

Supporting Information

Rare-earth metal ethylene and ethyne complexes

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General procedure

All manipulations were performed with rigorous exclusion of air and water, using Schlenk techniques or an MBRAUN glovebox (Unilab Mbraun; <1 ppm O₂, <1 ppm H₂O). Toluene, THF, and hexane were purified using Grubbs-type columns (MBraun SPS-800, solvent purification system), then further dried over fresh Na chips and stored in a glovebox. The AlEt₃ (1 mol L⁻¹ in hexane) was purchased from J&K Co., Ltd and used without purification. Benzene-d₆ was obtained from J&K Co., Ltd and dried by using sodium chips. The combustion method was used for the carbon, hydrogen, and nitrogen analyses on an Elementar Vario EL III analyzer at Fudan University (China).

Experimental section

Syntheses of complexes 1-5.

[[PhCH₂]₂NC(NC₆H₃^{*i*}Pr₂-2,6)₂]Y(μ₂-η¹:η²-Et)(Et)₂ (1-Y). A toluene solution (2 mL) of AlEt₃ (1.0 mL, 1 M in hexane, 1 mmol) was added slowly to a stirred solution of [(PhCH₂)₂NC(NC₆H₃^{*i*}Pr₂-2,6)₂]Y(o-CH₂C₆H₄NMe₂)₂ (0.46 g, 0.50 mmol) in toluene (10 mL) at ambient temperature. The reaction mixture was allowed to stir for 3 h, and a large amount of white powder precipitated. Then, the white residue was collected by filtration. The white powder was washed twice with toluene/hexane, and dried. Crystallization in toluene yields **1-Y** (0.25 g, 71%) as colorless crystals. ¹H NMR (400 MHz, C₆D₆, 25 °C): δ (ppm) = 0.59 (q, ³J_{H-H} = 8 Hz, 8H, CH₂CH₃), 1.16 (d, ³J_{H-H} = 8 Hz, 24H, CHMe₂), 1.44 (d, ³J_{H-H} = 8 Hz, 24H, CHMe₂), 1.51 (t, ³J_{H-H} = 8 Hz, 12H, CH₂CH₃), 3.92 (m, 8H, CHMe₂), 4.07 (s, 8H, CH₂Ph), 6.85-7.00 (m, 24H, Ar), 7.06-7.08 (m, 8H, Ar). ¹³C{¹H} NMR (100 MHz, C₆D₆, 25 °C): δ (ppm) = 13.1 (s, CH₂CH₃), 24.5 (s, CHMe₂), 26.5 (s, CHMe₂), 28.2 (s, CHMe₂), 40.9 (s, CH₂CH₃), 51.4 (s, CH₂Ph), 124.3 (s, Ar), 124.4 (s, Ar), 127.4 (s, Ar), 128.4 (s, Ar), 129.1 (s, Ar), 136.6 (s, Ar), 142.4 (s, Ar), 144.3 (s, Ar), 164.9 (s, NCN). Anal. Calcd for C₈₆H₁₁₆N₆Y₂ (%): C, 73.17; H, 8.28; N, 5.95; Found: C, 73.02; H, 8.20; N, 6.05.

[[PhCH₂]₂NC(NC₆H₃^{*i*}Pr₂-2,6)₂]Lu(μ₂-η¹:η²-Et)(Et)₂ (1-Lu). A toluene solution (2 mL) of AlEt₃ (1.0 mL, 1 M in hexane, 1 mmol) was added slowly to a stirred solution of [(PhCH₂)₂NC(NC₆H₃^{*i*}Pr₂-2,6)₂]Lu(o-CH₂C₆H₄NMe₂)₂ (0.50 g, 0.5 mmol) in toluene (10 mL) at ambient temperature. The reaction mixture was allowed to stir for 3 h, and a large amount of white powder precipitated. Then, the white residue was collected by filtration. The white powder was washed twice with toluene/hexane, and dried. Crystallization in toluene to yields **1-Lu** (0.31 g, 78%) as colorless crystals. ¹H NMR (400 MHz, C₆D₆, 25 °C): δ (ppm) = 0.86 (br, 8H, CH₂CH₃), 1.16 (d, ³J_{H-H} = 4 Hz, 24H, CHMe₂), 1.46 (d, ³J_{H-H} = 4 Hz, 24H, CHMe₂), 1.51 (br, 12H, CH₂CH₃), 3.95 (m, 8H, CHMe₂), 4.07 (s, 8H, CH₂Ph), 6.85-6.87 (m, 7H, Ar), 6.93-6.98 (m, 16H, Ar), 7.06-7.08 (m, 9H, Ar). ¹³C{¹H} NMR (100 MHz, C₆D₆, 25 °C): δ (ppm) = 13.4 (s, CH₂CH₃), 24.7 (s, CHMe₂), 26.8 (s, CHMe₂), 28.2 (s, CHMe₂), 51.5 (s, CH₂CH₃), 51.6 (s, CH₂Ph), 124.5 (s, Ar), 124.6 (s, Ar), 127.5 (s, Ar), 128.5 (s, Ar), 129.3 (s, Ar), 136.6 (s, Ar), 142.7 (s, Ar), 144.0 (s, Ar), 164.9 (s, NCN). Anal. Calcd for C₈₆H₁₁₆N₆Lu₂ (%): C, 65.22; H, 7.38; N, 5.31; Found: C, 65.10; H, 7.26; N, 5.06.

[(PhCH₂)₂NC(NC₆H₃^{*i*}Pr₂-2,6)₂]Y(Et)(μ₂-η¹:η²-Et)(μ₂-η¹-Et)(AlEt₂) (2-Y). A toluene solution (2 mL) of AlEt₃ (1.5 mL, 1 M in hexane, 1.5 mmol) was added slowly to a stirred solution of [(PhCH₂)₂NC(NC₆H₃^{*i*}Pr₂-2,6)₂]Y(o-CH₂C₆H₄NMe₂)₂ (0.46 g, 0.5 mmol) in toluene (10 mL) at ambient temperature. The reaction mixture was allowed to stir at ambient temperature for 3 h. The toluene was removed under vacuum, and the oily yellow residue turned to white powder after washing twice with hexane (2 mL), which was collected by filtration and dried. Crystallization in toluene and stored at -35 °C to yield **2-Y** (0.34 g, 83%) as colorless crystals. ¹H NMR (400 MHz, C₆D₆, 25 °C): δ (ppm) = 0.33 (q, 8H, ³J_{H-H} = 8 Hz, [AlCH₂CH₃]⁻), 0.85 (q, ³J_{H-H} = 8 Hz, 2H, YCH₂CH₃), 1.13 (d, ³J_{H-H} = 4 Hz, 12H, CHMe₂), 1.30 (t, ³J_{H-H} = 8 Hz, 12H, [AlCH₂CH₃]⁻), 1.35 (d, ³J_{H-H} = 8 Hz, 12H, CHMe₂), 1.78 (t, ³J_{H-H} = 8 Hz, 3H, YCH₂CH₃), 3.82 (br, 4H, CHMe₂), 4.00 (s, 4H, CH₂Ph), 6.82-6.84 (m, 4H, Ar), 6.95-7.03 (m, 8H, Ar), 7.07-7.08 (m, 4H, Ar). ¹³C{¹H} NMR (100 MHz, C₆D₆, 25 °C): δ (ppm)

= 10.5 (s, [AlCH₂CH₃]⁻), 10.8 (s, [AlCH₂CH₃]⁻), 14.1 (s, YCH₂CH₃), 24.4 (s, CHMe₂), 26.6 (s, CHMe₂), 28.5 (s, CHMe₂), 39.1 (d, *J*_{Y-C} = 56 Hz, YCH₂CH₃), 51.4 (s, CH₂Ph), 124.7 (s, Ar), 125.1 (s, Ar), 127.7 (s, Ar), 128.6 (s, Ar), 129.0 (s, Ar), 136.2 (s, Ar), 142.6 (s, Ar), 142.8 (s, Ar), 164.9 (s, NCN). ⁸⁹Y NMR (24.5 MHz, C₆D₆, 25 °C): δ = 850.1 ppm. Anal. Calcd for C₄₉H₇₃N₃AlY (%): C, 71.77; H, 8.97; N, 5.12; Found: C, 71.62; H, 9.10; N, 5.05.

[(PhCH₂)₂NC(NC₆H₃ⁱPr₂-2,6)]Lu(Et)(μ₂-η¹:η²-Et)(μ₂-η¹-Et)(AlEt₂) (2-Lu). A toluene solution (2 mL) of AlEt₃ (1.5 mL, 1 M in hexane, 1.5 mmol) was added slowly to a stirred solution of [(PhCH₂)₂NC(NC₆H₃ⁱPr₂-2,6)]Lu(*o*-CH₂C₆H₄NMe₂)₂ (0.50 g, 0.5 mmol) in toluene (10 mL) at ambient temperature. The reaction mixture was allowed to stir at ambient temperature for 3 h. The toluene was removed under vacuum, and the oily yellow residue turned to white powder after washing twice with hexane (2 mL), which was collected by filtration and dried. Crystallization in toluene and stored at -35 °C to yield **2-Lu** (0.41 g, 90%) as colorless crystals. ¹H NMR (400 MHz, C₆D₆, 25 °C): δ (ppm) = 0.53 (q, ³*J*_{H-H} = 8 Hz, 8H, [AlCH₂CH₃]⁻), 0.86 (q, ³*J*_{H-H} = 8 Hz, 2H, LuCH₂CH₃), 1.12 (br, 12H, CHMe₂), 1.28 (t, ³*J*_{H-H} = 8 Hz, 12H, [AlCH₂CH₃]⁻), 1.37 (br, 12H, CHMe₂), 1.84 (t, ³*J*_{H-H} = 8 Hz, 3H, LuCH₂CH₃), 3.82 (br, 4H, CHMe₂), 3.99 (s, 4H, CH₂Ph), 6.81-6.83 (m, 4H, Ar), 6.94-7.02 (m, 8H, Ar), 7.07-7.09 (m, 4H, Ar). ¹³C{¹H} NMR (100 MHz, C₆D₆, 25 °C): δ (ppm) = 10.9 (s, [AlCH₂CH₃]⁻), 12.8 (s, [AlCH₂CH₃]⁻), 14.4 (s, LuCH₂CH₃), 24.4 (s, CHMe₂), 26.6 (s, CHMe₂), 28.4 (s, CHMe₂), 44.2 (s, LuCH₂CH₃), 51.3 (s, CH₂Ph), 124.7 (s, Ar), 125.3 (s, Ar), 127.7 (s, Ar), 128.7 (s, Ar), 129.0 (s, Ar), 136.1 (s, Ar), 142.7 (s, Ar), 164.6 (s, NCN). Anal. Calcd for C₄₉H₇₃N₃AlLu (%): C, 64.95; H, 8.12; N, 4.64; Found: C, 65.02; H, 8.20; N, 4.60.

[[PhCH₂)₂NC(NC₆H₃ⁱPr₂-2,6)]Y(μ₂-η¹-Et)₂(AlEt)₂(μ₄-η¹:η¹:η²:η²-CHCH) (3-Y).

A toluene solution (2 mL) of AlEt₃ (1.5 mL, 1 M in hexane, 1.5 mmol) was added slowly to a stirred toluene solution (10 mL) of [(PhCH₂)₂NC(NC₆H₃ⁱPr₂-2,6)]Y(*o*-CH₂C₆H₄NMe₂)₂ (0.46 g, 0.5 mmol) at ambient temperature. The solution changed red from colorless when the reaction mixture was allowed to stir at ambient temperature for three days. The toluene was removed under vacuum, and the pale red residue turned to orange powder after washing twice with hexane (2 mL), which was collected by filtration and dried. Crystallization in toluene/hexane and stored at -35 °C to yield **3-Y** (0.15 g, 38%) as red crystals. ¹H NMR (400 MHz, C₆D₆, 25 °C): δ (ppm) = 0.33 (br, 12H, [AlCH₂CH₃]⁻), 1.19 (d, ³*J*_{H-H} = 8 Hz, 24H, CHMe₂), 1.34 (d, ³*J*_{H-H} = 8 Hz, 24H, CHMe₂), 1.40 (t, ³*J*_{H-H} = 8 Hz, 18H, [AlCH₂CH₃]⁻), 2.66 (s, 2H, μ₄-CH-CH), 3.80 (m, 8H, CHMe₂), 4.08 (s, 8H, CH₂Ph), 6.74-6.79 (m, 8H, Ar), 6.91-6.93 (m, 12H, Ar), 7.00-7.04 (m, 4H, Ar), 7.09-7.11 (m, 8H, Ar). ¹³C{¹H} NMR (100 MHz, C₆D₆, 25 °C): δ (ppm) = 11.4 (s, [AlCH₂CH₃]⁻), 11.7 (s, [AlCH₂CH₃]⁻), 24.2 (s, CHMe₂), 26.9 (s, CHMe₂), 28.5 (s, CHMe₂), 51.9 (s, CH₂Ph), 89.8 (s, μ₄-CH-CH), 124.1 (s, Ar), 124.2 (s, Ar), 124.3 (s, Ar), 127.4 (s, Ar), 127.8 (s, Ar), 128.0 (s, Ar), 128.3 (s, Ar), 129.4 (s, Ar), 129.5 (s, Ar), 136.7 (s, Ar), 142.3 (s, Ar), 144.0 (s, Ar), 165.6 (s, NCN). Anal. Calcd for C₉₂H₁₂₈N₆Al₂Y₂ (%): C, 71.30; H, 8.32; N, 5.42; Found: C, 71.64; H, 8.47; N, 5.54.

[(PhCH₂)₂NC(NC₆H₃ⁱPr₂-2,6)]Y(μ₃-η¹:η¹:η²-CH₂CH₂)[(μ₂-η¹-Et)(AlEt₂)(μ₂-η¹-Et)₂(AlEt)] (4-Y). A frozen toluene solution (2 mL) of AlEt₃ (2.0 mL, 1 M in hexane, 2 mmol) was added slowly to a stirred frozen toluene solution (10 mL) of [(PhCH₂)₂NC(NC₆H₃ⁱPr₂-2,6)]Y(*o*-CH₂C₆H₄NMe₂)₂ (0.46 g, 0.5 mmol) at ambient temperature. The reaction mixture was allowed to stir at 50 °C for 24 h. The toluene was removed under vacuum, and the oily yellow residue turned to white powder

after washing twice with hexane (2 mL), which was collected by filtration and dried. Crystallization in toluene and stored at -35 °C to yield **4-Y** (0.36 g, 81%) as colorless crystals. ¹H NMR (400 MHz, C₆D₆, 25 °C): δ (ppm) = 0.30 (q, ³J_{H-H} = 8 Hz, 12H, [AlCH₂CH₃]⁻), 0.81 (br, 4H, μ₃-CH₂CH₂), 1.08 (d, ³J_{H-H} = 8 Hz, 12H, CHMe₂), 1.28 (t, ³J_{H-H} = 8 Hz, 30H, CHMe₂ and [AlCH₂CH₃]⁻), 3.68 (br, 4H, CHMe₂), 3.97 (s, 4H, CH₂Ph), 6.82 (br, 4H, Ar), 6.95-7.06 (m, 12H, Ar). ¹³C{¹H} NMR (100 MHz, C₆D₆, 25 °C): δ (ppm) = 7.0 (s, [AlCH₂CH₃]⁻), 11.1 (s, [AlCH₂CH₃]⁻), 13.3 (d, J_{Y-C} = 7 Hz, μ₃-CH₂-CH₂), 25.3 (s, CHMe₂), 26.6 (s, CHMe₂), 28.4 (s, CHMe₂), 51.9 (s, CH₂Ph), 125.1 (s, Ar), 125.3 (s, Ar), 127.9 (s, Ar), 128.1 (s, Ar), 128.4 (s, Ar), 129.0 (s, Ar), 129.8 (s, Ar), 136.1 (s, Ar), 142.7 (s, Ar), 142.8 (s, Ar), 166.4 (s, NCN). ⁸⁹Y NMR (24.5 MHz, C₆D₆, 25 °C): δ = 326.4 ppm. Anal. Calcd for C₅₃H₈₂N₃Al₂Y (%): C, 70.41; H, 9.14; N, 4.65; Found: C, 70.19; H, 9.20; N, 4.47.

[(PhCH₂)₂NC(NC₆H₃ⁱPr₂-2,6)₂]Y[(μ₂-η¹-Et)₂(AlEt₂)₂] (5-Y). A toluene solution (2 mL) of AlEt₃ (2.0 mL, 1 M in hexane, 2.0 mmol) was added slowly to a stirred solution of [(PhCH₂)₂NC(NC₆H₃ⁱPr₂-2,6)₂]Y(o-CH₂C₆H₄NMe₂)₂ (0.46 g, 0.5 mmol) in toluene (10 mL) at -10 °C. The reaction mixture was allowed to stir at -10 °C for 3 h. The toluene was removed under vacuum, and the oily yellow residue turned to white powder after washing twice with hexane (2 mL), which was collected by filtration and dried. Crystallization in toluene and stored at -35 °C to yield **5-Y** (0.43 g, 92%) as colorless crystals. ¹H NMR (400 MHz, C₆D₆, 25 °C): δ (ppm) = 0.53 (q, ³J_{H-H} = 8 Hz, 16H, [AlCH₂CH₃]⁻), 1.06 (d, ³J_{H-H} = 8 Hz, 12H, CHMe₂), 1.37 (t, ³J_{H-H} = 8 Hz, 36H, CHMe₂ and [AlCH₂CH₃]⁻), 3.76 (m, 4H, CHMe₂), 4.00 (s, 4H, CH₂Ph), 6.78 (m, 4H, Ar), 6.80-7.05 (m, 12H, Ar). ¹³C{¹H} NMR (100 MHz, C₆D₆, 25 °C): δ (ppm) = 11.3 (s, [AlCH₂CH₃]⁻), 25.2 (s, CHMe₂), 26.2 (s, CHMe₂), 28.5 (s, CHMe₂), 51.8 (s, CH₂Ph), 125.0 (s, Ar), 125.4 (s, Ar), 127.8 (s, Ar), 128.1 (s, Ar), 128.3 (s, Ar), 128.5 (s, Ar), 129.4 (s, Ar), 135.8 (s, Ar), 142.7 (s, Ar), 142.8 (s, Ar), 165.3 (s, NCN). Anal. Calcd for C₅₅H₈₈N₃YAl₂ (%): C, 70.71; H, 9.50; N, 4.50; Found: C, 71.01; H, 9.26; N, 4.37.

NMR spectra of complexes 1-5.

The solid samples were dissolved in C_6D_6 , and then transferred into a J-Young NMR tube in the glove-box. The 1H , $^{13}C\{^1H\}$, ^{13}C DEPT-135 and HMQC-NMR spectra were recorded on a AVANCE III HD-400 NMR spectrometer (FT, 400 MHz for 1H ; 100 MHz for ^{13}C) in C_6D_6 at room temperature. The 1H VT NMR spectra were recorded on a AVANCE III HD-500 NMR spectrometer (FT, 500 MHz for 1H) in $tol-d_8$. And the ^{89}Y NMR spectra recorded on a in C_6D_6 at room temperature. ^{89}Y NMR spectra were obtained on a AVANCE NEO-500 NMR spectrometer (FT, 24.5 MHz for ^{89}Y) and were externally referenced to YCl_3 in D_2O .

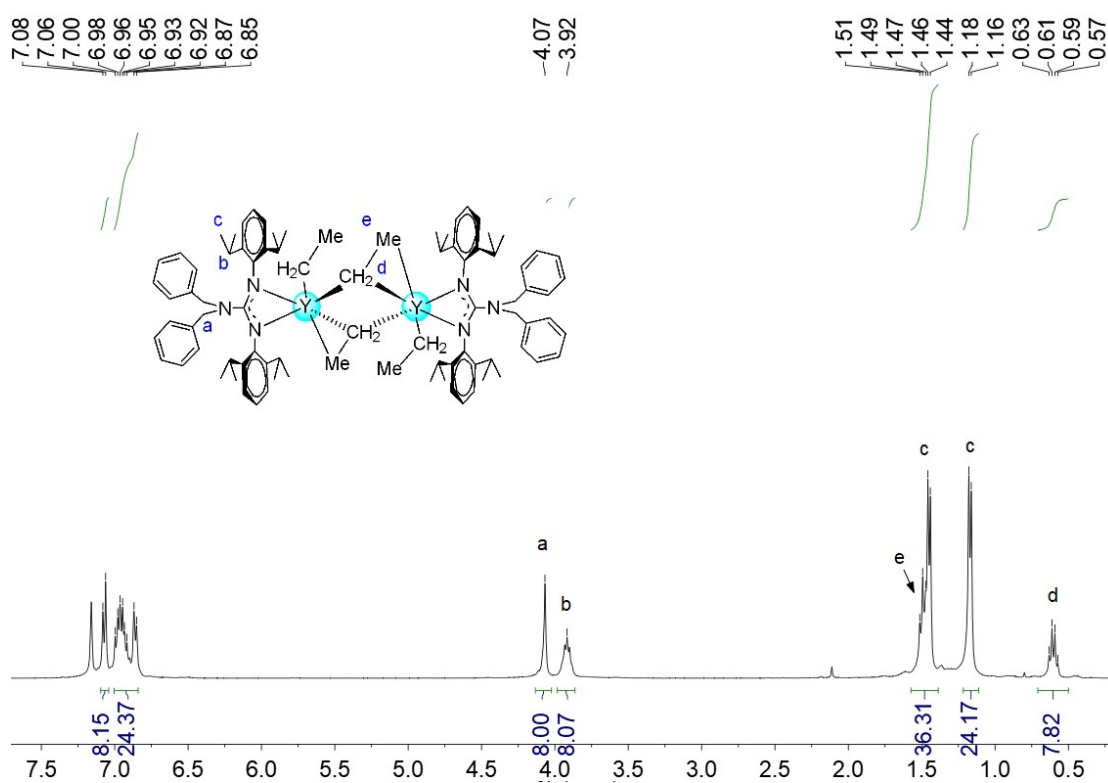


Figure S1. 1H NMR spectrum of 1-Y obtained in C_6D_6 at room temperature.

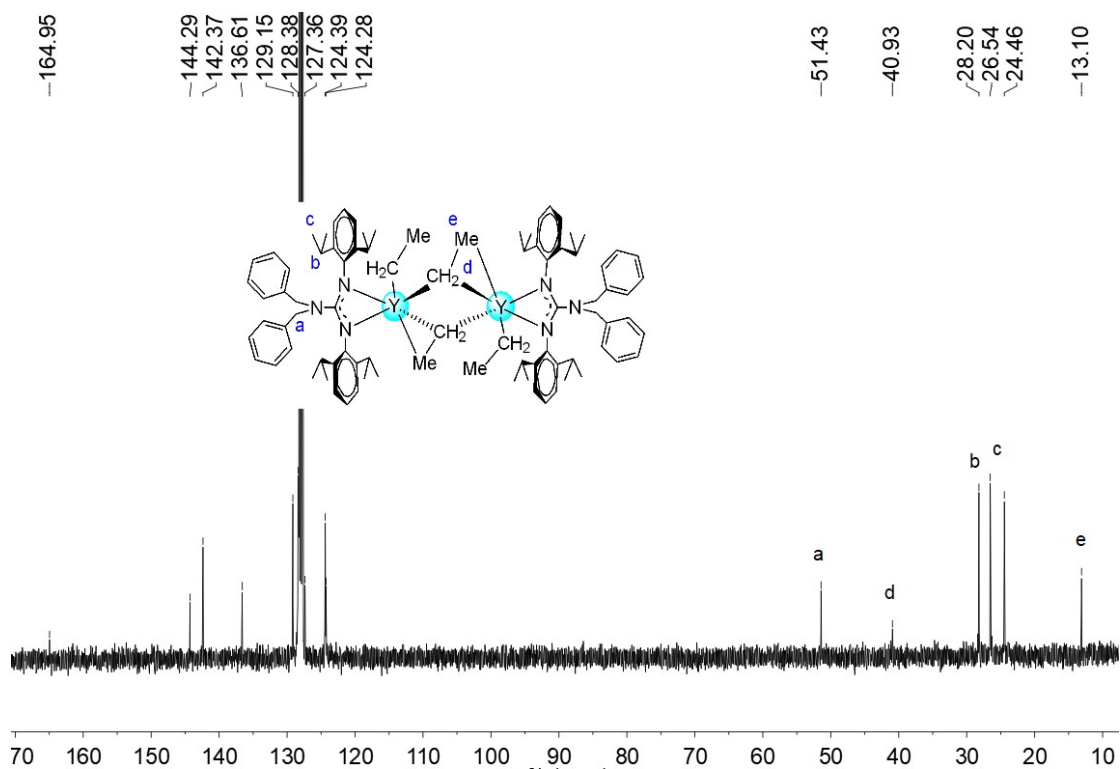


Figure S2. ¹³C{¹H} NMR spectrum of **1-Y** obtained in C₆D₆ at room temperature.

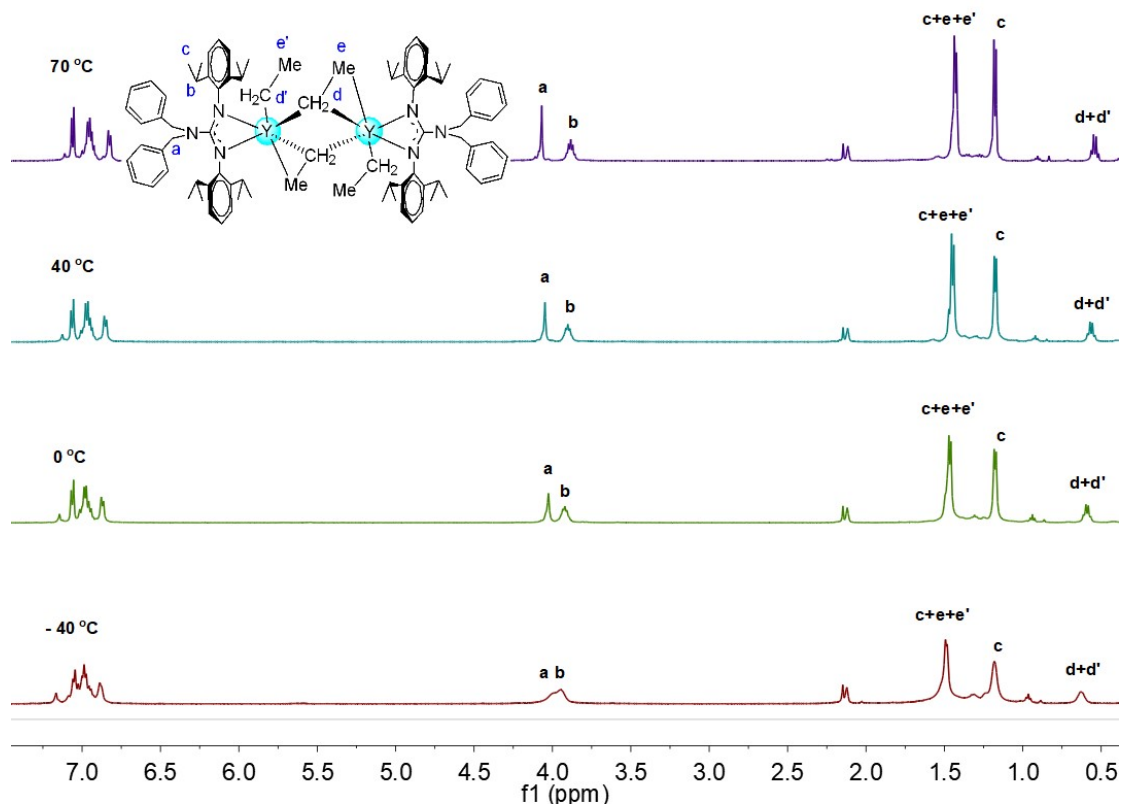


Figure S3. The ¹H VT NMR spectra (500 MHz) of **1-Y** in toluene-d₈.

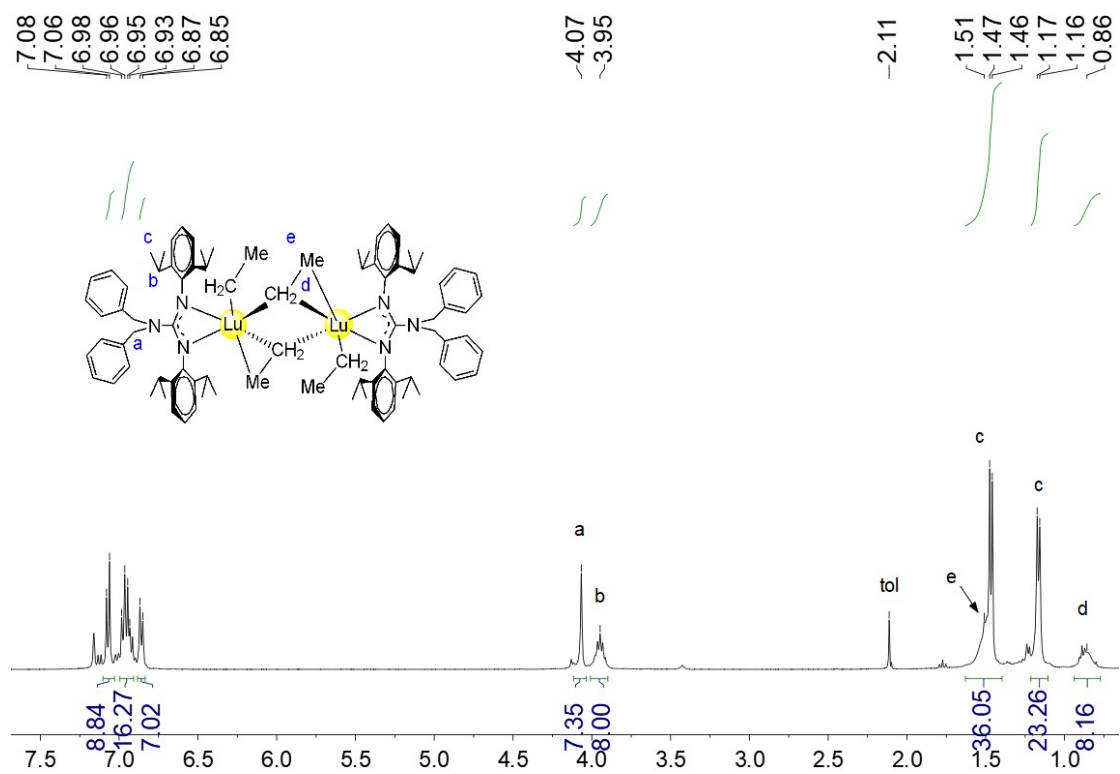


Figure S4. ¹H NMR spectrum of **1-Lu** obtained in C₆D₆ at room temperature.

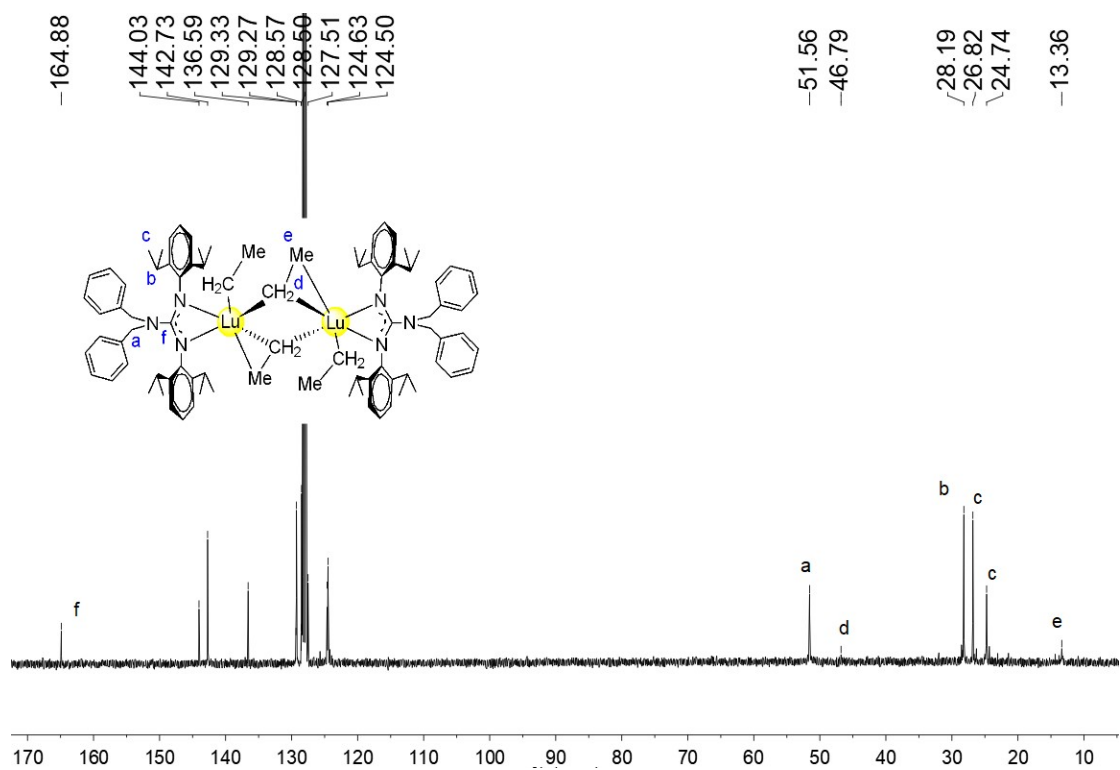


Figure S5. ¹³C{¹H} NMR spectrum of **1-Lu** obtained in C₆D₆ at room temperature.

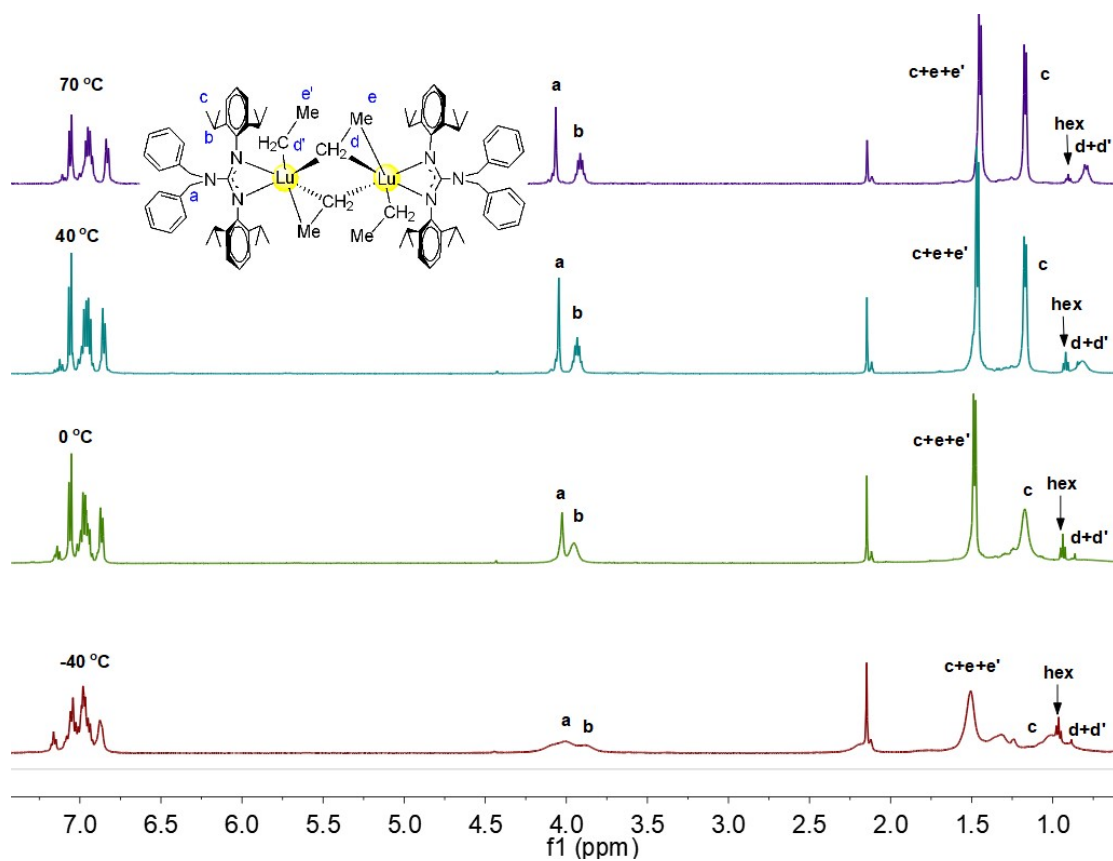


Figure S6. The ^1H VT NMR spectra (500 MHz) of **1-Lu** in toluene-d_8 .

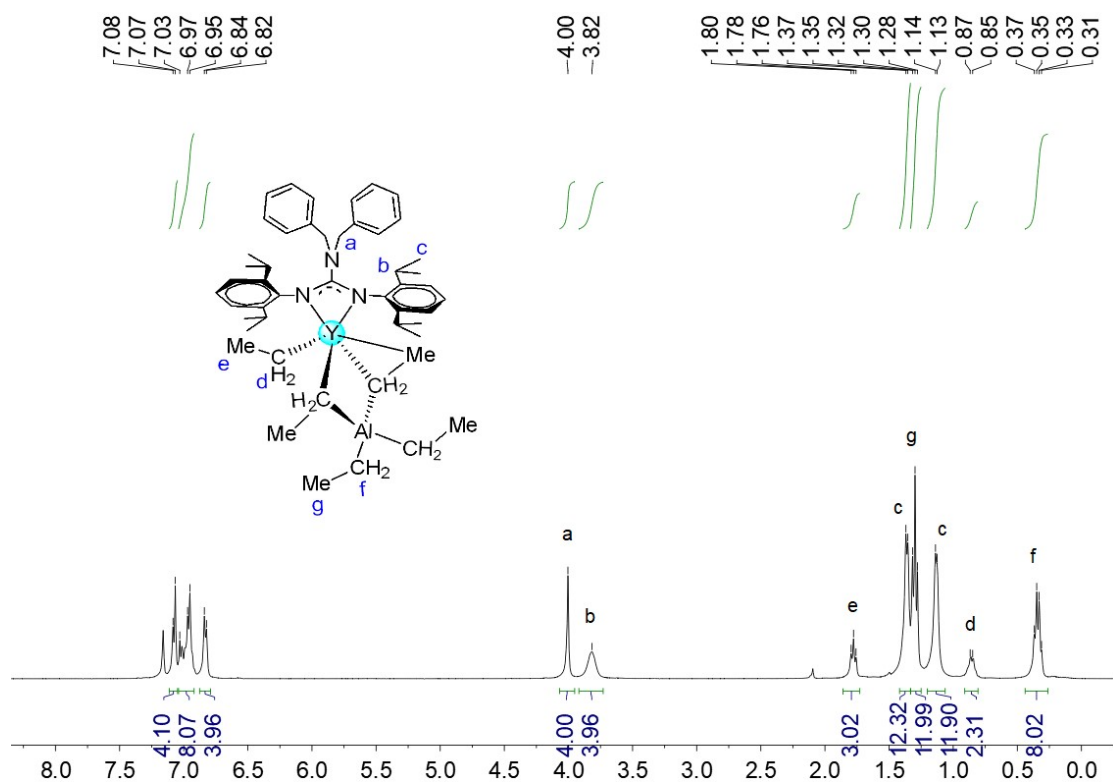


Figure S7. ^1H NMR spectrum of **2-Y** obtained in C_6D_6 at room temperature.

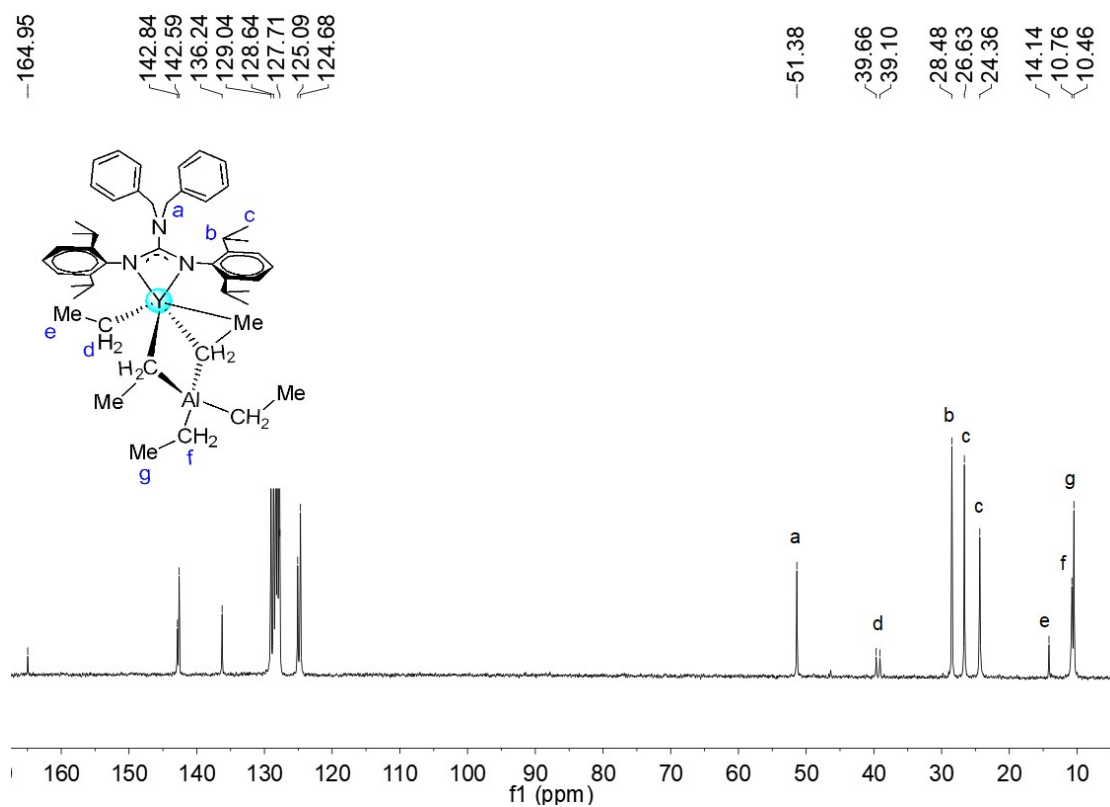


Figure S8. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2-Y** obtained in C_6D_6 at room temperature.

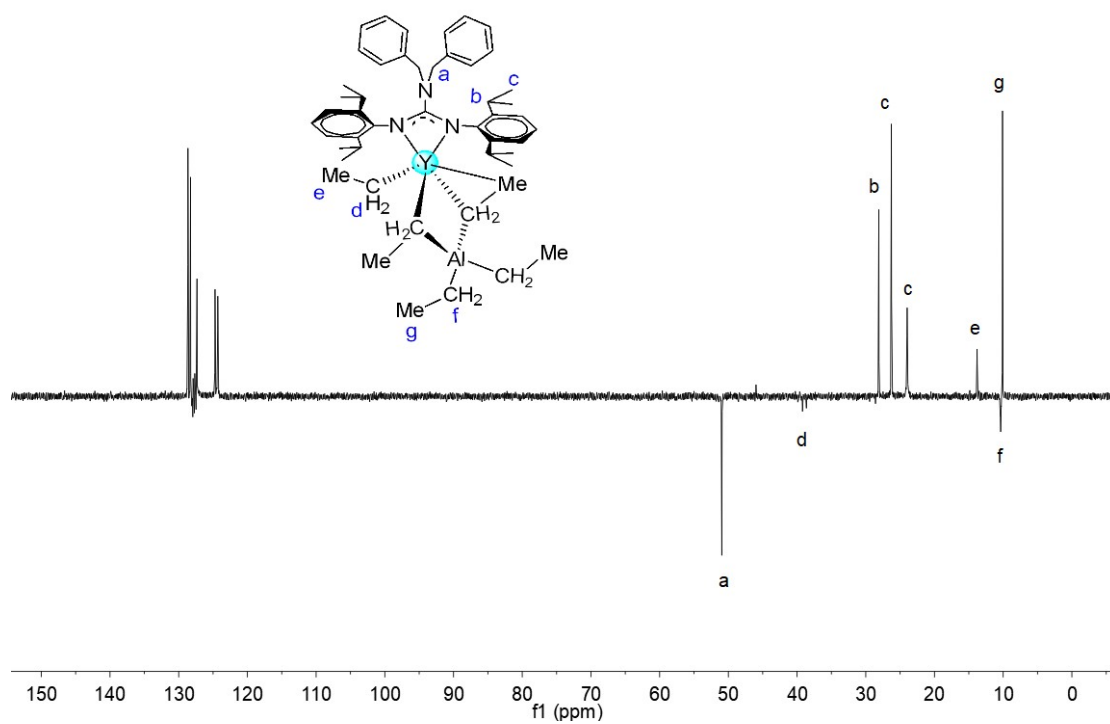


Figure S9. ^{13}C DEPT-135 NMR spectrum of **2-Y** obtained in C_6D_6 at room temperature.

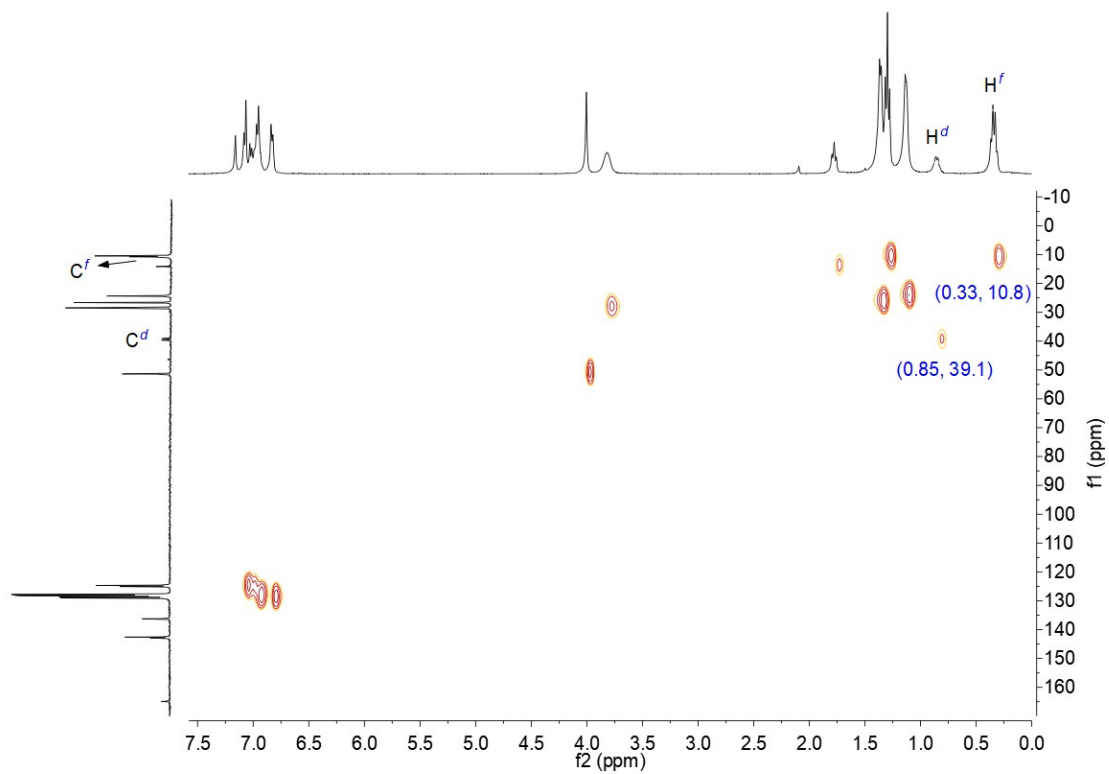


Figure S10. Two-dimensional ^1H - ^{13}C HMQC NMR spectrum of **2-Y** in C_6D_6 at room temperature.

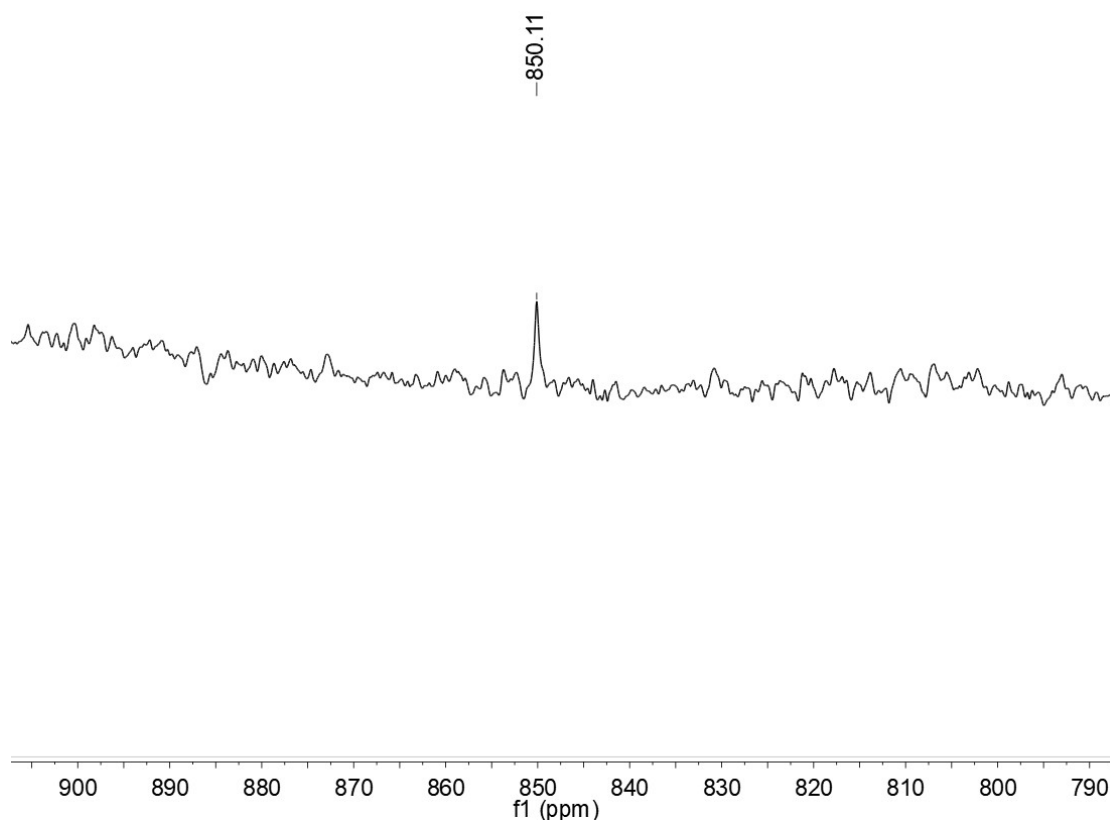


Figure S11. The ^{89}Y NMR spectrum (24.5 MHz) of **2-Y** in C_6D_6 at room temperature.

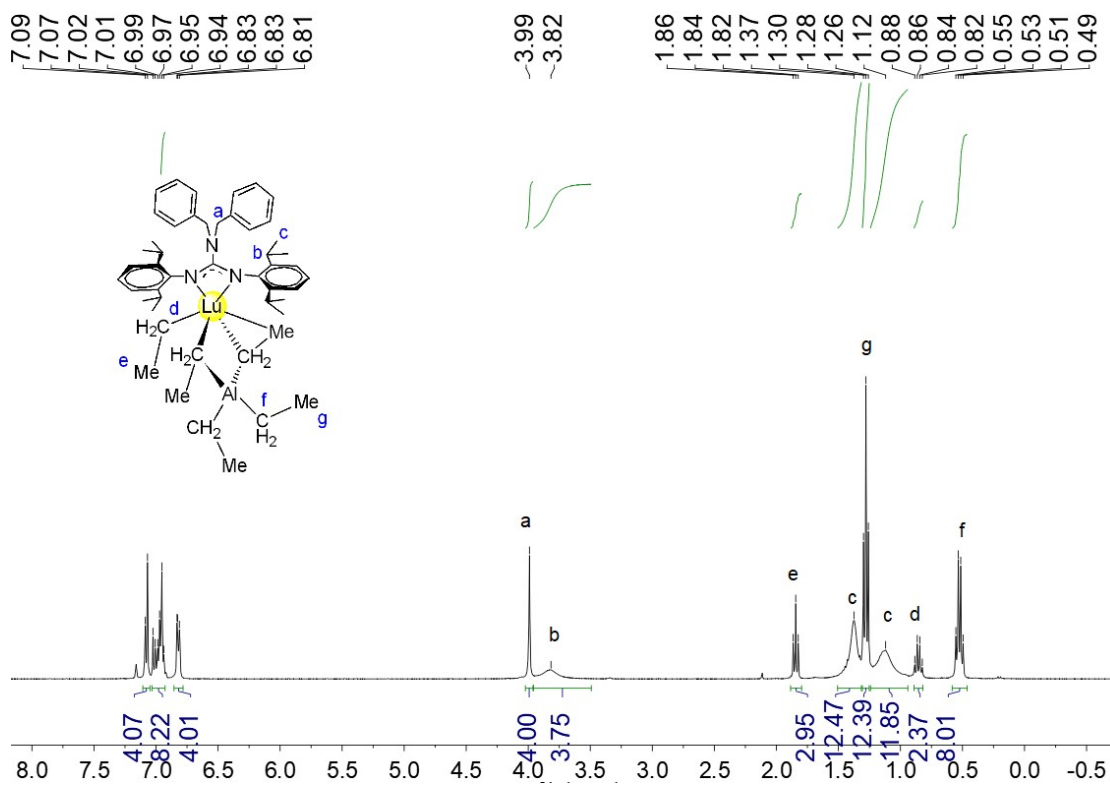


Figure S12. ¹H NMR spectrum of **2-Lu** obtained in C₆D₆ at room temperature.

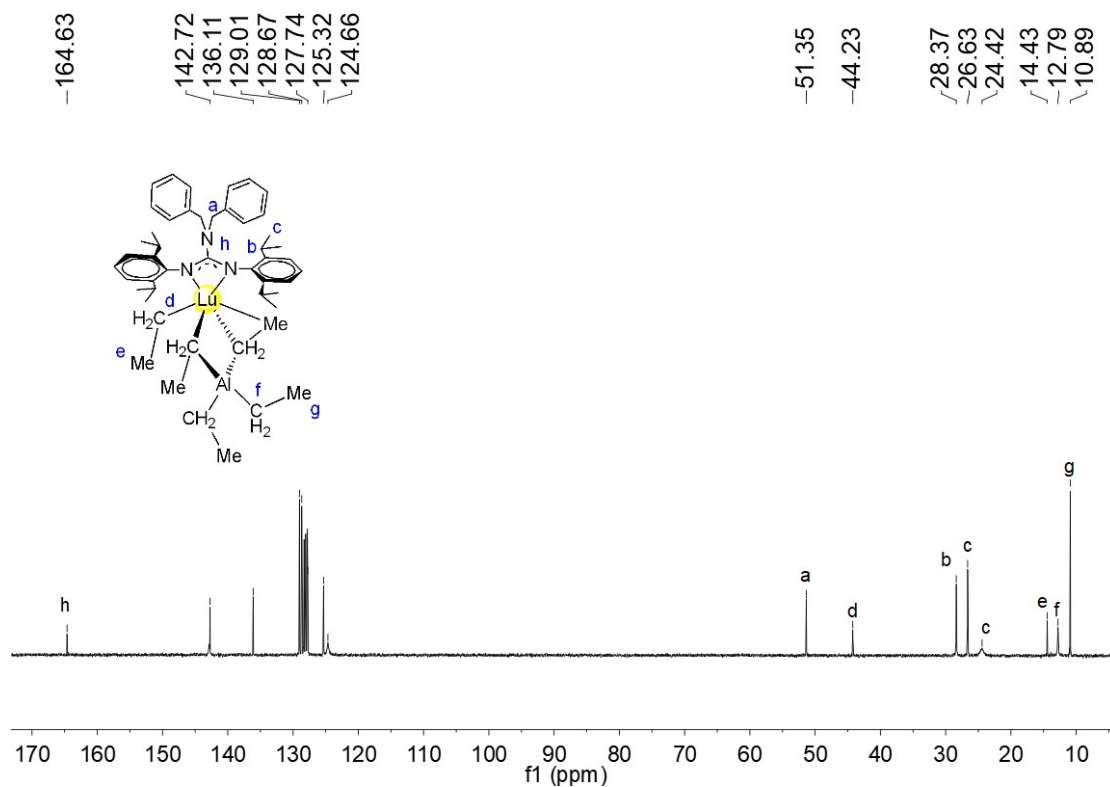


Figure S13. ¹³C{¹H} NMR spectrum of **2-Lu** obtained in C₆D₆ at room temperature.

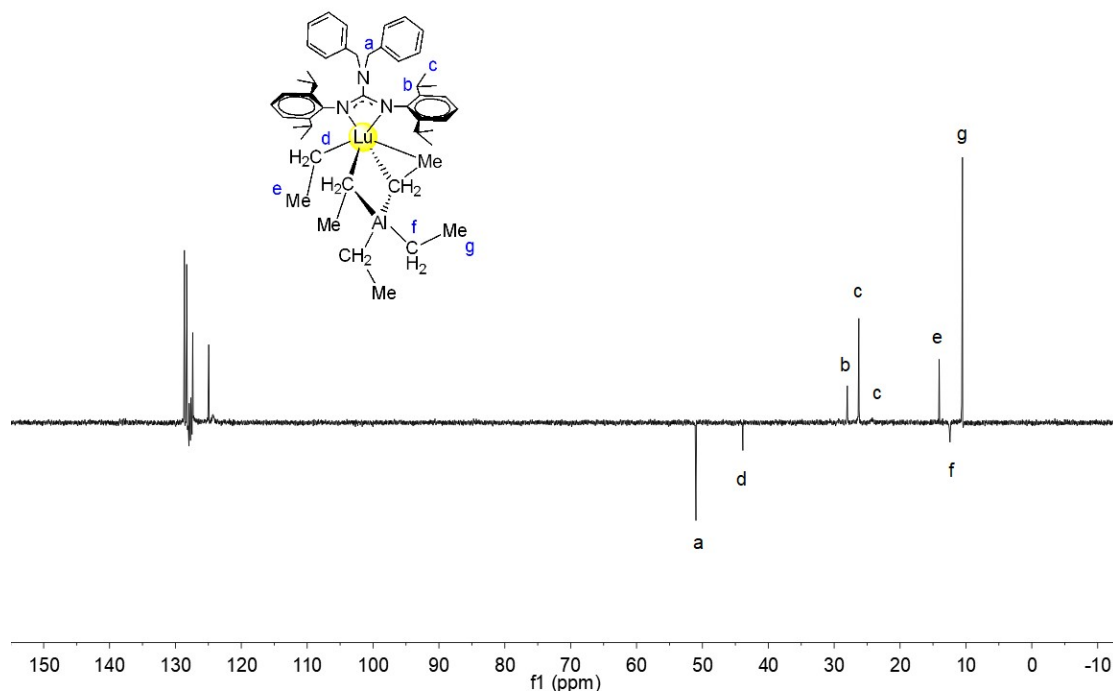


Figure S14. ^{13}C DEPT-135 NMR spectrum of **2-Lu** obtained in C_6D_6 at room temperature.

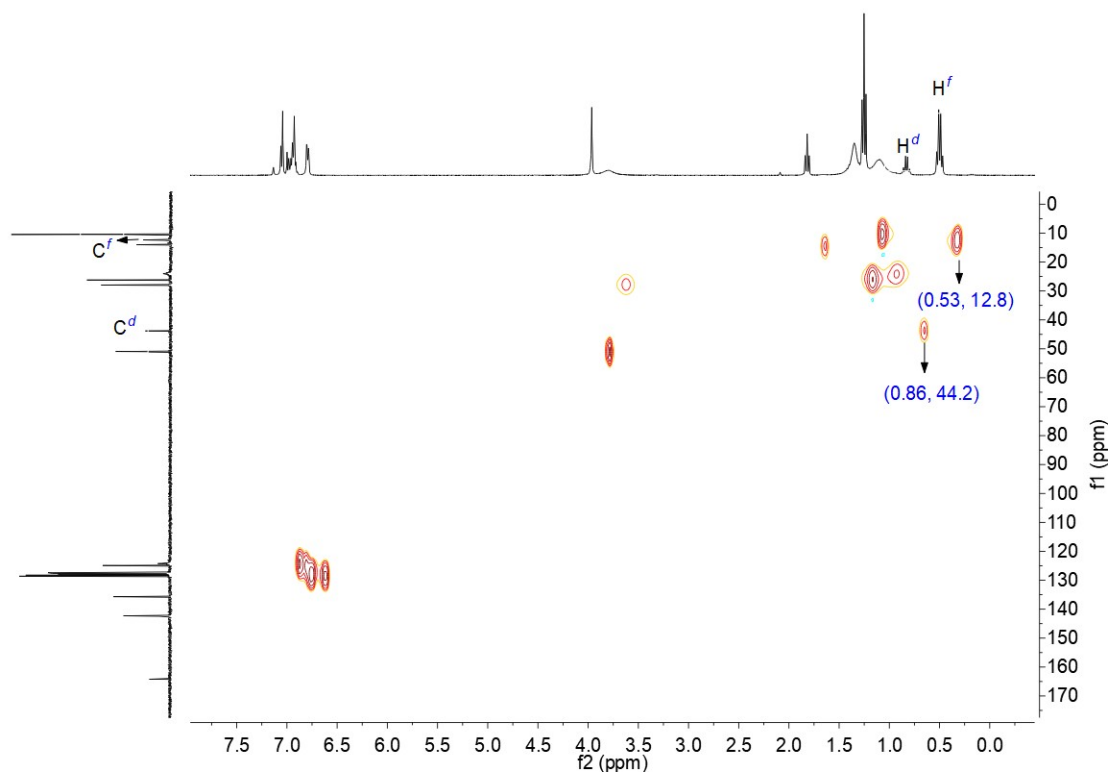


Figure S15. Two-dimensional ^1H - ^{13}C HMQC NMR spectrum of **2-Lu** in C_6D_6 at room temperature.

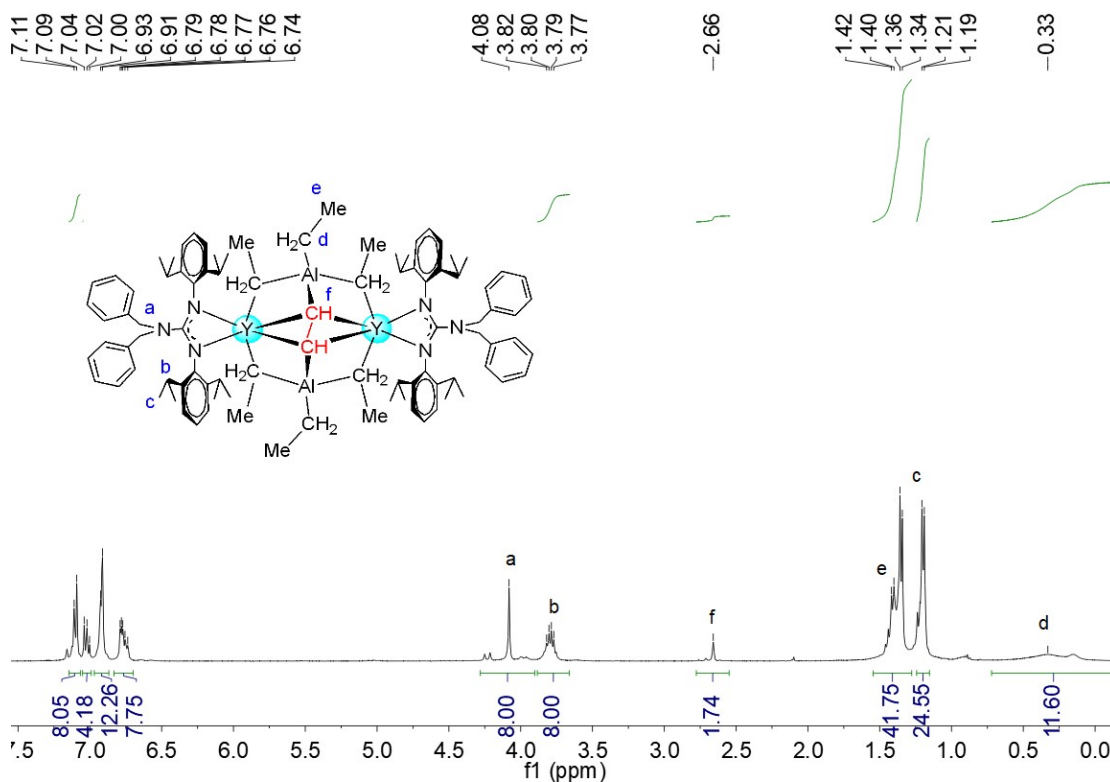


Figure S16. ¹H NMR spectrum of **3-Y** obtained in C₆D₆ at room temperature.

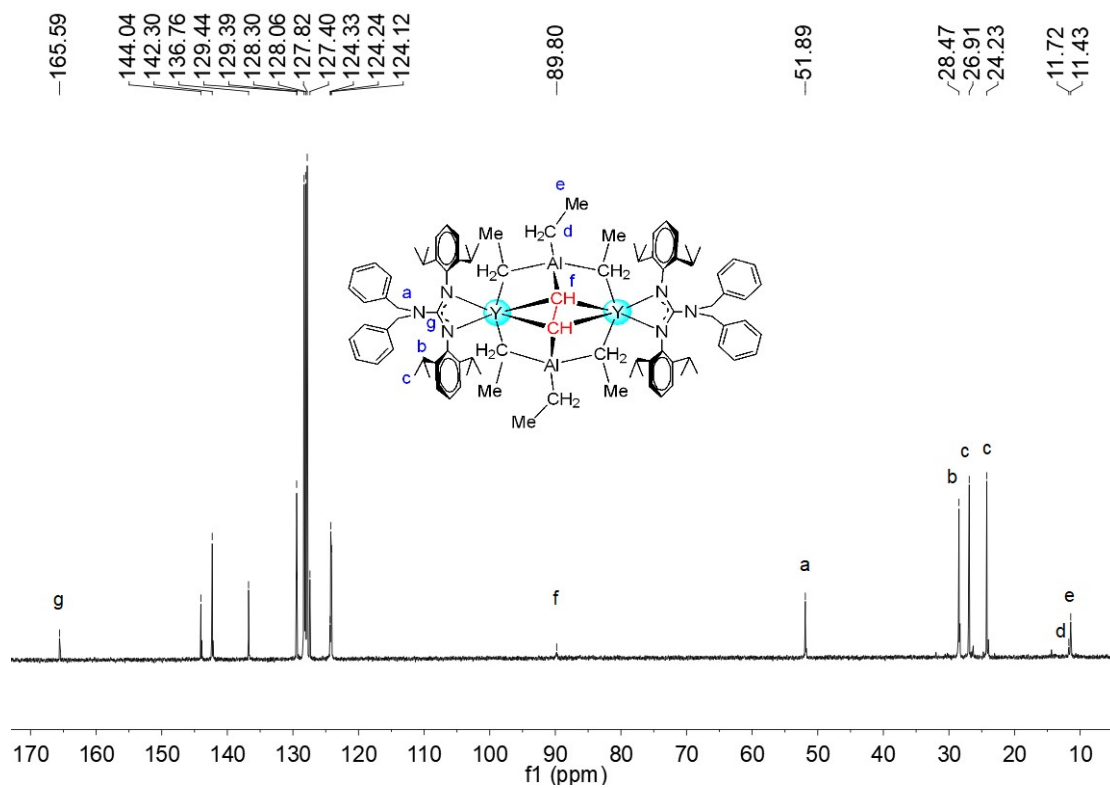


Figure S17. ¹³C{¹H} NMR spectrum of **3-Y** obtained in C₆D₆ at room temperature.

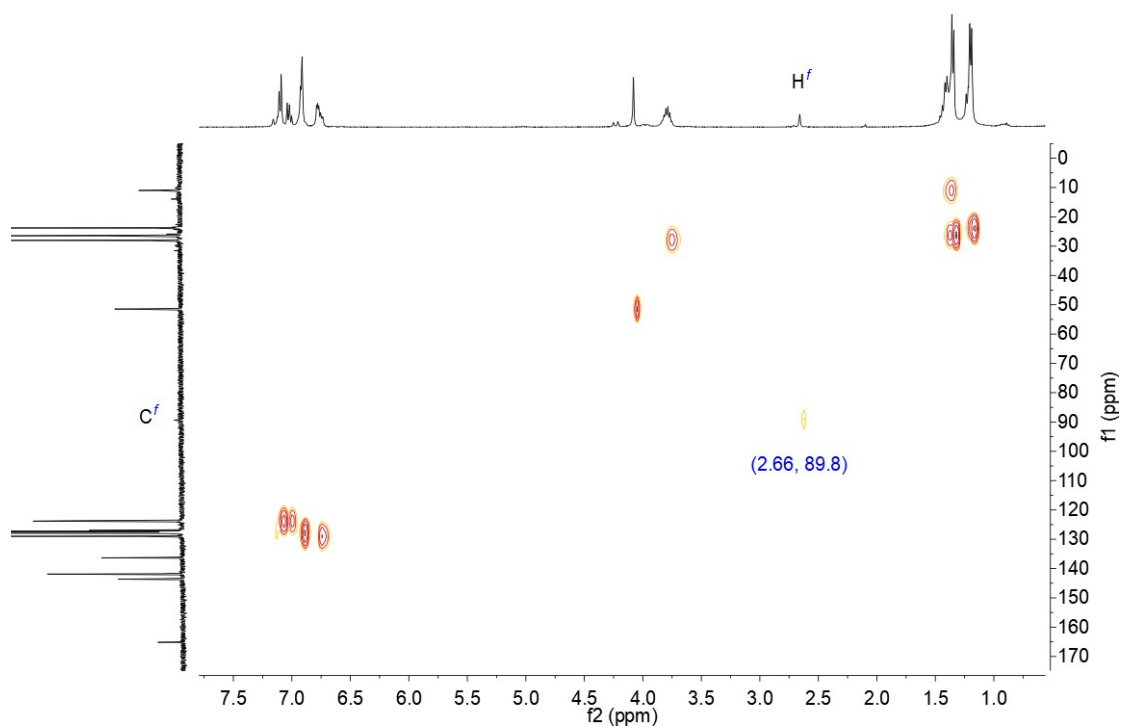


Figure S18. Two-dimensional ^1H - ^{13}C HMQC NMR spectrum of complex **3-Y** in C_6D_6 at room temperature.

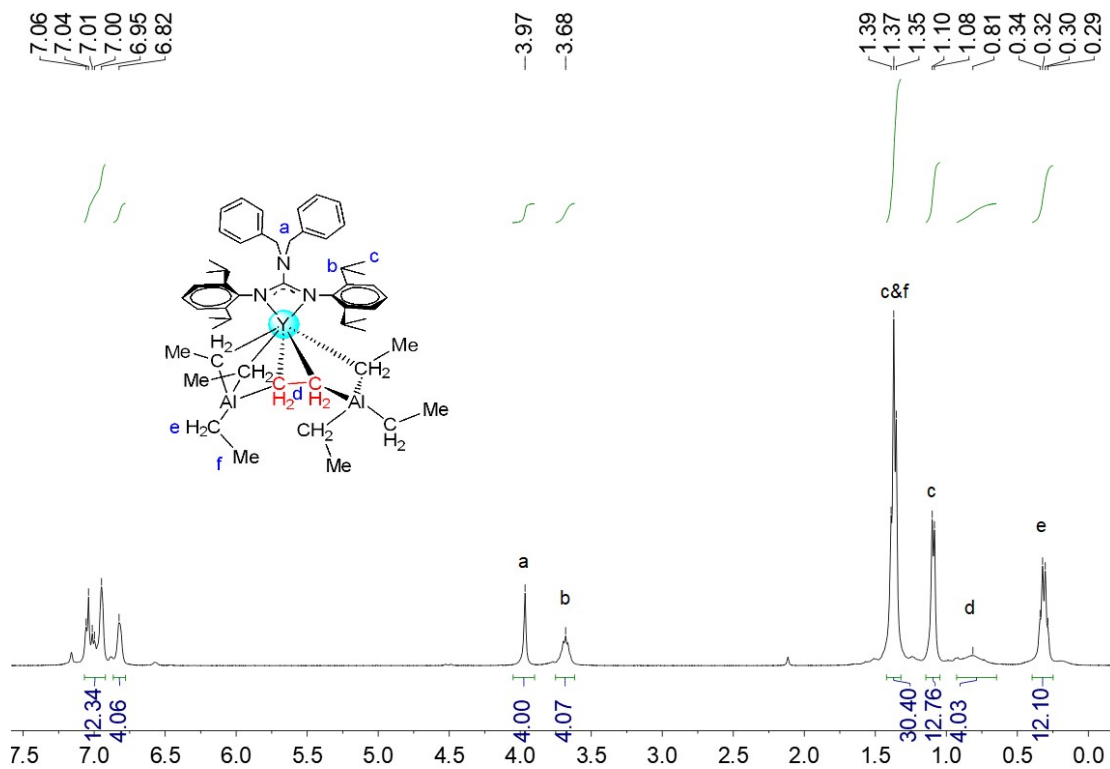


Figure S19. ^1H NMR spectrum of **4-Y** obtained in C_6D_6 at room temperature.

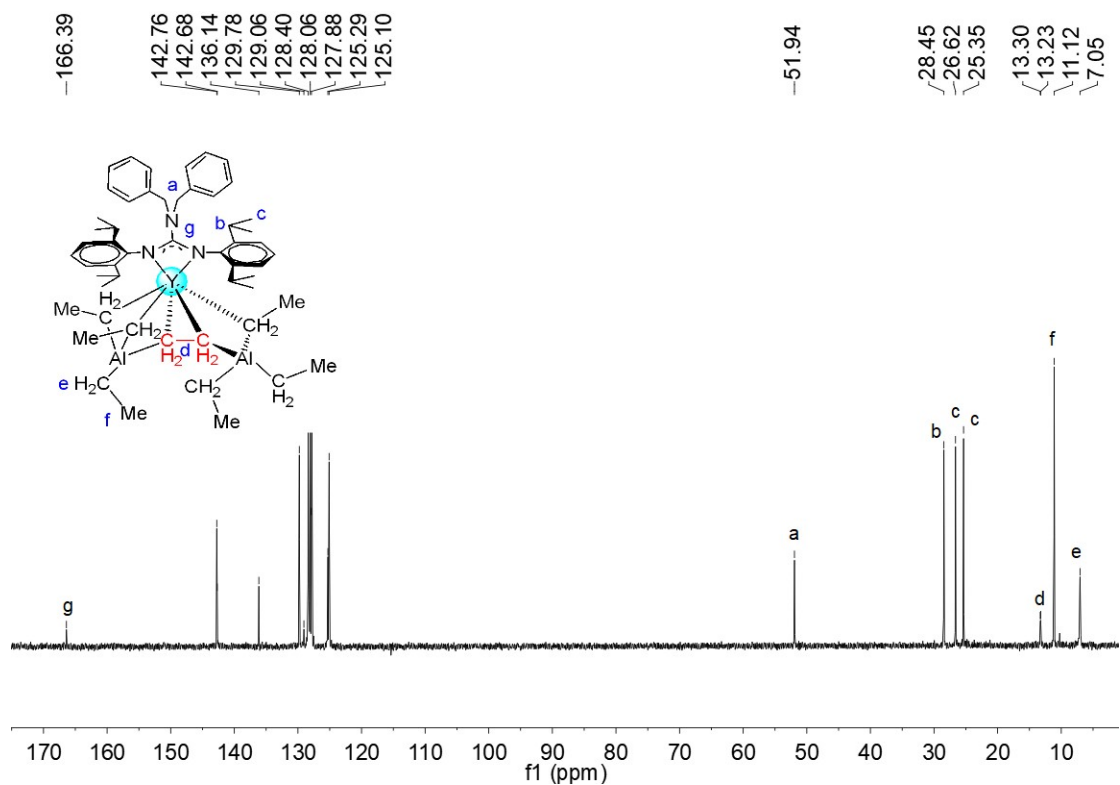


Figure S20. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4-Y** obtained in C_6D_6 at room temperature.

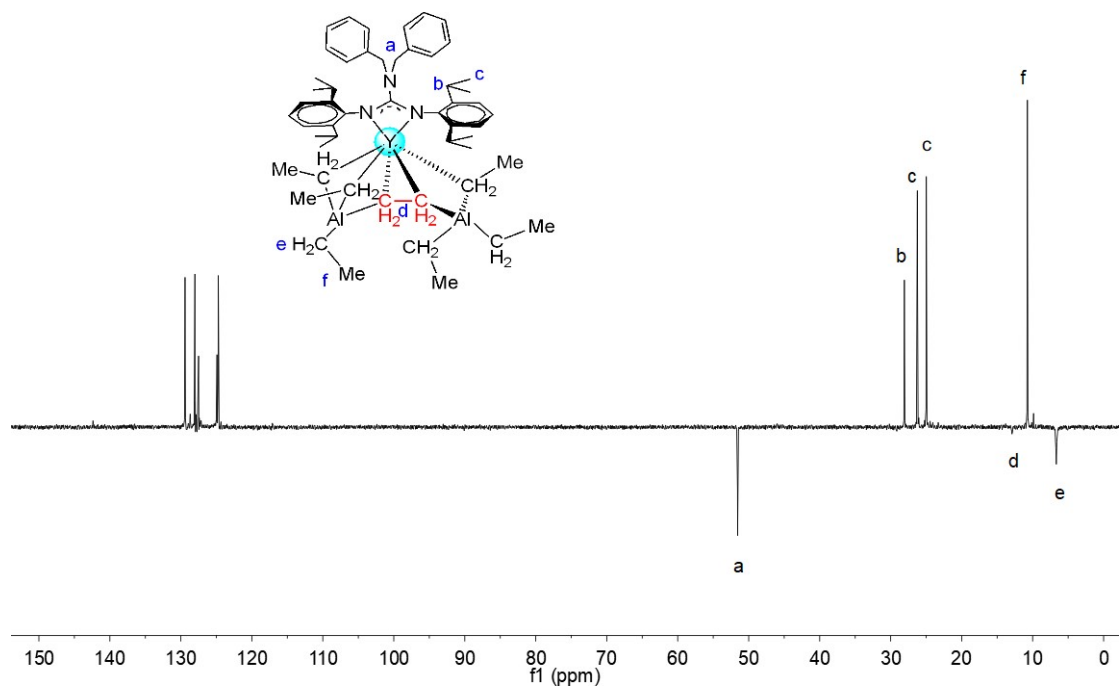


Figure S21. ^{13}C DEPT-135 NMR spectrum of **4-Y** obtained in C_6D_6 at room temperature.

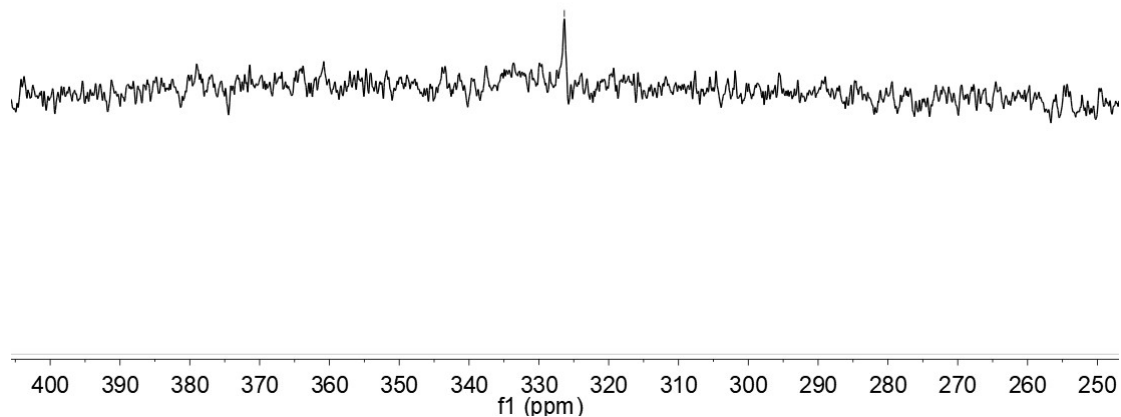


Figure S22. The ^{89}Y NMR spectrum (24.5 MHz) of **4-Y** in C_6D_6 at room temperature.

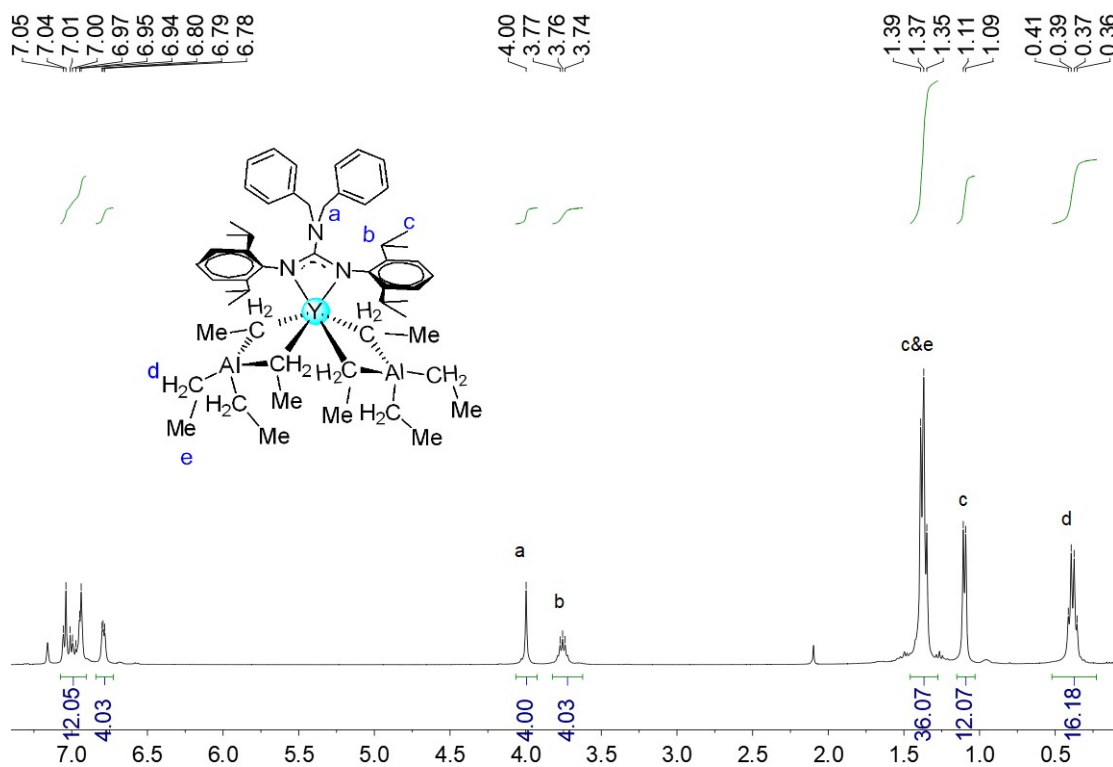


Figure S23. ^1H NMR spectrum of **5-Y** obtained in C_6D_6 at room temperature.

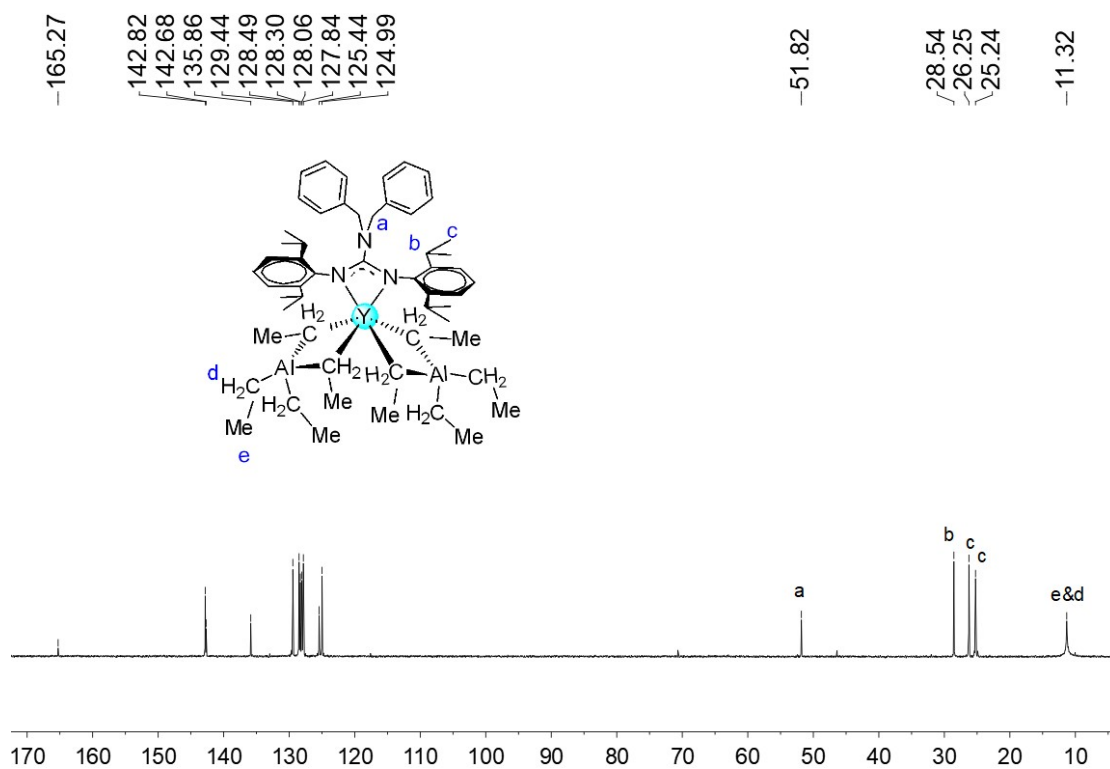


Figure S24. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **5-Y** obtained in C_6D_6 at room temperature.

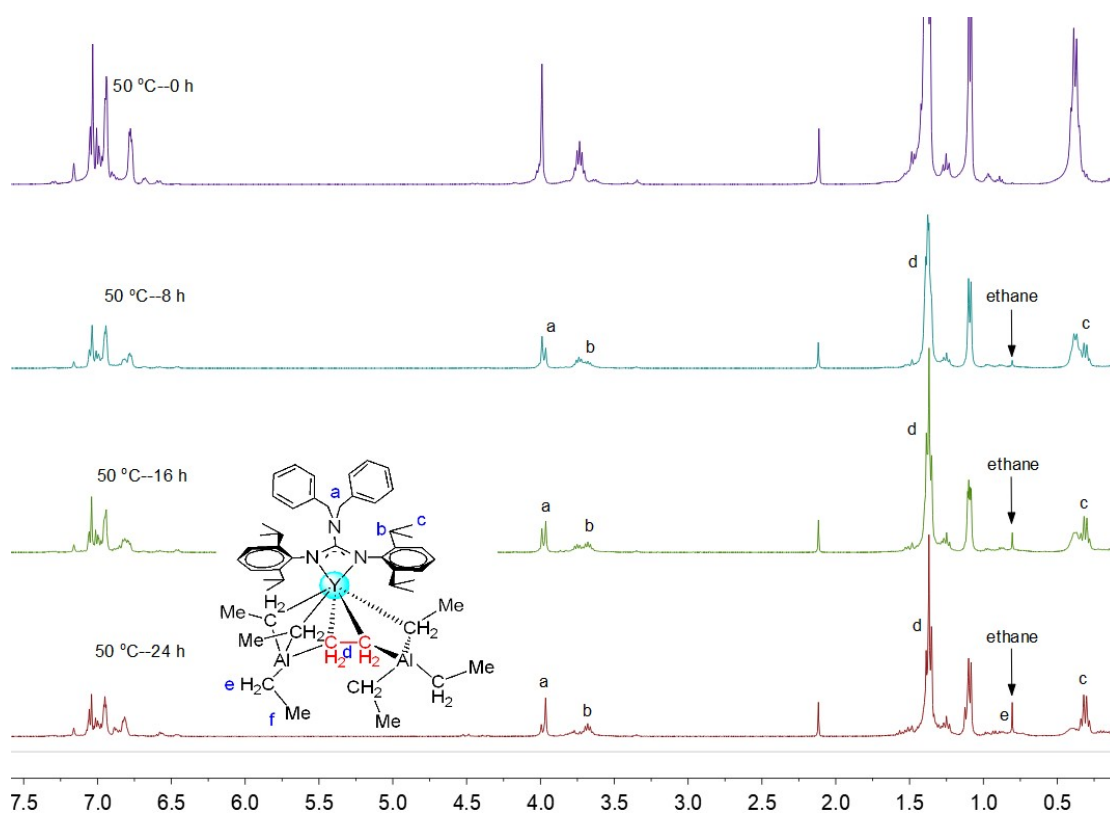


Figure S25. The *in situ* ^1H NMR spectrum was carried out on conversion of **4-Y** from **5-Y** in C_6D_6 at room temperature.

X-ray Crystallographic structure determinations

All crystals for X-ray analysis were obtained as described in the preparations. In the glovebox, the suitable crystals were sealed in dried immersion oil. Data collections were performed on a Bruker SMART APEX or Bruker SMART APEX II (at 173 K or 298 K) diffractometer with CCD area detector using graphite-monochromated Mo/Ga K α radiation ($\lambda = 0.71073 \text{ \AA}$ / $\lambda = 1.34138 \text{ \AA}$). The determination of crystal class and unit cell was carried out by using the SMART program package. The raw frame data were processed using SAINT^[1] and SADABS^[2] to yield the reflection data file. The structure was solved by using the SHELXTL program^[3] Refinement was performed on F^2 anisotropically by the full-matrix least-squares method for all the non-hydrogen atoms. The analytical scattering factors for neutral atoms were used throughout the analysis. Except for the hydrogen atoms on bridging carbons, hydrogen atoms were placed at the calculated positions and included in the structure calculation without further refinement of the parameters. The hydrogen atoms on bridging carbons were located by difference Fourier syntheses and their coordinates and isotropic parameters were refined. The residual electron densities were of no chemical significance. Crystal data, data collection, and processing parameters: 2259604 (for **1-Lu**), 2259606 (for **2-Y**), 2259605 (for **2-Lu**), 2259607 (for **3-Y**), 2259608 (for **4-Y**) and 2259609 (for **5-Y**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via <https://www.ccdc.cam.ac.uk/Community/Depositastructure/CSDCommunications/>

Crystal data of selected complexes

Table S1. Crystal data and refinement details of complexes **1-Lu**, **2-Y** and **2-Lu**.

	1-Lu	2-Y	2-Lu
Formula	C ₈₆ H ₁₁₆ N ₆ Lu ₂	C ₄₉ H ₇₃ N ₃ AlY	C ₄₉ H ₇₃ N ₃ AlLu
Molecular weight	1583.84	820.03	906.09
Crystal system	Triclinic	Monoclinic	Monoclinic
Space group	P-1	P2 ₁ /c	P2 ₁ /c
<i>a</i> / (Å)	10.8568(4)	11.4571(12)	11.4749(4)
<i>b</i> / (Å)	19.2449(8)	19.681(3)	19.6122(7)
<i>c</i> / (Å)	21.6617(7)	21.041(3)	20.9790(9)
<i>V</i> / (Å ³)	4417.0(3)	4679.6(10)	4662.0(3)
<i>Z</i>	2	4	4
ρ_c / (mg. m ⁻³)	1.260	1.154	1.291
μ (Mo-K α)/(mm ⁻¹)	2.267	1.299	2.170
Limiting indices	-13<= <i>h</i> <=13	-13<= <i>h</i> <=13	-14<= <i>h</i> <=14
	-24<= <i>k</i> <=24	-23<= <i>k</i> <=23	-24<= <i>k</i> <=24
	-27<= <i>l</i> <=27	-25<= <i>l</i> <=25	-26<= <i>l</i> <=26
Collected reflections	307106	92292	111964
Unique	18302 [R(int) = 0.1023]	8690 [R(int) = 0.1745]	9667 [R(int) = 0.1165]
Parameters	968	547	528
Goodness of fit on <i>F</i> ²	1.022	1.028	1.010
<i>R</i> ₁ ^a , <i>wR</i> ₂ ^a [<i>I</i> > 2 σ (<i>I</i>)]	<i>R</i> ₁ = 0.0311	<i>R</i> ₁ = 0.0412	<i>R</i> ₁ = 0.0277
	<i>wR</i> ₂ = 0.0670	<i>wR</i> ₂ = 0.0974	<i>wR</i> ₂ = 0.0602
<i>R</i> ₁ , <i>wR</i> ₂ indices (all data)	<i>R</i> ₁ = 0.0470	<i>R</i> ₁ = 0.0748	<i>R</i> ₁ = 0.0441
	<i>wR</i> ₂ = 0.0726	<i>wR</i> ₂ = 0.1101	<i>wR</i> ₂ = 0.0661
Max/min residual density (e Å ⁻³)	1.11 and -0.91	0.87 and -0.45	0.59 and -0.52

^a $R_1 = \sum || F_0 | - | F_c ||$ (based on reflections with $F_o^2 > 2\sigma F^2$). $wR_2 = [\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]]^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (0.095P)^2]$; $P = [\max(F_o^2, 0) + 2F_c^2] / 3$ (also with $F_o^2 > 2\sigma F^2$).

Table S2. Crystal data and refinement details of complexes **3-Y**, **4-Y** and **5-Y**.

	3-Y	4-Y	5-Y
Formula	C ₉₂ H ₁₂₈ N ₆ Al ₂ Y ₂	C ₅₃ H ₈₂ N ₃ Al ₂ Y	C ₅₅ H ₈₈ N ₃ YAl ₂
Molecular weight	1549.84	904.12	934.19
Crystal system	Triclinic	Monoclinic	Monoclinic
Space group	P-1	P2 ₁	P2 ₁ /c
<i>a</i> / (Å)	13.5651(5)	21.3577(8)	21.5841(6)
<i>b</i> / (Å)	18.5143(7)	11.1948(4)	30.8815(9)
<i>c</i> / (Å)	19.5102(7)	21.4820(9)	16.1320(5)
<i>V</i> / (Å ³)	4240.7(3)	5136.2(3)	10725.0(5)
<i>Z</i>	2	2	4
ρ_c / (mg. m ⁻³)	1.214	1.167	1.157
μ (Mo-K α)/(mm ⁻¹)	1.583	1.460	1.400
Limiting indices	-17<= <i>h</i> <=17 -23<= <i>k</i> <=23 -24<= <i>l</i> <=24	-27<= <i>h</i> <=27 -14<= <i>k</i> <=14 -27<= <i>l</i> <=27	-26<= <i>h</i> <=26 -37<= <i>k</i> <=37 -17<= <i>l</i> <=19
Collected reflections	93876	76031	210709
Unique	17937 [R(int) = 0.0846]	22242 [R(int) = 0.0932]	20088 [R(int) = 0.0590]
Parameters	1130	1116	1224
Goodness of fit on <i>F</i> ²	1.038	1.009	1.021
<i>R</i> ₁ ^a , <i>wR</i> ₂ ^a [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0557 <i>wR</i> ₂ = 0.1494	<i>R</i> ₁ = 0.0687 <i>wR</i> ₂ = 0.1773	<i>R</i> ₁ = 0.0478 <i>wR</i> ₂ = 0.1220
<i>R</i> ₁ , <i>wR</i> ₂ indices (all data)	<i>R</i> ₁ = 0.0698 <i>wR</i> ₂ = 0.1610	<i>R</i> ₁ = 0.0832 <i>wR</i> ₂ = 0.1910	<i>R</i> ₁ = 0.0553 <i>wR</i> ₂ = 0.1290
Max/min residual density(e Å ⁻³)	1.60 and -0.92	1.57 and -1.23	1.75 and -1.12

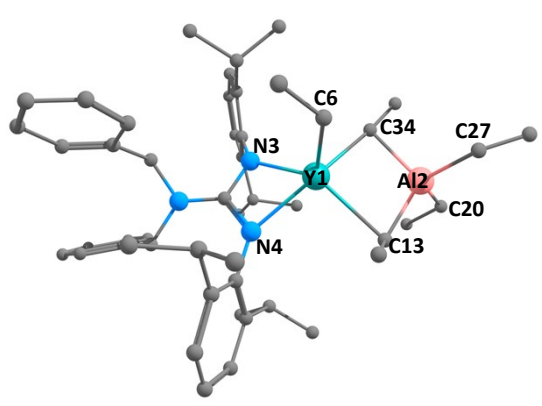
^a $R_1 = \sum || F_0| - |F_c||$ (based on reflections with $F_o^2 > 2\sigma F^2$). $wR_2 = [\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]]^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (0.095P)^2]$; $P = [\max(F_o^2, 0) + 2F_c^2]/3$ (also with $F_o^2 > 2\sigma F^2$).

Computational details

The optimization of reactants, transition states, IRC, and products were carried out by employing DFT hybrid functional (B3PW91)⁴ along with small core pseudopotential Stuttgart basis set⁵ for yttrium, aluminum atoms (additional polarization⁶ for aluminum atoms) and Pople basis set⁷ (6-31G**) for the rest of the atoms. Frequency calculations were performed to locate saddle points for transition state structures, minima for the rest of the structures, and for obtaining thermal corrections over the energies. Dispersion corrections were included in our calculations by employing the D3 version of Grimme's dispersion with Becke-Johnson damping.⁸ Solvent corrections using the SMD model⁹ were included by considering the reaction in toluene. All the calculations were performed using the Gaussian 09 suite of programs.¹⁰

Table S3. Comparison of structural parameters of DFT optimized geometry and X-ray structure **2-Y**

Atom labels	X-ray	DFT	
		Dispersion	No dispersion
Y1-N3	2.27	2.32	2.36
Y1-N4	2.34	2.35	2.37
Y1-C6	2.34	2.40	2.41
Y1-C13	2.51	2.56	2.67
Y1-C34	2.53	2.55	2.67
Al2-C13	2.10	2.12	2.14
Al2-C20	1.96	1.99	2.01
Al2-C27	1.98	2.00	2.01
Al2-C34	2.09	2.11	2.10



Optimized geometries

Y-1

Y	16.595357000	-0.156696000	19.712176000
N	17.560380000	1.735809000	18.610503000
N	18.684086000	3.560981000	19.720619000
N	15.090060000	-0.909823000	17.643152000
C	17.996863000	2.365876000	19.716677000
C	19.245680000	4.143369000	18.498653000
H	18.604609000	4.957436000	18.143934000
H	19.246043000	3.378906000	17.725084000
C	20.649212000	4.672473000	18.660825000

C	21.697308000	3.846995000	19.076172000
H	21.499768000	2.804987000	19.301681000
C	22.989660000	4.349507000	19.202825000
H	23.792876000	3.696356000	19.532203000
C	23.253914000	5.685394000	18.901555000
H	24.262227000	6.077709000	18.999074000
C	22.217507000	6.512978000	18.473218000
H	22.412264000	7.555750000	18.239276000
C	20.924051000	6.008530000	18.360486000
H	20.110412000	6.661515000	18.056851000
C	17.498985000	2.122008000	17.264816000
C	18.181900000	1.297532000	16.330175000
C	18.018482000	1.541692000	14.965694000
H	18.534294000	0.916538000	14.244390000
C	17.207309000	2.576840000	14.511005000
H	17.088941000	2.752034000	13.445428000
C	16.558179000	3.391722000	15.430809000
H	15.933629000	4.203508000	15.071099000
C	16.687627000	3.188818000	16.807340000
C	19.087551000	0.183289000	16.828663000
H	18.527724000	-0.376300000	17.590178000
C	20.333390000	0.740873000	17.525594000
H	20.919557000	1.367896000	16.844758000
H	20.975232000	-0.076523000	17.870869000
H	20.058403000	1.338249000	18.396076000
C	19.500382000	-0.819716000	15.754481000
H	20.164248000	-0.368647000	15.007773000
H	18.640196000	-1.243705000	15.226538000
H	20.047853000	-1.647706000	16.216201000
C	15.945533000	4.084790000	17.781677000
H	16.521448000	4.096200000	18.710463000
C	14.563076000	3.522498000	18.119011000
H	13.947535000	3.426989000	17.217784000
H	14.037100000	4.179161000	18.820647000
H	14.643084000	2.538370000	18.582014000
C	15.822968000	5.531486000	17.301242000
H	16.792341000	5.956161000	17.022311000
H	15.396103000	6.154915000	18.092958000
H	15.155658000	5.619419000	16.437216000
C	14.164050000	0.068999000	20.131344000
H	13.730789000	0.297538000	21.109473000
H	13.964954000	0.928614000	19.478875000

C	13.641991000	-1.198686000	19.597162000
C	14.122355000	-1.722572000	18.365704000
C	13.716310000	-2.973930000	17.908738000
H	14.101803000	-3.366273000	16.973996000
C	12.831951000	-3.752021000	18.655442000
H	12.536747000	-4.732544000	18.294453000
C	12.358314000	-3.268452000	19.871996000
H	11.677064000	-3.868263000	20.470173000
C	12.755470000	-2.015357000	20.325599000
H	12.375689000	-1.639459000	21.273333000
C	14.423572000	0.172604000	16.895035000
H	13.850828000	-0.242488000	16.052816000
H	15.171577000	0.869317000	16.507732000
H	13.733558000	0.711473000	17.542016000
C	15.922955000	-1.661302000	16.700018000
H	16.412181000	-2.489975000	17.210547000
H	16.677113000	-0.983663000	16.296592000
H	15.339840000	-2.047027000	15.851108000
N	17.672590000	1.667299000	20.819667000
C	18.924121000	4.316462000	20.951222000
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H	18.269112000	3.924650000	21.725766000
C	18.683519000	5.799576000	20.821532000
C	17.476902000	6.305149000	20.332219000
H	16.698797000	5.618043000	20.019778000
C	17.266748000	7.678894000	20.242004000
H	16.325300000	8.056517000	19.853013000
C	18.258889000	8.567232000	20.655984000
H	18.095319000	9.638972000	20.586826000
C	19.460555000	8.071543000	21.159331000
H	20.241232000	8.755024000	21.481019000
C	19.670587000	6.696959000	21.235146000
H	20.619378000	6.311704000	21.598724000
C	18.056082000	1.791016000	22.162144000
C	17.015624000	1.974793000	23.112174000
C	17.325126000	1.934358000	24.472593000
H	16.535627000	2.068525000	25.205001000
C	18.630701000	1.728219000	24.907722000
H	18.855383000	1.696815000	25.970166000
C	19.647766000	1.576298000	23.972632000
H	20.666496000	1.429844000	24.317480000
C	19.390011000	1.605381000	22.599510000

C	15.598721000	2.237162000	22.631568000
H	15.388768000	1.516359000	21.831308000
C	15.471769000	3.630462000	22.004572000
H	15.725705000	4.414635000	22.726344000
H	14.445426000	3.803267000	21.663227000
H	16.129404000	3.733856000	21.140325000
C	14.527441000	2.051805000	23.703331000
H	14.589487000	2.822277000	24.480765000
H	14.592359000	1.074596000	24.192627000
H	13.534726000	2.131224000	23.248920000
C	20.525483000	1.419401000	21.609440000
H	20.237282000	1.929371000	20.686640000
C	20.731347000	-0.055676000	21.259452000
H	20.968573000	-0.641711000	22.154011000
H	21.556133000	-0.174556000	20.548336000
H	19.837173000	-0.481324000	20.802712000
C	21.844255000	2.034334000	22.081410000
H	21.728650000	3.082453000	22.374384000
H	22.587627000	1.989975000	21.279609000
H	22.265630000	1.490475000	22.933703000
N	16.702322000	-1.823081000	21.825335000
C	17.976841000	-2.186537000	19.334015000
H	18.381376000	-2.465056000	18.355981000
H	18.831261000	-1.938196000	19.976066000
C	17.130098000	-3.253991000	19.889403000
C	16.450694000	-3.071340000	21.124326000
C	15.559098000	-4.026996000	21.605474000
H	15.039540000	-3.863724000	22.543451000
C	15.298777000	-5.187596000	20.877689000
H	14.588059000	-5.915823000	21.256434000
C	15.941466000	-5.385651000	19.658313000
H	15.741831000	-6.281093000	19.075130000
C	16.840084000	-4.436866000	19.181520000
H	17.343256000	-4.601147000	18.230855000
C	17.979316000	-1.874874000	22.560344000
H	17.904828000	-2.575402000	23.405196000
H	18.226450000	-0.881382000	22.943331000
H	18.780709000	-2.216412000	21.907285000
C	15.654005000	-1.440610000	22.775282000
H	14.682861000	-1.437423000	22.281082000
H	15.880009000	-0.438365000	23.143078000
H	15.618146000	-2.112866000	23.645422000

Int-1

Y	16.298274000	0.338177000	19.831374000
N	17.356143000	2.098286000	18.631073000
N	18.731700000	3.824493000	19.608061000
N	14.630611000	-0.271576000	17.803697000
C	17.932030000	2.705567000	19.684908000
C	19.255874000	4.321301000	18.333897000
H	18.662851000	5.175408000	17.991252000
H	19.140815000	3.537836000	17.588688000
C	20.705980000	4.732090000	18.382618000
C	21.696791000	3.875528000	18.868189000
H	21.420375000	2.894672000	19.238212000
C	23.032108000	4.271175000	18.883429000
H	23.790275000	3.596550000	19.271226000
C	23.395428000	5.527060000	18.398322000
H	24.436786000	5.836238000	18.409959000
C	22.414694000	6.382818000	17.899301000
H	22.687034000	7.365280000	17.524301000
C	21.079720000	5.987202000	17.897154000
H	20.311782000	6.667176000	17.537941000
C	17.268466000	2.447908000	17.276849000
C	17.838299000	1.543348000	16.341481000
C	17.616147000	1.752521000	14.979449000
H	18.040350000	1.065114000	14.254988000
C	16.858406000	2.830699000	14.531903000
H	16.689656000	2.976015000	13.468645000
C	16.330217000	3.728697000	15.452447000
H	15.751548000	4.574483000	15.094432000
C	16.522676000	3.563646000	16.826740000
C	18.694371000	0.388294000	16.836507000
H	18.157470000	-0.087228000	17.669024000
C	20.025149000	0.886173000	17.412068000
H	20.605985000	1.426020000	16.656327000
H	20.627976000	0.042178000	17.764020000
H	19.862733000	1.551649000	18.261159000
C	18.956949000	-0.692821000	15.791051000
H	19.600871000	-0.327986000	14.982681000
H	18.035093000	-1.073428000	15.339633000
H	19.471995000	-1.538842000	16.257027000
C	15.922824000	4.557073000	17.805884000
H	16.536874000	4.530010000	18.709909000
C	14.503467000	4.164790000	18.223211000

H	13.842152000	4.092843000	17.353369000
H	14.082062000	4.908868000	18.907758000
H	14.495809000	3.203656000	18.738885000
C	15.935222000	5.994129000	17.281714000
H	16.928708000	6.297291000	16.937119000
H	15.625729000	6.685439000	18.071627000
H	15.234952000	6.130585000	16.450803000
C	13.894734000	0.721042000	20.325894000
H	13.511189000	1.018730000	21.302688000
H	13.863928000	1.599146000	19.669881000
C	13.194310000	-0.425317000	19.774639000
C	13.570011000	-0.965131000	18.510760000
C	12.977710000	-2.119242000	18.019488000
H	13.286291000	-2.519790000	17.059860000
C	11.996301000	-2.799509000	18.751273000
H	11.555711000	-3.707731000	18.353905000
C	11.626264000	-2.317147000	19.997075000
H	10.897557000	-2.850219000	20.598723000
C	12.193660000	-1.130654000	20.492436000
H	11.970319000	-0.813310000	21.509809000
C	14.080970000	0.883493000	17.065379000
H	13.451162000	0.538276000	16.234095000
H	14.896907000	1.489604000	16.666262000
H	13.464909000	1.492377000	17.723098000
C	15.358471000	-1.109156000	16.844585000
H	15.708456000	-2.020217000	17.329326000
H	16.210624000	-0.537405000	16.476093000
H	14.738952000	-1.375038000	15.975749000
N	17.623343000	2.057951000	20.821906000
C	19.104035000	4.597432000	20.796797000
H	20.115074000	4.327205000	21.119254000
H	18.429976000	4.325744000	21.605811000
C	19.043424000	6.090372000	20.595541000
C	17.879439000	6.718095000	20.145387000
H	17.000550000	6.120306000	19.930504000
C	17.840904000	8.098668000	19.968301000
H	16.931737000	8.571334000	19.607484000
C	18.965036000	8.872243000	20.257166000
H	18.936437000	9.949331000	20.118397000
C	20.124417000	8.256051000	20.725134000
H	21.006303000	8.849595000	20.948903000
C	20.162544000	6.873314000	20.886056000

H	21.077678000	6.389762000	21.217321000
C	18.054515000	2.222858000	22.144468000
C	17.069024000	2.566440000	23.105785000
C	17.426930000	2.604244000	24.454602000
H	16.683114000	2.868183000	25.199347000
C	18.725321000	2.311990000	24.861838000
H	18.987587000	2.344749000	25.915595000
C	19.687770000	1.986505000	23.912160000
H	20.700174000	1.768924000	24.237999000
C	19.379413000	1.936040000	22.550429000
C	15.662469000	2.911620000	22.646327000
H	15.371661000	2.156776000	21.904068000
C	15.623748000	4.265063000	21.926688000
H	15.968861000	5.070746000	22.583929000
H	14.601770000	4.499954000	21.610796000
H	16.252541000	4.257211000	21.034446000
C	14.613734000	2.884722000	23.754849000
H	14.759966000	3.698764000	24.474118000
H	14.617016000	1.941751000	24.310733000
H	13.616754000	3.011411000	23.322225000
C	20.439542000	1.571117000	21.527625000
H	20.176062000	2.084817000	20.599001000
C	20.431424000	0.073148000	21.217576000
H	20.641110000	-0.516745000	22.116331000
H	21.190771000	-0.171016000	20.466511000
H	19.462742000	-0.237296000	20.823300000
C	21.845383000	2.024736000	21.920074000
H	21.877887000	3.090558000	22.167021000
H	22.540756000	1.846958000	21.093628000
H	22.228881000	1.466741000	22.780929000
N	16.332063000	-1.236329000	22.017567000
C	17.423753000	-1.839886000	19.477406000
H	17.723751000	-2.191491000	18.485425000
H	18.337730000	-1.721885000	20.070875000
C	16.433557000	-2.741296000	20.090803000
C	15.847432000	-2.430338000	21.348717000
C	14.822650000	-3.213686000	21.878039000
H	14.381390000	-2.955914000	22.834392000
C	14.335476000	-4.316895000	21.179007000
H	13.526200000	-4.907976000	21.596597000
C	14.884801000	-4.636012000	19.939227000
H	14.510021000	-5.488613000	19.379168000

C	15.913999000	-3.862774000	19.414398000
H	16.345261000	-4.122660000	18.450087000
C	17.628940000	-1.471580000	22.677927000
H	17.499344000	-2.133660000	23.546544000
H	18.044910000	-0.519104000	23.016408000
H	18.328604000	-1.944592000	21.991257000
C	15.417723000	-0.686272000	23.022182000
H	14.433506000	-0.521485000	22.585699000
H	15.826725000	0.265923000	23.364498000
H	15.323152000	-1.342479000	23.900030000
Al	10.183554000	0.230746000	19.823351000
C	8.732381000	-0.886291000	20.617080000
H	7.941686000	-0.183671000	20.928116000
H	9.079938000	-1.340835000	21.557050000
C	8.116904000	-1.958908000	19.714286000
H	7.678465000	-1.517562000	18.811103000
H	8.864973000	-2.683432000	19.370364000
H	7.318867000	-2.532816000	20.207265000
C	10.629842000	1.850912000	20.896409000
H	11.570270000	2.301889000	20.554915000
H	9.849408000	2.583151000	20.627225000
C	10.650403000	1.687671000	22.418118000
H	9.717729000	1.247140000	22.791998000
H	10.786728000	2.638284000	22.953882000
H	11.461376000	1.024915000	22.747339000
C	10.307274000	0.407951000	17.845750000
H	11.135685000	-0.211692000	17.479591000
H	9.405773000	-0.022770000	17.386088000
C	10.486791000	1.852712000	17.363167000
H	9.614093000	2.472196000	17.605294000
H	10.635870000	1.929738000	16.276280000
H	11.346541000	2.339854000	17.838725000

TS-1

Y	16.200685000	0.254757000	19.800521000
N	17.265735000	2.068680000	18.660561000
N	18.607230000	3.779876000	19.710937000
N	14.553887000	-0.273971000	17.734349000
C	17.825826000	2.644682000	19.739705000
C	19.139995000	4.329132000	18.462024000
H	18.537833000	5.185583000	18.140977000
H	19.048040000	3.570419000	17.688550000

C	20.582890000	4.759874000	18.545396000
C	21.580630000	3.897514000	19.005723000
H	21.314634000	2.897228000	19.328353000
C	22.909556000	4.311379000	19.054889000
H	23.673153000	3.631620000	19.422582000
C	23.260089000	5.591855000	18.627965000
H	24.296551000	5.915077000	18.665733000
C	22.272816000	6.453680000	18.152861000
H	22.534836000	7.454888000	17.822725000
C	20.943780000	6.039671000	18.118110000
H	20.170653000	6.723423000	17.777693000
C	17.191115000	2.469744000	17.319370000
C	17.788350000	1.614577000	16.355614000
C	17.595591000	1.886370000	14.999983000
H	18.043295000	1.237540000	14.254270000
C	16.838022000	2.977805000	14.585991000
H	16.693871000	3.172950000	13.527055000
C	16.278223000	3.825299000	15.535459000
H	15.699864000	4.682364000	15.204919000
C	16.442416000	3.597376000	16.904341000
C	18.638418000	0.442505000	16.816424000
H	18.081839000	-0.068267000	17.612867000
C	19.954591000	0.915278000	17.444578000
H	20.552917000	1.488607000	16.728012000
H	20.549825000	0.056485000	17.772893000
H	19.770847000	1.542007000	18.318786000
C	18.921840000	-0.593979000	15.732425000
H	19.579960000	-0.198406000	14.950155000
H	18.007258000	-0.955515000	15.251307000
H	19.428652000	-1.458321000	16.173392000
C	15.815582000	4.536203000	17.918961000
H	16.435024000	4.496822000	18.818813000
C	14.414990000	4.077986000	18.327191000
H	13.744044000	4.044967000	17.462450000
H	13.983261000	4.762307000	19.063941000
H	14.441588000	3.083721000	18.774761000
C	15.774796000	5.991130000	17.450424000
H	16.756818000	6.345951000	17.122492000
H	15.436434000	6.638924000	18.265072000
H	15.071289000	6.132373000	16.623023000
C	13.781637000	0.569405000	20.313561000
H	13.406872000	0.775514000	21.318809000

H	13.658541000	1.473221000	19.709307000
C	13.177267000	-0.631342000	19.724452000
C	13.577551000	-1.088016000	18.433255000
C	13.109410000	-2.292997000	17.924920000
H	13.431950000	-2.633615000	16.947268000
C	12.241470000	-3.098054000	18.668968000
H	11.894783000	-4.041086000	18.258842000
C	11.855223000	-2.691192000	19.938755000
H	11.207187000	-3.320144000	20.541719000
C	12.310574000	-1.476939000	20.453038000
H	12.035785000	-1.183328000	21.461620000
C	13.908459000	0.880102000	17.080549000
H	13.301251000	0.542005000	16.229602000
H	14.671802000	1.573550000	16.721040000
H	13.253143000	1.394280000	17.780607000
C	15.317615000	-0.994726000	16.710360000
H	15.783243000	-1.882248000	17.138348000
H	16.089327000	-0.322868000	16.331363000
H	14.688874000	-1.289175000	15.857542000
N	17.519744000	1.951542000	20.850691000
C	18.946390000	4.521980000	20.928788000
H	19.961131000	4.268419000	21.252725000
H	18.272521000	4.204864000	21.721216000
C	18.848316000	6.019521000	20.779491000
C	17.668754000	6.635271000	20.354187000
H	16.804424000	6.025314000	20.116989000
C	17.595327000	8.020348000	20.230853000
H	16.673662000	8.483542000	19.890048000
C	18.700154000	8.810046000	20.548749000
H	18.644165000	9.890729000	20.452701000
C	19.875463000	8.205261000	20.991115000
H	20.742467000	8.811695000	21.237398000
C	19.948090000	6.818670000	21.098824000
H	20.875155000	6.345491000	21.411221000
C	17.925377000	2.077848000	22.185416000
C	16.913143000	2.352016000	23.142493000
C	17.241500000	2.326680000	24.498958000
H	16.475298000	2.532772000	25.239340000
C	18.538478000	2.046883000	24.919305000
H	18.777983000	2.030296000	25.978829000
C	19.529430000	1.802745000	23.974665000
H	20.542015000	1.600399000	24.309566000

C	19.250404000	1.812294000	22.605670000
C	15.511330000	2.703344000	22.672843000
H	15.242541000	1.987797000	21.884892000
C	15.475644000	4.092538000	22.024504000
H	15.814805000	4.862613000	22.725992000
H	14.457107000	4.343994000	21.711821000
H	16.112339000	4.129172000	21.138594000
C	14.439520000	2.605064000	23.755127000
H	14.559260000	3.380474000	24.520606000
H	14.443613000	1.633008000	24.258687000
H	13.450511000	2.744306000	23.307542000
C	20.344879000	1.530575000	21.592663000
H	20.078243000	2.066466000	20.678023000
C	20.409327000	0.046444000	21.227629000
H	20.622570000	-0.567594000	22.109307000
H	21.196747000	-0.136777000	20.488313000
H	19.465203000	-0.289780000	20.797088000
C	21.721496000	2.028199000	22.033994000
H	21.701038000	3.081154000	22.332400000
H	22.439808000	1.924413000	21.214669000
H	22.114697000	1.447062000	22.875022000
N	16.303324000	-1.425583000	21.882967000
C	17.402599000	-1.854457000	19.311797000
H	17.718519000	-2.150697000	18.307032000
H	18.314925000	-1.681909000	19.897509000
C	16.510506000	-2.860489000	19.911241000
C	15.923986000	-2.645173000	21.187697000
C	15.006264000	-3.547713000	21.721607000
H	14.563035000	-3.363073000	22.694241000
C	14.626514000	-4.682212000	21.005551000
H	13.900066000	-5.370607000	21.426623000
C	15.169824000	-4.904926000	19.742709000
H	14.874319000	-5.778536000	19.167390000
C	16.093327000	-4.010236000	19.213137000
H	16.519218000	-4.194069000	18.229117000
C	17.611803000	-1.580092000	22.545734000
H	17.531036000	-2.282526000	23.388093000
H	17.951176000	-0.611886000	22.922185000
H	18.348457000	-1.972886000	21.847322000
C	15.343480000	-0.983503000	22.899386000
H	14.346223000	-0.904376000	22.468259000
H	15.661882000	-0.004525000	23.262571000

H	15.312748000	-1.663592000	23.763190000
Al	10.646521000	0.757128000	19.627722000
C	9.805468000	0.415550000	21.399094000
H	9.131934000	1.275870000	21.551155000
H	10.554704000	0.513322000	22.198092000
C	9.009294000	-0.879091000	21.569341000
H	8.204828000	-0.954554000	20.827984000
H	9.638941000	-1.764857000	21.432110000
H	8.539916000	-0.968377000	22.559172000
C	11.178122000	2.661924000	19.391326000
H	11.890543000	2.809841000	18.570477000
H	10.242819000	3.119849000	19.020720000
C	11.640644000	3.420635000	20.636555000
H	10.931636000	3.307088000	21.465630000
H	11.756832000	4.499933000	20.464525000
H	12.605035000	3.045591000	20.994605000
C	10.065405000	-0.200253000	17.989837000
H	10.740438000	-1.044444000	17.801948000
H	9.087988000	-0.663304000	18.193553000
C	9.969882000	0.674719000	16.735267000
H	9.233280000	1.479712000	16.849953000
H	9.678405000	0.105026000	15.841200000
H	10.925781000	1.159893000	16.504212000

Int-2

Y	15.963791000	0.225301000	19.675952000
N	17.139915000	1.963056000	18.558561000
N	18.458393000	3.678508000	19.638013000
N	14.561388000	-0.152021000	17.533641000
C	17.662343000	2.556720000	19.651353000
C	19.046436000	4.214628000	18.403595000
H	18.441577000	5.049538000	18.036330000
H	19.013397000	3.438620000	17.643747000
C	20.472572000	4.679309000	18.560403000
C	21.483911000	3.800222000	18.956308000
H	21.239929000	2.764425000	19.165740000
C	22.797889000	4.242038000	19.085176000
H	23.572573000	3.548617000	19.400331000
C	23.120090000	5.569766000	18.804746000
H	24.145352000	5.914821000	18.904494000
C	22.120558000	6.449675000	18.393722000
H	22.360820000	7.486501000	18.176561000

C	20.805236000	6.006331000	18.279346000
H	20.020389000	6.701000000	17.992866000
C	17.139217000	2.372565000	17.211678000
C	17.817229000	1.544147000	16.279989000
C	17.734595000	1.846487000	14.919256000
H	18.250872000	1.220104000	14.199390000
C	16.993275000	2.933322000	14.468013000
H	16.930707000	3.150040000	13.405417000
C	16.345735000	3.749844000	15.387446000
H	15.783825000	4.606918000	15.030328000
C	16.411885000	3.500186000	16.761106000
C	18.627928000	0.356812000	16.769633000
H	18.029581000	-0.145580000	17.538162000
C	19.923699000	0.805816000	17.452352000
H	20.555767000	1.378792000	16.765208000
H	20.496039000	-0.062201000	17.796039000
H	19.710959000	1.428082000	18.323354000
C	18.933654000	-0.679056000	15.690818000
H	19.640522000	-0.298751000	14.944580000
H	18.031549000	-1.005250000	15.163313000
H	19.392955000	-1.562517000	16.146071000
C	15.730740000	4.441037000	17.738004000
H	16.292369000	4.385718000	18.674308000
C	14.299172000	4.014858000	18.056943000
H	13.675969000	4.006139000	17.157076000
H	13.845049000	4.699114000	18.779001000
H	14.273011000	3.015009000	18.490060000
C	15.743066000	5.899777000	17.276328000
H	16.748742000	6.243329000	17.014719000
H	15.358767000	6.547269000	18.070708000
H	15.096539000	6.054466000	16.406333000
C	13.289905000	0.699033000	20.025872000
H	13.408351000	0.848739000	21.100192000
H	13.745229000	1.484412000	19.423386000
C	13.291280000	-0.696745000	19.558766000
C	13.838373000	-1.125323000	18.321316000
C	13.716065000	-2.459692000	17.914668000
H	14.144401000	-2.776091000	16.971863000
C	13.069905000	-3.392191000	18.709201000
H	13.000102000	-4.424514000	18.384508000
C	12.533037000	-2.993701000	19.934301000
H	12.026480000	-3.712616000	20.570283000

C	12.643445000	-1.677915000	20.341872000
H	12.185507000	-1.361234000	21.272581000
C	13.667489000	0.833052000	16.893011000
H	13.082150000	0.346387000	16.102375000
H	14.275162000	1.626802000	16.454284000
H	12.969623000	1.259073000	17.610291000
C	15.387793000	-0.739040000	16.472212000
H	16.072620000	-1.476716000	16.889357000
H	15.958195000	0.063998000	16.006577000
H	14.770323000	-1.210963000	15.696014000
N	17.284822000	1.898321000	20.764891000
C	18.793060000	4.411588000	20.861067000
H	19.814675000	4.169652000	21.169353000
H	18.136319000	4.069487000	21.656660000
C	18.671388000	5.910041000	20.743820000
C	17.538701000	6.519466000	20.201290000
H	16.726652000	5.904759000	19.831668000
C	17.446193000	7.907116000	20.122406000
H	16.562104000	8.363926000	19.686619000
C	18.483161000	8.705426000	20.602785000
H	18.412903000	9.787702000	20.541152000
C	19.611034000	8.105736000	21.161881000
H	20.426395000	8.719034000	21.534942000
C	19.704472000	6.718252000	21.224917000
H	20.599448000	6.252203000	21.628688000
C	17.723528000	1.982451000	22.097008000
C	16.734891000	2.253906000	23.081505000
C	17.066599000	2.130957000	24.431508000
H	16.313226000	2.328264000	25.186879000
C	18.350439000	1.769936000	24.826587000
H	18.592116000	1.670274000	25.880860000
C	19.327619000	1.564021000	23.860736000
H	20.334366000	1.306428000	24.173839000
C	19.047112000	1.669769000	22.495515000
C	15.360553000	2.754038000	22.667613000
H	15.024701000	2.153996000	21.811470000
C	15.461255000	4.205125000	22.178398000
H	15.944585000	4.836559000	22.931371000
H	14.470468000	4.620791000	21.976526000
H	16.041598000	4.269116000	21.256534000
C	14.288855000	2.640520000	23.749446000
H	14.472185000	3.334480000	24.576986000

H	14.219291000	1.631515000	24.168546000
H	13.313034000	2.893333000	23.325620000
C	20.161734000	1.430647000	21.491151000
H	19.891736000	1.949274000	20.568115000
C	20.319664000	-0.051394000	21.144317000
H	20.507252000	-0.648772000	22.043094000
H	21.161637000	-0.199019000	20.459327000
H	19.426554000	-0.442405000	20.655604000
C	21.506267000	1.995481000	21.959322000
H	21.428905000	3.040608000	22.273833000
H	22.240483000	1.941298000	21.150165000
H	21.916748000	1.423445000	22.797998000
N	16.051117000	-1.412731000	21.845923000
C	17.184813000	-1.841651000	19.294149000
H	17.524870000	-2.167412000	18.305800000
H	18.092919000	-1.546432000	19.842736000
C	16.474021000	-2.939950000	19.987111000
C	15.873410000	-2.729769000	21.250682000
C	15.183708000	-3.748010000	21.903827000
H	14.728978000	-3.565270000	22.872060000
C	15.052787000	-5.005496000	21.314387000
H	14.507733000	-5.791332000	21.829000000
C	15.616562000	-5.232208000	20.061826000
H	15.516791000	-6.203821000	19.584886000
C	16.307866000	-4.212497000	19.413819000
H	16.746645000	-4.396304000	18.435673000
C	17.337063000	-1.389348000	22.572208000
H	17.303652000	-2.089506000	23.419160000
H	17.537312000	-0.385750000	22.947623000
H	18.146412000	-1.695659000	21.912266000
C	15.001227000	-1.025775000	22.793285000
H	14.021164000	-1.116286000	22.326072000
H	15.176198000	0.008698000	23.094107000
H	15.015364000	-1.635230000	23.707870000
Al	11.182722000	1.233834000	19.870090000
C	10.422390000	0.649692000	21.652822000
H	9.942593000	1.534299000	22.102062000
H	11.232592000	0.396028000	22.355760000
C	9.400621000	-0.491770000	21.616696000
H	8.532390000	-0.228255000	20.999802000
H	9.819972000	-1.404188000	21.174832000
H	9.010755000	-0.765322000	22.609107000

C	11.187880000	3.231257000	19.687234000
H	11.599317000	3.540295000	18.715661000
H	10.144830000	3.585365000	19.678081000
C	11.946939000	3.930249000	20.815793000
H	11.495190000	3.716186000	21.792981000
H	11.987642000	5.027196000	20.724318000
H	12.984266000	3.578853000	20.868743000
C	10.424512000	0.285270000	18.260795000
H	11.129964000	-0.472548000	17.891260000
H	9.546488000	-0.293658000	18.585918000
C	10.008459000	1.201890000	17.104789000
H	9.244670000	1.925169000	17.417045000
H	9.594432000	0.657512000	16.242268000
H	10.849842000	1.796496000	16.725349000

Int-3

Y	16.948430000	-0.269106000	19.659548000
N	18.107397000	1.473297000	18.602878000
N	19.042202000	3.401767000	19.712936000
N	11.974263000	-1.258140000	18.718425000
C	18.382046000	2.197304000	19.704817000
C	19.559868000	3.979400000	18.454445000
H	18.726487000	4.297426000	17.823128000
H	20.085738000	3.196204000	17.913573000
C	20.493660000	5.148573000	18.637176000
C	21.857340000	4.947643000	18.872335000
H	22.244745000	3.936276000	18.929850000
C	22.722349000	6.028885000	19.020400000
H	23.778561000	5.853737000	19.204260000
C	22.234505000	7.331259000	18.920034000
H	22.907882000	8.176160000	19.033667000
C	20.882596000	7.543182000	18.655625000
H	20.496108000	8.553774000	18.559714000
C	20.020474000	6.458890000	18.511191000
H	18.968415000	6.628759000	18.304820000
C	18.510395000	1.629185000	17.250371000
C	19.676332000	0.953714000	16.807709000
C	20.046627000	1.035186000	15.464297000
H	20.948967000	0.526721000	15.135746000
C	19.288390000	1.748410000	14.544949000
H	19.593577000	1.806690000	13.504085000
C	18.121981000	2.366554000	14.972537000

H	17.506101000	2.899379000	14.253426000
C	17.706707000	2.307108000	16.306065000
C	20.554169000	0.151508000	17.747455000
H	20.077283000	0.162213000	18.729611000
C	21.940945000	0.786707000	17.877663000
H	22.468988000	0.786096000	16.917792000
H	22.556249000	0.234752000	18.595532000
H	21.874967000	1.824109000	18.215895000
C	20.670042000	-1.313216000	17.319333000
H	21.109901000	-1.410044000	16.320900000
H	19.691389000	-1.798012000	17.306826000
H	21.310075000	-1.863544000	18.017861000
C	16.368042000	2.920242000	16.659509000
H	16.218319000	2.782063000	17.735783000
C	15.251618000	2.175733000	15.917821000
H	15.304432000	2.371992000	14.841527000
H	14.264275000	2.497355000	16.265912000
H	15.334241000	1.095624000	16.053937000
C	16.291606000	4.416288000	16.341952000
H	17.062570000	4.993720000	16.858463000
H	15.316661000	4.819668000	16.635691000
H	16.409447000	4.596112000	15.268335000
C	14.340306000	0.337544000	18.539362000
H	13.821263000	0.560075000	17.598752000
H	15.069526000	1.162943000	18.587261000
C	13.383829000	0.482404000	19.666397000
C	12.260643000	-0.369112000	19.795554000
C	11.453158000	-0.293875000	20.932705000
H	10.611042000	-0.970202000	21.038360000
C	11.683636000	0.667411000	21.916786000
H	11.028810000	0.727075000	22.781416000
C	12.722221000	1.577328000	21.750116000
H	12.871320000	2.375585000	22.469020000
C	13.566873000	1.468793000	20.645887000
H	14.382860000	2.177468000	20.522055000
C	11.256364000	-0.574556000	17.644890000
H	10.234350000	-0.292773000	17.951747000
H	11.191331000	-1.227981000	16.771037000
H	11.781181000	0.337246000	17.353475000
C	11.277650000	-2.478593000	19.087173000
H	11.795553000	-2.972563000	19.911993000
H	11.276405000	-3.156935000	18.229223000

H	10.225702000	-2.312859000	19.377440000
N	17.881308000	1.609370000	20.826670000
C	18.874029000	4.346801000	20.810299000
H	19.845923000	4.793621000	21.038376000
H	18.574705000	3.802182000	21.704285000
C	17.878511000	5.448429000	20.542776000
C	16.798445000	5.275440000	19.677173000
H	16.677678000	4.332733000	19.154421000
C	15.877864000	6.302790000	19.474699000
H	15.046815000	6.153309000	18.791759000
C	16.025527000	7.516074000	20.143186000
H	15.310395000	8.318084000	19.984641000
C	17.099388000	7.694108000	21.016046000
H	17.225465000	8.638393000	21.538471000
C	18.020736000	6.668911000	21.208604000
H	18.869283000	6.818203000	21.871701000
C	18.432277000	1.723296000	22.123333000
C	17.556310000	1.964592000	23.219114000
C	18.073719000	2.064343000	24.510753000
H	17.399367000	2.265745000	25.335638000
C	19.430147000	1.909531000	24.767906000
H	19.815206000	1.996573000	25.779813000
C	20.276849000	1.623850000	23.709724000
H	21.336032000	1.474306000	23.899593000
C	19.811653000	1.513016000	22.395274000
C	16.062452000	2.132033000	23.014326000
H	15.758864000	1.421751000	22.234996000
C	15.737080000	3.534958000	22.500054000
H	16.119462000	4.297085000	23.187325000
H	14.657145000	3.687220000	22.405280000
H	16.187690000	3.709601000	21.524032000
C	15.238395000	1.823011000	24.266165000
H	15.329387000	2.615817000	25.016789000
H	15.532641000	0.881138000	24.739647000
H	14.180225000	1.745922000	24.007581000
C	20.846678000	1.174342000	21.339882000
H	20.335109000	1.040337000	20.385673000
C	21.588818000	-0.129995000	21.657476000
H	22.228111000	-0.018962000	22.539900000
H	22.236694000	-0.409076000	20.819648000
H	20.902773000	-0.959117000	21.841613000
C	21.860155000	2.311840000	21.191024000

H	21.373160000	3.248287000	20.918749000
H	22.602832000	2.072491000	20.423993000
H	22.400685000	2.476199000	22.129538000
N	16.299933000	-1.680424000	21.839833000
C	18.704163000	-1.726468000	20.392132000
H	19.620292000	-1.880612000	19.820450000
H	18.946276000	-1.144041000	21.289067000
C	18.014266000	-2.990256000	20.694720000
C	16.776616000	-2.982261000	21.389911000
C	16.071794000	-4.159886000	21.628723000
H	15.126094000	-4.132823000	22.159782000
C	16.562908000	-5.381705000	21.169735000
H	16.001993000	-6.293460000	21.350997000
C	17.765833000	-5.414064000	20.465859000
H	18.152586000	-6.358447000	20.092175000
C	18.471215000	-4.238908000	20.230224000
H	19.408278000	-4.270019000	19.679496000
C	16.962063000	-1.336435000	23.112100000
H	16.650416000	-2.034221000	23.902209000
H	16.697729000	-0.323648000	23.405814000
H	18.045300000	-1.391553000	23.007773000
C	14.845749000	-1.593109000	22.029142000
H	14.325637000	-1.890905000	21.117468000
H	14.578451000	-0.559663000	22.261258000
H	14.492995000	-2.221172000	22.858702000
Al	14.821386000	-1.501961000	17.558336000
C	13.987705000	-1.354201000	15.732326000
H	14.736920000	-1.030635000	14.997425000
H	13.232335000	-0.556151000	15.728948000
C	13.342904000	-2.654104000	15.240103000
H	14.085042000	-3.453978000	15.129184000
H	12.593126000	-3.030083000	15.947613000
H	12.840840000	-2.551975000	14.266595000
C	16.912515000	-1.426057000	17.324565000
H	17.469974000	-0.474254000	17.340491000
H	17.433834000	-2.105451000	18.025933000
C	17.173631000	-1.980326000	15.915391000
H	16.587798000	-2.883029000	15.713519000
H	18.228614000	-2.234936000	15.753205000
H	16.902378000	-1.242388000	15.155736000
C	14.540866000	-3.276137000	18.452687000
H	14.623868000	-3.231265000	19.545934000

H	13.500015000	-3.562899000	18.259765000
C	15.461205000	-4.391224000	17.945177000
H	15.344235000	-4.548642000	16.865529000
H	15.265754000	-5.358526000	18.428083000
H	16.517865000	-4.166630000	18.123957000

TS-2

Y	18.001531000	0.233481000	19.478749000
N	19.466411000	1.894633000	18.695310000
N	20.236592000	3.747396000	19.999413000
N	11.197223000	-0.747708000	16.960914000
C	19.426672000	2.661290000	19.807543000
C	21.487132000	3.919077000	19.259776000
H	21.595800000	4.982821000	19.029402000
H	21.419095000	3.395052000	18.309177000
C	22.682367000	3.422455000	20.036886000
C	22.848947000	2.050069000	20.257184000
H	22.113811000	1.355170000	19.863338000
C	23.947610000	1.573991000	20.965588000
H	24.071929000	0.505140000	21.113563000
C	24.891859000	2.466632000	21.476588000
H	25.748796000	2.095019000	22.031082000
C	24.732545000	3.834436000	21.267299000
H	25.464099000	4.535303000	21.659443000
C	23.634673000	4.306485000	20.547144000
H	23.522055000	5.372113000	20.365319000
C	19.795800000	2.292406000	17.385771000
C	20.679520000	1.477981000	16.638128000
C	20.945159000	1.801063000	15.304454000
H	21.628033000	1.175029000	14.735978000
C	20.364230000	2.906694000	14.700880000
H	20.586646000	3.151215000	13.666042000
C	19.486894000	3.699217000	15.435680000
H	19.024285000	4.555116000	14.956280000
C	19.175265000	3.411308000	16.764765000
C	21.367739000	0.271832000	17.247309000
H	21.058786000	0.216330000	18.296300000
C	22.893069000	0.415523000	17.202239000
H	23.264405000	0.385321000	16.172005000
H	23.374969000	-0.401525000	17.751101000
H	23.222949000	1.358560000	17.646126000
C	20.935451000	-1.028338000	16.560869000

H	21.200152000	-1.019120000	15.497642000
H	19.854315000	-1.184043000	16.627864000
H	21.430009000	-1.892223000	17.018172000
C	18.133055000	4.235105000	17.500395000
H	18.491615000	4.396651000	18.518603000
C	16.812154000	3.466891000	17.581955000
H	16.408834000	3.281260000	16.582625000
H	16.060822000	4.029018000	18.145806000
H	16.942046000	2.498776000	18.072405000
C	17.890348000	5.617690000	16.900041000
H	18.815163000	6.196872000	16.819875000
H	17.200045000	6.179435000	17.535763000
H	17.430608000	5.558696000	15.907403000
C	13.043124000	-0.574540000	19.054366000
H	13.697176000	-0.206576000	19.852957000
H	12.999794000	-1.665605000	19.174505000
C	11.707750000	0.070142000	19.182487000
C	10.785884000	-0.003244000	18.111013000
C	9.573753000	0.686456000	18.167636000
H	8.876659000	0.626452000	17.337698000
C	9.254531000	1.471431000	19.276265000
H	8.310857000	2.009300000	19.303256000
C	10.150804000	1.559824000	20.337253000
H	9.916868000	2.173388000	21.203437000
C	11.356215000	0.861104000	20.283309000
H	12.061742000	0.939227000	21.107618000
C	10.542587000	-0.393435000	15.709915000
H	9.504338000	-0.760132000	15.651392000
H	10.542334000	0.687509000	15.576012000
C	11.105513000	-2.195880000	17.154907000
H	11.591017000	-2.494519000	18.083152000
H	11.602725000	-2.704634000	16.325060000
H	10.055247000	-2.527001000	17.194018000
N	18.500901000	2.219300000	20.676052000
C	20.070429000	4.679622000	21.112808000
H	20.958257000	4.622405000	21.752951000
H	19.220829000	4.363736000	21.712328000
C	19.858342000	6.104605000	20.666315000
C	18.612454000	6.512768000	20.180303000
H	17.801275000	5.793399000	20.126231000
C	18.401950000	7.829819000	19.783065000
H	17.426425000	8.134301000	19.415186000

C	19.439394000	8.759036000	19.866314000
H	19.276144000	9.787241000	19.556400000
C	20.681840000	8.365488000	20.358383000
H	21.491125000	9.086213000	20.435160000
C	20.885896000	7.045947000	20.760533000
H	21.848270000	6.743235000	21.164948000
C	18.262746000	2.465074000	22.041924000
C	16.981300000	2.969357000	22.378985000
C	16.570610000	2.944259000	23.713625000
H	15.580337000	3.309014000	23.972670000
C	17.413878000	2.472080000	24.714585000
H	17.078258000	2.443946000	25.747320000
C	18.711689000	2.090004000	24.388351000
H	19.393759000	1.787308000	25.178212000
C	19.168994000	2.101374000	23.067521000
C	16.098408000	3.593660000	21.312887000
H	16.733328000	3.733191000	20.431754000
C	15.582038000	4.969322000	21.747436000
H	14.843156000	4.891491000	22.552382000
H	15.089949000	5.471633000	20.907334000
H	16.393380000	5.612562000	22.101458000
C	14.929859000	2.698431000	20.894294000
H	14.313545000	2.423475000	21.757242000
H	15.272475000	1.773853000	20.424298000
H	14.283978000	3.206864000	20.171538000
C	20.625744000	1.799972000	22.772244000
H	20.833223000	2.148731000	21.760347000
C	20.953477000	0.308204000	22.802642000
H	20.692392000	-0.139325000	23.767839000
H	22.024178000	0.152237000	22.636584000
H	20.414099000	-0.227956000	22.019780000
C	21.565727000	2.568210000	23.706491000
H	21.294316000	3.625726000	23.774648000
H	22.592942000	2.501695000	23.335169000
H	21.553883000	2.157855000	24.722241000
N	17.199151000	-1.131480000	21.541994000
C	19.358669000	-1.776438000	19.806597000
H	20.087225000	-2.120782000	19.070857000
H	19.847689000	-1.660406000	20.775527000
C	18.139717000	-2.587507000	19.810926000
C	17.036782000	-2.268394000	20.656651000
C	15.827388000	-2.962286000	20.565755000

H	15.001112000	-2.700619000	21.217075000
C	15.656794000	-3.968437000	19.621690000
H	14.708390000	-4.491192000	19.550783000
C	16.708894000	-4.279169000	18.756839000
H	16.581224000	-5.049253000	18.001312000
C	17.915212000	-3.602152000	18.851678000
H	18.728926000	-3.850151000	18.174592000
C	17.996209000	-1.456922000	22.734620000
H	17.431946000	-2.135318000	23.390436000
H	18.221338000	-0.537856000	23.279718000
H	18.926265000	-1.948213000	22.454196000
C	15.944158000	-0.515143000	21.987111000
H	15.290843000	-0.322596000	21.134515000
H	16.179057000	0.427817000	22.485465000
H	15.397525000	-1.149664000	22.699167000
Al	13.811788000	-0.155906000	17.222761000
C	14.147234000	-1.489382000	15.766745000
H	14.896977000	-1.054392000	15.088089000
H	13.246956000	-1.603057000	15.145775000
C	14.629912000	-2.866108000	16.227456000
H	15.541093000	-2.790774000	16.830669000
H	13.889311000	-3.364996000	16.864328000
H	14.851937000	-3.556259000	15.398877000
C	13.734654000	1.790606000	16.733680000
H	13.915503000	2.345053000	17.668894000
H	14.634174000	1.971531000	16.124650000
C	12.538010000	2.421571000	16.022194000
H	12.340548000	1.936899000	15.058603000
H	12.681776000	3.492147000	15.809910000
H	11.624419000	2.339992000	16.621792000
C	15.984899000	-0.070077000	18.094597000
H	15.524836000	0.861731000	18.414450000
H	15.687153000	-1.001590000	18.571002000
C	16.924606000	-0.095871000	16.917482000
H	16.864966000	-1.040823000	16.371798000
H	18.026426000	0.008752000	17.128488000
H	16.737322000	0.713626000	16.206372000
H	11.101993000	-0.843997000	14.884726000

Int-4

Y	0.562308000	-1.377071000	0.087234000
N	2.009086000	0.300693000	-0.739357000

N	2.653864000	2.257139000	0.489071000
N	-6.506408000	-2.018740000	-2.371317000
C	1.901423000	1.121466000	0.327303000
C	3.923597000	2.447735000	-0.209512000
H	3.985649000	3.495108000	-0.519440000
H	3.927343000	1.848861000	-1.117681000
C	5.111610000	2.084857000	0.648853000
C	5.305089000	0.757751000	1.049639000
H	4.596986000	-0.002420000	0.734540000
C	6.400923000	0.406111000	1.832364000
H	6.545839000	-0.630246000	2.123952000
C	7.316706000	1.380758000	2.233048000
H	8.171703000	1.107110000	2.844669000
C	7.132458000	2.703930000	1.839047000
H	7.842191000	3.467605000	2.144697000
C	6.035878000	3.051075000	1.049223000
H	5.898043000	4.081349000	0.731658000
C	2.421151000	0.615499000	-2.045450000
C	3.382073000	-0.221440000	-2.663864000
C	3.731024000	0.004617000	-3.997711000
H	4.472526000	-0.637848000	-4.465550000
C	3.159380000	1.037186000	-4.727227000
H	3.444228000	1.205436000	-5.762042000
C	2.214598000	1.857199000	-4.117489000
H	1.764663000	2.659438000	-4.693087000
C	1.820900000	1.666012000	-2.792287000
C	4.066197000	-1.344943000	-1.909835000
H	3.675595000	-1.334270000	-0.886774000
C	5.582414000	-1.131973000	-1.845573000
H	6.038767000	-1.224629000	-2.837652000
H	6.051571000	-1.879618000	-1.195875000
H	5.834894000	-0.142478000	-1.455276000
C	3.745782000	-2.711829000	-2.522955000
H	4.116628000	-2.778037000	-3.552041000
H	2.668679000	-2.900512000	-2.551796000
H	4.217151000	-3.516043000	-1.947644000
C	0.719194000	2.525452000	-2.197960000
H	0.953063000	2.687888000	-1.143863000
C	-0.625129000	1.795106000	-2.268576000
H	-0.905300000	1.597429000	-3.308857000
H	-1.418599000	2.398018000	-1.813722000
H	-0.591497000	0.835880000	-1.748649000

C	0.601811000	3.908621000	-2.835154000
H	1.553112000	4.448923000	-2.815470000
H	-0.134266000	4.506208000	-2.289048000
H	0.256669000	3.854818000	-3.873382000
C	-4.495019000	-2.240555000	-0.505787000
H	-3.723304000	-1.890949000	0.183502000
H	-4.399603000	-3.334169000	-0.552530000
C	-5.854517000	-1.829349000	-0.040462000
C	-6.881773000	-1.701481000	-0.999006000
C	-8.156587000	-1.262558000	-0.654004000
H	-8.931217000	-1.171466000	-1.408786000
C	-8.432067000	-0.912202000	0.667447000
H	-9.422862000	-0.558762000	0.937478000
C	-7.430133000	-1.010887000	1.630800000
H	-7.636556000	-0.729546000	2.660012000
C	-6.162040000	-1.467988000	1.277590000
H	-5.382295000	-1.539007000	2.032254000
C	-7.232380000	-1.259960000	-3.399432000
H	-8.279378000	-1.576324000	-3.484523000
H	-7.192543000	-0.195429000	-3.168843000
C	-6.659583000	-3.466180000	-2.627877000
H	-6.071193000	-4.032174000	-1.904910000
H	-6.301407000	-3.693390000	-3.633786000
H	-7.712201000	-3.763274000	-2.540096000
N	0.979852000	0.677477000	1.193324000
C	2.422325000	3.211756000	1.571947000
H	3.251512000	3.154779000	2.287966000
H	1.518791000	2.925488000	2.103380000
C	2.274477000	4.629516000	1.080735000
C	1.110624000	5.026946000	0.415862000
H	0.314130000	4.305405000	0.260174000
C	0.963873000	6.334898000	-0.035979000
H	0.052601000	6.630778000	-0.547634000
C	1.982215000	7.265634000	0.173598000
H	1.868339000	8.286654000	-0.179335000
C	3.140329000	6.882974000	0.846860000
H	3.933352000	7.604649000	1.021829000
C	3.282378000	5.571294000	1.298819000
H	4.179572000	5.272079000	1.834255000
C	0.628384000	1.027852000	2.505679000
C	-0.668939000	1.565072000	2.691315000
C	-1.180942000	1.663159000	3.986493000

H	-2.180631000	2.060252000	4.138447000
C	-0.421849000	1.271207000	5.086216000
H	-0.836162000	1.338186000	6.088293000
C	0.891417000	0.847299000	4.899562000
H	1.503746000	0.611522000	5.765415000
C	1.448147000	0.743237000	3.622011000
C	-1.443657000	2.062786000	1.485365000
H	-0.696149000	2.282316000	0.713676000
C	-2.216576000	3.351458000	1.770954000
H	-3.065608000	3.179979000	2.441797000
H	-2.623652000	3.758778000	0.839256000
H	-1.576943000	4.114662000	2.225653000
C	-2.373172000	0.999097000	0.899983000
H	-3.120956000	0.680905000	1.634063000
H	-1.820634000	0.114641000	0.568607000
H	-2.900575000	1.385688000	0.024636000
C	2.913512000	0.402776000	3.434028000
H	3.207197000	0.796629000	2.458905000
C	3.178674000	-1.101285000	3.396278000
H	2.898869000	-1.578316000	4.341782000
H	4.241990000	-1.298124000	3.222000000
H	2.615115000	-1.580986000	2.592599000
C	3.809713000	1.082578000	4.470125000
H	3.586689000	2.150728000	4.556572000
H	4.859012000	0.978847000	4.177636000
H	3.699502000	0.636245000	5.464717000
N	-0.430289000	-2.645579000	2.162909000
C	1.808342000	-3.465621000	0.576220000
H	2.561692000	-3.872369000	-0.100299000
H	2.223308000	-3.358712000	1.578490000
C	0.522485000	-4.142684000	0.466334000
C	-0.614885000	-3.740297000	1.231927000
C	-1.875128000	-4.300025000	1.002823000
H	-2.723980000	-3.981268000	1.596555000
C	-2.070174000	-5.228364000	-0.012425000
H	-3.058769000	-5.639229000	-0.191145000
C	-0.984637000	-5.607464000	-0.806895000
H	-1.124483000	-6.317668000	-1.617281000
C	0.273510000	-5.082295000	-0.564344000
H	1.113183000	-5.384150000	-1.185774000
C	0.286740000	-3.035450000	3.385327000
H	-0.345934000	-3.689644000	4.002605000

H	0.533670000	-2.137976000	3.956587000
H	1.202810000	-3.572687000	3.146076000
C	-1.661684000	-1.962939000	2.557922000
H	-2.251681000	-1.707988000	1.677191000
H	-1.398510000	-1.045395000	3.088989000
H	-2.283481000	-2.579842000	3.223666000
Al	-4.401015000	-1.519094000	-2.377524000
C	-3.717129000	-2.549717000	-3.936062000
H	-2.896825000	-1.960993000	-4.372265000
H	-4.488528000	-2.563467000	-4.723436000
C	-3.226527000	-3.976591000	-3.671109000
H	-2.430104000	-3.987821000	-2.920194000
H	-4.025339000	-4.621373000	-3.283954000
H	-2.830738000	-4.470437000	-4.570466000
C	-4.434944000	0.469005000	-2.548892000
H	-3.387555000	0.800867000	-2.486722000
H	-4.742565000	0.744850000	-3.569740000
C	-5.265697000	1.260590000	-1.531937000
H	-6.341119000	1.081576000	-1.645931000
H	-5.117252000	2.347804000	-1.610628000
H	-5.029018000	0.977269000	-0.501131000
C	-1.190298000	-1.672610000	-1.539114000
H	-1.909298000	-0.863540000	-1.726451000
H	-1.766872000	-2.576217000	-1.297764000
C	-0.324456000	-1.921279000	-2.777767000
H	-0.866803000	-2.307571000	-3.653468000
H	0.459308000	-2.673194000	-2.582724000
H	0.193689000	-1.012255000	-3.112881000
H	-6.743484000	-1.431073000	-4.361782000

Int-5

Y	0.953824000	0.055643000	-0.852322000
N	-1.051817000	-1.018871000	-0.147692000
N	-3.103426000	0.195249000	0.252832000
N	2.450102000	-1.960106000	-0.191505000
C	-1.800064000	0.094344000	-0.176594000
C	-3.865488000	-0.966608000	0.706395000
H	-3.800874000	-1.059098000	1.795848000
H	-3.417332000	-1.862093000	0.281121000
C	-5.319693000	-0.913420000	0.312374000
C	-5.699651000	-0.762028000	-1.023805000
H	-4.934620000	-0.652210000	-1.783345000

C	-7.044478000	-0.746990000	-1.380926000
H	-7.323879000	-0.626906000	-2.423943000
C	-8.030133000	-0.891285000	-0.403559000
H	-9.080206000	-0.880507000	-0.681496000
C	-7.660517000	-1.048985000	0.930427000
H	-8.421504000	-1.161305000	1.697689000
C	-6.311723000	-1.056462000	1.284816000
H	-6.022849000	-1.173412000	2.326341000
C	-1.229142000	-2.273361000	0.462605000
C	-1.243299000	-3.403367000	-0.397485000
C	-1.237835000	-4.682752000	0.161141000
H	-1.246887000	-5.550238000	-0.490772000
C	-1.218377000	-4.865476000	1.540325000
H	-1.205488000	-5.867293000	1.959954000
C	-1.236166000	-3.755544000	2.376289000
H	-1.244397000	-3.899134000	3.452548000
C	-1.252497000	-2.454334000	1.865553000
C	-1.312359000	-3.207584000	-1.902521000
H	-0.663410000	-2.357843000	-2.148670000
C	-2.733626000	-2.813141000	-2.319100000
H	-3.455835000	-3.580628000	-2.020170000
H	-2.801796000	-2.687987000	-3.404602000
H	-3.026791000	-1.870355000	-1.855085000
C	-0.840640000	-4.409044000	-2.718529000
H	-1.535287000	-5.252711000	-2.640123000
H	0.149068000	-4.760230000	-2.410317000
H	-0.784221000	-4.136436000	-3.777231000
C	-1.303329000	-1.275154000	2.815946000
H	-1.720082000	-0.428539000	2.269175000
C	0.091870000	-0.856194000	3.278172000
H	0.598980000	-1.673658000	3.802363000
H	0.029080000	-0.001846000	3.960614000
H	0.710737000	-0.560148000	2.429756000
C	-2.211980000	-1.514576000	4.022973000
H	-3.191164000	-1.903435000	3.726316000
H	-2.368531000	-0.573499000	4.557119000
H	-1.773563000	-2.225303000	4.732313000
C	2.653943000	0.678175000	0.868501000
H	2.841522000	1.698635000	1.202954000
H	2.374009000	0.041523000	1.704293000
C	3.655582000	0.165368000	-0.034928000
C	3.569639000	-1.144459000	-0.603746000

C	4.442764000	-1.548591000	-1.614538000
H	4.355700000	-2.545851000	-2.031009000
C	5.410330000	-0.688420000	-2.126496000
H	6.074526000	-1.020990000	-2.916424000
C	5.509749000	0.603824000	-1.607839000
H	6.238016000	1.301986000	-2.010026000
C	4.666791000	1.012971000	-0.572542000
H	4.699104000	2.042669000	-0.226954000
C	2.588802000	-2.517191000	1.164316000
H	3.323160000	-3.334564000	1.164029000
H	1.621556000	-2.903992000	1.493932000
H	2.932203000	-1.756599000	1.862857000
C	2.104051000	-3.046603000	-1.108626000
H	1.943750000	-2.663007000	-2.118727000
H	1.185222000	-3.508436000	-0.745161000
H	2.880845000	-3.823485000	-1.147003000
N	-1.110498000	1.138677000	-0.692896000
C	-3.651710000	1.476644000	0.710072000
H	-4.707576000	1.502166000	0.429626000
H	-3.162289000	2.286507000	0.175515000
C	-3.503220000	1.683521000	2.197612000
C	-2.247068000	1.976909000	2.740693000
H	-1.386304000	2.039221000	2.082480000
C	-2.096926000	2.191348000	4.107529000
H	-1.117935000	2.432291000	4.511917000
C	-3.204190000	2.105873000	4.953909000
H	-3.089177000	2.275842000	6.020579000
C	-4.456577000	1.803231000	4.424022000
H	-5.321887000	1.732960000	5.077190000
C	-4.603486000	1.594950000	3.052219000
H	-5.581800000	1.369558000	2.636047000
C	-1.604452000	2.298937000	-1.312279000
C	-1.084314000	3.548432000	-0.892911000
C	-1.528589000	4.719054000	-1.512348000
H	-1.133686000	5.675739000	-1.181654000
C	-2.462401000	4.679749000	-2.538437000
H	-2.810027000	5.598300000	-3.002638000
C	-2.935437000	3.447824000	-2.980529000
H	-3.640830000	3.418701000	-3.804582000
C	-2.511715000	2.249439000	-2.404598000
C	-0.018039000	3.637357000	0.180593000
H	0.037230000	2.655936000	0.663974000

C	-0.335418000	4.672301000	1.262115000
H	-0.306465000	5.693534000	0.867211000
H	0.403005000	4.615682000	2.069582000
H	-1.325747000	4.509706000	1.696780000
C	1.349154000	3.926836000	-0.453787000
H	1.340996000	4.898566000	-0.959920000
H	1.620640000	3.181275000	-1.210972000
H	2.140191000	3.944501000	0.303005000
C	-2.940470000	0.923687000	-3.005085000
H	-3.063961000	0.211562000	-2.186734000
C	-1.835665000	0.386710000	-3.921085000
H	-1.652356000	1.078612000	-4.750689000
H	-2.115661000	-0.583718000	-4.343633000
H	-0.893754000	0.266585000	-3.381909000
C	-4.268619000	0.979805000	-3.758440000
H	-5.066238000	1.418244000	-3.150758000
H	-4.576169000	-0.031719000	-4.045692000
H	-4.188561000	1.558722000	-4.684816000
Al	6.718156000	0.515559000	0.988964000
C	6.952154000	2.466901000	1.310601000
H	7.723508000	2.554110000	2.093777000
H	6.043875000	2.892435000	1.761973000
C	7.379123000	3.303179000	0.099868000
H	8.287967000	2.903872000	-0.366944000
H	6.605958000	3.317528000	-0.679261000
H	7.585476000	4.352847000	0.352059000
C	5.760357000	-0.564768000	2.353508000
H	4.823872000	-0.070355000	2.642345000
H	5.473577000	-1.533823000	1.923372000
C	6.635141000	-0.786563000	3.596191000
H	7.573994000	-1.299225000	3.349919000
H	6.138930000	-1.392781000	4.367668000
H	6.910383000	0.163208000	4.072629000
C	8.195142000	-0.409050000	0.023719000
H	8.347190000	0.019027000	-0.976152000
H	9.118316000	-0.164774000	0.575531000
C	8.053927000	-1.930589000	-0.073857000
H	7.966784000	-2.390749000	0.917979000
H	8.906358000	-2.410735000	-0.575415000
H	7.152741000	-2.213127000	-0.630297000
C	1.698271000	0.261629000	-3.144719000
H	1.151183000	1.139946000	-3.536350000

H	2.741400000	0.613690000	-3.040174000
C	1.670258000	-0.841656000	-4.205881000
H	0.669343000	-1.279503000	-4.327568000
H	2.343093000	-1.667996000	-3.938997000
H	1.983435000	-0.511245000	-5.209083000

TS-3

Y	-0.988183000	-0.115083000	1.084796000
N	0.915501000	-1.033393000	0.004994000
N	2.976942000	0.188188000	-0.300772000
N	-2.616541000	-1.924523000	0.135634000
C	1.696535000	0.043163000	0.180248000
C	3.670344000	-0.890706000	-1.004606000
H	3.529576000	-0.789744000	-2.086641000
H	3.225169000	-1.838531000	-0.709934000
C	5.147399000	-0.927617000	-0.705323000
C	5.608666000	-1.080064000	0.604997000
H	4.891399000	-1.156922000	1.413640000
C	6.972652000	-1.124875000	0.876325000
H	7.315112000	-1.239300000	1.901004000
C	7.896716000	-1.024717000	-0.164516000
H	8.961745000	-1.058301000	0.046713000
C	7.446398000	-0.882727000	-1.475264000
H	8.159602000	-0.806494000	-2.291298000
C	6.078267000	-0.832219000	-1.741889000
H	5.725971000	-0.713985000	-2.763536000
C	1.017726000	-2.164091000	-0.821309000
C	1.042220000	-3.427353000	-0.173328000
C	0.978710000	-4.587626000	-0.947014000
H	0.997452000	-5.556736000	-0.459139000
C	0.890146000	-4.523446000	-2.334100000
H	0.835613000	-5.435660000	-2.921474000
C	0.888377000	-3.283650000	-2.962769000
H	0.837880000	-3.237089000	-4.046460000
C	0.957554000	-2.093297000	-2.233349000
C	1.188737000	-3.503604000	1.337735000
H	0.565098000	-2.710672000	1.770677000
C	2.633870000	-3.197756000	1.746519000
H	3.326897000	-3.911045000	1.287180000
H	2.754114000	-3.258508000	2.833153000
H	2.924401000	-2.193613000	1.434048000
C	0.743489000	-4.830340000	1.948995000

H	1.420993000	-5.649055000	1.682550000
H	-0.265831000	-5.117033000	1.637514000
H	0.745915000	-4.753687000	3.040928000
C	0.968463000	-0.760852000	-2.956411000
H	1.462175000	-0.035726000	-2.307555000
C	-0.447139000	-0.235375000	-3.196542000
H	-1.032208000	-0.929238000	-3.809686000
H	-0.415889000	0.729885000	-3.712852000
H	-0.973382000	-0.089031000	-2.251786000
C	1.755406000	-0.791686000	-4.267198000
H	2.743227000	-1.246425000	-4.140468000
H	1.898305000	0.228003000	-4.635120000
H	1.229409000	-1.351367000	-5.048496000
C	-2.758982000	0.908204000	-0.308322000
H	-2.915309000	1.986115000	-0.359711000
H	-2.595648000	0.506137000	-1.305120000
C	-3.749121000	0.224161000	0.516764000
C	-3.687804000	-1.187750000	0.767026000
C	-4.519247000	-1.778439000	1.717617000
H	-4.464511000	-2.846901000	1.890085000
C	-5.401438000	-1.018061000	2.482199000
H	-6.031650000	-1.502777000	3.220680000
C	-5.452053000	0.360494000	2.294808000
H	-6.116936000	0.972454000	2.897113000
C	-4.657845000	0.960570000	1.324850000
H	-4.673683000	2.039186000	1.206889000
C	-2.799799000	-2.154469000	-1.305016000
H	-3.589699000	-2.898149000	-1.477280000
H	-1.862361000	-2.521897000	-1.729275000
H	-3.082847000	-1.235111000	-1.808329000
C	-2.293617000	-3.204818000	0.769165000
H	-2.102804000	-3.068535000	1.835919000
H	-1.397638000	-3.598183000	0.286745000
H	-3.096656000	-3.945232000	0.645694000
N	1.067837000	0.989899000	0.915316000
C	3.543697000	1.517355000	-0.549500000
H	4.618141000	1.457957000	-0.358935000
H	3.133953000	2.222509000	0.169387000
C	3.290938000	2.010102000	-1.953412000
C	1.999825000	2.387591000	-2.340586000
H	1.186564000	2.307784000	-1.626097000
C	1.754655000	2.862776000	-3.625513000

H	0.749863000	3.164939000	-3.906733000
C	2.799410000	2.957984000	-4.546856000
H	2.609437000	3.329663000	-5.549721000
C	4.085631000	2.574217000	-4.173948000
H	4.902831000	2.643451000	-4.886635000
C	4.328270000	2.104923000	-2.882584000
H	5.333254000	1.815608000	-2.587076000
C	1.612386000	2.031643000	1.686087000
C	1.064910000	3.329493000	1.526392000
C	1.544542000	4.378893000	2.313921000
H	1.125140000	5.372436000	2.180791000
C	2.541902000	4.175986000	3.257067000
H	2.912971000	5.003672000	3.854827000
C	3.046334000	2.892938000	3.443112000
H	3.802929000	2.729288000	4.203582000
C	2.592997000	1.808402000	2.690619000
C	-0.067215000	3.606425000	0.556345000
H	-0.203474000	2.707883000	-0.055630000
C	0.234098000	4.774434000	-0.386557000
H	0.275181000	5.727337000	0.152286000
H	-0.549349000	4.863195000	-1.147466000
H	1.190380000	4.639812000	-0.899355000
C	-1.373385000	3.860425000	1.320747000
H	-1.278632000	4.742830000	1.963155000
H	-1.642808000	3.020259000	1.971439000
H	-2.205717000	4.034311000	0.630853000
C	3.069015000	0.408613000	3.031587000
H	3.061953000	-0.182096000	2.113651000
C	2.090041000	-0.244446000	4.013144000
H	2.056370000	0.315510000	4.954623000
H	2.390889000	-1.272933000	4.239604000
H	1.074938000	-0.265506000	3.611003000
C	4.490899000	0.356212000	3.590293000
H	5.205690000	0.864020000	2.935768000
H	4.809994000	-0.685709000	3.701381000
H	4.556780000	0.810193000	4.584745000
Al	-5.897111000	0.665712000	-1.217342000
C	-6.252853000	2.607242000	-0.959849000
H	-6.608739000	2.966332000	-1.939450000
H	-5.308469000	3.146847000	-0.797348000
C	-7.275686000	2.986794000	0.113492000
H	-8.240371000	2.494625000	-0.059555000

H	-6.949157000	2.682068000	1.114708000
H	-7.471471000	4.067342000	0.157226000
C	-5.005026000	0.218654000	-2.942862000
H	-4.077454000	0.785752000	-3.092623000
H	-4.737439000	-0.843313000	-2.997060000
C	-5.991429000	0.536638000	-4.080117000
H	-6.934245000	-0.015756000	-3.970293000
H	-5.593157000	0.281006000	-5.071972000
H	-6.250146000	1.602284000	-4.109142000
C	-7.226817000	-0.674244000	-0.604591000
H	-7.378110000	-0.616880000	0.479698000
H	-8.184930000	-0.344996000	-1.042095000
C	-6.954909000	-2.121990000	-1.022647000
H	-6.817124000	-2.214641000	-2.107132000
H	-7.768509000	-2.807571000	-0.745655000
H	-6.042192000	-2.505155000	-0.553716000
C	-1.548444000	-0.350708000	3.435240000
H	-0.989658000	0.455429000	3.947055000
H	-2.603442000	-0.024133000	3.483094000
C	-1.406713000	-1.642706000	4.244364000
H	-0.386009000	-2.048450000	4.208175000
H	-2.068222000	-2.430203000	3.857721000
H	-1.656226000	-1.539279000	5.312678000

Int-6

Y	1.056044000	-1.163656000	-0.630850000
N	-0.862442000	-0.919556000	0.698995000
N	-2.710235000	0.507478000	0.073049000
N	2.596514000	-1.909896000	1.283641000
C	-1.518806000	-0.127645000	-0.167231000
C	-3.495595000	0.252877000	1.282692000
H	-3.248155000	0.988326000	2.054526000
H	-3.221646000	-0.726066000	1.670291000
C	-4.981789000	0.292682000	1.033560000
C	-5.595041000	-0.634639000	0.186500000
H	-4.991641000	-1.391833000	-0.301269000
C	-6.968087000	-0.592674000	-0.035729000
H	-7.429479000	-1.318510000	-0.699335000
C	-7.749941000	0.375775000	0.595137000
H	-8.821579000	0.409528000	0.420842000
C	-7.150233000	1.295832000	1.452203000
H	-7.752349000	2.049740000	1.951413000

C	-5.773201000	1.252710000	1.668139000
H	-5.303437000	1.971147000	2.335138000
C	-1.042798000	-1.194738000	2.069815000
C	-1.244242000	-2.557067000	2.413550000
C	-1.272600000	-2.921746000	3.760643000
H	-1.429839000	-3.961169000	4.030551000
C	-1.100546000	-1.973663000	4.764259000
H	-1.117781000	-2.272317000	5.808573000
C	-0.921946000	-0.639200000	4.420843000
H	-0.804704000	0.101292000	5.206186000
C	-0.896581000	-0.222190000	3.086765000
C	-1.481358000	-3.587042000	1.323773000
H	-0.852731000	-3.310945000	0.468525000
C	-2.933939000	-3.510111000	0.840736000
H	-3.627591000	-3.707883000	1.665340000
H	-3.125021000	-4.243780000	0.050849000
H	-3.158464000	-2.519063000	0.440170000
C	-1.124799000	-5.017653000	1.719817000
H	-1.820851000	-5.422610000	2.462521000
H	-0.113940000	-5.091343000	2.132876000
H	-1.176507000	-5.670112000	0.842586000
C	-0.708951000	1.246683000	2.766903000
H	-1.110309000	1.426818000	1.768919000
C	0.768505000	1.630611000	2.729017000
H	1.247812000	1.472271000	3.700186000
H	0.883224000	2.684964000	2.463658000
H	1.316106000	1.041625000	1.991084000
C	-1.457390000	2.179626000	3.722075000
H	-2.499309000	1.876688000	3.867196000
H	-1.451481000	3.196295000	3.319892000
H	-0.983731000	2.216395000	4.709112000
C	3.193151000	0.505162000	-0.221578000
H	2.908129000	1.102871000	-1.089249000
H	2.478139000	0.573540000	0.599296000
C	3.788108000	-0.800288000	-0.543378000
C	3.574840000	-1.978742000	0.224658000
C	4.210398000	-3.178637000	-0.115363000
H	4.044112000	-4.064360000	0.486564000
C	5.033025000	-3.255125000	-1.229211000
H	5.516541000	-4.193229000	-1.482451000
C	5.221806000	-2.119684000	-2.022333000
H	5.853439000	-2.168818000	-2.904419000

C	4.613332000	-0.924296000	-1.682458000
H	4.782322000	-0.038602000	-2.287222000
C	3.054561000	-1.156362000	2.463597000
H	3.797299000	-1.742252000	3.020752000
H	2.199185000	-0.952691000	3.111403000
H	3.514618000	-0.215321000	2.170264000
C	2.068230000	-3.200941000	1.728759000
H	1.701748000	-3.782449000	0.879373000
H	1.240796000	-3.010990000	2.414364000
H	2.823338000	-3.798744000	2.257558000
N	-0.846147000	-0.026554000	-1.339575000
C	-3.049533000	1.759895000	-0.614374000
H	-4.138524000	1.810606000	-0.676160000
H	-2.678164000	1.721536000	-1.635367000
C	-2.507248000	2.983549000	0.081707000
C	-1.132630000	3.247529000	0.057074000
H	-0.471693000	2.555992000	-0.454960000
C	-0.613296000	4.380457000	0.675537000
H	0.454641000	4.575439000	0.637211000
C	-1.467563000	5.267922000	1.333259000
H	-1.065189000	6.155189000	1.813474000
C	-2.836735000	5.012350000	1.367033000
H	-3.506237000	5.699782000	1.876471000
C	-3.352679000	3.874711000	0.744760000
H	-4.422133000	3.681863000	0.760515000
C	-1.349493000	0.321351000	-2.606465000
C	-0.627540000	1.274056000	-3.366544000
C	-1.098381000	1.647550000	-4.627382000
H	-0.546608000	2.387042000	-5.200584000
C	-2.254116000	1.091815000	-5.156136000
H	-2.619663000	1.403408000	-6.130396000
C	-2.924385000	0.107925000	-4.436043000
H	-3.803809000	-0.353466000	-4.872506000
C	-2.485865000	-0.312819000	-3.179505000
C	0.690179000	1.841666000	-2.881271000
H	0.769578000	1.612704000	-1.811635000
C	0.804586000	3.359131000	-3.029696000
H	0.836760000	3.662721000	-4.081247000
H	1.728698000	3.715050000	-2.562120000
H	-0.037483000	3.871775000	-2.556514000
C	1.847715000	1.142990000	-3.609458000
H	1.790168000	1.332257000	-4.686735000

H	1.822348000	0.053063000	-3.486064000
H	2.817305000	1.509848000	-3.259712000
C	-3.156897000	-1.493856000	-2.501425000
H	-3.195329000	-1.291554000	-1.429045000
C	-2.309389000	-2.753981000	-2.706566000
H	-2.215705000	-2.988532000	-3.772885000
H	-2.766070000	-3.615388000	-2.208723000
H	-1.301990000	-2.623738000	-2.308442000
C	-4.592166000	-1.746292000	-2.960553000
H	-5.215462000	-0.851689000	-2.869996000
H	-5.042663000	-2.536989000	-2.351052000
H	-4.634122000	-2.090384000	-3.999386000
Al	4.682420000	1.900169000	0.516926000
C	4.510043000	3.419538000	-0.792909000
H	4.951875000	4.327805000	-0.354377000
H	3.441834000	3.664064000	-0.920030000
C	5.148493000	3.170477000	-2.161637000
H	6.231304000	3.020811000	-2.071110000
H	4.756506000	2.262083000	-2.639787000
H	4.997255000	3.988561000	-2.882133000
C	4.163753000	2.490912000	2.372060000
H	3.248287000	3.099103000	2.320142000
H	3.922245000	1.666580000	3.058288000
C	5.287008000	3.333163000	2.993335000
H	6.206514000	2.746998000	3.115555000
H	5.034403000	3.739294000	3.984550000
H	5.547791000	4.191317000	2.359847000
C	6.465757000	0.985338000	0.469601000
H	6.707755000	0.639331000	-0.545601000
H	7.219234000	1.760025000	0.687468000
C	6.646294000	-0.177491000	1.450017000
H	6.401527000	0.115628000	2.479535000
H	7.671278000	-0.577910000	1.471530000
H	5.989057000	-1.017133000	1.195523000
C	1.273257000	-3.037160000	-2.091201000
H	0.764712000	-2.717882000	-3.019990000
H	2.347073000	-3.035482000	-2.349324000
C	0.850580000	-4.473169000	-1.770238000
H	-0.213058000	-4.542967000	-1.509023000
H	1.409596000	-4.878453000	-0.916124000
H	1.011732000	-5.179082000	-2.599650000

Int-7

Y	16.915135000	0.025318000	19.203481000
N	18.361096000	1.744849000	18.620777000
N	18.935670000	3.633349000	20.005561000
N	11.490182000	0.907433000	19.179058000
C	18.301426000	2.434067000	19.782156000
C	19.800800000	4.243113000	18.978564000
H	19.195042000	4.867663000	18.315174000
H	20.216619000	3.444570000	18.370595000
C	20.935776000	5.078924000	19.517090000
C	22.082479000	4.481625000	20.049256000
H	22.153780000	3.400932000	20.085229000
C	23.136956000	5.258960000	20.521490000
H	24.017741000	4.777617000	20.937242000
C	23.066316000	6.649620000	20.448525000
H	23.888709000	7.257912000	20.814693000
C	21.941621000	7.254471000	19.890611000
H	21.880857000	8.336670000	19.820092000
C	20.885350000	6.473157000	19.428642000
H	20.005731000	6.949015000	19.005602000
C	18.781210000	2.093806000	17.323431000
C	19.849473000	1.343395000	16.769556000
C	20.219979000	1.578177000	15.444565000
H	21.040106000	1.015624000	15.010416000
C	19.554109000	2.521144000	14.667121000
H	19.855218000	2.690464000	13.637221000
C	18.498658000	3.241615000	15.213451000
H	17.977893000	3.970340000	14.599667000
C	18.091611000	3.043836000	16.535106000
C	20.588474000	0.327302000	17.624099000
H	19.839576000	-0.173359000	18.248672000
C	21.553149000	1.013222000	18.596613000
H	22.291114000	1.618279000	18.058694000
H	22.091185000	0.269278000	19.194283000
H	21.009231000	1.660841000	19.287295000
C	21.306018000	-0.753405000	16.819432000
H	22.175343000	-0.356174000	16.283782000
H	20.642166000	-1.221836000	16.085980000
H	21.672452000	-1.535612000	17.492286000
C	16.911943000	3.814029000	17.096098000
H	17.018179000	3.819717000	18.184978000
C	15.589501000	3.114531000	16.776251000

H	15.409185000	3.099435000	15.696876000
H	14.751200000	3.631545000	17.256028000
H	15.582005000	2.076764000	17.115149000
C	16.853388000	5.266334000	16.619386000
H	17.786711000	5.804993000	16.809877000
H	16.042768000	5.797757000	17.128713000
H	16.645011000	5.327525000	15.546577000
C	14.310373000	0.496179000	18.971806000
H	14.864046000	1.402829000	19.275664000
H	13.587187000	0.936641000	18.269853000
C	13.523301000	-0.048420000	20.128031000
C	12.119493000	0.135046000	20.191681000
C	11.386205000	-0.459762000	21.223896000
H	10.309572000	-0.326459000	21.258202000
C	12.014196000	-1.205255000	22.219305000
H	11.423807000	-1.653166000	23.013646000
C	13.396150000	-1.361506000	22.192198000
H	13.906622000	-1.936770000	22.958750000
C	14.125049000	-0.797501000	21.147124000
H	15.197519000	-0.987458000	21.129301000
C	11.687649000	2.342170000	19.325988000
H	11.089757000	2.765834000	20.151594000
H	11.399967000	2.850493000	18.399037000
H	12.738960000	2.562284000	19.522518000
C	10.110005000	0.584058000	18.881729000
H	9.998653000	-0.496414000	18.761375000
H	9.832680000	1.063485000	17.937103000
H	9.394382000	0.927583000	19.649974000
N	17.525254000	1.788758000	20.679727000
C	18.690632000	4.444066000	21.198051000
H	19.600143000	4.476100000	21.806431000
H	17.937034000	3.947276000	21.803968000
C	18.248803000	5.862555000	20.941741000
C	17.379747000	6.204369000	19.906367000
H	17.011375000	5.430978000	19.244904000
C	16.996415000	7.529132000	19.705550000
H	16.332064000	7.778683000	18.883015000
C	17.466472000	8.529727000	20.554007000
H	17.171659000	9.563402000	20.397203000
C	18.319668000	8.193962000	21.605417000
H	18.694296000	8.966102000	22.271480000
C	18.711587000	6.871907000	21.790950000

H	19.405362000	6.618247000	22.588378000
C	17.570721000	1.872652000	22.085538000
C	16.375542000	2.220275000	22.770030000
C	16.390239000	2.310083000	24.161541000
H	15.482151000	2.588261000	24.686117000
C	17.546798000	2.048540000	24.890170000
H	17.544322000	2.135491000	25.973101000
C	18.694065000	1.648594000	24.220086000
H	19.587876000	1.408156000	24.789487000
C	18.727259000	1.526654000	22.827178000
C	15.108385000	2.511234000	21.988412000
H	15.061111000	1.760749000	21.195604000
C	15.162303000	3.877353000	21.299519000
H	15.298253000	4.686722000	22.024559000
H	14.232928000	4.071562000	20.751833000
H	15.985204000	3.920189000	20.585060000
C	13.826640000	2.367900000	22.803506000
H	13.724927000	3.160523000	23.553687000
H	13.776167000	1.400623000	23.310821000
H	12.959533000	2.436106000	22.140334000
C	20.001588000	1.013967000	22.181751000
H	19.794262000	0.842266000	21.121042000
C	20.458570000	-0.317114000	22.792093000
H	20.813582000	-0.181839000	23.819626000
H	21.292005000	-0.729481000	22.212154000
H	19.656082000	-1.056666000	22.802838000
C	21.139636000	2.029643000	22.296146000
H	20.882025000	2.980554000	21.832162000
H	22.048492000	1.652309000	21.814545000
H	21.380665000	2.226309000	23.346911000
C	17.962361000	-1.507112000	20.692345000
H	19.042834000	-1.381150000	20.498993000
H	17.805182000	-1.008091000	21.663929000
Al	14.558627000	-0.970305000	17.450618000
C	13.001736000	-2.189128000	17.661141000
H	12.831393000	-2.647603000	16.673316000
H	12.111168000	-1.572925000	17.847961000
C	13.094316000	-3.289561000	18.722004000
H	13.974522000	-3.928157000	18.570221000
H	13.178421000	-2.868170000	19.728725000
H	12.220128000	-3.956637000	18.726865000
C	14.654813000	-0.086301000	15.662462000

H	15.572166000	0.502477000	15.521371000
H	14.736340000	-0.908318000	14.932176000
C	13.427440000	0.763152000	15.317097000
H	12.505888000	0.170491000	15.373646000
H	13.466294000	1.198441000	14.308060000
H	13.298403000	1.599089000	16.015962000
C	16.317988000	-2.041053000	17.683436000
H	16.570268000	-2.454926000	18.671347000
H	15.837946000	-2.903889000	17.197252000
C	17.601219000	-1.749882000	16.891123000
H	17.372140000	-1.541572000	15.841852000
H	18.319433000	-2.577227000	16.927711000
H	18.183755000	-0.868763000	17.215511000
C	17.650783000	-2.997089000	20.841471000
H	17.911777000	-3.560224000	19.935521000
H	18.187761000	-3.483242000	21.671616000
H	16.581676000	-3.178287000	21.020198000

TS-4

Y	18.090217000	0.323507000	19.022426000
N	19.542298000	2.027020000	18.432355000
N	20.150780000	3.833238000	19.877534000
N	11.158458000	-0.953427000	17.472770000
C	19.412940000	2.713119000	19.594407000
C	21.487862000	4.012361000	19.299301000
H	21.622842000	5.076347000	19.090564000
H	21.533965000	3.493391000	18.345524000
C	22.584272000	3.518221000	20.211515000
C	22.812225000	2.145064000	20.355632000
H	22.191000000	1.442815000	19.808566000
C	23.833181000	1.677060000	21.177763000
H	24.006141000	0.608439000	21.269583000
C	24.634222000	2.580020000	21.878663000
H	25.431794000	2.216748000	22.520450000
C	24.407216000	3.948600000	21.750874000
H	25.026443000	4.656812000	22.294400000
C	23.389119000	4.413746000	20.918578000
H	23.215926000	5.481174000	20.811478000
C	19.943850000	2.537756000	17.185040000
C	20.970893000	1.861823000	16.485365000
C	21.332548000	2.302858000	15.210294000
H	22.124188000	1.785702000	14.674858000

C	20.703019000	3.392287000	14.623292000
H	21.000603000	3.732294000	13.635419000
C	19.675920000	4.038480000	15.305963000
H	19.172387000	4.873797000	14.830126000
C	19.266584000	3.624849000	16.575110000
C	21.667860000	0.660429000	17.091836000
H	21.338630000	0.596610000	18.133960000
C	23.191955000	0.800202000	17.084033000
H	23.592254000	0.793388000	16.064520000
H	23.656496000	-0.032267000	17.623845000
H	23.512051000	1.730056000	17.562692000
C	21.235888000	-0.632126000	16.390429000
H	21.548037000	-0.631013000	15.339998000
H	20.147006000	-0.753354000	16.400112000
H	21.677788000	-1.509124000	16.875134000
C	18.055387000	4.261395000	17.234650000
H	18.243012000	4.314356000	18.310552000
C	16.814441000	3.386642000	17.023420000
H	16.608919000	3.258092000	15.955938000
H	15.929374000	3.833103000	17.486324000
H	16.941008000	2.388235000	17.451665000
C	17.765969000	5.684753000	16.756071000
H	18.660223000	6.315281000	16.780874000
H	17.004848000	6.146236000	17.393351000
H	17.375359000	5.697754000	15.732931000
C	13.150052000	-0.691597000	19.377902000
H	13.890212000	-0.297285000	20.084444000
H	13.106706000	-1.774720000	19.563341000
C	11.832977000	-0.033615000	19.605497000
C	10.828290000	-0.150382000	18.616244000
C	9.617833000	0.530850000	18.738558000
H	8.857678000	0.432649000	17.969783000
C	9.381875000	1.355714000	19.839087000
H	8.439085000	1.889266000	19.922037000
C	10.359996000	1.489219000	20.820741000
H	10.188169000	2.132607000	21.679777000
C	11.563939000	0.795923000	20.701193000
H	12.327790000	0.906597000	21.466933000
C	10.413289000	-0.651393000	16.255584000
H	9.373259000	-1.011711000	16.295968000
H	10.408360000	0.421367000	16.073328000
C	11.033240000	-2.388099000	17.756002000

H	11.586887000	-2.654245000	18.655140000
H	11.435996000	-2.960651000	16.917316000
H	9.979435000	-2.669932000	17.903212000
N	18.490508000	2.156715000	20.395953000
C	19.904399000	4.635418000	21.073238000
H	20.524993000	4.283626000	21.905154000
H	18.867015000	4.497035000	21.370619000
C	20.146865000	6.107022000	20.857096000
C	19.593594000	6.771914000	19.759541000
H	19.023226000	6.206292000	19.031538000
C	19.781742000	8.140676000	19.592639000
H	19.346930000	8.644214000	18.733776000
C	20.523121000	8.864091000	20.527452000
H	20.670394000	9.932524000	20.398411000
C	21.074931000	8.209094000	21.626647000
H	21.654769000	8.765093000	22.358063000
C	20.889674000	6.836311000	21.787495000
H	21.326216000	6.322870000	22.640610000
C	18.086520000	2.464327000	21.712674000
C	16.807953000	3.044983000	21.882695000
C	16.326179000	3.253219000	23.177320000
H	15.348922000	3.708718000	23.312746000
C	17.081229000	2.898705000	24.288920000
H	16.694080000	3.064772000	25.290266000
C	18.343441000	2.340261000	24.111323000
H	18.936123000	2.077539000	24.982329000
C	18.869042000	2.117162000	22.837085000
C	15.990354000	3.504167000	20.690557000
H	16.519346000	3.174021000	19.792164000
C	15.915293000	5.033794000	20.634977000
H	15.408523000	5.437570000	21.518448000
H	15.354990000	5.361164000	19.752368000
H	16.910673000	5.487914000	20.590712000
C	14.592464000	2.883093000	20.668954000
H	13.999564000	3.189698000	21.537181000
H	14.639401000	1.790022000	20.672071000
H	14.041461000	3.188276000	19.774262000
C	20.246027000	1.507441000	22.671925000
H	20.611940000	1.780098000	21.678369000
C	20.170223000	-0.020754000	22.730598000
H	19.822355000	-0.355150000	23.714713000
H	21.152750000	-0.469413000	22.547089000

H	19.479762000	-0.418377000	21.981946000
C	21.263141000	2.034151000	23.684530000
H	21.299893000	3.128044000	23.692469000
H	22.262959000	1.671407000	23.432925000
H	21.038796000	1.698853000	24.702853000
C	19.136524000	-1.736440000	19.637596000
H	20.231630000	-1.639080000	19.726770000
H	18.801773000	-2.062502000	20.637524000
Al	13.643273000	-0.396535000	17.425068000
C	13.908068000	-1.875660000	16.092648000
H	14.576425000	-1.515254000	15.296128000
H	12.964597000	-2.102618000	15.575727000
C	14.482736000	-3.169834000	16.677320000
H	15.455035000	-3.000430000	17.159577000
H	13.829682000	-3.593701000	17.450589000
H	14.640610000	-3.961108000	15.929295000
C	13.539116000	1.533474000	16.851340000
H	13.801799000	2.090628000	17.765118000
H	14.394415000	1.694961000	16.176290000
C	12.309524000	2.198518000	16.233504000
H	12.018321000	1.721043000	15.290241000
H	12.470876000	3.263415000	16.006435000
H	11.446668000	2.149921000	16.907345000
C	15.919908000	-0.188258000	17.986392000
H	15.498546000	0.737025000	18.375429000
H	15.775932000	-1.103349000	18.557152000
C	16.663714000	-0.215114000	16.680894000
H	16.684413000	-1.222388000	16.257381000
H	17.751786000	0.094037000	16.683353000
H	16.235477000	0.451761000	15.926503000
H	10.907664000	-1.144676000	15.413850000
C	18.798576000	-2.846840000	18.627853000
H	19.135492000	-2.605539000	17.610177000
H	19.248424000	-3.822872000	18.868633000
H	17.715853000	-3.023105000	18.561994000

Int-8

Y	0.413469000	-1.744700000	0.045124000
N	1.803594000	-0.002161000	-0.659983000
N	2.396181000	1.893376000	0.679898000
N	-6.594029000	-2.631745000	-2.288652000
C	1.693394000	0.730300000	0.473708000

C	3.683353000	2.121893000	0.017747000
H	3.757133000	3.188111000	-0.209202000
H	3.687369000	1.595114000	-0.933424000
C	4.868272000	1.686873000	0.846411000
C	5.148703000	0.325479000	1.011100000
H	4.494216000	-0.411047000	0.555973000
C	6.257566000	-0.087933000	1.743306000
H	6.470045000	-1.148012000	1.849530000
C	7.097850000	0.858228000	2.333231000
H	7.964169000	0.537056000	2.904500000
C	6.820020000	2.215304000	2.185535000
H	7.468913000	2.957214000	2.642703000
C	5.712808000	2.625164000	1.442267000
H	5.503009000	3.683640000	1.313893000
C	2.144890000	0.442996000	-1.948661000
C	3.131503000	-0.280963000	-2.660495000
C	3.423680000	0.074228000	-3.979530000
H	4.181877000	-0.483848000	-4.522424000
C	2.769184000	1.128736000	-4.601316000
H	3.012409000	1.401641000	-5.624316000
C	1.788718000	1.828849000	-3.903531000
H	1.266297000	2.639552000	-4.400844000
C	1.447414000	1.500704000	-2.590723000
C	3.867897000	-1.440930000	-2.019751000
H	3.583563000	-1.451891000	-0.962585000
C	5.387936000	-1.279062000	-2.100698000
H	5.744896000	-1.339707000	-3.134567000
H	5.888981000	-2.071984000	-1.534348000
H	5.711460000	-0.317826000	-1.691644000
C	3.432343000	-2.778413000	-2.627819000
H	3.697260000	-2.831458000	-3.689892000
H	2.348841000	-2.921854000	-2.561937000
H	3.915540000	-3.617141000	-2.115600000
C	0.287018000	2.197503000	-1.903586000
H	0.553975000	2.326770000	-0.852208000
C	-0.964995000	1.317402000	-1.958140000
H	-1.263469000	1.128106000	-2.994096000
H	-1.804029000	1.794718000	-1.443365000
H	-0.792201000	0.348813000	-1.484319000
C	-0.027325000	3.584608000	-2.462801000
H	0.862810000	4.220105000	-2.506343000
H	-0.771084000	4.081090000	-1.830376000

H	-0.454824000	3.531158000	-3.469878000
C	-4.751229000	-2.659833000	-0.243572000
H	-3.990796000	-2.271923000	0.439332000
H	-4.825355000	-3.739979000	-0.043999000
C	-6.062780000	-1.981527000	-0.011816000
C	-6.997514000	-1.950119000	-1.066974000
C	-8.211211000	-1.278200000	-0.949385000
H	-8.917017000	-1.266037000	-1.773965000
C	-8.512909000	-0.595709000	0.228932000
H	-9.454779000	-0.062235000	0.317854000
C	-7.599884000	-0.599174000	1.281320000
H	-7.825144000	-0.061825000	2.198657000
C	-6.394592000	-1.287573000	1.158992000
H	-5.682468000	-1.283742000	1.979832000
C	-7.148200000	-2.048780000	-3.517826000
H	-8.220343000	-2.256467000	-3.625513000
H	-6.987258000	-0.970580000	-3.517156000
C	-6.946181000	-4.064892000	-2.221363000
H	-6.501975000	-4.513388000	-1.332090000
H	-6.560658000	-4.573902000	-3.107098000
H	-8.035239000	-4.192133000	-2.173985000
N	0.820862000	0.185284000	1.333346000
C	2.137344000	2.744899000	1.839554000
H	2.777062000	2.457169000	2.681922000
H	1.106776000	2.583907000	2.152173000
C	2.335330000	4.210834000	1.549663000
C	1.620464000	4.842097000	0.527818000
H	0.935214000	4.259530000	-0.077957000
C	1.789939000	6.200724000	0.279477000
H	1.228646000	6.677506000	-0.519257000
C	2.674966000	6.949407000	1.056872000
H	2.807856000	8.009986000	0.863288000
C	3.385287000	6.330184000	2.082840000
H	4.074754000	6.905886000	2.694065000
C	3.216758000	4.966947000	2.324604000
H	3.777344000	4.480944000	3.118917000
C	0.510746000	0.469143000	2.677324000
C	-0.820252000	0.859261000	2.959015000
C	-1.208168000	1.045495000	4.288018000
H	-2.226499000	1.357683000	4.504634000
C	-0.311714000	0.848626000	5.330867000
H	-0.625343000	0.997540000	6.360361000

C	0.995340000	0.464141000	5.046351000
H	1.694323000	0.315550000	5.863615000
C	1.430991000	0.269678000	3.734314000
C	-1.809329000	1.125892000	1.840818000
H	-1.321950000	0.836587000	0.905530000
C	-2.130002000	2.620433000	1.738583000
H	-2.613626000	2.986366000	2.651335000
H	-2.807521000	2.817243000	0.900348000
H	-1.221565000	3.213151000	1.587097000
C	-3.084851000	0.292795000	1.982374000
H	-3.645184000	0.556832000	2.886234000
H	-2.855935000	-0.776921000	2.036880000
H	-3.748238000	0.450877000	1.127045000
C	2.855931000	-0.161388000	3.454254000
H	3.127738000	0.219336000	2.467848000
C	2.967886000	-1.687015000	3.391531000
H	2.696509000	-2.138028000	4.352852000
H	3.992563000	-1.990624000	3.150612000
H	2.309791000	-2.110010000	2.627580000
C	3.871869000	0.411563000	4.441502000
H	3.761219000	1.494925000	4.554592000
H	4.885856000	0.215391000	4.083352000
H	3.781778000	-0.040555000	5.435271000
C	1.533376000	-3.776082000	0.694331000
H	2.633930000	-3.720625000	0.651929000
H	1.305614000	-4.016416000	1.748495000
Al	-4.411351000	-2.429023000	-2.214674000
C	-3.814934000	-3.940892000	-3.371336000
H	-2.913540000	-3.613218000	-3.907721000
H	-4.558972000	-4.106605000	-4.167636000
C	-3.520106000	-5.269018000	-2.667513000
H	-2.752119000	-5.149341000	-1.893188000
H	-4.405645000	-5.675550000	-2.163412000
H	-3.160136000	-6.050641000	-3.351856000
C	-4.199452000	-0.588510000	-2.956402000
H	-3.139315000	-0.458669000	-3.216507000
H	-4.726755000	-0.520244000	-3.920194000
C	-4.637445000	0.567338000	-2.051380000
H	-5.705711000	0.518415000	-1.809622000
H	-4.453517000	1.557390000	-2.493454000
H	-4.107896000	0.544469000	-1.091553000
C	-1.544285000	-2.216876000	-1.240366000

H	-2.263278000	-1.389067000	-1.235236000
H	-2.081170000	-3.147149000	-1.026696000
C	-0.772278000	-2.301392000	-2.560778000
H	-0.511336000	-3.336747000	-2.806897000
H	0.193780000	-1.743201000	-2.570054000
H	-1.300097000	-1.888674000	-3.430945000
H	-6.627634000	-2.484726000	-4.374514000
C	1.044556000	-4.936417000	-0.188273000
H	1.309273000	-4.789846000	-1.244924000
H	1.451953000	-5.921601000	0.090544000
H	-0.049451000	-5.042095000	-0.159092000

1-Y

Y	9.800001000	19.246619000	9.049026000
C	12.156255000	19.536631000	8.554636000
H	12.309022000	19.265601000	7.496320000
H	12.427514000	20.604898000	8.603172000
C	13.145053000	18.732996000	9.407640000
H	12.992937000	18.888097000	10.483195000
H	14.205233000	18.964539000	9.211360000
H	13.033001000	17.655770000	9.242630000
C	9.893353000	18.032316000	11.269271000
H	10.359236000	17.422751000	10.478124000
H	10.762546000	18.444240000	11.811918000
C	9.177146000	17.020199000	12.171897000
H	9.862809000	16.349422000	12.704520000
H	8.571906000	17.470246000	12.982890000
H	8.489772000	16.398369000	11.591873000
C	8.775322000	17.689465000	6.946970000
C	8.229628000	19.947274000	6.022902000
C	6.918092000	20.487134000	6.067084000
C	6.550139000	21.468764000	5.146402000
H	5.538562000	21.863852000	5.170398000
C	7.451613000	21.948703000	4.203758000
H	7.151594000	22.715942000	3.495456000
C	8.743142000	21.440747000	4.186055000
H	9.456855000	21.826295000	3.463349000
C	9.155751000	20.446685000	5.079287000
C	10.593958000	19.979342000	5.016442000
H	10.712200000	19.142623000	5.709549000
C	11.538719000	21.102265000	5.460468000
H	11.491635000	21.949040000	4.766170000

H	12.574641000	20.749663000	5.494061000
H	11.279781000	21.476108000	6.455654000
C	10.976472000	19.480329000	3.621919000
H	10.359698000	18.631398000	3.315977000
H	12.018177000	19.151906000	3.607458000
H	10.865660000	20.267630000	2.868525000
C	5.890853000	19.991317000	7.063312000
H	6.433047000	19.402974000	7.807910000
C	4.864978000	19.073941000	6.388520000
H	4.350272000	19.597347000	5.574665000
H	4.103865000	18.750998000	7.106435000
H	5.324184000	18.176762000	5.964126000
C	5.181164000	21.138217000	7.786593000
H	5.895077000	21.827025000	8.247110000
H	4.530634000	20.747226000	8.575690000
H	4.547794000	21.719197000	7.107361000
C	8.915274000	15.897972000	8.601810000
C	7.548498000	15.558515000	8.812522000
C	7.231202000	14.306272000	9.340966000
H	6.189985000	14.041996000	9.492509000
C	8.219258000	13.397755000	9.708695000
H	7.949400000	12.428967000	10.119458000
C	9.550389000	13.755716000	9.559791000
H	10.329394000	13.060209000	9.860593000
C	9.920988000	14.989086000	9.014521000
C	11.400284000	15.288861000	8.866841000
H	11.483139000	16.304033000	8.466805000
C	12.128859000	15.240661000	10.214567000
H	11.701365000	15.943196000	10.933901000
H	13.188185000	15.488804000	10.089633000
H	12.077116000	14.239483000	10.655993000
C	12.077171000	14.326255000	7.884302000
H	12.075808000	13.303599000	8.278270000
H	13.119739000	14.617333000	7.716072000
H	11.577838000	14.308673000	6.913326000
C	6.447040000	16.585855000	8.613441000
H	6.651783000	17.154314000	7.702017000
C	5.046008000	15.992359000	8.471104000
H	4.994716000	15.227209000	7.692703000
H	4.335540000	16.779906000	8.207080000
H	4.697907000	15.547589000	9.409542000
C	6.453538000	17.563038000	9.793396000

H	6.211759000	17.037588000	10.722018000
H	5.718016000	18.360238000	9.657327000
H	7.442536000	18.017244000	9.923834000
C	7.803244000	17.345032000	4.682291000
H	8.485936000	17.501973000	3.836655000
H	7.353042000	18.313188000	4.891208000
C	6.708455000	16.386518000	4.274015000
C	6.212803000	15.415518000	5.145998000
H	6.656894000	15.312395000	6.130799000
C	5.169277000	14.578630000	4.753193000
H	4.800597000	13.821487000	5.439910000
C	4.603627000	14.708865000	3.486964000
H	3.789769000	14.057647000	3.181171000
C	5.093555000	15.678194000	2.610955000
H	4.660779000	15.785492000	1.620073000
C	6.142627000	16.506120000	3.000786000
H	6.525750000	17.257481000	2.313500000
C	9.375970000	15.718363000	5.608114000
H	8.781381000	15.009321000	5.027063000
H	9.590878000	15.237752000	6.560126000
C	10.656512000	16.029042000	4.872963000
C	11.705848000	16.691504000	5.521787000
H	11.576547000	17.011040000	6.550633000
C	12.910471000	16.923514000	4.866393000
H	13.718522000	17.428968000	5.387858000
C	13.077846000	16.509966000	3.543438000
H	14.018908000	16.689302000	3.031023000
C	12.031480000	15.873019000	2.880606000
H	12.151830000	15.556998000	1.848078000
C	10.828550000	15.631600000	3.545362000
H	10.017327000	15.118262000	3.034009000
N	8.591190000	19.011870000	7.019973000
N	9.273355000	17.162140000	8.094980000
N	8.544562000	16.900660000	5.846893000
Y	8.414059000	19.886649000	12.155520000
C	6.057795000	19.596713000	12.649879000
H	5.904948000	19.867907000	13.708141000
H	5.786427000	18.528473000	12.601443000
C	5.069191000	20.400367000	11.796660000
H	5.221352000	20.245043000	10.721147000
H	4.008954000	20.169049000	11.992905000
H	5.181418000	21.477608000	11.961467000

C	8.320726000	21.100969000	9.935287000
H	7.854829000	21.710554000	10.726416000
H	7.451541000	20.689049000	9.392614000
C	9.036976000	22.113052000	9.032652000
H	8.351347000	22.783905000	8.500084000
H	9.642116000	21.662958000	8.221612000
H	9.724447000	22.734800000	9.612651000
C	9.438768000	21.443756000	14.257615000
C	9.984364000	19.185875000	15.181612000
C	11.295876000	18.645954000	15.137393000
C	11.663785000	17.664246000	16.058005000
H	12.675343000	17.269113000	16.033974000
C	10.762292000	17.184292000	17.000626000
H	11.062278000	16.416995000	17.708878000
C	9.470796000	17.692330000	17.018382000
H	8.757073000	17.306788000	17.741082000
C	9.058234000	18.686477000	16.125220000
C	7.620071000	19.153962000	16.188150000
H	7.501838000	19.990591000	15.494932000
C	6.675157000	18.031061000	15.744398000
H	6.722254000	17.184380000	16.438811000
H	5.639260000	18.383741000	15.710872000
H	6.933956000	17.657063000	14.749236000
C	7.237763000	19.653233000	17.582632000
H	7.854650000	20.502162000	17.888353000
H	6.196090000	19.981751000	17.597158000
H	7.348589000	18.866055000	18.336152000
C	12.323159000	19.141794000	14.141226000
H	11.781023000	19.730232000	13.396661000
C	13.349078000	20.059053000	14.816110000
H	13.863660000	19.535591000	15.630008000
H	14.110289000	20.381903000	14.098260000
H	12.889943000	20.956291000	15.240461000
C	13.032801000	17.994895000	13.417883000
H	12.318869000	17.306143000	12.957314000
H	13.683364000	18.385899000	12.628818000
H	13.666128000	17.413845000	14.097097000
C	9.298777000	23.235322000	12.602874000
C	10.665543000	23.574864000	12.392244000
C	10.982796000	24.827141000	11.863859000
H	12.024005000	25.091477000	11.712362000
C	9.994704000	25.735624000	11.496134000

H	10.264532000	26.704446000	11.085431000
C	8.663586000	25.377597000	11.644992000
H	7.884558000	26.073089000	11.344211000
C	8.293031000	24.144179000	12.190191000
C	6.813747000	23.844337000	12.337883000
H	6.730939000	22.829174000	12.737957000
C	6.085158000	23.892443000	10.990161000
H	6.512714000	23.189934000	10.270837000
H	5.025855000	23.644204000	11.115111000
H	6.136797000	24.893614000	10.548708000
C	6.136819000	24.806944000	13.320387000
H	6.138162000	25.829587000	12.926390000
H	5.094257000	24.515839000	13.488608000
H	6.636138000	24.824565000	14.291371000
C	11.767019000	22.547559000	12.591353000
H	11.562319000	21.979165000	13.502828000
C	13.168051000	23.141082000	12.733563000
H	13.219389000	23.906242000	13.511950000
H	13.878564000	22.353557000	12.997534000
H	13.516048000	23.585853000	11.795088000
C	11.760442000	21.570297000	11.411466000
H	12.002279000	22.095684000	10.482825000
H	12.495895000	20.773038000	11.547585000
H	10.771398000	21.116179000	11.281053000
C	10.411008000	21.788238000	16.522229000
H	9.728397000	21.631444000	17.367956000
H	10.861117000	20.820027000	16.313371000
C	11.505901000	22.746727000	16.930292000
C	12.001385000	23.717751000	16.058241000
H	11.557119000	23.820899000	15.073522000
C	13.044987000	24.554631000	16.450871000
H	13.413533000	25.311794000	15.764105000
C	13.610895000	24.424352000	17.716980000
H	14.424811000	25.075562000	18.022634000
C	13.121144000	23.454990000	18.593050000
H	13.554124000	23.347651000	19.583838000
C	12.071994000	22.627079000	18.203401000
H	11.689014000	21.875696000	18.890744000
C	8.838164000	23.414847000	15.596497000
H	9.432749000	24.123921000	16.177515000
H	8.623210000	23.895429000	14.644482000
C	7.557668000	23.104125000	16.331705000

C	6.508336000	22.441596000	15.682953000
H	6.637595000	22.122037000	14.654109000
C	5.303762000	22.209532000	16.338421000
H	4.495706000	21.704032000	15.817009000
C	5.136431000	22.623102000	17.661374000
H	4.195404000	22.443722000	18.173837000
C	6.182804000	23.260107000	18.324144000
H	6.062496000	23.576140000	19.356672000
C	7.385684000	23.501571000	17.659317000
H	8.196902000	24.014982000	18.170605000
N	9.622839000	20.121349000	14.184605000
N	8.940730000	21.971111000	13.109619000
N	9.669582000	22.232562000	15.357686000

2-Y

Y	7.857263000	5.903980000	7.686465000
Al	8.753013000	8.449649000	6.374786000
N	7.361031000	5.420710000	9.897779000
N	5.819132000	4.944499000	8.355138000
N	5.477876000	4.140105000	10.609103000
C	9.433452000	4.309819000	6.838010000
H	9.119608000	4.050077000	5.812295000
H	10.354536000	4.902871000	6.690494000
C	9.793859000	3.024523000	7.589072000
H	10.270210000	3.240782000	8.552782000
H	10.491756000	2.370031000	7.042641000
H	8.909456000	2.415145000	7.809433000
C	6.906426000	7.502311000	5.926822000
H	6.654242000	8.384228000	5.322502000
H	6.099030000	7.508962000	6.681417000
C	6.750292000	6.275544000	5.012904000
H	7.455054000	6.320907000	4.177877000
H	6.942179000	5.296864000	5.492459000
H	5.737789000	6.175004000	4.606229000
C	8.336913000	10.395197000	6.396428000
H	9.244372000	10.974391000	6.619157000
H	8.058327000	10.688530000	5.371858000
C	7.219360000	10.799099000	7.363356000
H	6.285779000	10.263112000	7.149315000
H	6.980936000	11.871924000	7.332055000
H	7.483685000	10.565089000	8.401304000
C	10.060078000	7.745719000	5.035381000

H	9.934152000	6.656506000	4.936315000
H	9.793279000	8.151872000	4.046869000
C	11.535241000	8.046039000	5.326283000
H	11.726208000	9.124816000	5.390788000
H	12.215948000	7.649734000	4.559385000
H	11.853150000	7.610402000	6.281948000
C	9.411265000	7.835839000	8.278485000
H	10.048402000	6.930509000	8.241625000
H	8.702296000	7.673341000	9.112396000
C	10.312787000	8.988786000	8.742008000
H	11.078900000	9.228960000	7.997663000
H	10.829927000	8.751502000	9.680281000
H	9.729224000	9.898601000	8.910539000
C	6.174356000	4.813257000	9.639519000
C	4.731600000	4.402877000	7.634674000
C	3.641188000	5.257869000	7.336279000
C	2.581333000	4.767441000	6.572699000
H	1.735770000	5.416055000	6.360674000
C	2.590292000	3.466825000	6.080936000
H	1.758435000	3.098112000	5.487414000
C	3.680094000	2.647496000	6.346023000
H	3.698454000	1.638366000	5.943940000
C	4.760548000	3.090921000	7.114771000
C	5.943899000	2.167299000	7.318214000
H	6.619447000	2.639381000	8.038098000
C	5.539341000	0.806621000	7.887789000
H	5.057895000	0.902168000	8.865060000
H	6.421211000	0.174678000	8.019002000
H	4.849698000	0.278647000	7.220516000
C	6.701400000	1.989343000	5.996909000
H	6.063303000	1.511272000	5.245270000
H	7.588084000	1.362651000	6.134932000
H	7.029115000	2.949668000	5.588088000
C	3.590803000	6.677352000	7.863551000
H	4.585472000	6.900124000	8.258003000
C	2.592389000	6.808597000	9.018320000
H	1.580027000	6.544900000	8.692155000
H	2.563692000	7.838380000	9.390980000
H	2.846219000	6.154853000	9.857546000
C	3.277109000	7.699660000	6.767988000
H	3.938884000	7.581278000	5.905310000
H	3.401481000	8.718161000	7.152383000

H	2.244881000	7.611516000	6.411914000
C	7.728346000	6.036466000	11.110415000
C	6.917987000	7.042397000	11.699687000
C	7.365285000	7.671591000	12.862672000
H	6.749811000	8.439220000	13.319935000
C	8.593427000	7.357425000	13.437345000
H	8.920466000	7.864216000	14.340788000
C	9.397466000	6.399525000	12.836096000
H	10.362052000	6.153620000	13.272347000
C	8.987088000	5.730592000	11.680009000
C	9.892859000	4.677811000	11.077030000
H	9.372656000	4.279748000	10.201067000
C	10.140476000	3.522560000	12.052047000
H	10.715194000	3.858043000	12.922478000
H	10.709307000	2.721635000	11.567369000
H	9.204079000	3.091849000	12.416553000
C	11.223199000	5.271309000	10.604171000
H	11.070146000	6.085844000	9.890755000
H	11.838088000	4.505628000	10.118373000
H	11.798195000	5.674422000	11.445153000
C	5.646428000	7.523955000	11.022824000
H	5.139170000	6.662873000	10.578691000
C	4.652972000	8.190272000	11.975571000
H	5.001537000	9.175565000	12.303732000
H	4.475401000	7.585988000	12.870461000
H	3.694233000	8.341082000	11.470844000
C	5.998830000	8.493627000	9.889631000
H	6.544908000	9.356613000	10.283520000
H	5.099887000	8.861209000	9.385009000
H	6.638668000	8.024131000	9.135203000
C	6.199186000	3.501085000	11.715628000
H	5.552950000	3.530908000	12.595741000
H	7.083492000	4.088639000	11.950396000
C	6.583940000	2.077049000	11.400321000
C	5.916762000	1.003132000	11.993096000
H	5.100719000	1.200097000	12.683837000
C	6.294965000	-0.309749000	11.709694000
H	5.768737000	-1.136937000	12.178015000
C	7.350408000	-0.558601000	10.834974000
H	7.651898000	-1.580049000	10.620819000
C	8.017191000	0.509212000	10.232296000
H	8.840273000	0.324683000	9.547594000

C	7.628422000	1.816063000	10.507014000
H	8.146412000	2.645884000	10.038181000
C	4.158795000	3.565965000	10.362294000
H	4.247475000	2.532004000	10.008862000
H	3.679615000	4.129370000	9.564704000
C	3.272671000	3.605601000	11.580807000
C	2.513292000	2.487292000	11.929685000
H	2.600898000	1.578445000	11.339363000
C	1.651685000	2.529877000	13.025398000
H	1.065878000	1.652839000	13.286183000
C	1.548978000	3.691481000	13.788169000
H	0.881939000	3.724828000	14.644854000
C	2.309603000	4.810791000	13.448288000
H	2.235746000	5.719761000	14.038848000
C	3.164559000	4.766877000	12.351047000
H	3.767292000	5.630210000	12.090650000

TS-5

Y	7.880415000	6.141682000	7.949283000
Al	8.834056000	8.418539000	6.248717000
N	7.283193000	5.481645000	10.095743000
N	5.797274000	4.992184000	8.491913000
N	5.446429000	4.082347000	10.697606000
C	9.750229000	4.488810000	7.338557000
H	10.628423000	4.251456000	7.951334000
H	8.991885000	3.755622000	7.662539000
C	10.073355000	4.303043000	5.858095000
H	9.219203000	4.525491000	5.207723000
H	10.393127000	3.280432000	5.621818000
H	10.879844000	4.978076000	5.553588000
C	6.876129000	7.566284000	6.069596000
H	6.617785000	8.447373000	5.465937000
H	6.097172000	7.608721000	6.854070000
C	6.654301000	6.322068000	5.190657000
H	7.305894000	6.352241000	4.312811000
H	6.872980000	5.356373000	5.686354000
H	5.618936000	6.210719000	4.848351000
C	8.588295000	10.363600000	6.632904000
H	9.581698000	10.832910000	6.702007000
H	8.108171000	10.844871000	5.766223000
C	7.792583000	10.685680000	7.900559000
H	6.771119000	10.287221000	7.848189000

H	7.696792000	11.763721000	8.098313000
H	8.261483000	10.244739000	8.789674000
C	9.668423000	8.014450000	4.472260000
H	10.008335000	6.969219000	4.431770000
H	8.884617000	8.090434000	3.701256000
C	10.825845000	8.944092000	4.086693000
H	10.507307000	9.993762000	4.070983000
H	11.247213000	8.725481000	3.094470000
H	11.655096000	8.882302000	4.801946000
C	9.805000000	7.375205000	7.758240000
H	9.831271000	5.837775000	7.597791000
H	9.495713000	7.718125000	8.780317000
C	11.298861000	7.634623000	7.598658000
H	11.643271000	7.302034000	6.612210000
H	11.904011000	7.091124000	8.340758000
H	11.577777000	8.694355000	7.686520000
C	6.133592000	4.826682000	9.771353000
C	4.785363000	4.393138000	7.717354000
C	3.699034000	5.209294000	7.313299000
C	2.732020000	4.678961000	6.458598000
H	1.890729000	5.298002000	6.159749000
C	2.828567000	3.376303000	5.981682000
H	2.070823000	2.979164000	5.312172000
C	3.906046000	2.588300000	6.367678000
H	3.988015000	1.574975000	5.985093000
C	4.891682000	3.070186000	7.233400000
C	6.067102000	2.181916000	7.587237000
H	6.598800000	2.642546000	8.424938000
C	5.639873000	0.784691000	8.038390000
H	5.000271000	0.823710000	8.924518000
H	6.516764000	0.185129000	8.293106000
H	5.094549000	0.252612000	7.251887000
C	7.034385000	2.086666000	6.401137000
H	6.560702000	1.575158000	5.555710000
H	7.936652000	1.526984000	6.671107000
H	7.340317000	3.075578000	6.045433000
C	3.552874000	6.625295000	7.834541000
H	4.523410000	6.906328000	8.253736000
C	2.526116000	6.695595000	8.970644000
H	1.542122000	6.353692000	8.630437000
H	2.414612000	7.724956000	9.328565000
H	2.812191000	6.075561000	9.825390000

C	3.203473000	7.628536000	6.733499000
H	3.894153000	7.553112000	5.888881000
H	3.254224000	8.651897000	7.121137000
H	2.187954000	7.478775000	6.351047000
C	7.554544000	6.060111000	11.352673000
C	6.684772000	7.029380000	11.917919000
C	7.027569000	7.607270000	13.141346000
H	6.365213000	8.343860000	13.584320000
C	8.212804000	7.281767000	13.794704000
H	8.459983000	7.749978000	14.743199000
C	9.080593000	6.366700000	13.214222000
H	10.014485000	6.121305000	13.712514000
C	8.771269000	5.744533000	12.001732000
C	9.743553000	4.749731000	11.400417000
H	9.233854000	4.293299000	10.545508000
C	10.120173000	3.637016000	12.381788000
H	10.697352000	4.025404000	13.227790000
H	10.737070000	2.879541000	11.885894000
H	9.234956000	3.135892000	12.784589000
C	10.992850000	5.458214000	10.866635000
H	10.731026000	6.220525000	10.127387000
H	11.674412000	4.743786000	10.391692000
H	11.540204000	5.954259000	11.676128000
C	5.467276000	7.529123000	11.159193000
H	5.010612000	6.685152000	10.633516000
C	4.389171000	8.152358000	12.047708000
H	4.700984000	9.128400000	12.434777000
H	4.139026000	7.521086000	12.904823000
H	3.474182000	8.312120000	11.470173000
C	5.897530000	8.560647000	10.109893000
H	6.326177000	9.443807000	10.594364000
H	5.049623000	8.884931000	9.498600000
H	6.668843000	8.174047000	9.435660000
C	6.148050000	3.436121000	11.812132000
H	5.499986000	3.486668000	12.690472000
H	7.042181000	4.007420000	12.044457000
C	6.505649000	1.998912000	11.524222000
C	5.702531000	0.955551000	11.992325000
H	4.806871000	1.189065000	12.562940000
C	6.049094000	-0.372470000	11.744936000
H	5.416962000	-1.174166000	12.116536000
C	7.209941000	-0.670225000	11.033955000

H	7.487499000	-1.704444000	10.851412000
C	8.013981000	0.365188000	10.556154000
H	8.920736000	0.140623000	10.001253000
C	7.656580000	1.689507000	10.792093000
H	8.282040000	2.495422000	10.421823000
C	4.128983000	3.528415000	10.421982000
H	4.209395000	2.483816000	10.098719000
H	3.690374000	4.075658000	9.590263000
C	3.187470000	3.621703000	11.595945000
C	2.218999000	2.632818000	11.784530000
H	2.193001000	1.776013000	11.115189000
C	1.289314000	2.741604000	12.817190000
H	0.538973000	1.967423000	12.951547000
C	1.325859000	3.836150000	13.679930000
H	0.604410000	3.918724000	14.487738000
C	2.298376000	4.820044000	13.504289000
H	2.339090000	5.672489000	14.176787000
C	3.221350000	4.712470000	12.467398000
H	3.989771000	5.466344000	12.334733000

Int-9

Y	7.369801000	6.738781000	7.996196000
Al	9.113437000	8.270713000	6.233447000
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N	5.676988000	5.212726000	8.504408000
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C	6.954929000	8.549542000	6.267874000
H	7.092975000	9.526339000	5.785436000
H	6.272860000	8.823583000	7.102668000
C	6.215755000	7.617711000	5.294292000
H	6.823387000	7.438884000	4.401959000
H	6.000703000	6.614455000	5.705556000
H	5.243126000	8.003690000	4.967332000
C	9.748794000	9.576289000	7.630262000
H	10.807628000	9.382702000	7.857625000
H	9.717179000	10.604168000	7.238768000
C	8.943896000	9.527565000	8.933267000
H	7.892646000	9.802188000	8.771419000
H	9.311174000	10.197017000	9.724781000
H	8.965680000	8.527657000	9.403722000
C	9.634394000	8.619397000	4.337945000
H	9.247886000	7.822623000	3.686077000

H	9.168301000	9.549148000	3.977217000
C	11.156277000	8.717154000	4.168270000
H	11.575935000	9.534221000	4.769057000
H	11.467345000	8.895471000	3.128559000
H	11.659317000	7.798332000	4.495862000
C	9.288927000	6.318301000	6.853025000
H	10.110161000	6.272601000	7.595730000
C	9.604012000	5.390497000	5.674750000
H	8.770261000	5.341762000	4.959970000
H	9.791152000	4.352730000	5.990188000
H	10.483259000	5.688723000	5.081075000
C	6.004358000	5.069315000	9.800097000
C	4.823341000	4.472765000	7.663342000
C	3.711422000	5.152343000	7.107067000
C	2.906527000	4.486710000	6.180231000
H	2.048390000	4.996405000	5.753701000
C	3.185250000	3.179859000	5.796646000
H	2.550323000	2.674675000	5.074249000
C	4.280841000	2.521866000	6.345030000
H	4.492251000	1.501370000	6.042943000
C	5.116068000	3.145463000	7.274409000
C	6.321731000	2.422331000	7.839874000
H	6.467929000	2.771478000	8.865540000
C	6.144901000	0.907262000	7.913386000
H	5.222508000	0.632053000	8.435679000
H	6.979413000	0.463414000	8.462006000
H	6.124767000	0.445084000	6.920379000
C	7.586051000	2.784551000	7.055404000
H	7.492730000	2.490954000	6.004199000
H	8.462840000	2.277676000	7.473631000
H	7.786855000	3.860503000	7.086430000
C	3.361698000	6.554415000	7.569990000
H	4.306591000	7.072374000	7.776696000
C	2.588255000	6.500455000	8.892685000
H	1.664282000	5.923754000	8.776271000
H	2.316775000	7.506469000	9.230593000
H	3.177952000	6.028780000	9.681144000
C	2.592671000	7.378919000	6.539886000
H	3.070114000	7.352686000	5.556307000
H	2.539101000	8.423944000	6.862833000
H	1.562004000	7.026419000	6.423491000
C	7.355643000	6.411498000	11.399164000

C	6.443385000	7.258004000	12.080692000
C	6.842657000	7.858149000	13.275361000
H	6.147355000	8.502360000	13.804038000
C	8.120362000	7.666367000	13.793386000
H	8.411398000	8.147461000	14.722750000
C	9.020150000	6.863216000	13.105351000
H	10.022177000	6.719031000	13.500332000
C	8.661459000	6.227066000	11.914089000
C	9.674327000	5.353802000	11.199507000
H	9.150814000	4.875667000	10.364816000
C	10.229450000	4.257672000	12.114086000
H	10.842808000	4.681166000	12.916937000
H	10.864482000	3.568355000	11.546923000
H	9.430497000	3.673396000	12.579193000
C	10.817347000	6.190561000	10.614017000
H	10.451382000	6.965584000	9.933946000
H	11.515259000	5.558747000	10.054249000
H	11.380775000	6.693719000	11.407955000
C	5.092847000	7.587051000	11.473134000
H	4.731010000	6.694385000	10.957257000
C	4.030330000	7.985550000	12.497716000
H	4.229575000	8.972568000	12.928787000
H	3.972426000	7.267717000	13.321678000
H	3.046762000	8.037726000	12.019317000
C	5.239324000	8.693017000	10.423091000
H	5.623850000	9.613183000	10.875325000
H	4.282130000	8.916534000	9.941258000
H	5.944472000	8.400001000	9.638281000
C	6.063925000	3.745354000	11.890487000
H	5.365530000	3.795969000	12.730036000
H	6.890079000	4.411821000	12.121722000
C	6.572597000	2.333434000	11.727385000
C	5.905151000	1.256572000	12.315074000
H	5.005951000	1.441555000	12.896683000
C	6.381841000	-0.044677000	12.158426000
H	5.851289000	-0.873292000	12.619258000
C	7.539924000	-0.280288000	11.420663000
H	7.916430000	-1.292601000	11.304704000
C	8.215615000	0.790084000	10.833084000
H	9.122886000	0.615924000	10.261497000
C	7.729218000	2.086064000	10.980605000
H	8.252286000	2.917159000	10.518409000

C	4.180026000	3.475301000	10.343118000
H	4.455973000	2.454598000	10.051624000
H	3.715105000	3.934403000	9.473277000
C	3.163964000	3.417591000	11.455515000
C	2.491554000	2.222462000	11.719193000
H	2.743955000	1.332437000	11.148004000
C	1.510049000	2.163842000	12.707541000
H	0.994629000	1.227357000	12.901644000
C	1.196603000	3.301487000	13.449378000
H	0.436416000	3.256312000	14.224027000
C	1.868350000	4.497262000	13.194856000
H	1.632324000	5.388552000	13.769662000
C	2.842588000	4.553485000	12.202378000
H	3.372706000	5.478927000	12.009104000

3-Y

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Y	14.836305000	12.055579000	14.819846000
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Al	14.865812000	9.062577000	14.651615000
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N	11.221408000	6.706310000	9.598767000
N	16.874836000	12.957654000	13.957509000
N	15.875522000	14.035034000	15.630943000
N	17.876852000	15.008335000	14.775184000
C	13.525584000	11.447510000	12.949893000
H	13.642709000	12.019584000	12.022626000
C	14.569575000	10.346769000	13.156075000
H	15.353707000	10.295516000	12.391067000
C	11.740638000	7.480797000	10.612075000
C	12.876911000	9.273142000	9.277526000
C	11.981148000	10.126463000	8.595278000
C	12.438375000	10.853373000	7.493520000
H	11.751011000	11.515155000	6.974639000
C	13.751079000	10.750232000	7.052036000
H	14.086824000	11.318358000	6.189030000
C	14.631683000	9.918783000	7.732936000
H	15.659458000	9.838758000	7.392999000
C	14.225282000	9.185091000	8.849506000
C	10.557975000	10.325268000	9.066486000
H	10.314410000	9.515801000	9.760852000

C	9.527921000	10.277478000	7.938742000
H	9.671576000	11.090066000	7.218758000
H	8.519516000	10.377136000	8.347496000
H	9.568145000	9.331463000	7.391295000
C	10.467384000	11.650449000	9.826591000
H	11.183367000	11.686171000	10.654002000
H	9.462959000	11.807354000	10.231522000
H	10.701624000	12.492634000	9.165817000
C	15.211424000	8.256717000	9.530803000
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C	16.599485000	8.875530000	9.695606000
H	17.063039000	9.109412000	8.731168000
H	17.269246000	8.178133000	10.206795000
H	16.566038000	9.794204000	10.284885000
C	15.308518000	6.929532000	8.769255000
H	15.677451000	7.093664000	7.750176000
H	14.340864000	6.426803000	8.689232000
H	16.002211000	6.245042000	9.269252000
C	11.349805000	5.931020000	12.472208000
C	12.307077000	4.902049000	12.248671000
C	12.141735000	3.670027000	12.882826000
H	12.869888000	2.884538000	12.708841000
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H	10.981426000	2.462902000	14.241005000
C	10.180588000	4.450047000	14.010889000
H	9.360401000	4.283308000	14.704543000
C	10.293890000	5.694996000	13.386969000
C	13.570345000	5.168817000	11.452106000
H	13.316972000	5.781748000	10.583965000
C	14.549883000	5.969487000	12.311513000
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H	14.816599000	5.406292000	13.210610000
C	14.262771000	3.909297000	10.930420000
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H	15.050883000	4.183390000	10.222769000
H	13.568469000	3.235770000	10.418281000
C	9.274697000	6.765873000	13.711695000
H	9.543280000	7.643504000	13.118282000
C	9.325020000	7.157680000	15.192522000
H	9.008507000	6.325043000	15.831014000
H	8.658409000	8.003616000	15.395056000

H	10.336857000	7.437306000	15.500898000
C	7.855166000	6.342783000	13.321599000
H	7.795584000	6.043475000	12.271994000
H	7.148478000	7.166210000	13.476050000
H	7.514169000	5.496751000	13.928806000
C	9.960299000	5.984996000	9.801953000
H	9.881254000	5.696005000	10.847059000
H	10.005524000	5.062679000	9.218122000
C	8.757658000	6.796982000	9.391195000
C	8.094766000	6.550187000	8.186991000
H	8.458316000	5.762524000	7.531486000
C	6.972589000	7.298885000	7.830232000
H	6.462598000	7.096064000	6.892490000
C	6.501947000	8.299678000	8.677850000
H	5.623530000	8.877513000	8.404596000
C	7.165047000	8.559680000	9.878270000
H	6.806191000	9.340314000	10.543398000
C	8.287804000	7.815806000	10.226279000
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C	11.549097000	6.928074000	8.196717000
H	10.814710000	7.594881000	7.729221000
H	12.509279000	7.436188000	8.142207000
C	11.644200000	5.651227000	7.400747000
C	11.196816000	5.623592000	6.078007000
H	10.735111000	6.511331000	5.652063000
C	11.337975000	4.471029000	5.306419000
H	10.987078000	4.463611000	4.278177000
C	11.918506000	3.328799000	5.855256000
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C	16.916601000	14.022655000	14.767450000
C	17.784023000	12.483910000	12.986363000
C	19.000691000	11.844690000	13.321899000
C	19.778943000	11.290240000	12.301253000
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C	19.393705000	11.362228000	10.969505000
H	20.013928000	10.924545000	10.192397000
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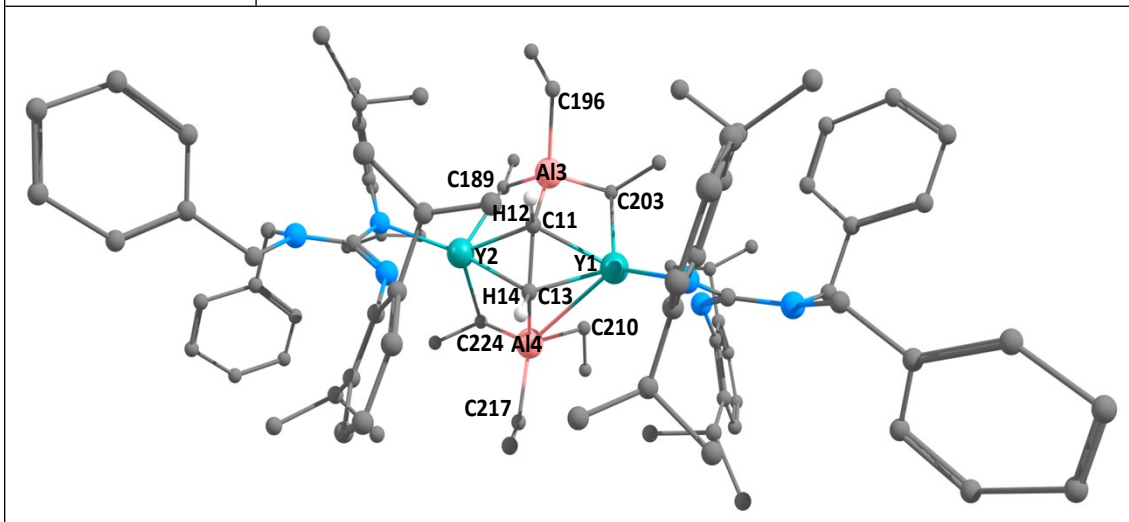
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H	18.842663000	12.331227000	15.381707000
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H	21.184929000	12.148389000	16.013077000
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H	21.630059000	11.503564000	14.429261000
C	19.339826000	10.256162000	15.222128000
H	18.320551000	9.895140000	15.089829000
H	19.608842000	10.161493000	16.280269000
H	19.998472000	9.596836000	14.646174000
C	16.124356000	13.295456000	11.216335000
H	15.478041000	13.347828000	12.095852000
C	15.339908000	12.588386000	10.111773000
H	15.879484000	12.579064000	9.159144000
H	14.387775000	13.099365000	9.933738000
H	15.116458000	11.552352000	10.376482000
C	16.465128000	14.732387000	10.805094000
H	16.917986000	15.289593000	11.630112000
H	15.567534000	15.273036000	10.485750000
H	17.176801000	14.741649000	9.971701000
C	15.226947000	15.143016000	16.196754000
C	14.734873000	16.220985000	15.411471000
C	13.991863000	17.225134000	16.034938000
H	13.612137000	18.049665000	15.439997000
C	13.703993000	17.187299000	17.396363000
H	13.118901000	17.979572000	17.854818000
C	14.166778000	16.121139000	18.156016000
H	13.941893000	16.078860000	19.218751000
C	14.925033000	15.098749000	17.581735000
C	14.901850000	16.236991000	13.902709000
H	15.872009000	15.797246000	13.661752000
C	13.818667000	15.378635000	13.246719000
H	13.851026000	14.335236000	13.577813000
H	13.926341000	15.367579000	12.158059000
H	12.825809000	15.766137000	13.488592000
C	14.875783000	17.639820000	13.293521000
H	13.874154000	18.081810000	13.331031000
H	15.160401000	17.593750000	12.236957000
H	15.563177000	18.320854000	13.804790000
C	15.411065000	13.959969000	18.455389000
H	16.005704000	13.305727000	17.812071000

C	14.244469000	13.137057000	19.011754000
H	13.622661000	13.736997000	19.685793000
H	14.610611000	12.273409000	19.578397000
H	13.592919000	12.770511000	18.212729000
C	16.311832000	14.457164000	19.589442000
H	17.145708000	15.052106000	19.207015000
H	16.730558000	13.613312000	20.149457000
H	15.753003000	15.079773000	20.297101000
C	18.935759000	15.068086000	13.771046000
H	18.568007000	14.604019000	12.858034000
H	19.805963000	14.490275000	14.095934000
C	19.369333000	16.480410000	13.472099000
C	20.711163000	16.845635000	13.596497000
H	21.435032000	16.105292000	13.927480000
C	21.122807000	18.146904000	13.308579000
H	22.170056000	18.417598000	13.411283000
C	20.191938000	19.097780000	12.895973000
H	20.508966000	20.113180000	12.675496000
C	18.849099000	18.739667000	12.767624000
H	18.117443000	19.474329000	12.442790000
C	18.443742000	17.439534000	13.052524000
H	17.400128000	17.162130000	12.962888000
C	18.191053000	15.708522000	16.022996000
H	17.281500000	15.814340000	16.611171000
H	18.519278000	16.717481000	15.762815000
C	19.258064000	15.013875000	16.834801000
C	18.981185000	13.797098000	17.468142000
H	17.996671000	13.354725000	17.355427000
C	19.947754000	13.162379000	18.242032000
H	19.713478000	12.222801000	18.734721000
C	21.213304000	13.733939000	18.386456000
H	21.968805000	13.240697000	18.991444000
C	21.502820000	14.938484000	17.749347000
H	22.486613000	15.387670000	17.853788000
C	20.528455000	15.574103000	16.979264000
H	20.750560000	16.518810000	16.489681000
C	12.215525000	12.502071000	15.807831000
H	12.906904000	13.365599000	15.900686000
H	12.689790000	11.662548000	16.344321000
C	10.974973000	12.873049000	16.631934000
H	10.453085000	13.733988000	16.207168000
H	11.220461000	13.125416000	17.672294000

H	10.257810000	12.044752000	16.665550000
C	10.943704000	13.503594000	12.829960000
H	11.719832000	13.941232000	12.186578000
H	10.206617000	13.089389000	12.131223000
C	10.266642000	14.614021000	13.640239000
H	9.386149000	14.238843000	14.176767000
H	9.918747000	15.448411000	13.013526000
H	10.933782000	15.043205000	14.397176000
C	10.440836000	10.424893000	13.980399000
H	9.916332000	10.934999000	14.801515000
H	10.645315000	9.449372000	14.453268000
C	9.434216000	10.252876000	12.835311000
H	9.051771000	11.226572000	12.518831000
H	8.572091000	9.631010000	13.106792000
H	9.872187000	9.803100000	11.930526000
C	13.098309000	8.032181000	15.086630000
H	12.403174000	7.583191000	14.352698000
H	12.469557000	8.697949000	15.699664000
C	13.517300000	6.825933000	15.943637000
H	14.025305000	6.072741000	15.334788000
H	12.658951000	6.332231000	16.416958000
H	14.209883000	7.107301000	16.746178000
C	16.480629000	7.919513000	14.453736000
H	17.136222000	8.062719000	15.324941000
H	16.190258000	6.861411000	14.492557000
C	17.264958000	8.183343000	13.165370000
H	16.642879000	7.989623000	12.288411000
H	18.164370000	7.558220000	13.068972000
H	17.589502000	9.225724000	13.081119000
C	15.069208000	10.098877000	16.519830000
H	14.283857000	10.750591000	16.943333000
H	14.835269000	9.155058000	17.032637000
C	16.445676000	10.558588000	17.029875000
H	16.884165000	11.398698000	16.469085000
H	17.169366000	9.746423000	16.940931000
H	16.424210000	10.866085000	18.082719000

Table S4. Computed natural charges for **3-Y**

	Natural charges
Y1	1.60923
Y2	1.54166
Al3	1.77746
Al4	1.77467
C11	-1.41005
H12	0.29223
C13	-1.40166
H14	0.29622
C189	-1.04480
C196	-1.08474
C203	-1.10306
C210	-1.06059
C217	-1.09717
C224	-1.09661

**Table S5.** Computed Wiberg bond index for **3-Y**

Atom Label	Wiberg bond index	Atom Label	Wiberg bond index	Atom Label	Wiberg bond index
Y1	0.0000	Y1	0.0000	Y1	0.0000
C11	0.3577	C13	0.4073	C203	0.2152
Atom Label	Wiberg bond index	Atom Label	Wiberg bond index	Atom Label	Wiberg bond index
Y1	0.0000	Y1	0.0000	Y1	0.0000
C210	0.2175	Al3	0.1096	Al4	0.1121
Atom Label	Wiberg bond index	Atom Label	Wiberg bond index	Atom Label	Wiberg bond index

Y2	0.0000	Y2	0.0000	Y2	0.0000
C11	0.4230	C13	0.3878	C189	0.2160
Atom Label	Wiberg bond index	Atom Label	Wiberg bond index	Atom Label	Wiberg bond index
Y2	0.0000	Y2	0.0000	Y2	0.0000
C224	0.2568	Al3	0.0995	Al4	0.1194
Atom Label	Wiberg bond index	Atom Label	Wiberg bond index	Atom Label	Wiberg bond index
C11	0.0000	Al3	0.0000	Al3	0.0000
C13	1.0170	C189	0.3797	C196	0.4980
Atom Label	Wiberg bond index	Atom Label	Wiberg bond index	Atom Label	Wiberg bond index
Al3	0.0000	Al4	0.0000	Al4	0.0000
C203	0.3537	C210	0.3674	C217	0.4942
Atom Label	Wiberg bond index				
Al4	0.0000				
C224	0.3281				

Bonding orbitals in Y_2Al_2 core for **3-Y**

(1.74314) BD (1) Al3-C11

(13.19%) 0.3632*Al3 s(40.63%) p 1.45(58.98%) d 0.01(0.38%)

(86.81%) 0.9317*C11 s(47.48%) p 1.11(52.52%) d 0.00(0.00%)

(1.74246) BD (1) Al4-C13

(13.10%) 0.3620*Al4 s(45.89%) p 1.17(53.78%) d 0.01(0.33%)

(86.90%) 0.9322* C13 s(47.30%) p 1.11(52.70%) d 0.00(0.00%)

(1.94161) BD (1) C11-C13

(50.09%) 0.7078* C11 s(27.65%) p 2.62(72.31%) d 0.00(0.04%)

(49.91%) 0.7065* C13 s(27.57%) p 2.63(72.39%) d 0.00(0.04%)

Table S6. DFT computed NBO second order perturbation analysis for **3-Y**

Donor NBO	Acceptor NBO	E(2) kcal/mol
(1.74314) BD (1)Al3-C11 (13.19%) 0.3632*Al3 s(40.63%) p 1.45(58.98%) d 0.01(0.38%) (86.81%) 0.9317*C11 s(47.48%) p 1.11(52.52%) d 0.00(0.00%)	(0.31853) LP*(1) Y1 s(0.25%) p3 0.48(7.52%) d 99.99(92.23%)	23.98

(1.74314) BD (1)AI3-C11 (13.19%) 0.3632*AI3 s(40.63%) p 1.45(58.98%) d 0.01(0.38%) (86.81%) 0.9317*C11 s(47.48%) p 1.11(52.52%) d 0.00(0.00%)	(0.18233) LP*(2) Y1 s(9.42%) p 1.67(15.68%) d 7.95(74.90%)	23.87
(1.74314) BD (1)AI3-C11 (13.19%) 0.3632*AI3 s(40.63%) p 1.45(58.98%) d 0.01(0.38%) (86.81%) 0.9317*C11 s(47.48%) p 1.11(52.52%) d 0.00(0.00%)	(0.17054) LP*(3) Y1 s(4.41%) p 6.57(28.99%) d 15.09(66.59%)	9.19
(1.74314) BD (1)AI3-C11 (13.19%) 0.3632*AI3 s(40.63%) p 1.45(58.98%) d 0.01(0.38%) (86.81%) 0.9317*C11 s(47.48%) p 1.11(52.52%) d 0.00(0.00%)	(0.13155) LP*(4) Y1 s(5.92%) p 5.06(29.94%) d 10.84(64.14%)	6.18
(1.74246) BD (1)AI4-C13 (13.10%) 0.3620*AI4 s(45.89%) p 1.17(53.78%) d 0.01(0.33%) (86.90%) 0.9322* C13 s(47.30%) p 1.11(52.70%) d 0.00(0.00%)	(0.31853) LP*(1) Y1 s(0.25%) p 30.48(7.52%) d 99.99(92.23%)	29.13
(1.74246) BD (1)AI4-C13 (13.10%) 0.3620*AI4 s(45.89%) p 1.17(53.78%) d 0.01(0.33%) (86.90%) 0.9322* C13 s(47.30%) p 1.11(52.70%) d 0.00(0.00%)	(0.18233) LP*(2) Y1 s(9.42%) p 1.67(15.68%) d 7.95(74.90%)	26.24
(1.74246) BD (1)AI4-C13 (13.10%) 0.3620*AI4 s(45.89%) p 1.17(53.78%) d 0.01(0.33%) (86.90%) 0.9322* C13 s(47.30%) p 1.11(52.70%) d 0.00(0.00%)	(0.12239) LP*(5) Y1 s(3.16%) p 15.16(47.92%) d 15.47(48.92%)	7.54
(1.92270) BD (1) C11-H12 (63.98%) 0.7999* C11 s(24.61%) p 3.06(75.35%) d 0.00(0.04%) (36.02%) 0.6001* H12 s(99.96%) p 0.00(0.04%)	(0.18233) LP*(2) Y1 s(9.42%) p 1.67(15.68%) d 7.95(74.90%)	5.91
(1.94161) BD (1) C11-C13 (50.09%) 0.7078* C11 s(27.65%) p 2.62(72.31%) d 0.00(0.04%) (49.91%) 0.7065* C13 s(27.57%) p 2.63(72.39%) d 0.00(0.04%)	(0.18233) LP*(2) Y1 s(9.42%) p 1.67(15.68%) d 7.95(74.90%)	19.93

(1.92249) BD (1) C13-H14 (64.26%) 0.8016* C13 s(24.93%) p 3.01(75.03%) d 0.00(0.04%) (35.74%) 0.5979* H14 s(99.96%) p 0.00(0.04%)	(0.18233) LP*(2) Y1 s(9.42%) p 1.67(15.68%) d 7.95(74.90%)	3.75
(1.65430) LP (1) C11 s(0.18%) p 99.99(99.82%) d 0.02(0.00%)	(0.31853) LP*(1) Y1 s(0.25%) p 30.48(7.52%) d 99.99(92.23%)	10.30
(1.64076) LP (1) C13 s(0.11%) p 99.99(99.88%) d 0.04(0.00%)	(0.31853) LP*(1) Y1 s(0.25%) p 30.48(7.52%) d 99.99(92.23%)	18.83
(1.74314) BD (1)A13-C11 (13.19%) 0.3632*A13 s(40.63%) p 1.45(58.98%) d 0.01(0.38%) (86.81%) 0.9317* C11 s(47.48%) p 1.11(52.52%) d 0.00(0.00%)	(0.32916) LP*(1) Y2 s(0.11%) p 74.33(8.12%) d 99.99(91.77%)	31.74
(1.74314) BD (1)A13-C11 (13.19%) 0.3632*A13 s(40.63%) p 1.45(58.98%) d 0.01(0.38%) (86.81%) 0.9317* C11 s(47.48%) p 1.11(52.52%) d 0.00(0.00%)	(0.20549) LP*(2) Y2 s(5.05%) p 3.26(16.46%) d15.53(78.49%)	10.70
(1.74314) BD (1)A13-C11 (13.19%) 0.3632*A13 s(40.63%) p 1.45(58.98%) d 0.01(0.38%) (86.81%) 0.9317* C11 s(47.48%) p 1.11(52.52%) d 0.00(0.00%)	(0.19382) LP*(3) Y2 s(2.83%) p 2.38(6.72%) d 31.99(90.45%)	36.32
(1.74314) BD (1)A13-C11 (13.19%) 0.3632*A13 s(40.63%) p 1.45(58.98%) d 0.01(0.38%) (86.81%) 0.9317* C11 s(47.48%) p 1.11(52.52%) d 0.00(0.00%)	(0.16938) LP*(4) Y2 s(0.31%) p 85.25(26.25%) d 99.99(73.45%)	6.11
(1.74314) BD (1)A13-C11 (13.19%) 0.3632*A13 s(40.63%) p 1.45(58.98%) d 0.01(0.38%) (86.81%) 0.9317* C11 s(47.48%) p 1.11(52.52%) d 0.00(0.00%)	(0.11134) LP*(6) Y2 s(2.98%) p 15.15(45.10%) d 17.44(51.92%)	5.44
(1.74246) BD (1)A14-C13 (13.10%) 0.3620*A14 s(45.89%) p 1.17(53.78%) d 0.01(0.33%) (86.90%) 0.9322* C13 s(47.30%) p 1.11(52.70%) d 0.00(0.00%)	(0.32916) LP*(1) Y2 s(0.11%) p 74.33(8.12%) d 99.99(91.77%)	37.65
(1.74246) BD (1) A14-C13 (13.10%) 0.3620*A14 s(45.89%) p 1.17(53.78%) d 0.01(0.33%)	(0.20549) LP*(2) Y2 s(5.05%) p 3.26(16.46%) d 15.53(78.49%)	41.51

(86.90%) 0.9322* C13 s(47.30%) p 1.11(52.70%) d 0.00(0.00%)		
(1.74246) BD (1) AI4-C13 (13.10%) 0.3620*AI4 s(45.89%) p 1.17(53.78%) d 0.01(0.33%) (86.90%) 0.9322* C13 s(47.30%) p 1.11(52.70%) d 0.00(0.00%)	(0.19382) LP*(3) Y2 s(2.83%) p 2.38(6.72%) d 31.99(90.45%)	9.18
(1.92270) BD (1) C11-H12 (63.98%) 0.7999* C11 s(24.61%) p 3.06(75.35%) d 0.00(0.04%) (36.02%) 0.6001* H12 s(99.96%) p 0.00(0.04%)	(0.11134) LP*(6) Y2 s(2.98%) p 15.15(45.10%) d 17.44(51.92%)	4.86
(1.94161) BD (1) C11-C13 (50.09%) 0.7078* C11 s(27.65%) p 2.62(72.31%) d 0.00(0.04%) (49.91%) 0.7065* C13 s(27.57%) p 2.63(72.39%) d 0.00(0.04%)	(0.20549) LP*(2) Y2 s(5.05%) p 3.26(16.46%) d 15.53(78.49%)	9.23
(1.94161) BD (1) C11-C13 (50.09%) 0.7078* C11 s(27.65%) p 2.62(72.31%) d 0.00(0.04%) (49.91%) 0.7065* C13 s(27.57%) p 2.63(72.39%) d 0.00(0.04%)	(0.19382) LP*(3) Y2 s(2.83%) p 2.38(6.72%) d 31.99(90.45%)	13.86
(1.92249) BD (1) C13-H14 (64.26%) 0.8016* C13 s(24.93%) p 3.01(75.03%) d 0.00(0.04%) (35.74%) 0.5979* H14 s(99.96%) p 0.00(0.04%)	(0.11134) LP*(6) Y2 s(2.98%) p 15.15(45.10%) d 17.44(51.92%)	7.37
(1.65430) LP (1) C11 s(0.18%) p 99.99(99.82%) d 0.02(0.00%)	(0.32916) LP*(1) Y2 s(0.11%) p 74.33(8.12%) d 99.99(91.77%)	16.20
(1.65430) LP (1) C11 s(0.18%) p 99.99(99.82%) d 0.02(0.00%)	(0.09513) LP*(7) Y2 s(64.33%) p 0.24(15.28%) d 0.32(20.39%)	4.80
(1.64076) LP (1) C13 s(0.11%) p 99.99(99.88%) d 0.04(0.00%)	(0.32916) LP*(1) Y2 s(0.11%) p 74.33(8.12%) d 99.99(91.77%)	10.15
(1.64076) LP (1) C13 s(0.11%) p 99.99(99.88%) d 0.04(0.00%)	(0.09513) LP*(7) Y2 s(64.33%) p 0.24(15.28%) d 0.32(20.39%)	4.85
(1.65430) LP (1) C11 s(0.18%) p99.99(99.82%) d 0.02(0.00%)	(0.28853) LP*(2) AI3 s(0.28%) p 99.99(99.13%) d 2.12(0.59%)	12.35
(1.64076) LP (1) C13 s(0.11%) p 99.99(99.88%) d 0.04(0.00%)	(0.30753) LP*(2) AI4 s(1.58%) p 62.01(97.70%) d 0.46(0.72%)	13.03
(1.64921) LP (1) C189 s(17.85%) p 4.60(82.15%) d 0.00(0.00%)	(0.32916) LP*(1) Y2 s(0.11%) p 74.33(8.12%) d 99.99(91.77%)	4.15

(1.64921) LP (1) C189 s(17.85%) p 4.60(82.15%) d 0.00(0.00%)	(0.16938) LP*(4) Y2 s(0.31%) p 85.25(26.25%) d 99.99(73.45%)	7.85
(1.64921) LP (1) C189 s(17.85%) p 4.60(82.15%) d 0.00(0.00%)	(0.38375) LP*(1) AI3 s(56.83%) p 0.76(43.00%) d 0.00(0.17%)	45.70
(1.64921) LP (1) C189 s(17.85%) p 4.60(82.15%) d 0.00(0.00%)	(0.28853) LP*(2) AI3 s(0.28%) p 99.99(99.13%) d 2.12(0.59%)	31.55
(1.64921) LP (1) C189 s(17.85%) p 4.60(82.15%) d 0.00(0.00%)	(0.21757) LP*(3) AI3 s(2.22%) p 43.98(97.62%) d 0.07(0.16%)	30.24
(1.64239) LP (1) C196 s(17.87%) p 4.60(82.13%) d 0.00(0.00%)	(0.38375) LP*(1) AI3 s(56.83%) p 0.76(43.00%) d 0.00(0.17%)	136.80
(1.64239) LP (1) C196 s(17.87%) p 4.60(82.13%) d 0.00(0.00%)	(0.21757) LP*(3) AI3 s(2.22%) p 43.98(97.62%) d 0.07(0.16%)	24.38
(1.64800) LP (1) C203 s(17.11%) p 4.84(82.89%) d 0.00(0.00%)	(0.17054) LP*(3) Y1 s(4.41%) p 6.57(28.99%) d 15.09(66.59%)	4.48
(1.64800) LP (1) C203 s(17.11%) p 4.84(82.89%) d 0.00(0.00%)	(0.12239) LP*(5) Y1 s(3.16%) p 15.16(47.92%) d 15.47(48.92%)	4.48
(1.64800) LP (1) C203 s(17.11%) p 4.84(82.89%) d 0.00(0.00%)	(0.38375) LP*(1) AI3 s(56.83%) p 0.76(43.00%) d 0.00(0.17%)	20.10
(1.64800) LP (1) C203 s(17.11%) p 4.84(82.89%) d 0.00(0.00%)	(0.28853) LP*(2) AI3 s(0.28%) p 99.99(99.13%) d 2.12(0.59%)	38.92
(1.64800) LP (1) C203 s(17.11%) p 4.84(82.89%) d 0.00(0.00%)	(0.21757) LP*(3) AI3 s(2.22%) p 43.98(97.62%) d 0.07(0.16%)	23.83
(1.63348) LP (1) C 210 s(17.51%) p 4.71(82.49%) d 0.00(0.00%)	(0.13155) LP*(4) Y1 s(5.92%) p 5.06(29.94%) d 10.84(64.14%)	6.83
(1.63348) LP (1) C210 s(17.51%) p 4.71(82.49%) d 0.00(0.00%)	(0.35821) LP*(1) AI4 s(48.89%) p 1.04(50.95%) d 0.00(0.16%)	34.26
(1.63348) LP (1) C210 s(17.51%) p 4.71(82.49%) d 0.00(0.00%)	(0.30753) LP*(2) AI4 s(1.58%) p 62.01(97.70%) d 0.46(0.72%)	23.51
(1.63348) LP (1) C210 s(17.51%) p 4.71(82.49%) d 0.00(0.00%)	(0.20922) LP*(3) AI4 s(3.65%) p 26.37(96.18%) d 0.05(0.17%)	33.09
(1.64131) LP (1) C217 s(17.58%) p 4.69(82.42%) d 0.00(0.00%)	(0.35821) LP*(1) AI4 s(48.89%) p 1.04(50.95%) d 0.00(0.16%)	136.11
(1.64131) LP (1) C217 s(17.58%) p 4.69(82.42%) d 0.00(0.00%)	(0.30753) LP*(2) AI4 s(1.58%) p 62.01(97.70%) d 0.46(0.72%)	7.77
(1.64131) LP (1) C217 s(17.58%) p 4.69(82.42%) d 0.00(0.00%)	(0.20922) LP*(3) AI4 s(3.65%) p 26.37(96.18%) d 0.05(0.17%)	14.59
(1.64018) LP (1) C224 s(17.41%) p 4.74(82.59%) d 0.00(0.00%)	(0.20549) LP*(2) Y2 s(5.05%) p 3.26(16.46%) d 15.53(78.49%)	5.31
(1.64018) LP (1) C224 s(17.41%) p 4.74(82.59%) d 0.00(0.00%)	(0.19382) LP*(3) Y2 s(2.83%) p 2.38(6.72%) d 31.99(90.45%)	11.97
(1.64018) LP (1) C224 s(17.41%) p 4.74(82.59%) d 0.00(0.00%)	(0.35821) LP*(1) AI4 s(48.89%) p 1.04(50.95%) d 0.00(0.16%)	7.95

(1.64018) LP (1) C224 s(17.41%) p 4.74(82.59%) d 0.00(0.00%)	(0.30753) LP*(2) A14 s(1.58%) p 62.01(97.70%) d 0.46(0.72%)	37.68
(1.64018) LP (1) C224 s(17.41%) p 4.74(82.59%) d 0.00(0.00%)	(0.20922) LP*(3) A14 s(3.65%) p 26.37(96.18%) d 0.05(0.17%)	25.16

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