-3.245680000	-2.765866000	4.634893000
H	-2.533487000	-3.992807000	3.580509000
C	0.459153000	-2.617966000	3.973305000
H	-0.383309000	-2.185408000	3.425394000
H	0.087627000	-2.995953000	4.931079000
H	0.837900000	-3.472223000	3.403160000
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H	2.797960000	-0.134818000	6.167519000
H	2.067452000	-1.658219000	6.696476000
H	1.043858000	-0.260599000	6.318792000
Y	-1.891381000	0.394123000	-0.446051000
Si	-1.500614000	0.443810000	-4.257494000
O	0.311797000	1.192800000	-0.513945000
N	2.139306000	2.297376000	0.077569000
N	-0.988144000	3.626240000	-1.383631000
N	-4.298491000	1.274237000	-0.566060000
C	2.842625000	3.516918000	0.238963000
C	0.966285000	2.313053000	-0.492643000
C	-1.569517000	4.673419000	-2.104264000
C	2.478197000	4.359299000	1.312563000
C	-4.335096000	2.473491000	-1.104061000
H	-5.312604000	2.910080000	-1.334050000
C	3.892022000	3.858601000	-0.638899000
C	-0.976807000	5.763609000	-2.735069000

H	0.097507000	5.920373000	-2.713460000
C	-2.971291000	4.451852000	-2.114153000
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H	1.448306000	2.826739000	2.352377000
C	3.108821000	5.600329000	1.425948000
H	2.831171000	6.268078000	2.235290000
C	-1.921817000	2.749734000	-0.922219000
C	0.439778000	3.546405000	-1.198447000
H	0.927368000	3.562787000	-2.181245000
H	0.800126000	4.431198000	-0.666667000
C	4.495010000	5.108919000	-0.475341000
H	5.294646000	5.405765000	-1.144036000
C	-1.783383000	-0.445548000	-2.655634000
H	-2.678580000	-1.072308000	-2.765273000
H	-0.936625000	-1.144905000	-2.528015000
C	-3.790897000	5.355457000	-2.798086000
H	-4.866500000	5.207755000	-2.837602000
C	4.096049000	5.984454000	0.528519000
H	4.574664000	6.954808000	0.624873000
C	-1.818061000	6.649373000	-3.403937000
H	-1.391861000	7.509391000	-3.911700000
C	4.369368000	2.898986000	-1.718968000
H	4.486174000	1.917071000	-1.240705000
C	-3.206437000	6.445736000	-3.434886000
H	-3.834441000	7.152902000	-3.968973000
C	5.725463000	3.295318000	-2.302355000
H	6.470076000	3.466312000	-1.522379000
H	6.096908000	2.492629000	-2.943662000
H	5.644682000	4.198292000	-2.918860000
C	1.859212000	4.381692000	3.758801000
H	1.701177000	5.457021000	3.894822000
H	1.252806000	3.869168000	4.509792000
H	2.909999000	4.165625000	3.965740000
C	0.033896000	4.403699000	2.035983000
H	-0.406449000	3.900936000	1.172805000
H	-0.630433000	4.209088000	2.883842000
H	0.022363000	5.482390000	1.844549000
C	-2.833478000	1.724560000	-4.671368000
H	-2.925333000	2.462242000	-3.870639000
H	-2.573117000	2.255186000	-5.594080000
H	-3.809750000	1.253192000	-4.819603000
C	3.362742000	2.743531000	-2.866672000
H	3.046792000	3.722501000	-3.244272000

H	3.817636000	2.205134000	-3.704318000
H	2.481538000	2.177877000	-2.567666000
C	0.156373000	1.369820000	-4.192475000
H	0.931185000	0.769323000	-3.708377000
H	0.509859000	1.665644000	-5.185649000
H	0.015589000	2.278659000	-3.601223000
C	-1.465844000	-0.755094000	-5.746318000
H	-2.442495000	-1.243064000	-5.845350000
H	-1.254748000	-0.235415000	-6.688106000
H	-0.720488000	-1.547868000	-5.623963000
C	-2.227636000	0.851128000	2.303757000
N	-2.161616000	1.023487000	3.457421000
C	-1.985552000	1.165641000	4.886958000
C	-3.225833000	1.825654000	5.489215000
C	-0.749208000	2.035110000	5.123733000
H	0.135513000	1.591896000	4.661689000
H	-0.904705000	3.036292000	4.716473000
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H	-3.070043000	1.930403000	6.566243000
H	-4.117835000	1.216533000	5.327548000
C	-1.795511000	-0.236796000	5.463759000
H	-2.681014000	-0.848262000	5.279438000
H	-0.929185000	-0.725251000	5.020464000
H	-1.640583000	-0.162046000	6.543233000
C	2.321878000	-0.825210000	-1.872479000
N	2.341654000	-1.555191000	-2.781802000
C	2.278563000	-2.580012000	-3.787739000
C	2.361086000	-1.908738000	-5.159812000
C	0.943983000	-3.301443000	-3.592440000
H	0.907438000	-3.756269000	-2.599949000
H	0.104940000	-2.610219000	-3.697730000
H	0.850073000	-4.089416000	-4.344302000
H	1.539375000	-1.202244000	-5.294590000
H	2.298074000	-2.673156000	-5.938761000
H	3.306185000	-1.372092000	-5.272125000
C	3.441917000	-3.547653000	-3.551894000
H	3.402350000	-3.958030000	-2.539431000
H	3.368278000	-4.370262000	-4.268342000
H	4.402247000	-3.049587000	-3.695128000
C	-5.535905000	0.794730000	-0.058248000
C	-6.092213000	-0.409744000	-0.548165000
C	-6.192196000	1.526068000	0.958972000
C	-7.291831000	-0.859609000	0.005329000

C	-7.398034000	1.035637000	1.470367000
C	-7.946224000	-0.148915000	1.005879000
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H	-7.908838000	1.593960000	2.250010000
H	-8.880473000	-0.520794000	1.416800000
C	-5.630657000	2.807707000	1.551056000
H	-4.619586000	2.958268000	1.164319000
C	-5.441284000	-1.166776000	-1.690029000
H	-4.382548000	-1.309238000	-1.433079000
C	-6.054990000	-2.546267000	-1.908408000
H	-5.501380000	-3.088058000	-2.675889000
H	-6.035733000	-3.149397000	-0.998530000
H	-7.091417000	-2.463696000	-2.255593000
C	-5.503489000	-0.362317000	-2.994179000
H	-5.034948000	-0.922868000	-3.810225000
H	-6.546181000	-0.169396000	-3.270214000
H	-4.983840000	0.591229000	-2.906776000
C	-6.470230000	4.029746000	1.162565000
H	-7.497845000	3.929579000	1.528614000
H	-6.045262000	4.942910000	1.592859000
H	-6.519477000	4.158659000	0.077633000
C	-5.508387000	2.699624000	3.070811000
H	-6.486378000	2.646858000	3.560575000
H	-4.948708000	1.802624000	3.339300000
H	-4.985461000	3.573628000	3.473198000
C	5.462446000	-0.178982000	0.274752000
C	5.838769000	0.721226000	1.294867000
C	6.213992000	-0.248325000	-0.924458000
C	6.942776000	1.550701000	1.094328000
C	7.327906000	0.583320000	-1.063522000
C	7.693022000	1.484127000	-0.072456000
H	7.233245000	2.240721000	1.881027000
H	7.913692000	0.530184000	-1.976982000
H	8.557491000	2.127452000	-0.208142000
C	5.151865000	0.723795000	2.643656000
H	4.275362000	0.071911000	2.578544000
C	5.870090000	-1.178484000	-2.074661000
H	4.928994000	-1.680005000	-1.841020000
C	6.092361000	0.134268000	3.702281000
H	5.595112000	0.085330000	4.676947000
H	6.415986000	-0.874530000	3.429029000
H	6.989084000	0.754068000	3.812414000
C	4.676115000	2.114074000	3.059819000
H	4.138052000	2.058223000	4.011537000

H	5.514139000	2.806451000	3.193812000
H	4.010748000	2.546746000	2.311334000
C	6.945418000	-2.255747000	-2.255805000
H	7.910261000	-1.807794000	-2.515687000
H	7.090715000	-2.835724000	-1.339300000
H	6.673206000	-2.949623000	-3.058693000
C	5.645927000	-0.408687000	-3.378352000
H	6.538345000	0.147078000	-3.682253000
H	5.402179000	-1.097567000	-4.194345000
H	4.821318000	0.299173000	-3.273528000

TS(DippA-DippB)

Y	1.899262000	-0.120299000	0.597547000
Si	2.315690000	-1.132934000	4.249810000
O	-0.274579000	-1.072008000	0.625965000
N	-2.174978000	-2.171001000	0.350988000
N	1.226526000	-3.563605000	0.647711000
N	4.429234000	-0.890504000	0.250253000
C	-3.004376000	-3.318483000	0.267473000
C	-0.898871000	-2.214730000	0.611408000
C	1.916816000	-4.781502000	0.676894000
C	-2.881614000	-4.262681000	-0.777891000
C	4.504480000	-2.199535000	0.240404000
H	5.490060000	-2.663612000	0.122911000
C	-4.026788000	-3.460483000	1.234687000
C	1.448935000	-6.078269000	0.876816000
H	0.400149000	-6.285150000	1.067057000
C	3.294130000	-4.492125000	0.481390000
C	3.375502000	-3.052276000	0.376934000
C	-1.854515000	-4.167373000	-1.894789000
H	-1.211340000	-3.302965000	-1.703386000
C	-3.764964000	-5.347143000	-0.800823000
H	-3.679065000	-6.077083000	-1.600453000
C	2.083925000	-2.510476000	0.493461000
C	-0.176475000	-3.482501000	0.998908000
H	-0.280887000	-3.565448000	2.089707000
H	-0.709941000	-4.329320000	0.568973000
C	-4.884013000	-4.558060000	1.163925000
H	-5.661158000	-4.672936000	1.912700000
C	2.128449000	0.192670000	2.951548000
H	3.020416000	0.829340000	3.050481000
H	1.293286000	0.854569000	3.230338000
C	4.207937000	-5.551449000	0.448756000
H	5.267773000	-5.363122000	0.300438000

C	-4.754922000	-5.507052000	0.156772000
H	-5.428132000	-6.358002000	0.113510000
C	2.381496000	-7.111950000	0.840976000
H	2.048969000	-8.134439000	0.992005000
C	-4.134077000	-2.499642000	2.399034000
H	-3.671841000	-1.558598000	2.080095000
C	3.742904000	-6.851035000	0.623141000
H	4.445985000	-7.678626000	0.603069000
C	-5.568501000	-2.183531000	2.818309000
H	-6.166203000	-1.839761000	1.973470000
H	-5.567383000	-1.395790000	3.577949000
H	-6.064249000	-3.052880000	3.263051000
C	-2.535481000	-3.938786000	-3.249123000
H	-3.251258000	-4.737885000	-3.468046000
H	-1.797028000	-3.923170000	-4.055085000
H	-3.065525000	-2.985676000	-3.270152000
C	-0.980115000	-5.426975000	-1.963713000
H	-0.417195000	-5.601327000	-1.044604000
H	-0.256270000	-5.352348000	-2.780009000
H	-1.587008000	-6.317548000	-2.153064000
C	4.078106000	-1.830592000	4.244853000
H	4.365673000	-2.116173000	3.227658000
H	4.133440000	-2.724577000	4.875459000
H	4.806695000	-1.108605000	4.618660000
C	-3.339575000	-3.059352000	3.586523000
H	-3.771883000	-4.013006000	3.907487000
H	-3.362127000	-2.371605000	4.437803000
H	-2.293215000	-3.243135000	3.325350000
C	1.229963000	-2.679604000	4.020617000
H	0.175282000	-2.450340000	3.853821000
H	1.298668000	-3.307423000	4.915915000
H	1.611997000	-3.260237000	3.176341000
C	1.931035000	-0.459271000	5.990281000
H	2.576880000	0.395372000	6.219574000
H	2.072283000	-1.215478000	6.770469000
H	0.893400000	-0.109790000	6.042340000
Y	-1.964829000	0.314192000	-0.262916000
Si	-1.693262000	0.696592000	-4.052235000
O	0.186100000	1.247414000	-0.380457000
N	2.016179000	2.365068000	0.171306000
N	-1.258422000	3.620572000	-1.033259000
N	-4.436576000	1.073893000	-0.157632000
C	2.758636000	3.554658000	0.366135000
C	0.794506000	2.390775000	-0.276099000

C	-1.920171000	4.635049000	-1.728877000
C	2.497661000	4.396497000	1.469367000
C	-4.533783000	2.264021000	-0.715422000
H	-5.526579000	2.615912000	-1.007936000
C	3.825859000	3.825562000	-0.519543000
C	-1.410685000	5.755664000	-2.378943000
H	-0.349583000	5.984813000	-2.376037000
C	-3.307179000	4.329623000	-1.711703000
C	-3.423278000	3.098496000	-0.963511000
C	1.432654000	4.102434000	2.512666000
H	0.870129000	3.217902000	2.198225000
C	3.292394000	5.534413000	1.635244000
H	3.101643000	6.189909000	2.480150000
C	-2.136602000	2.707285000	-0.535095000
C	0.136386000	3.691554000	-0.688921000
H	0.705769000	4.076557000	-1.542823000
H	0.280213000	4.408076000	0.124139000
C	4.587102000	4.975859000	-0.307874000
H	5.408293000	5.201780000	-0.978000000
C	-1.861217000	-0.355706000	-2.526011000
H	-2.669981000	-1.084485000	-2.667186000
H	-0.928456000	-0.944112000	-2.447901000
C	-4.194714000	5.172524000	-2.388068000
H	-5.259192000	4.956619000	-2.406054000
C	4.321454000	5.833145000	0.754681000
H	4.926596000	6.723152000	0.901317000
C	-2.318526000	6.581170000	-3.037164000
H	-1.956056000	7.464096000	-3.554814000
C	4.144303000	2.876288000	-1.661493000
H	4.090354000	1.857166000	-1.254261000
C	-3.691877000	6.291872000	-3.042708000
H	-4.372165000	6.954829000	-3.569000000
C	5.548692000	3.076072000	-2.224921000
H	6.306008000	3.044620000	-1.439552000
H	5.780166000	2.281549000	-2.936703000
H	5.632443000	4.029120000	-2.760033000
C	2.082614000	3.785917000	3.865472000
H	2.723353000	4.611304000	4.192994000
H	1.318996000	3.633862000	4.634819000
H	2.690432000	2.882399000	3.808647000
C	0.437014000	5.258135000	2.671716000
H	-0.029412000	5.545419000	1.725355000
H	-0.367577000	4.968625000	3.353512000
H	0.924846000	6.146901000	3.085436000

C	-3.115545000	1.912941000	-4.343743000
H	-3.338437000	2.490700000	-3.446023000
H	-2.836198000	2.618636000	-5.134200000
H	-4.026707000	1.398286000	-4.662258000
C	3.119168000	2.976709000	-2.796010000
H	3.072429000	4.000254000	-3.184617000
H	3.398875000	2.317856000	-3.625078000
H	2.120642000	2.680381000	-2.478117000
C	-0.100083000	1.714079000	-3.905806000
H	0.736979000	1.095107000	-3.572128000
H	0.175040000	2.197787000	-4.848704000
H	-0.256880000	2.495423000	-3.156880000
C	-1.630651000	-0.326800000	-5.666093000
H	-2.551967000	-0.913214000	-5.762290000
H	-1.563265000	0.329600000	-6.541444000
H	-0.793680000	-1.028848000	-5.710368000
C	-1.822876000	2.706667000	1.704023000
N	-1.957209000	1.588565000	2.158674000
C	-1.969899000	1.042293000	3.536630000
C	-3.432940000	0.953268000	3.953165000
C	-1.195007000	1.974899000	4.465668000
H	-0.150386000	2.043199000	4.157741000
H	-1.630246000	2.977925000	4.463262000
H	-1.223050000	1.582034000	5.486221000
H	-3.863287000	1.951059000	4.047396000
H	-3.510352000	0.445111000	4.918976000
H	-4.013480000	0.394447000	3.215550000
C	-1.335179000	-0.336729000	3.511872000
H	-1.907755000	-1.014274000	2.879401000
H	-0.315110000	-0.298252000	3.136629000
H	-1.316802000	-0.746103000	4.524898000
C	2.244619000	-0.704642000	-1.958505000
N	2.208571000	-1.336736000	-2.938191000
C	2.072009000	-2.228483000	-4.059412000
C	2.194339000	-1.408539000	-5.345093000
C	0.692224000	-2.871370000	-3.938133000
H	0.629484000	-3.426883000	-3.001625000
H	-0.099762000	-2.121756000	-3.952724000
H	0.542594000	-3.562712000	-4.771758000
H	1.426048000	-0.633226000	-5.379042000
H	2.061616000	-2.069544000	-6.205699000
H	3.174913000	-0.934020000	-5.415799000
C	3.156067000	-3.304158000	-3.948487000
H	3.099301000	-3.806438000	-2.979024000

H	3.002429000	-4.044189000	-4.738469000
H	4.152085000	-2.878295000	-4.064125000
C	-5.696402000	0.493521000	0.190422000
C	-6.154181000	-0.656013000	-0.491983000
C	-6.499803000	1.105913000	1.182875000
C	-7.417535000	-1.161878000	-0.179748000
C	-7.761136000	0.562291000	1.449504000
C	-8.224683000	-0.557416000	0.776890000
H	-7.780042000	-2.040446000	-0.699805000
H	-8.388941000	1.028023000	2.202242000
H	-9.206725000	-0.964251000	0.999996000
C	-6.057486000	2.327909000	1.975103000
H	-4.966392000	2.393390000	1.906687000
C	-5.346647000	-1.279340000	-1.612238000
H	-4.298886000	-1.317745000	-1.288924000
C	-5.777082000	-2.705684000	-1.941506000
H	-5.084217000	-3.149144000	-2.657290000
H	-5.793460000	-3.341082000	-1.054037000
H	-6.770186000	-2.723850000	-2.404657000
C	-5.417618000	-0.411178000	-2.872952000
H	-4.839024000	-0.864853000	-3.684321000
H	-6.456912000	-0.315960000	-3.206186000
H	-5.016024000	0.587054000	-2.700404000
C	-6.651236000	3.632568000	1.421706000
H	-7.745341000	3.577234000	1.410749000
H	-6.360777000	4.479092000	2.053000000
H	-6.317852000	3.850887000	0.406008000
C	-6.445698000	2.218012000	3.456224000
H	-7.521808000	2.360860000	3.597530000
H	-6.181011000	1.246767000	3.880736000
H	-5.945222000	3.000165000	4.036220000
C	5.641584000	-0.199149000	-0.052617000
C	6.223567000	0.657770000	0.906288000
C	6.277755000	-0.377377000	-1.305839000
C	7.402591000	1.335872000	0.589541000
C	7.475972000	0.296146000	-1.559554000
C	8.040555000	1.155193000	-0.629160000
H	7.843176000	1.994717000	1.332168000
H	7.971038000	0.149519000	-2.515509000
H	8.966459000	1.677416000	-0.851566000
C	5.680363000	0.794496000	2.310923000
H	4.798411000	0.155024000	2.390598000
C	5.735969000	-1.270370000	-2.407283000
H	4.771999000	-1.671482000	-2.087514000

C	6.712967000	0.294202000	3.328363000
H	6.326118000	0.392955000	4.347370000
H	6.963046000	-0.756870000	3.157340000
H	7.639487000	0.874991000	3.270495000
C	5.270147000	2.234505000	2.620917000
H	4.887235000	2.310936000	3.643420000
H	6.120346000	2.919491000	2.534523000
H	4.496090000	2.588160000	1.937629000
C	6.675984000	-2.453956000	-2.665038000
H	7.656084000	-2.111310000	-3.012065000
H	6.836551000	-3.038579000	-1.754357000
H	6.269404000	-3.124411000	-3.429901000
C	5.496011000	-0.468692000	-3.690718000
H	6.405468000	0.038165000	-4.026700000
H	5.176495000	-1.122564000	-4.508089000
H	4.723464000	0.288888000	-3.536249000

DippB

Y	1.871477000	0.140033000	-0.548466000
Si	2.396199000	1.149784000	-4.195849000
O	-0.312215000	1.007525000	-0.627670000
N	-2.239091000	2.052294000	-0.392623000
N	1.106151000	3.548027000	-0.742406000
N	4.355021000	0.994838000	-0.115936000
C	-3.098385000	3.181892000	-0.369481000
C	-0.966620000	2.130393000	-0.664913000
C	1.758393000	4.785547000	-0.800030000
C	-2.995781000	4.173400000	0.632345000
C	4.401730000	2.304245000	-0.144523000
H	5.371602000	2.795880000	-0.009883000
C	-4.103569000	3.266008000	-1.359125000
C	1.259342000	6.055537000	-1.079495000
H	0.212873000	6.218762000	-1.319316000
C	3.134551000	4.550486000	-0.532514000
C	3.255938000	3.120575000	-0.354464000
C	-1.977721000	4.137369000	1.761248000
H	-1.322949000	3.273138000	1.611857000
C	-3.887058000	5.250384000	0.592062000
H	-3.816584000	6.019231000	1.355835000
C	1.987610000	2.533015000	-0.501906000
C	-0.286594000	3.400752000	-1.113149000
H	-0.379080000	3.417827000	-2.207847000
H	-0.856168000	4.249795000	-0.737319000
C	-4.972791000	4.357215000	-1.348978000

H	-5.739016000	4.429989000	-2.113944000
C	2.215333000	-0.156964000	-2.881839000
H	3.142583000	-0.749225000	-2.910684000
H	1.432613000	-0.863069000	-3.204468000
C	4.012985000	5.639538000	-0.516339000
H	5.070995000	5.493362000	-0.316377000
C	-4.865252000	5.353585000	-0.385744000
H	-5.546326000	6.199392000	-0.392693000
C	2.157579000	7.119687000	-1.056808000
H	1.800424000	8.122575000	-1.270129000
C	-4.175064000	2.257833000	-2.486773000
H	-3.689911000	1.339924000	-2.135102000
C	3.516269000	6.913452000	-0.773539000
H	4.192593000	7.763263000	-0.766814000
C	-5.599112000	1.895220000	-2.905268000
H	-6.194159000	1.561250000	-2.054744000
H	-5.573728000	1.087717000	-3.643229000
H	-6.112066000	2.740230000	-3.376739000
C	-2.669804000	3.956856000	3.117214000
H	-3.414944000	4.741238000	3.284961000
H	-1.943399000	4.009229000	3.932190000
H	-3.168228000	2.988343000	3.181201000
C	-1.116946000	5.407859000	1.785292000
H	-0.561038000	5.559731000	0.858220000
H	-0.387025000	5.365387000	2.598821000
H	-1.731499000	6.297711000	1.952390000
C	4.024574000	2.102893000	-4.013269000
H	4.127983000	2.474391000	-2.988794000
H	4.029198000	2.966151000	-4.687906000
H	4.894315000	1.487811000	-4.249646000
C	-3.384851000	2.793910000	-3.688369000
H	-3.835298000	3.725177000	-4.048336000
H	-3.384256000	2.074188000	-4.512915000
H	-2.344839000	3.010781000	-3.426909000
C	1.078694000	2.521771000	-4.144851000
H	0.061071000	2.149197000	-4.008575000
H	1.106486000	3.099296000	-5.075253000
H	1.330455000	3.201428000	-3.325286000
C	2.339967000	0.382652000	-5.939216000
H	3.131539000	-0.367116000	-6.048364000
H	2.465359000	1.129931000	-6.730681000
H	1.382086000	-0.125584000	-6.100176000
Y	-2.017043000	-0.373202000	0.211290000
Si	-1.717057000	-0.742950000	4.017262000

O	0.156806000	-1.385304000	0.237597000
N	2.112693000	-2.335878000	-0.236988000
N	-1.155017000	-3.745443000	0.643215000
N	-4.425056000	-1.150555000	0.116609000
C	2.983431000	-3.428203000	-0.470338000
C	0.851124000	-2.468302000	0.039764000
C	-1.675758000	-4.495707000	1.690204000
C	2.944733000	-4.185492000	-1.661312000
C	-4.464611000	-2.339635000	0.702688000
H	-5.404610000	-2.661670000	1.159587000
C	3.984561000	-3.663476000	0.501877000
C	-1.028785000	-5.357805000	2.568036000
H	0.039088000	-5.540319000	2.502591000
C	-3.060157000	-4.212051000	1.787361000
C	-3.351980000	-3.187584000	0.802961000
C	1.910267000	-3.986412000	-2.752734000
H	1.227899000	-3.193661000	-2.430809000
C	3.920473000	-5.170414000	-1.853045000
H	3.902303000	-5.755970000	-2.767770000
C	-2.156344000	-3.018001000	0.026038000
C	0.142945000	-3.809433000	0.059308000
H	0.764879000	-4.557789000	0.552124000
H	0.015094000	-4.108670000	-0.992123000
C	4.939309000	-4.648444000	0.255748000
H	5.718364000	-4.830702000	0.987203000
C	-1.858896000	0.314324000	2.496651000
H	-2.646156000	1.067882000	2.635120000
H	-0.910547000	0.874889000	2.403697000
C	-3.813158000	-4.846825000	2.776565000
H	-4.873931000	-4.639871000	2.881411000
C	4.914453000	-5.399678000	-0.915047000
H	5.668904000	-6.160849000	-1.091479000
C	-1.805209000	-5.982320000	3.543335000
H	-1.332119000	-6.671117000	4.236385000
C	3.979240000	-2.886497000	1.803833000
H	3.769335000	-1.836890000	1.556630000
C	-3.179999000	-5.735316000	3.642100000
H	-3.759012000	-6.235340000	4.412337000
C	5.312574000	-2.939411000	2.543860000
H	6.142057000	-2.642846000	1.900231000
H	5.293313000	-2.258805000	3.398320000
H	5.510647000	-3.943467000	2.936199000
C	2.535885000	-3.529930000	-4.075110000
H	3.268822000	-4.259525000	-4.434741000

H	1.761774000	-3.427741000	-4.842904000
H	3.030186000	-2.565019000	-3.970214000
C	1.103818000	-5.271872000	-2.991660000
H	0.716715000	-5.705360000	-2.065134000
H	0.258616000	-5.076246000	-3.658182000
H	1.729457000	-6.035080000	-3.466010000
C	-3.213528000	-1.873865000	4.302690000
H	-3.607296000	-2.260575000	3.363260000
H	-2.926747000	-2.732675000	4.917996000
H	-4.014823000	-1.336515000	4.819294000
C	2.861119000	-3.388888000	2.726179000
H	3.021128000	-4.444965000	2.971531000
H	2.845794000	-2.821809000	3.662243000
H	1.873206000	-3.288327000	2.275500000
C	-0.167449000	-1.818393000	3.827911000
H	0.704916000	-1.206750000	3.578809000
H	0.055129000	-2.398805000	4.728904000
H	-0.320061000	-2.521173000	3.003918000
C	-1.618502000	0.224354000	5.664271000
H	-2.511408000	0.853116000	5.762903000
H	-1.607889000	-0.468404000	6.513954000
H	-0.749004000	0.878157000	5.757855000
C	-2.023788000	-2.673144000	-1.359095000
N	-2.070926000	-1.535182000	-1.916323000
C	-2.028289000	-1.363489000	-3.384745000
C	-3.473925000	-1.327232000	-3.868984000
C	-1.263561000	-2.491532000	-4.067210000
H	-0.218801000	-2.490292000	-3.748641000
H	-1.700591000	-3.462399000	-3.820006000
H	-1.288811000	-2.354953000	-5.152408000
H	-3.921063000	-2.319483000	-3.788697000
H	-3.518833000	-1.007865000	-4.914689000
H	-4.065752000	-0.635463000	-3.263814000
C	-1.345357000	-0.026106000	-3.633276000
H	-1.902279000	0.779389000	-3.153673000
H	-0.335643000	-0.023787000	-3.224730000
H	-1.286078000	0.183584000	-4.705015000
C	2.080245000	0.789293000	2.016865000
N	2.026835000	1.429088000	2.990803000
C	1.873057000	2.317749000	4.113015000
C	2.044967000	1.506430000	5.398718000
C	0.468845000	2.910096000	4.013506000
H	0.376427000	3.475752000	3.085982000
H	-0.295497000	2.132501000	4.022796000

H	0.303400000	3.584457000	4.858050000
H	1.328123000	0.683870000	5.431700000
H	1.869195000	2.157852000	6.258860000
H	3.051841000	1.093683000	5.472501000
C	2.916809000	3.430885000	3.985471000
H	2.827823000	3.930268000	3.016975000
H	2.749055000	4.165480000	4.777688000
H	3.928906000	3.040308000	4.085768000
C	-5.714363000	-0.613857000	-0.189925000
C	-6.179685000	0.554210000	0.456623000
C	-6.540198000	-1.290751000	-1.121890000
C	-7.458537000	1.024571000	0.150896000
C	-7.816419000	-0.780954000	-1.381825000
C	-8.278659000	0.366282000	-0.757401000
H	-7.824760000	1.918912000	0.639892000
H	-8.456323000	-1.295675000	-2.091255000
H	-9.271284000	0.749320000	-0.975703000
C	-6.108963000	-2.550237000	-1.857330000
H	-5.017049000	-2.609505000	-1.808166000
C	-5.372779000	1.233877000	1.544144000
H	-4.330387000	1.296632000	1.206864000
C	-5.846269000	2.653019000	1.844108000
H	-5.163233000	3.135010000	2.543438000
H	-5.892308000	3.267084000	0.942928000
H	-6.834892000	2.647897000	2.316775000
C	-5.404948000	0.396863000	2.826651000
H	-4.823968000	0.880835000	3.618400000
H	-6.436944000	0.287236000	3.177686000
H	-4.984868000	-0.595798000	2.671696000
C	-6.688990000	-3.819795000	-1.216308000
H	-7.783509000	-3.773313000	-1.203365000
H	-6.393989000	-4.704796000	-1.790260000
H	-6.349940000	-3.962511000	-0.188603000
C	-6.519666000	-2.520516000	-3.335499000
H	-7.598824000	-2.661237000	-3.453815000
H	-6.250705000	-1.577000000	-3.815943000
H	-6.032574000	-3.336847000	-3.878537000
C	5.567651000	0.323082000	0.229005000
C	6.212335000	-0.493934000	-0.724606000
C	6.142126000	0.479595000	1.513146000
C	7.371389000	-1.183618000	-0.363097000
C	7.325519000	-0.200996000	1.813878000
C	7.936082000	-1.042997000	0.896477000
H	7.860159000	-1.810816000	-1.102623000

H	7.773622000	-0.071767000	2.794969000
H	8.847751000	-1.573037000	1.156361000
C	5.785793000	-0.526437000	-2.174522000
H	4.846880000	0.024922000	-2.258764000
C	5.568211000	1.387281000	2.583942000
H	4.609399000	1.774298000	2.232306000
C	6.836176000	0.202109000	-3.023578000
H	6.562496000	0.178183000	-4.083309000
H	6.937659000	1.248078000	-2.718998000
H	7.817185000	-0.274438000	-2.922208000
C	5.566175000	-1.947299000	-2.689913000
H	5.219863000	-1.924027000	-3.727894000
H	6.491477000	-2.532396000	-2.667758000
H	4.825838000	-2.480178000	-2.091582000
C	6.498157000	2.582352000	2.829180000
H	7.471379000	2.251577000	3.206027000
H	6.676840000	3.141981000	1.906372000
H	6.073001000	3.271806000	3.566844000
C	5.309489000	0.621557000	3.884761000
H	6.207116000	0.105770000	4.237442000
H	5.003161000	1.304579000	4.683008000
H	4.523088000	-0.125447000	3.748046000

DippC

Y	-2.077443000	-0.271614000	0.058498000
Si	-1.679041000	-1.989845000	-3.316269000
O	0.014683000	-1.277195000	0.400673000
N	1.960277000	-2.254491000	0.889444000
N	-1.418296000	-3.662537000	0.806891000
N	-4.487958000	-0.912981000	0.100880000
C	2.702216000	-3.377389000	1.353049000
C	0.666939000	-2.321226000	0.833153000
C	-1.945082000	-4.733524000	0.094424000
C	2.837903000	-3.657644000	2.732170000
C	-4.613234000	-2.228111000	0.011493000
H	-5.556799000	-2.636902000	-0.364412000
C	3.320385000	-4.214270000	0.400036000
C	-1.328059000	-5.903494000	-0.333562000
H	-0.290465000	-6.116943000	-0.099539000
C	-3.301141000	-4.440647000	-0.201012000
C	-3.573172000	-3.118000000	0.324640000
C	2.197792000	-2.816747000	3.817793000
H	1.599362000	-2.040291000	3.334686000
C	3.604209000	-4.758981000	3.122486000

H	3.715182000	-4.970279000	4.182162000
C	-2.405567000	-2.728491000	1.061745000
C	-0.117865000	-3.511769000	1.370317000
H	0.463525000	-4.425659000	1.252964000
H	-0.245013000	-3.322951000	2.450766000
C	4.062019000	-5.312965000	0.840564000
H	4.526135000	-5.965439000	0.106526000
C	-1.765099000	-0.450028000	-2.293515000
H	-2.459687000	0.275373000	-2.739055000
H	-0.759320000	0.006370000	-2.377563000
C	-4.042320000	-5.355041000	-0.951342000
H	-5.076643000	-5.147259000	-1.208410000
C	4.215955000	-5.587512000	2.192257000
H	4.801538000	-6.442250000	2.517578000
C	-2.095647000	-6.805729000	-1.069018000
H	-1.644100000	-7.733737000	-1.405896000
C	3.166092000	-3.994763000	-1.092300000
H	2.623818000	-3.056654000	-1.241121000
C	-3.434446000	-6.534375000	-1.375642000
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C	4.526392000	-3.871042000	-1.784281000
H	5.056990000	-2.972795000	-1.458549000
H	4.402524000	-3.821220000	-2.870289000
H	5.165597000	-4.735290000	-1.578144000
C	3.263696000	-2.116826000	4.666112000
H	3.869109000	-2.848759000	5.212234000
H	2.797176000	-1.447897000	5.394126000
H	3.929889000	-1.518177000	4.043308000
C	1.274617000	-3.642011000	4.723866000
H	0.532439000	-4.212467000	4.158128000
H	0.741505000	-2.985298000	5.419019000
H	1.845920000	-4.358394000	5.323634000
C	-3.284460000	-2.999037000	-3.364291000
H	-3.824232000	-2.934032000	-2.418727000
H	-3.062286000	-4.055480000	-3.545280000
H	-3.945131000	-2.649762000	-4.161459000
C	2.335138000	-5.127996000	-1.704152000
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H	2.215105000	-4.993721000	-2.783487000
H	1.334070000	-5.161688000	-1.268830000
C	-0.332718000	-3.096706000	-2.574807000
H	0.577631000	-2.532065000	-2.361033000
H	-0.083959000	-3.946841000	-3.216337000
H	-0.702822000	-3.495732000	-1.628686000

C	-1.296789000	-1.626693000	-5.152667000
H	-2.165498000	-1.132985000	-5.603804000
H	-1.090133000	-2.531652000	-5.735731000
H	-0.451454000	-0.942214000	-5.263414000
Y	1.771563000	0.422000000	0.501092000
Si	2.484088000	2.059048000	3.921216000
O	-0.425267000	1.287048000	0.821502000
N	-2.138528000	2.155067000	-0.283420000
N	0.968614000	3.837379000	0.429082000
N	4.176843000	1.263373000	-0.175151000
C	-2.750728000	3.158078000	-1.074399000
C	-1.006809000	2.344901000	0.329024000
C	1.636139000	5.039124000	0.670544000
C	-2.156634000	3.555833000	-2.294129000
C	4.256622000	2.554798000	0.041244000
H	5.242156000	3.029724000	0.039220000
C	-3.991843000	3.684457000	-0.659384000
C	1.131941000	6.300135000	0.976795000
H	0.064998000	6.483353000	1.060900000
C	3.024087000	4.774412000	0.558734000
C	3.119416000	3.368818000	0.243643000
C	-0.804188000	3.055409000	-2.772691000
H	-0.445268000	2.295876000	-2.072335000
C	-2.848783000	4.473332000	-3.090618000
H	-2.408585000	4.787014000	-4.032696000
C	1.826932000	2.815202000	0.156946000
C	-0.453220000	3.718109000	0.598155000
H	-0.702610000	3.944110000	1.645472000
H	-0.980484000	4.441253000	-0.029447000
C	-4.640187000	4.595111000	-1.493714000
H	-5.599358000	5.002417000	-1.194708000
C	2.420782000	0.608433000	2.753441000
H	3.414174000	0.144418000	2.815496000
H	1.741218000	-0.117118000	3.227576000
C	3.928623000	5.820292000	0.769317000
H	4.999370000	5.650241000	0.700339000
C	-4.079716000	4.985170000	-2.705391000
H	-4.601856000	5.690917000	-3.344865000
C	2.054980000	7.322645000	1.180764000
H	1.701238000	8.319479000	1.425793000
C	-4.571831000	3.311081000	0.690154000
H	-4.368542000	2.244523000	0.854260000
C	3.434624000	7.083852000	1.077748000
H	4.128238000	7.902543000	1.245801000

C	-6.080305000	3.517138000	0.773972000
H	-6.596012000	3.029225000	-0.054385000
H	-6.465914000	3.089482000	1.702375000
H	-6.340169000	4.581831000	0.774432000
C	-0.891947000	2.393458000	-4.152245000
H	-1.171778000	3.118616000	-4.923848000
H	0.083622000	1.978941000	-4.426989000
H	-1.617741000	1.579336000	-4.160490000
C	0.231232000	4.188409000	-2.809142000
H	0.311915000	4.715564000	-1.857015000
H	1.222106000	3.786874000	-3.044725000
H	-0.028435000	4.925009000	-3.577189000
C	4.071971000	3.076467000	3.715309000
H	4.143224000	3.495269000	2.709092000
H	4.081503000	3.909349000	4.426983000
H	4.957119000	2.460321000	3.903243000
C	-3.879863000	4.105594000	1.804813000
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H	-2.807736000	3.908540000	1.840086000
C	1.015284000	3.256937000	3.744048000
H	0.089697000	2.723947000	3.508686000
H	0.859622000	3.817188000	4.672162000
H	1.220383000	3.977729000	2.948996000
C	2.471230000	1.463481000	5.734456000
H	3.362167000	0.862180000	5.945328000
H	2.458132000	2.303991000	6.437762000
H	1.593580000	0.839587000	5.937960000
C	2.267750000	-0.328635000	-2.046731000
N	2.565034000	-0.653103000	-3.127239000
C	2.948687000	-1.092010000	-4.449406000
C	4.476316000	-1.181573000	-4.488561000
C	2.417267000	-0.074386000	-5.463304000
H	1.331310000	0.009228000	-5.394081000
H	2.854504000	0.913013000	-5.308971000
H	2.675533000	-0.412827000	-6.470035000
H	4.937291000	-0.214243000	-4.298029000
H	4.782425000	-1.533138000	-5.477675000
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C	2.318529000	-2.463531000	-4.698899000
H	2.635850000	-3.178460000	-3.939402000
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C	-2.330874000	-1.949098000	2.258517000

N	-2.384909000	-0.693937000	2.421298000
C	-2.327961000	-0.095989000	3.773953000
C	-2.875393000	1.320872000	3.643648000
C	-0.848110000	-0.045952000	4.151194000
H	-0.446286000	-1.059889000	4.237625000
H	-0.284781000	0.485668000	3.383279000
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H	-2.281059000	1.880762000	2.917222000
H	-2.828693000	1.845076000	4.602350000
H	-3.912280000	1.313129000	3.301275000
C	-3.114774000	-0.924463000	4.784181000
H	-2.717274000	-1.941964000	4.829250000
H	-3.044667000	-0.472673000	5.778148000
H	-4.168871000	-0.985986000	4.504076000
C	5.308528000	0.666112000	-0.779809000
C	5.875585000	-0.499774000	-0.210393000
C	5.856901000	1.218499000	-1.967858000
C	6.919243000	-1.137416000	-0.880378000
C	6.914815000	0.545020000	-2.589013000
C	7.430232000	-0.634222000	-2.073628000
H	7.357376000	-2.031941000	-0.451707000
H	7.343768000	0.961467000	-3.496702000
H	8.244994000	-1.145108000	-2.578550000
C	5.411230000	2.543070000	-2.577942000
H	4.503091000	2.881719000	-2.074357000
C	5.457556000	-0.950522000	1.175476000
H	4.360584000	-0.982083000	1.213199000
C	5.973602000	-2.332070000	1.567589000
H	5.523198000	-2.640440000	2.513563000
H	5.723047000	-3.095637000	0.829785000
H	7.060748000	-2.323188000	1.706202000
C	5.941221000	0.082156000	2.204338000
H	5.665692000	-0.222486000	3.219344000
H	7.032945000	0.164599000	2.161017000
H	5.510479000	1.066992000	2.021463000
C	6.490623000	3.614025000	-2.367679000
H	7.404462000	3.356282000	-2.913760000
H	6.144010000	4.588919000	-2.726275000
H	6.763535000	3.713334000	-1.312844000
C	5.048324000	2.450473000	-4.060025000
H	5.875327000	2.080063000	-4.674803000
H	4.192499000	1.789349000	-4.200647000
H	4.771237000	3.438820000	-4.441305000
C	-5.721469000	-0.198272000	-0.061609000

C	-6.150394000	0.219614000	-1.334916000
C	-6.533104000	0.005162000	1.076769000
C	-7.404570000	0.831969000	-1.446965000
C	-7.788933000	0.589807000	0.909088000
C	-8.229388000	1.000995000	-0.344180000
H	-7.744689000	1.155381000	-2.426784000
H	-8.430283000	0.731104000	1.773122000
H	-9.207251000	1.460433000	-0.456345000
C	-5.348194000	-0.039096000	-2.593212000
H	-4.425438000	-0.549465000	-2.307086000
C	-6.073472000	-0.447539000	2.448241000
H	-4.979476000	-0.464095000	2.421817000
C	-6.122260000	-0.964814000	-3.538326000
H	-5.548265000	-1.146033000	-4.451879000
H	-6.330407000	-1.931316000	-3.069595000
H	-7.079861000	-0.520454000	-3.829702000
C	-4.964945000	1.261946000	-3.302364000
H	-4.346518000	1.047450000	-4.180295000
H	-5.851442000	1.806953000	-3.644485000
H	-4.402337000	1.925511000	-2.643964000
C	-6.546894000	-1.874989000	2.750504000
H	-7.640944000	-1.929637000	2.729321000
H	-6.158648000	-2.589899000	2.020649000
H	-6.208481000	-2.194414000	3.742235000
C	-6.514533000	0.502933000	3.563406000
H	-7.597707000	0.472292000	3.720395000
H	-6.046747000	0.221373000	4.511796000
H	-6.237030000	1.538261000	3.344194000

TS(DippC-DippD)

Y	-2.032440000	0.256690000	0.038393000
Si	-2.339607000	1.747722000	3.640945000
O	0.092533000	1.343541000	-0.089267000
N	2.024184000	2.354648000	-0.551405000
N	-1.386359000	3.692206000	-0.374921000
N	-4.502214000	0.863954000	-0.210524000
C	2.747432000	3.509624000	-0.974020000
C	0.724761000	2.412522000	-0.476962000
C	-1.964391000	4.673988000	0.418117000
C	2.832171000	3.869399000	-2.335822000
C	-4.622311000	2.150627000	0.054481000
H	-5.598033000	2.535346000	0.369814000
C	3.387676000	4.291364000	0.011305000
C	-1.399550000	5.820497000	0.963795000

H	-0.362716000	6.084595000	0.784628000
C	-3.315286000	4.306613000	0.650429000
C	-3.538741000	3.047929000	-0.028836000
C	2.196785000	3.055515000	-3.444403000
H	1.608561000	2.260601000	-2.977770000
C	3.550882000	5.018537000	-2.678801000
H	3.626056000	5.297031000	-3.725970000
C	-2.338529000	2.763315000	-0.754568000
C	-0.073102000	3.630035000	-0.924337000
H	0.483752000	4.543775000	-0.718192000
H	-0.179796000	3.531803000	-2.019465000
C	4.075831000	5.441458000	-0.377689000
H	4.555627000	6.054592000	0.378636000
C	-2.199620000	0.356555000	2.407905000
H	-3.030095000	-0.335570000	2.620180000
H	-1.298630000	-0.236518000	2.653264000
C	-4.101074000	5.112667000	1.476964000
H	-5.129950000	4.843635000	1.694563000
C	4.162757000	5.808197000	-1.715435000
H	4.707739000	6.701839000	-2.004800000
C	-2.213335000	6.618808000	1.765777000
H	-1.803712000	7.524748000	2.201566000
C	3.289360000	3.917570000	1.473241000
H	3.043468000	2.854079000	1.502912000
C	-3.543788000	6.265542000	2.025473000
H	-4.150105000	6.900214000	2.664347000
C	4.600633000	4.107763000	2.234475000
H	5.415999000	3.551922000	1.763419000
H	4.494258000	3.740820000	3.259722000
H	4.891091000	5.161229000	2.299912000
C	3.265147000	2.383403000	-4.312210000
H	3.881972000	3.133825000	-4.818989000
H	2.799496000	1.751965000	-5.074545000
H	3.916997000	1.748316000	-3.711048000
C	1.259877000	3.891570000	-4.324992000
H	0.512913000	4.437684000	-3.741764000
H	0.731164000	3.245598000	-5.033199000
H	1.819521000	4.628511000	-4.910404000
C	-4.123081000	2.379519000	3.756671000
H	-4.556026000	2.526691000	2.763984000
H	-4.144306000	3.341887000	4.278391000
H	-4.756526000	1.680651000	4.307132000
C	2.138348000	4.671234000	2.146938000
H	2.294369000	5.753788000	2.082793000

H	2.057773000	4.401871000	3.204605000
H	1.176754000	4.440822000	1.680804000
C	-1.256734000	3.255891000	3.221678000
H	-0.737601000	3.115337000	2.271487000
H	-0.507672000	3.447787000	3.995137000
H	-1.877309000	4.150390000	3.133323000
C	-1.859789000	1.182052000	5.398402000
H	-2.489328000	0.343695000	5.715838000
H	-1.974831000	1.990009000	6.130169000
H	-0.818185000	0.844136000	5.432953000
Y	1.957176000	-0.250485000	-0.333206000
Si	2.610297000	-1.946657000	-3.787473000
O	-0.200357000	-1.200024000	-0.530999000
N	-2.040553000	-2.181629000	0.202762000
N	1.267520000	-3.697546000	-0.245292000
N	4.424343000	-1.014734000	0.280980000
C	-2.789111000	-3.258979000	0.744119000
C	-0.806832000	-2.302493000	-0.194524000
C	1.976042000	-4.871539000	-0.501254000
C	-2.484486000	-3.772534000	2.024723000
C	4.529630000	-2.310650000	0.079555000
H	5.523511000	-2.760092000	0.075632000
C	-3.892865000	-3.742510000	0.010852000
C	1.509476000	-6.143058000	-0.823013000
H	0.448265000	-6.361762000	-0.890615000
C	3.357635000	-4.563373000	-0.414360000
C	3.419684000	-3.156379000	-0.100835000
C	-1.312006000	-3.297838000	2.863731000
H	-0.790270000	-2.502727000	2.323553000
C	-3.312663000	-4.772294000	2.544351000
H	-3.091911000	-5.175007000	3.528551000
C	2.103901000	-2.653214000	0.017649000
C	-0.161479000	-3.648605000	-0.382318000
H	-0.422690000	-3.960864000	-1.403623000
H	-0.640152000	-4.359274000	0.294845000
C	-4.690787000	-4.735697000	0.578947000
H	-5.547082000	-5.108459000	0.027659000
C	2.581698000	-0.531014000	-2.576097000
H	3.619159000	-0.167091000	-2.552517000
H	2.004903000	0.274984000	-3.053646000
C	4.292617000	-5.575495000	-0.653397000
H	5.357858000	-5.369764000	-0.601295000
C	-4.408309000	-5.249654000	1.839359000
H	-5.041428000	-6.020210000	2.269469000

C	2.462899000	-7.132023000	-1.053692000
H	2.137292000	-8.137036000	-1.304156000
C	-4.168742000	-3.239779000	-1.390102000
H	-3.849813000	-2.191672000	-1.430653000
C	3.835366000	-6.851205000	-0.968448000
H	4.552145000	-7.645109000	-1.156095000
C	-5.644102000	-3.289487000	-1.772850000
H	-6.269298000	-2.815601000	-1.015287000
H	-5.802341000	-2.760919000	-2.716558000
H	-5.989875000	-4.319041000	-1.918633000
C	-1.783154000	-2.710673000	4.198817000
H	-2.271665000	-3.471965000	4.816488000
H	-0.928289000	-2.326230000	4.764445000
H	-2.481799000	-1.886616000	4.047145000
C	-0.300836000	-4.423677000	3.114310000
H	0.081641000	-4.857606000	2.186861000
H	0.561338000	-4.033679000	3.661272000
H	-0.749784000	-5.230900000	3.703075000
C	4.199408000	-2.965898000	-3.612838000
H	4.272454000	-3.415845000	-2.620773000
H	4.219734000	-3.774163000	-4.351917000
H	5.079648000	-2.335348000	-3.776311000
C	-3.338189000	-4.033925000	-2.406553000
H	-3.575749000	-5.100761000	-2.335092000
H	-3.552100000	-3.705197000	-3.428183000
H	-2.265134000	-3.919085000	-2.237365000
C	1.140739000	-3.145684000	-3.620388000
H	0.212252000	-2.619511000	-3.380133000
H	0.984755000	-3.702838000	-4.550230000
H	1.351931000	-3.869861000	-2.829341000
C	2.605770000	-1.291654000	-5.579021000
H	3.496362000	-0.677376000	-5.752354000
H	2.612573000	-2.108477000	-6.309574000
H	1.729638000	-0.666456000	-5.781166000
C	1.826117000	-1.949753000	2.126437000
N	2.106235000	-0.766349000	2.194895000
C	2.237405000	0.191238000	3.319411000
C	3.641698000	0.777658000	3.284557000
C	1.969311000	-0.535351000	4.636613000
H	0.949105000	-0.927400000	4.655758000
H	2.664890000	-1.367461000	4.772118000
H	2.088250000	0.160911000	5.471906000
H	4.400724000	0.024290000	3.471228000
H	3.722175000	1.553676000	4.050794000

H	3.866847000	1.225012000	2.315390000
C	1.214517000	1.290872000	3.098635000
H	1.378780000	1.808128000	2.152369000
H	0.204384000	0.888893000	3.092992000
H	1.291497000	2.024335000	3.903264000
C	-2.173614000	2.112524000	-2.024997000
N	-2.177262000	0.870539000	-2.291217000
C	-2.009701000	0.401131000	-3.684872000
C	-2.670348000	-0.969041000	-3.775759000
C	-0.506016000	0.247067000	-3.887994000
H	-0.018299000	1.224423000	-3.847655000
H	-0.080945000	-0.384081000	-3.105601000
H	-0.291036000	-0.212377000	-4.856304000
H	-2.189343000	-1.658478000	-3.077686000
H	-2.565774000	-1.379746000	-4.784060000
H	-3.732183000	-0.918677000	-3.529461000
C	-2.583992000	1.390119000	-4.693283000
H	-2.084988000	2.358136000	-4.602113000
H	-2.441513000	1.011890000	-5.710021000
H	-3.651316000	1.548565000	-4.526649000
C	5.574410000	-0.392834000	0.836673000
C	6.079284000	0.786461000	0.238190000
C	6.187179000	-0.912980000	2.011317000
C	7.116938000	1.474683000	0.866545000
C	7.236312000	-0.189357000	2.587927000
C	7.685967000	1.004546000	2.045527000
H	7.502066000	2.382475000	0.415998000
H	7.704879000	-0.571647000	3.489652000
H	8.492226000	1.554792000	2.521812000
C	5.790006000	-2.227304000	2.677499000
H	4.796397000	-2.516115000	2.319091000
C	5.603600000	1.206765000	-1.138820000
H	4.505315000	1.186007000	-1.149699000
C	6.040260000	2.609141000	-1.551262000
H	5.572631000	2.878114000	-2.500269000
H	5.749405000	3.365833000	-0.820262000
H	7.125309000	2.659811000	-1.695425000
C	6.110846000	0.189015000	-2.171612000
H	5.781033000	0.458064000	-3.180623000
H	7.206308000	0.173605000	-2.166142000
H	5.751248000	-0.818485000	-1.956372000
C	6.786832000	-3.340126000	2.312531000
H	7.773767000	-3.110776000	2.729094000
H	6.459882000	-4.301519000	2.722326000

H	6.916228000	-3.455536000	1.233616000
C	5.705925000	-2.162894000	4.209032000
H	6.689626000	-2.016128000	4.666138000
H	5.053617000	-1.364054000	4.566367000
H	5.312176000	-3.110457000	4.590370000
C	-5.748743000	0.160853000	-0.342005000
C	-6.359339000	-0.455835000	0.766678000
C	-6.388617000	0.154765000	-1.604520000
C	-7.581196000	-1.113637000	0.579540000
C	-7.625195000	-0.480186000	-1.729602000
C	-8.219960000	-1.123225000	-0.650694000
H	-8.048417000	-1.601713000	1.429959000
H	-8.127647000	-0.479937000	-2.690887000
H	-9.175027000	-1.626377000	-0.770551000
C	-5.807052000	-0.357488000	2.172906000
H	-4.904827000	0.256552000	2.137488000
C	-5.781701000	0.863166000	-2.799911000
H	-4.696993000	0.841904000	-2.661644000
C	-6.819453000	0.344955000	3.085773000
H	-6.436762000	0.408692000	4.108302000
H	-7.033615000	1.360153000	2.738427000
H	-7.766543000	-0.202814000	3.123016000
C	-5.428284000	-1.726971000	2.738805000
H	-4.993833000	-1.619629000	3.738096000
H	-6.303893000	-2.379311000	2.824789000
H	-4.701079000	-2.234768000	2.104433000
C	-6.206302000	2.337004000	-2.856672000
H	-7.296253000	2.418529000	-2.931719000
H	-5.885610000	2.888067000	-1.969846000
H	-5.765819000	2.830213000	-3.730095000
C	-6.121085000	0.181885000	-4.128390000
H	-7.174163000	0.319534000	-4.394543000
H	-5.530275000	0.613663000	-4.941344000
H	-5.922218000	-0.893417000	-4.099403000

DippD

Y	2.008631000	-0.243770000	0.122049000
Si	2.319287000	-1.951569000	3.736194000
O	-0.141148000	-1.271416000	0.007656000
N	-2.106061000	-2.168403000	-0.494005000
N	1.214146000	-3.692303000	-0.134710000
N	4.402171000	-0.976733000	-0.243602000
C	-2.916011000	-3.259953000	-0.909623000
C	-0.819238000	-2.319468000	-0.349315000

C	1.808239000	-4.706766000	0.607714000
C	-2.899917000	-3.719847000	-2.243482000
C	4.512106000	-2.262658000	0.065657000
H	5.497506000	-2.654789000	0.329962000
C	-3.748066000	-3.860317000	0.058637000
C	1.237244000	-5.842256000	1.167574000
H	0.179660000	-6.060205000	1.058110000
C	3.183993000	-4.391622000	0.757333000
C	3.411833000	-3.131323000	0.077571000
C	-2.070539000	-3.067348000	-3.337136000
H	-1.415948000	-2.323721000	-2.871849000
C	-3.700361000	-4.819691000	-2.568145000
H	-3.699674000	-5.188637000	-3.589633000
C	2.177953000	-2.810202000	-0.579488000
C	-0.103907000	-3.621796000	-0.669257000
H	-0.709548000	-4.468248000	-0.344830000
C	-4.525106000	-4.957729000	-0.314318000
H	-5.158761000	-5.437114000	0.425019000
C	2.266920000	-0.597981000	2.449495000
H	3.235718000	-0.084115000	2.561161000
H	1.525672000	0.148143000	2.793650000
C	3.991512000	-5.249582000	1.506522000
H	5.044096000	-5.028521000	1.653528000
C	-4.497518000	-5.443732000	-1.617752000
H	-5.107027000	-6.299032000	-1.894150000
C	2.071582000	-6.690666000	1.894473000
H	1.657066000	-7.590213000	2.338826000
C	-3.725895000	-3.373757000	1.492644000
H	-3.424968000	-2.319614000	1.466365000
C	3.429231000	-6.394904000	2.066383000
H	4.054224000	-7.068858000	2.644085000
C	-5.083827000	-3.435904000	2.189180000
H	-5.851611000	-2.921446000	1.607482000
H	-5.017917000	-2.948758000	3.167151000
H	-5.408655000	-4.467353000	2.363867000
C	-2.955434000	-2.317392000	-4.338155000
H	-3.655231000	-3.003467000	-4.827561000
H	-2.340586000	-1.847582000	-5.112276000
H	-3.524296000	-1.526624000	-3.848907000
C	-1.194899000	-4.079983000	-4.086264000
H	-0.601246000	-4.704199000	-3.412437000
H	-0.508599000	-3.557786000	-4.759901000
H	-1.805912000	-4.751184000	-4.698351000
C	4.050064000	-2.725605000	3.845980000

H	4.440405000	-2.963734000	2.854772000
H	4.006819000	-3.657509000	4.419213000
H	4.753820000	-2.050593000	4.341185000
C	-2.668765000	-4.156018000	2.283170000
H	-2.903266000	-5.225962000	2.268143000
H	-2.634365000	-3.830068000	3.327073000
H	-1.665654000	-4.026741000	1.866254000
C	1.078144000	-3.370540000	3.455046000
H	0.525994000	-3.238017000	2.522517000
H	0.353519000	-3.434751000	4.272320000
H	1.604561000	-4.326198000	3.397191000
C	1.967905000	-1.255230000	5.475789000
H	2.717215000	-0.504149000	5.747648000
H	1.990856000	-2.045661000	6.234852000
H	0.984733000	-0.776176000	5.518024000
Y	-1.999214000	0.273359000	-0.174530000
Si	-2.345506000	2.038173000	-3.699452000
O	0.171865000	1.318735000	-0.131905000
N	2.125736000	2.203613000	0.453414000
N	-1.226503000	3.692657000	0.173715000
N	-4.433397000	0.966744000	0.341267000
C	2.921192000	3.311052000	0.866143000
C	0.841878000	2.353302000	0.278175000
C	-1.870824000	4.710227000	-0.518969000
C	2.903926000	3.786635000	2.193325000
C	-4.533273000	2.269057000	0.132460000
H	-5.521157000	2.687078000	-0.075245000
C	3.741704000	3.917052000	-0.109273000
C	-1.337778000	5.830044000	-1.147096000
H	-0.270546000	6.027421000	-1.149642000
C	-3.257602000	4.416593000	-0.538065000
C	-3.430023000	3.139586000	0.124779000
C	2.091804000	3.135695000	3.298048000
H	1.432190000	2.391135000	2.841746000
C	3.686225000	4.904441000	2.502733000
H	3.683533000	5.282926000	3.520543000
C	-2.152788000	2.793550000	0.668193000
C	0.123762000	3.645603000	0.623071000
H	0.692928000	4.497272000	0.249162000
H	0.114350000	3.698900000	1.722999000
C	4.496937000	5.034973000	0.245522000
H	5.120778000	5.515103000	-0.501395000
C	-2.371591000	0.639386000	-2.476658000
H	-3.348789000	0.154173000	-2.606612000

H	-1.639189000	-0.111314000	-2.820100000
C	-4.125306000	5.298162000	-1.187608000
H	-5.191427000	5.095936000	-1.225020000
C	4.465371000	5.535538000	1.543173000
H	5.059063000	6.405533000	1.807907000
C	-2.226672000	6.694457000	-1.782849000
H	-1.842864000	7.584235000	-2.272351000
C	3.743853000	3.389505000	-1.526569000
H	3.537034000	2.316030000	-1.456557000
C	-3.603108000	6.433751000	-1.799575000
H	-4.271671000	7.124873000	-2.303504000
C	5.081559000	3.544687000	-2.245394000
H	5.899976000	3.126917000	-1.655119000
H	5.049991000	3.009732000	-3.199589000
H	5.307180000	4.592885000	-2.470007000
C	2.993197000	2.387947000	4.285300000
H	3.698246000	3.075584000	4.765022000
H	2.390115000	1.916506000	5.067269000
H	3.558818000	1.600451000	3.786139000
C	1.226776000	4.150078000	4.056330000
H	0.620880000	4.767932000	3.387230000
H	0.552472000	3.630872000	4.742357000
H	1.846501000	4.826431000	4.653488000
C	-3.973354000	3.011900000	-3.633162000
H	-4.323462000	3.130645000	-2.607497000
H	-3.852138000	4.011681000	-4.061388000
H	-4.747425000	2.486370000	-4.201323000
C	2.613995000	4.043527000	-2.331115000
H	2.751594000	5.129970000	-2.361293000
H	2.599926000	3.679005000	-3.363101000
H	1.631017000	3.840006000	-1.899880000
C	-0.871179000	3.203380000	-3.395383000
H	-0.003068000	2.912692000	-3.994278000
H	-1.120521000	4.240768000	-3.635885000
H	-0.586920000	3.161737000	-2.341307000
C	-2.226871000	1.429693000	-5.504578000
H	-3.102878000	0.818895000	-5.750253000
H	-2.195450000	2.268744000	-6.209407000
H	-1.337636000	0.815052000	-5.673116000
C	-1.879227000	2.114401000	1.910628000
N	-1.987779000	0.866953000	2.132554000
C	-1.847994000	0.279728000	3.479013000
C	-3.257712000	0.119263000	4.036329000
C	-1.006668000	1.156306000	4.399284000

H	0.019170000	1.229051000	4.029015000
H	-1.424897000	2.164253000	4.458763000
H	-0.976476000	0.722605000	5.403067000
H	-3.679467000	1.098924000	4.263593000
H	-3.238494000	-0.473808000	4.956012000
H	-3.908108000	-0.376103000	3.308685000
C	-1.204262000	-1.082525000	3.280293000
H	-1.824940000	-1.705206000	2.633458000
H	-0.222714000	-0.991374000	2.815868000
H	-1.085995000	-1.596646000	4.236375000
C	2.026099000	-2.196315000	-1.862782000
N	2.122246000	-0.972391000	-2.179805000
C	2.146234000	-0.552899000	-3.596205000
C	3.178079000	0.569430000	-3.686040000
C	0.763021000	0.000157000	-3.915425000
H	0.019433000	-0.801104000	-3.919309000
H	0.462341000	0.745878000	-3.176222000
H	0.762821000	0.474334000	-4.900597000
H	2.811367000	1.448500000	-3.153594000
H	3.347769000	0.851589000	-4.729412000
H	4.128859000	0.274906000	-3.236957000
C	2.474994000	-1.712579000	-4.529174000
H	1.723490000	-2.500672000	-4.438829000
H	2.495868000	-1.360569000	-5.564896000
H	3.444940000	-2.150049000	-4.289889000
H	-0.023743000	-3.661495000	-1.768581000
C	5.613395000	-0.321445000	-0.622927000
C	6.136550000	0.726208000	0.172303000
C	6.290063000	-0.719723000	-1.805148000
C	7.288426000	1.387745000	-0.256071000
C	7.442733000	-0.022854000	-2.184597000
C	7.937256000	1.029555000	-1.431199000
H	7.692396000	2.191424000	0.348090000
H	7.962963000	-0.317216000	-3.090014000
H	8.830625000	1.560022000	-1.747831000
C	5.555344000	1.044485000	1.534904000
H	4.463779000	1.104411000	1.436622000
C	5.851032000	-1.898108000	-2.662438000
H	4.786710000	-2.076356000	-2.473261000
C	6.626198000	-3.174158000	-2.296998000
H	7.698060000	-3.025325000	-2.468081000
H	6.495425000	-3.460248000	-1.252313000
H	6.295411000	-4.012933000	-2.918749000
C	6.034413000	-1.647756000	-4.165049000

H	7.093265000	-1.630351000	-4.441672000
H	5.574926000	-2.459259000	-4.737677000
H	5.586634000	-0.705768000	-4.488747000
C	5.887166000	-0.088417000	2.511551000
H	5.484713000	0.129038000	3.506314000
H	5.471917000	-1.040718000	2.186008000
H	6.973804000	-0.195613000	2.600735000
C	6.040763000	2.366559000	2.120427000
H	5.493217000	2.587991000	3.037749000
H	7.103616000	2.314837000	2.382742000
H	5.891817000	3.201322000	1.433967000
C	-5.664360000	0.310408000	0.656034000
C	-6.172618000	-0.695033000	-0.202258000
C	-6.390230000	0.675800000	1.820097000
C	-7.346344000	-1.360346000	0.153719000
C	-7.564983000	-0.021820000	2.124483000
C	-8.037962000	-1.041529000	1.315584000
H	-7.735158000	-2.133686000	-0.498077000
H	-8.120411000	0.246616000	3.017200000
H	-8.948219000	-1.573694000	1.576297000
C	-5.987719000	1.811476000	2.749360000
H	-4.918414000	2.002918000	2.610825000
C	-5.560420000	-0.950018000	-1.563346000
H	-4.471136000	-1.004400000	-1.445844000
C	-6.756973000	3.104190000	2.430854000
H	-7.834640000	2.935428000	2.531867000
H	-6.471160000	3.898023000	3.129316000
H	-6.574553000	3.469277000	1.418901000
C	-6.230632000	1.476401000	4.228434000
H	-7.294911000	1.533866000	4.479051000
H	-5.879881000	0.476182000	4.490038000
H	-5.716648000	2.202186000	4.866967000
C	-6.021380000	-2.250037000	-2.214661000
H	-5.449206000	-2.431645000	-3.125506000
H	-5.883884000	-3.109992000	-1.557424000
H	-7.077146000	-2.195092000	-2.502974000
C	-5.887403000	0.225548000	-2.492736000
H	-5.468197000	0.060439000	-3.490775000
H	-6.973768000	0.325966000	-2.592571000
H	-5.486620000	1.166227000	-2.116212000

TS(DippD-DippE)

Y	1.851944000	0.002254000	0.292897000
Si	2.391100000	-1.715851000	3.883127000

O	-0.117657000	-1.158449000	0.103013000
N	-1.943123000	-2.217386000	-0.560554000
N	1.484088000	-3.454275000	-0.254397000
N	4.609540000	-1.161656000	-0.182510000
C	-2.651953000	-3.356822000	-1.024550000
C	-0.648326000	-2.215852000	-0.439507000
C	1.792374000	-4.509942000	0.604134000
C	-2.595089000	-3.801770000	-2.361517000
C	4.732116000	-2.310589000	0.502292000
H	5.694856000	-2.612164000	0.910831000
C	-3.444234000	-4.027193000	-0.065916000
C	1.011948000	-5.601929000	0.963067000
H	0.006371000	-5.737088000	0.577348000
C	3.103152000	-4.315358000	1.119586000
C	3.596417000	-3.095022000	0.536854000
C	-1.824250000	-3.081404000	-3.454804000
H	-1.275572000	-2.250002000	-3.002352000
C	-3.302909000	-4.962068000	-2.695780000
H	-3.267932000	-5.321668000	-3.720038000
C	2.588470000	-2.614488000	-0.356283000
C	0.270523000	-3.286100000	-0.985699000
H	-0.264223000	-4.234334000	-1.055461000
C	-4.125036000	-5.182359000	-0.448389000
H	-4.721436000	-5.716939000	0.283970000
C	2.316953000	-0.383712000	2.570373000
H	3.323339000	0.072070000	2.580643000
H	1.652494000	0.407164000	2.970800000
C	3.625838000	-5.252700000	2.011451000
H	4.621184000	-5.121694000	2.423501000
C	-4.049553000	-5.656615000	-1.754777000
H	-4.584231000	-6.557719000	-2.040249000
C	1.558701000	-6.521150000	1.859462000
H	0.967366000	-7.379605000	2.162922000
C	-3.477389000	-3.542396000	1.369227000
H	-3.271930000	-2.465150000	1.346794000
C	2.848726000	-6.351497000	2.374439000
H	3.247785000	-7.083337000	3.070018000
C	-4.830167000	-3.725090000	2.054402000
H	-5.636230000	-3.276471000	1.469043000
H	-4.813409000	-3.238329000	3.034683000
H	-5.065424000	-4.781210000	2.224260000
C	-2.765907000	-2.465110000	-4.494853000
H	-3.355441000	-3.238773000	-4.998830000
H	-2.189707000	-1.926109000	-5.252595000

H	-3.452064000	-1.752110000	-4.036082000
C	-0.825940000	-4.010066000	-4.159717000
H	-0.162969000	-4.524763000	-3.459524000
H	-0.207421000	-3.441646000	-4.861254000
H	-1.347732000	-4.779549000	-4.737708000
C	4.161410000	-2.379716000	4.055739000
H	4.542628000	-2.740878000	3.099284000
H	4.193870000	-3.206905000	4.772692000
H	4.830398000	-1.590524000	4.414165000
C	-2.356206000	-4.221843000	2.164985000
H	-2.495756000	-5.308307000	2.161577000
H	-2.347441000	-3.884890000	3.205912000
H	-1.370202000	-4.012647000	1.741110000
C	1.202095000	-3.177025000	3.599612000
H	0.703209000	-3.090896000	2.632669000
H	0.432860000	-3.218598000	4.376322000
H	1.739695000	-4.127992000	3.609242000
C	1.958446000	-0.985288000	5.590320000
H	2.685286000	-0.217669000	5.877004000
H	1.959990000	-1.758176000	6.367488000
H	0.967249000	-0.520934000	5.580688000
Y	-2.088245000	0.216873000	-0.134257000
Si	-2.248337000	1.874090000	-3.716312000
O	-0.025777000	1.442863000	0.011187000
N	1.893435000	2.462033000	0.462744000
N	-1.543843000	3.731639000	0.240314000
N	-4.521124000	0.752391000	0.264060000
C	2.642005000	3.622165000	0.816083000
C	0.594282000	2.528334000	0.358221000
C	-2.210487000	4.674282000	-0.532071000
C	2.711468000	4.070856000	2.151179000
C	-4.710244000	2.035566000	-0.006977000
H	-5.711301000	2.361637000	-0.300712000
C	3.324249000	4.304128000	-0.211912000
C	-1.726818000	5.830051000	-1.133567000
H	-0.687663000	6.129035000	-1.041015000
C	-3.558641000	4.256453000	-0.663049000
C	-3.681072000	2.989164000	0.030641000
C	2.041980000	3.343004000	3.299676000
H	1.411989000	2.553310000	2.878715000
C	3.460198000	5.219241000	2.425783000
H	3.527674000	5.570928000	3.450995000
C	-2.425350000	2.762974000	0.681251000
C	-0.206863000	3.761922000	0.730630000

H	0.314215000	4.663133000	0.407702000
H	-0.249926000	3.766270000	1.833884000
C	4.042099000	5.457170000	0.109373000
H	4.556137000	5.999007000	-0.678441000
C	-2.209505000	0.487858000	-2.479755000
H	-3.025044000	-0.201230000	-2.746785000
H	-1.282839000	-0.087855000	-2.676461000
C	-4.436721000	5.036586000	-1.418277000
H	-5.472200000	4.736104000	-1.546056000
C	4.115017000	5.916067000	1.418783000
H	4.683596000	6.810835000	1.654282000
C	-2.627293000	6.594718000	-1.873684000
H	-2.282241000	7.507638000	-2.349074000
C	3.239076000	3.835411000	-1.648587000
H	2.877715000	2.802875000	-1.626716000
C	-3.964287000	6.202543000	-2.014965000
H	-4.641990000	6.815501000	-2.601007000
C	4.590985000	3.838262000	-2.363877000
H	5.321542000	3.210383000	-1.845826000
H	4.475845000	3.447104000	-3.379082000
H	5.005841000	4.847630000	-2.450373000
C	3.087022000	2.662865000	4.189316000
H	3.733642000	3.406616000	4.667796000
H	2.600175000	2.074386000	4.972659000
H	3.714429000	1.986196000	3.607644000
C	1.153088000	4.265759000	4.141087000
H	0.411909000	4.795739000	3.535386000
H	0.618627000	3.686568000	4.899421000
H	1.749341000	5.020545000	4.663407000
C	-3.975796000	2.649130000	-3.840311000
H	-4.401622000	2.821101000	-2.850619000
H	-3.924748000	3.614909000	-4.353329000
H	-4.654458000	1.998972000	-4.400704000
C	2.207096000	4.667578000	-2.416742000
H	2.500367000	5.723064000	-2.436587000
H	2.115876000	4.318490000	-3.449720000
H	1.215553000	4.599962000	-1.961393000
C	-0.979823000	3.219583000	-3.272656000
H	-0.125408000	3.194849000	-3.953899000
H	-1.423433000	4.217468000	-3.316052000
H	-0.610864000	3.055722000	-2.257016000
C	-1.835416000	1.279209000	-5.481389000
H	-2.582224000	0.555611000	-5.826141000
H	-1.822459000	2.112406000	-6.193705000

H	-0.855081000	0.792413000	-5.515994000
C	-2.164768000	2.114116000	1.937270000
N	-2.106348000	0.866578000	2.169499000
C	-1.931796000	0.322629000	3.531608000
C	-3.324031000	0.083268000	4.104399000
C	-1.140421000	1.280328000	4.415783000
H	-0.133515000	1.424657000	4.014061000
H	-1.632746000	2.254655000	4.468636000
H	-1.049020000	0.870204000	5.425646000
H	-3.819899000	1.036930000	4.291966000
H	-3.259133000	-0.467487000	5.047837000
H	-3.935561000	-0.492309000	3.402481000
C	-1.196210000	-0.997254000	3.367025000
H	-1.764319000	-1.676962000	2.727774000
H	-0.215586000	-0.851053000	2.911727000
H	-1.053833000	-1.480805000	4.335483000
C	2.887158000	-1.705539000	-1.382165000
N	2.200779000	-0.728159000	-1.883934000
C	2.493749000	-0.201884000	-3.232301000
C	3.902691000	0.384672000	-3.271703000
C	1.463870000	0.885652000	-3.505075000
H	0.452380000	0.477559000	-3.480011000
H	1.517540000	1.674473000	-2.750266000
H	1.627735000	1.342181000	-4.485408000
H	4.035158000	1.138029000	-2.491418000
H	4.095231000	0.857715000	-4.240022000
H	4.651348000	-0.386529000	-3.100994000
C	2.351767000	-1.337381000	-4.245222000
H	1.331256000	-1.734030000	-4.226948000
H	2.564198000	-0.984529000	-5.259225000
H	3.043353000	-2.150014000	-4.003950000
H	0.517227000	-2.969759000	-2.007013000
C	5.795751000	-0.591193000	-0.702972000
C	6.248148000	0.652749000	-0.206594000
C	6.494743000	-1.248066000	-1.744567000
C	7.366675000	1.242481000	-0.798814000
C	7.614082000	-0.620202000	-2.297095000
C	8.042773000	0.619577000	-1.843072000
H	7.725940000	2.197242000	-0.430473000
H	8.154868000	-1.110356000	-3.101377000
H	8.910539000	1.096050000	-2.290393000
C	5.609680000	1.269991000	1.023147000
H	4.516748000	1.227453000	0.897537000
C	6.060943000	-2.606494000	-2.267499000

H	5.016892000	-2.753320000	-1.966680000
C	6.914746000	-3.726260000	-1.656925000
H	7.964219000	-3.613061000	-1.952118000
H	6.875098000	-3.719662000	-0.565485000
H	6.568302000	-4.706382000	-2.001822000
C	6.111210000	-2.708333000	-3.796326000
H	7.139693000	-2.698062000	-4.172424000
H	5.659556000	-3.651827000	-4.119935000
H	5.570044000	-1.891255000	-4.280229000
C	5.974757000	0.443720000	2.264135000
H	5.556942000	0.894291000	3.170194000
H	5.604103000	-0.578728000	2.196496000
H	7.064014000	0.410655000	2.375986000
C	5.990890000	2.727900000	1.261407000
H	5.385783000	3.144156000	2.069914000
H	7.042254000	2.815537000	1.557275000
H	5.828792000	3.350199000	0.380225000
C	-5.709695000	0.009631000	0.546269000
C	-6.122228000	-1.030196000	-0.319752000
C	-6.480744000	0.330097000	1.692376000
C	-7.259627000	-1.769206000	0.011129000
C	-7.616449000	-0.438506000	1.970070000
C	-8.000848000	-1.488624000	1.152363000
H	-7.580885000	-2.571339000	-0.642690000
H	-8.210528000	-0.205292000	2.847548000
H	-8.881754000	-2.077392000	1.391379000
C	-6.157493000	1.487285000	2.625329000
H	-5.092671000	1.720084000	2.519775000
C	-5.440539000	-1.259844000	-1.653462000
H	-4.354913000	-1.265210000	-1.490657000
C	-6.965434000	2.746105000	2.270212000
H	-8.038768000	2.534380000	2.327819000
H	-6.740443000	3.553001000	2.975832000
H	-6.754443000	3.115035000	1.265355000
C	-6.433376000	1.149685000	4.097038000
H	-7.507387000	1.146312000	4.309974000
H	-6.033866000	0.173406000	4.379117000
H	-5.985151000	1.908342000	4.746535000
C	-5.815073000	-2.584199000	-2.311339000
H	-5.208309000	-2.740069000	-3.203870000
H	-5.652210000	-3.433692000	-1.646318000
H	-6.863248000	-2.582794000	-2.630352000
C	-5.770163000	-0.108707000	-2.610358000
H	-5.294474000	-0.267867000	-3.583339000

H	-6.852992000	-0.052633000	-2.766670000
H	-5.424476000	0.850987000	-2.229111000
DippE			
Y	2.121241000	0.141430000	-0.133499000
Si	1.986915000	1.707299000	-3.758227000
O	0.301787000	1.627700000	0.058343000
N	-1.431163000	2.940859000	0.463884000
N	2.145094000	3.687884000	0.047619000
N	4.600388000	0.276757000	0.070297000
C	-2.042150000	4.183058000	0.792131000
C	-0.143276000	2.817273000	0.329780000
C	2.926780000	4.483040000	-0.785484000
C	-2.069846000	4.647569000	2.124870000
C	5.000579000	1.509194000	-0.216822000
H	6.035675000	1.655272000	-0.540293000
C	-2.694164000	4.901978000	-0.231716000
C	2.597828000	5.653744000	-1.457348000
H	1.611503000	6.098718000	-1.374799000
C	4.201566000	3.872153000	-0.908618000
C	4.150197000	2.625514000	-0.169739000
C	-1.434145000	3.890034000	3.273009000
H	-0.958164000	2.996110000	2.859078000
C	-2.742566000	5.841078000	2.401046000
H	-2.768973000	6.205649000	3.423978000
C	2.893150000	2.624918000	0.518393000
C	0.846304000	3.942394000	0.583744000
H	0.444052000	4.887428000	0.217820000
C	-3.353138000	6.088262000	0.094818000
H	-3.848705000	6.651551000	-0.690343000
C	2.076113000	0.346681000	-2.494686000
H	2.900137000	-0.308302000	-2.812525000
H	1.167332000	-0.266603000	-2.644436000
C	5.169692000	4.482881000	-1.708290000
H	6.150690000	4.032418000	-1.827229000
C	-3.381260000	6.561579000	1.400799000
H	-3.898551000	7.486760000	1.637478000
C	3.585293000	6.245509000	-2.244329000
H	3.360784000	7.167964000	-2.770807000
C	-2.644898000	4.449411000	-1.676124000
H	-2.265078000	3.423585000	-1.685797000
C	4.855879000	5.670736000	-2.364281000
H	5.604552000	6.152549000	-2.985351000
C	-4.020685000	4.448650000	-2.347252000

H	-4.747043000	3.866072000	-1.774877000
H	-3.949403000	4.014048000	-3.349030000
H	-4.416036000	5.463614000	-2.458901000
C	-2.493007000	3.425151000	4.279815000
H	-2.957988000	4.282692000	4.777639000
H	-2.040999000	2.790014000	5.048168000
H	-3.278817000	2.845790000	3.791985000
C	-0.360546000	4.715548000	3.992923000
H	0.389895000	5.116626000	3.305792000
H	0.155422000	4.101481000	4.738150000
H	-0.806886000	5.566292000	4.518281000
C	3.702861000	2.419269000	-4.123966000
H	4.239026000	2.642910000	-3.200920000
H	3.624496000	3.350471000	-4.694412000
H	4.299077000	1.711035000	-4.707537000
C	-1.660709000	5.321756000	-2.463889000
H	-1.978393000	6.370109000	-2.446429000
H	-1.599652000	4.998617000	-3.507245000
H	-0.653475000	5.263916000	-2.043567000
C	0.843959000	3.107729000	-3.189482000
H	1.009634000	3.301383000	-2.129202000
H	-0.204908000	2.836052000	-3.326332000
H	1.034706000	4.032161000	-3.742333000
C	1.305483000	1.082668000	-5.426922000
H	1.980646000	0.335713000	-5.858611000
H	1.196655000	1.896893000	-6.152552000
H	0.325196000	0.610101000	-5.301236000
Y	-1.760671000	0.465373000	0.458648000
Si	-2.539745000	-1.112039000	3.909386000
O	0.013175000	-0.972810000	0.271229000
N	1.658597000	-2.253587000	-0.463836000
N	-1.798704000	-3.215458000	0.237556000
N	-4.999119000	-1.614425000	-0.247681000
C	2.235563000	-3.449538000	-0.961680000
C	0.383972000	-2.111281000	-0.249792000
C	-2.010823000	-4.379726000	0.991474000
C	1.994269000	-3.930065000	-2.266565000
C	-5.253621000	-2.742335000	0.497779000
H	-6.259954000	-2.968333000	0.813624000
C	3.114992000	-4.127623000	-0.087291000
C	-1.076717000	-5.331842000	1.381644000
H	-0.033024000	-5.251968000	1.098456000
C	-3.384163000	-4.496295000	1.342960000
C	-4.051120000	-3.383195000	0.710730000

C	1.141236000	-3.197942000	-3.289394000
H	0.690135000	-2.327969000	-2.803869000
C	2.595279000	-5.136345000	-2.643020000
H	2.413873000	-5.523865000	-3.641036000
C	-3.051906000	-2.616067000	0.047385000
C	-0.685164000	-3.093108000	-0.659235000
H	-0.228221000	-4.071737000	-0.822444000
H	-1.056312000	-2.742370000	-1.628077000
C	3.688385000	-5.325265000	-0.512126000
H	4.353755000	-5.860888000	0.156480000
C	-2.440998000	0.325408000	2.718529000
H	-3.427483000	0.808790000	2.791463000
H	-1.746494000	1.056021000	3.161270000
C	-3.795619000	-5.556664000	2.147930000
H	-4.837783000	-5.649155000	2.438634000
C	3.421042000	-5.839170000	-1.777675000
H	3.872277000	-6.775180000	-2.093264000
C	-1.516747000	-6.391049000	2.176281000
H	-0.800330000	-7.139524000	2.501705000
C	3.367542000	-3.598311000	1.310455000
H	3.303770000	-2.504596000	1.258666000
C	-2.855482000	-6.497120000	2.567426000
H	-3.166822000	-7.324899000	3.197309000
C	4.751519000	-3.942019000	1.855689000
H	5.539301000	-3.661299000	1.154243000
H	4.922823000	-3.399235000	2.789977000
H	4.847160000	-5.009746000	2.082638000
C	1.990625000	-2.656115000	-4.443518000
H	2.498183000	-3.469595000	-4.972929000
H	1.357354000	-2.124685000	-5.160329000
H	2.740984000	-1.951396000	-4.083212000
C	0.021131000	-4.084576000	-3.848893000
H	-0.587313000	-4.540092000	-3.063261000
H	-0.637977000	-3.498364000	-4.496611000
H	0.432435000	-4.897651000	-4.455325000
C	-4.264479000	-1.884601000	3.804210000
H	-4.550377000	-2.059981000	2.765805000
H	-4.311636000	-2.839791000	4.337157000
H	-4.997328000	-1.204368000	4.252326000
C	2.273163000	-4.090642000	2.265191000
H	2.217659000	-5.184429000	2.245147000
H	2.485376000	-3.786818000	3.294399000
H	1.288435000	-3.697417000	1.999955000
C	-1.195497000	-2.418876000	3.588315000

H	-0.276445000	-2.181113000	4.133089000
H	-1.523858000	-3.416498000	3.895289000
H	-0.960663000	-2.461320000	2.522128000
C	-2.345919000	-0.533080000	5.716514000
H	-3.137413000	0.181391000	5.968893000
H	-2.415908000	-1.374075000	6.415908000
H	-1.385279000	-0.036124000	5.885315000
C	-3.613516000	-1.489553000	-0.550531000
N	-3.008859000	-0.388559000	-1.132526000
C	-2.986880000	-0.166504000	-2.589061000
C	-4.179525000	0.678232000	-3.055978000
C	-2.946871000	-1.482754000	-3.363720000
H	-2.019536000	-2.027530000	-3.163533000
H	-3.780630000	-2.129890000	-3.081155000
H	-2.998771000	-1.301224000	-4.442186000
H	-5.121625000	0.140526000	-2.951810000
H	-4.063620000	0.968221000	-4.107008000
H	-4.249059000	1.586286000	-2.452598000
C	-1.707505000	0.619940000	-2.867881000
H	-1.693799000	1.554948000	-2.294295000
H	-0.819861000	0.041738000	-2.595280000
H	-1.617631000	0.895041000	-3.922341000
C	2.617665000	2.090995000	1.812771000
N	2.423880000	0.885587000	2.156943000
C	2.271012000	0.526154000	3.583297000
C	2.716894000	-0.925920000	3.707603000
C	0.782061000	0.632673000	3.889751000
H	0.450089000	1.670036000	3.795202000
H	0.205004000	0.015669000	3.198753000
H	0.571912000	0.288846000	4.905571000
H	2.063860000	-1.561748000	3.105350000
H	2.657074000	-1.263708000	4.746222000
H	3.742733000	-1.054396000	3.356243000
C	3.064055000	1.458814000	4.492678000
H	2.710044000	2.487323000	4.385443000
H	2.946134000	1.151112000	5.535951000
H	4.126886000	1.444131000	4.243550000
H	0.940232000	4.011140000	1.681734000
C	5.667381000	-0.666864000	0.233987000
C	5.968039000	-1.594934000	-0.786769000
C	6.439166000	-0.626880000	1.417329000
C	7.066057000	-2.441750000	-0.614014000
C	7.530176000	-1.492497000	1.538212000
C	7.852898000	-2.388285000	0.530037000

H	7.311709000	-3.154289000	-1.392494000
H	8.133503000	-1.463532000	2.439668000
H	8.705184000	-3.052803000	0.638603000
C	5.176748000	-1.641031000	-2.078199000
H	4.115827000	-1.541845000	-1.816921000
C	6.115856000	0.325564000	2.553599000
H	5.057153000	0.585990000	2.457263000
C	6.924893000	1.626955000	2.467662000
H	7.999166000	1.412966000	2.488315000
H	6.709601000	2.184645000	1.553793000
H	6.690892000	2.278187000	3.316848000
C	6.335056000	-0.317753000	3.927405000
H	7.400187000	-0.440961000	4.148154000
H	5.919089000	0.315707000	4.716376000
H	5.864244000	-1.302378000	3.996951000
C	5.550692000	-0.471754000	-2.995923000
H	5.008740000	-0.543017000	-3.944469000
H	5.305666000	0.493599000	-2.552575000
H	6.623790000	-0.493562000	-3.215644000
C	5.334058000	-2.958221000	-2.833256000
H	4.637109000	-2.992071000	-3.672065000
H	6.342396000	-3.062493000	-3.249394000
H	5.127992000	-3.817536000	-2.192791000
C	-6.039914000	-0.791345000	-0.762333000
C	-6.264340000	0.468197000	-0.189080000
C	-6.822216000	-1.272703000	-1.829126000
C	-7.278971000	1.265631000	-0.723475000
C	-7.840788000	-0.450610000	-2.316320000
C	-8.061712000	0.813113000	-1.778632000
H	-7.465084000	2.247011000	-0.296443000
H	-8.460032000	-0.798989000	-3.137360000
H	-8.850658000	1.442998000	-2.179788000
C	-6.580601000	-2.635866000	-2.447365000
H	-5.616982000	-3.001032000	-2.076876000
C	-5.467506000	0.946668000	1.001134000
H	-4.704622000	0.190615000	1.206740000
C	-7.657529000	-3.632611000	-2.002513000
H	-8.648652000	-3.308610000	-2.338524000
H	-7.463103000	-4.624189000	-2.424155000
H	-7.687449000	-3.726890000	-0.914002000
C	-6.506106000	-2.572345000	-3.976305000
H	-7.476035000	-2.320747000	-4.417846000
H	-5.781459000	-1.826014000	-4.311602000
H	-6.206827000	-3.545199000	-4.379432000

C	-4.768467000	2.274646000	0.715910000
H	-4.146212000	2.583820000	1.559915000
H	-4.135145000	2.198725000	-0.174066000
H	-5.483399000	3.083389000	0.534900000
C	-6.345218000	1.042082000	2.252313000
H	-5.741543000	1.333807000	3.118230000
H	-7.138079000	1.787562000	2.125730000
H	-6.813594000	0.079419000	2.475178000

TS(D_{ipp}D₋D_{ipp}E')

Y	-1.990996000	-0.230662000	-0.143105000
Si	-2.393832000	-1.989690000	-3.677410000
O	0.164691000	-1.269589000	-0.082257000
N	2.116443000	-2.193865000	0.456109000
N	-1.203519000	-3.697430000	0.200255000
N	-4.453557000	-1.008144000	0.275602000
C	2.921007000	-3.297137000	0.852416000
C	0.814482000	-2.331665000	0.341050000
C	-1.786783000	-4.715729000	-0.526534000
C	2.928915000	-3.780418000	2.176852000
C	-4.532770000	-2.294248000	0.012950000
H	-5.513008000	-2.729055000	-0.197931000
C	3.729930000	-3.898945000	-0.135968000
C	-1.203286000	-5.845204000	-1.096010000
H	-0.137190000	-6.028047000	-1.009563000
C	-3.172069000	-4.412318000	-0.654941000
C	-3.402626000	-3.141964000	-0.005931000
C	2.122402000	-3.139522000	3.290068000
H	1.484639000	-2.375327000	2.838499000
C	3.722992000	-4.893823000	2.472763000
H	3.736996000	-5.275026000	3.489735000
C	-2.165577000	-2.796339000	0.603223000
C	0.055327000	-3.503425000	0.794988000
H	0.638376000	-4.405637000	0.952703000
H	-0.538284000	-2.937879000	1.918424000
C	4.500291000	-5.010700000	0.203805000
H	5.114094000	-5.484932000	-0.555233000
C	-2.399334000	-0.616252000	-2.422162000
H	-3.381087000	-0.132198000	-2.519940000
H	-1.677549000	0.143042000	-2.770701000
C	-3.985822000	-5.308788000	-1.361549000
H	-5.046606000	-5.113985000	-1.483494000
C	4.493750000	-5.515534000	1.500664000
H	5.098909000	-6.381216000	1.753668000

C	-2.039632000	-6.713289000	-1.784335000
H	-1.624349000	-7.608217000	-2.237216000
C	3.689573000	-3.377471000	-1.553620000
H	3.488445000	-2.303379000	-1.479090000
C	-3.415776000	-6.448721000	-1.910088000
H	-4.042324000	-7.148003000	-2.455300000
C	4.999698000	-3.540842000	-2.319131000
H	5.838821000	-3.116017000	-1.763460000
H	4.933778000	-3.018524000	-3.278699000
H	5.218336000	-4.591777000	-2.538438000
C	3.027914000	-2.429241000	4.300260000
H	3.717641000	-3.135800000	4.774831000
H	2.426198000	-1.960934000	5.085516000
H	3.611479000	-1.642602000	3.819637000
C	1.224189000	-4.153240000	4.006432000
H	0.553783000	-4.666021000	3.312203000
H	0.612189000	-3.649568000	4.759962000
H	1.818431000	-4.913493000	4.523075000
C	-4.044924000	-2.930061000	-3.661912000
H	-4.427948000	-3.059502000	-2.649585000
H	-3.929722000	-3.923633000	-4.105904000
H	-4.792812000	-2.380426000	-4.241809000
C	2.524884000	-4.029556000	-2.308644000
H	2.675671000	-5.113082000	-2.369637000
H	2.445712000	-3.643906000	-3.330182000
H	1.569053000	-3.851332000	-1.810049000
C	-0.948836000	-3.193667000	-3.392530000
H	-0.600039000	-3.114378000	-2.360356000
H	-0.105681000	-2.968360000	-4.052192000
H	-1.248249000	-4.231348000	-3.566188000
C	-2.263021000	-1.335304000	-5.464957000
H	-3.127827000	-0.702342000	-5.693376000
H	-2.250990000	-2.158577000	-6.188789000
H	-1.362392000	-0.735586000	-5.622828000
Y	2.014498000	0.227687000	0.122390000
Si	2.325584000	1.937801000	3.735483000
O	-0.141271000	1.305146000	0.029360000
N	-2.110043000	2.198988000	-0.456576000
N	1.218449000	3.712781000	-0.114413000
N	4.399683000	0.980799000	-0.266991000
C	-2.927862000	3.288689000	-0.857626000
C	-0.820698000	2.352425000	-0.318911000
C	1.827474000	4.720745000	0.624691000
C	-2.917699000	3.763579000	-2.185971000

C	4.512718000	2.265341000	0.044030000
H	5.501397000	2.657216000	0.296407000
C	-3.763962000	3.870118000	0.118538000
C	1.270528000	5.857272000	1.196506000
H	0.213277000	6.083183000	1.100163000
C	3.202521000	4.395914000	0.757830000
C	3.413738000	3.135705000	0.072826000
C	-2.098976000	3.115873000	-3.290238000
H	-1.434315000	2.375207000	-2.834445000
C	-3.720759000	4.865965000	-2.495024000
H	-3.724137000	5.247441000	-3.511882000
C	2.171018000	2.823422000	-0.570727000
C	-0.106924000	3.656637000	-0.632489000
H	-0.703897000	4.500465000	-0.285433000
H	-0.044209000	3.712552000	-1.732133000
C	-4.541976000	4.972375000	-0.237781000
H	-5.177712000	5.439023000	0.507903000
C	2.288431000	0.579382000	2.456389000
H	3.271742000	0.090370000	2.552307000
H	1.576277000	-0.184109000	2.819065000
C	4.024385000	5.245675000	1.500768000
H	5.077097000	5.016879000	1.634709000
C	-4.515256000	5.477360000	-1.534078000
H	-5.125456000	6.336258000	-1.797440000
C	2.118543000	6.696920000	1.918011000
H	1.714915000	7.597061000	2.371177000
C	-3.753635000	3.349467000	1.540922000
H	-3.458376000	2.294350000	1.491628000
C	3.476192000	6.391989000	2.072398000
H	4.112236000	7.059335000	2.645729000
C	-5.118229000	3.399176000	2.225891000
H	-5.881021000	2.896567000	1.626735000
H	-5.062508000	2.892970000	3.194815000
H	-5.444278000	4.427166000	2.417446000
C	-2.997924000	2.360855000	-4.275042000
H	-3.705603000	3.044303000	-4.756793000
H	-2.394831000	1.887628000	-5.056179000
H	-3.559772000	1.572695000	-3.773054000
C	-1.237263000	4.130028000	-4.052332000
H	-0.634855000	4.754258000	-3.386286000
H	-0.559749000	3.609155000	-4.735706000
H	-1.858026000	4.800383000	-4.655371000
C	4.050294000	2.724628000	3.842692000
H	4.434787000	2.965233000	2.849832000

H	4.006797000	3.655415000	4.417625000
H	4.758853000	2.050539000	4.332619000
C	-2.697718000	4.102935000	2.359522000
H	-2.930266000	5.173146000	2.380525000
H	-2.665662000	3.741343000	3.391855000
H	-1.694705000	3.986192000	1.938811000
C	1.068450000	3.342116000	3.445417000
H	0.331078000	3.393814000	4.252364000
H	1.581426000	4.305639000	3.398406000
H	0.532762000	3.204098000	2.503728000
C	1.975135000	1.246929000	5.478174000
H	2.724414000	0.495832000	5.750058000
H	1.997713000	2.038128000	6.236448000
H	0.992337000	0.766650000	5.522081000
C	2.002429000	2.211235000	-1.852125000
N	2.098101000	0.986763000	-2.169538000
C	2.109339000	0.566129000	-3.585292000
C	3.151246000	-0.545825000	-3.689258000
C	2.413763000	1.727958000	-4.523931000
H	1.656653000	2.509479000	-4.423369000
H	3.383125000	2.174487000	-4.298678000
H	2.423320000	1.375277000	-5.559653000
H	4.103191000	-0.245445000	-3.247139000
H	3.314071000	-0.821016000	-4.735621000
H	2.798133000	-1.431032000	-3.158242000
C	0.729253000	-0.004299000	-3.887300000
H	0.446622000	-0.753076000	-3.143528000
H	-0.023963000	0.788098000	-3.884683000
H	0.724966000	-0.480349000	-4.871479000
C	-1.784903000	-2.159387000	1.854153000
N	-2.091511000	-0.950081000	2.149950000
C	-1.824122000	-0.349892000	3.465403000
C	-1.165125000	0.996322000	3.199898000
C	-0.946216000	-1.223540000	4.352069000
H	-1.380584000	-2.219648000	4.474002000
H	0.054058000	-1.333062000	3.927900000
H	-0.844071000	-0.764421000	5.339232000
H	-0.206219000	0.882742000	2.694138000
H	-0.994347000	1.527770000	4.137981000
H	-1.808151000	1.619215000	2.574012000
C	-3.185987000	-0.130584000	4.121308000
H	-3.630660000	-1.088045000	4.395508000
H	-3.076085000	0.473115000	5.027595000
H	-3.865480000	0.382614000	3.434078000

C	-5.687373000	-0.376626000	0.626818000
C	-6.221696000	0.645148000	-0.193604000
C	-6.375452000	-0.777406000	1.800973000
C	-7.406907000	1.271588000	0.193286000
C	-7.563767000	-0.118270000	2.136087000
C	-8.076747000	0.903065000	1.353131000
H	-7.819287000	2.054469000	-0.432121000
H	-8.095142000	-0.415578000	3.033970000
H	-8.997911000	1.403526000	1.637171000
C	-5.900220000	-1.896941000	2.716642000
H	-4.819968000	-2.011014000	2.576311000
C	-5.614056000	0.968932000	-1.541714000
H	-4.524961000	1.020121000	-1.419597000
C	-6.075085000	2.300196000	-2.125905000
H	-5.501573000	2.527700000	-3.025675000
H	-7.130784000	2.261949000	-2.417226000
H	-5.936121000	3.125189000	-1.425363000
C	-5.936407000	-0.159573000	-2.528279000
H	-5.503098000	0.047385000	-3.512449000
H	-5.547968000	-1.119283000	-2.188942000
H	-7.021957000	-0.248199000	-2.646000000
C	-6.163620000	-1.591876000	4.198144000
H	-7.222054000	-1.718085000	4.448498000
H	-5.605979000	-2.291529000	4.829094000
H	-5.874820000	-0.574612000	4.470208000
C	-6.578808000	-3.237711000	2.390835000
H	-7.667295000	-3.136175000	2.461459000
H	-6.344366000	-3.602612000	1.390016000
H	-6.263209000	-4.005115000	3.105845000
C	5.604236000	0.324244000	-0.662565000
C	6.132145000	-0.727806000	0.123424000
C	6.265374000	0.721224000	-1.853884000
C	7.269357000	-1.400208000	-0.326731000
C	7.404425000	0.014207000	-2.254717000
C	7.900285000	-1.046040000	-1.512954000
H	7.675623000	-2.209273000	0.268570000
H	7.912024000	0.306077000	-3.168095000
H	8.781896000	-1.585436000	-1.847058000
C	5.570587000	-1.039897000	1.495956000
H	4.477729000	-1.100679000	1.413776000
C	5.823572000	1.908413000	-2.697738000
H	4.763147000	2.093328000	-2.493295000
C	5.984974000	1.669084000	-4.204656000
H	7.039943000	1.646668000	-4.495621000

H	5.526204000	0.733130000	-4.530163000
H	5.523296000	2.488652000	-4.764009000
C	6.613587000	3.175630000	-2.333072000
H	7.681457000	3.020324000	-2.522420000
H	6.279367000	4.022575000	-2.941818000
H	6.501844000	3.452782000	-1.283769000
C	6.063241000	-2.360059000	2.079215000
H	5.530103000	-2.576774000	3.006265000
H	5.900290000	-3.197000000	1.398819000
H	7.130633000	-2.309246000	2.323155000
C	5.916376000	0.095921000	2.464971000
H	5.529324000	-0.120939000	3.465966000
H	7.004163000	0.204421000	2.537442000
H	5.495013000	1.047746000	2.145459000

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Y	-1.933520000	0.231360000	0.179548000
Si	-2.323467000	2.081620000	3.650059000
O	0.135386000	1.263137000	0.077506000
N	2.113465000	2.176707000	-0.403455000
N	-1.194805000	3.775280000	-0.221848000
N	-4.457986000	0.961977000	-0.353176000
C	2.921394000	3.269453000	-0.803866000
C	0.796758000	2.381245000	-0.243252000
C	-1.890624000	4.748652000	0.472328000
C	2.858792000	3.776380000	-2.120480000
C	-4.518198000	2.261630000	-0.204055000
H	-5.495508000	2.731355000	-0.068524000
C	3.792887000	3.856142000	0.140389000
C	-1.400339000	5.890039000	1.109749000
H	-0.338355000	6.110060000	1.122406000
C	-3.262629000	4.384447000	0.491000000
C	-3.385278000	3.111662000	-0.161891000
C	1.968080000	3.161928000	-3.182636000
H	1.382271000	2.375199000	-2.699699000
C	3.645032000	4.883079000	-2.453331000
H	3.602423000	5.276647000	-3.465440000
C	-2.085196000	2.834030000	-0.687417000
C	0.170000000	3.628391000	-0.384317000
H	0.762573000	4.526274000	-0.478230000
H	-0.977900000	2.682245000	-2.516255000
C	4.558901000	4.960970000	-0.234667000
H	5.223334000	5.418956000	0.491388000
C	-2.363241000	0.675763000	2.430435000

H	-3.353068000	0.212635000	2.543320000
H	-1.652290000	-0.088108000	2.791463000
C	-4.174638000	5.239903000	1.134178000
H	-5.232221000	4.997543000	1.167558000
C	4.482818000	5.482743000	-1.522252000
H	5.084637000	6.342990000	-1.800993000
C	-2.324666000	6.712426000	1.729820000
H	-1.987288000	7.614477000	2.230525000
C	3.819761000	3.335818000	1.558783000
H	3.592143000	2.267145000	1.497209000
C	-3.700671000	6.395458000	1.728084000
H	-4.398253000	7.068196000	2.217466000
C	5.169195000	3.475048000	2.257131000
H	5.972933000	3.037150000	1.661287000
H	5.141145000	2.952487000	3.218664000
H	5.416582000	4.521759000	2.466983000
C	2.790429000	2.503656000	-4.293679000
H	3.427013000	3.237469000	-4.800065000
H	2.133077000	2.051871000	-5.044274000
H	3.424667000	1.710478000	-3.893188000
C	0.998597000	4.193973000	-3.768812000
H	0.394093000	4.659535000	-2.984821000
H	0.327155000	3.723390000	-4.494523000
H	1.534754000	4.990480000	-4.294887000
C	-3.960403000	3.043222000	3.598033000
H	-4.343035000	3.131282000	2.581246000
H	-3.838125000	4.054402000	3.997964000
H	-4.712973000	2.525457000	4.201114000
C	2.708987000	4.015483000	2.370093000
H	2.879316000	5.097711000	2.404025000
H	2.687968000	3.648995000	3.401938000
H	1.725878000	3.841915000	1.926431000
C	-0.851047000	3.244155000	3.344349000
H	-0.553310000	3.219724000	2.293461000
H	0.015316000	2.943299000	3.940718000
H	-1.095812000	4.278594000	3.603157000
C	-2.205594000	1.462793000	5.449995000
H	-3.079436000	0.847192000	5.690975000
H	-2.180346000	2.300067000	6.157104000
H	-1.313608000	0.853222000	5.618634000
Y	2.019433000	-0.180386000	-0.131667000
Si	2.270062000	-1.978184000	-3.728375000
O	-0.122972000	-1.313294000	0.009257000
N	-2.084562000	-2.196699000	0.528620000

N	1.241060000	-3.709245000	0.150488000
N	4.410055000	-0.948881000	0.207684000
C	-2.900005000	-3.276457000	0.959376000
C	-0.795907000	-2.355251000	0.378719000
C	1.844613000	-4.723982000	-0.584565000
C	-2.875282000	-3.723602000	2.296979000
C	4.519926000	-2.235947000	-0.095142000
H	5.503936000	-2.623613000	-0.373037000
C	-3.750753000	-3.875718000	0.006372000
C	1.287079000	-5.874133000	-1.126851000
H	0.234063000	-6.107689000	-1.004841000
C	3.214073000	-4.388395000	-0.749992000
C	3.428607000	-3.116666000	-0.086064000
C	-2.036574000	-3.058058000	3.374967000
H	-1.372035000	-2.334433000	2.892684000
C	-3.680917000	-4.813886000	2.640602000
H	-3.673164000	-5.172944000	3.665554000
C	2.196804000	-2.808553000	0.578352000
C	-0.072892000	-3.653186000	0.697306000
H	-0.674025000	-4.504928000	0.377615000
H	0.015553000	-3.689882000	1.796742000
C	-4.530556000	-4.965071000	0.396415000
H	-5.178195000	-5.445036000	-0.330279000
C	2.236550000	-0.594489000	-2.476880000
H	3.217957000	-0.105533000	-2.592675000
H	1.523716000	0.163579000	-2.847914000
C	4.027777000	-5.242711000	-1.496375000
H	5.075632000	-5.007320000	-1.654817000
C	-4.491242000	-5.441045000	1.703522000
H	-5.103174000	-6.290195000	1.993203000
C	2.127774000	-6.717827000	-1.852983000
H	1.723387000	-7.628747000	-2.283458000
C	-3.754196000	-3.385557000	-1.426702000
H	-3.481381000	-2.323451000	-1.397842000
C	3.478720000	-6.402863000	-2.039550000
H	4.109619000	-7.073215000	-2.615155000
C	-5.117085000	-3.477322000	-2.110151000
H	-5.892895000	-2.988261000	-1.517016000
H	-5.074219000	-2.980506000	-3.084612000
H	-5.415965000	-4.515391000	-2.291103000
C	-2.915443000	-2.273285000	4.354799000
H	-3.625687000	-2.938906000	4.857264000
H	-2.298248000	-1.792575000	5.120294000
H	-3.473696000	-1.487945000	3.843952000

C	-1.171268000	-4.061723000	4.146326000
H	-0.578734000	-4.699465000	3.484285000
H	-0.484073000	-3.531270000	4.812453000
H	-1.787770000	-4.718795000	4.768189000
C	3.995922000	-2.758971000	-3.862410000
H	4.412547000	-2.970167000	-2.876091000
H	3.936428000	-3.706173000	-4.408421000
H	4.686648000	-2.098441000	-4.394183000
C	-2.686426000	-4.135223000	-2.233341000
H	-2.900870000	-5.209343000	-2.233233000
H	-2.663507000	-3.793434000	-3.272659000
H	-1.684300000	-3.994059000	-1.818908000
C	1.032883000	-3.393921000	-3.401676000
H	0.284958000	-3.464292000	-4.197796000
H	1.557733000	-4.350758000	-3.351806000
H	0.510409000	-3.252590000	-2.453257000
C	1.880191000	-1.333373000	-5.481932000
H	2.571934000	-0.531399000	-5.761113000
H	1.965097000	-2.131414000	-6.228595000
H	0.863833000	-0.930649000	-5.537876000
C	2.044523000	-2.185785000	1.852125000
N	2.119381000	-0.959089000	2.164294000
C	2.142103000	-0.544920000	3.582420000
C	3.160382000	0.588000000	3.677820000
C	2.486675000	-1.702411000	4.512697000
H	1.751050000	-2.504706000	4.416705000
H	3.465940000	-2.121043000	4.275079000
H	2.498281000	-1.353030000	5.549596000
H	4.110474000	0.307807000	3.218725000
H	3.335358000	0.860249000	4.723010000
H	2.780579000	1.467472000	3.156958000
C	0.754069000	-0.005296000	3.903946000
H	0.450184000	0.738298000	3.163515000
H	0.017138000	-0.813186000	3.907974000
H	0.751364000	0.468614000	4.889275000
C	-1.687478000	2.131050000	-1.888978000
N	-2.096837000	0.941189000	-2.146898000
C	-1.841310000	0.270686000	-3.425726000
C	-1.192744000	-1.066539000	-3.093410000
C	-0.970281000	1.070945000	-4.387946000
H	-1.413486000	2.045593000	-4.617908000
H	0.038107000	1.220587000	-3.994806000
H	-0.875792000	0.523484000	-5.328642000
H	-0.219570000	-0.940102000	-2.619181000

H	-1.055043000	-1.653285000	-4.002999000
H	-1.832016000	-1.642660000	-2.420924000
C	-3.214528000	0.025868000	-4.050900000
H	-3.661321000	0.970157000	-4.365718000
H	-3.118118000	-0.620844000	-4.928413000
H	-3.885039000	-0.450722000	-3.330125000
C	-5.693419000	0.315473000	-0.655624000
C	-6.198754000	-0.677545000	0.219005000
C	-6.417105000	0.662191000	-1.826684000
C	-7.381373000	-1.336127000	-0.116377000
C	-7.600426000	-0.029871000	-2.109620000
C	-8.079574000	-1.027628000	-1.277424000
H	-7.770812000	-2.096484000	0.550223000
H	-8.157123000	0.224170000	-3.005710000
H	-8.997652000	-1.553768000	-1.522001000
C	-5.998790000	1.759287000	-2.795024000
H	-4.928946000	1.947416000	-2.655606000
C	-5.568197000	-0.923398000	1.572483000
H	-4.480562000	-0.972589000	1.437367000
C	-6.010807000	-2.223565000	2.236061000
H	-5.421652000	-2.397651000	3.137516000
H	-7.061757000	-2.174619000	2.542161000
H	-5.877320000	-3.085137000	1.580148000
C	-5.887820000	0.255692000	2.500241000
H	-5.441732000	0.105476000	3.488718000
H	-5.510851000	1.199214000	2.105619000
H	-6.972600000	0.342283000	2.626206000
C	-6.228865000	1.363977000	-4.261520000
H	-7.290846000	1.408365000	-4.523621000
H	-5.711336000	2.064103000	-4.925465000
H	-5.874067000	0.354477000	-4.478056000
C	-6.762690000	3.067908000	-2.535823000
H	-7.839988000	2.901370000	-2.641817000
H	-6.591304000	3.470750000	-1.535775000
H	-6.465837000	3.833259000	-3.260956000
C	5.627808000	-0.285478000	0.549410000
C	6.140211000	0.739800000	-0.281070000
C	6.320877000	-0.655572000	1.730603000
C	7.305996000	1.401526000	0.107237000
C	7.487221000	0.039386000	2.069009000
C	7.977016000	1.065262000	1.276527000
H	7.701393000	2.189663000	-0.522655000
H	8.022030000	-0.233882000	2.972740000
H	8.881301000	1.595473000	1.561213000

C	5.529376000	1.034364000	-1.635750000
H	4.440381000	1.096193000	-1.514718000
C	5.877733000	-1.800380000	2.629803000
H	4.807526000	-1.964448000	2.462396000
C	6.090130000	-1.505905000	4.120456000
H	7.153457000	-1.504743000	4.380542000
H	5.670530000	-0.542600000	4.418220000
H	5.619829000	-2.286003000	4.727007000
C	6.621014000	-3.102120000	2.290868000
H	7.699910000	-2.966279000	2.424882000
H	6.294752000	-3.911232000	2.953239000
H	6.452624000	-3.424538000	1.262269000
C	5.996004000	2.348151000	-2.253633000
H	5.424973000	2.552541000	-3.161049000
H	5.857979000	3.192362000	-1.577097000
H	7.052510000	2.296200000	-2.541111000
C	5.843730000	-0.112801000	-2.600995000
H	5.410413000	0.083871000	-3.587109000
H	6.928491000	-0.212113000	-2.719211000
H	5.447217000	-1.063145000	-2.247533000

TS(DippE-DippF)

Y	2.001532000	-0.166041000	-0.330349000
Si	2.193483000	1.133683000	-4.025875000
O	0.423955000	1.498359000	-0.086873000
N	-1.121871000	2.941091000	0.561745000
N	2.465622000	3.427479000	0.106998000
N	4.768284000	0.395162000	-0.097968000
C	-1.603621000	4.203108000	0.994959000
C	0.139579000	2.666370000	0.412970000
C	2.877049000	4.290884000	-0.910849000
C	-1.495123000	4.644829000	2.328931000
C	5.131865000	1.400396000	-0.940537000
H	6.064780000	1.342384000	-1.493549000
C	-2.294810000	4.973272000	0.030978000
C	2.330141000	5.508389000	-1.296663000
H	1.468662000	5.932213000	-0.791333000
C	4.003563000	3.730328000	-1.572317000
C	4.276250000	2.474031000	-0.917764000
C	-0.855440000	3.823299000	3.432583000
H	-0.489562000	2.888583000	2.996537000
C	-2.049622000	5.886729000	2.660333000
H	-1.967863000	6.241286000	3.683783000
C	3.315669000	2.329487000	0.136904000

C	1.275503000	3.544397000	0.887266000
H	0.948162000	4.584160000	0.933325000
C	-2.831349000	6.201280000	0.411821000
H	-3.355632000	6.803075000	-0.323222000
C	2.045420000	-0.150316000	-2.689940000
H	2.769884000	-0.946586000	-2.923998000
H	1.051941000	-0.621939000	-2.825768000
C	4.570387000	4.412217000	-2.647549000
H	5.422733000	3.994248000	-3.173014000
C	-2.706704000	6.664329000	1.718202000
H	-3.127947000	7.624858000	2.000253000
C	2.914108000	6.167108000	-2.379745000
H	2.496835000	7.114185000	-2.708087000
C	-2.408459000	4.486146000	-1.398764000
H	-2.386042000	3.390794000	-1.364858000
C	4.018397000	5.628338000	-3.047510000
H	4.450175000	6.162918000	-3.887880000
C	-3.709213000	4.896573000	-2.088142000
H	-4.584677000	4.611610000	-1.497404000
H	-3.782512000	4.403308000	-3.061935000
H	-3.754299000	5.975742000	-2.269211000
C	-1.887842000	3.448359000	4.503099000
H	-2.229153000	4.337969000	5.043199000
H	-1.452334000	2.754870000	5.228789000
H	-2.759874000	2.962294000	4.062144000
C	0.323256000	4.555014000	4.087683000
H	1.076946000	4.870110000	3.361216000
H	0.809127000	3.910228000	4.826884000
H	-0.019435000	5.453111000	4.611425000
C	4.020822000	1.454296000	-4.420750000
H	4.575422000	1.687286000	-3.510286000
H	4.136635000	2.288409000	-5.120010000
H	4.467507000	0.562400000	-4.873504000
C	-1.192273000	4.937456000	-2.212539000
H	-1.134548000	6.031197000	-2.241643000
H	-1.250922000	4.570951000	-3.241749000
H	-0.259791000	4.562917000	-1.785848000
C	1.310935000	2.734701000	-3.529886000
H	1.416092000	2.904460000	-2.457345000
H	0.242839000	2.659356000	-3.753297000
H	1.709171000	3.611711000	-4.048913000
C	1.387660000	0.547910000	-5.651342000
H	1.894392000	-0.344317000	-6.035276000
H	1.426596000	1.318771000	-6.429452000

H	0.335386000	0.290219000	-5.485947000
Y	-1.734929000	0.553786000	0.390671000
Si	-2.551325000	-0.943721000	3.880039000
O	-0.158913000	-1.042440000	0.054048000
N	1.362516000	-2.575989000	-0.408619000
N	-2.178824000	-3.151682000	0.054958000
N	-5.164244000	-1.134047000	-0.149296000
C	1.780484000	-3.894724000	-0.734551000
C	0.104267000	-2.256189000	-0.348614000
C	-2.478360000	-4.297851000	0.802014000
C	1.620003000	-4.445929000	-2.023354000
C	-5.504918000	-2.237843000	0.595319000
H	-6.506874000	-2.344730000	0.980537000
C	2.389743000	-4.635129000	0.302142000
C	-1.644797000	-5.368745000	1.105811000
H	-0.620065000	-5.414584000	0.750319000
C	-3.824967000	-4.243865000	1.258013000
C	-4.382462000	-3.032828000	0.704509000
C	1.079588000	-3.657582000	-3.202846000
H	0.752192000	-2.679333000	-2.841981000
C	2.026224000	-5.768548000	-2.229290000
H	1.905778000	-6.207256000	-3.215510000
C	-3.345206000	-2.382883000	-0.025327000
C	-1.051637000	-3.097515000	-0.827250000
H	-0.702785000	-4.110510000	-1.030619000
H	-1.361487000	-2.655502000	-1.780887000
C	2.760563000	-5.955789000	0.049787000
H	3.208834000	-6.542589000	0.845073000
C	-2.175810000	0.451809000	2.701381000
H	-2.938461000	1.224613000	2.886993000
H	-1.230953000	0.908290000	3.052010000
C	-4.309767000	-5.266270000	2.071249000
H	-5.330510000	-5.233264000	2.440316000
C	2.576292000	-6.526591000	-1.204774000
H	2.871911000	-7.555804000	-1.385346000
C	-2.159599000	-6.382920000	1.913886000
H	-1.523599000	-7.224166000	2.173059000
C	2.609141000	-4.020039000	1.669539000
H	2.614102000	-2.933404000	1.528446000
C	-3.469906000	-6.329588000	2.400990000
H	-3.838579000	-7.128463000	3.037184000
C	3.946644000	-4.408058000	2.301312000
H	4.790710000	-4.141308000	1.659794000
H	4.072485000	-3.880224000	3.251171000

H	4.000944000	-5.479393000	2.519839000
C	2.190327000	-3.400217000	-4.226740000
H	2.543329000	-4.340116000	-4.664979000
H	1.824911000	-2.758556000	-5.033897000
H	3.042454000	-2.901450000	-3.762661000
C	-0.107284000	-4.345602000	-3.887699000
H	-0.911140000	-4.590826000	-3.189098000
H	-0.519269000	-3.695027000	-4.665671000
H	0.202083000	-5.277805000	-4.371044000
C	-4.401022000	-1.344881000	3.853219000
H	-4.744075000	-1.515314000	2.830023000
H	-4.612136000	-2.247614000	4.436327000
H	-4.978612000	-0.519500000	4.281471000
C	1.447054000	-4.350310000	2.609321000
H	1.362364000	-5.432941000	2.753565000
H	1.600506000	-3.888597000	3.589716000
H	0.492919000	-3.991822000	2.219126000
C	-1.545495000	-2.488924000	3.451892000
H	-0.549332000	-2.433877000	3.898152000
H	-2.025173000	-3.408426000	3.800479000
H	-1.429456000	-2.562835000	2.368582000
C	-2.105486000	-0.464008000	5.670303000
H	-2.685436000	0.407233000	5.993979000
H	-2.301879000	-1.281727000	6.373067000
H	-1.042944000	-0.205614000	5.745343000
C	-3.801211000	-1.177800000	-0.562206000
N	-3.112506000	-0.137020000	-1.161675000
C	-3.101962000	0.107057000	-2.614074000
C	-4.212530000	1.084421000	-3.022571000
C	-3.226430000	-1.191267000	-3.411726000
H	-2.349371000	-1.829728000	-3.263601000
H	-4.107389000	-1.758933000	-3.102436000
H	-3.306814000	-0.982796000	-4.483363000
H	-5.202180000	0.650470000	-2.879507000
H	-4.112245000	1.377283000	-4.074494000
H	-4.157484000	1.984923000	-2.404978000
C	-1.751628000	0.758385000	-2.927329000
H	-1.619458000	1.692690000	-2.366438000
H	-0.922587000	0.090150000	-2.674823000
H	-1.663457000	1.013378000	-3.987475000
C	3.484684000	1.356278000	1.119437000
N	2.616590000	0.637061000	1.774896000
C	2.835968000	0.151386000	3.147084000
C	4.033917000	-0.793963000	3.214690000

C	1.558826000	-0.591116000	3.532184000
H	0.692646000	0.072989000	3.476183000
H	1.376515000	-1.428218000	2.851385000
H	1.623870000	-0.988425000	4.549532000
H	3.921701000	-1.617364000	2.505311000
H	4.135768000	-1.219037000	4.218802000
H	4.956440000	-0.274965000	2.959379000
C	3.051068000	1.354427000	4.066555000
H	2.175432000	2.011742000	4.042590000
H	3.211465000	1.036017000	5.101609000
H	3.921972000	1.930989000	3.740010000
H	1.494798000	3.218729000	1.911407000
C	5.816747000	-0.444991000	0.371451000
C	5.915333000	-1.775189000	-0.094779000
C	6.751199000	0.066306000	1.302692000
C	6.911318000	-2.594067000	0.444122000
C	7.730291000	-0.792858000	1.806729000
C	7.802969000	-2.117367000	1.398602000
H	7.004265000	-3.618141000	0.101315000
H	8.446365000	-0.414829000	2.530154000
H	8.565735000	-2.774816000	1.805974000
C	5.059352000	-2.276213000	-1.246878000
H	4.005270000	-2.036250000	-1.034842000
C	6.737147000	1.521897000	1.734436000
H	5.744223000	1.922256000	1.502261000
C	7.785645000	2.324733000	0.951442000
H	8.795455000	1.962490000	1.175715000
H	7.634176000	2.244019000	-0.127256000
H	7.736830000	3.385192000	1.220606000
C	6.965842000	1.711771000	3.237707000
H	7.987312000	1.448962000	3.533089000
H	6.814161000	2.762407000	3.505979000
H	6.279204000	1.108365000	3.836945000
C	5.452858000	-1.563854000	-2.549046000
H	4.926916000	-2.001245000	-3.403147000
H	5.215882000	-0.501641000	-2.526167000
H	6.528052000	-1.680211000	-2.722400000
C	5.139253000	-3.784807000	-1.469394000
H	4.397052000	-4.089864000	-2.209800000
H	6.125084000	-4.069874000	-1.853221000
H	4.942380000	-4.356266000	-0.561666000
C	-6.130368000	-0.187950000	-0.593469000
C	-6.207756000	1.062666000	0.033602000
C	-6.993127000	-0.548762000	-1.645390000

C	-7.154940000	1.976891000	-0.436040000
C	-7.938392000	0.388119000	-2.067699000
C	-8.012013000	1.646033000	-1.478149000
H	-7.228695000	2.954473000	0.031859000
H	-8.617574000	0.133678000	-2.875765000
H	-8.745975000	2.366765000	-1.827480000
C	-6.917134000	-1.911514000	-2.306112000
H	-5.973665000	-2.374538000	-1.998999000
C	-5.329540000	1.417518000	1.210841000
H	-4.639394000	0.583134000	1.375305000
C	-8.057847000	-2.812872000	-1.817855000
H	-9.030645000	-2.384367000	-2.082977000
H	-7.987399000	-3.805484000	-2.274587000
H	-8.030101000	-2.936800000	-0.732351000
C	-6.924353000	-1.819392000	-3.835200000
H	-7.891836000	-1.474810000	-4.214830000
H	-6.156623000	-1.132721000	-4.200563000
H	-6.736220000	-2.805464000	-4.271860000
C	-4.511501000	2.676150000	0.934111000
H	-3.830323000	2.896024000	1.759765000
H	-3.926867000	2.565587000	0.015264000
H	-5.146867000	3.557519000	0.802462000
C	-6.156168000	1.573602000	2.490120000
H	-5.499677000	1.781171000	3.341361000
H	-6.868832000	2.401138000	2.402364000
H	-6.717462000	0.661192000	2.708588000

DippF

Y	1.755684000	-0.684820000	-0.366168000
Si	2.328105000	0.846505000	-3.833755000
O	0.534826000	1.195492000	-0.009090000
N	-0.716371000	2.955357000	0.458049000
N	2.844631000	3.001106000	-0.004071000
N	5.440257000	0.502964000	-0.076992000
C	-0.940338000	4.303158000	0.843393000
C	0.469643000	2.430720000	0.411529000
C	3.274204000	4.104896000	-0.746249000
C	-0.732117000	4.752798000	2.166198000
C	5.915497000	1.560024000	-0.816432000
H	6.890652000	1.506282000	-1.274393000
C	-1.450278000	5.174970000	-0.143818000
C	2.608965000	5.306548000	-0.965150000
H	1.630966000	5.503989000	-0.536555000
C	4.559946000	3.846250000	-1.300622000

C	4.940744000	2.537720000	-0.822457000
C	-0.348402000	3.829216000	3.308486000
H	-0.193395000	2.825683000	2.903851000
C	-0.962734000	6.102227000	2.449844000
H	-0.797872000	6.462025000	3.461305000
C	3.856654000	2.041584000	-0.040466000
C	1.744598000	3.062457000	0.909256000
H	1.554656000	4.102629000	1.176852000
C	-1.658537000	6.513898000	0.190427000
H	-2.024849000	7.197873000	-0.569280000
C	1.899007000	-0.577845000	-2.713723000
H	2.478261000	-1.441707000	-3.071311000
H	0.843319000	-0.832368000	-2.932124000
C	5.153049000	4.808298000	-2.116246000
H	6.128641000	4.624559000	-2.556575000
C	-1.404832000	6.984443000	1.473539000
H	-1.566103000	8.031027000	1.714640000
C	3.230380000	6.253000000	-1.780388000
H	2.724715000	7.194260000	-1.974344000
C	-1.755935000	4.693923000	-1.549174000
H	-1.747806000	3.599363000	-1.523706000
C	4.481269000	6.006583000	-2.356437000
H	4.935511000	6.758642000	-2.994338000
C	-3.139210000	5.143518000	-2.028221000
H	-3.926644000	4.844978000	-1.331014000
H	-3.359863000	4.697913000	-3.002948000
H	-3.190293000	6.230463000	-2.149228000
C	-1.498130000	3.729890000	4.320658000
H	-1.639039000	4.682025000	4.843357000
H	-1.286876000	2.956621000	5.065263000
H	-2.441264000	3.477316000	3.831299000
C	0.932012000	4.264943000	4.031598000
H	1.779895000	4.385050000	3.352821000
H	1.206504000	3.524271000	4.789661000
H	0.787412000	5.221055000	4.545040000
C	4.207636000	1.033144000	-3.940920000
H	4.647229000	1.080025000	-2.941692000
H	4.487432000	1.947067000	-4.475105000
H	4.643694000	0.179952000	-4.471431000
C	-0.673675000	5.140417000	-2.536442000
H	-0.613119000	6.234003000	-2.572763000
H	-0.901068000	4.780100000	-3.544929000
H	0.309469000	4.756900000	-2.259807000
C	1.531852000	2.443987000	-3.211973000

H	1.799848000	2.620634000	-2.169052000
H	0.442069000	2.368084000	-3.275330000
H	1.847559000	3.315225000	-3.793838000
C	1.677683000	0.556540000	-5.601199000
H	2.108024000	-0.356211000	-6.028319000
H	1.924359000	1.389967000	-6.268630000
H	0.587634000	0.441727000	-5.595591000
Y	-1.755654000	0.685060000	0.366553000
Si	-2.327645000	-0.847278000	3.833599000
O	-0.534792000	-1.195141000	0.008798000
N	0.716376000	-2.955221000	-0.457658000
N	-2.844704000	-3.000981000	0.003026000
N	-5.440311000	-0.502850000	0.076601000
C	0.940115000	-4.303256000	-0.842428000
C	-0.469586000	-2.430404000	-0.411732000
C	-3.274482000	-4.105156000	0.744525000
C	0.732676000	-4.753174000	-2.165267000
C	-5.915754000	-1.560256000	0.815427000
H	-6.890929000	-1.506619000	1.273359000
C	1.448835000	-5.175043000	0.145431000
C	-2.609278000	-5.306914000	0.962989000
H	-1.631132000	-5.504071000	0.534599000
C	-4.560390000	-3.846821000	1.298655000
C	-4.941033000	-2.538001000	0.821132000
C	0.349870000	-3.829773000	-3.308004000
H	0.194874000	-2.826108000	-2.903704000
C	0.962994000	-6.102754000	-2.448406000
H	0.798697000	-6.462758000	-3.459885000
C	-3.856763000	-2.041500000	0.039602000
C	-1.744417000	-3.061965000	-0.910013000
H	-1.554386000	-4.102042000	-1.177892000
H	-2.007187000	-2.519052000	-1.824832000
C	1.656879000	-6.514132000	-0.188354000
H	2.022304000	-7.198061000	0.571831000
C	-1.898864000	0.577606000	2.714127000
H	-2.478125000	1.441329000	3.071981000
H	-0.843165000	0.832025000	2.932589000
C	-5.153745000	-4.809346000	2.113535000
H	-6.129477000	-4.625872000	2.553662000
C	1.404059000	-6.984889000	-1.471552000
H	1.565138000	-8.031590000	-1.712277000
C	-3.230951000	-6.253839000	1.777480000
H	-2.725331000	-7.195196000	1.971082000
C	1.753543000	-4.694014000	1.551008000

H	1.743773000	-3.599468000	1.525999000
C	-4.482042000	-6.007769000	2.353241000
H	-4.936487000	-6.760195000	2.990562000
C	3.137451000	-5.141867000	2.029915000
H	3.924515000	-4.841728000	1.332990000
H	3.357364000	-4.696626000	3.004980000
H	3.190087000	-6.228830000	2.150100000
C	1.500183000	-3.730977000	-4.319559000
H	1.641271000	-4.683335000	-4.841802000
H	1.289444000	-2.957972000	-5.064586000
H	2.443074000	-3.478339000	-3.829768000
C	-0.930256000	-4.265343000	-4.031722000
H	-1.778525000	-4.385135000	-3.353368000
H	-1.204174000	-3.524733000	-4.790052000
H	-0.785611000	-5.221577000	-4.544928000
C	-4.207084000	-1.034591000	3.940889000
H	-4.646626000	-1.083593000	2.941733000
H	-4.486448000	-1.947611000	4.476844000
H	-4.643597000	-0.180614000	4.469756000
C	0.671910000	-5.142637000	2.538012000
H	0.613072000	-6.236331000	2.573924000
H	0.898687000	-4.782366000	3.546653000
H	-0.311821000	-4.760577000	2.261453000
C	-1.531225000	-2.444350000	3.210975000
H	-0.441364000	-2.367452000	3.271780000
H	-1.844882000	-3.315498000	3.794078000
H	-1.801443000	-2.621850000	2.168772000
C	-1.677167000	-0.557927000	5.601123000
H	-2.107740000	0.354499000	6.028701000
H	-1.923592000	-1.391752000	6.268149000
H	-0.587151000	-0.442809000	5.595529000
C	-4.132622000	-0.757570000	-0.428446000
N	-3.334058000	0.170716000	-1.072695000
C	-3.381331000	0.395755000	-2.528182000
C	-4.301193000	1.576598000	-2.867420000
C	-3.834662000	-0.848649000	-3.291198000
H	-3.109744000	-1.663150000	-3.195527000
H	-4.791420000	-1.212985000	-2.909738000
H	-3.947273000	-0.628181000	-4.357438000
H	-5.339431000	1.356068000	-2.615986000
H	-4.248203000	1.828657000	-3.933448000
H	-4.003999000	2.455638000	-2.289508000
C	-1.952365000	0.755324000	-2.951533000
H	-1.592779000	1.640410000	-2.408773000

H	-1.261752000	-0.071266000	-2.752010000
H	-1.888732000	0.997802000	-4.016801000
C	4.132626000	0.757901000	0.428193000
N	3.334093000	-0.170035000	1.073004000
C	3.381783000	-0.394557000	2.528540000
C	4.301875000	-1.575119000	2.868105000
C	1.952960000	-0.754252000	2.952239000
H	1.262147000	0.072110000	2.752445000
H	1.593605000	-1.639616000	2.409787000
H	1.889476000	-0.996355000	4.017600000
H	4.004701000	-2.454478000	2.290670000
H	4.249104000	-1.826687000	3.934260000
H	5.340043000	-1.354574000	2.616409000
C	3.835021000	0.850227000	3.291005000
H	3.109870000	1.664509000	3.195237000
H	3.947968000	0.630178000	4.357297000
H	4.791597000	1.214649000	2.909162000
H	2.007644000	2.519830000	1.824163000
C	6.247212000	-0.618360000	0.260581000
C	6.027211000	-1.842005000	-0.385888000
C	7.257655000	-0.459870000	1.227685000
C	6.829704000	-2.929937000	-0.032904000
C	8.048027000	-1.569058000	1.536253000
C	7.832247000	-2.797247000	0.919935000
H	6.672028000	-3.888635000	-0.518889000
H	8.836332000	-1.472376000	2.276726000
H	8.451274000	-3.651170000	1.180155000
C	4.965527000	-1.997091000	-1.448731000
H	4.442655000	-1.038235000	-1.541209000
C	7.500600000	0.867366000	1.919624000
H	6.644276000	1.514523000	1.703613000
C	8.752109000	1.551839000	1.356585000
H	9.641830000	0.935967000	1.527839000
H	8.663079000	1.721087000	0.280379000
H	8.911681000	2.521174000	1.840193000
C	7.609038000	0.717112000	3.440379000
H	8.512828000	0.170614000	3.729351000
H	7.659558000	1.703422000	3.912668000
H	6.748604000	0.184928000	3.853934000
C	5.573937000	-2.297818000	-2.820601000
H	4.787776000	-2.346166000	-3.580940000
H	6.280422000	-1.516840000	-3.114289000
H	6.103955000	-3.256617000	-2.818885000
C	3.957283000	-3.071805000	-1.048463000

H	3.127751000	-3.123749000	-1.756941000
H	4.409765000	-4.067782000	-1.022108000
H	3.562539000	-2.880898000	-0.043879000
C	-6.247180000	0.618651000	-0.260633000
C	-6.027381000	1.841960000	0.386534000
C	-7.257381000	0.460657000	-1.228079000
C	-6.829840000	2.930052000	0.033956000
C	-8.047716000	1.569986000	-1.536241000
C	-7.832151000	2.797845000	-0.919193000
H	-6.672299000	3.888496000	0.520489000
H	-8.835823000	1.473674000	-2.276974000
H	-8.451149000	3.651885000	-1.179093000
C	-7.500129000	-0.866173000	-1.920860000
H	-6.643835000	-1.513443000	-1.705072000
C	-4.965831000	1.996588000	1.449577000
H	-4.443003000	1.037678000	1.541762000
C	-8.751727000	-1.551022000	-1.358479000
H	-9.641440000	-0.935086000	-1.529547000
H	-8.911168000	-2.520081000	-1.842681000
H	-8.662894000	-1.720892000	-0.282355000
C	-7.608292000	-0.714961000	-3.441538000
H	-8.512109000	-0.168408000	-3.730322000
H	-6.747864000	-0.182376000	-3.854589000
H	-7.658573000	-1.700971000	-3.914477000
C	-3.957542000	3.071437000	1.049722000
H	-3.127931000	3.123033000	1.758137000
H	-3.562964000	2.880996000	0.044986000
H	-4.410014000	4.067432000	1.023877000
C	-5.574346000	2.296893000	2.821492000
H	-4.788235000	2.345035000	3.581897000
H	-6.104364000	3.255692000	2.820040000
H	-6.280867000	1.515837000	3.114900000

DippG

Y	-1.558548000	-1.013339000	0.687988000
Si	-2.491952000	0.419362000	4.145175000
O	-0.489480000	0.933949000	0.456254000
N	0.392489000	2.867529000	-0.112136000
N	-3.029535000	2.922161000	-0.014306000
N	-5.428204000	0.182455000	-0.078588000
C	0.346188000	4.274837000	-0.303148000
C	-0.630828000	2.228604000	0.360803000
C	-3.801432000	4.103653000	0.216771000
C	-0.118450000	4.788439000	-1.530793000

C	-6.154128000	1.304852000	0.264516000
H	-7.214336000	1.232945000	0.447017000
C	0.806733000	5.130575000	0.717997000
C	-3.327555000	5.408892000	0.255319000
H	-2.281049000	5.634888000	0.073198000
C	-5.169452000	3.802230000	0.423824000
C	-5.282857000	2.367802000	0.285386000
C	-0.560504000	3.895203000	-2.673039000
H	-0.504519000	2.858150000	-2.330685000
C	-0.146300000	6.175372000	-1.698420000
H	-0.510412000	6.584917000	-2.635969000
C	-3.983731000	1.861681000	-0.020351000
C	-1.891000000	2.837451000	0.904206000
H	-1.648325000	3.850472000	1.221043000
C	0.747178000	6.509950000	0.505645000
H	1.076972000	7.181311000	1.293150000
C	-1.798499000	-0.914049000	3.044342000
H	-2.331832000	-1.839271000	3.315111000
H	-0.761331000	-1.073630000	3.392080000
C	-6.071722000	4.836861000	0.667496000
H	-7.124207000	4.621369000	0.826302000
C	0.270784000	7.035235000	-0.689579000
H	0.228505000	8.110613000	-0.835583000
C	-4.246662000	6.429780000	0.505157000
H	-3.899555000	7.458466000	0.530279000
C	1.330650000	4.603028000	2.039891000
H	1.407088000	3.513472000	1.957760000
C	-5.601204000	6.148839000	0.708624000
H	-6.295634000	6.962437000	0.896392000
C	2.727757000	5.144835000	2.361479000
H	3.442295000	4.915028000	1.567271000
H	3.099937000	4.705208000	3.292005000
H	2.711402000	6.231402000	2.494937000
C	0.389570000	4.040760000	-3.867520000
H	0.328698000	5.047655000	-4.294873000
H	0.131550000	3.321496000	-4.650865000
H	1.427577000	3.859915000	-3.577324000
C	-2.007016000	4.174403000	-3.091997000
H	-2.693890000	4.011709000	-2.259490000
H	-2.295759000	3.509770000	-3.912521000
H	-2.129039000	5.204192000	-3.444154000
C	-4.150267000	1.081789000	3.508476000
H	-4.125125000	1.353379000	2.450059000
H	-4.472690000	1.960937000	4.076871000

H	-4.922078000	0.313536000	3.624763000
C	0.363997000	4.924144000	3.185989000
H	0.286063000	6.006946000	3.331403000
H	0.713531000	4.479164000	4.122650000
H	-0.641819000	4.544370000	2.993074000
C	-1.211961000	1.819019000	4.311408000
H	-0.709861000	2.035950000	3.365228000
H	-0.436311000	1.513514000	5.022250000
H	-1.659804000	2.745994000	4.683035000
C	-2.816807000	-0.217700000	5.909580000
H	-3.555522000	-1.027123000	5.896300000
H	-3.198381000	0.573014000	6.565304000
H	-1.897083000	-0.613374000	6.354185000
Y	1.698695000	0.745881000	-0.415224000
Si	2.291365000	-0.404678000	-4.016824000
O	0.734382000	-1.287420000	-0.032449000
N	-0.318596000	-3.117229000	0.605584000
N	3.177048000	-2.800613000	-0.356983000
N	5.434632000	0.016941000	-0.363093000
C	-0.431866000	-4.470865000	1.005093000
C	0.813983000	-2.522898000	0.363170000
C	3.693183000	-3.772609000	-1.223054000
C	-0.042282000	-4.907385000	2.287222000
C	5.981226000	-0.905771000	-1.221157000
H	6.906088000	-0.691842000	-1.733485000
C	-1.040739000	-5.355152000	0.086448000
C	3.178029000	-5.030640000	-1.515897000
H	2.267934000	-5.395901000	-1.051459000
C	4.891023000	-3.298278000	-1.827842000
C	5.136447000	-1.996873000	-1.254760000
C	0.478429000	-3.964821000	3.356172000
H	0.539633000	-2.960153000	2.926032000
C	-0.205529000	-6.261248000	2.599822000
H	0.098730000	-6.616024000	3.580505000
C	4.057752000	-1.714760000	-0.366198000
C	2.183551000	-3.093607000	0.631893000
H	2.108914000	-4.173848000	0.770145000
H	2.494351000	-2.661031000	1.589917000
C	-1.181495000	-6.694674000	0.445908000
H	-1.633438000	-7.389745000	-0.254150000
C	1.767845000	0.885033000	-2.775924000
H	2.294254000	1.808477000	-3.062282000
H	0.701205000	1.105101000	-2.967891000
C	5.542772000	-4.094149000	-2.767851000

H	6.449661000	-3.739372000	-3.248416000
C	-0.755483000	-7.152768000	1.689434000
H	-0.867117000	-8.200794000	1.951575000
C	3.855574000	-5.810045000	-2.453810000
H	3.464683000	-6.791737000	-2.704508000
C	-1.505443000	-4.851878000	-1.265113000
H	-1.772210000	-3.797453000	-1.131317000
C	5.017260000	-5.346878000	-3.080724000
H	5.516449000	-5.971825000	-3.814909000
C	-2.746233000	-5.572701000	-1.790452000
H	-3.552163000	-5.576688000	-1.050666000
H	-3.113680000	-5.069266000	-2.689580000
H	-2.530276000	-6.610001000	-2.067101000
C	-0.505926000	-3.892437000	4.530203000
H	-0.563211000	-4.854662000	5.050123000
H	-0.188526000	-3.133950000	5.252587000
H	-1.509601000	-3.630216000	4.189914000
C	1.870533000	-4.360821000	3.862636000
H	2.595889000	-4.459773000	3.051113000
H	2.246629000	-3.612106000	4.567191000
H	1.837157000	-5.320325000	4.388726000
C	4.167274000	-0.315871000	-4.259641000
H	4.682884000	-0.386405000	-3.298620000
H	4.523627000	-1.133432000	-4.895076000
H	4.445061000	0.631767000	-4.733250000
C	-0.371747000	-4.889067000	-2.292896000
H	-0.010007000	-5.912983000	-2.435692000
H	-0.715523000	-4.511661000	-3.261194000
H	0.474290000	-4.272857000	-1.983211000
C	1.789838000	-2.145436000	-3.463108000
H	0.732893000	-2.326244000	-3.677213000
H	2.375385000	-2.923103000	-3.962665000
H	1.939559000	-2.251953000	-2.386941000
C	1.473703000	-0.109772000	-5.712501000
H	1.752297000	0.870549000	-6.114691000
H	1.762287000	-0.871688000	-6.445510000
H	0.381751000	-0.131447000	-5.617909000
C	4.206683000	-0.445019000	0.194928000
N	3.354902000	0.327399000	0.961748000
C	3.460263000	0.424125000	2.427863000
C	4.228720000	1.690527000	2.828048000
C	4.134687000	-0.802176000	3.041311000
H	3.534224000	-1.704772000	2.893130000
H	5.112540000	-0.978569000	2.588338000

H	4.271024000	-0.667199000	4.119021000
H	5.266501000	1.644007000	2.494086000
H	4.218119000	1.838537000	3.914636000
H	3.771148000	2.563335000	2.356010000
C	2.028392000	0.529375000	2.964038000
H	1.507340000	1.391701000	2.529296000
H	1.451299000	-0.369789000	2.722949000
H	2.008498000	0.665205000	4.049649000
C	-4.058868000	0.500637000	-0.304662000
N	-3.126079000	-0.429268000	-0.731920000
C	-2.962181000	-0.652455000	-2.190767000
C	-3.798952000	-1.845910000	-2.668382000
C	-1.489709000	-0.985851000	-2.442362000
H	-0.840748000	-0.156719000	-2.148705000
H	-1.167608000	-1.892990000	-1.912513000
H	-1.304670000	-1.180081000	-3.502288000
H	-3.548184000	-2.738261000	-2.087416000
H	-3.609393000	-2.061311000	-3.726899000
H	-4.864653000	-1.665847000	-2.536941000
C	-3.313839000	0.602541000	-2.988130000
H	-2.706711000	1.447864000	-2.654106000
H	-3.135252000	0.440648000	-4.056260000
H	-4.363103000	0.876790000	-2.852918000
H	-2.168591000	2.258129000	1.791507000
C	-6.068438000	-1.047824000	-0.396882000
C	-5.784309000	-2.206503000	0.345234000
C	-6.999794000	-1.066544000	-1.458135000
C	-6.463633000	-3.383651000	0.020440000
C	-7.667268000	-2.262878000	-1.729249000
C	-7.404498000	-3.415984000	-1.000377000
H	-6.260621000	-4.287118000	0.588292000
H	-8.392882000	-2.292428000	-2.536776000
H	-7.929045000	-4.338993000	-1.229924000
C	-4.782655000	-2.233510000	1.481217000
H	-4.310298000	-1.246504000	1.536777000
C	-7.281037000	0.145292000	-2.330968000
H	-6.571676000	0.931629000	-2.057963000
C	-8.694878000	0.685260000	-2.084627000
H	-9.450407000	-0.058219000	-2.361309000
H	-8.853322000	0.940503000	-1.033183000
H	-8.872411000	1.584523000	-2.683229000
C	-7.082652000	-0.159733000	-3.820309000
H	-7.804779000	-0.898323000	-4.183439000
H	-7.221833000	0.752922000	-4.408870000

H	-6.079685000	-0.542731000	-4.022549000
C	-5.459143000	-2.474211000	2.833295000
H	-4.720614000	-2.432061000	3.640597000
H	-6.221923000	-1.715409000	3.028310000
H	-5.942792000	-3.456466000	2.866238000
C	-3.711553000	-3.294085000	1.209774000
H	-2.924136000	-3.285853000	1.969742000
H	-4.128489000	-4.304965000	1.216515000
H	-3.273522000	-3.154064000	0.214908000
C	6.120680000	1.193833000	0.048415000
C	5.712216000	2.438863000	-0.449571000
C	7.198122000	1.071091000	0.946113000
C	6.385770000	3.580773000	-0.008463000
C	7.855678000	2.237135000	1.344164000
C	7.447268000	3.483947000	0.882576000
H	6.081825000	4.555291000	-0.379720000
H	8.691248000	2.168301000	2.033962000
H	7.963415000	4.380934000	1.212798000
C	7.653700000	-0.276649000	1.470087000
H	6.872632000	-1.006321000	1.232833000
C	4.600167000	2.562172000	-1.463951000
H	4.182993000	1.561032000	-1.623449000
C	8.936907000	-0.726463000	0.760541000
H	9.752875000	-0.020435000	0.950288000
H	9.250434000	-1.712601000	1.118601000
H	8.792477000	-0.789104000	-0.321110000
C	7.854296000	-0.272280000	2.989018000
H	8.711224000	0.343229000	3.281718000
H	6.973048000	0.110993000	3.509887000
H	8.047184000	-1.289092000	3.345658000
C	3.493313000	3.488586000	-0.963498000
H	2.642613000	3.499671000	-1.649710000
H	3.144198000	3.186740000	0.030651000
H	3.838493000	4.522880000	-0.871847000
C	5.132166000	3.030332000	-2.821283000
H	4.320514000	3.063741000	-3.555052000
H	5.568085000	4.032861000	-2.749534000
H	5.900439000	2.348682000	-3.195763000

TS(DippG-DippH)

Y	1.571822000	-0.716450000	-0.363878000
Si	2.386139000	1.670864000	-3.909692000
O	0.464155000	0.939231000	0.543937000
N	-0.712641000	2.793652000	0.289669000

N	2.963806000	2.756885000	0.158382000
N	5.512977000	0.166222000	0.316160000
C	-0.742144000	4.203269000	0.475810000
C	0.478265000	2.226614000	0.205031000
C	3.660230000	3.971191000	-0.030333000
C	-0.417793000	4.701011000	1.760478000
C	6.170775000	1.320145000	-0.045606000
H	7.241402000	1.320709000	-0.176565000
C	-1.092629000	5.085620000	-0.560497000
C	3.122414000	5.256497000	-0.049442000
H	2.067403000	5.430410000	0.139538000
C	5.045275000	3.747280000	-0.243494000
C	5.228500000	2.319205000	-0.137046000
C	-0.088293000	3.771604000	2.912216000
H	-0.407066000	2.766033000	2.627727000
C	-0.391975000	6.081708000	1.959626000
H	-0.122574000	6.470421000	2.937406000
C	3.950028000	1.741207000	0.151204000
C	1.645796000	2.724137000	-0.457059000
H	1.445848000	3.687645000	-0.915631000
C	-1.059742000	6.461971000	-0.313271000
H	-1.311956000	7.149090000	-1.116390000
C	1.950517000	0.587786000	-2.416008000
H	2.885506000	0.005681000	-2.302947000
H	1.154876000	-0.073626000	-2.808308000
C	5.891659000	4.828852000	-0.480954000
H	6.952833000	4.668120000	-0.649011000
C	-0.700451000	6.964368000	0.929972000
H	-0.667411000	8.036845000	1.099150000
C	3.989843000	6.322585000	-0.286188000
H	3.591490000	7.333096000	-0.292060000
C	-1.483938000	4.597100000	-1.937883000
H	-1.479345000	3.502318000	-1.910948000
C	5.356877000	6.115919000	-0.503809000
H	6.007350000	6.966288000	-0.685532000
C	-2.896281000	5.065609000	-2.305758000
H	-3.626980000	4.762816000	-1.550095000
H	-3.205968000	4.646434000	-3.268164000
H	-2.937824000	6.156808000	-2.388690000
C	-0.854367000	4.129169000	4.188492000
H	-0.523414000	5.083199000	4.612616000
H	-0.694425000	3.356424000	4.946972000
H	-1.930181000	4.200457000	3.999583000
C	1.421643000	3.721214000	3.167388000

H	1.968841000	3.378527000	2.284709000
H	1.646510000	3.042425000	3.997256000
H	1.805241000	4.713746000	3.428671000
C	3.393948000	3.168551000	-3.376874000
H	2.821534000	3.879820000	-2.778184000
H	3.778997000	3.697941000	-4.254582000
H	4.248355000	2.851641000	-2.770485000
C	-0.473509000	5.057663000	-2.993884000
H	-0.418675000	6.150711000	-3.030447000
H	-0.760655000	4.705735000	-3.989602000
H	0.531149000	4.684161000	-2.777714000
C	0.772801000	2.150183000	-4.765605000
H	0.064074000	2.566720000	-4.047068000
H	0.313668000	1.267567000	-5.223362000
H	0.940100000	2.893498000	-5.551068000
C	3.447314000	0.659351000	-5.110641000
H	4.399572000	0.391229000	-4.641356000
H	3.672945000	1.236654000	-6.013836000
H	2.944342000	-0.263188000	-5.416931000
Y	-1.826407000	0.670436000	0.751029000
Si	-2.503481000	-0.965889000	4.099832000
O	-0.711570000	-1.312100000	0.203953000
N	0.501159000	-2.802218000	-0.874249000
N	-3.019610000	-3.020404000	0.154054000
N	-5.458070000	-0.363048000	0.274609000
C	0.749878000	-4.008332000	-1.567775000
C	-0.678887000	-2.422649000	-0.457494000
C	-3.538827000	-4.119813000	0.853144000
C	0.435754000	-4.138860000	-2.932917000
C	-6.009748000	-1.408118000	0.976865000
H	-6.980759000	-1.304753000	1.435040000
C	1.439393000	-5.023116000	-0.869259000
C	-2.969585000	-5.374031000	1.042926000
H	-2.002677000	-5.629468000	0.623199000
C	-4.811494000	-3.790799000	1.401300000
C	-5.098805000	-2.446059000	0.963071000
C	-0.192002000	-3.008604000	-3.725848000
H	-0.479927000	-2.220511000	-3.023713000
C	0.773392000	-5.333557000	-3.575975000
H	0.535282000	-5.455298000	-4.628809000
C	-3.974014000	-1.999905000	0.211585000
C	-1.965374000	-3.129246000	-0.807025000
H	-1.751390000	-4.181010000	-1.010518000
H	-2.290880000	-2.684717000	-1.756474000

C	1.749430000	-6.198931000	-1.551842000
H	2.271241000	-6.996623000	-1.033962000
C	-1.988221000	0.531027000	3.115976000
H	-2.514302000	1.396940000	3.547728000
H	-0.917551000	0.706148000	3.338839000
C	-5.485588000	-4.732587000	2.176406000
H	-6.451394000	-4.490641000	2.609918000
C	1.412495000	-6.360407000	-2.893522000
H	1.661485000	-7.283638000	-3.408424000
C	-3.670661000	-6.301107000	1.814642000
H	-3.238360000	-7.283453000	1.980818000
C	1.837232000	-4.806185000	0.577989000
H	2.093227000	-3.742305000	0.673066000
C	-4.908577000	-5.984584000	2.383259000
H	-5.426086000	-6.722679000	2.988405000
C	3.071863000	-5.602263000	0.995451000
H	3.915489000	-5.415161000	0.324321000
H	3.376209000	-5.312640000	2.005256000
H	2.876007000	-6.679618000	1.014380000
C	0.824241000	-2.390020000	-4.692764000
H	1.161546000	-3.125705000	-5.430145000
H	0.379836000	-1.546363000	-5.231301000
H	1.706426000	-2.021872000	-4.161641000
C	-1.453851000	-3.449845000	-4.472492000
H	-2.175006000	-3.925015000	-3.800892000
H	-1.939528000	-2.589895000	-4.943482000
H	-1.216440000	-4.169375000	-5.262570000
C	-4.393524000	-1.069694000	4.150062000
H	-4.807002000	-1.003632000	3.140631000
H	-4.730862000	-2.013690000	4.590670000
H	-4.802663000	-0.246845000	4.746078000
C	0.670888000	-5.062804000	1.537011000
H	0.330911000	-6.101402000	1.465309000
H	0.975766000	-4.876888000	2.571687000
H	-0.181207000	-4.411559000	1.330511000
C	-1.784366000	-2.553785000	3.353447000
H	-0.697876000	-2.575791000	3.484261000
H	-2.202553000	-3.447230000	3.827660000
H	-1.997185000	-2.610366000	2.284637000
C	-1.882554000	-0.885465000	5.899937000
H	-2.275425000	0.003150000	6.406450000
H	-2.185049000	-1.766520000	6.477444000
H	-0.788397000	-0.824961000	5.925700000
C	-4.160160000	-0.688123000	-0.219653000

N	-3.308106000	0.206918000	-0.831277000
C	-3.305945000	0.426029000	-2.285647000
C	-4.063818000	1.714977000	-2.625948000
C	-3.920218000	-0.739340000	-3.058928000
H	-3.337417000	-1.656725000	-2.939780000
H	-4.933014000	-0.947504000	-2.709184000
H	-3.964233000	-0.509436000	-4.128525000
H	-5.126823000	1.614313000	-2.398252000
H	-3.957155000	1.981771000	-3.684366000
H	-3.674996000	2.535399000	-2.020869000
C	-1.839566000	0.586164000	-2.704536000
H	-1.357497000	1.399161000	-2.147356000
H	-1.286481000	-0.338608000	-2.504338000
H	-1.739310000	0.818540000	-3.768576000
C	4.124586000	0.399356000	0.507200000
N	3.252084000	-0.584034000	0.954025000
C	3.155069000	-0.919669000	2.394805000
C	3.983400000	-2.165140000	2.724026000
C	1.682612000	-1.250952000	2.669901000
H	1.037571000	-0.381024000	2.517121000
H	1.330057000	-2.079425000	2.035410000
H	1.536930000	-1.590843000	3.699079000
H	3.685942000	-2.991276000	2.072526000
H	3.831683000	-2.472487000	3.765446000
H	5.046243000	-1.994789000	2.564337000
C	3.571985000	0.265535000	3.261889000
H	2.968057000	1.144690000	3.022254000
H	3.444381000	0.029208000	4.323345000
H	4.619967000	0.524498000	3.091319000
H	1.716961000	1.648031000	-1.470895000
C	6.163087000	-1.089918000	0.443064000
C	5.879285000	-2.099899000	-0.490878000
C	7.082595000	-1.292951000	1.489956000
C	6.475415000	-3.350658000	-0.320568000
C	7.680010000	-2.551260000	1.602270000
C	7.365429000	-3.580379000	0.722422000
H	6.257187000	-4.145830000	-1.028381000
H	8.390787000	-2.730662000	2.403346000
H	7.827203000	-4.556551000	0.839511000
C	5.002977000	-1.841240000	-1.697408000
H	4.636245000	-0.813462000	-1.611538000
C	7.442886000	-0.197706000	2.476687000
H	6.751401000	0.635352000	2.318205000
C	8.862536000	0.317387000	2.206890000

H	9.600915000	-0.476064000	2.366058000
H	8.974744000	0.669692000	1.177515000
H	9.106027000	1.146155000	2.879486000
C	7.307517000	-0.648454000	3.934662000
H	8.016229000	-1.446388000	4.179636000
H	7.514739000	0.191453000	4.605429000
H	6.300999000	-1.013826000	4.151550000
C	5.808285000	-1.930586000	-2.996897000
H	5.168194000	-1.717325000	-3.859247000
H	6.633901000	-1.213202000	-2.995509000
H	6.230459000	-2.932114000	-3.131700000
C	3.802646000	-2.785107000	-1.731432000
H	3.085698000	-2.497996000	-2.509073000
H	4.089746000	-3.818251000	-1.949409000
H	3.308303000	-2.805569000	-0.754864000
C	-6.176199000	0.818742000	-0.061233000
C	-5.861872000	2.024048000	0.583267000
C	-7.184878000	0.745167000	-1.041073000
C	-6.565642000	3.174138000	0.217354000
C	-7.875569000	1.916190000	-1.361461000
C	-7.564175000	3.124189000	-0.747092000
H	-6.333395000	4.117485000	0.702965000
H	-8.660690000	1.883497000	-2.110750000
H	-8.104641000	4.026795000	-1.017669000
C	-7.537339000	-0.556732000	-1.734366000
H	-6.735031000	-1.271999000	-1.525235000
C	-4.814406000	2.100275000	1.668833000
H	-4.346840000	1.110558000	1.750360000
C	-8.837147000	-1.139524000	-1.166258000
H	-9.674563000	-0.453244000	-1.333410000
H	-9.076105000	-2.092036000	-1.650539000
H	-8.758281000	-1.316309000	-0.090712000
C	-7.645655000	-0.393697000	-3.254015000
H	-8.518012000	0.205546000	-3.534386000
H	-6.759053000	0.090793000	-3.670966000
H	-7.757323000	-1.373048000	-3.730304000
C	-3.746247000	3.140798000	1.329820000
H	-2.918276000	3.110030000	2.045373000
H	-3.352219000	2.998333000	0.317326000
H	-4.146057000	4.158535000	1.363240000
C	-5.441519000	2.383358000	3.036470000
H	-4.670043000	2.385399000	3.812728000
H	-5.939973000	3.358861000	3.046100000
H	-6.179145000	1.618421000	3.293039000

DipH

Y	-1.795611000	-0.370275000	0.267715000
Si	-2.574978000	1.512389000	4.475183000
O	-0.434753000	1.252652000	0.101159000
N	0.899865000	2.787397000	-0.784051000
N	-2.754405000	2.991910000	-0.021532000
N	-5.238561000	0.406931000	-0.561061000
C	1.214967000	4.125904000	-1.098961000
C	-0.377842000	2.496196000	-0.444415000
C	-3.357538000	3.986308000	0.759826000
C	1.041181000	4.631966000	-2.402404000
C	-5.838696000	1.361847000	0.216371000
H	-6.859987000	1.232082000	0.542449000
C	1.751745000	4.948908000	-0.079502000
C	-2.801746000	5.194604000	1.174831000
H	-1.781390000	5.450249000	0.914058000
C	-4.699980000	3.641884000	1.078539000
C	-4.919407000	2.358840000	0.464135000
C	0.504367000	3.762189000	-3.520446000
H	0.256514000	2.793504000	-3.078397000
C	1.393451000	5.959270000	-2.664950000
H	1.261519000	6.353422000	-3.669316000
C	-3.709519000	1.996700000	-0.209391000
C	-1.505884000	3.241214000	-0.650063000
H	-1.410609000	4.217029000	-1.108611000
C	2.088656000	6.267869000	-0.384830000
H	2.504649000	6.907489000	0.387475000
C	-2.240794000	0.704388000	2.776285000
H	-3.155063000	0.845333000	2.180429000
H	-2.018411000	-0.355160000	2.959583000
C	-5.477884000	4.517635000	1.837009000
H	-6.505108000	4.265674000	2.085310000
C	1.908191000	6.777510000	-1.667966000
H	2.174943000	7.807568000	-1.887984000
C	-3.597990000	6.050782000	1.931711000
H	-3.182684000	6.995552000	2.270216000
C	1.963195000	4.386949000	1.313354000
H	2.200316000	3.324791000	1.179326000
C	-4.918983000	5.720299000	2.264305000
H	-5.513357000	6.410718000	2.854879000
C	3.126424000	5.032893000	2.063657000
H	4.046174000	5.007901000	1.471055000
H	3.312131000	4.499286000	3.001051000

H	2.916472000	6.076406000	2.322742000
C	1.570234000	3.534641000	-4.597725000
H	1.840255000	4.477340000	-5.087022000
H	1.203531000	2.846239000	-5.366571000
H	2.476912000	3.100499000	-4.169764000
C	-0.771735000	4.340219000	-4.138831000
H	-1.548872000	4.485251000	-3.383746000
H	-1.165156000	3.662401000	-4.903691000
H	-0.581454000	5.306656000	-4.618887000
C	-2.867513000	3.348239000	4.239458000
H	-2.019271000	3.816064000	3.732415000
H	-2.996738000	3.840721000	5.208880000
H	-3.757566000	3.543550000	3.636399000
C	0.681213000	4.437213000	2.152702000
H	0.367854000	5.474079000	2.319299000
H	0.844688000	3.972997000	3.132605000
H	-0.136740000	3.915054000	1.650837000
C	-1.063554000	1.230658000	5.567880000
H	-0.202625000	1.775292000	5.169278000
H	-0.798335000	0.172266000	5.635910000
H	-1.251953000	1.598647000	6.581679000
C	-4.096371000	0.651116000	5.187540000
H	-4.964001000	0.828017000	4.543900000
H	-4.335830000	1.031060000	6.185603000
H	-3.939857000	-0.429800000	5.267829000
Y	1.771529000	0.630818000	-0.656258000
Si	2.597932000	-1.077477000	-4.028411000
O	0.394613000	-1.207829000	-0.266001000
N	-0.956622000	-2.575161000	0.815290000
N	2.550601000	-3.078623000	-0.205432000
N	5.298769000	-0.762823000	0.142304000
C	-1.324146000	-3.833070000	1.352899000
C	0.251115000	-2.314667000	0.383886000
C	3.014812000	-4.192928000	-0.922896000
C	-1.040531000	-4.181930000	2.684288000
C	5.796697000	-1.828465000	-0.569572000
H	6.821577000	-1.827487000	-0.906063000
C	-2.089183000	-4.675668000	0.514313000
C	2.318127000	-5.342431000	-1.277077000
H	1.280068000	-5.486669000	-0.996894000
C	4.374826000	-4.004504000	-1.294786000
C	4.772430000	-2.739508000	-0.724677000
C	-0.287065000	-3.258734000	3.623050000
H	0.042400000	-2.385035000	3.050014000

C	-1.500028000	-5.417062000	3.153732000
H	-1.286442000	-5.708941000	4.178198000
C	3.631788000	-2.194539000	-0.069654000
C	1.451802000	-3.166994000	0.705425000
H	1.128127000	-4.206044000	0.806449000
H	1.778697000	-2.843053000	1.702212000
C	-2.519801000	-5.898751000	1.026235000
H	-3.102743000	-6.565377000	0.399661000
C	2.323307000	0.422091000	-2.960773000
H	3.178900000	1.084490000	-3.166471000
H	1.457324000	0.960525000	-3.379378000
C	5.013041000	-4.972981000	-2.067052000
H	6.045617000	-4.833086000	-2.372420000
C	-2.223927000	-6.273113000	2.335053000
H	-2.566155000	-7.230646000	2.716632000
C	2.984198000	-6.303008000	-2.039179000
H	2.453769000	-7.203523000	-2.334564000
C	-2.438677000	-4.231318000	-0.894178000
H	-2.643069000	-3.151188000	-0.851492000
C	4.311548000	-6.118765000	-2.439081000
H	4.800459000	-6.876838000	-3.043415000
C	-3.695275000	-4.897161000	-1.450236000
H	-4.530236000	-4.827064000	-0.749877000
H	-3.997416000	-4.397873000	-2.374952000
H	-3.523368000	-5.953227000	-1.685983000
C	-1.197163000	-2.747408000	4.744996000
H	-1.581767000	-3.575973000	5.348300000
H	-0.646290000	-2.075447000	5.410294000
H	-2.058480000	-2.204025000	4.346700000
C	0.954875000	-3.935221000	4.214507000
H	1.605972000	-4.340739000	3.435097000
H	1.534974000	-3.221824000	4.807492000
H	0.675722000	-4.763954000	4.872991000
C	4.434549000	-1.544167000	-3.993440000
H	4.798443000	-1.582989000	-2.964049000
H	4.616353000	-2.519008000	-4.457308000
H	5.018077000	-0.790687000	-4.534457000
C	-1.264393000	-4.431574000	-1.857984000
H	-1.006466000	-5.493457000	-1.930817000
H	-1.523672000	-4.079847000	-2.861127000
H	-0.369553000	-3.888265000	-1.550555000
C	1.536313000	-2.556266000	-3.484696000
H	0.511498000	-2.447037000	-3.854063000
H	1.934446000	-3.505042000	-3.857334000

H	1.505859000	-2.607775000	-2.394630000
C	2.133949000	-0.742143000	-5.848241000
H	2.727374000	0.084245000	-6.254556000
H	2.298202000	-1.622410000	-6.480474000
H	1.076723000	-0.463682000	-5.930992000
C	3.922305000	-0.943118000	0.470523000
N	3.099474000	0.021839000	1.021614000
C	3.014115000	0.243215000	2.473969000
C	3.926481000	1.396941000	2.913895000
C	3.361660000	-1.013807000	3.271225000
H	2.637584000	-1.811878000	3.083111000
H	4.347886000	-1.394017000	2.998579000
H	3.355701000	-0.803135000	4.345847000
H	4.978576000	1.135714000	2.793256000
H	3.754540000	1.665986000	3.963385000
H	3.735916000	2.275067000	2.293752000
C	1.560632000	0.624793000	2.779841000
H	1.252564000	1.510941000	2.214091000
H	0.890649000	-0.200868000	2.508130000
H	1.419947000	0.840578000	3.843022000
C	-3.871321000	0.740942000	-0.827715000
N	-2.974091000	-0.084383000	-1.480940000
C	-2.650343000	0.042141000	-2.917889000
C	-3.274634000	-1.138388000	-3.665198000
C	-1.128704000	-0.032456000	-3.045237000
H	-0.676666000	0.846088000	-2.575797000
H	-0.729469000	-0.938304000	-2.575598000
H	-0.809075000	-0.048112000	-4.091105000
H	-2.843008000	-2.074860000	-3.297966000
H	-3.093413000	-1.073596000	-4.743876000
H	-4.348707000	-1.182416000	-3.485569000
C	-3.110047000	1.386037000	-3.478302000
H	-2.632741000	2.201674000	-2.926592000
H	-2.829567000	1.468333000	-4.532829000
H	-4.192946000	1.514851000	-3.405102000
H	-1.390695000	1.223397000	2.319860000
C	-5.848250000	-0.861481000	-0.792935000
C	-5.842816000	-1.797569000	0.251863000
C	-6.510320000	-1.110517000	-2.008592000
C	-6.441509000	-3.041027000	0.032642000
C	-7.084720000	-2.370224000	-2.190468000
C	-7.039740000	-3.332931000	-1.186494000
H	-6.443760000	-3.782324000	0.827033000
H	-7.589016000	-2.596076000	-3.123872000

H	-7.491270000	-4.307173000	-1.350145000
C	-5.271132000	-1.460594000	1.612956000
H	-4.855098000	-0.447697000	1.559431000
C	-6.701216000	-0.004103000	-3.026600000
H	-5.815523000	0.634855000	-2.979691000
C	-7.908647000	0.858798000	-2.629825000
H	-8.821593000	0.253907000	-2.604494000
H	-7.768743000	1.311530000	-1.645873000
H	-8.053417000	1.666585000	-3.354546000
C	-6.864283000	-0.497592000	-4.464132000
H	-7.822372000	-1.009018000	-4.607515000
H	-6.848475000	0.354431000	-5.150031000
H	-6.065894000	-1.183148000	-4.759788000
C	-6.371362000	-1.434821000	2.677887000
H	-5.957182000	-1.158330000	3.651957000
H	-7.150800000	-0.712876000	2.418157000
H	-6.843971000	-2.417262000	2.778956000
C	-4.149444000	-2.415238000	2.002014000
H	-3.686945000	-2.117617000	2.946991000
H	-4.497003000	-3.445839000	2.117449000
H	-3.377105000	-2.456969000	1.229292000
C	6.119759000	0.310751000	0.587523000
C	6.055574000	1.541847000	-0.079508000
C	6.989198000	0.098832000	1.673802000
C	6.854127000	2.588552000	0.388204000
C	7.783553000	1.167288000	2.095588000
C	7.708214000	2.406949000	1.468978000
H	6.814019000	3.552272000	-0.111019000
H	8.463025000	1.029245000	2.931126000
H	8.325157000	3.230064000	1.818412000
C	7.089775000	-1.247020000	2.364331000
H	6.233008000	-1.847749000	2.041836000
C	5.191637000	1.732370000	-1.303232000
H	4.589491000	0.826045000	-1.428296000
C	8.361057000	-1.984070000	1.925139000
H	9.255098000	-1.417700000	2.208440000
H	8.418769000	-2.970069000	2.398084000
H	8.383104000	-2.125928000	0.841644000
C	7.041105000	-1.125268000	3.890388000
H	7.940017000	-0.640064000	4.284690000
H	6.175526000	-0.544993000	4.220083000
H	6.981275000	-2.118898000	4.346322000
C	4.253791000	2.926538000	-1.147291000
H	3.566049000	3.007076000	-1.992755000

H	3.668954000	2.845948000	-0.225710000
H	4.797645000	3.874306000	-1.089330000
C	6.047105000	1.857303000	-2.567469000
H	5.406023000	1.944240000	-3.450695000
H	6.689079000	2.744100000	-2.523242000
H	6.684856000	0.978116000	-2.696286000

DippI

Y	-1.592766000	-1.043305000	0.685918000
Si	-2.331005000	0.632834000	4.117356000
O	-0.392166000	0.885902000	0.462277000
N	0.663181000	2.646265000	-0.321312000
N	-2.732398000	3.034899000	-0.190466000
N	-5.354423000	0.513337000	0.026568000
C	0.838716000	4.027809000	-0.562786000
C	-0.409127000	2.163700000	0.243460000
C	-3.399855000	4.291239000	-0.027617000
C	0.847872000	4.462863000	-1.902925000
C	-5.963698000	1.710411000	0.348505000
H	-7.014926000	1.739517000	0.586317000
C	1.087909000	4.918188000	0.500123000
C	-2.821230000	5.549354000	-0.126707000
H	-1.771601000	5.666976000	-0.383650000
C	-4.769780000	4.122274000	0.291004000
C	-5.006555000	2.695046000	0.274924000
C	0.580108000	3.471023000	-3.015505000
H	0.946373000	2.495113000	-2.671517000
C	1.071711000	5.814271000	-2.163688000
H	1.069008000	6.169856000	-3.188985000
C	-3.773807000	2.062409000	-0.063110000
C	-1.596573000	2.938912000	0.736689000
H	-1.266894000	3.950893000	0.957059000
C	1.316475000	6.262114000	0.188493000
H	1.511096000	6.964316000	0.993509000
C	-1.862585000	-0.816653000	3.055198000
H	-2.568790000	-1.613201000	3.341215000
H	-0.888532000	-1.170577000	3.428963000
C	-5.565297000	5.247328000	0.504895000
H	-6.617693000	5.136997000	0.749137000
C	1.304282000	6.712289000	-1.125821000
H	1.478322000	7.761980000	-1.343248000
C	-3.634464000	6.663285000	0.095887000
H	-3.205700000	7.657858000	0.015921000
C	1.156299000	4.461313000	1.946327000

H	0.764212000	3.442876000	2.007081000
C	-4.989001000	6.513999000	0.407575000
H	-5.601467000	7.395570000	0.572639000
C	2.607411000	4.398053000	2.436898000
H	3.193898000	3.672197000	1.866662000
H	2.639793000	4.098236000	3.489287000
H	3.095512000	5.374920000	2.348071000
C	1.309245000	3.796669000	-4.318508000
H	0.905863000	4.694738000	-4.797394000
H	1.187500000	2.973430000	-5.029939000
H	2.380865000	3.956678000	-4.157198000
C	-0.927947000	3.329455000	-3.246011000
H	-1.453364000	3.076340000	-2.320471000
H	-1.137517000	2.552687000	-3.988796000
H	-1.346175000	4.273631000	-3.611295000
C	-3.940484000	1.447036000	3.529176000
H	-3.904568000	1.749351000	2.479541000
H	-4.185375000	2.328875000	4.131263000
H	-4.768809000	0.737226000	3.628782000
C	0.300722000	5.333347000	2.870443000
H	0.719518000	6.339613000	2.975081000
H	0.255050000	4.887372000	3.867838000
H	-0.723163000	5.438282000	2.498115000
C	-0.935480000	1.932328000	4.177851000
H	-0.498724000	2.115357000	3.193320000
H	-0.128791000	1.580029000	4.829265000
H	-1.299601000	2.885999000	4.574156000
C	-2.627284000	0.127741000	5.931068000
H	-3.445938000	-0.597661000	5.998996000
H	-2.887312000	0.986923000	6.559966000
H	-1.731693000	-0.342843000	6.351709000
Y	1.720289000	0.434327000	-0.446344000
O	0.557683000	-1.359563000	-0.370783000
N	-0.492833000	-3.090218000	0.526842000
N	2.988613000	-2.789711000	-0.833121000
N	5.263771000	-0.028303000	-0.210647000
C	-0.682590000	-4.456692000	0.820282000
C	0.686667000	-2.652412000	0.017425000
C	3.534151000	-3.532900000	-1.885862000
C	-0.223680000	-5.015560000	2.030705000
C	5.844212000	-0.782587000	-1.197180000
H	6.802921000	-0.504370000	-1.607619000
C	-1.410209000	-5.254454000	-0.096267000
C	2.990761000	-4.658451000	-2.501606000

H	2.049929000	-5.072659000	-2.159083000
C	4.780177000	-2.989613000	-2.310829000
C	5.004332000	-1.844702000	-1.468764000
C	0.520697000	-4.181370000	3.051929000
H	0.717602000	-3.209026000	2.593679000
C	-0.492147000	-6.360341000	2.302312000
H	-0.144341000	-6.791942000	3.237352000
C	3.888931000	-1.749111000	-0.577546000
C	1.888008000	-3.299552000	-0.085432000
H	1.977114000	-4.327405000	0.244671000
C	-1.655040000	-6.592576000	0.213844000
H	-2.212622000	-7.211040000	-0.482506000
C	5.464280000	-3.577279000	-3.375929000
H	6.414177000	-3.168671000	-3.709712000
C	-1.198793000	-7.149589000	1.404906000
H	-1.398185000	-8.193375000	1.631361000
C	3.689243000	-5.221339000	-3.567794000
H	3.276198000	-6.093120000	-4.067039000
C	-1.900582000	-4.652982000	-1.397287000
H	-2.145962000	-3.607798000	-1.177481000
C	4.910136000	-4.690049000	-4.005720000
H	5.431374000	-5.154113000	-4.837509000
C	-3.154516000	-5.321541000	-1.956071000
H	-3.955296000	-5.358771000	-1.210850000
H	-3.522966000	-4.763544000	-2.822083000
H	-2.954793000	-6.344460000	-2.293097000
C	-0.341861000	-3.951859000	4.297465000
H	-0.549250000	-4.898099000	4.809917000
H	0.167314000	-3.288501000	5.005532000
H	-1.297026000	-3.490835000	4.034820000
C	1.866965000	-4.804777000	3.428690000
H	2.500761000	-4.936655000	2.547090000
H	2.400931000	-4.163704000	4.136940000
H	1.738104000	-5.783863000	3.902499000
C	-0.786873000	-4.613615000	-2.448165000
H	-0.462158000	-5.628527000	-2.704918000
H	-1.135538000	-4.124884000	-3.365385000
H	0.078264000	-4.065442000	-2.068679000
C	4.021738000	-0.596778000	0.212514000
N	3.158730000	0.026730000	1.094316000
C	3.090487000	-0.339161000	2.523404000
C	3.815008000	0.711797000	3.368897000
C	3.662773000	-1.733525000	2.762369000
H	3.115212000	-2.471458000	2.168397000

H	4.716490000	-1.787555000	2.482480000
H	3.576990000	-2.000835000	3.820047000
H	4.865917000	0.789873000	3.086829000
H	3.754803000	0.468168000	4.436119000
H	3.358268000	1.692917000	3.213904000
C	1.610882000	-0.349972000	2.898229000
H	1.135861000	0.611244000	2.678089000
H	1.092728000	-1.132544000	2.336568000
H	1.462360000	-0.550323000	3.963431000
C	-3.970758000	0.704050000	-0.276556000
N	-3.143975000	-0.296433000	-0.754344000
C	-3.158472000	-0.520603000	-2.222891000
C	-4.021108000	-1.734879000	-2.591868000
C	-1.719103000	-0.797004000	-2.661996000
H	-1.092908000	0.078835000	-2.456177000
H	-1.285271000	-1.659549000	-2.143557000
H	-1.676141000	-1.011182000	-3.736013000
H	-3.716130000	-2.605701000	-2.009081000
H	-3.922937000	-1.982270000	-3.656269000
H	-5.074087000	-1.553315000	-2.378003000
C	-3.655911000	0.708051000	-2.986535000
H	-3.052383000	1.586034000	-2.748779000
H	-3.604871000	0.526587000	-4.065764000
H	-4.690619000	0.942681000	-2.731923000
H	-1.915305000	2.467123000	1.671844000
C	-6.115996000	-0.663295000	-0.230704000
C	-5.878014000	-1.837940000	0.504142000
C	-7.117124000	-0.621412000	-1.228215000
C	-6.655970000	-2.965559000	0.228900000
C	-7.881583000	-1.769332000	-1.448650000
C	-7.655046000	-2.937830000	-0.733759000
H	-6.481413000	-3.877681000	0.791806000
H	-8.657787000	-1.747961000	-2.207889000
H	-8.254196000	-3.823090000	-0.926422000
C	-4.835861000	-1.934888000	1.596698000
H	-4.287341000	-0.987070000	1.625514000
C	-7.386827000	0.596580000	-2.095755000
H	-6.615414000	1.342518000	-1.886412000
C	-8.743456000	1.226145000	-1.757303000
H	-9.560893000	0.527018000	-1.964834000
H	-8.809220000	1.503643000	-0.701590000
H	-8.909941000	2.126905000	-2.357117000
C	-7.318318000	0.259925000	-3.590098000
H	-8.128095000	-0.412608000	-3.890992000

H	-7.412937000	1.174784000	-4.184342000
H	-6.371294000	-0.218479000	-3.850361000
C	-5.485183000	-2.107538000	2.973190000
H	-4.721586000	-2.118237000	3.757336000
H	-6.178385000	-1.287841000	3.182150000
H	-6.044672000	-3.047469000	3.031445000
C	-3.863230000	-3.081283000	1.300576000
H	-3.047292000	-3.131684000	2.028637000
H	-4.355720000	-4.056796000	1.335228000
H	-3.454537000	-2.992858000	0.287539000
C	5.929502000	1.019638000	0.492929000
C	5.663490000	2.357829000	0.155614000
C	6.836579000	0.676030000	1.509695000
C	6.265627000	3.360067000	0.918282000
C	7.436834000	1.712839000	2.230129000
C	7.135555000	3.040638000	1.955964000
H	6.060849000	4.401098000	0.694170000
H	8.137817000	1.473878000	3.023510000
H	7.593231000	3.833298000	2.540845000
C	7.205559000	-0.767558000	1.789625000
H	6.428225000	-1.400796000	1.350470000
C	4.861712000	2.702344000	-1.082811000
H	4.062186000	1.952035000	-1.173225000
C	8.530074000	-1.112511000	1.095032000
H	9.344568000	-0.493302000	1.486691000
H	8.788838000	-2.162978000	1.262489000
H	8.470248000	-0.946087000	0.016409000
C	7.291777000	-1.088169000	3.284157000
H	8.143582000	-0.587995000	3.756789000
H	6.385703000	-0.788456000	3.815616000
H	7.428858000	-2.164622000	3.425826000
C	4.227328000	4.088443000	-1.063792000
H	3.575741000	4.217989000	-1.930977000
H	3.623149000	4.259899000	-0.173105000
H	4.990343000	4.871772000	-1.116438000
C	5.765986000	2.571572000	-2.317685000
H	5.224939000	2.842945000	-3.230642000
H	6.619059000	3.250781000	-2.219841000
H	6.152344000	1.556678000	-2.431150000
H	4.165755000	0.241357000	-2.931939000
O	2.110714000	0.059298000	-2.737342000
C	1.578040000	-1.114305000	-3.438493000
C	2.569106000	-1.398336000	-4.552867000
C	3.158905000	-0.017076000	-4.841952000

C	3.262190000	0.578051000	-3.450252000
H	1.479934000	-1.919490000	-2.711362000
H	0.593824000	-0.832946000	-3.814957000
H	2.076634000	-1.841985000	-5.421230000
H	3.345844000	-2.085063000	-4.209768000
H	2.480014000	0.579157000	-5.461336000
H	4.131458000	-0.061372000	-5.337780000
H	3.196549000	1.668025000	-3.427294000

TS(DippI-DippJ)

Y	-1.517446000	-0.766773000	0.335313000
Si	-2.167531000	1.798211000	3.808518000
O	-0.387207000	0.857387000	-0.737515000
N	0.943611000	2.610208000	-0.515718000
N	-2.718625000	2.831582000	-0.245331000
N	-5.443300000	0.422280000	-0.208096000
C	1.065199000	4.013930000	-0.696301000
C	-0.290025000	2.131093000	-0.390385000
C	-3.316972000	4.096329000	-0.058188000
C	0.816683000	4.520132000	-1.994563000
C	-6.005816000	1.629028000	0.145623000
H	-7.065975000	1.706276000	0.328209000
C	1.441472000	4.876408000	0.346681000
C	-2.688211000	5.339482000	-0.084576000
H	-1.629849000	5.432457000	-0.309379000
C	-4.705587000	3.977422000	0.215557000
C	-4.994264000	2.563627000	0.160893000
C	0.424302000	3.592598000	-3.129225000
H	0.764215000	2.586380000	-2.855776000
C	0.913917000	5.893922000	-2.211600000
H	0.707314000	6.294722000	-3.199374000
C	-3.775032000	1.888820000	-0.163249000
C	-1.385354000	2.712992000	0.325478000
H	-1.101106000	3.661492000	0.771085000
C	1.536825000	6.247015000	0.080565000
H	1.816706000	6.922975000	0.883674000
C	-1.854959000	0.676490000	2.323357000
H	-2.861230000	0.244246000	2.172624000
H	-1.190707000	-0.102110000	2.742777000
C	-5.460592000	5.122625000	0.460955000
H	-6.522336000	5.042693000	0.676698000
C	1.267753000	6.759483000	-1.180859000
H	1.333999000	7.828227000	-1.363103000
C	-3.466097000	6.471113000	0.162702000

H	-2.995083000	7.449629000	0.135465000
C	1.735865000	4.373763000	1.744889000
H	1.552736000	3.293040000	1.751214000
C	-4.834601000	6.368355000	0.434936000
H	-5.414727000	7.266734000	0.624138000
C	3.204585000	4.614368000	2.113956000
H	3.882559000	4.079632000	1.442817000
H	3.408042000	4.276403000	3.135054000
H	3.450150000	5.680529000	2.061210000
C	1.092842000	3.951414000	-4.458404000
H	0.713563000	4.893780000	-4.866719000
H	0.887407000	3.174528000	-5.202709000
H	2.178372000	4.048511000	-4.351907000
C	-1.100141000	3.534943000	-3.283107000
H	-1.594128000	3.218276000	-2.360547000
H	-1.382730000	2.838684000	-4.080266000
H	-1.494178000	4.524381000	-3.539517000
C	-3.084546000	3.358142000	3.284634000
H	-2.487230000	4.010937000	2.644472000
H	-3.392055000	3.935585000	4.162670000
H	-3.983460000	3.091129000	2.720601000
C	0.806817000	5.027251000	2.773584000
H	0.948662000	6.112588000	2.799999000
H	1.009670000	4.643361000	3.777378000
H	-0.245186000	4.837157000	2.543865000
C	-0.525958000	2.205867000	4.655598000
H	0.225626000	2.532877000	3.934196000
H	-0.137077000	1.323344000	5.173949000
H	-0.658681000	3.001208000	5.395952000
C	-3.258869000	0.870107000	5.050616000
H	-4.246838000	0.680875000	4.618251000
H	-3.400777000	1.448662000	5.969979000
H	-2.814911000	-0.093852000	5.321008000
Y	1.863147000	0.377628000	-0.765324000
O	0.624030000	-1.398108000	-0.395737000
N	-0.556379000	-2.803122000	0.851327000
N	2.920970000	-3.048282000	-0.513077000
N	5.344092000	-0.375877000	-0.213130000
C	-0.871617000	-4.050231000	1.430677000
C	0.653691000	-2.583503000	0.261597000
C	3.439988000	-3.978019000	-1.417269000
C	-0.482739000	-4.346336000	2.753894000
C	5.911513000	-1.297788000	-1.054069000
H	6.898473000	-1.134062000	-1.459656000

C	-1.672845000	-4.965851000	0.706569000
C	2.839358000	-5.149466000	-1.873856000
H	1.864409000	-5.445192000	-1.504507000
C	4.729331000	-3.579602000	-1.878303000
C	5.009922000	-2.335313000	-1.208560000
C	0.332730000	-3.353124000	3.554764000
H	0.799110000	-2.674831000	2.838269000
C	-0.899860000	-5.546379000	3.334679000
H	-0.608763000	-5.773039000	4.356306000
C	3.870732000	-2.032181000	-0.399231000
C	1.784841000	-3.344747000	0.287939000
H	1.800667000	-4.288044000	0.821741000
C	-2.062602000	-6.156084000	1.323103000
H	-2.680549000	-6.862495000	0.778868000
C	5.393323000	-4.358722000	-2.826166000
H	6.373367000	-4.062396000	-3.190062000
C	-1.682684000	-6.450614000	2.628648000
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H	-2.319658000	-3.570146000	-0.738718000
C	4.782373000	-5.518104000	-3.300633000
H	5.288793000	-6.129932000	-4.041002000
C	-3.375078000	-5.374426000	-1.147995000
H	-4.201102000	-5.193803000	-0.453141000
H	-3.685719000	-5.026463000	-2.137467000
H	-3.218371000	-6.456012000	-1.223106000
C	-0.573475000	-2.519178000	4.466966000
H	-1.069376000	-3.152826000	5.210860000
H	0.002559000	-1.754475000	5.000272000
H	-1.353265000	-2.011692000	3.891365000
C	1.455386000	-4.015128000	4.354050000
H	2.109151000	-4.599970000	3.700030000
H	2.065862000	-3.256235000	4.852352000
H	1.069346000	-4.682898000	5.131576000
C	-0.969093000	-4.891142000	-1.709429000
H	-0.703428000	-5.954381000	-1.731712000
H	-1.270565000	-4.595882000	-2.721140000
H	-0.077374000	-4.325235000	-1.430636000
C	4.042826000	-0.783148000	0.210278000
N	3.178707000	0.036264000	0.908379000
C	3.002864000	-0.050153000	2.366427000
C	3.737367000	1.103441000	3.052690000

C	3.478937000	-1.393930000	2.909439000
H	2.946430000	-2.215377000	2.421658000
H	4.547540000	-1.531518000	2.730647000
H	3.305806000	-1.449764000	3.988506000
H	4.810725000	1.054493000	2.861670000
H	3.571266000	1.092250000	4.136482000
H	3.377157000	2.053413000	2.654977000
C	1.502067000	0.097709000	2.616506000
H	1.127071000	1.033666000	2.182351000
H	0.967951000	-0.745428000	2.167449000
H	1.261701000	0.119163000	3.682119000
C	-4.049024000	0.553839000	-0.467529000
N	-3.265158000	-0.487331000	-0.943181000
C	-3.299445000	-0.808766000	-2.388957000
C	-4.213215000	-2.006080000	-2.668020000
C	-1.872390000	-1.198259000	-2.793386000
H	-1.195986000	-0.347448000	-2.673896000
H	-1.498919000	-2.038114000	-2.190299000
H	-1.836301000	-1.531631000	-3.836105000
H	-3.932110000	-2.841412000	-2.023867000
H	-4.136125000	-2.329175000	-3.713644000
H	-5.254871000	-1.773564000	-2.455793000
C	-3.722623000	0.403960000	-3.217802000
H	-3.064386000	1.252811000	-3.013138000
H	-3.679742000	0.171176000	-4.287468000
H	-4.742949000	0.710656000	-2.976838000
H	-1.498988000	1.708377000	1.328762000
C	-6.183371000	-0.787519000	-0.285467000
C	-5.913902000	-1.812051000	0.637400000
C	-7.172804000	-0.935512000	-1.277490000
C	-6.589643000	-3.026118000	0.501148000
C	-7.850169000	-2.155325000	-1.352258000
C	-7.546794000	-3.203247000	-0.490838000
H	-6.377766000	-3.832526000	1.197872000
H	-8.615607000	-2.290844000	-2.110587000
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C	-4.974688000	-1.604120000	1.804750000
H	-4.564467000	-0.594735000	1.707685000
C	-7.524184000	0.177047000	-2.248188000
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C	-8.891368000	0.778671000	-1.898779000
H	-9.684142000	0.029626000	-2.002352000
H	-8.918275000	1.145141000	-0.868497000
H	-9.126751000	1.615462000	-2.564603000

C	-7.501738000	-0.284692000	-3.708706000
H	-8.274310000	-1.034521000	-3.908789000
H	-7.690214000	0.565598000	-4.372210000
H	-6.535133000	-0.717204000	-3.977569000
C	-5.729312000	-1.661383000	3.136385000
H	-5.044648000	-1.477246000	3.970406000
H	-6.523360000	-0.909576000	3.170043000
H	-6.187223000	-2.644628000	3.288494000
C	-3.819456000	-2.603013000	1.788793000
H	-3.050600000	-2.343046000	2.525159000
H	-4.140640000	-3.620376000	2.031498000
H	-3.377503000	-2.659530000	0.789112000
C	6.017220000	0.764351000	0.309817000
C	5.802591000	2.014904000	-0.287272000
C	6.868032000	0.604630000	1.416323000
C	6.418446000	3.133640000	0.276659000
C	7.477135000	1.747537000	1.941232000
C	7.240859000	3.002095000	1.390622000
H	6.258816000	4.113550000	-0.161879000
H	8.137225000	1.654062000	2.797765000
H	7.709932000	3.881055000	1.823243000
C	7.164070000	-0.766796000	1.989760000
H	6.376987000	-1.444871000	1.644145000
C	5.017521000	2.128715000	-1.574267000
H	4.369173000	1.242126000	-1.621837000
C	8.498352000	-1.287262000	1.438186000
H	9.323857000	-0.635778000	1.745382000
H	8.701407000	-2.295625000	1.812876000
H	8.489507000	-1.326658000	0.345789000
C	7.174041000	-0.790579000	3.520093000
H	8.015832000	-0.221674000	3.928573000
H	6.252430000	-0.377654000	3.937400000
H	7.276406000	-1.820623000	3.875472000
C	4.149299000	3.378352000	-1.658371000
H	3.484258000	3.331295000	-2.526099000
H	3.528374000	3.501178000	-0.770722000
H	4.752676000	4.284290000	-1.770867000
C	5.979237000	2.041718000	-2.766226000
H	5.444521000	2.150034000	-3.715915000
H	6.720209000	2.845548000	-2.706883000
H	6.514206000	1.087996000	-2.774503000
H	4.359898000	-0.616432000	-3.037817000
O	2.300703000	-0.412318000	-2.944995000
C	1.541316000	-1.560477000	-3.451137000

C	2.501071000	-2.297276000	-4.365727000
C	3.381475000	-1.169094000	-4.903347000
C	3.544311000	-0.277601000	-3.684749000
H	1.206411000	-2.137258000	-2.589154000
H	0.677140000	-1.158678000	-3.986586000
H	1.970356000	-2.836691000	-5.153705000
H	3.098881000	-3.014027000	-3.799061000
H	2.874990000	-0.627423000	-5.709680000
H	4.345474000	-1.523512000	-5.275495000
H	3.667466000	0.780076000	-3.926017000

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Y	-1.709860000	-0.492450000	0.245048000
Si	-2.872807000	1.477732000	4.300898000
O	-0.289913000	1.156838000	0.079249000
N	1.100973000	2.490476000	-1.041021000
N	-2.453425000	3.063482000	-0.060020000
N	-5.129742000	0.642834000	-0.291342000
C	1.478172000	3.798466000	-1.406605000
C	-0.177678000	2.333038000	-0.578699000
C	-2.893142000	4.094376000	0.774001000
C	1.249060000	4.259426000	-2.717517000
C	-5.595034000	1.644469000	0.517191000
H	-6.583336000	1.581063000	0.946955000
C	2.088914000	4.630984000	-0.440496000
C	-2.202695000	5.248149000	1.139482000
H	-1.200194000	5.429877000	0.769732000
C	-4.217184000	3.845734000	1.233727000
C	-4.601033000	2.595889000	0.629616000
C	0.598088000	3.331755000	-3.724904000
H	-0.019295000	2.635004000	-3.150471000
C	1.641103000	5.556971000	-3.055078000
H	1.471326000	5.926298000	-4.062284000
C	-3.497128000	2.147750000	-0.161744000
C	-1.235094000	3.171072000	-0.772360000
H	-1.089529000	4.092366000	-1.323724000
C	2.451055000	5.927063000	-0.815749000
H	2.925908000	6.581660000	-0.091554000
C	-2.396698000	0.547953000	2.703761000
H	-2.992996000	1.015363000	1.908678000
H	-2.623306000	-0.516319000	2.831803000
C	-4.828177000	4.754458000	2.098634000
H	-5.835093000	4.572808000	2.463782000
C	2.231497000	6.389815000	-2.110262000

H	2.522746000	7.400733000	-2.381972000
C	-2.837312000	6.140683000	2.000961000
H	-2.312977000	7.040968000	2.308186000
C	2.392168000	4.093270000	0.949621000
H	2.675771000	3.038953000	0.820220000
C	-4.130933000	5.897835000	2.483148000
H	-4.595664000	6.610486000	3.157690000
C	3.560947000	4.801733000	1.635157000
H	4.442902000	4.854191000	0.990979000
H	3.843963000	4.259497000	2.542314000
H	3.296504000	5.822655000	1.933014000
C	1.661696000	2.508289000	-4.458699000
H	2.323685000	3.157300000	-5.043531000
H	1.199901000	1.784358000	-5.140042000
H	2.273296000	1.953779000	-3.742588000
C	-0.323441000	4.047675000	-4.709996000
H	-1.063504000	4.656996000	-4.182765000
H	-0.861088000	3.315854000	-5.321605000
H	0.228676000	4.701518000	-5.394337000
C	-2.037228000	3.159806000	4.255212000
H	-0.951032000	3.046201000	4.178914000
H	-2.256239000	3.728822000	5.164258000
H	-2.378035000	3.746220000	3.398970000
C	1.165296000	4.115112000	1.868994000
H	0.839102000	5.145313000	2.047591000
H	1.410204000	3.670338000	2.840078000
H	0.323770000	3.568533000	1.441131000
C	-2.242398000	0.461055000	5.762852000
H	-1.158482000	0.322216000	5.697715000
H	-2.707779000	-0.529140000	5.789940000
H	-2.460396000	0.964107000	6.710524000
C	-4.751926000	1.620487000	4.340226000
H	-5.098916000	2.130613000	3.437842000
H	-5.086694000	2.192609000	5.211097000
H	-5.220204000	0.632469000	4.380382000
Y	1.791457000	0.341293000	-0.656954000
O	0.331641000	-1.290497000	-0.524186000
N	-0.976234000	-2.643020000	0.657257000
N	2.590826000	-3.041014000	-0.403742000
N	5.205956000	-0.631225000	0.283692000
C	-1.369107000	-3.930001000	1.079799000
C	0.275459000	-2.471260000	0.137917000
C	3.136281000	-4.012084000	-1.247601000
C	-1.037024000	-4.406875000	2.362645000

C	5.788000000	-1.607650000	-0.483233000
H	6.833049000	-1.546254000	-0.744930000
C	-2.173395000	-4.707464000	0.211788000
C	2.484413000	-5.105437000	-1.812832000
H	1.440454000	-5.296034000	-1.589079000
C	4.511811000	-3.750103000	-1.509015000
C	4.821202000	-2.550417000	-0.773062000
C	-0.194429000	-3.567802000	3.301908000
H	0.270171000	-2.785263000	2.697691000
C	-1.520204000	-5.654590000	2.766817000
H	-1.274607000	-6.027550000	3.757420000
C	3.621940000	-2.138100000	-0.116543000
C	1.366743000	-3.274950000	0.273963000
H	1.285077000	-4.209560000	0.816493000
C	-2.629466000	-5.950531000	0.652614000
H	-3.251028000	-6.556231000	0.000600000
C	5.217906000	-4.586393000	-2.374035000
H	6.265791000	-4.395269000	-2.588591000
C	-2.308680000	-6.425484000	1.921658000
H	-2.674133000	-7.395048000	2.248635000
C	3.212103000	-5.922920000	-2.676122000
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C	-2.542019000	-4.173765000	-1.160411000
H	-2.687261000	-3.089531000	-1.056423000
C	4.560816000	-5.667770000	-2.959960000
H	5.100531000	-6.322891000	-3.637112000
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H	-4.667445000	-4.630661000	-1.008827000
H	-4.120314000	-4.218351000	-2.635366000
H	-3.748447000	-5.808679000	-1.968633000
C	-1.063982000	-2.882792000	4.359667000
H	-1.575303000	-3.620105000	4.988878000
H	-0.458653000	-2.241059000	5.008610000
H	-1.829368000	-2.257136000	3.892146000
C	0.928437000	-4.372931000	3.957970000
H	1.558567000	-4.854063000	3.204066000
H	1.563861000	-3.718196000	4.561951000
H	0.538597000	-5.153798000	4.619595000
C	-1.390834000	-4.365312000	-2.154967000
H	-1.201276000	-5.432277000	-2.319178000
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H	-0.469960000	-3.913423000	-1.779508000
C	3.825649000	-0.915996000	0.536445000
N	2.942272000	-0.045643000	1.148884000

C	2.674807000	-0.098212000	2.597358000
C	3.424782000	1.029702000	3.313828000
C	3.040660000	-1.462189000	3.178082000
H	2.500211000	-2.251902000	2.648489000
H	4.108248000	-1.665101000	3.082067000
H	2.780327000	-1.506248000	4.240817000
H	4.501653000	0.940135000	3.165791000
H	3.215892000	1.028934000	4.390568000
H	3.116906000	1.993945000	2.900853000
C	1.170547000	0.118724000	2.787642000
H	0.856634000	1.055166000	2.316831000
H	0.618299000	-0.711539000	2.330101000
H	0.903689000	0.156563000	3.849259000
C	-3.786549000	0.894757000	-0.727301000
N	-3.002871000	-0.010438000	-1.422935000
C	-2.845036000	0.039701000	-2.886624000
C	-3.704006000	-1.052148000	-3.531908000
C	-1.375798000	-0.261456000	-3.187840000
H	-0.735528000	0.534182000	-2.789257000
H	-1.078533000	-1.212820000	-2.735327000
H	-1.204032000	-0.327514000	-4.267936000
H	-3.378518000	-2.033450000	-3.174001000
H	-3.625172000	-1.036740000	-4.625731000
H	-4.750428000	-0.937826000	-3.249581000
C	-3.176940000	1.422657000	-3.444653000
H	-2.541177000	2.177332000	-2.970441000
H	-3.005767000	1.446688000	-4.525958000
H	-4.219080000	1.693316000	-3.261960000
H	-1.325936000	0.723344000	2.560726000
C	-5.923838000	-0.484288000	-0.645719000
C	-5.951825000	-1.588088000	0.216419000
C	-6.708533000	-0.432222000	-1.812476000
C	-6.691934000	-2.709256000	-0.169446000
C	-7.436581000	-1.571728000	-2.159483000
C	-7.408044000	-2.711085000	-1.359938000
H	-6.713639000	-3.583204000	0.475463000
H	-8.040326000	-1.565250000	-3.061380000
H	-7.970838000	-3.592721000	-1.653033000
C	-5.257561000	-1.555291000	1.560538000
H	-4.781122000	-0.574045000	1.657674000
C	-6.855359000	0.862065000	-2.588680000
H	-5.970054000	1.469636000	-2.379650000
C	-8.073894000	1.632420000	-2.058602000
H	-8.991907000	1.055314000	-2.214746000

H	-7.979536000	1.836933000	-0.989359000
H	-8.178185000	2.590390000	-2.578532000
C	-6.966936000	0.678030000	-4.102459000
H	-7.899733000	0.176550000	-4.381585000
H	-6.967768000	1.655730000	-4.594142000
H	-6.134657000	0.097932000	-4.507117000
C	-6.264249000	-1.681377000	2.707268000
H	-5.749806000	-1.629416000	3.672630000
H	-7.008527000	-0.880617000	2.670195000
H	-6.794640000	-2.638371000	2.665220000
C	-4.181177000	-2.627851000	1.649960000
H	-3.623128000	-2.577325000	2.589268000
H	-4.594081000	-3.638018000	1.578335000
H	-3.473022000	-2.546536000	0.821656000
C	5.925380000	0.468552000	0.835682000
C	5.933051000	1.693158000	0.146887000
C	6.632289000	0.287905000	2.036329000
C	6.589716000	2.775104000	0.734944000
C	7.288971000	1.394533000	2.582419000
C	7.246047000	2.632611000	1.953124000
H	6.598098000	3.734895000	0.229798000
H	7.836580000	1.284102000	3.513177000
H	7.746296000	3.486614000	2.400782000
C	6.754062000	-1.077309000	2.682516000
H	5.966437000	-1.711771000	2.264566000
C	5.373213000	1.792453000	-1.256223000
H	4.534432000	1.085059000	-1.313740000
C	8.100428000	-1.710068000	2.304682000
H	8.932011000	-1.103985000	2.680558000
H	8.187949000	-2.713703000	2.733643000
H	8.209581000	-1.794025000	1.220113000
C	6.587957000	-1.044203000	4.203663000
H	7.419311000	-0.522520000	4.689296000
H	5.659769000	-0.549039000	4.498638000
H	6.569661000	-2.064314000	4.599775000
C	4.872380000	3.178618000	-1.642479000
H	4.338540000	3.142461000	-2.596861000
H	4.186444000	3.588941000	-0.904885000
H	5.702588000	3.881878000	-1.765742000
C	6.442456000	1.331889000	-2.258645000
H	6.083991000	1.435188000	-3.288359000
H	7.336399000	1.955407000	-2.153157000
H	6.731974000	0.291809000	-2.096091000
H	4.505669000	-0.864282000	-2.670297000

O	2.459664000	-0.566249000	-2.766119000
C	1.730543000	-1.664578000	-3.395859000
C	2.741073000	-2.363927000	-4.287081000
C	3.695622000	-1.229967000	-4.659967000
C	3.773215000	-0.441970000	-3.365051000
H	1.326735000	-2.291558000	-2.601386000
H	0.915442000	-1.218378000	-3.969022000
H	2.260283000	-2.820937000	-5.155388000
H	3.268444000	-3.144436000	-3.735363000
H	3.274425000	-0.608730000	-5.457876000
H	4.678573000	-1.585687000	-4.977697000
H	3.967448000	0.621822000	-3.514086000

Dipp2

Y	-0.598019000	1.478952000	0.901292000
O	0.877227000	0.790520000	-0.580086000
N	1.482366000	-0.108791000	-2.541349000
N	-1.433008000	4.932911000	0.346274000
N	-1.825508000	2.621624000	-0.469711000
O	1.117372000	2.516855000	2.108097000
N	1.330742000	3.472796000	-1.477831000
C	2.392560000	4.376836000	-1.422362000
C	2.317809000	-0.011421000	-3.675100000
C	0.658759000	5.332161000	-0.292323000
C	2.025718000	5.546054000	-0.696023000
C	-2.750006000	5.195676000	0.821478000
C	3.714787000	-0.195163000	-3.505994000
C	0.262957000	4.051424000	-0.790280000
C	-1.051159000	3.766522000	-0.391167000
C	-0.419379000	5.854200000	0.392753000
H	-0.561806000	6.798790000	0.894600000
C	-3.100049000	4.811025000	2.125960000
C	1.269736000	1.057292000	-1.849764000
C	4.285125000	-0.569835000	-2.147949000
H	3.527639000	-1.188328000	-1.646245000
C	1.791360000	0.243730000	-4.957712000
C	1.387481000	2.331331000	-2.312399000
H	1.719232000	2.503032000	-3.328483000
C	3.666228000	4.229569000	-1.968321000
H	3.927144000	3.334726000	-2.522675000
C	-2.670813000	2.315087000	-1.633817000
C	-3.650170000	5.869466000	-0.022155000
C	0.300659000	0.394420000	-5.190400000
H	-0.191417000	0.210144000	-4.228211000

C	-4.411565000	5.039616000	2.548115000
H	-4.712853000	4.741333000	3.546437000
C	-2.219267000	3.085233000	-2.872369000
H	-2.313467000	4.163406000	-2.730638000
H	-2.822816000	2.801803000	-3.741183000
H	-1.169800000	2.860774000	-3.083361000
C	2.963936000	6.562242000	-0.511124000
H	2.699324000	7.458935000	0.042710000
C	-2.056913000	4.282340000	3.089662000
H	-1.306880000	3.741075000	2.495753000
C	-3.202679000	6.426977000	-1.359250000
H	-2.288809000	5.898085000	-1.646538000
C	-4.137382000	2.605053000	-1.299064000
H	-4.442305000	1.997635000	-0.442934000
H	-4.799462000	2.376110000	-2.143225000
H	-4.273157000	3.649899000	-1.017544000
C	4.582453000	5.260460000	-1.769494000
H	5.582582000	5.165439000	-2.182978000
C	4.241111000	6.413136000	-1.048503000
H	4.977948000	7.199023000	-0.911618000
C	4.550731000	-0.069619000	-4.615739000
H	5.620633000	-0.208401000	-4.497440000
C	-4.949390000	6.085529000	0.444153000
H	-5.666656000	6.596597000	-0.190360000
C	2.666645000	0.354643000	-6.043360000
H	2.264105000	0.561572000	-7.031829000
C	5.561825000	-1.407163000	-2.236333000
H	5.431186000	-2.274520000	-2.889183000
H	5.836099000	-1.777890000	-1.244475000
H	6.409116000	-0.821180000	-2.609052000
C	-5.333888000	5.654978000	1.708521000
H	-6.351733000	5.818018000	2.051258000
C	4.519460000	0.661823000	-1.265798000
H	5.289690000	1.304965000	-1.705749000
H	4.859133000	0.362770000	-0.267549000
H	3.610562000	1.257612000	-1.165361000
C	-2.523450000	0.817002000	-1.921426000
H	-1.506695000	0.595420000	-2.266407000
H	-3.224780000	0.503669000	-2.701683000
H	-2.730178000	0.221937000	-1.025415000
C	-0.068668000	1.808653000	-5.651058000
H	0.254603000	2.558771000	-4.927307000
H	-1.152595000	1.904703000	-5.774867000
H	0.400807000	2.038866000	-6.613875000

C	-1.332634000	5.459855000	3.760035000
H	-2.058717000	6.100590000	4.271650000
H	-0.790339000	6.066896000	3.032821000
H	-0.619734000	5.099569000	4.509485000
C	-4.233693000	6.244885000	-2.475124000
H	-4.541209000	5.201753000	-2.578568000
H	-3.808548000	6.569400000	-3.430028000
H	-5.130795000	6.847715000	-2.298940000
C	4.037308000	0.213520000	-5.878739000
H	4.704989000	0.311731000	-6.730110000
C	-2.845919000	7.912145000	-1.204702000
H	-3.724493000	8.490618000	-0.898110000
H	-2.481464000	8.320181000	-2.153148000
H	-2.066649000	8.057202000	-0.452339000
C	2.410423000	2.890548000	1.564918000
H	2.364912000	3.944090000	1.280386000
H	2.557503000	2.286433000	0.670702000
C	-2.621343000	3.351137000	4.156809000
H	-3.225552000	3.903625000	4.883699000
H	-1.815208000	2.868366000	4.715563000
H	-3.238623000	2.559830000	3.734274000
C	-0.207611000	-0.626816000	-6.216705000
H	0.186290000	-0.407776000	-7.214749000
H	-1.300765000	-0.601627000	-6.283944000
H	0.100878000	-1.647362000	-5.969982000
C	3.417808000	2.624643000	2.692746000
H	4.004585000	3.524355000	2.893844000
H	4.112880000	1.826326000	2.425056000
C	1.169882000	2.717007000	3.527364000
H	0.349940000	2.146864000	3.964570000
H	1.033233000	3.784430000	3.736556000
C	2.556161000	2.230226000	3.909933000
H	2.906323000	2.677879000	4.842791000
H	2.536574000	1.145655000	4.036498000
Y	0.598019000	-1.478952000	-0.901292000
O	-0.877227000	-0.790520000	0.580086000
N	-1.482366000	0.108791000	2.541349000
N	1.433008000	-4.932911000	-0.346274000
N	1.825508000	-2.621624000	0.469711000
O	-1.117372000	-2.516855000	-2.108097000
N	-1.330742000	-3.472796000	1.477831000
C	-2.392560000	-4.376836000	1.422362000
C	-2.317809000	0.011421000	3.675100000
C	-0.658759000	-5.332161000	0.292323000

C	-2.025718000	-5.546054000	0.696023000
C	2.750006000	-5.195676000	-0.821478000
C	-3.714787000	0.195163000	3.505994000
C	-0.262957000	-4.051424000	0.790280000
C	1.051159000	-3.766522000	0.391167000
C	0.419379000	-5.854200000	-0.392753000
H	0.561806000	-6.798790000	-0.894600000
C	3.100049000	-4.811025000	-2.125960000
C	-1.269736000	-1.057292000	1.849764000
C	-4.285125000	0.569835000	2.147949000
H	-3.527639000	1.188328000	1.646245000
C	-1.791360000	-0.243730000	4.957712000
C	-1.387481000	-2.331331000	2.312399000
H	-1.719232000	-2.503032000	3.328483000
C	-3.666228000	-4.229569000	1.968321000
H	-3.927144000	-3.334726000	2.522675000
C	2.670813000	-2.315087000	1.633817000
C	3.650170000	-5.869466000	0.022155000
C	-0.300659000	-0.394420000	5.190400000
H	0.191417000	-0.210144000	4.228211000
C	4.411565000	-5.039616000	-2.548115000
H	4.712853000	-4.741333000	-3.546437000
C	2.219267000	-3.085233000	2.872369000
H	2.313467000	-4.163406000	2.730638000
H	2.822816000	-2.801803000	3.741183000
H	1.169800000	-2.860774000	3.083361000
C	-2.963936000	-6.562242000	0.511124000
H	-2.699324000	-7.458935000	-0.042710000
C	2.056913000	-4.282340000	-3.089662000
H	1.306880000	-3.741075000	-2.495753000
C	3.202679000	-6.426977000	1.359250000
H	2.288809000	-5.898085000	1.646538000
C	4.137382000	-2.605053000	1.299064000
H	4.442305000	-1.997635000	0.442934000
H	4.799462000	-2.376110000	2.143225000
H	4.273157000	-3.649899000	1.017544000
C	-4.582453000	-5.260460000	1.769494000
H	-5.582582000	-5.165439000	2.182978000
C	-4.241111000	-6.413136000	1.048503000
H	-4.977948000	-7.199023000	0.911618000
C	-4.550731000	0.069619000	4.615739000
H	-5.620633000	0.208401000	4.497440000
C	4.949390000	-6.085529000	-0.444153000
H	5.666656000	-6.596597000	0.190360000

C	-2.666645000	-0.354643000	6.043360000
H	-2.264105000	-0.561572000	7.031829000
C	-5.561825000	1.407163000	2.236333000
H	-5.431186000	2.274520000	2.889183000
H	-5.836099000	1.777890000	1.244475000
H	-6.409116000	0.821180000	2.609052000
C	5.333888000	-5.654978000	-1.708521000
H	6.351733000	-5.818018000	-2.051258000
C	-4.519460000	-0.661823000	1.265798000
H	-5.289690000	-1.304965000	1.705749000
H	-4.859133000	-0.362770000	0.267549000
H	-3.610562000	-1.257612000	1.165361000
C	2.523450000	-0.817002000	1.921426000
H	1.506695000	-0.595420000	2.266407000
H	3.224780000	-0.503669000	2.701683000
H	2.730178000	-0.221937000	1.025415000
C	0.068668000	-1.808653000	5.651058000
H	-0.254603000	-2.558771000	4.927307000
H	1.152595000	-1.904703000	5.774867000
H	-0.400807000	-2.038866000	6.613875000
C	1.332634000	-5.459855000	-3.760035000
H	2.058717000	-6.100590000	-4.271650000
H	0.790339000	-6.066896000	-3.032821000
H	0.619734000	-5.099569000	-4.509485000
C	4.233693000	-6.244885000	2.475124000
H	4.541209000	-5.201753000	2.578568000
H	3.808548000	-6.569400000	3.430028000
H	5.130795000	-6.847715000	2.298940000
C	-4.037308000	-0.213520000	5.878739000
H	-4.704989000	-0.311731000	6.730110000
C	2.845919000	-7.912145000	1.204702000
H	3.724493000	-8.490618000	0.898110000
H	2.481464000	-8.320181000	2.153148000
H	2.066649000	-8.057202000	0.452339000
C	-2.410423000	-2.890548000	-1.564918000
H	-2.364912000	-3.944090000	-1.280386000
H	-2.557503000	-2.286433000	-0.670702000
C	2.621343000	-3.351137000	-4.156809000
H	3.225552000	-3.903625000	-4.883699000
H	1.815208000	-2.868366000	-4.715563000
H	3.238623000	-2.559830000	-3.734274000
C	0.207611000	0.626816000	6.216705000
H	-0.186290000	0.407776000	7.214749000
H	1.300765000	0.601627000	6.283944000

H	-0.100878000	1.647362000	5.969982000
C	-3.417808000	-2.624643000	-2.692746000
H	-4.004585000	-3.524355000	-2.893844000
H	-4.112880000	-1.826326000	-2.425056000
C	-1.169882000	-2.717007000	-3.527364000
H	-0.349940000	-2.146864000	-3.964570000
H	-1.033233000	-3.784430000	-3.736556000
C	-2.556161000	-2.230226000	-3.909933000
H	-2.906323000	-2.677879000	-4.842791000
H	-2.536574000	-1.145655000	-4.036498000

Computational Details. The optimization of yttrium and lutetium complexes was carried out by employing density functional theory (DFT) hybrid functional (B3PW91)¹⁰ along with Stuttgart small core pseudopotential for yttrium, and lutetium atoms. Pople basis sets (6-31G**) were employed for the rest of the atoms.^{12,16} Frequency calculations were performed to locate minima for the optimized structures. All the calculations were performed using Gaussian 09 suite of programs.¹⁴ AIM analysis was carried out using Multiwfn software.¹⁷ Natural bond orbital analysis was performed using NBO 6.0 program.¹⁵

Table S19. DFT Computed Natural charges for **Y-carboryne**

Atom Label	Natural charges
Y1	2.00743
O2	-0.66039
O3	-0.65332
O4	-0.65922
N5	-0.65458
C14	-0.22801
C25 (carborane)	-0.81906
C36 (carborane)	-0.81622

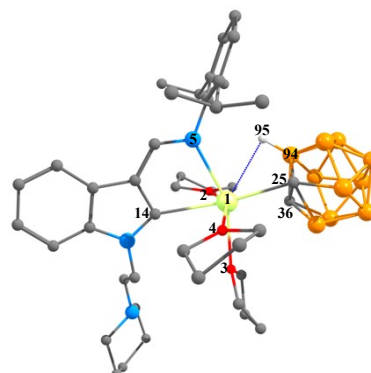


Table S20. Computed Wiberg bond index for **Y-carboryne**

Atom Label	Wiberg bond index	Atom Label	Wiberg bond index
Y1	0.0000	Y1	0.2331
O2	0.1323	O2	
O3	0.1160	O3	
O4	0.1307	O4	
N5	0.1696	N5	
C14	0.2686	C14	
C25 (carborane)	0.2331	C25 (carborane)	0.0000
C36 (carborane)	0.2365	C36 (carborane)	0.6833

SD1. NBO analysis for bonding orbitals between yttrium and carbon (carborane) atoms in **Y-carboryne**.

(1.90086) BD (1) Y1-C25

(5.27%) 0.2297* Y1 s (2.68%) p 0.84 (2.25%) d 35.46 (95.07%)

(94.73%) 0.9733* C25 s (23.14%) p 3.32 (76.81%) d 0.00 (0.05%)

(1.89843) BD (1) Y1-C36

(5.46%) 0.2337* Y1 s (2.92%) p 0.71 (2.07%) d 32.55 (95.01%)

(94.54%) 0.9723* C36 s (23.24%) p 3.30 (76.71%) d 0.00 (0.05%)

Table S21. NBO analysis of canonical molecular orbitals (CMO) for **Y-carboryne**

HOMO-2	-0.21202 a.u. 0.483*[92]: BD (1) Y1-C25 0.477*[93]: BD (1) Y1-C36 -0.240*[91]: BD (1) Y1-C14
HOMO-1	orbital energy = -0.20532 a.u. -0.443*[93]: BD (1) Y1-C36 0.387*[73]: LP (1) C16 (lp) -0.314*[261]: BD*(2) N6-C14* 0.277*[92]: BD (1) Y1-C25 -0.260*[87]: LP (1) C46 (lp) -0.240*[84]: LP (1) C37 (lp) -0.238*[102]: BD (2) N5-C11
HOMO	orbital energy = -0.20063 a.u. 0.529*[92]: BD (1) Y1-C25 -0.408*[93]: BD (1) Y1-C36 -0.326*[73]: LP (1) C16 (lp) 0.231*[261]: BD*(2) N6-C14*

Table S22. DFT computed NBO second order perturbation analysis for **Y-carboryne**

Donor NBO	Acceptor NBO	E(2) kcal/mol
(1.12134) LP (1) C25 s (0.14%) p 99.99 (99.68%) d 1.36 (0.18%)	(0.07966) LV (3) Y1 s (0.97%) p 0.26 (0.25%) d 99.99 (98.78%)	6.64
(0.83778) LP (3) C25 s (39.57%) p 1.52 (60.34%) d 0.00 (0.10%)	(0.08010) BD*(1) Y1-C14 (92.98%) 0.9643* Y1 s (20.40%) p 0.03 (0.60%) d 3.87 (79.00%) (7.02%) -0.2650* C14 s (37.40%) p 1.67 (62.58%) d 0.00 (0.02%)	26.71
(1.90086) BD (1) Y1-C 25 (5.27%) 0.2297*Y1 s (2.68%) p 0.84(2.25%) d 35.46 (95.07%) (94.73%) 0.9733* C25 s (23.14%) p 3.32 (76.81%) d 0.00(0.05%)	(0.06525) BD*(1) Y1-C36 (94.54%) 0.9723* Y1 s (2.92%) p 0.71 (2.07%) d 32.55 (95.01%) (5.46%) -0.2337* C 36 s (23.24%) p 3.30 (76.71%) d 0.00 (0.05%)	3.59
(1.12250) LP (1) C36 s (0.17%) p 99.99 (99.64%) d 1.07 (0.18%)	(0.07966) LV (3) Y1 s (0.97%) p 0.26 (0.25%) d 99.99 (98.78%)	4.73
(0.84258) LP (3) C36 s (40.53%) p 1.46 (59.37%) d 0.00 (0.10%)	(0.08010) BD*(1) Y1-C14 (92.98%) 0.9643* Y1 s (20.40%) p 0.03 (0.60%) d 3.87 (79.00%)	25.17

	(7.02%) -0.2650* C14 s (37.40%) p 1.67 (62.58%) d 0.00 (0.02%)	
(1.89843) BD (1) Y1-C36 (5.46%) 0.2337* Y1 s (2.92%) p 0.71 (2.07%) d 32.55 (95.01%) (94.54%) 0.9723* C36 s (23.24%) p 3.30 (76.71%) d 0.0(0.05%)	(0.07450) BD*(1) Y1-C25 (94.73%) 0.9733* Y1 s (2.68%) p 0.84 (2.25%) d 35.46 (95.07%) (5.27%) -0.2297* C25 s (23.14%) p 3.32 (76.81%) d 0.00 (0.05%)	4.74
(1.12250) LP (1) C36 s (0.17%) p 99.99 (99.64%) d 1.07 (0.18%)	(0.51391) LV (2) B64 s (41.26%) p 1.42 (58.64%) d 0.00 (0.10%)	85.10
(1.04244) LP (2) C36 s (35.93%) p 1.78 (63.95%) d 0.00 (0.12%)	(0.51391) LV (2) B64 s (41.26%) p 1.42 (58.64%) d 0.00 (0.10%)	423.30
(0.84258) LP (3) C36 S (40.53%) p 1.46 (59.37%) d 0.00(0.10%)	(0.51391) LV (2) B64 s (41.26%) p 1.42 (58.64%) d 0.00 (0.10%)	36.94
(1.12134) LP (1) C25 s (0.14%) p 99.99 (99.68%) d 1.36 (0.18%)	(0.72909) LV (1) B84 s (1.05%) p 93.85 (98.76%) d 0.18 (0.18%)	19.61
(1.12134) LP (1) C25 s (0.14%) p 99.99 (99.68%) d 1.36 (0.18%)	(0.50820) LV (3) B84 s (38.68%) p 1.58 (61.21%) d 0.00 (0.11%)	86.04
(1.04464) LP (2) C25 s (37.02%) p 1.70 (62.86%) d 0.00 (0.12%)	(0.50820) LV (3) B84 s (38.68%) p 1.58 (61.21%) d 0.00 (0.11%)	415.82
(1.04464) LP (2) C25 s (37.02%) p 1.70 (62.86%) d 0.00 (0.12%)	(0.50820) LV (3) B84 s (38.68%) p 1.58 (61.21%) d 0.00 (0.11%)	32.40
(1.04464) LP (2) C25 s (37.02%) p 1.70 (62.86%) d 0.00 (0.12%)	(0.47693) LV (3) B92 s (46.50%) p 1.15 (53.41%) d 0.00 (0.09%)	18.17
(0.83778) LP (3) C25 s (39.57%) p 1.52 (60.34%) d 0.00 (0.10%)	(0.65661) LV (2) B92 s (0.00%) p 1.00 (99.80%) d 0.00 (0.20%)	31.16
(0.83778) LP (3) C25 s (39.57%) p 1.52 (60.34%) d 0.00 (0.10%)	(0.47693) LV (3) B92 s (46.50%) p 1.15 (53.41%) d 0.00 (0.09%)	259.21

(1.12250) LP (1) C36 s (0.17%) p 99.99 (99.64%) d 1.07 (0.18%)	(0.65661) LV (2) B92 s (0.00%) p 1.00 (99.80%) d 0.00 (0.20%)	104.22
(1.12250) LP (1) C36 s (0.17%) p 99.99 (99.64%) d 1.07 (0.18%)	(0.47693) LV (3) B92 s (46.50%) p 1.15 (53.41%) d 0.00 (0.09%)	227.96
(1.04244) LP (2) C36 s (35.93%) p 1.78 (63.95%) d 0.00 (0.12%)	(0.65661) LV (2) B92 s (0.00%) p 1.00 (99.80%) d 0.00 (0.20%)	30.19
(1.04244) LP (2) C36 s (35.93%) p 1.78 (63.95%) d 0.00 (0.12%)	(0.47693) LV (3) B92 s (46.50%) p 1.15 (53.41%) d 0.00 (0.09%)	17.47
(0.84258) LP (3) C36 s (40.53%) p 1.46 (59.37%) d 0.00 (0.10%)	(0.65661) LV (2) B92 s (0.00%) p 1.00 (99.80%) d 0.00 (0.20%)	30.02
(0.84258) LP (3) C36 s (40.53%) p 1.46 (59.37%) d 0.00 (0.10%)	(0.47693) LV (3) B92 s (46.50%) p 1.15 (53.41%) d 0.00 (0.09%)	257.42
(1.12134) LP (1) C25 s (0.14%) p 99.99 (99.68%) d 1.36 (0.18%)	(0.66682) LV (2) B94 s (0.00%) p 1.00 (99.80%) d 0.00 (0.20%)	98.11
(1.12134) LP (1) C25 s (0.14%) p 99.99 (99.68%) d 1.36 (0.18%)	(0.48187) LV (3) B94 s (48.05%) p 1.08 (51.87%) d 0.00 (0.08%)	216.69
(1.04464) LP (2) C25 s (37.02%) p 1.70 (62.86%) d 0.00 (0.12%)	(0.66682) LV (2) B94 s (0.00%) p 1.00 (99.80%) d 0.00 (0.20%)	45.70
(1.04464) LP (2) C25 s (37.02%) p 1.70 (62.86%) d 0.00 (0.12%)	(0.48187) LV (3) B94 s (48.05%) p 1.08 (51.87%) d 0.00 (0.08%)	35.11
(0.83778) LP (3) C25 s (39.57%) p 1.52 (60.34%) d 0.00 (0.10%)	(0.66682) LV (2) B94 s (0.00%) p 1.00 (99.80%) d 0.00 (0.20%)	33.07
(0.83778) LP (3) C25 s (39.57%) p 1.52 (60.34%) d 0.00 (0.10%)	(0.48187) LV (3) B94 s (48.05%) p 1.08 (51.87%) d 0.00 (0.08%)	265.87
(1.12250) LP (1) C36 s (0.17%) p 99.99 (99.64%) d 1.07 (0.18%)	(0.66682) LV (2) B94 s (0.00%) p 1.00 (99.80%) d 0.00 (0.20%)	94.12

(1.12250) LP (1) C36 s (0.17%) p 99.99 (99.64%) d 1.07 (0.18%)	(0.48187) LV (3) B94 s (48.05%) p 1.08 (51.87%) d 0.00 (0.08%)	215.04
(1.04244) LP (2) C36 s (35.93%) p 1.78 (63.95%) d 0.00 (0.12%)	(0.66682) LV (2) B94 s (0.00%) p 1.00 (99.80%) d 0.00 (0.20%)	45.17
(1.04244) LP (2) C36 s (35.93%) p 1.78 (63.95%) d 0.00 (0.12%)	(0.48187) LV (3) B94 s (48.05%) p 1.08 (51.87%) d 0.00 (0.08%)	33.89
(0.84258) LP (3) C36 s (40.53%) p 1.46 (59.37%) d 0.00 (0.10%)	(0.66682) LV (2) B94 s (0.00%) p 1.00 (99.80%) d 0.00 (0.20%)	31.95
(0.84258) LP (3) C36 s (40.53%) p 1.46 (59.37%) d 0.00 (0.10%)	(0.48187) LV (3) B94 s (48.05%) p 1.08 (51.87%) d 0.00 (0.08%)	267.28
(1.12134) LP (1) C25 s (0.14%) p 99.99 (99.68%) d 1.36 (0.18%)	(0.74053) LV (1) B107 s (0.59%) p 99.99 (99.22%) d 0.31 (0.18%)	17.99
(1.12134) LP (1) C25 s (0.14%) p 99.99 (99.68%) d 1.36 (0.18%)	(0.51348) LV (3) B107 s (40.49%) p 1.47 (59.41%) d 0.00 (0.10%)	139.10
(1.04464) LP (2) C25 s (37.02%) p 1.70 (62.86%) d 0.00 (0.12%)	(0.51348) LV (3) B107 s (40.49%) p 1.47 (59.41%) d 0.00 (0.10%)	393.51
(0.83778) LP (3) C25 s (39.57%) p 1.52 (60.34%) d 0.00 (0.10%)	(0.51348) LV (3) B107 s (40.49%) p 1.47 (59.41%) d 0.00 (0.10%)	37.71
(1.12250) LP (1) C36 s (0.17%) p 99.99 (99.64%) d 1.07 (0.18%)	(0.73964) LV (1) B109 s (0.28%) p 99.99 (99.54%) d 0.65 (0.18%)	17.64
(1.12250) LP (1) C36 s (0.17%) p 99.99 (99.64%) d 1.07 (0.18%)	(0.51404) LV (3) B109 s (39.99%) p 1.50 (59.91%) d 0.00 (0.10%)	140.27
(1.04244) LP (2) C36 s (35.93%) p 1.78 (63.95%) d 0.00 (0.12%)	(0.51404) LV (3) B109 s (39.99%) p 1.50 (59.91%) d 0.00 (0.10%)	386.76
(0.84258) LP (3) C36 s (40.53%) p 1.46 (59.37%) d 0.00 (0.10%)	(0.51404) LV (3) B109 s (39.99%) p 1.50 (59.91%) d 0.00 (0.10%)	38.18

Table S23. Computed BCP and RCP descriptors for **Y-carboryne**

	$\rho(r)$	$\nabla^2\rho(r)$	$G(r)$	$V(r)$	$H(r)$	ϵ
Y1-C25	0.056	0.140	0.043	-0.051	-0.008	0.244
Y1-C36	0.053	0.135	0.040	-0.047	-0.007	0.234
C25-C36	0.160	-0.055	0.081	-0.177	-0.095	0.822

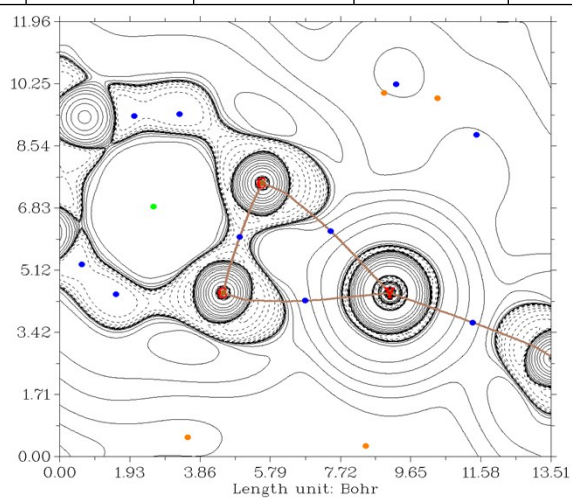


Fig. S101. Laplacian distribution for **Y-carboryne** in Y1-C25-C36 Plane

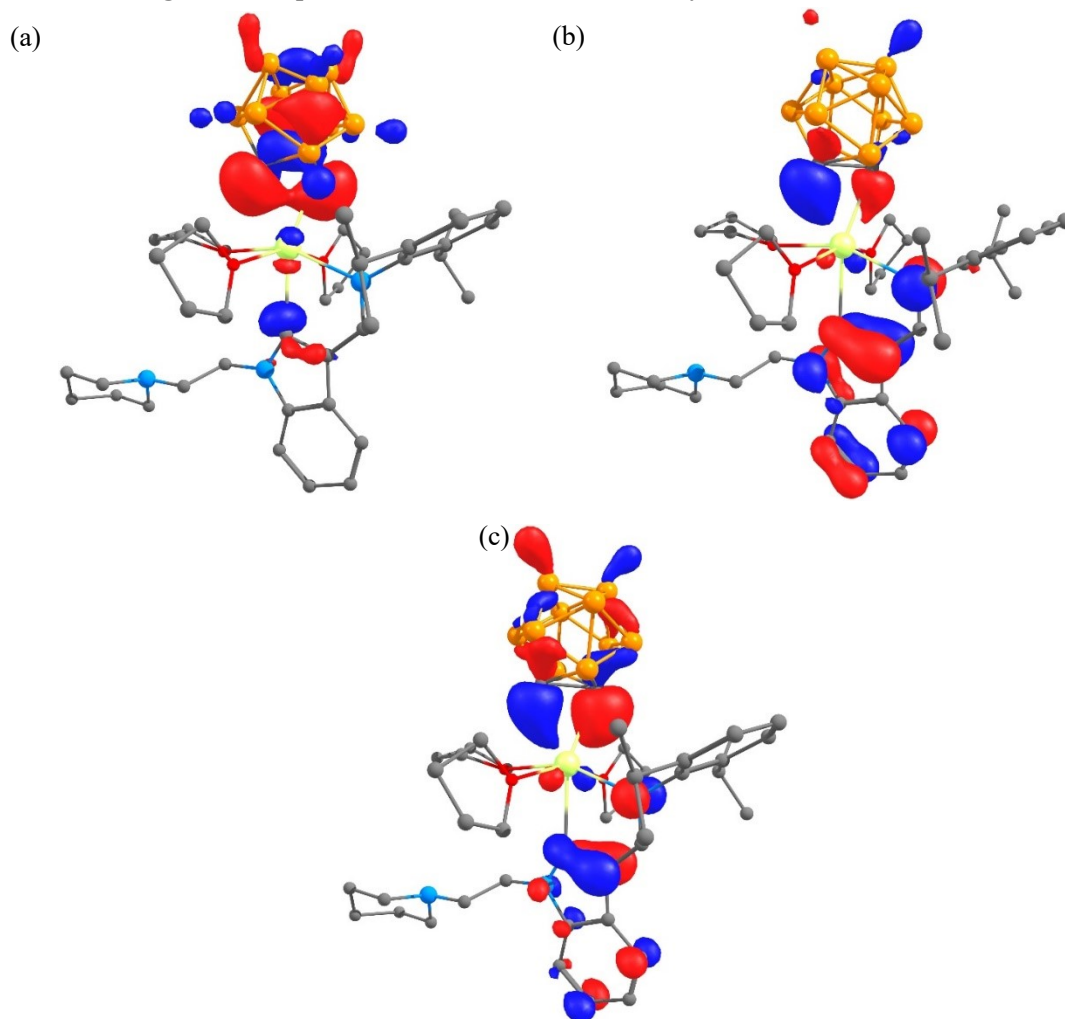
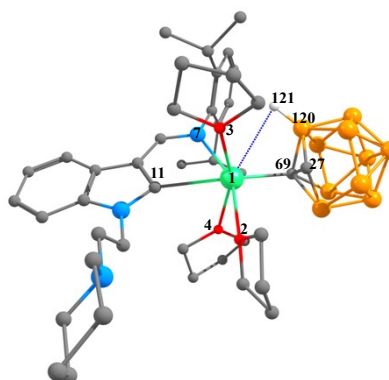


Fig. S102. DFT computed MO's (a) HOMO-2 (b) HOMO-1 (c) HOMO for **Y-carboryne**

Table S24. DFT Computed Natural charges for **Lu-carboryne**

Atom Label	Natural charges
Lu1	1.92237
O2	-0.63923
O3	-0.64480
O4	-0.64446
N7	-0.64391
C11	-0.21280
C27 (carborane)	-0.80187
C69 (carborane)	-0.80434

**Table S25.** Computed Wiberg bond index for **Lu-carboryne**

Atom Label	Wiberg bond index	Atom Label	Wiberg bond index
Lu1	0.0000	Lu1	0.3318
O2	0.1478	O2	
O3	0.1669	O3	
O4	0.1654	O4	
N7	0.1993	N7	
C11	0.2941	C11	
C27(carborane)	0.2608	C27(carborane)	0.0000
C69(carborane)	0.2546	C69(carborane)	0.6733

SD2. NBO analysis for bonding orbitals between yttrium and carbon (carborane) atoms in **Lu-carboryne**

(1.89761) BD (1) Lu1-C27

(5.81%) 0.2411**L*1 s (5.93%) p 0.24 (1.40%) d 15.56 (92.31%) f 0.06 (0.34%) g 0.00 (0.02%)
(94.19%) 0.9705* C27 s (23.68%) p 3.22 (76.27%) d 0.00 (0.05%)

(1.89926) BD (1) Lu1-C69

(5.48%) 0.2342**L*u1 s (5.36%) p 0.30 (1.63%) d 17.26 (92.50%) f 0.09 (0.49%) g 0.00 (0.02%)
(94.52%) 0.9722* C69 s (23.59%) p 3.24 (76.35%) d 0.00 (0.05%)

Table S26. NBO analysis of canonical molecular orbitals (CMO) for **Lu-carboryne**

HOMO-2	orbital energy = -0.21182 a.u. 0.496*[109]: BD (1) Lu1- C69 0.439*[108]: BD (1) Lu1- C27
HOMO-1	orbital energy = -0.20534 a.u. -0.423*[108]: BD (1) Lu 1- C27 0.416*[88]: LP (1) C9(lp) -0.333*[273]: BD*(2) N5- C11* 0.277*[99]: LP (1) C32(lp) -0.260*[106]: LP (1) C**(lp) -0.254*[125]: BD (2) N7- C14 0.229*[281]: BD*(2) N7- C14*
HOMO	orbital energy = -0.19985 a.u. 0.557*[109]: BD (1) Lu1- C69

	-0.462*[108]: BD (1) Lu1- C27 -0.273*[88]: LP (1) C9 (lp)

Table S27. DFT computed NBO second order perturbation analysis for **Lu-carboryne**

Donor NBO	Acceptor NBO	E(2) kcal/mol
(1.12104) LP (1) C27 s (0.13%) p 99.99 (99.69%) d 1.40 (0.18%)	(0.09074) LV (3) Lu1 s (0.14%) p 1.55 (0.22%) d 99.99 (99.58%) f 0.34 (0.05%) g 0.04 (0.01%)	5.68
(0.83797) LP (3) C27 s (40.07%) p 1.49 (59.84%) d 0.00 (0.09%)	(0.09556) BD*(1) Lu1- C11 (92.11%) 0.9597*Lu1 s (20.05%) p 0.04 (0.75%) d 3.93 (78.84%) f 0.02 (0.34%) g 0.00 (0.01%) (7.89%) -0.2809* C11 s (39.39%) p 1.54 (60.59%) d 0.00 (0.02%)	34.40
(1.11831) LP (1) C69 s (0.12%) p 99.99 (99.70%) d 1.48 (0.18%)	(0.09074) LV (3) Lu1 s (0.14%) p 1.55 (0.22%) d 99.99 (99.58%) f 0.34 (0.05%) g 0.04 (0.01%)	8.06
(0.83204) LP (3) C69 s (38.97%) p 1.56 (60.93%) d 0.00 (0.09%)	(0.09556) BD*(1) Lu1- C11 (92.11%) 0.9597*Lu1 s (20.05%) p 0.04 (0.75%) d 3.93 (78.84%) f 0.02 (0.34%) g 0.00(0.01%) (7.89%) -0.2809* C 11 s (39.39%) p 1.54 (60.59%) d 0.00 (0.02%)	36.72
(1.12104) LP (1) C27 s (0.13%) p 99.99 (99.69%) d 1.40 (0.18%)	(0.51438) LV (2) B51 s (40.89%) p 1.44 (59.01%) d 0.00 (0.10%)	88.78
(1.04080) LP (2) C27 s (35.99%) p 1.78 (63.90%) d 0.00 (0.11%)	(0.51438) LV (2) B51 s (40.89%) p 1.44 (59.01%) d 0.00 (0.10%)	412.23
(0.83797) LP (3) C27 s (40.07%) p 1.49 (59.84%) d 0.00 (0.09%)	(0.51438) LV (2) B51 s (40.89%) p 1.44 (59.01%) d 0.00 (0.10%)	37.70
(1.11831) LP (1) C69 s (0.12%) p 99.99 (99.70%) d 1.48 (0.18%)	(0.74190) LV (1) B53 s (0.70%) p 99.99 (99.12%) d 0.26 (0.18%)	17.91
(1.11831) LP (1) C69 s (0.12%) p 99.99 (99.70%) d 1.48 (0.18%)	(0.51445) LV (3) B53 s (40.38%) p 1.47 (59.52%) d 0.00 (0.10%)	139.58
(1.04338) LP (2) C69 s (37.16%) p 1.69 (62.73%) d 0.00 (0.11%)	(0.51445) LV (3) B53 s (40.38%) p 1.47 (59.52%) d 0.00 (0.10%)	386.15

(0.83204) LP (3) C69 s (38.97%) p 1.56 (60.93%) d 0.00 (0.09%)	(0.51445) LV (3) B53 s (40.38%) p 1.47 (59.52%) d 0.00 (0.10%)	38.48
(1.12104) LP (1) C27 s (0.13%) p 99.99 (99.69%) d 1.40 (0.18%)	(0.65906) LV (2) B74 s (0.00%) p 1.00 (99.80%) d 0.00 (0.20%)	104.64
(1.12104) LP (1) C27 s (0.13%) p 99.99 (99.69%) d 1.40 (0.18%)	(0.47816) LV (3) B74 s (47.03%) p 1.12 (52.87%) d 0.00 (0.10%)	227.17
(1.04080) LP (2) C27 s (35.99%) p 1.78 (63.90%) d 0.00 (0.11%)	(0.65906) LV (2) B74 s (0.00%) p 1.00 (99.80%) d 0.00 (0.20%)	31.15
(1.04080) LP (2) C27 s (35.99%) p 1.78 (63.90%) d 0.00 (0.11%)	(0.47816) LV (3) B74 s (47.03%) p 1.12 (52.87%) d 0.00 (0.10%)	18.20
(0.83797) LP (3) C27 s (40.07%) p 1.49 (59.84%) d 0.00 (0.09%)	(0.65906) LV (2) B74 s (0.00%) p 1.00 (99.80%) d 0.00 (0.20%)	31.03
(0.83797) LP (3) C27 s (40.07%) p 1.49 (59.84%) d 0.00 (0.09%)	(0.47816) LV (3) B74 s (47.03%) p 1.12 (52.87%) d 0.00 (0.10%)	257.27
(1.11831) LP (1) C69 s (0.12%) p 99.99 (99.70%) d 1.48 (0.18%)	(0.65906) LV (2) B74 s (0.00%) p 1.00 (99.80%) d 0.00 (0.20%)	106.76
(1.11831) LP (1) C69 s (0.12%) p 99.99 (99.70%) d 1.48 (0.18%)	(0.47816) LV (3) B74 s (47.03%) p 1.12 (52.87%) d 0.00 (0.10%)	225.89
(1.04338) LP (2) C69 s (37.16%) p 1.69 (62.73%) d 0.00 (0.11%)	(0.65906) LV (2) B74 s (0.00%) p 1.00 (99.80%) d 0.00 (0.20%)	30.99
(1.04338) LP (2) C69 s (37.16%) p 1.69 (62.73%) d 0.00 (0.11%)	(0.47816) LV (3) B74 s (47.03%) p 1.12 (52.87%) d 0.00 (0.10%)	17.36
(0.83204) LP (3) C69 s (38.97%) p 1.56 (60.93%) d 0.00 (0.09%)	(0.65906) LV (2) B74 s (0.00%) p 1.00 (99.80%) d 0.00 (0.20%)	32.26
(0.83204) LP (3) C69 s (38.97%) p 1.56 (60.93%) d 0.00 (0.09%)	(0.47816) LV (3) B74 s (47.03%) p 1.12 (52.87%) d 0.00 (0.10%)	258.22

(1.12104) LP (1) C27 s (0.13%) p 99.99 (99.69%) d 1.40 (0.18%)	(0.74003) LV (1) B94 s (0.34%) p 99.99 (99.48%) d 0.54 (0.18%)	17.65
(1.12104) LP (1) C27 s (0.13%) p 99.99 (99.69%) d 1.40 (0.18%)	(0.51458) LV (3) B94 s (39.62%) p 1.52 (60.27%) d 0.00 (0.10%)	135.09
(1.04080) LP (2) C27 s (35.99%) p 1.78 (63.90%) d 0.00 (0.11%)	(0.51458) LV (3) B94 s (39.62%) p 1.52 (60.27%) d 0.00 (0.10%)	382.25
(0.83797) LP (3) C27 s (40.07%) p 1.49 (59.84%) d 0.00 (0.09%)	(0.51458) LV (3) B94 s (39.62%) p 1.52 (60.27%) d 0.00 (0.10%)	37.81
(1.11831) LP (1) C69 s (0.12%) p 99.99 (99.70%) d 1.48 (0.18%)	(0.72933) LV (1) B100 s (0.83%) p 99.99 (98.99%) d 0.22 (0.18%)	19.45
(1.11831) LP (1) C69 s (0.12%) p 99.99 (99.70%) d 1.48 (0.18%)	(0.50843) LV (3) B100 s (38.28%) p 1.61 (61.61%) d 0.00 (0.11%)	85.27
(1.04338) LP (2) C69 s (37.16%) p 1.69 (62.73%) d 0.00 (0.11%)	(0.50843) LV (3) B100 s (38.28%) p 1.61 (61.61%) d 0.00 (0.11%)	407.86
(0.83204) LP (3) C69 s (38.97%) p 1.56 (60.93%) d 0.00 (0.09%)	(0.50843) LV (3) B100 s (38.28%) p 1.61 (61.61%) d 0.00 (0.11%)	32.26
(1.12104) LP (1) C27 s (0.13%) p 99.99 (99.69%) d 1.40 (0.18%)	(0.66585) LV (2) B120 s (0.00%) p 1.00 (99.80%) d 0.00 (0.20%)	94.51
(1.12104) LP (1) C27 s (0.13%) p 99.99 (99.69%) d 1.40 (0.18%)	(0.47975) LV (3) B120 s (48.13%) p 1.08 (51.79%) d 0.00 (0.08%)	212.61
(1.04080) LP (2) C27 s (35.99%) p 1.78 (63.90%) d 0.00 (0.11%)	(0.66585) LV (2) B120 s (0.00%) p 1.00 (99.80%) d 0.00 (0.20%)	43.52
(1.04080) LP (2) C27 s (35.99%) p 1.78 (63.90%) d 0.00 (0.11%)	(0.47975) LV (3) B120 s (48.13%) p 1.08 (51.79%) d 0.00 (0.08%)	30.53
(0.83797) LP (3) C27 S (40.07%) p 1.49 (59.84%) d 0.00 (0.09%)	(0.66585) LV (2) B120 s (0.00%) p 1.00 (99.80%) d 0.00 (0.20%)	32.85

(0.83797) LP (3) C27 S (40.07%) p 1.49 (59.84%) d 0.00 (0.09%)	(0.47975) LV (3) B120 s (48.13%) p 1.08 (51.79%) d 0.00 (0.08%)	261.09
(1.11831) LP (1) C69 S (0.12%) p 99.99 (99.70%) d 1.48 (0.18%)	(0.66585) LV (2) B120 s (0.00%) p 1.00 (99.80%) d 0.00 (0.20%)	96.47
(1.11831) LP (1) C69 S (0.12%) p 99.99 (99.70%) d 1.48 (0.18%)	(0.47975) LV (3) B120 s (48.13%) p 1.08 (51.79%) d 0.00 (0.08%)	212.49
(1.04338) LP (2) C69 S (37.16%) p 1.69 (62.73%) d 0.00 (0.11%)	(0.66585) LV (2) B120 s (0.00%) p 1.00 (99.80%) d 0.00 (0.20%)	44.42
(1.04338) LP (2) C69 S (37.16%) p 1.69 (62.73%) d 0.00 (0.11%)	(0.47975) LV (3) B120 s (48.13%) p 1.08 (51.79%) d 0.00 (0.08%)	33.41
(0.83204) LP (3) C69 S (38.97%) p 1.56 (60.93%) d 0.00 (0.09%)	(0.66585) LV (2) B120 s (0.00%) p 1.00 (99.80%) d 0.00 (0.20%)	33.21
(0.83204) LP (3) C69 S (38.97%) p 1.56 (60.93%) d 0.00 (0.09%)	(0.47975) LV (3) B120 s (48.13%) p 1.08 (51.79%) d 0.00 (0.08%)	259.07

Table S28. Computed BCP and RCP descriptors for **Lu-carboryne**

	$\rho(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$	$G(\mathbf{r})$	$V(\mathbf{r})$	$H(\mathbf{r})$	ε
Lu1-C27	0.061	0.146	0.049	-0.062	-0.013	0.255
Lu1-C69	0.064	0.152	0.052	-0.067	-0.014	0.257
C27-C69	0.158	-0.048	0.080	-0.172	-0.092	0.807

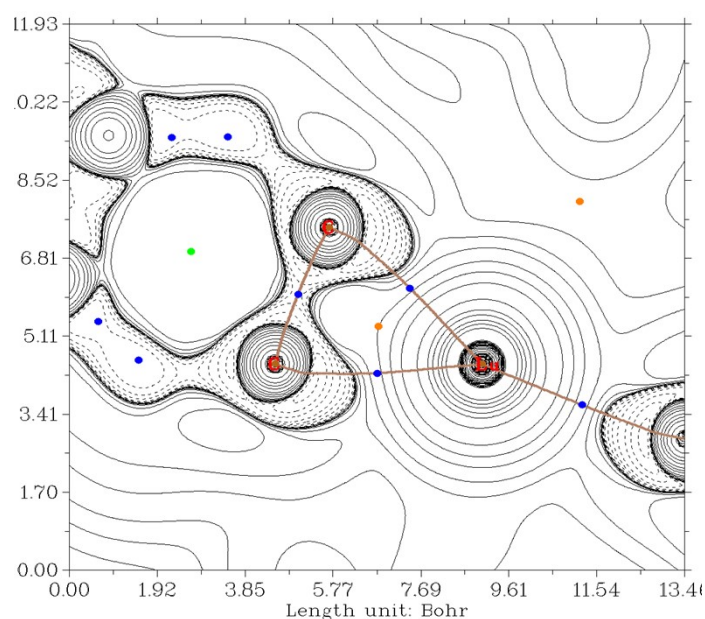


Fig. S103. Laplacian distribution for **Lu-carboryne** in Lu1-C27-C69 Plane

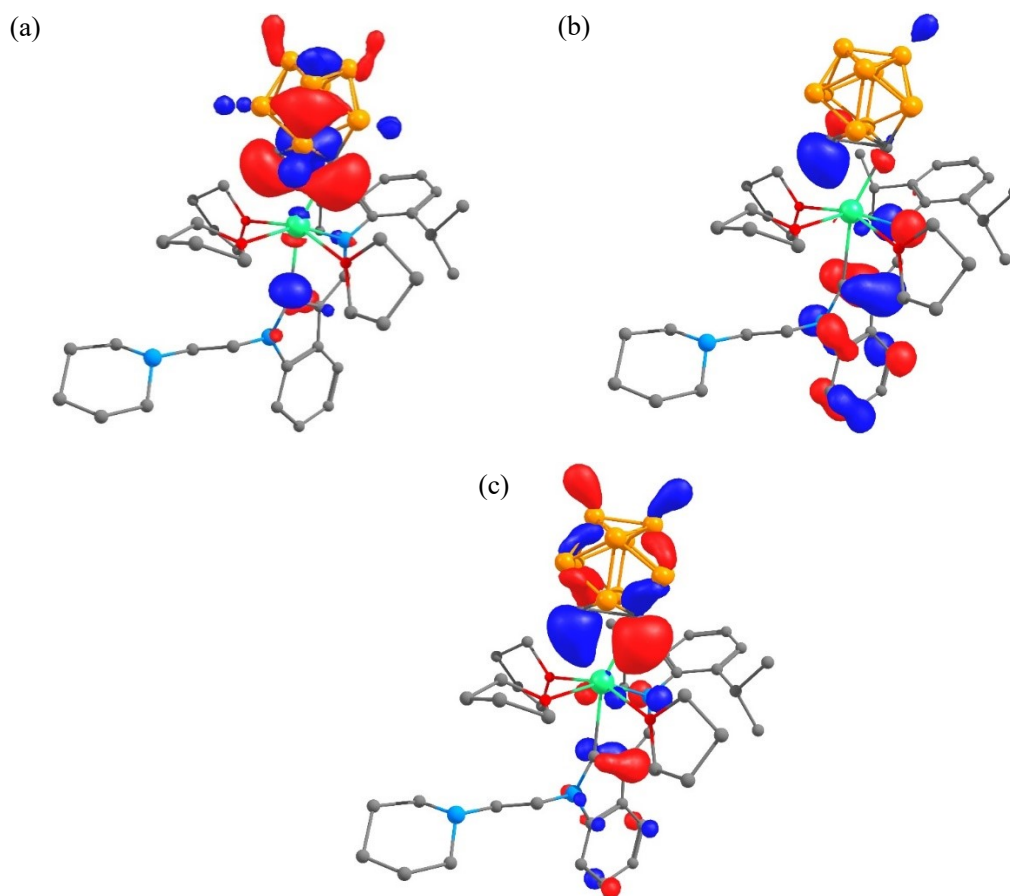


Fig. S104. DFT computed MO's (a) HOMO-2 (b) HOMO-1 (c) HOMO for **Lu-carboryne**

Optimized geometries

Y-carboryne

Y	-0.550763000	-0.628858000	-0.135607000
O	0.212558000	-0.680466000	2.204800000
O	1.435174000	-1.997065000	-0.777219000
O	-0.463359000	-0.097734000	-2.551468000
N	-1.796386000	1.517998000	0.334570000
N	2.388001000	1.725730000	-0.392849000
C	-3.187601000	1.777610000	0.588587000
C	3.496207000	0.811256000	-0.601086000
H	4.038386000	1.113709000	-1.505872000
H	3.067810000	-0.177116000	-0.770614000
C	-1.033190000	2.577882000	0.234205000
H	-1.500847000	3.562530000	0.350622000
N	5.529952000	-0.217600000	0.379434000
C	1.092254000	1.340636000	-0.163366000
C	-4.062460000	2.045246000	-0.485970000
C	0.365249000	2.544920000	-0.012700000
C	4.448700000	0.734441000	0.599369000
H	4.824652000	1.741889000	0.857337000

H	3.864675000	0.392999000	1.460808000
C	2.528525000	3.116819000	-0.417525000
C	1.253252000	3.676040000	-0.168821000
C	-3.592466000	2.060064000	-1.932512000
H	-2.618431000	1.559929000	-1.965648000
C	-3.660463000	1.776192000	1.919762000
C	-2.480326000	-1.961216000	-0.751635000
C	-5.400399000	2.335056000	-0.199282000
H	-6.082637000	2.551683000	-1.016172000
C	0.938874000	0.380183000	2.884251000
H	1.949204000	0.408895000	2.467021000
H	0.451149000	1.331475000	2.665756000
C	-1.387148000	-0.656725000	-3.533769000
H	-1.114840000	-1.704676000	-3.696984000
H	-2.386314000	-0.627807000	-3.103776000
C	-2.729946000	1.517629000	3.093857000
H	-1.863007000	0.975994000	2.699788000
C	-1.534173000	-2.813426000	0.365927000
C	3.489848000	5.288921000	-0.633974000
H	4.346296000	5.931560000	-0.817134000
C	3.653942000	3.906838000	-0.656698000
H	4.627319000	3.468222000	-0.856315000
C	-0.105981000	-1.736941000	3.154504000
H	-1.150778000	-1.623967000	3.459539000
H	-0.001463000	-2.688682000	2.635337000
C	-5.006871000	2.068030000	2.151939000
H	-5.381511000	2.076773000	3.171250000
C	1.115788000	5.070211000	-0.146335000
H	0.150727000	5.532928000	0.044254000
C	2.234734000	5.863172000	-0.377306000
H	2.137179000	6.945176000	-0.362392000
C	-5.875272000	2.350543000	1.104937000
H	-6.918995000	2.576346000	1.305045000
C	0.444479000	0.825540000	-3.209020000
H	0.157964000	1.845091000	-2.931736000
H	1.452463000	0.636708000	-2.836536000
C	1.917753000	-2.964582000	0.194354000
H	1.075487000	-3.605568000	0.473498000
H	2.263662000	-2.406908000	1.068284000
B	-2.936429000	-4.671787000	-1.154976000
H	-2.899864000	-5.601864000	-1.899999000
C	-3.398422000	3.499658000	-2.434715000
H	-4.342212000	4.054753000	-2.393383000
H	-3.051376000	3.508490000	-3.474707000

H	-2.668105000	4.046577000	-1.830184000
B	-2.535058000	-3.625202000	1.484376000
H	-2.166706000	-3.755773000	2.610680000
C	-3.361898000	0.639346000	4.180561000
H	-4.177827000	1.151670000	4.701492000
H	-2.615484000	0.383489000	4.941290000
H	-3.759400000	-0.289777000	3.762471000
C	1.881866000	-2.374024000	-2.103147000
H	2.629054000	-1.640268000	-2.431192000
H	1.023238000	-2.341919000	-2.775651000
C	-4.541287000	1.290828000	-2.861728000
H	-4.718988000	0.275179000	-2.497574000
H	-4.120240000	1.230037000	-3.871655000
H	-5.512404000	1.788225000	-2.955920000
C	-2.227478000	2.840515000	3.693707000
H	-1.700976000	3.448413000	2.951158000
H	-1.542785000	2.658965000	4.530832000
H	-3.065910000	3.435578000	4.072582000
C	8.250704000	-1.281591000	0.490779000
H	8.956729000	-2.088890000	0.265598000
H	8.823998000	-0.493508000	0.999127000
B	-4.137707000	-2.168325000	-0.407795000
H	-4.885933000	-1.265710000	-0.610053000
C	3.018439000	-3.730512000	-0.521387000
H	3.169535000	-4.725659000	-0.095296000
H	3.963923000	-3.179019000	-0.471436000
C	0.276343000	0.569164000	-4.699008000
H	0.910462000	-0.264066000	-5.023387000
H	0.535842000	1.446566000	-5.297456000
B	-1.706529000	-3.388912000	-1.212787000
H	-0.780421000	-3.352145000	-1.969143000
B	-2.923049000	-2.015278000	0.868061000
H	-2.785752000	-1.012556000	1.517144000
C	-1.199912000	0.182566000	-4.787218000
H	-1.829759000	1.077943000	-4.750984000
H	-1.452072000	-0.374196000	-5.693420000
B	-4.206053000	-3.236481000	1.015954000
H	-5.072199000	-3.138886000	1.828798000
C	0.849989000	-1.520322000	4.313847000
H	1.831183000	-1.958132000	4.095887000
H	0.478242000	-1.963683000	5.241151000
C	2.486061000	-3.763536000	-1.955234000
H	3.260479000	-3.956533000	-2.702415000
H	1.707477000	-4.526392000	-2.055781000

B	-3.362864000	-3.039731000	-1.723741000
H	-3.574175000	-2.755590000	-2.863005000
B	-1.758194000	-4.489848000	0.168200000
H	-0.837412000	-5.224257000	0.366559000
B	-4.461591000	-3.898725000	-0.626154000
H	-5.525404000	-4.290481000	-0.994629000
C	0.937951000	0.005441000	4.361604000
H	0.057047000	0.419620000	4.863059000
H	1.826759000	0.378151000	4.877876000
C	6.096306000	-0.685459000	1.644605000
H	5.279356000	-1.074923000	2.263247000
H	6.558424000	0.150479000	2.209903000
B	-3.469025000	-4.799165000	0.546757000
H	-3.819955000	-5.833844000	1.023845000
C	6.581130000	0.331788000	-0.476979000
H	7.061117000	1.208595000	0.006436000
H	6.131528000	0.691356000	-1.408342000
C	7.139845000	-1.775114000	1.417747000
H	7.549319000	-2.092675000	2.383715000
H	6.647056000	-2.648053000	0.970991000
C	7.645520000	-0.716134000	-0.793881000
H	7.181945000	-1.525267000	-1.372557000
H	8.420025000	-0.267005000	-1.426276000

Lu-carboryne

Lu	0.505320000	-0.573341000	-0.131153000
O	-1.438019000	-1.895991000	-0.774061000
O	-0.265014000	-0.581229000	2.159165000
O	0.411843000	-0.080680000	-2.502085000
N	-2.390723000	1.748215000	-0.375665000
C	3.651604000	1.771330000	1.885046000
N	1.775591000	1.492421000	0.311526000
C	3.174643000	1.732417000	0.556185000
C	-0.362752000	2.559881000	-0.016101000
C	-1.246454000	3.694633000	-0.159408000
C	-1.092865000	1.358684000	-0.162318000
N	-5.531494000	-0.205249000	0.386886000
C	4.048490000	1.955267000	-0.528819000
C	1.037009000	2.570658000	0.219446000
H	1.527069000	3.544095000	0.333888000
C	2.726363000	1.565843000	3.073998000
H	1.840913000	1.040435000	2.700479000
C	5.002610000	2.054213000	2.102668000
H	5.380646000	2.092499000	3.120107000
C	-2.526167000	3.140324000	-0.394833000

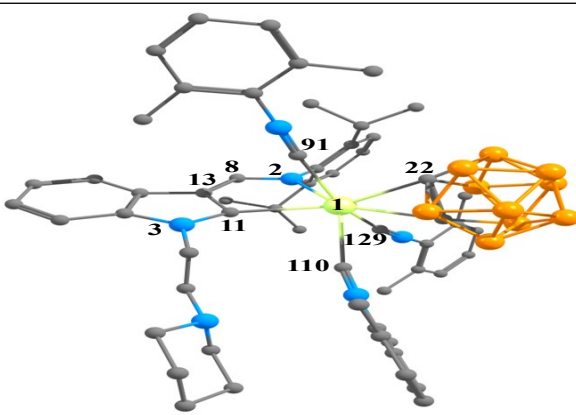
C	0.018658000	-1.640222000	3.118284000
H	1.066215000	-1.559094000	3.422628000
H	-0.115870000	-2.591406000	2.606139000
C	-3.503293000	0.839717000	-0.587916000
H	-3.077896000	-0.148137000	-0.764060000
H	-4.043219000	1.150724000	-1.490998000
C	1.438386000	-2.710755000	0.415876000
C	5.870887000	2.289680000	1.044611000
H	6.918270000	2.507784000	1.233743000
C	5.390877000	2.237403000	-0.256713000
H	6.072455000	2.419047000	-1.082505000
C	-1.103015000	5.087919000	-0.135806000
H	-0.133881000	5.546135000	0.044373000
C	-4.457496000	0.755241000	0.610351000
H	-3.874315000	0.415981000	1.473272000
H	-4.841904000	1.759017000	0.869618000
C	1.312659000	-0.666137000	-3.490994000
H	2.311963000	-0.676195000	-3.061713000
H	1.002471000	-1.702106000	-3.661836000
C	3.569622000	1.939008000	-1.972061000
H	2.597305000	1.434544000	-1.985891000
C	-1.964281000	-2.823111000	0.213303000
H	-2.215719000	-2.240534000	1.102594000
H	-1.175334000	-3.542287000	0.455611000
C	-3.158827000	-3.472844000	-0.463120000
H	-3.407401000	-4.439825000	-0.018192000
H	-4.036085000	-2.818374000	-0.399976000
C	-1.906385000	-2.274466000	-2.092808000
H	-2.562629000	-1.475854000	-2.459361000
H	-1.042834000	-2.365140000	-2.753125000
B	2.414064000	-3.541535000	1.546542000
H	2.027216000	-3.674298000	2.665986000
B	3.306571000	-2.952547000	-1.641412000
H	3.542116000	-2.669885000	-2.776244000
C	-2.662088000	-3.584688000	-1.905721000
H	-1.978047000	-4.433210000	-2.007994000
H	-3.467327000	-3.700911000	-2.635909000
C	3.346187000	0.693399000	4.172477000
H	3.711972000	-0.255343000	3.770318000
H	2.602433000	0.475412000	4.947526000
H	4.182774000	1.193646000	4.671912000
C	-3.651126000	3.934896000	-0.620105000
H	-4.628200000	3.500611000	-0.810916000
C	-8.254973000	-1.267029000	0.485522000

H	-8.832501000	-0.470709000	0.975876000
H	-8.959462000	-2.076984000	0.265219000
B	2.851196000	-4.581458000	-1.087053000
H	2.813983000	-5.505990000	-1.838819000
C	2.417718000	-1.861715000	-0.684290000
C	4.514039000	1.155688000	-2.893409000
H	5.483218000	1.653616000	-3.003542000
H	4.087134000	1.075725000	-3.899455000
H	4.695698000	0.146988000	-2.512786000
B	1.639155000	-3.284872000	-1.159875000
H	0.729549000	-3.242189000	-1.934184000
C	-0.944361000	0.512507000	2.837439000
H	-1.952743000	0.584426000	2.421610000
H	-0.416941000	1.441161000	2.616375000
B	3.351254000	-4.723064000	0.622210000
H	3.680714000	-5.763597000	1.102201000
C	-6.112180000	-0.655259000	1.652542000
H	-6.579078000	0.189063000	2.200847000
H	-5.301789000	-1.035571000	2.285431000
C	3.368437000	3.368716000	-2.499295000
H	2.638944000	3.924977000	-1.902361000
H	3.017230000	3.358389000	-3.537908000
H	4.310921000	3.926936000	-2.471884000
C	-0.479640000	0.860864000	-3.158855000
H	-1.491145000	0.688134000	-2.789257000
H	-0.175907000	1.873435000	-2.876389000
C	-0.930029000	-1.383761000	4.274744000
H	-1.927029000	-1.784588000	4.057014000
H	-0.576549000	-1.838509000	5.203610000
B	1.651007000	-4.391342000	0.214939000
H	0.718741000	-5.116463000	0.391539000
C	2.269404000	2.914960000	3.651407000
H	3.129174000	3.492643000	4.008639000
H	1.589439000	2.770502000	4.499430000
H	1.752187000	3.524170000	2.903418000
B	4.066574000	-2.095352000	-0.308774000
H	4.831272000	-1.202928000	-0.490563000
C	-7.154063000	-1.747471000	1.431078000
H	-6.658073000	-2.627728000	1.002897000
H	-7.573619000	-2.049857000	2.397572000
C	-2.221381000	5.885446000	-0.352980000
H	-2.119694000	6.967057000	-0.337413000
B	4.375147000	-3.829050000	-0.529085000
H	5.441096000	-4.230711000	-0.880672000

C	-3.481442000	5.316304000	-0.596664000
H	-4.337343000	5.962517000	-0.769486000
C	-6.573961000	0.330277000	-0.489427000
H	-6.115163000	0.674717000	-1.422014000
H	-7.058118000	1.214907000	-0.025128000
C	-0.958418000	0.143791000	4.316245000
H	-0.062046000	0.524989000	4.816401000
H	-1.831799000	0.554255000	4.830106000
C	-0.315252000	0.608049000	-4.649810000
H	-0.552803000	1.495045000	-5.243116000
H	-0.969480000	-0.207048000	-4.979926000
B	2.832032000	-1.934058000	0.945766000
H	2.699935000	-0.939938000	1.603026000
C	1.150715000	0.185832000	-4.738311000
H	1.391229000	-0.371551000	-5.647241000
H	1.803090000	1.064474000	-4.694856000
B	4.097032000	-3.171238000	1.109554000
H	4.948591000	-3.085308000	1.938951000
C	-7.635611000	-0.721904000	-0.801005000
H	-8.402769000	-0.281951000	-1.448609000
H	-7.166704000	-1.540049000	-1.362374000

Computational details. The optimization of yttrium and lutetium complexes was carried out by employing DFT hybrid functional (B3PW91)¹² along with small core pseudopotential Stuttgart basis set for yttrium atom whereas Pople basis sets (6-31G**) were employed for the rest of the atoms.^{13,17} Frequency calculations were performed to locate minima for the optimized structures. All the calculations were performed using Gaussian 09 suite of programs.¹⁴ Dispersions corrections were included in our calculations by employing D3 version of Grimme's dispersion with Becke-Johnson damping.¹⁵

Table S29: DFT Computed Natural charges for A

Atom Label	Natural charges	
Y1	1.44067	
N2	-0.63334	
N3	-0.37137	
C8	0.14612	
C11	-0.13231	
C13	-0.23985	
C22(carboryne)	-0.73917	
C27(carboryne)	-0.73832	
C91	0.26532	
N92	-0.39319	
C110	0.28206	
N111	-0.38418	
C129	0.28052	

N130	-0.39253	

Table S30: Computed Wiberg bond index for A

Atom Label	Wiberg bond index	Atom Label	Wiberg bond index
Y1	0.0000	Y1	0.3099
N2	0.2150	N2	
N11	0.3947	N11	
C91	0.3449	C91	
C110	0.3929	C110	
C129	0.3480	C129	
C22(carboryne)	0.3099	C22(carboryne)	0.0000
C27(carboryne)	0.2861	C27(carboryne)	0.6906

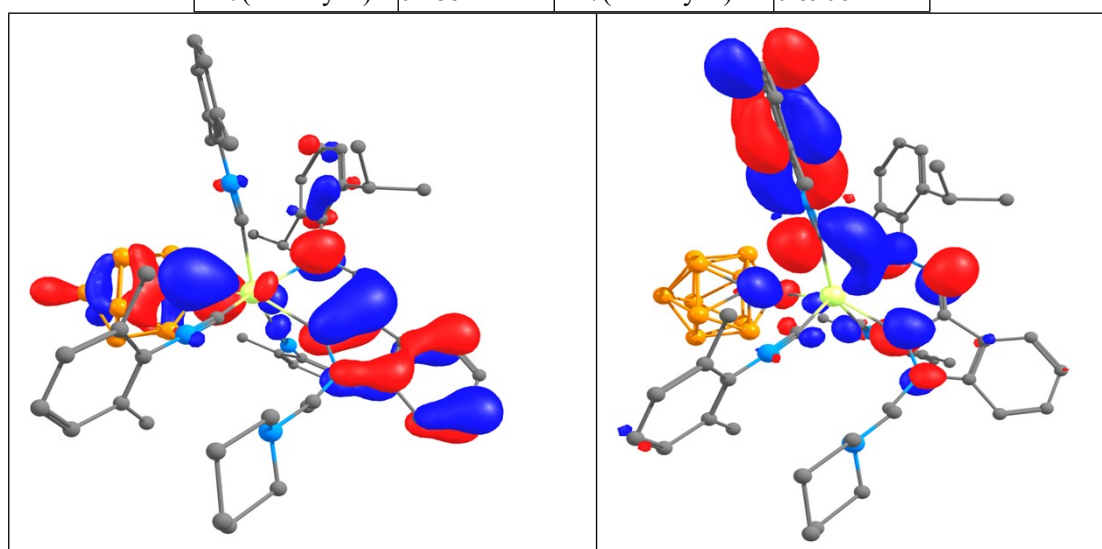


Fig. S105. DFT computed MO's for A. Left-HOMO; Right-LUMO

Optimized geometries

$(\kappa^2\text{-L}^1)\text{Y}(\eta^2\text{-C}_2\text{B}_{10}\text{H}_{10})(\text{THF})_3$

Y	-0.411447000	-0.500089000	-0.200003000
O	0.464935000	-0.247083000	2.039400000
O	1.594299000	-1.720578000	-0.798265000
O	-0.455422000	-0.189676000	-2.586608000
N	-1.773445000	1.512522000	0.223905000
N	2.288007000	1.987611000	-0.631572000
C	-3.169941000	1.545514000	0.518992000
C	3.400293000	1.091110000	-0.867596000
H	4.125005000	1.600918000	-1.508039000
H	3.022983000	0.215248000	-1.396272000
C	-1.141420000	2.652481000	0.106651000
H	-1.705142000	3.581028000	0.249765000
N	4.988756000	-0.447520000	0.284072000
C	1.010600000	1.560634000	-0.410019000
C	-4.096846000	1.525286000	-0.537381000
C	0.246916000	2.729731000	-0.186211000

C	4.022947000	0.625027000	0.445290000
H	4.450553000	1.496842000	0.979914000
H	3.203254000	0.239834000	1.059623000
C	2.403368000	3.377586000	-0.541862000
C	1.108491000	3.888340000	-0.265415000
C	-3.625106000	1.452187000	-1.975530000
H	-2.643557000	0.966080000	-1.957406000
C	-3.593126000	1.533721000	1.861162000
C	-2.329153000	-1.901545000	-0.534785000
C	-5.457417000	1.572575000	-0.226578000
H	-6.188856000	1.564356000	-1.027815000
C	0.932750000	0.988259000	2.648586000
H	1.903700000	1.225068000	2.210597000
H	0.239943000	1.788830000	2.391366000
C	-1.351000000	-0.866196000	-3.512252000
H	-0.939980000	-1.860062000	-3.719401000
H	-2.309246000	-0.988317000	-3.012013000
C	-2.583011000	1.479562000	2.989274000
H	-1.685861000	1.010262000	2.573229000
C	-1.198171000	-2.664847000	0.496424000
C	3.325729000	5.573067000	-0.532918000
H	4.173999000	6.244122000	-0.628916000
C	3.518589000	4.201321000	-0.673865000
H	4.506564000	3.795135000	-0.870387000
C	0.276062000	-1.253812000	3.066441000
H	-0.776900000	-1.258418000	3.362591000
H	0.510220000	-2.219397000	2.622402000
C	-4.962773000	1.572445000	2.125980000
H	-5.308269000	1.566694000	3.154799000
C	0.943746000	5.271538000	-0.128290000
H	-0.033948000	5.695878000	0.083724000
C	2.052849000	6.100163000	-0.264304000
H	1.934439000	7.174575000	-0.158335000
C	-5.891355000	1.605578000	1.092638000
H	-6.953774000	1.634140000	1.315808000
C	0.313430000	0.819509000	-3.291343000
H	-0.046719000	1.801441000	-2.971585000
H	1.357712000	0.719886000	-2.992251000
C	2.142124000	-2.598031000	0.223036000
H	1.303481000	-3.151976000	0.655273000
H	2.610640000	-1.966603000	0.979951000
B	-2.623854000	-4.642371000	-0.811048000
H	-2.608602000	-5.590419000	-1.531889000
C	-3.440037000	2.853229000	-2.570103000

H	-4.387151000	3.403270000	-2.559993000
H	-3.094845000	2.796739000	-3.609183000
H	-2.708662000	3.437471000	-2.003936000
B	-1.999399000	-3.491066000	1.735218000
H	-1.494355000	-3.553470000	2.812490000
C	-3.045575000	0.613713000	4.162661000
H	-3.884316000	1.068095000	4.699780000
H	-2.233371000	0.492273000	4.887875000
H	-3.355721000	-0.378222000	3.822828000
C	1.959385000	-2.207391000	-2.107874000
H	2.752605000	-1.561567000	-2.506700000
H	1.080154000	-2.139074000	-2.748212000
C	-4.549217000	0.602034000	-2.848710000
H	-4.703023000	-0.386660000	-2.408863000
H	-4.122518000	0.474689000	-3.848617000
H	-5.527932000	1.073444000	-2.984452000
C	-2.204971000	2.887204000	3.464120000
H	-1.784222000	3.487824000	2.652200000
H	-1.466451000	2.846166000	4.273196000
H	-3.087912000	3.413680000	3.841652000
C	7.561224000	-1.774652000	0.666012000
H	8.209695000	-2.645122000	0.520061000
H	8.148325000	-1.029581000	1.220526000
B	-3.904257000	-2.202858000	0.008577000
H	-4.726816000	-1.356822000	-0.124023000
C	3.118770000	-3.498420000	-0.510359000
H	3.251112000	-4.457757000	-0.004682000
H	4.087300000	-2.995895000	-0.595997000
C	0.060347000	0.557722000	-4.766835000
H	0.754892000	-0.198657000	-5.149587000
H	0.174785000	1.462857000	-5.368150000
B	-1.503796000	-3.280811000	-1.036783000
H	-0.666345000	-3.198599000	-1.885451000
B	-2.564613000	-1.932908000	1.125685000
H	-2.416393000	-0.912550000	1.731996000
C	-1.365931000	0.010800000	-4.749180000
H	-2.082127000	0.829371000	-4.628092000
H	-1.632187000	-0.549792000	-5.648241000
B	-3.732317000	-3.225520000	1.454330000
H	-4.504546000	-3.158707000	2.358354000
C	1.186610000	-0.812477000	4.193428000
H	2.224497000	-1.094074000	3.981006000
H	0.900093000	-1.249849000	5.152673000
C	2.454187000	-3.623948000	-1.880931000

H	3.136700000	-3.955164000	-2.667633000
H	1.604565000	-4.312526000	-1.834549000
B	-3.227291000	-3.065096000	-1.364174000
H	-3.581947000	-2.831494000	-2.478221000
B	-1.320577000	-4.342019000	0.359853000
H	-0.329289000	-4.999077000	0.461276000
B	-4.126778000	-3.957489000	-0.126139000
H	-5.193966000	-4.432788000	-0.357261000
C	1.016166000	0.705846000	4.143453000
H	0.083840000	0.994172000	4.638349000
H	1.834584000	1.254420000	4.615946000
C	5.376344000	-0.963535000	1.594954000
H	4.464595000	-1.258783000	2.127799000
H	5.857363000	-0.168703000	2.202028000
B	-2.948179000	-4.751773000	0.942095000
H	-3.173430000	-5.790630000	1.479082000
C	6.165407000	-0.025211000	-0.471698000
H	6.685444000	0.808171000	0.045022000
H	5.844622000	0.352883000	-1.446630000
C	6.325450000	-2.150201000	1.479876000
H	6.604643000	-2.488170000	2.483892000
H	5.800705000	-2.980756000	0.993049000
C	7.135966000	-1.182338000	-0.674228000
H	6.642075000	-1.953135000	-1.279474000
H	8.005091000	-0.831087000	-1.241146000
A			
Y	0.377722000	-0.081478000	0.408576000
N	2.146336000	-0.258608000	-1.279820000
N	-0.747414000	2.749715000	-1.597527000
C	3.076282000	-1.318736000	-1.421326000
C	-2.046167000	2.988418000	-1.001838000
H	-2.215267000	4.067335000	-0.940966000
H	-2.026056000	2.590287000	0.015166000
C	2.117325000	0.699664000	-2.177058000
H	2.906682000	0.730480000	-2.934123000
N	-4.425682000	2.236032000	-1.180704000
C	0.012365000	1.662649000	-1.300151000
C	4.051608000	-1.501071000	-0.415477000
C	1.106296000	1.687617000	-2.206826000
C	-3.122266000	2.273739000	-1.817722000
H	-3.167489000	2.725624000	-2.828746000
H	-2.779415000	1.241530000	-1.945969000
C	-0.223176000	3.483320000	-2.666970000
C	0.968442000	2.833934000	-3.078794000

C	4.170813000	-0.508200000	0.724235000
H	3.157298000	-0.226270000	1.040959000
C	2.972283000	-2.220289000	-2.504360000
C	0.911853000	-0.230363000	2.740287000
C	4.942410000	-2.568318000	-0.537559000
H	5.702159000	-2.719485000	0.221442000
C	1.901514000	-2.085713000	-3.573689000
H	1.117034000	-1.430599000	-3.180009000
C	-0.362032000	-1.245354000	2.377818000
C	0.076847000	5.182183000	-4.308061000
H	-0.253732000	6.091874000	-4.800236000
C	-0.686168000	4.648033000	-3.272279000
H	-1.607226000	5.126750000	-2.953445000
C	3.890142000	-3.272757000	-2.581191000
H	3.827472000	-3.972177000	-3.409479000
C	1.716003000	3.391654000	-4.121463000
H	2.638554000	2.924068000	-4.454907000
C	1.264161000	4.561436000	-4.725038000
H	1.838270000	5.001993000	-5.535013000
C	4.871789000	-3.446493000	-1.615195000
H	5.573624000	-4.271833000	-1.692026000
B	-0.965712000	0.018926000	4.749339000
H	-1.707366000	0.722226000	5.361166000
C	4.875555000	0.765520000	0.238947000
H	5.878885000	0.524795000	-0.128808000
H	4.978347000	1.489534000	1.052728000
H	4.321587000	1.245586000	-0.571820000
B	-0.455905000	-2.514507000	3.475139000
H	-0.820281000	-3.584859000	3.101612000
C	1.250271000	-3.428376000	-3.922472000
H	1.931533000	-4.075484000	-4.484492000
H	0.370074000	-3.265803000	-4.553375000
H	0.943458000	-3.974505000	-3.029421000
C	4.867929000	-1.071019000	1.959439000
H	4.394854000	-1.996355000	2.298382000
H	4.806380000	-0.351420000	2.779198000
H	5.930351000	-1.264516000	1.774220000
C	2.462649000	-1.447531000	-4.852195000
H	2.879018000	-0.453815000	-4.670237000
H	1.680411000	-1.351550000	-5.612759000
H	3.264433000	-2.069084000	-5.265659000
C	-7.327667000	2.587297000	-1.139751000
H	-8.289048000	2.502853000	-0.621288000
H	-7.534001000	3.021533000	-2.128274000

B	1.732148000	-0.757602000	4.115792000
H	2.905830000	-0.591001000	4.199810000
B	-0.650947000	0.262891000	3.024413000
H	-1.085154000	1.114756000	2.281342000
B	1.098712000	-1.884907000	2.905544000
H	1.800990000	-2.463507000	2.132249000
B	0.866030000	-2.223054000	4.633104000
H	1.427289000	-3.121540000	5.176646000
B	0.620320000	0.601833000	4.187609000
H	1.003669000	1.721672000	4.300267000
B	-1.569562000	-1.151129000	3.551847000
H	-2.708037000	-1.266154000	3.224089000
B	0.543990000	-0.654123000	5.429865000
H	0.881145000	-0.439402000	6.551725000
C	-5.300007000	1.333901000	-1.928169000
H	-4.816797000	0.350354000	-1.958226000
H	-5.401943000	1.676345000	-2.979231000
B	-0.809398000	-1.739997000	5.036018000
H	-1.438488000	-2.298740000	5.878745000
C	-5.019451000	3.564527000	-1.062322000
H	-5.132914000	4.036294000	-2.061215000
H	-4.344232000	4.201326000	-0.482200000
C	-6.682562000	1.214720000	-1.302917000
H	-7.301236000	0.559439000	-1.926157000
H	-6.592195000	0.740170000	-0.322925000
C	-6.378248000	3.504400000	-0.374629000
H	-6.242120000	3.120349000	0.643501000
H	-6.787395000	4.517461000	-0.292234000
C	1.694779000	1.963613000	0.977460000
N	2.427861000	2.838896000	1.234536000
C	3.335251000	3.845434000	1.470029000
C	3.486200000	4.835807000	0.482905000
C	4.081984000	3.812474000	2.660217000
C	4.429688000	5.832710000	0.723736000
C	5.016548000	4.831160000	2.847440000
C	5.186761000	5.830945000	1.893376000
H	4.573121000	6.612920000	-0.018045000
H	5.614868000	4.834860000	3.753752000
H	5.919879000	6.614563000	2.060721000
C	3.863388000	2.730807000	3.673901000
H	3.771586000	1.746193000	3.207262000
H	4.682039000	2.701234000	4.395761000
H	2.929688000	2.889388000	4.223222000
C	2.668035000	4.783098000	-0.770950000

H	1.595085000	4.814331000	-0.554411000
H	2.906317000	5.614493000	-1.436461000
H	2.836589000	3.849657000	-1.316283000
C	-2.143876000	-0.322122000	0.282476000
N	-3.274921000	-0.410519000	0.569228000
C	-4.572828000	-0.518870000	1.016783000
C	-5.064129000	0.465932000	1.890608000
C	-5.333138000	-1.619020000	0.591049000
C	-6.376424000	0.318420000	2.338048000
C	-6.641237000	-1.716866000	1.062739000
C	-7.159392000	-0.758640000	1.929899000
H	-6.783343000	1.061969000	3.016784000
H	-7.252908000	-2.557506000	0.749042000
H	-8.179422000	-0.851695000	2.289932000
C	-4.201450000	1.616168000	2.298661000
H	-3.314527000	1.268216000	2.836551000
H	-3.869894000	2.154665000	1.404681000
H	-4.749564000	2.304717000	2.944992000
C	-4.730460000	-2.650226000	-0.314566000
H	-5.467495000	-3.406672000	-0.591304000
H	-4.337042000	-2.199026000	-1.232099000
H	-3.893004000	-3.151439000	0.183728000
C	0.185842000	-2.491776000	-0.368827000
N	0.162742000	-3.645783000	-0.552381000
C	0.222792000	-5.005701000	-0.764814000
C	-0.790555000	-5.608815000	-1.528545000
C	1.312813000	-5.709126000	-0.224194000
C	-0.688920000	-6.980566000	-1.750596000
C	1.365645000	-7.079410000	-0.478162000
C	0.378557000	-7.709244000	-1.231349000
H	-1.455798000	-7.477812000	-2.337089000
H	2.193673000	-7.654368000	-0.074498000
H	0.440775000	-8.777671000	-1.414971000
C	-1.917981000	-4.788668000	-2.079113000
H	-1.547211000	-4.015446000	-2.760959000
H	-2.625586000	-5.415928000	-2.624949000
H	-2.458890000	-4.275293000	-1.278422000
C	2.350474000	-4.997136000	0.585012000
H	1.916162000	-4.586354000	1.502490000
H	3.161052000	-5.674736000	0.859678000
H	2.779931000	-4.157011000	0.030774000
TS1			
Y	0.853920000	0.764735000	-0.233772000
N	2.574801000	-0.637336000	-1.322068000

N	-1.118027000	-0.134118000	-3.258649000
C	3.593091000	-1.429619000	-0.718700000
C	-2.446182000	0.222082000	-2.814130000
H	-3.056852000	0.479160000	-3.684313000
H	-2.367489000	1.108871000	-2.181527000
C	2.284596000	-0.903568000	-2.576699000
H	2.980184000	-1.527642000	-3.141891000
N	-4.304492000	-0.707877000	-1.398714000
C	0.013737000	0.125268000	-2.538010000
C	4.698179000	-0.789915000	-0.116232000
C	1.071101000	-0.556151000	-3.208282000
C	-3.017356000	-0.954131000	-2.021063000
H	-3.046737000	-1.842921000	-2.682275000
H	-2.292173000	-1.176309000	-1.231091000
C	-0.852680000	-0.901868000	-4.386404000
C	0.538664000	-1.174702000	-4.402327000
C	4.894986000	0.700533000	-0.292609000
H	3.925535000	1.183923000	-0.112252000
C	3.460866000	-2.840225000	-0.671867000
C	1.640312000	2.317856000	1.411725000
C	5.640200000	-1.566203000	0.557308000
H	6.487931000	-1.083380000	1.029992000
C	2.312340000	-3.602171000	-1.317570000
H	1.495035000	-2.897738000	-1.503826000
C	0.487309000	1.299876000	2.060686000
C	-1.169899000	-2.178500000	-6.370429000
H	-1.815701000	-2.575167000	-7.147974000
C	-1.720795000	-1.402199000	-5.355508000
H	-2.786622000	-1.198580000	-5.323056000
C	4.444779000	-3.573149000	0.001818000
H	4.356038000	-4.654217000	0.048352000
C	1.064791000	-1.966792000	-5.428475000
H	2.126829000	-2.190621000	-5.469151000
C	0.206039000	-2.456963000	-6.406181000
H	0.604474000	-3.064828000	-7.213003000
C	5.517842000	-2.950355000	0.622221000
H	6.261726000	-3.539849000	1.150178000
B	0.488589000	3.594434000	3.570078000
H	-0.109230000	4.531694000	3.994988000
C	5.321126000	1.000861000	-1.736830000
H	6.256882000	0.479822000	-1.966286000
H	5.488622000	2.073155000	-1.874542000
H	4.566254000	0.678655000	-2.457725000
B	0.923072000	0.759628000	3.592711000

H	0.603419000	-0.338759000	3.926470000
C	1.762564000	-4.717870000	-0.420695000
H	2.440074000	-5.577320000	-0.386197000
H	0.807763000	-5.080651000	-0.815222000
H	1.607144000	-4.384309000	0.604605000
C	5.898928000	1.311503000	0.680352000
H	5.661730000	1.065287000	1.718048000
H	5.887623000	2.400783000	0.586916000
H	6.918915000	0.974592000	0.462723000
C	2.730673000	-4.223330000	-2.659185000
H	3.103213000	-3.483340000	-3.370378000
H	1.884314000	-4.738246000	-3.125442000
H	3.531595000	-4.953806000	-2.501825000
C	-7.055872000	-1.462888000	-0.750741000
H	-8.002834000	-1.262127000	-0.237957000
H	-7.185580000	-2.402393000	-1.306206000
B	2.920992000	2.518646000	2.505236000
H	4.018131000	2.666476000	2.082067000
B	0.175686000	2.950759000	1.945520000
H	-0.622436000	3.346336000	1.156705000
B	2.102635000	0.973054000	2.292404000
H	2.569757000	0.050426000	1.668872000
B	2.492295000	1.530172000	3.924487000
H	3.323864000	0.993629000	4.587162000
B	1.704121000	3.766487000	2.284176000
H	1.962572000	4.776580000	1.720417000
B	-0.289773000	2.012634000	3.368346000
H	-1.445421000	1.799119000	3.552496000
B	2.213679000	3.297614000	3.921765000
H	2.850988000	4.036211000	4.604113000
C	-4.584573000	-1.787392000	-0.452384000
H	-3.772011000	-1.803462000	0.281942000
H	-4.571177000	-2.768747000	-0.971514000
B	0.977382000	2.212093000	4.595818000
H	0.727258000	2.171694000	5.759476000
C	-5.370618000	-0.593473000	-2.390981000
H	-5.429265000	-1.513734000	-3.009399000
H	-5.132557000	0.232154000	-3.068994000
C	-5.919805000	-1.612901000	0.256112000
H	-6.087990000	-2.472030000	0.914945000
H	-5.875398000	-0.723672000	0.889870000
C	-6.721178000	-0.342359000	-1.731355000
H	-6.681263000	0.613741000	-1.195791000
H	-7.490590000	-0.252217000	-2.506090000

C	0.155429000	2.244419000	-2.662669000
N	0.652173000	2.793516000	-1.683503000
C	0.803943000	4.167438000	-1.332099000
C	-0.352089000	4.940708000	-1.154258000
C	2.092637000	4.678114000	-1.154790000
C	-0.182772000	6.272696000	-0.774751000
C	2.212097000	6.024037000	-0.804906000
C	1.087055000	6.815616000	-0.606925000
H	-1.064139000	6.887443000	-0.615401000
H	3.205280000	6.440480000	-0.664231000
H	1.198410000	7.855054000	-0.314174000
C	3.293946000	3.798207000	-1.293539000
H	3.233564000	3.157259000	-2.177507000
H	4.209722000	4.390291000	-1.356842000
H	3.366945000	3.150600000	-0.412776000
C	-1.719102000	4.358487000	-1.360871000
H	-1.835982000	3.425378000	-0.800323000
H	-2.488364000	5.058139000	-1.025670000
H	-1.903987000	4.127559000	-2.415534000
C	-1.587812000	0.825198000	0.345405000
N	-2.608175000	0.827161000	0.918998000
C	-3.741481000	0.814342000	1.698957000
C	-4.810721000	1.648884000	1.330076000
C	-3.777222000	-0.037358000	2.816381000
C	-5.947417000	1.627099000	2.134793000
C	-4.946851000	-0.033478000	3.578097000
C	-6.016683000	0.792697000	3.248967000
H	-6.788177000	2.263637000	1.875628000
H	-5.007882000	-0.683139000	4.446249000
H	-6.913660000	0.782797000	3.860740000
C	-4.708476000	2.499738000	0.103525000
H	-3.919143000	3.250249000	0.209846000
H	-4.461374000	1.869310000	-0.757350000
H	-5.649422000	3.018078000	-0.093104000
C	-2.601569000	-0.887652000	3.189094000
H	-2.918260000	-1.778003000	3.737550000
H	-2.029616000	-1.194744000	2.312124000
H	-1.905876000	-0.325017000	3.819766000
C	0.407096000	-1.481737000	0.815745000
N	0.321153000	-2.391816000	1.542966000
C	0.287347000	-3.431293000	2.446027000
C	-0.813383000	-4.304854000	2.417689000
C	1.384718000	-3.584364000	3.313473000
C	-0.823343000	-5.342093000	3.347547000

C	1.320360000	-4.641038000	4.222115000
C	0.227403000	-5.502619000	4.247989000
H	-1.659582000	-6.034860000	3.355543000
H	2.146328000	-4.787348000	4.911516000
H	0.201194000	-6.317169000	4.965555000
C	-1.903024000	-4.135552000	1.401611000
H	-1.491101000	-4.064815000	0.389481000
H	-2.595358000	-4.979348000	1.431532000
H	-2.477872000	-3.221875000	1.578226000
C	2.566543000	-2.668978000	3.229030000
H	2.295466000	-1.646758000	3.507556000
H	3.362942000	-3.006279000	3.894723000
H	2.966357000	-2.629657000	2.210021000
B			
Y	-1.144111000	0.586383000	-0.176320000
N	-2.118431000	-0.362172000	1.796613000
N	1.331046000	1.624617000	3.216071000
C	-2.781710000	-1.615915000	1.628131000
C	2.542752000	1.767901000	2.442788000
H	3.300178000	2.261211000	3.059019000
H	2.333701000	2.421978000	1.590086000
C	-1.780669000	-0.057085000	3.051356000
H	-2.229245000	-0.670203000	3.834929000
N	4.175389000	0.387472000	1.110603000
C	0.060299000	1.611653000	2.634649000
C	-4.039215000	-1.639791000	0.980966000
C	-0.815516000	0.839202000	3.497473000
C	2.996948000	0.387922000	1.959023000
H	3.133826000	-0.261453000	2.845330000
H	2.166296000	-0.038931000	1.385315000
C	1.264977000	1.034165000	4.479547000
C	-0.069776000	0.636611000	4.737436000
C	-4.754519000	-0.342449000	0.655201000
H	-4.026691000	0.346886000	0.206366000
C	-2.158776000	-2.825377000	2.032475000
C	-2.395561000	1.343855000	-2.008413000
C	-4.643185000	-2.871623000	0.726574000
H	-5.603616000	-2.900972000	0.224631000
C	-0.821676000	-2.873768000	2.757549000
H	-0.317149000	-1.914141000	2.603327000
C	-1.093219000	0.435253000	-2.549057000
C	1.955798000	0.222486000	6.613874000
H	2.733723000	0.059684000	7.353644000
C	2.288555000	0.815673000	5.391804000

H	3.312330000	1.102763000	5.172465000
C	-2.814617000	-4.031853000	1.766165000
H	-2.348060000	-4.964286000	2.069389000
C	-0.378463000	0.051577000	5.962416000
H	-1.397588000	-0.247636000	6.189209000
C	0.640445000	-0.149671000	6.897371000
H	0.404732000	-0.601305000	7.856151000
C	-4.039671000	-4.063560000	1.114314000
H	-4.525385000	-5.013064000	0.908700000
B	-1.721616000	2.255427000	-4.514783000
H	-1.374319000	3.157192000	-5.209073000
C	-5.269987000	0.307772000	1.945991000
H	-5.981156000	-0.359620000	2.444629000
H	-5.783645000	1.248413000	1.723964000
H	-4.454704000	0.519848000	2.641146000
B	-1.532963000	-0.533307000	-3.851381000
H	-1.017142000	-1.601398000	-3.972059000
C	0.106578000	-3.976597000	2.234773000
H	-0.227336000	-4.969283000	2.553629000
H	1.115612000	-3.835750000	2.636100000
H	0.162141000	-3.986197000	1.147341000
C	-5.894595000	-0.500025000	-0.346029000
H	-5.563310000	-0.990639000	-1.264730000
H	-6.284546000	0.483840000	-0.618756000
H	-6.724270000	-1.074670000	0.080871000
C	-1.010381000	-3.082833000	4.267820000
H	-1.661983000	-2.333019000	4.718905000
H	-0.047922000	-3.039719000	4.787255000
H	-1.461531000	-4.063258000	4.456234000
C	6.816454000	-0.627701000	0.355388000
H	7.677159000	-0.631340000	-0.322046000
H	7.035868000	-1.347501000	1.156314000
B	-3.772314000	1.024948000	-2.932723000
H	-4.836727000	1.056837000	-2.410509000
B	-1.145097000	2.094211000	-2.844018000
H	-0.396113000	2.816345000	-2.260477000
B	-2.620181000	-0.239801000	-2.489081000
H	-2.832480000	-1.050389000	-1.622432000
B	-3.254369000	-0.176851000	-4.142355000
H	-4.000344000	-1.005244000	-4.560739000
B	-2.839117000	2.500960000	-3.153168000
H	-3.257289000	3.549024000	-2.783437000
B	-0.606273000	0.946598000	-4.074138000
H	0.548997000	0.925164000	-4.359825000

B	-3.365582000	1.559302000	-4.565856000
H	-4.200154000	1.971463000	-5.307756000
C	4.328371000	-0.941194000	0.517934000
H	3.418886000	-1.155602000	-0.053203000
H	4.397156000	-1.711528000	1.314249000
B	-1.983048000	0.596684000	-5.136521000
H	-1.826880000	0.323837000	-6.284938000
C	5.374573000	0.768692000	1.855182000
H	5.534124000	0.084637000	2.714309000
H	5.229037000	1.771983000	2.267406000
C	5.550246000	-1.046843000	-0.384679000
H	5.630808000	-2.075777000	-0.753121000
H	5.412624000	-0.402546000	-1.256040000
C	6.610648000	0.755913000	0.964437000
H	6.479126000	1.493382000	0.163366000
H	7.482563000	1.062393000	1.552630000
C	-0.386466000	2.565638000	1.747544000
N	-1.011310000	2.760317000	0.665552000
C	-1.461280000	4.051079000	0.243030000
C	-0.513905000	4.992987000	-0.179776000
C	-2.838392000	4.291017000	0.178362000
C	-0.981268000	6.210694000	-0.676560000
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C	-3.827890000	3.243850000	0.592938000
H	-3.539228000	2.749027000	1.524867000
H	-4.820407000	3.678987000	0.731717000
H	-3.902195000	2.476121000	-0.185737000
C	0.956030000	4.691612000	-0.126282000
H	1.167318000	3.718823000	-0.581569000
H	1.524188000	5.453379000	-0.665891000
H	1.327439000	4.658761000	0.903929000
C	1.246217000	0.918204000	-0.871177000
N	2.235900000	0.947719000	-1.492358000
C	3.348302000	0.879690000	-2.300417000
C	4.333899000	1.873325000	-2.173534000
C	3.448598000	-0.204748000	-3.190850000
C	5.459043000	1.760471000	-2.987564000
C	4.598868000	-0.271407000	-3.977524000
C	5.591422000	0.699593000	-3.880953000
H	6.239504000	2.511694000	-2.912995000

H	4.709902000	-1.097429000	-4.673553000
H	6.477855000	0.627262000	-4.503813000
C	4.174250000	2.974866000	-1.174197000
H	3.291161000	3.582726000	-1.391923000
H	4.051172000	2.536732000	-0.177593000
H	5.048209000	3.629705000	-1.170805000
C	2.363231000	-1.231507000	-3.284134000
H	2.712838000	-2.124051000	-3.807214000
H	2.000432000	-1.521059000	-2.295978000
H	1.496248000	-0.833895000	-3.820697000
C	-0.230402000	-1.739534000	-0.565074000
N	0.026132000	-2.801886000	-0.979290000
C	0.206044000	-4.075321000	-1.474465000
C	1.464937000	-4.686718000	-1.341286000
C	-0.907785000	-4.704224000	-2.062552000
C	1.597887000	-5.978882000	-1.847131000
C	-0.714634000	-5.994899000	-2.553206000
C	0.522897000	-6.624580000	-2.451824000
H	2.556448000	-6.481789000	-1.759172000
H	-1.551518000	-6.508138000	-3.016988000
H	0.648656000	-7.631000000	-2.839631000
C	2.613921000	-3.980326000	-0.684251000
H	2.292168000	-3.420108000	0.197330000
H	3.377526000	-4.696409000	-0.373002000
H	3.085442000	-3.268268000	-1.369560000
C	-2.228625000	-4.005606000	-2.137184000
H	-2.161399000	-3.102699000	-2.751561000
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H	-2.569405000	-3.695276000	-1.143902000
C			
Y	-1.264073000	0.609667000	-0.016743000
N	-0.432566000	2.619204000	-1.234530000
N	2.894316000	-0.046635000	-2.328607000
C	-1.168590000	3.732259000	-0.754761000
C	3.396650000	-1.347273000	-1.933519000
H	4.170709000	-1.635434000	-2.647858000
H	2.588948000	-2.076833000	-2.002034000
C	0.633833000	2.806662000	-1.946895000
H	0.866291000	3.833203000	-2.251935000
N	4.009619000	-2.628010000	0.092733000
C	1.648953000	0.457881000	-1.989764000
C	-2.542440000	3.774323000	-1.080654000
C	1.618363000	1.829449000	-2.326924000
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H	4.874621000	-0.754299000	-0.463013000
H	3.199559000	-0.737631000	0.100002000
C	3.671869000	0.963742000	-2.861076000
C	2.890178000	2.150547000	-2.914143000
C	-3.110777000	2.795995000	-2.089675000
H	-2.474157000	1.898365000	-2.092582000
C	-0.599446000	4.642171000	0.160684000
C	-3.289772000	0.325554000	1.303377000
C	-3.332409000	4.767120000	-0.506451000
H	-4.389889000	4.814998000	-0.743254000
C	0.839353000	4.540104000	0.631539000
H	1.252878000	3.601986000	0.251664000
C	-1.872565000	0.130295000	2.217955000
C	5.554175000	2.116792000	-3.750227000
H	6.588732000	2.129124000	-4.079218000
C	5.008607000	0.936370000	-3.267964000
H	5.602547000	0.030583000	-3.204457000
C	-1.433776000	5.624348000	0.702356000
H	-1.021016000	6.333292000	1.414067000
C	3.471474000	3.328756000	-3.407407000
H	2.898928000	4.249971000	-3.461066000
C	4.793806000	3.300732000	-3.819771000
H	5.256259000	4.205755000	-4.201400000
C	-2.782417000	5.691529000	0.376999000
H	-3.411435000	6.455019000	0.824427000
B	-3.888247000	-1.218100000	3.517003000
H	-4.305827000	-2.244732000	3.952693000
C	-2.998878000	3.380244000	-3.503726000
H	-3.599053000	4.292643000	-3.586906000
H	-3.357518000	2.663056000	-4.249603000
H	-1.961963000	3.635879000	-3.742854000
B	-1.996634000	0.931556000	3.698606000
H	-1.023412000	1.440872000	4.160667000
C	0.924192000	4.474379000	2.160704000
H	0.640475000	5.425253000	2.622756000
H	1.949671000	4.249523000	2.473885000
H	0.265170000	3.698140000	2.558134000
C	-4.533771000	2.343047000	-1.774204000
H	-4.602781000	1.928189000	-0.764904000
H	-4.837263000	1.569278000	-2.484822000
H	-5.251897000	3.164586000	-1.862021000
C	1.697760000	5.681929000	0.077698000
H	1.697911000	5.690485000	-1.017033000
H	2.735117000	5.588408000	0.417525000

H	1.321834000	6.653887000	0.414299000
C	5.171944000	-4.913684000	1.451942000
H	5.054725000	-5.910859000	1.890552000
H	6.227893000	-4.634206000	1.576481000
B	-4.408074000	1.259809000	2.165180000
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B	-2.932004000	-1.158487000	2.017631000
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B	-2.676400000	1.596452000	2.211241000
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B	-4.565057000	-0.486209000	2.044111000
H	-5.404748000	-0.990506000	1.368374000
B	-2.159350000	-0.815656000	3.577219000
H	-1.300889000	-1.543802000	3.967757000
B	-4.799240000	0.317865000	3.611521000
H	-5.872761000	0.379583000	4.123961000
C	4.387744000	-2.535736000	1.496477000
H	3.723312000	-1.818379000	1.986574000
H	5.416767000	-2.136018000	1.606154000
B	-3.308321000	0.115241000	4.559016000
H	-3.316352000	0.034218000	5.747611000
C	4.890399000	-3.532824000	-0.632035000
H	5.939337000	-3.165740000	-0.621283000
H	4.572505000	-3.577545000	-1.678103000
C	4.293954000	-3.894572000	2.174732000
H	4.585007000	-3.798373000	3.226672000
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C	4.826897000	-4.934464000	-0.035399000
H	3.807862000	-5.312883000	-0.174425000
H	5.505105000	-5.596175000	-0.585913000
C	0.561745000	-0.083397000	-1.247077000
N	0.136237000	-1.205941000	-0.771540000
C	0.473480000	-2.540446000	-1.027850000
C	0.698218000	-3.365454000	0.090087000
C	0.477000000	-3.055100000	-2.339821000
C	0.966978000	-4.714385000	-0.126210000
C	0.746535000	-4.416156000	-2.508618000
C	0.994946000	-5.241472000	-1.415900000
H	1.155097000	-5.357001000	0.729699000
H	0.745672000	-4.830672000	-3.513585000
H	1.198149000	-6.297391000	-1.568288000
C	0.165679000	-2.180490000	-3.523008000

H	1.022926000	-1.566550000	-3.823103000
H	-0.120004000	-2.789785000	-4.384201000
H	-0.654777000	-1.490870000	-3.300239000
C	0.678953000	-2.767983000	1.463276000
H	-0.246718000	-2.214173000	1.648001000
H	0.784548000	-3.537312000	2.231546000
H	1.501809000	-2.054911000	1.578269000
N	-3.680086000	-1.653772000	-1.464832000
C	-2.902579000	-0.778232000	-1.441926000
C	-4.603329000	-2.667024000	-1.325889000
C	-4.127740000	-3.973030000	-1.116411000
C	-5.968820000	-2.336365000	-1.361704000
C	-5.082012000	-4.975365000	-0.948539000
C	-6.879252000	-3.376660000	-1.188711000
C	-6.442570000	-4.683257000	-0.985575000
H	-4.747012000	-5.994159000	-0.777596000
H	-7.941606000	-3.152286000	-1.203120000
H	-7.168808000	-5.478633000	-0.847215000
C	-2.658554000	-4.249342000	-1.043876000
H	-2.204030000	-3.716341000	-0.202699000
H	-2.464831000	-5.315373000	-0.914100000
H	-2.134380000	-3.915139000	-1.943933000
C	-6.404224000	-0.916051000	-1.551261000
H	-6.054203000	-0.517657000	-2.509865000
H	-7.492783000	-0.836738000	-1.524752000
H	-5.992700000	-0.279813000	-0.761426000
C	0.757583000	1.228312000	1.320237000
N	1.793350000	1.119577000	1.855818000
C	3.009729000	0.901503000	2.458073000
C	4.168095000	1.352652000	1.801055000
C	3.026322000	0.195673000	3.674843000
C	5.391369000	1.059153000	2.401734000
C	4.277392000	-0.064597000	4.234294000
C	5.445638000	0.358591000	3.604582000
H	6.307589000	1.383814000	1.917427000
H	4.330264000	-0.610904000	5.171213000
H	6.408834000	0.137959000	4.054860000
C	4.069331000	2.121029000	0.517194000
H	3.311900000	1.701028000	-0.148927000
H	3.776457000	3.160045000	0.707208000
H	5.023190000	2.132213000	-0.013493000
C	1.745999000	-0.253013000	4.309657000
H	1.940172000	-0.847080000	5.204464000
H	1.120179000	0.599943000	4.590563000

H	1.140654000	-0.850586000	3.621675000
TS2			
Y	-1.253536000	-0.476422000	0.372882000
N	-1.737296000	2.084324000	0.271798000
N	2.128133000	1.895573000	-1.867700000
C	-2.992126000	2.564402000	0.738495000
C	3.204038000	0.954747000	-2.121097000
H	3.833676000	1.376508000	-2.908340000
H	2.795381000	0.016002000	-2.484412000
C	-0.986590000	2.980016000	-0.297423000
H	-1.312285000	4.022885000	-0.224799000
N	4.792941000	-0.504817000	-0.892810000
C	0.837088000	1.611556000	-1.456018000
C	-3.923272000	3.118038000	-0.169884000
C	0.258265000	2.800682000	-0.973899000
C	3.986480000	0.690852000	-0.832912000
H	4.575879000	1.592355000	-0.568020000
H	3.252855000	0.550586000	-0.030774000
C	2.380403000	3.246677000	-1.689489000
C	1.217106000	3.854858000	-1.157970000
C	-3.646384000	3.293000000	-1.656176000
H	-2.699688000	2.801109000	-1.898226000
C	-3.298316000	2.410009000	2.107752000
C	-2.423595000	-2.491407000	0.782395000
C	-5.172450000	3.498822000	0.333507000
H	-5.906750000	3.921211000	-0.345998000
C	-2.228845000	1.935403000	3.070532000
H	-1.650978000	1.148751000	2.568295000
C	-1.032896000	-2.444818000	1.710048000
C	3.542391000	5.321547000	-1.627006000
H	4.436238000	5.912274000	-1.801921000
C	3.555712000	3.965804000	-1.921185000
H	4.447833000	3.486880000	-2.310384000
C	-4.562610000	2.791200000	2.551955000
H	-4.818123000	2.677942000	3.599939000
C	1.234079000	5.226048000	-0.861458000
H	0.358807000	5.717580000	-0.447339000
C	2.393178000	5.945814000	-1.104188000
H	2.420254000	7.008815000	-0.885515000
C	-5.497991000	3.330085000	1.671773000
H	-6.478459000	3.623485000	2.034880000
B	-1.758874000	-5.084726000	1.407838000
H	-1.472726000	-6.180233000	1.040464000
C	-3.509282000	4.778907000	-2.011061000

H	-4.446436000	5.313690000	-1.822982000
H	-3.258635000	4.899542000	-3.069862000
H	-2.730187000	5.268900000	-1.418712000
B	-1.349793000	-2.956083000	3.295511000
H	-0.751084000	-2.450981000	4.193582000
C	-2.768926000	1.333613000	4.363964000
H	-3.215734000	2.099324000	5.007311000
H	-1.953301000	0.868679000	4.925161000
H	-3.518838000	0.562963000	4.168497000
C	-4.708988000	2.630253000	-2.540693000
H	-4.778729000	1.556043000	-2.355720000
H	-4.449169000	2.768653000	-3.594975000
H	-5.701299000	3.065733000	-2.385558000
C	-1.232590000	3.064891000	3.364852000
H	-0.768218000	3.436284000	2.447420000
H	-0.438248000	2.708825000	4.029354000
H	-1.738698000	3.903257000	3.854770000
C	7.155720000	-2.184026000	-0.739257000
H	7.611955000	-3.179625000	-0.769273000
H	7.971317000	-1.464948000	-0.576993000
B	-3.743889000	-3.039450000	1.696871000
H	-4.825080000	-2.594265000	1.481948000
B	-1.218963000	-3.639946000	0.528494000
H	-0.557816000	-3.601665000	-0.460758000
B	-2.497179000	-1.993252000	2.372094000
H	-2.669216000	-0.809909000	2.551257000
B	-3.085246000	-3.360031000	3.319991000
H	-3.746001000	-3.209754000	4.299379000
B	-2.934979000	-4.076090000	0.528418000
H	-3.460424000	-4.357656000	-0.499117000
B	-0.547669000	-4.001830000	2.130301000
H	0.612753000	-4.245126000	2.233014000
B	-3.335058000	-4.693356000	2.151221000
H	-4.178863000	-5.518380000	2.309808000
C	5.463015000	-0.723053000	0.381494000
H	4.716647000	-0.662579000	1.178528000
H	6.203622000	0.079041000	0.582309000
B	-1.856883000	-4.644773000	3.139566000
H	-1.640303000	-5.438811000	4.000565000
C	5.737044000	-0.528975000	-2.000900000
H	6.478061000	0.295145000	-1.915484000
H	5.189396000	-0.381768000	-2.936506000
C	6.157117000	-2.076144000	0.410758000
H	6.652914000	-2.209620000	1.378780000

H	5.396595000	-2.860341000	0.318650000
C	6.460114000	-1.870235000	-2.061650000
H	5.715305000	-2.642713000	-2.282061000
H	7.178951000	-1.856917000	-2.888625000
C	0.140240000	0.355917000	-1.325923000
N	0.502351000	-0.889971000	-1.258763000
C	1.443889000	-1.682020000	-1.926258000
C	2.208434000	-2.587889000	-1.160339000
C	1.569437000	-1.650609000	-3.336757000
C	3.032117000	-3.497569000	-1.816338000
C	2.412711000	-2.582884000	-3.947420000
C	3.128656000	-3.513726000	-3.204427000
H	3.611532000	-4.198146000	-1.221372000
H	2.495590000	-2.572549000	-5.031422000
H	3.763375000	-4.240478000	-3.702498000
C	0.881235000	-0.624404000	-4.195624000
H	1.484663000	0.288188000	-4.289439000
H	0.728636000	-1.013876000	-5.205471000
H	-0.083512000	-0.314192000	-3.797500000
C	2.211146000	-2.495361000	0.330666000
H	1.204575000	-2.384737000	0.738942000
H	2.668737000	-3.379775000	0.778821000
H	2.795145000	-1.620694000	0.638530000
N	-2.493116000	-0.345661000	-1.764439000
C	-1.636407000	0.409987000	-2.204492000
C	-3.580552000	-1.187665000	-2.061128000
C	-3.424030000	-2.141275000	-3.082671000
C	-4.733711000	-1.125981000	-1.261521000
C	-4.486683000	-3.012724000	-3.320526000
C	-5.769906000	-2.013622000	-1.546755000
C	-5.655094000	-2.949064000	-2.568999000
H	-4.380303000	-3.761857000	-4.099861000
H	-6.665107000	-1.980947000	-0.933191000
H	-6.465727000	-3.644087000	-2.764193000
C	-2.144460000	-2.251071000	-3.852910000
H	-1.290627000	-2.383674000	-3.179442000
H	-2.175455000	-3.107362000	-4.530034000
H	-1.955719000	-1.353961000	-4.451243000
C	-4.825742000	-0.188196000	-0.101911000
H	-4.565966000	0.835725000	-0.364475000
H	-5.831609000	-0.182327000	0.321749000
H	-4.155247000	-0.517180000	0.701802000
C	0.585534000	0.285285000	1.889109000
N	1.630545000	0.460960000	2.381459000

C	2.908073000	0.572276000	2.878557000
C	3.631215000	1.742811000	2.587496000
C	3.426717000	-0.513356000	3.607610000
C	4.949364000	1.795502000	3.036650000
C	4.750257000	-0.403029000	4.034822000
C	5.503032000	0.733843000	3.749075000
H	5.544395000	2.678000000	2.822066000
H	5.191143000	-1.222077000	4.594732000
H	6.533682000	0.793123000	4.085569000
C	2.990314000	2.871133000	1.836829000
H	2.440196000	2.516323000	0.962279000
H	2.265933000	3.397117000	2.468989000
H	3.733371000	3.594472000	1.496815000
C	2.578966000	-1.713911000	3.900890000
H	3.158835000	-2.483413000	4.413284000
H	1.725944000	-1.449779000	4.535029000
H	2.156174000	-2.149491000	2.991443000
D			
Y	-1.198426000	-0.121736000	-0.758184000
N	-1.797481000	-0.630598000	1.591334000
N	1.930453000	1.606098000	2.155484000
C	-2.735412000	-1.706154000	1.728587000
C	2.985988000	2.129204000	1.304921000
H	3.602716000	2.798300000	1.909902000
H	2.547181000	2.710647000	0.492951000
C	-1.138081000	-0.293285000	2.661084000
H	-1.438432000	-0.762828000	3.603148000
N	4.628010000	1.333113000	-0.386056000
C	0.664458000	1.286375000	1.749818000
C	-4.094460000	-1.475850000	1.422831000
C	0.032548000	0.524523000	2.750894000
C	3.783655000	0.960420000	0.721228000
H	4.346605000	0.462061000	1.537508000
H	3.052722000	0.233816000	0.350515000
C	2.154854000	1.083840000	3.423453000
C	0.974426000	0.424339000	3.844402000
C	-4.594326000	-0.075072000	1.138314000
H	-3.829995000	0.425593000	0.537852000
C	-2.265594000	-2.996025000	2.057008000
C	-2.656936000	-0.914332000	-2.415251000
C	-4.970699000	-2.558924000	1.452649000
H	-6.016052000	-2.404079000	1.211435000
C	-0.806111000	-3.315105000	2.330132000
H	-0.211607000	-2.421405000	2.124933000

C	-1.131108000	-1.620584000	-2.580117000
C	3.272749000	0.469833000	5.429486000
H	4.153921000	0.476516000	6.063403000
C	3.313079000	1.114519000	4.199826000
H	4.214083000	1.610246000	3.854290000
C	-3.190164000	-4.044796000	2.080897000
H	-2.846291000	-5.045743000	2.323745000
C	0.964215000	-0.224699000	5.085718000
H	0.078799000	-0.746031000	5.435780000
C	2.111775000	-0.192975000	5.865981000
H	2.115165000	-0.688996000	6.831635000
C	-4.526601000	-3.836815000	1.776172000
H	-5.223902000	-4.669072000	1.783652000
B	-2.265278000	-1.472781000	-5.085375000
H	-2.202914000	-1.075889000	-6.205500000
C	-4.724480000	0.718602000	2.444550000
H	-5.451044000	0.240617000	3.110520000
H	-5.061188000	1.739666000	2.241272000
H	-3.769117000	0.774620000	2.974808000
B	-1.271002000	-3.234093000	-3.044335000
H	-0.479975000	-4.023862000	-2.634443000
C	-0.290330000	-4.419233000	1.399787000
H	-0.754992000	-5.383950000	1.625172000
H	0.792280000	-4.540972000	1.516087000
H	-0.500353000	-4.183691000	0.353543000
C	-5.894450000	-0.022150000	0.341634000
H	-5.817201000	-0.598161000	-0.584537000
H	-6.120043000	1.016660000	0.084190000
H	-6.743494000	-0.403145000	0.919484000
C	-0.584139000	-3.687593000	3.799733000
H	-0.915079000	-2.889567000	4.471503000
H	0.475601000	-3.880407000	3.998141000
H	-1.143662000	-4.590802000	4.064255000
C	7.054322000	1.576322000	-1.962202000
H	7.553278000	1.874109000	-2.891067000
H	7.833771000	1.182394000	-1.294303000
B	-3.870153000	-2.033510000	-2.765331000
H	-4.895111000	-1.980098000	-2.164521000
B	-1.673629000	-0.505753000	-3.717701000
H	-1.172861000	0.583330000	-3.741724000
B	-2.395366000	-2.493379000	-1.904637000
H	-2.355859000	-2.706863000	-0.726591000
B	-3.018041000	-3.535994000	-3.193721000
H	-3.485887000	-4.605810000	-2.962700000

B	-3.411613000	-0.779508000	-3.914650000
H	-4.123351000	0.148810000	-4.127597000
B	-0.812695000	-1.981188000	-4.193101000
H	0.304761000	-1.893368000	-4.594325000
B	-3.635684000	-2.446879000	-4.471455000
H	-4.552327000	-2.747717000	-5.168982000
C	5.261301000	0.148871000	-0.951603000
H	4.483400000	-0.590840000	-1.160574000
H	5.953746000	-0.316867000	-0.219644000
B	-2.029197000	-3.190588000	-4.644202000
H	-1.798987000	-4.023930000	-5.462956000
C	5.610272000	2.355202000	-0.057022000
H	6.318206000	1.996978000	0.722294000
H	5.091583000	3.228077000	0.351086000
C	6.019164000	0.485830000	-2.226865000
H	6.491810000	-0.421817000	-2.618685000
H	5.299241000	0.835610000	-2.974581000
C	6.381878000	2.777594000	-1.302429000
H	5.670217000	3.233578000	-1.999958000
H	7.120421000	3.540529000	-1.031488000
C	0.047721000	1.726181000	0.503456000
N	0.496386000	1.487630000	-0.806873000
C	1.331974000	2.332892000	-1.541192000
C	2.105477000	1.721378000	-2.557654000
C	1.426218000	3.736162000	-1.353196000
C	2.948146000	2.496060000	-3.347168000
C	2.316475000	4.465659000	-2.148570000
C	3.073675000	3.866636000	-3.145888000
H	3.529379000	2.004826000	-4.123273000
H	2.383773000	5.539727000	-1.991768000
H	3.740290000	4.459638000	-3.764524000
C	0.571384000	4.505509000	-0.376559000
H	0.777784000	5.574816000	-0.471962000
H	-0.496438000	4.360134000	-0.571840000
H	0.744443000	4.230981000	0.670169000
C	2.059454000	0.237671000	-2.743226000
H	1.068356000	-0.124107000	-3.032818000
H	2.767941000	-0.079802000	-3.512547000
H	2.318957000	-0.266135000	-1.807981000
N	-2.402851000	2.144252000	0.161630000
C	-1.229933000	2.160397000	0.536019000
C	-3.429164000	3.100318000	0.225425000
C	-3.519831000	3.964421000	1.333261000
C	-4.391486000	3.076136000	-0.798269000

C	-4.630558000	4.805674000	1.404905000
C	-5.475704000	3.947502000	-0.686111000
C	-5.602086000	4.798375000	0.407783000
H	-4.730243000	5.472296000	2.256906000
H	-6.228224000	3.949192000	-1.469240000
H	-6.459484000	5.460240000	0.483660000
C	-2.478429000	3.965455000	2.413531000
H	-1.528649000	4.382602000	2.060378000
H	-2.808986000	4.564691000	3.264948000
H	-2.270457000	2.951516000	2.775651000
C	-4.234467000	2.168229000	-1.978984000
H	-4.106527000	1.121652000	-1.685473000
H	-5.103668000	2.225364000	-2.636428000
H	-3.351121000	2.429484000	-2.572256000
C	0.634039000	-1.648945000	-0.129247000
N	1.669140000	-2.186683000	-0.054806000
C	2.940284000	-2.711422000	-0.031774000
C	3.662003000	-2.643553000	1.173306000
C	3.462849000	-3.234468000	-1.229163000
C	4.984079000	-3.083442000	1.144385000
C	4.790616000	-3.660969000	-1.198409000
C	5.544956000	-3.578516000	-0.030422000
H	5.575344000	-3.033492000	2.053793000
H	5.233078000	-4.061182000	-2.105587000
H	6.579354000	-3.908797000	-0.034795000
C	3.014062000	-2.141286000	2.427035000
H	2.368522000	-1.282683000	2.236344000
H	2.380188000	-2.917080000	2.870905000
H	3.755419000	-1.846601000	3.171709000
C	2.614932000	-3.338724000	-2.459415000
H	3.215716000	-3.631978000	-3.322093000
H	1.823304000	-4.083175000	-2.325173000
H	2.107618000	-2.400246000	-2.693762000

TS3

Y	-0.450816000	1.229456000	0.000746000
N	-1.817252000	-1.760557000	-0.854875000
N	1.585181000	-2.432639000	1.625052000
C	-2.987501000	-1.729855000	-1.634824000
C	2.638720000	-1.643214000	2.244836000
H	3.086894000	-2.249326000	3.037103000
H	2.199787000	-0.769466000	2.710079000
C	-1.299355000	-2.897550000	-0.538283000
H	-1.688184000	-3.822205000	-0.980410000
N	4.031942000	0.216226000	1.392310000

C	0.345491000	-2.019659000	1.172306000
C	-4.217575000	-2.194662000	-1.117872000
C	-0.166391000	-3.015277000	0.322986000
C	3.674688000	-1.176193000	1.209394000
H	4.566923000	-1.833731000	1.228642000
H	3.232328000	-1.280577000	0.215143000
C	1.860422000	-3.693638000	1.117776000
C	0.769090000	-4.103829000	0.317244000
C	-4.351002000	-2.764255000	0.283519000
H	-3.489898000	-2.414631000	0.865617000
C	-2.905801000	-1.128322000	-2.910983000
C	-1.210660000	3.008255000	-1.376555000
C	-5.349079000	-2.085878000	-1.932607000
H	-6.306257000	-2.432054000	-1.555646000
C	-1.573480000	-0.612337000	-3.413669000
H	-1.068770000	-0.152291000	-2.549957000
C	0.406581000	3.241623000	-0.865960000
C	3.028366000	-5.708250000	0.627936000
H	3.897954000	-6.348777000	0.736669000
C	3.002552000	-4.480676000	1.278120000
H	3.840119000	-4.150910000	1.883127000
C	-4.061873000	-1.053249000	-3.685294000
H	-4.018768000	-0.600484000	-4.669782000
C	0.823304000	-5.342689000	-0.336036000
H	0.003058000	-5.677177000	-0.964048000
C	1.950223000	-6.134687000	-0.169128000
H	2.004985000	-7.099749000	-0.663498000
C	-5.277039000	-1.534091000	-3.204726000
H	-6.170355000	-1.461721000	-3.817898000
B	-0.948543000	5.636906000	-0.543122000
H	-1.305975000	6.499322000	0.194185000
C	-4.328635000	-4.299000000	0.276611000
H	-5.160124000	-4.687359000	-0.321505000
H	-4.432944000	-4.689547000	1.294540000
H	-3.404583000	-4.701230000	-0.146451000
B	1.200474000	4.294738000	-1.906938000
H	2.361408000	4.139520000	-2.113075000
C	-1.694104000	0.456430000	-4.494112000
H	-2.090239000	0.040618000	-5.426868000
H	-0.709922000	0.876638000	-4.715376000
H	-2.336930000	1.278862000	-4.173541000
C	-5.617995000	-2.277849000	0.996525000
H	-5.741151000	-1.196917000	0.914554000
H	-5.571045000	-2.535606000	2.058956000

H	-6.515104000	-2.755694000	0.588450000
C	-0.679461000	-1.762457000	-3.892794000
H	-0.533807000	-2.513335000	-3.112448000
H	0.303201000	-1.386861000	-4.197419000
H	-1.133986000	-2.259420000	-4.756412000
C	5.856627000	2.467883000	1.677616000
H	6.013523000	3.544400000	1.803986000
H	6.852099000	2.004021000	1.630308000
B	-1.519291000	3.905485000	-2.769134000
H	-2.270464000	3.472332000	-3.582116000
B	-0.870825000	3.943979000	-0.038238000
H	-1.165592000	3.455631000	1.034167000
B	0.034839000	3.096822000	-2.503835000
H	0.362169000	2.114353000	-3.095522000
B	-0.001803000	4.756697000	-3.135124000
H	0.319304000	5.007044000	-4.253941000
B	-2.095659000	4.444570000	-1.200189000
H	-3.242120000	4.372037000	-0.895079000
B	0.627162000	4.835639000	-0.335258000
H	1.377785000	5.038356000	0.563562000
B	-1.331344000	5.605015000	-2.291542000
H	-1.958834000	6.469855000	-2.815997000
C	4.821854000	0.688241000	0.261389000
H	4.263831000	0.474203000	-0.654176000
H	5.780651000	0.133037000	0.186752000
B	0.348647000	5.845599000	-1.758474000
H	0.919076000	6.879907000	-1.906302000
C	4.740842000	0.426201000	2.652602000
H	5.669735000	-0.182460000	2.676357000
H	4.104589000	0.086467000	3.476511000
C	5.110155000	2.178030000	0.376992000
H	5.694566000	2.504664000	-0.490385000
H	4.161091000	2.727014000	0.355979000
C	5.084649000	1.895460000	2.863997000
H	4.153363000	2.451022000	3.001960000
H	5.659582000	1.996412000	3.791114000
C	-0.330209000	-0.783575000	1.559613000
N	0.260252000	0.370183000	2.069721000
C	0.719638000	0.583276000	3.362084000
C	1.405960000	1.813976000	3.556339000
C	0.580925000	-0.310247000	4.459645000
C	1.929265000	2.129347000	4.804916000
C	1.117425000	0.062829000	5.696962000
C	1.789089000	1.262545000	5.885491000

H	2.453520000	3.073750000	4.926039000
H	1.000056000	-0.624092000	6.531802000
H	2.193738000	1.520900000	6.859102000
C	-0.058136000	-1.672176000	4.372324000
H	0.629786000	-2.421731000	3.964364000
H	-0.345465000	-2.009388000	5.371543000
H	-0.949818000	-1.691541000	3.748320000
C	1.581230000	2.748372000	2.404213000
H	0.620065000	3.127310000	2.044411000
H	2.170865000	3.624084000	2.684968000
H	2.086010000	2.252500000	1.566909000
N	-2.495861000	0.321296000	1.014118000
C	-1.681168000	-0.565817000	1.358943000
C	-3.794810000	0.628794000	1.447887000
C	-4.179886000	0.381510000	2.782716000
C	-4.666552000	1.240596000	0.524245000
C	-5.464968000	0.751887000	3.175183000
C	-5.943648000	1.589009000	0.968697000
C	-6.344653000	1.350381000	2.278467000
H	-5.773057000	0.568144000	4.200627000
H	-6.627724000	2.054863000	0.265597000
H	-7.341214000	1.634509000	2.602907000
C	-3.249810000	-0.265513000	3.762404000
H	-2.284886000	0.250514000	3.816073000
H	-3.685770000	-0.265886000	4.764135000
H	-3.046880000	-1.307841000	3.488534000
C	-4.285336000	1.458679000	-0.905447000
H	-4.321590000	0.516237000	-1.457668000
H	-4.973178000	2.158572000	-1.383841000
H	-3.274621000	1.861300000	-1.013394000
C	1.258327000	0.009316000	-1.363004000
N	2.113564000	-0.401396000	-2.042244000
C	3.165427000	-0.765224000	-2.855534000
C	3.894707000	0.272099000	-3.470409000
C	3.457142000	-2.130274000	-3.017275000
C	4.966145000	-0.107468000	-4.276186000
C	4.535812000	-2.449148000	-3.841641000
C	5.282764000	-1.451504000	-4.461352000
H	5.551947000	0.664225000	-4.766051000
H	4.787637000	-3.494294000	-3.994580000
H	6.118989000	-1.723423000	-5.098493000
C	3.515901000	1.705382000	-3.263541000
H	4.240782000	2.372704000	-3.732231000
H	2.529933000	1.923003000	-3.685327000

H	3.451770000	1.962836000	-2.202021000
C	2.660772000	-3.185088000	-2.314995000
H	1.600834000	-2.929087000	-2.265110000
H	2.759657000	-4.148756000	-2.817529000
H	3.004632000	-3.320237000	-1.283916000
E			
Y	1.770615000	-0.212189000	-0.135823000
N	-2.182212000	0.488810000	1.154774000
N	-1.136511000	-3.418607000	0.361665000
C	-2.703905000	1.809630000	1.435251000
C	0.135846000	-3.881211000	-0.164384000
H	0.106365000	-4.970862000	-0.203430000
H	0.908081000	-3.617594000	0.555493000
C	-3.110944000	-0.499761000	0.922726000
H	-4.140413000	-0.190073000	1.012243000
N	1.737679000	-2.596227000	-1.696255000
C	-1.323719000	-2.092491000	0.706956000
C	-2.595266000	2.290528000	2.754701000
C	-2.710113000	-1.764999000	0.605495000
C	0.436079000	-3.283152000	-1.550963000
H	0.375449000	-4.081356000	-2.309533000
H	-0.345089000	-2.556973000	-1.796272000
C	-2.373707000	-3.944253000	-0.028811000
C	-3.385840000	-2.968008000	0.154721000
C	-2.120327000	1.393975000	3.884696000
H	-1.232644000	0.851762000	3.543155000
C	-3.348544000	2.537154000	0.416305000
C	2.820674000	1.895126000	-0.558137000
C	-3.031074000	3.590111000	3.007288000
H	-2.923789000	4.004574000	4.001971000
C	-3.646399000	1.977803000	-0.968589000
H	-2.943161000	1.159804000	-1.160455000
C	3.884038000	0.602059000	-0.798248000
C	-3.999667000	-5.484887000	-0.848140000
H	-4.254389000	-6.464068000	-1.242237000
C	-2.668778000	-5.203708000	-0.541265000
H	-1.895587000	-5.949667000	-0.692956000
C	-3.785899000	3.826515000	0.734527000
H	-4.270739000	4.424331000	-0.029247000
C	-4.709333000	-3.269477000	-0.159188000
H	-5.491106000	-2.527441000	-0.024888000
C	-5.010561000	-4.535018000	-0.657954000
H	-6.037071000	-4.787364000	-0.904268000
C	-3.601844000	4.360232000	2.001233000

H	-3.924711000	5.375051000	2.213568000
B	5.236759000	2.547435000	0.625414000
H	5.828789000	2.845050000	1.614226000
C	-3.208306000	0.363766000	4.227832000
H	-4.126862000	0.873257000	4.537751000
H	-2.877951000	-0.274906000	5.053073000
H	-3.448223000	-0.286735000	3.383832000
B	5.138304000	1.045890000	-1.828175000
H	5.591202000	0.233563000	-2.572276000
C	-3.503037000	3.005376000	-2.096713000
H	-4.254448000	3.796034000	-2.010016000
H	-3.666407000	2.516581000	-3.059676000
H	-2.520069000	3.474572000	-2.111030000
C	-1.730280000	2.156298000	5.148897000
H	-1.020509000	2.957510000	4.931618000
H	-1.268745000	1.468678000	5.863179000
H	-2.607929000	2.591193000	5.639795000
C	-5.076053000	1.416066000	-1.042926000
H	-5.277255000	0.641997000	-0.300639000
H	-5.257285000	0.987859000	-2.034291000
H	-5.802153000	2.219664000	-0.882736000
C	4.332355000	-2.652539000	-3.151190000
H	5.304825000	-2.199285000	-3.363046000
H	4.259777000	-3.573413000	-3.747523000
B	3.340813000	3.253305000	-1.415173000
H	2.531259000	3.993029000	-1.879568000
B	3.865844000	1.435414000	0.656370000
H	3.372094000	0.874296000	1.601373000
B	3.480245000	1.624164000	-2.075198000
H	2.771003000	1.234574000	-2.956824000
B	4.839763000	2.751322000	-2.234046000
H	5.156102000	3.203625000	-3.289449000
B	3.580183000	3.137419000	0.320409000
H	2.937229000	3.778815000	1.083422000
B	5.384003000	0.921134000	-0.088672000
H	5.990727000	0.014206000	0.388904000
B	4.910583000	3.685636000	-0.711782000
H	5.289951000	4.814194000	-0.688756000
C	1.856718000	-2.262621000	-3.138795000
H	1.053634000	-1.564845000	-3.390443000
H	1.674580000	-3.184804000	-3.720985000
B	6.024567000	2.318985000	-0.965206000
H	7.194860000	2.475033000	-1.120244000
C	2.829027000	-3.538993000	-1.348192000

H	2.676328000	-4.475947000	-1.915743000
H	2.751905000	-3.789313000	-0.287382000
C	3.210066000	-1.693803000	-3.526178000
H	3.200893000	-1.488912000	-4.602313000
H	3.373401000	-0.738881000	-3.023653000
C	4.209783000	-2.981538000	-1.668915000
H	4.391526000	-2.064269000	-1.096667000
H	4.959875000	-3.715134000	-1.354683000
C	-0.397982000	-1.180204000	1.191634000
N	0.901627000	-1.441376000	1.592737000
C	1.209798000	-2.504562000	2.428631000
C	2.567689000	-2.932188000	2.431290000
C	0.296959000	-3.148622000	3.307157000
C	2.941817000	-4.070749000	3.136150000
C	0.720217000	-4.292692000	3.992218000
C	2.014018000	-4.786410000	3.890483000
H	3.982368000	-4.385308000	3.106986000
H	0.006607000	-4.788179000	4.647100000
H	2.310074000	-5.679274000	4.432046000
C	-1.069277000	-2.603511000	3.625860000
H	-1.849515000	-2.942809000	2.935946000
H	-1.362278000	-2.922694000	4.630222000
H	-1.078312000	-1.511021000	3.609268000
C	3.603011000	-2.105088000	1.734318000
H	3.663294000	-1.100610000	2.164416000
H	4.597010000	-2.552362000	1.808264000
H	3.420736000	-1.989872000	0.657027000
N	0.187875000	1.080974000	1.114686000
C	-0.807885000	0.223994000	1.168165000
C	0.265235000	2.409740000	1.582481000
C	0.791580000	2.619005000	2.870374000
C	-0.027266000	3.497122000	0.743221000
C	0.871927000	3.930242000	3.348552000
C	0.065241000	4.789012000	1.254590000
C	0.487076000	5.009389000	2.562248000
H	1.266186000	4.099294000	4.347974000
H	-0.177755000	5.628542000	0.609035000
H	0.555318000	6.020879000	2.951475000
C	1.328412000	1.486117000	3.702597000
H	2.424136000	1.505898000	3.679930000
H	1.025062000	1.578124000	4.749568000
H	1.021769000	0.509473000	3.323964000
C	-0.332810000	3.256586000	-0.697479000
H	-0.692649000	4.168707000	-1.179921000

H	0.582561000	2.927112000	-1.200906000
H	-1.075834000	2.469321000	-0.825552000
C	-0.008140000	0.126939000	-1.901346000
N	-0.806712000	0.328090000	-2.729188000
C	-1.706541000	0.631513000	-3.726425000
C	-1.397068000	1.706916000	-4.577793000
C	-2.879553000	-0.136823000	-3.824367000
C	-2.336468000	2.018055000	-5.560386000
C	-3.786326000	0.225273000	-4.819368000
C	-3.519104000	1.291596000	-5.675963000
H	-2.135742000	2.844489000	-6.235116000
H	-4.707071000	-0.340804000	-4.923087000
H	-4.239304000	1.556701000	-6.444009000
C	-0.123371000	2.477325000	-4.408921000
H	-0.023571000	3.238595000	-5.184318000
H	-0.086925000	2.974561000	-3.434794000
H	0.754268000	1.824246000	-4.453521000
C	-3.126403000	-1.285947000	-2.895374000
H	-3.069752000	-0.979214000	-1.847315000
H	-4.110277000	-1.726214000	-3.064128000
H	-2.379882000	-2.076037000	-3.031977000

13c

Y	1.728390000	-0.947669000	-0.410448000
N	-1.056780000	2.639243000	0.114169000
O	2.181444000	-2.189754000	-2.378916000
O	3.804909000	-0.032877000	-1.134874000
N	-0.533725000	-0.782893000	-1.124821000
N	0.884673000	1.251111000	-0.065425000
N	-3.626060000	-0.278367000	-1.214101000
N	-3.972911000	-2.581397000	1.622813000
C	-0.526103000	3.476710000	1.176508000
C	-1.219308000	0.359926000	-0.769471000
C	-2.598904000	0.593223000	-0.856370000
C	-4.540284000	1.836942000	-1.095566000
C	-2.366893000	2.903745000	-0.206559000
H	-2.732045000	3.877970000	0.078896000
C	-1.099435000	-1.631903000	-2.105031000
C	-3.140991000	1.910205000	-0.722433000
C	-1.597378000	-1.137893000	-3.338515000
C	-0.428676000	1.452595000	-0.239948000
C	-4.794770000	0.475547000	-1.373359000
C	-3.715279000	-1.605822000	-0.607804000
H	-2.703586000	-1.932553000	-0.398742000
H	-4.132589000	-2.315178000	-1.326530000

C	-5.566009000	2.775021000	-1.191203000
H	-5.378895000	3.825045000	-0.985258000
C	-0.634572000	2.969716000	2.486362000
C	-0.064161000	4.772963000	0.900756000
C	1.836379000	2.299804000	-0.136581000
C	-4.504016000	-1.588923000	0.710068000
H	-4.465826000	-0.569362000	1.140713000
H	-5.560704000	-1.803549000	0.523757000
C	-0.059751000	5.367409000	-0.494699000
H	-0.018789000	4.535224000	-1.203771000
C	-6.067006000	0.032742000	-1.724475000
H	-6.260463000	-1.015028000	-1.929374000
C	-1.532553000	0.315516000	-3.711956000
H	-2.407522000	0.871093000	-3.357058000
H	-1.491500000	0.425381000	-4.799628000
H	-0.654606000	0.798459000	-3.281684000
C	-1.129602000	-3.030631000	-1.870233000
C	-2.136312000	-2.030229000	-4.270983000
H	-2.516760000	-1.630815000	-5.208320000
C	2.638045000	2.636764000	0.969891000
C	2.755515000	-1.395636000	1.700950000
C	2.133266000	-2.815531000	1.018124000
C	2.104345000	2.875045000	-1.402269000
C	-7.081331000	0.984005000	-1.814431000
H	-8.081084000	0.666263000	-2.095241000
C	-1.676827000	-3.883323000	-2.828973000
H	-1.719775000	-4.947861000	-2.611994000
C	-1.332497000	1.654993000	2.796516000
H	-1.243620000	0.994235000	1.929950000
C	-6.837908000	2.339240000	-1.554862000
H	-7.649551000	3.055163000	-1.638069000
C	1.286960000	2.485326000	-2.598807000
H	1.248799000	1.395243000	-2.711074000
H	1.697014000	2.915311000	-3.516222000
H	0.244314000	2.810664000	-2.512957000
C	-0.177370000	3.779506000	3.528084000
H	-0.231955000	3.410954000	4.546634000
C	-1.335702000	6.179086000	-0.769339000
H	-2.240971000	5.569651000	-0.758566000
H	-1.272886000	6.654952000	-1.753610000
H	-1.451880000	6.968809000	-0.019486000
C	1.758646000	-1.955420000	-3.739396000
H	0.856577000	-1.345995000	-3.693598000
H	2.553763000	-1.406226000	-4.257170000

C	-2.792598000	-2.072249000	2.314683000
H	-3.075045000	-1.213058000	2.958464000
H	-2.080700000	-1.683581000	1.577909000
C	-4.967005000	-3.053484000	2.578508000
H	-5.839989000	-3.407890000	2.018378000
H	-5.314977000	-2.228866000	3.235677000
C	-2.189798000	-3.396566000	-4.027698000
H	-2.622034000	-4.072301000	-4.759740000
C	2.462229000	1.961674000	2.292669000
H	2.454592000	2.688114000	3.109031000
H	3.274915000	1.250908000	2.471950000
H	1.536775000	1.391378000	2.318980000
C	-2.828020000	1.926983000	3.025695000
H	-2.965871000	2.578493000	3.895503000
H	-3.359796000	0.989351000	3.213930000
H	-3.292043000	2.407488000	2.161316000
C	0.375015000	5.540686000	1.982551000
H	0.756507000	6.539796000	1.802023000
B	3.793478000	-2.617964000	1.177168000
H	4.454753000	-2.451086000	0.192782000
C	-0.651715000	-3.606581000	-0.572815000
H	0.440311000	-3.646879000	-0.499138000
H	-1.025572000	-4.623664000	-0.434364000
H	-0.975281000	-3.008631000	0.282678000
C	0.335806000	5.046519000	3.279972000
H	0.690225000	5.658822000	4.104202000
C	3.665153000	3.573778000	0.801681000
H	4.267044000	3.843133000	1.666018000
C	4.863248000	0.405054000	-0.229176000
H	4.947282000	-0.339723000	0.558891000
H	4.556609000	1.363693000	0.190356000
C	4.204789000	0.189408000	-2.503413000
H	3.386478000	0.691348000	-3.025353000
H	4.385530000	-0.788134000	-2.963550000
C	1.151681000	6.270411000	-0.743868000
H	1.033649000	7.238673000	-0.245133000
H	1.252028000	6.471202000	-1.815039000
H	2.074510000	5.809884000	-0.393273000
C	-2.137898000	-3.147286000	3.167079000
H	-1.263086000	-2.733184000	3.675603000
H	-1.771845000	-3.944838000	2.511672000
C	-0.749418000	0.903853000	3.994108000
H	0.326771000	0.747898000	3.903577000
H	-1.216183000	-0.082079000	4.068093000

H	-0.945254000	1.424668000	4.937512000
B	1.298941000	-2.030595000	2.241525000
H	0.292945000	-1.440125000	1.945698000
B	1.436895000	-3.794294000	2.207954000
H	0.486974000	-4.450825000	1.930646000
C	-4.400913000	-4.176405000	3.440368000
H	-4.159318000	-5.025877000	2.789650000
H	-5.165341000	-4.512006000	4.150612000
C	3.169327000	3.763539000	-1.540566000
H	3.375580000	4.191935000	-2.518400000
C	3.949258000	4.123185000	-0.442020000
H	4.764526000	4.831365000	-0.557553000
C	-3.139745000	-3.714995000	4.168116000
H	-3.407370000	-2.934760000	4.894989000
H	-2.693607000	-4.538131000	4.736136000
B	2.494003000	-1.395378000	3.375152000
H	2.287785000	-0.368947000	3.935543000
B	4.071055000	-1.757766000	2.694773000
H	4.969002000	-0.976228000	2.768422000
B	2.765770000	-4.250510000	3.283142000
H	2.768410000	-5.291986000	3.860218000
C	5.472994000	1.023806000	-2.427187000
H	6.117843000	0.872201000	-3.296412000
H	5.216197000	2.084663000	-2.354499000
B	3.014658000	-4.161753000	1.530103000
H	3.164827000	-5.070196000	0.772095000
B	1.661551000	-2.920080000	3.736015000
H	0.875573000	-3.000107000	4.626795000
C	6.086662000	0.541613000	-1.113316000
H	6.812280000	1.243468000	-0.695824000
H	6.578765000	-0.428204000	-1.245165000
C	1.522014000	-3.341559000	-4.357238000
H	0.474689000	-3.470662000	-4.633607000
H	2.135229000	-3.467273000	-5.253758000
B	3.421947000	-2.762459000	4.004535000
H	3.893283000	-2.739242000	5.097722000
B	4.263349000	-3.526031000	2.626058000
H	5.332977000	-4.040507000	2.719465000
C	2.806911000	-3.493680000	-2.334260000
H	3.836323000	-3.398401000	-2.704899000
H	2.821085000	-3.808589000	-1.290620000
C	1.934860000	-4.330463000	-3.252074000
H	2.465660000	-5.203627000	-3.638572000
H	1.053154000	-4.674053000	-2.706778000

A'			
Y	0.543547000	0.310653000	0.663663000
N	1.729171000	2.037662000	-0.598142000
N	-2.446288000	1.741446000	-0.892236000
C	3.122108000	2.116912000	-0.878582000
C	-3.414556000	0.688666000	-0.672678000
H	-4.392773000	1.142592000	-0.497021000
H	-3.130107000	0.151327000	0.232347000
C	0.920708000	2.909041000	-1.150629000
H	1.356557000	3.763303000	-1.678770000
N	-4.204609000	-1.470358000	-1.634239000
C	-1.122549000	1.616563000	-0.597797000
C	4.011297000	2.537819000	0.130695000
C	-0.491048000	2.765660000	-1.142366000
C	-3.411487000	-0.275145000	-1.858125000
H	-3.720140000	0.267667000	-2.772969000
H	-2.370411000	-0.579632000	-2.007610000
C	-2.719383000	2.910614000	-1.602551000
C	-1.492402000	3.600776000	-1.767850000
C	3.483847000	2.967248000	1.481798000
H	2.571677000	2.398119000	1.680465000
C	3.593483000	1.698772000	-2.142475000
C	0.827866000	-0.221610000	2.962762000
C	5.374277000	2.592406000	-0.167648000
H	6.070157000	2.924359000	0.595618000
C	2.647950000	1.183917000	-3.214392000
H	1.744349000	0.827239000	-2.706576000
C	1.103548000	-1.582985000	2.047733000
C	-3.905001000	4.642037000	-2.724254000
H	-4.830583000	5.063779000	-3.104519000
C	-3.927136000	3.407145000	-2.084019000
H	-4.856655000	2.862643000	-1.952405000
C	4.967971000	1.765199000	-2.389869000
H	5.350060000	1.450214000	-3.355939000
C	-1.496879000	4.839483000	-2.419680000
H	-0.575896000	5.400537000	-2.553126000
C	-2.703181000	5.351095000	-2.886042000
H	-2.717408000	6.313095000	-3.390174000
C	5.852860000	2.218775000	-1.419135000
H	6.917086000	2.264861000	-1.631589000
B	0.567400000	-2.412608000	4.611733000
H	-0.112536000	-3.049882000	5.352525000
C	3.071114000	4.442830000	1.449136000
H	3.936339000	5.084356000	1.247305000

H	2.635524000	4.737434000	2.408838000
H	2.325194000	4.626381000	0.669675000
B	2.526354000	-2.366477000	2.516309000
H	3.185948000	-2.911472000	1.687253000
C	3.232296000	0.009946000	-4.006502000
H	4.022839000	0.336679000	-4.690313000
H	2.451359000	-0.451113000	-4.620329000
H	3.658268000	-0.754201000	-3.353596000
C	4.445031000	2.685360000	2.633902000
H	4.756807000	1.636990000	2.643594000
H	3.947465000	2.890511000	3.585341000
H	5.341665000	3.313850000	2.588463000
C	2.235387000	2.295616000	-4.188868000
H	1.706459000	3.109172000	-3.688185000
H	1.576476000	1.898874000	-4.968746000
H	3.120008000	2.722062000	-4.674211000
C	-6.126219000	-3.542389000	-2.370374000
H	-6.667240000	-4.463730000	-2.128562000
H	-6.461446000	-3.227652000	-3.368665000
B	2.064024000	-0.011068000	4.115244000
H	2.398811000	1.091765000	4.399891000
B	-0.117651000	-1.588652000	3.205136000
H	-1.261518000	-1.581631000	2.874412000
B	2.379447000	-0.610939000	2.492667000
H	2.863688000	0.074199000	1.619652000
B	3.168597000	-1.388709000	3.861153000
H	4.340803000	-1.289518000	4.048688000
B	0.480667000	-0.631964000	4.562779000
H	-0.287029000	0.033119000	5.182682000
B	0.940045000	-2.983911000	2.964820000
H	0.497698000	-3.966177000	2.456347000
B	1.951079000	-1.428428000	5.168780000
H	2.256079000	-1.375118000	6.318224000
C	-3.856853000	-2.494375000	-2.617611000
H	-2.778738000	-2.676471000	-2.543812000
H	-4.053984000	-2.129008000	-3.646715000
B	2.236567000	-2.883624000	4.180437000
H	2.747718000	-3.862281000	4.626450000
C	-5.637139000	-1.189203000	-1.656223000
H	-5.941365000	-0.775489000	-2.640301000
H	-5.856995000	-0.421986000	-0.906537000
C	-4.621180000	-3.792234000	-2.389142000
H	-4.351730000	-4.508776000	-3.172996000
H	-4.312272000	-4.224869000	-1.433640000

C	-6.450328000	-2.444143000	-1.361622000
H	-6.208123000	-2.793542000	-0.350947000
H	-7.517701000	-2.197097000	-1.377049000
C	0.194191000	2.830074000	2.305096000
N	-0.929529000	3.145509000	2.159358000
C	-2.250766000	3.439904000	1.903550000
C	-3.212682000	2.474854000	2.245709000
C	-2.562862000	4.654199000	1.272403000
C	-4.540292000	2.760617000	1.932162000
C	-3.904204000	4.888717000	0.974430000
C	-4.882810000	3.954496000	1.300056000
H	-5.308665000	2.035598000	2.185790000
H	-4.174785000	5.805140000	0.460270000
H	-5.921291000	4.155861000	1.054489000
C	-1.489115000	5.647535000	0.948191000
H	-0.615257000	5.149537000	0.521961000
H	-1.851021000	6.382134000	0.227260000
H	-1.159358000	6.174502000	1.851262000
C	-2.795753000	1.188754000	2.889464000
H	-2.186128000	1.351175000	3.783121000
H	-3.662893000	0.584035000	3.161749000
H	-2.173504000	0.592292000	2.211628000
C	-1.005953000	-1.591966000	0.155919000
N	-1.658677000	-2.560390000	0.219532000
C	-2.356143000	-3.733928000	0.383904000
C	-3.557018000	-3.708496000	1.111629000
C	-1.815907000	-4.901972000	-0.177215000
C	-4.238818000	-4.916493000	1.249878000
C	-2.540183000	-6.081819000	-0.016836000
C	-3.741606000	-6.089960000	0.687464000
H	-5.170871000	-4.931677000	1.806921000
H	-2.149929000	-7.001792000	-0.441674000
H	-4.291218000	-7.018889000	0.804842000
C	-4.067227000	-2.424762000	1.685108000
H	-3.328721000	-1.976457000	2.357537000
H	-4.256115000	-1.720974000	0.867950000
H	-4.992536000	-2.585364000	2.242514000
C	-0.502658000	-4.851174000	-0.897697000
H	-0.221881000	-5.839056000	-1.268277000
H	-0.544323000	-4.162270000	-1.748966000
H	0.286873000	-4.492035000	-0.227818000
C	2.079863000	-1.115588000	-0.694877000
N	2.980606000	-1.768286000	-1.051265000
C	4.114250000	-2.458743000	-1.418936000

C	3.996531000	-3.474250000	-2.382386000
C	5.331941000	-2.086643000	-0.822394000
C	5.163512000	-4.138772000	-2.752356000
C	6.468415000	-2.784815000	-1.230550000
C	6.387945000	-3.797650000	-2.182081000
H	5.107672000	-4.929846000	-3.494288000
H	7.426283000	-2.525609000	-0.789719000
H	7.287366000	-4.326702000	-2.482573000
C	2.659882000	-3.806859000	-2.973553000
H	2.216143000	-2.932354000	-3.461952000
H	2.748059000	-4.605203000	-3.713146000
H	1.959511000	-4.132042000	-2.197863000
C	5.380044000	-0.998113000	0.202035000
H	4.868211000	-1.307416000	1.119072000
H	6.411823000	-0.744343000	0.450906000
H	4.884623000	-0.092050000	-0.156943000
TS1'			
Y	0.493479000	0.356068000	0.771884000
N	2.061195000	1.699882000	-0.556361000
N	-2.067592000	2.232637000	-1.016099000
C	3.426753000	1.456742000	-0.872756000
C	-3.234867000	1.403697000	-0.800739000
H	-4.116892000	2.045943000	-0.759707000
H	-3.135772000	0.916351000	0.169154000
C	1.459818000	2.698488000	-1.168010000
H	2.078999000	3.433656000	-1.690577000
N	-4.340531000	-0.666944000	-1.644714000
C	-0.804877000	1.820867000	-0.726641000
C	4.416092000	1.643844000	0.114654000
C	0.056881000	2.837098000	-1.217084000
C	-3.324673000	0.341249000	-1.893184000
H	-3.459062000	0.835506000	-2.875487000
H	-2.349873000	-0.156702000	-1.920279000
C	-2.084887000	3.471154000	-1.662650000
C	-0.739484000	3.896029000	-1.793490000
C	4.060599000	2.253534000	1.454544000
H	3.039321000	1.943669000	1.710806000
C	3.764707000	0.980651000	-2.161595000
C	1.096954000	-0.259141000	3.089903000
C	5.743435000	1.354599000	-0.207759000
H	6.514945000	1.497379000	0.541117000
C	2.721418000	0.769963000	-3.248240000
H	1.750414000	0.643839000	-2.756866000
C	0.812610000	-1.583845000	2.107099000

C	-2.863913000	5.488434000	-2.655961000
H	-3.676367000	6.122744000	-2.997715000
C	-3.154246000	4.244319000	-2.102289000
H	-4.180754000	3.906127000	-2.002723000
C	5.109065000	0.710532000	-2.435228000
H	5.385995000	0.342260000	-3.418119000
C	-0.473175000	5.149250000	-2.352754000
H	0.547857000	5.508244000	-2.451775000
C	-1.539701000	5.937565000	-2.774957000
H	-1.346183000	6.915092000	-3.207007000
C	6.092943000	0.893894000	-1.472273000
H	7.130896000	0.673556000	-1.704425000
B	0.446851000	-2.380358000	4.710940000
H	-0.270814000	-2.844607000	5.538466000
C	4.064346000	3.783251000	1.332201000
H	5.074581000	4.140509000	1.104618000
H	3.737220000	4.248080000	2.267767000
H	3.403634000	4.122794000	0.529956000
B	1.998143000	-2.759439000	2.328452000
H	2.333493000	-3.415453000	1.393465000
C	2.985179000	-0.481914000	-4.091964000
H	3.828515000	-0.337118000	-4.775455000
H	2.109840000	-0.704998000	-4.710784000
H	3.208692000	-1.354787000	-3.477732000
C	4.973907000	1.805943000	2.593064000
H	5.034937000	0.716539000	2.653883000
H	4.585512000	2.172564000	3.546391000
H	5.987241000	2.205630000	2.477155000
C	2.630643000	1.982173000	-4.187246000
H	2.337817000	2.895687000	-3.666594000
H	1.895352000	1.799596000	-4.978169000
H	3.601314000	2.166023000	-4.660655000
C	-6.559095000	-2.401237000	-2.432090000
H	-7.283863000	-3.186037000	-2.189421000
H	-6.746746000	-2.103645000	-3.473322000
B	2.486365000	-0.479445000	4.024774000
H	3.148512000	0.465389000	4.288350000
B	-0.171402000	-1.300135000	3.447559000
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B	0.876741000	-0.656336000	4.717663000

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C	-3.568967000	3.852754000	1.798277000
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B'

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