

SUPPORTING INFORMATION

Multi-Electron Redox Reactivity of A Samarium(II) Hydrido Complex

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General remarks

All reactions were carried out under a dry and oxygen-free nitrogen atmosphere using Schlenk techniques and a Vigor glovebox. The nitrogen in the glovebox was constantly circulated through a copper/molecular sieves (4 Å) catalyst unit. The oxygen and moisture concentrations in the glovebox atmosphere were monitored using an O₂(GE)/H₂O (Xentaur) analyzer to ensure that both were always below 0.1 ppm. Toluene, hexane and Et₂O were purified by use of a Vigor VSPS-5 solvent purification system, and dried over fresh Na chips in the glovebox. Tetrahydropyran (THP), pentane and benzene-*d*₆ were distilled from Na/K alloy/benzophenone ketyl, degassed by the freeze-pump-thaw method (three times), and dried over fresh Na chips in the glovebox. [KCH(SiMe₃)₂]^[1], [SmI₂(THF)₅]^[2] and [(Cp^{Ar5})H] (Cp^{Ar5}=C₅Ar₅, Ar = 3,5-*i*-Pr₂-C₆H₃)^[3] were synthesized according to the published procedures. Other commercially available reagents were used without purification.

Samples for NMR spectroscopic measurements were prepared in the glovebox by use of J. Young valve NMR tubes. ¹H, ²H and ¹³C NMR spectra were recorded on a Bruker AV400 or AV500 spectrometer and referenced to the resonances of the solvent used. IR spectra of solid samples were measured with a Nicolet IS5 spectrometer and Diamond ATR accessory was placed in a glovebox (argon atmosphere). All magnetization data were recorded on a Quantum Design MPMS-XL7 SQUID magnetometer equipped with a 7 T magnet. Magnetic moments were collected with an external magnetic field of 1000 Oe at 300 K. The elemental analyses were performed on Elementar Vario EL cube (WO₃ was used as pro-oxidant) at National Analytical Research Centre of Changchun Institute of Applied Chemistry (CIAC).

Synthetic and analytical data for new complexes

Synthesis of $[(\text{Cp}^{\text{Ar5}})\text{K}(\text{THF})_2]$ (**1**)

Solid of KH (231 mg, 5.76 mmol) was added to a stirred solution of $(\text{Cp}^{\text{Ar5}})\text{H}$ (2.5 g, 2.88 mmol) in THF (30 mL). The mixture was stirred for 24 h at room temperature and then filtered. The filtrate was evaporated under reduced pressure to dryness and washed with cold hexane (5 mL x 3) to give complex **1** (2.66 g, 2.53 mmol, 88% yield) as colorless powder. Single crystals of complex **1** suitable for X-ray analysis were grown from hexane/toluene solution at $-30\text{ }^\circ\text{C}$ as colorless crystals. Crystal data of **1**: Triclinic, P-1; $a = 9.7490(18)\text{ \AA}$, $b = 14.689(3)\text{ \AA}$, $c = 23.623(4)\text{ \AA}$; $\alpha = 92.911(4)^\circ$, $\beta = 95.753(3)^\circ$, $\gamma = 93.301(4)^\circ$; $V = 3354.7(10)\text{ \AA}^3$, $Z = 2$, $R_{\text{int}} = 0.0286$, $R_{\text{sigma}} = 0.0138$.

^1H NMR (500 MHz, C_6D_6 , $25\text{ }^\circ\text{C}$): $\delta = 1.16$ (d, $^3J_{\text{HH}} = 7\text{ Hz}$, 60H, $\text{CH}(\text{CH}_3)_2$), 1.39 (m, 8H, THF), 2.71 (sept, $^3J_{\text{HH}} = 7\text{ Hz}$, 10H, $\text{CH}(\text{CH}_3)_2$), 3.44 (m, 8H, THF), 6.81 (s, 5H, aryl), 6.86 (d, $^3J_{\text{HH}} = 2\text{ Hz}$, 10H, aryl) ppm. ^{13}C $\{^1\text{H}\}$ NMR (125 MHz, C_6D_6 , $25\text{ }^\circ\text{C}$): $\delta = 24.02$ (s, $\text{CH}(\text{CH}_3)_2$), 25.35 (s, THF), 34.10 (s, $\text{CH}(\text{CH}_3)_2$), 67.50 (s, THF), 118.98 (s, aryl), 121.41 (s, Cp), 127.10 (s, aryl), 141.58 (s, aryl), 146.93 (s, aryl) ppm. Anal. calcd. for (**1**) $\text{C}_{73}\text{H}_{101}\text{O}_2\text{K}_1$ (1049.68): C, 83.53; H, 9.70 found: C, 83.77; H, 9.46. IR: 3496 (br), 2953 (s), 2868 (s), 1921 (w), 1726 (w), 1587 (s), 1468 (s), 1362 (m), 1330 (w), 1187 (m), 1132 (w), 1044 (s), 980 (m), 887 (s), 864 (s), 763 (w), 709 (s), 664 (m), 608 (m), 509 (s) cm^{-1} .

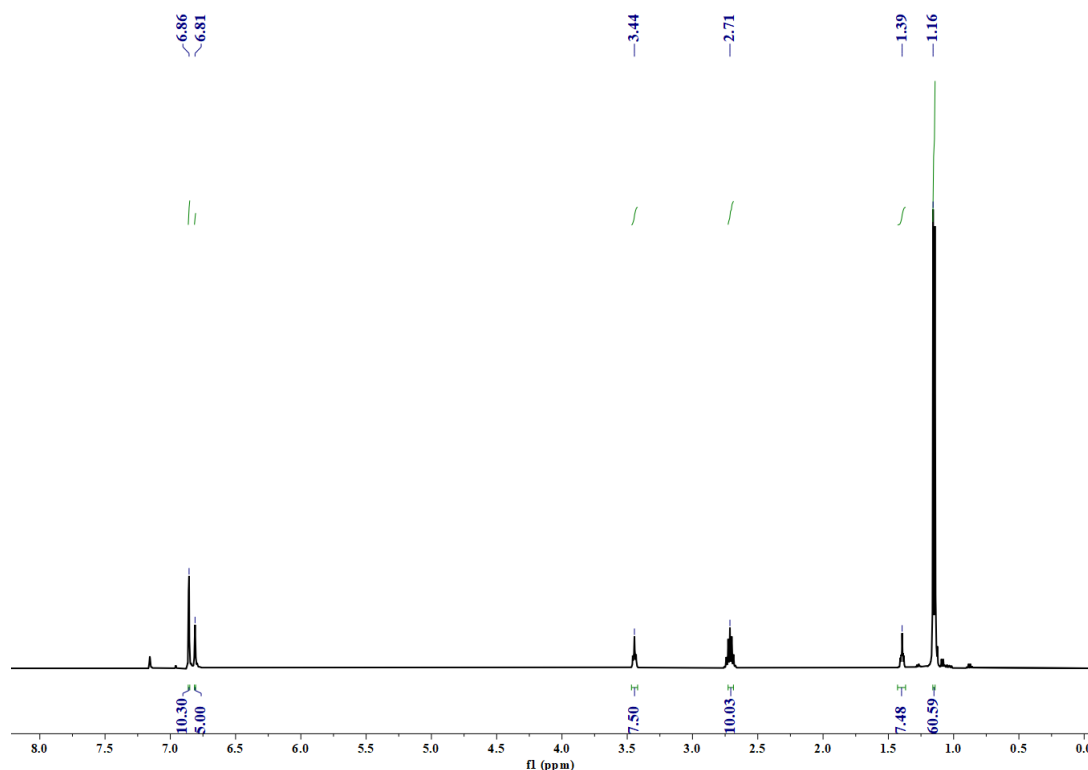


Figure S1. ^1H NMR spectrum (500 MHz) of $[(\text{Cp}^{\text{Ar5}})\text{K}(\text{THF})_2]$ (**1**) in C_6D_6 at $25\text{ }^\circ\text{C}$.

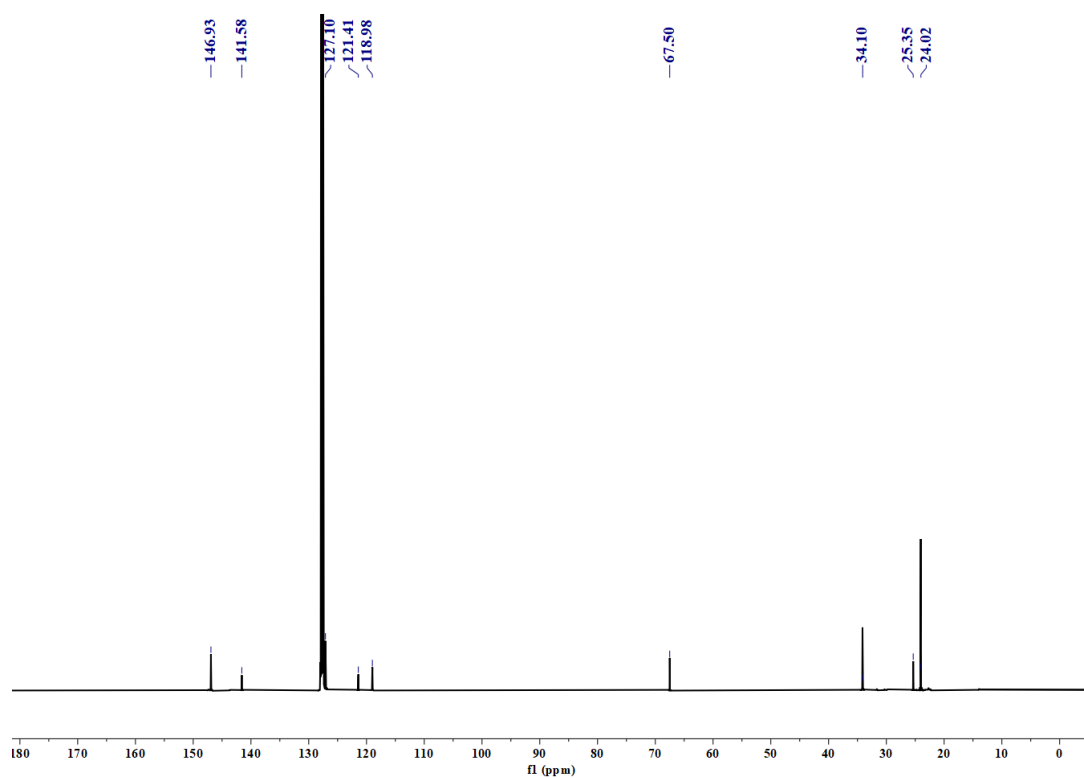


Figure S2. ^{13}C $\{^1\text{H}\}$ NMR spectrum (125 MHz) of $[(\text{Cp}^{\text{Ar5}})\text{K}(\text{THF})_2]$ (**1**) in C_6D_6 at 25 °C.

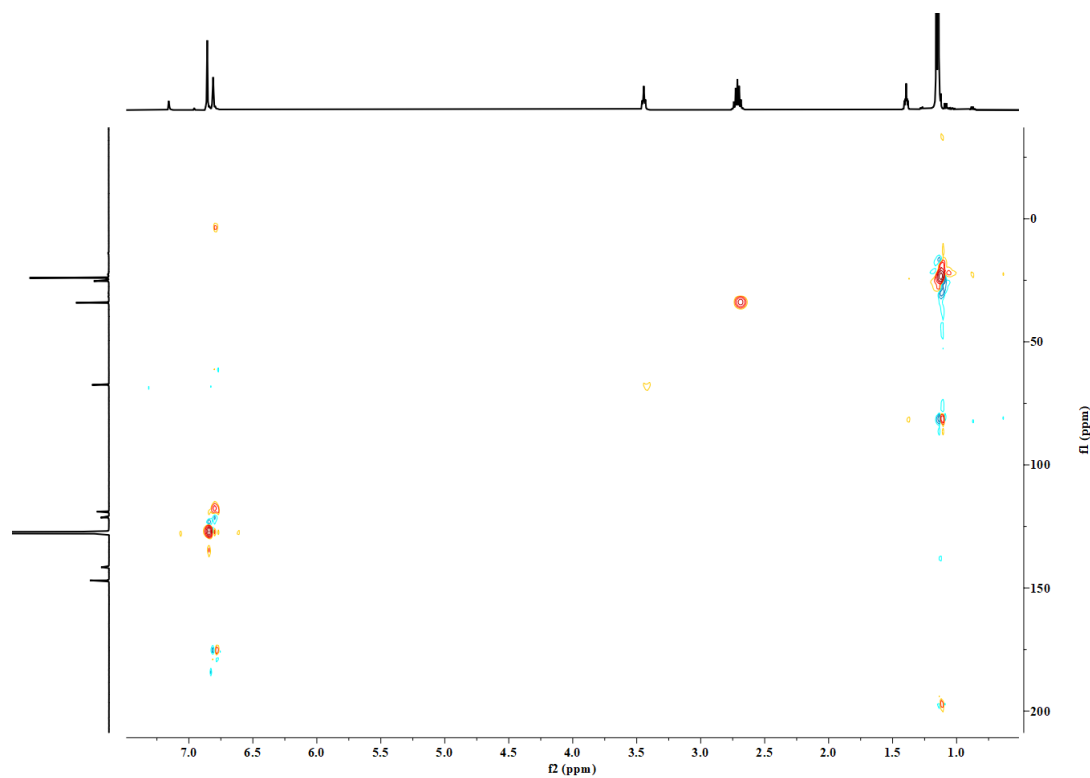


Figure S3. ^1H - ^{13}C HSQC NMR spectrum (500 MHz) of $[(\text{Cp}^{\text{Ar5}})\text{K}(\text{THF})_2]$ (**1**) in C_6D_6 at 25 °C.

Synthesis of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{II}}(\mu\text{-I})(\text{DABCO})]_2$ (2**)**

$[\text{SmI}_2(\text{THF})_5]$ (765 mg, 1.00 mmol) and $[\text{Cp}^{\text{Ar5}}\text{K}(\text{THF})_2]$ (**1**) (1.05 g, 1.00 mmol) were combined into a schlenk flask and dissolved in 30 mL of THF. The reaction mixture was heated to 80 °C and stirred for 12 h. Afterwards, the dark-green solution was filtered and all volatiles of the filtrate were removed *in vacuo*. To the residue was added a solution of DABCO (224 mg, 2.00 mmol) in benzene (10 mL) and stirred at room temperature for 30 minutes. The benzene solvent was evaporated under reduced pressure to give complex **2** (1.16 g, 0.46 mmol, 92% yield) as dark-green powder. Single crystals of **2**•(Hexane) suitable for X-ray analysis were grown from hexane/toluene solution at -30 °C as dark-green crystals.

^1H NMR (500 MHz, C_6D_6 , 25 °C): δ = -0.28, 0.43 (br, 12H, DABCO), 2.47 (br, 60H, $\text{CH}(\text{CH}_3)_2$), 3.83 (br, 10H, $\text{CH}(\text{CH}_3)_2$), 7.38 (br, 5H, aryl), 10.02 (br, 10H, aryl) ppm. ^{13}C $\{^1\text{H}\}$ NMR (125 MHz, C_6D_6 , 25 °C): δ = 25.24 (s, $\text{CH}(\text{CH}_3)_2$), 34.97 (s, $\text{CH}(\text{CH}_3)_2$), 53.59 (s, DABCO), 122.32 (s, aryl), 130.87, 152.38, 187.31 ppm. Detailed identification of the signals could not be performed due to paramagnetism of samarium(II). Magnetic moment (300K): $\mu_{\text{eff}} = 3.2 \mu_B$. Anal. calcd. for (**2**) $\text{C}_{142}\text{H}_{194}\text{I}_2\text{N}_4\text{Sm}_2$ (2511.50): C, 67.91; H, 7.79; N, 2.23; found: C, 67.76; H, 7.61; N, 2.30. IR: 2953 (s), 2866 (s), 1970 (w), 1590 (s), 1459 (s), 1321 (m), 1056 (s), 994 (m), 869 (s), 824 (w), 768 (s), 710 (s), 652 (m), 608 (m), 556 (m), 531 (m), 508 (s) cm^{-1} .

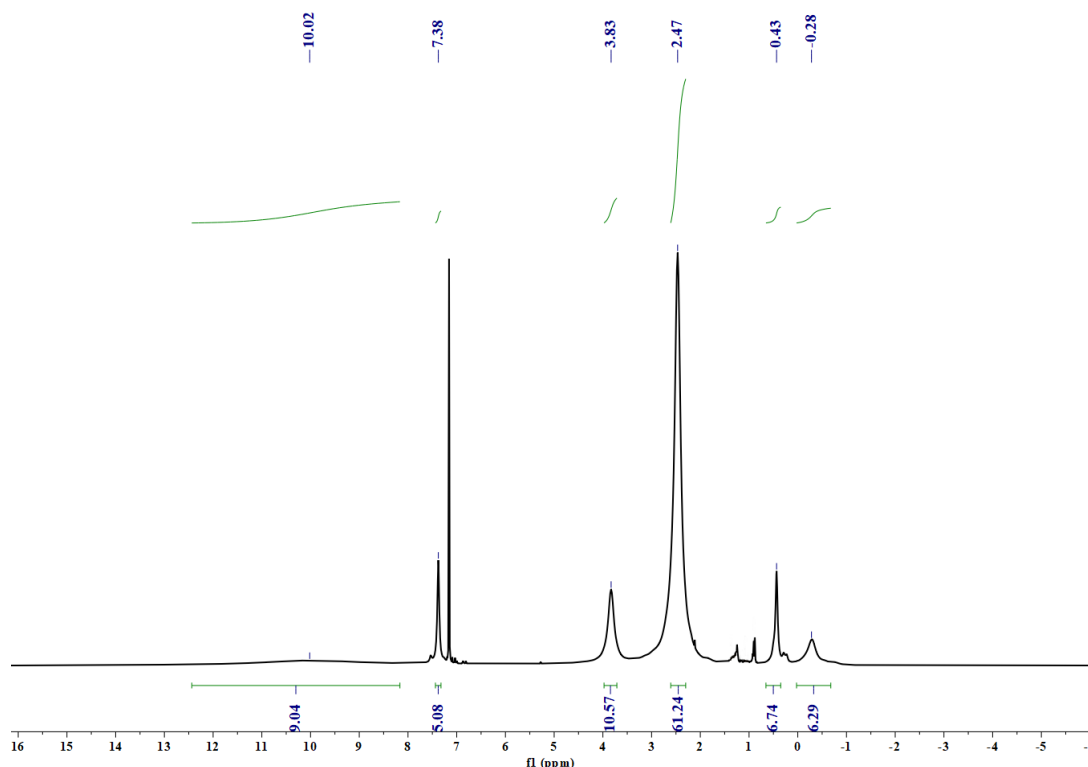


Figure S4. ^1H NMR spectrum (500 MHz) of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{II}}(\mu\text{-I})(\text{DABCO})]_2$ (**2**) in C_6D_6 at 25 °C.

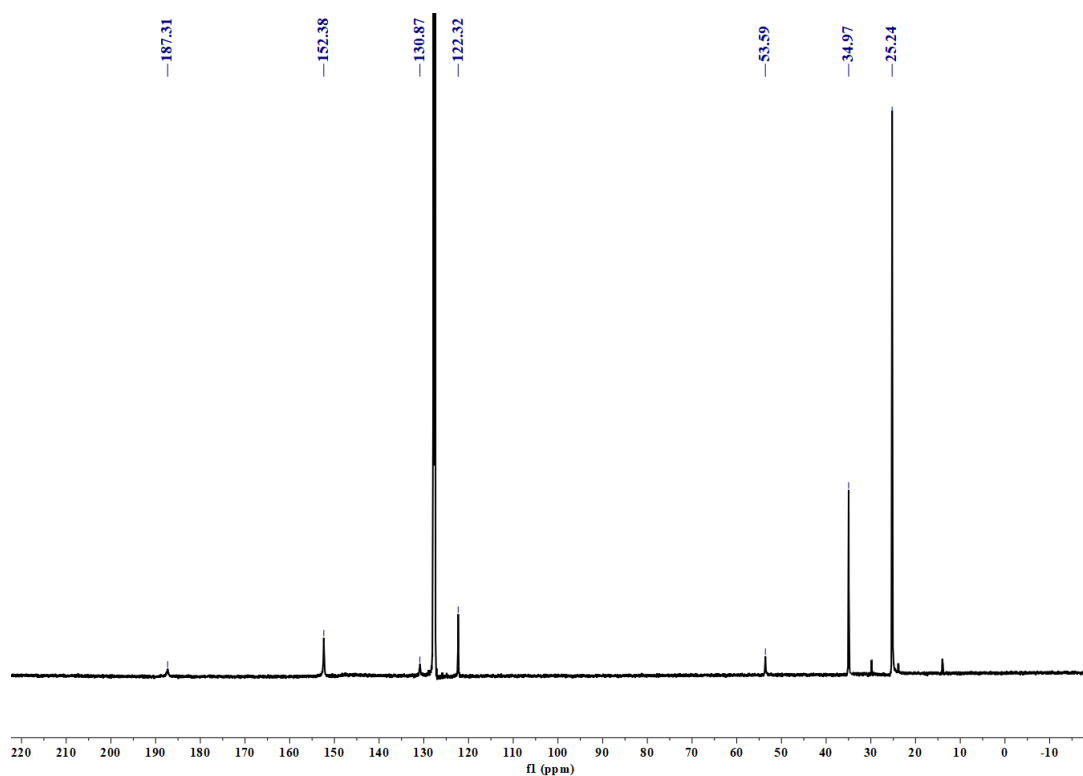


Figure S5. ^{13}C $\{^1\text{H}\}$ NMR spectrum (125 MHz) of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{II}}(\mu\text{-I})(\text{DABCO})]_2$ (**2**) in C_6D_6 at 25 °C.

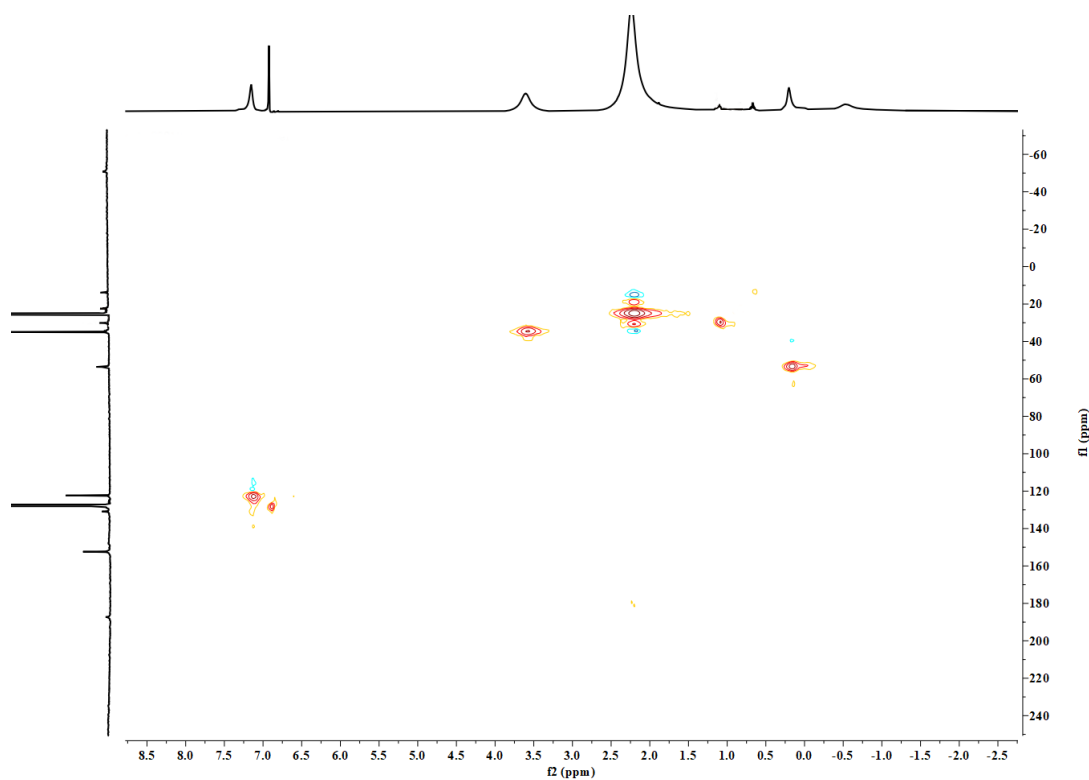


Figure S6. ^1H - ^{13}C HSQC NMR spectrum (500 MHz) of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{II}}(\mu\text{-I})(\text{DABCO})]_2$ (**2**) in C_6D_6 at 25 °C.

Synthesis of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{II}}\{\text{CH}(\text{SiMe}_3)_2\}(\text{DABCO})]$ (3**)**

Solid of $[\text{KCH}(\text{SiMe}_3)_2]$ (159 mg, 0.80 mmol) was added in several portions to a stirred solution of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{II}}(\mu\text{-I})(\text{DABCO})]_2$ (**2**) (1.0 g, 0.40 mmol) in benzene (15 mL) at $-30\text{ }^\circ\text{C}$. The mixture was stirred at $-30\text{ }^\circ\text{C}$ for 1 h and at room temperature for 2 h, then filtered. After evaporation of all the volatiles *in vacuo*, the residue was extracted twice with hexane (15 mLx2). The hexane solvent was removed under reduced pressure to give complex **3** (882 mg, 0.69 mmol, 86% yield) as dark-brown powder.

^1H NMR (500 MHz, C_6D_6 , $25\text{ }^\circ\text{C}$): $\delta = -2.31$ (br, 12H, DABCO), 3.25 (br, 60H, $\text{CH}(\text{CH}_3)_2$), 4.93 (br, 18H, $\text{Sm-CH}(\text{SiMe}_3)_2$), 5.94 (br, 10H, $\text{CH}(\text{CH}_3)_2$), 8.31 (s, 5H, aryl), 16.33 (br, 10H, aryl) ppm. ^{13}C $\{^1\text{H}\}$ NMR (125 MHz, C_6D_6 , $25\text{ }^\circ\text{C}$): $\delta = 25.86$ (s, $\text{CH}(\text{CH}_3)_2$), 37.16 (s, $\text{CH}(\text{CH}_3)_2$), 52.91 (s, DABCO), 125.77 (s, aryl), 150.33, 153.93, 183.17 ppm. Detailed identification of the signals could not be performed due to paramagnetism of samarium(II). Anal. calcd. for (**3**) $\text{C}_{78}\text{H}_{116}\text{N}_2\text{Si}_2\text{Sm}_1$ (1288.33): C, 72.72; H, 9.08; N, 2.17; found: C, 72.96; H, 9.21; N, 2.25. IR: 3625 (w), 2955 (s), 2869 (s), 2118 (w), 2064 (w), 1779 (w), 1593 (s), 1461 (s), 1379 (m), 1316 (m), 1250 (w), 1186 (w), 1106 (m), 1057 (s), 990 (w), 921 (w), 870 (s), 842 (m), 765 (m), 712 (m), 641 (w), 610 (w) cm^{-1} .

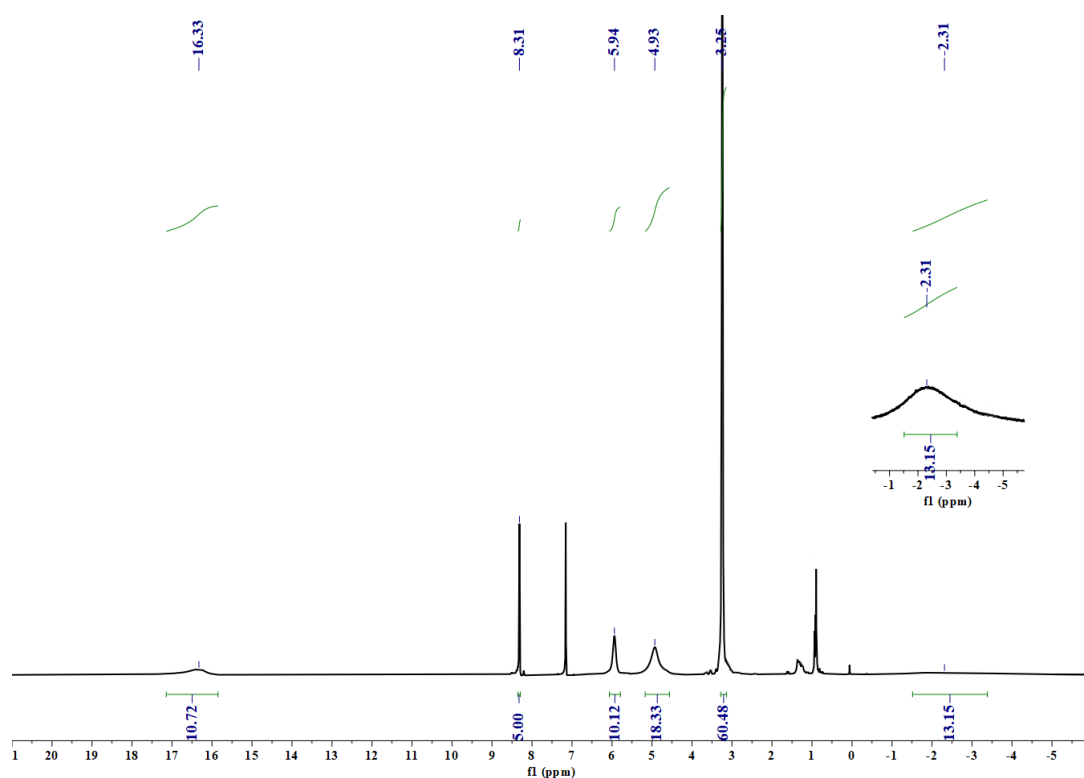


Figure S7. ^1H NMR spectrum (500 MHz) of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{II}}\{\text{CH}(\text{SiMe}_3)_2\}(\text{DABCO})]$ (**3**) in C_6D_6 at $25\text{ }^\circ\text{C}$.

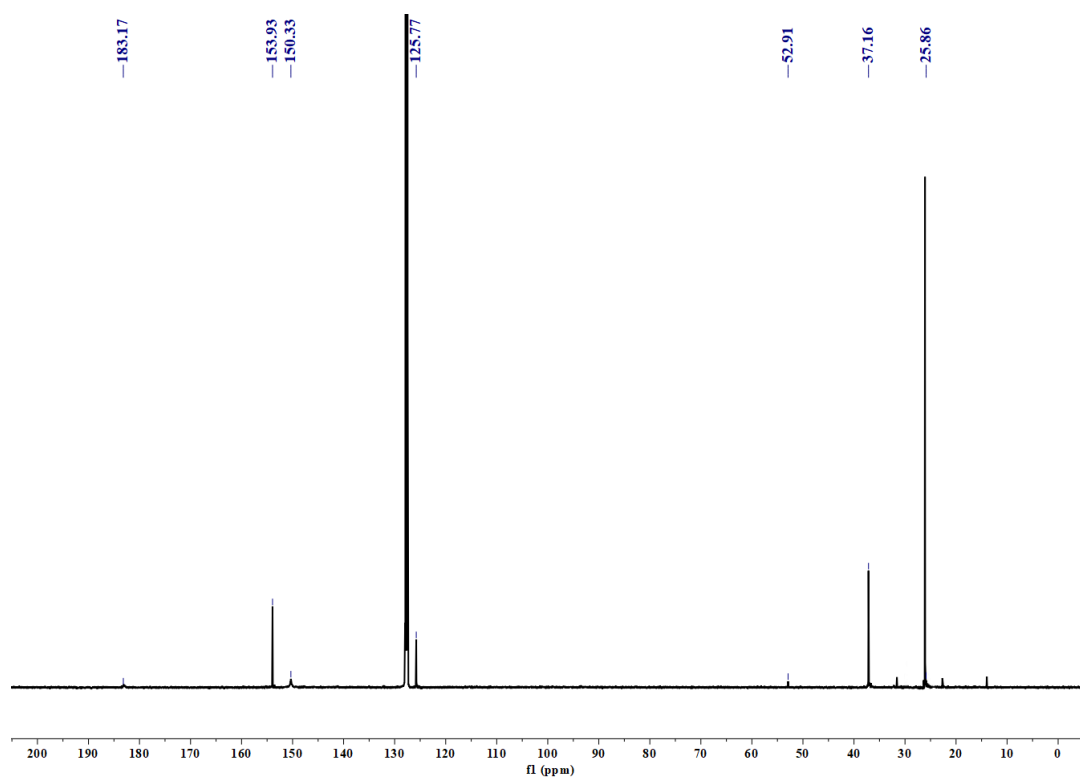


Figure S8. ^{13}C $\{^1\text{H}\}$ NMR spectrum (125 MHz) of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{II}}\{\text{CH}(\text{SiMe}_3)_2\}(\text{DABCO})]$ (**3**) in C_6D_6 at 25 °C.

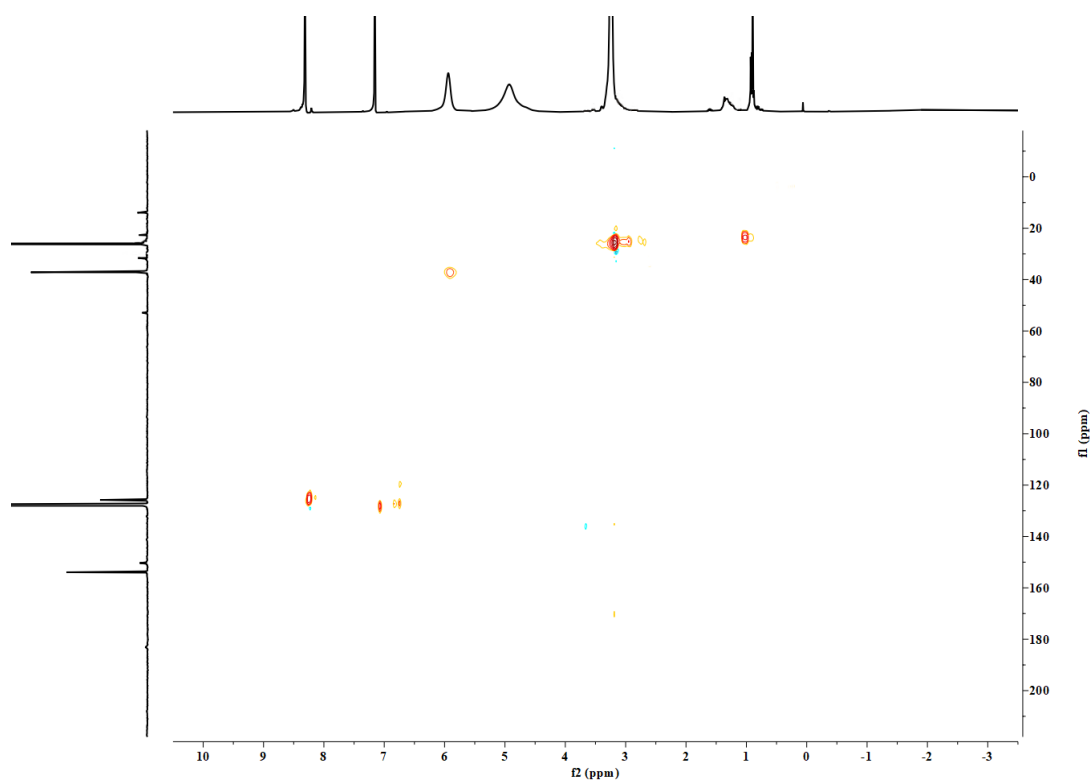


Figure S9. ^1H - ^{13}C HSQC NMR spectrum (500 MHz) of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{II}}\{\text{CH}(\text{SiMe}_3)_2\}(\text{DABCO})]$ (**3**) in C_6D_6 at 25 °C.

Synthesis of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{II}}(\mu\text{-H})(\text{DABCO})]_2$ (4**)**

A solution of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{II}}\{\text{CH}(\text{SiMe}_3)_2\}(\text{DABCO})]$ (**3**) (528 mg, 0.41 mmol) in hexane (5 mL) was added into a glass tube in a medium-pressure autoclave. The autoclave was transferred outside of the glovebox and pressurized with H_2 to 20 atm. The mixture was left standing at room temperature for 24 h to precipitate complex **4** (361 mg, 0.16 mmol, 78% yield) as dark-brown crystalline solid. Single crystals of complex **4**•(DABCO) suitable for X-ray analysis were grown from hexane solution containing free DABCO as dark-brown crystals at room temperature.

^1H NMR (500 MHz, C_6D_6 , 25 °C): δ = 1.63 (br, 1H, Sm-H), 1.81 (br, 12H, DABCO), 2.61 (br, 60H, $\text{CH}(\text{CH}_3)_2$), 5.32 (br, 10H, $\text{CH}(\text{CH}_3)_2$), 7.44 (br, 10H, aryl), 7.81 (br, 5H, aryl) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, C_6D_6 , 25 °C): δ = -25.08, 27.74 (s, $\text{CH}(\text{CH}_3)_2$), 35.21 (s, $\text{CH}(\text{CH}_3)_2$), 122.56 (s, aryl), 150.79, 152.11, 185.25 ppm. Detailed identification of the signals could not be performed due to paramagnetism of samarium(II). Magnetic moment (300K): $\mu_{\text{eff}} = 3.9 \mu_B$. Anal. calcd. for (**4**) $\text{C}_{142}\text{H}_{196}\text{N}_4\text{Sm}_2$ (2259.72): C, 75.47; H, 8.74; N, 2.48; found: C, 75.63; H, 8.81; N, 2.55. IR: 3622 (w), 2956 (s), 2869 (s), 1760 (w), 1593 (s), 1462 (s), 1379 (m), 1315 (s), 1255 (w), 1186 (w), 1103 (m), 1058 (s), 988 (w), 927 (m), 870 (s), 827 (w), 766 (m), 711(s), 639 (w), 521 (m) cm^{-1} .

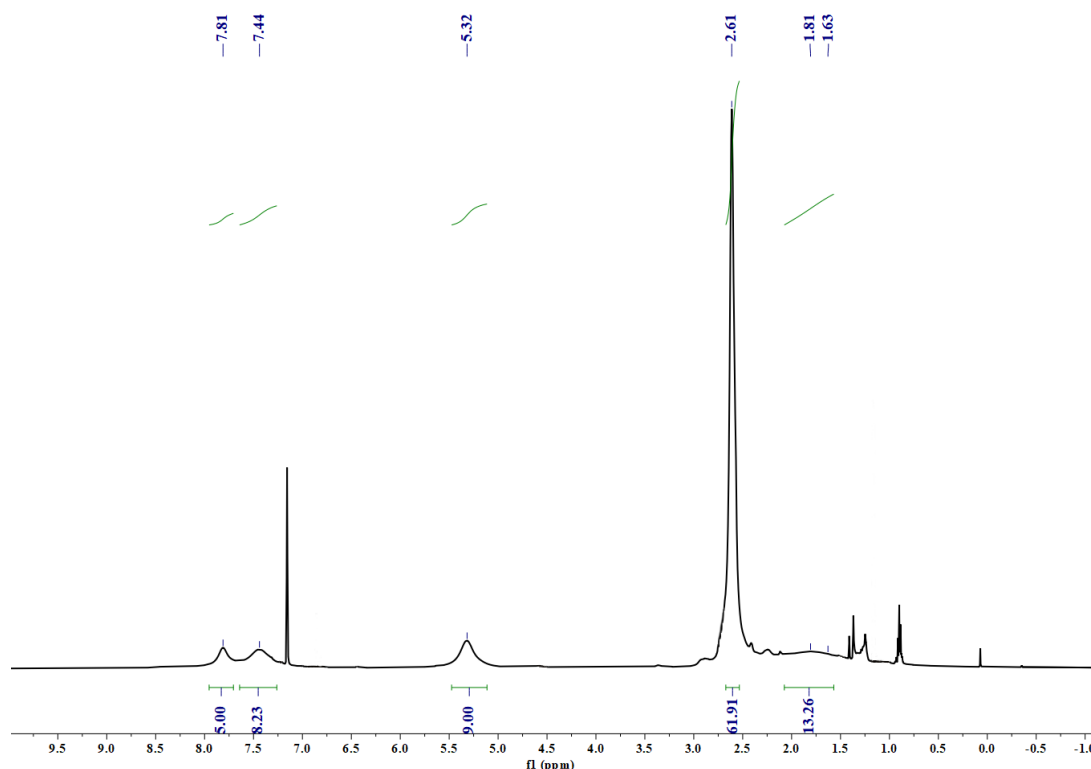


Figure S10. ^1H NMR spectrum (500 MHz) of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{II}}(\mu\text{-H})(\text{DABCO})]_2$ (**4**) in C_6D_6 at 25 °C.

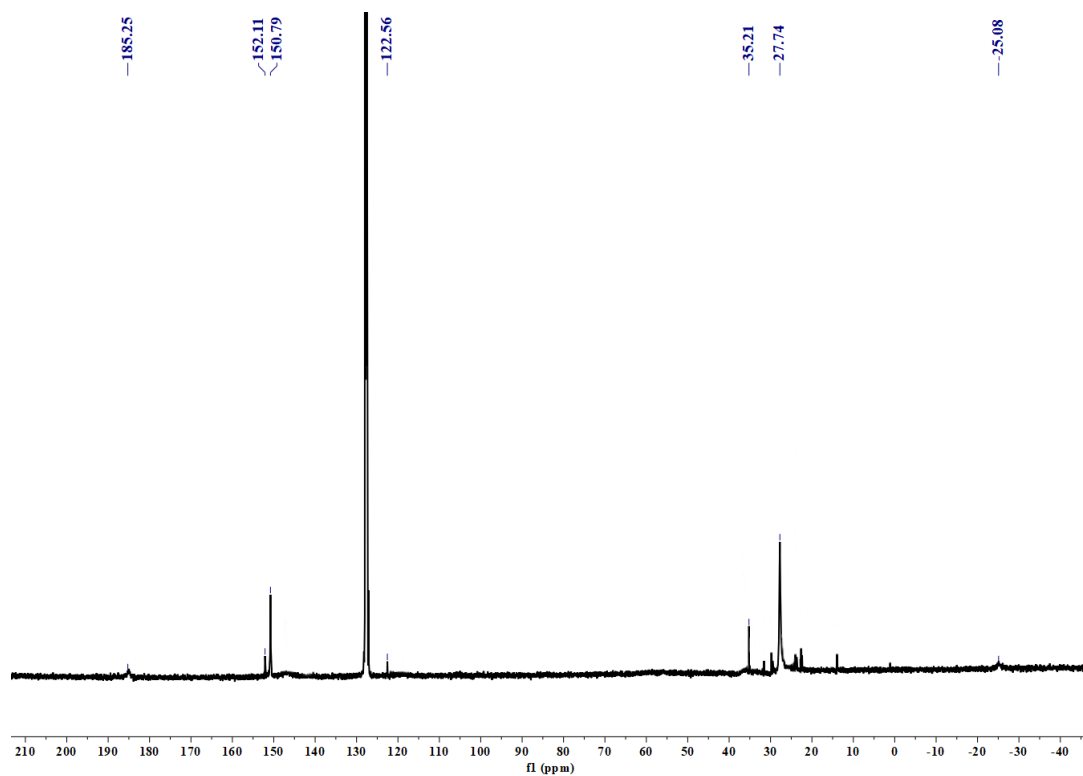


Figure S11. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (125 MHz) of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{II}}(\mu\text{-H})(\text{DABCO})_2]$ (**4**) in C_6D_6 at 25 °C.

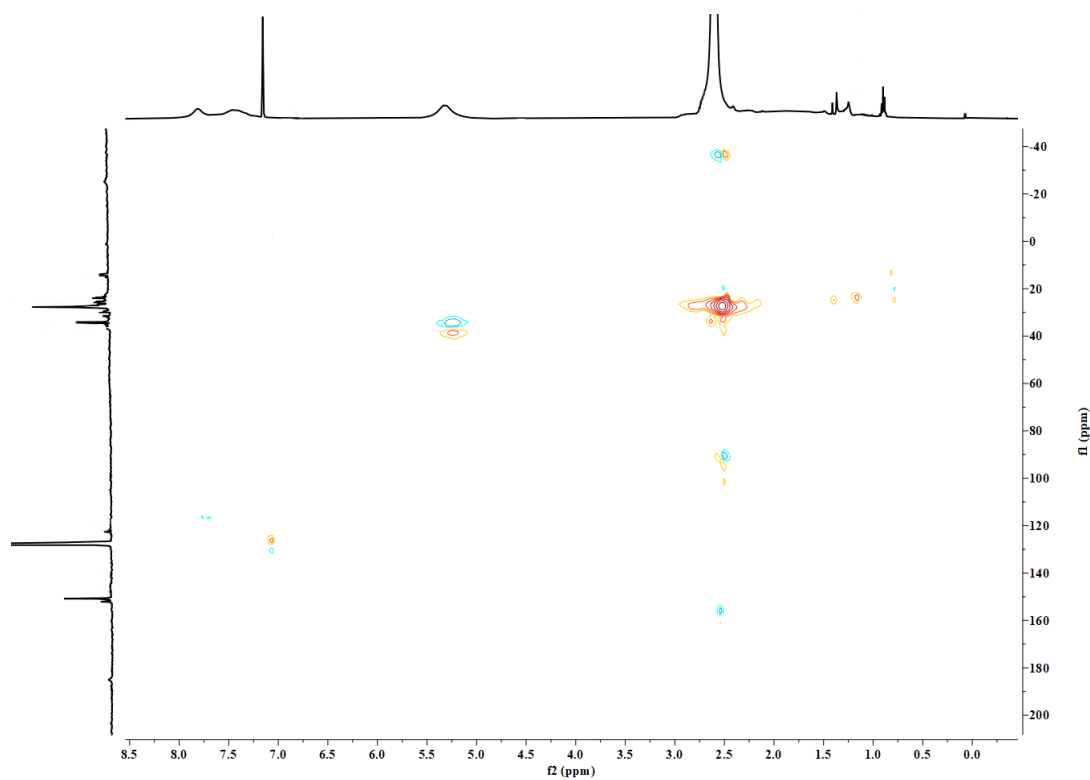


Figure S12. ^1H - ^{13}C HSQC NMR spectrum (500 MHz) of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{II}}(\mu\text{-H})(\text{DABCO})_2]$ (**4**) in C_6D_6 at 25 °C.

Syntheses of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{II}}(\mu\text{-D})(\text{DABCO})]_2$ (4-D**)**

The synthesis of complex **4-D** was analogous to that of complex **4** except for the use of deuteride gas D_2 (15 atm, 3 days).

^2H NMR (77 MHz, C_6D_6 , 25 °C) for $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{II}}(\mu\text{-D})(\text{DABCO})]_2$: $\delta = 1.63$ (br, Sm-D) ppm.
IR: 3622 (w), 2958 (s), 2870 (s), 1745 (w), 1593 (s), 1463 (s), 1379 (m), 1314 (m), 1254 (w), 1186 (w), 1107 (m), 1059 (s), 991 (w), 923 (m), 871 (s), 826 (w), 765 (m), 712 (s), 671 (w), 508 (m) cm^{-1} .

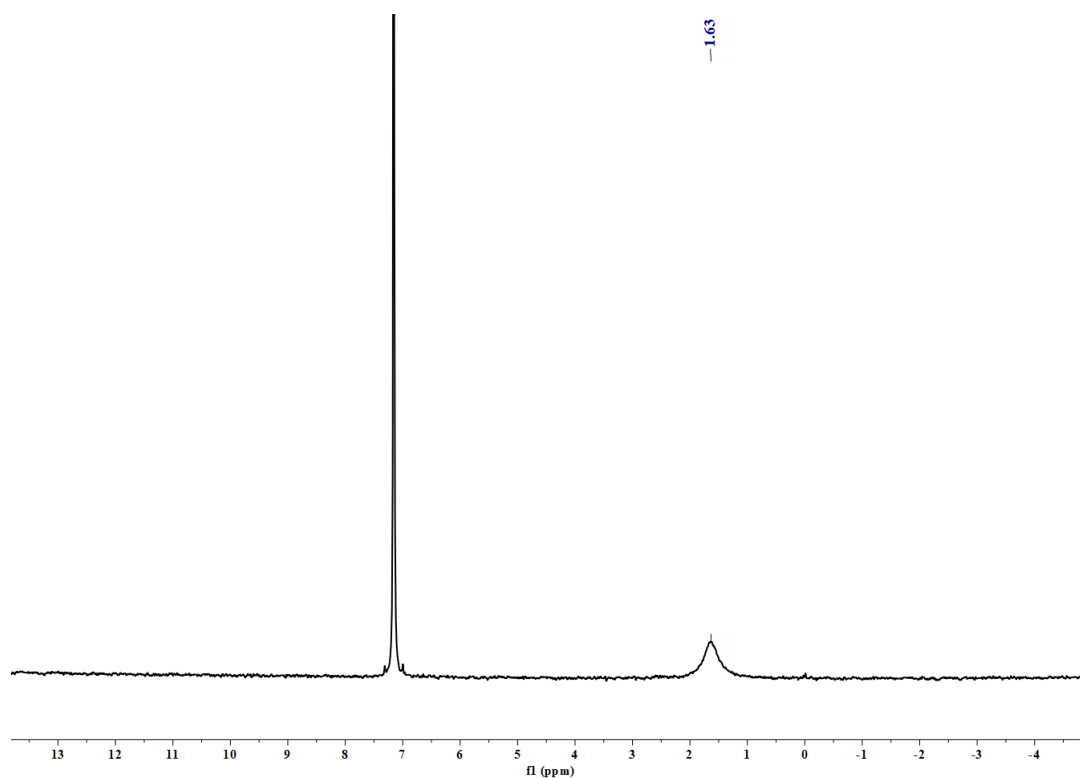


Figure S13. ^2H NMR spectrum (77 MHz) of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{II}}(\mu\text{-D})(\text{DABCO})]_2$ (**4-D**) in C_6H_6 at 25 °C.
(Drops of C_6D_6 were added as internal standard)

Synthesis of $[(\text{Cp}^{\text{Ar5}})_2\text{Sm}^{\text{II}}]$ (5**)**

A solution of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{II}}(\mu\text{-H})(\text{DABCO})]_2$ (**4**) (100 mg, 0.044 mmol) in THF (5 mL) was stirred at room temperature for 2 h. The resulting dark-purple mixture was filtered and all volatiles of the filtrate were removed under reduced pressure to give complex **5** (68 mg, 0.036 mmol, 82% yield) as dark-purple powder. Single crystals of complex **5** suitable for X-ray analysis were grown from hexane/toluene solution at $-30\text{ }^\circ\text{C}$ as dark-purple crystals.

^1H NMR (500 MHz, C_6D_6 , $25\text{ }^\circ\text{C}$): $\delta = 2.13$ (br, 60H, $\text{CH}(\text{CH}_3)_2$), 6.00 (br, 10H, $\text{CH}(\text{CH}_3)_2$), 8.21 (br, 5H, aryl) ppm. ^{13}C $\{^1\text{H}\}$ NMR (125 MHz, C_6D_6 , $25\text{ }^\circ\text{C}$): $\delta = -71.13$, 25.15 (s, $\text{CH}(\text{CH}_3)_2$), 35.55 (s, $\text{CH}(\text{CH}_3)_2$), 121.73, 153.24, 188.92 ppm. Detailed identification of the signals could not be performed due to paramagnetism of samarium(II). Anal. calcd. for (**5**) $\text{C}_{130}\text{H}_{170}\text{Sm}_1$ (1883.00): C, 82.92; H, 9.10; found: C, 83.08; H, 9.24. IR: 3131 (br), 2954 (s), 2867 (s), 2225 (w), 1909 (w), 1587(s), 1511 (m), 1458 (s), 1278 (s), 1089 (w), 1010 (m), 979 (m), 863 (s), 706 (s), 595 (m), 554 (m), 519 (w) cm^{-1} .

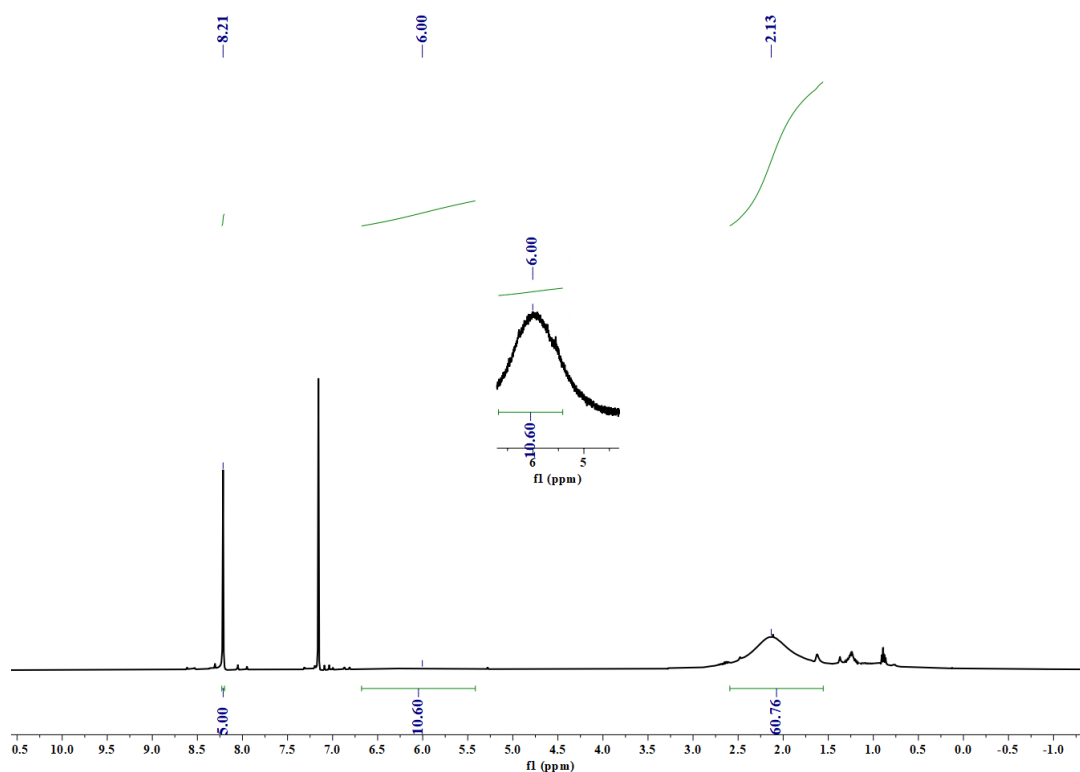


Figure S14. ^1H NMR spectrum (500 MHz) of $[(\text{Cp}^{\text{Ar5}})_2\text{Sm}^{\text{II}}]$ (**5**) in C_6D_6 at $25\text{ }^\circ\text{C}$.

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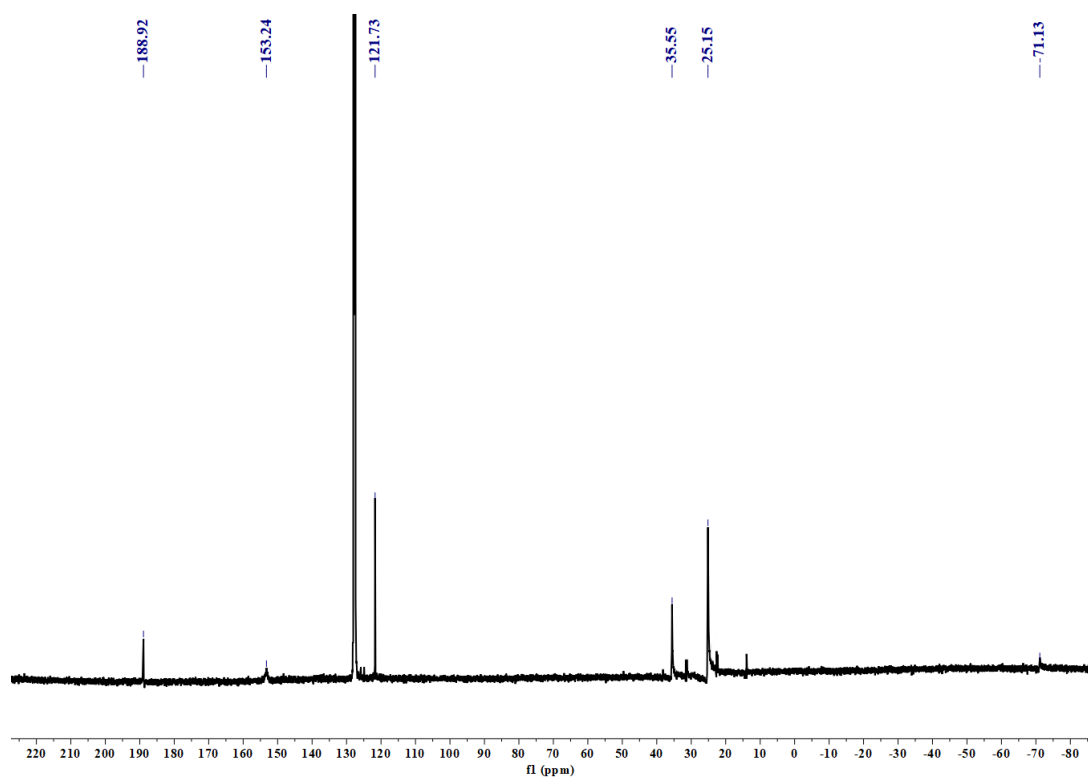


Figure S15. ^{13}C $\{^1\text{H}\}$ NMR spectrum (125 MHz) of $[(\text{Cp}^{\text{Ar5}})_2\text{Sm}^{\text{II}}]$ (**5**) in C_6D_6 at 25 °C.

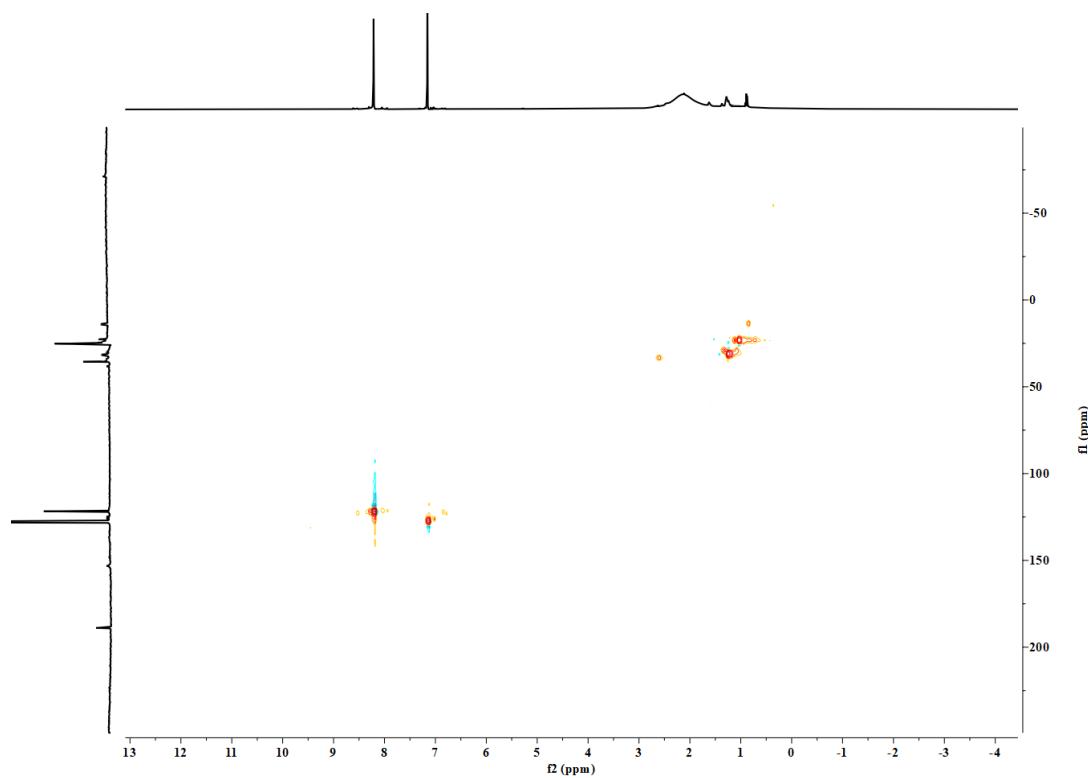


Figure S16. ^1H - ^{13}C HSQC NMR spectrum (500 MHz) of $[(\text{Cp}^{\text{Ar5}})_2\text{Sm}^{\text{II}}]$ (**5**) in C_6D_6 at 25 °C.

Synthesis of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{III}}(\mu\text{-Se})(\text{DABCO})]_2$ (6**)**

To a stirring solution of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{II}}(\mu\text{-H})(\text{DABCO})]_2$ (**4**) (85 mg, 0.038 mmol) in benzene (5 mL) was added powdery Se (6.3 mg, 0.08 mmol) at room temperature. After 2 h, the solution was filtered and all volatiles of the filtrate were removed under reduced pressure to give complex **6** (70 mg, 0.029 mmol, 77 % yield) as pale-brown powder. Single crystals of complex **6** • (0.5 x Hexane) suitable for X-ray analysis were grown from volatilization of a concentrated hexane/benzene solution at room temperature as pale-brown crystals.

^1H NMR (500 MHz, C_6D_6 , 25 °C): δ = 3.07 (br, 60H, $\text{CH}(\text{CH}_3)_2$), 5.12 (br, 10H, $\text{CH}(\text{CH}_3)_2$), 8.21 (br, 5H, aryl), 13.06 (br, 10H, aryl) ppm. ^{13}C $\{^1\text{H}\}$ NMR (125 MHz, C_6D_6 , 25 °C): δ = 24.89 (s, $\text{CH}(\text{CH}_3)_2$), 34.15 (s, $\text{CH}(\text{CH}_3)_2$), 121.48, 151.75 ppm. Detailed identification of the signals could not be performed due to paramagnetism of samarium(III). Anal. calcd. for (**6**) $\text{C}_{142}\text{H}_{194}\text{N}_4\text{Se}_2\text{Sm}_2$ (2415.62): C, 70.60; H, 8.09; N, 2.32; found: C, 70.72; H, 8.14; N, 2.30. IR: 3488 (br), 2954 (s), 2867 (s), 1776 (w), 1590 (s), 1461 (s), 1270 (m), 1187 (m), 1139 (m), 1100 (m), 1053 (m), 1000 (m), 964 (m), 932 (w), 868 (s), 826 (m), 770 (s), 708 (s), 660 (m), 604 (m), 547 (m), 508 (s) cm^{-1} .

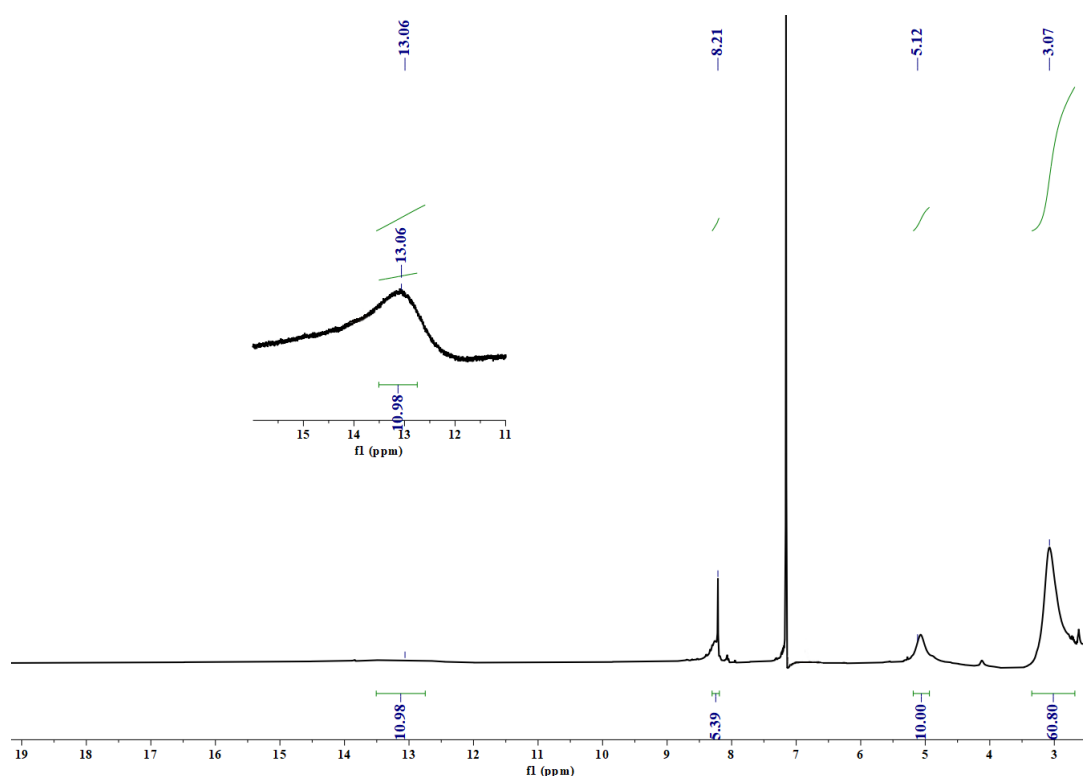


Figure S17. ^1H NMR spectrum (500 MHz) of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{III}}(\mu\text{-Se})(\text{DABCO})]_2$ (**6**) in C_6D_6 at 25 °C.

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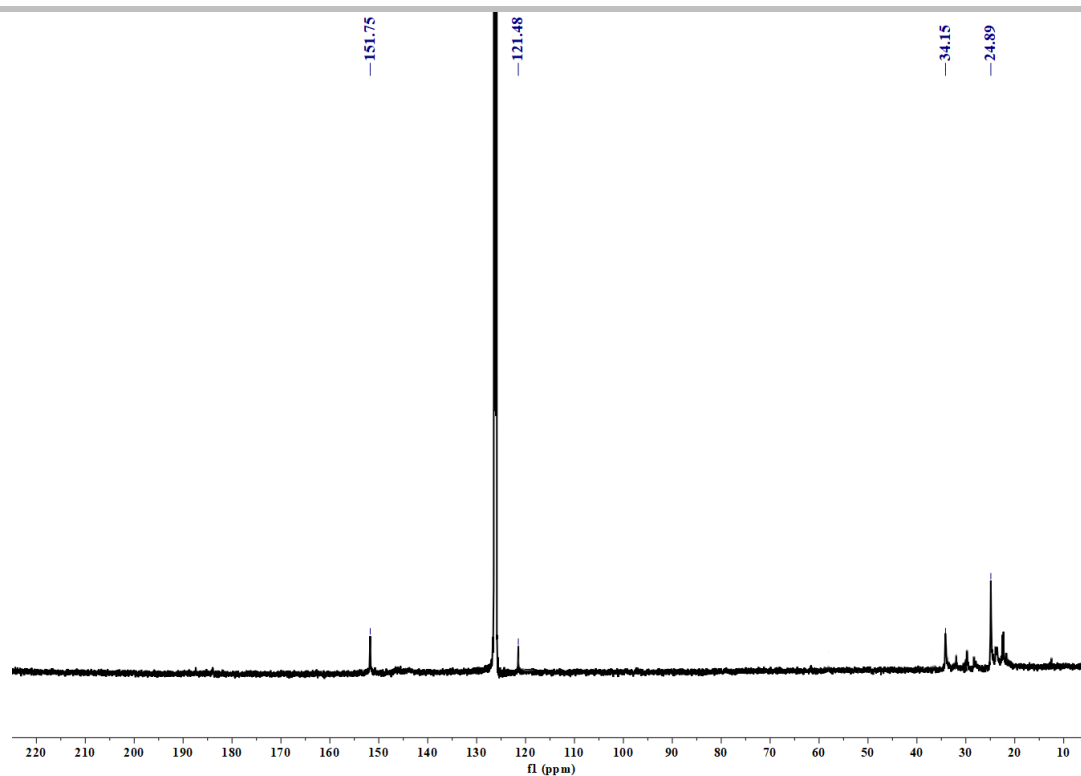


Figure S18. ^{13}C $\{^1\text{H}\}$ NMR spectrum (125 MHz) of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{III}}(\mu\text{-Se})(\text{DABCO})]_2$ (**6**) in C_6D_6 at 25°C .

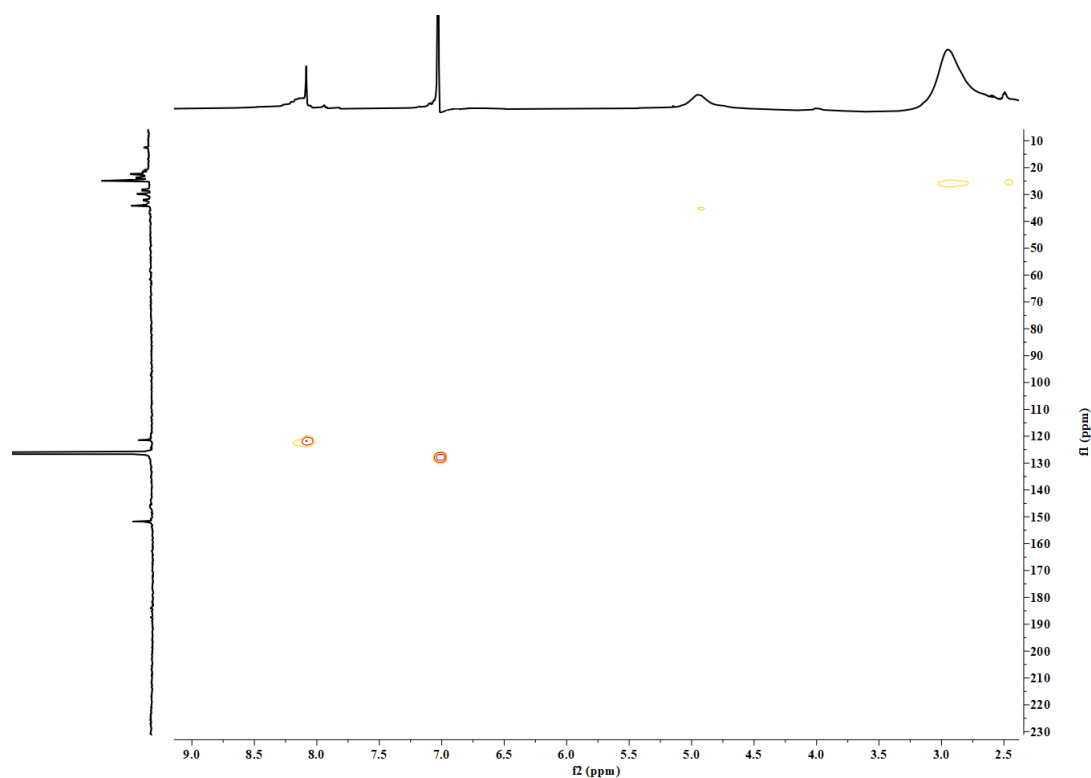


Figure S19. ^1H - ^{13}C HSQC NMR spectrum (500 MHz) of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{III}}(\mu\text{-Se})(\text{DABCO})]_2$ (**6**) in C_6D_6 at 25°C .

Synthesis of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{III}}(\mu\text{-PhN-NPh})_2]$ (7**)**

To a stirring solution of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{II}}(\mu\text{-H})(\text{DABCO})]_2$ (**4**) (110 mg, 0.049 mmol) in benzene (5 mL) was added azobenzene (16 mg, 0.098 mmol) at room temperature. Upon addition the solution immediately turned red-brown. After 2 h, the solution was filtered and all volatiles of the filtrate were removed under reduced pressure to give complex **7** (104 mg, 0.043 mmol, 89% yield) as red-brown powder. Single crystals of complex **7** suitable for X-ray analysis were grown from volatilization of a concentrated hexane/benzene solution at room temperature as red-brown crystals.

^1H NMR (500 MHz, C_6D_6 , 25 °C): δ = -1.96 (br, 2H, Ph), 0.79 (br, 60H, $\text{CH}(\text{CH}_3)_2$), 1.93 (br, 10H, $\text{CH}(\text{CH}_3)_2$), 3.50 (br, 2H, Ph), 6.54 (t, 2H, Ph), 13.05 (br, 2H, Ph) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, C_6D_6 , 25 °C): δ = 23.59 (s, $\text{CH}(\text{CH}_3)_2$), 29.85, 33.26 (s, $\text{CH}(\text{CH}_3)_2$), 112.97, 120.73, 126.48, 128.22, 148.30, 151.87 ppm. Detailed identification of the signals could not be performed due to paramagnetism of samarium(III). Anal. calcd. for (**7**) $\text{C}_{154}\text{H}_{190}\text{N}_4\text{Sm}_2$ (2397.78): C, 77.14; H, 7.99; N, 2.34; found: C, 77.31; H, 8.12; N, 2.29. IR: 3437 (br), 2957 (s), 2871 (s), 1595 (s), 1465 (s), 1378 (m), 1361 (m), 1306 (m), 1250 (m), 1098 (s), 1033 (m), 920 (m), 872 (s), 753 (m), 707 (m), 642 (w), 518 (w) cm^{-1} .

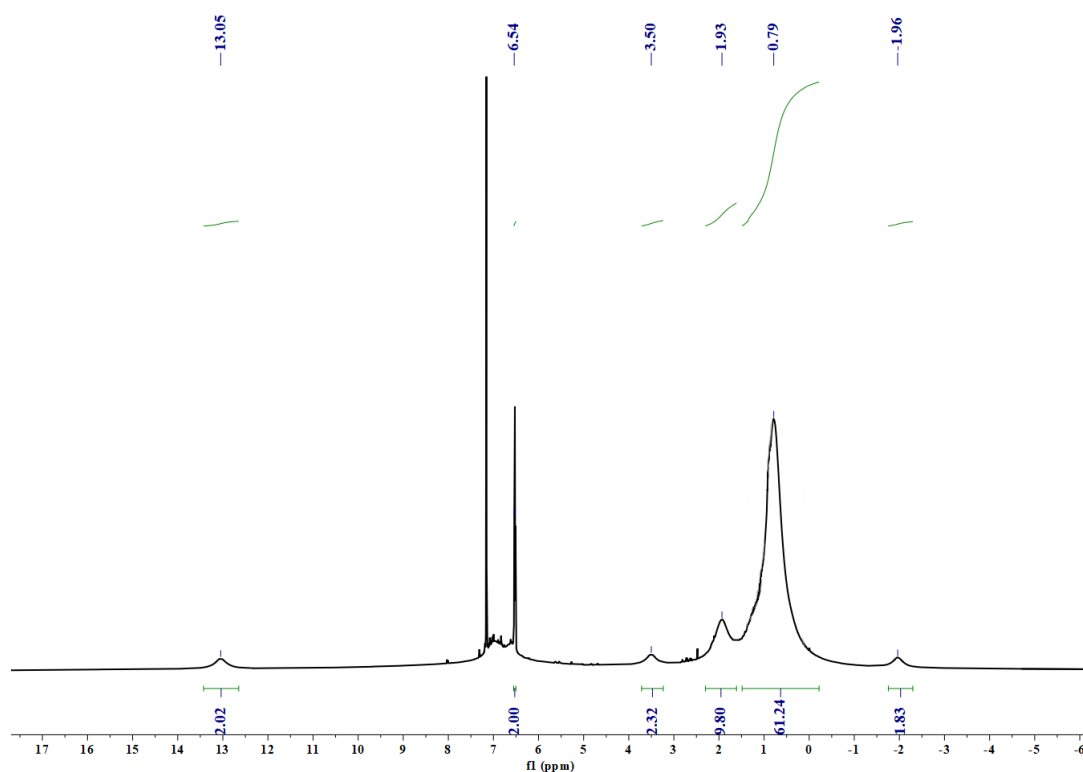


Figure S20. ^1H NMR spectrum (500 MHz) of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{III}}(\mu\text{-PhN-NPh})_2]$ (**7**) in C_6D_6 at 25 °C.

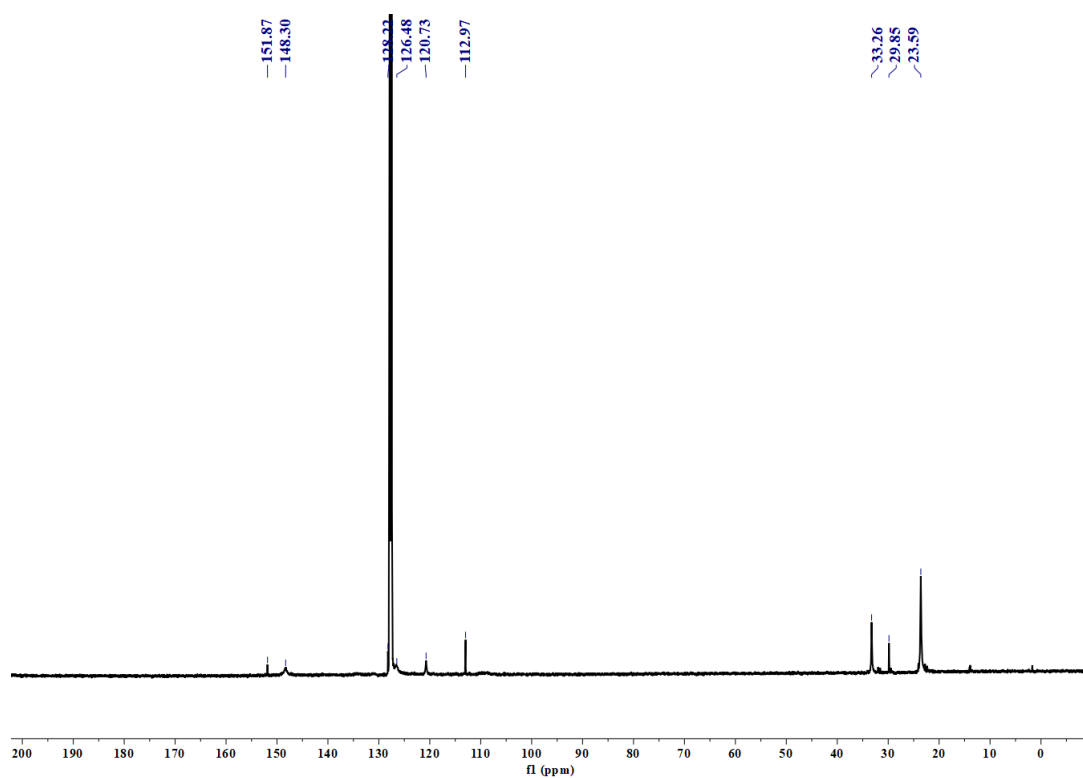


Figure S21. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (125 MHz) of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{III}}(\mu\text{-PhN-NPh})]_2$ (**7**) in C_6D_6 at 25 °C.

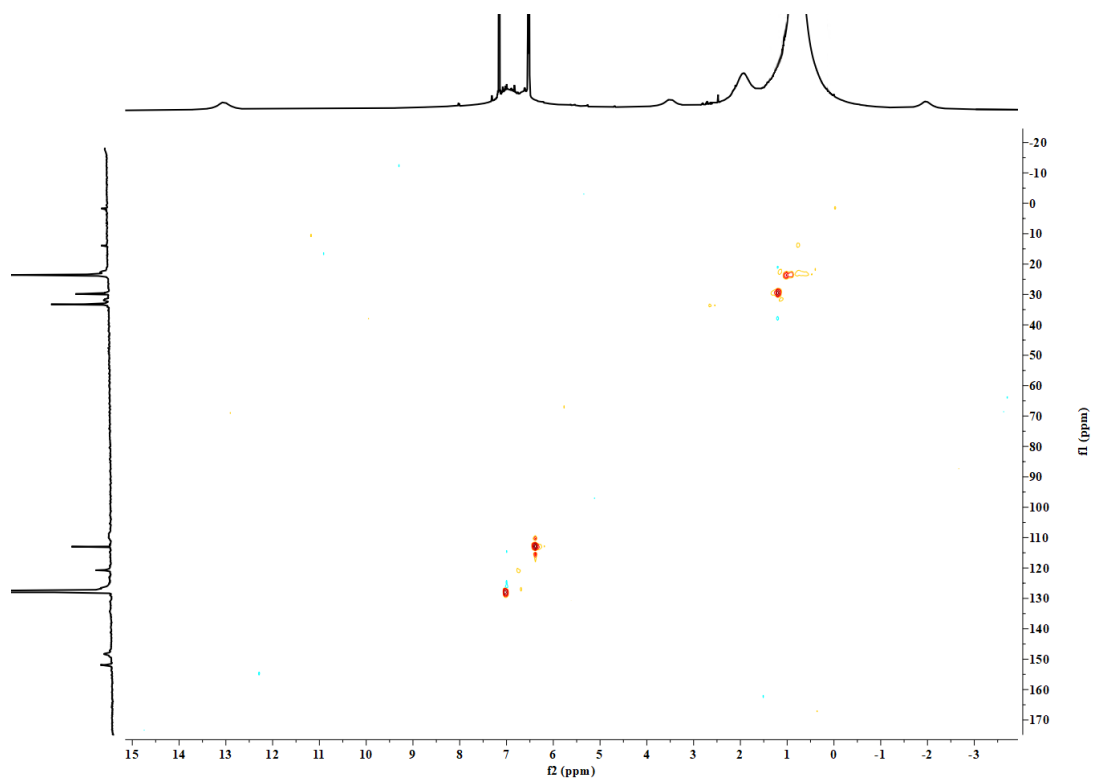


Figure S22. ^1H - ^{13}C HSQC NMR spectrum (500 MHz) of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{III}}(\mu\text{-PhN-NPh})]_2$ (**7**) in C_6D_6 at 25 °C.

Synthesis of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{III}}(\mu\text{-}\eta^2\text{:}\eta^1\text{-O}_2\text{CH})(\mu\text{-}\eta^2\text{:}\eta^2\text{-CO}_3)(\mu\text{-}\eta^1\text{:}\eta^1\text{-O}_2\text{CH})\text{Sm}^{\text{III}}(\text{Cp}^{\text{Ar5}})(\text{DABCO})]$ (8**)**

A solution of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{II}}(\mu\text{-H})(\text{DABCO})]_2$ (**4**) (100 mg, 0.044 mmol) in toluene (2 mL) was charged into J. Young valve NMR tube. The tube was frozen in liquid nitrogen, evacuated and backfilled with CO_2 (1 atm). Warmed up to room temperature, the solution changed from dark-brown to pale-yellow after 30 minutes. The resulting solution was added dropwise with pentane (2 mL) and slowly volatilized at room temperature overnight to give complex **8** (76 mg, 0.033 mmol, 75 % yield) as pale-yellow crystals. Single crystals of complex **8**•(0.5 x Benzene) suitable for X-ray analysis were grown from benzene/pentane solution at room temperature.

^1H NMR (500 MHz, C_6D_6 , 25 °C): δ = 0.78 (br, 60H, $\text{CH}(\text{CH}_3)_2$), 2.30 (sept, 10H, $\text{CH}(\text{CH}_3)_2$), 6.56 (br, 5H, aryl) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, C_6D_6 , 25 °C): δ = 23.82 (s, $\text{CH}(\text{CH}_3)_2$), 33.91 (s, $\text{CH}(\text{CH}_3)_2$), 44.87, 121.96, 126.65, 128.21, 141.06, 147.70 ppm. Detailed identification of the signals could not be performed due to paramagnetism of samarium(III). Anal. calcd. for (**8**) $\text{C}_{139}\text{H}_{184}\text{N}_2\text{O}_7\text{Sm}_2$ (2295.57): C, 72.72; H, 8.08; N, 1.22; found: C, 72.88; H, 8.21; N, 1.25. IR: 3482 (br), 2957 (s), 2871 (s), 2589 (w), 1761 (w), 1590 (s), 1463 (s), 1366 (s), 1331 (m), 1186 (w), 1060 (m), 918 (m), 871 (s), 825 (w), 777 (w), 711 (s), 678 (w), 593 (m) cm^{-1} .

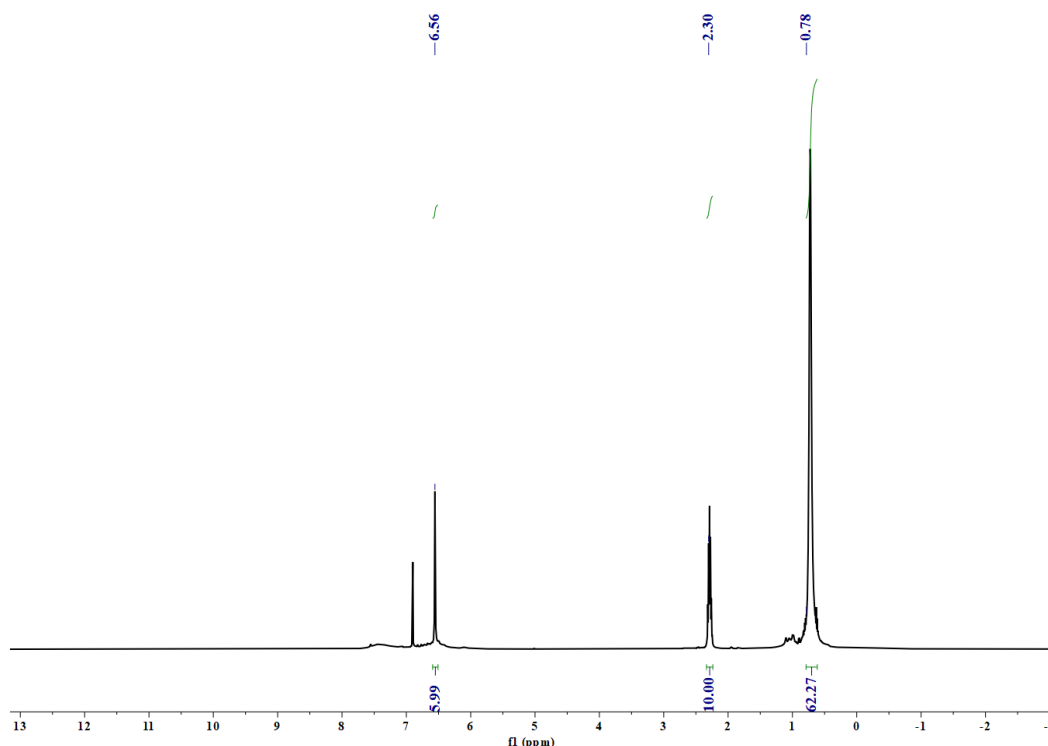


Figure S23. ^1H NMR spectrum (500 MHz) of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{III}}(\mu\text{-}\eta^2\text{:}\eta^1\text{-O}_2\text{CH})(\mu\text{-}\eta^2\text{:}\eta^2\text{-CO}_3)(\mu\text{-}\eta^1\text{:}\eta^1\text{-O}_2\text{CH})\text{Sm}^{\text{III}}(\text{Cp}^{\text{Ar5}})(\text{DABCO})]$ (**8**) in C_6D_6 at 25 °C.

SUPPORTING INFORMATION

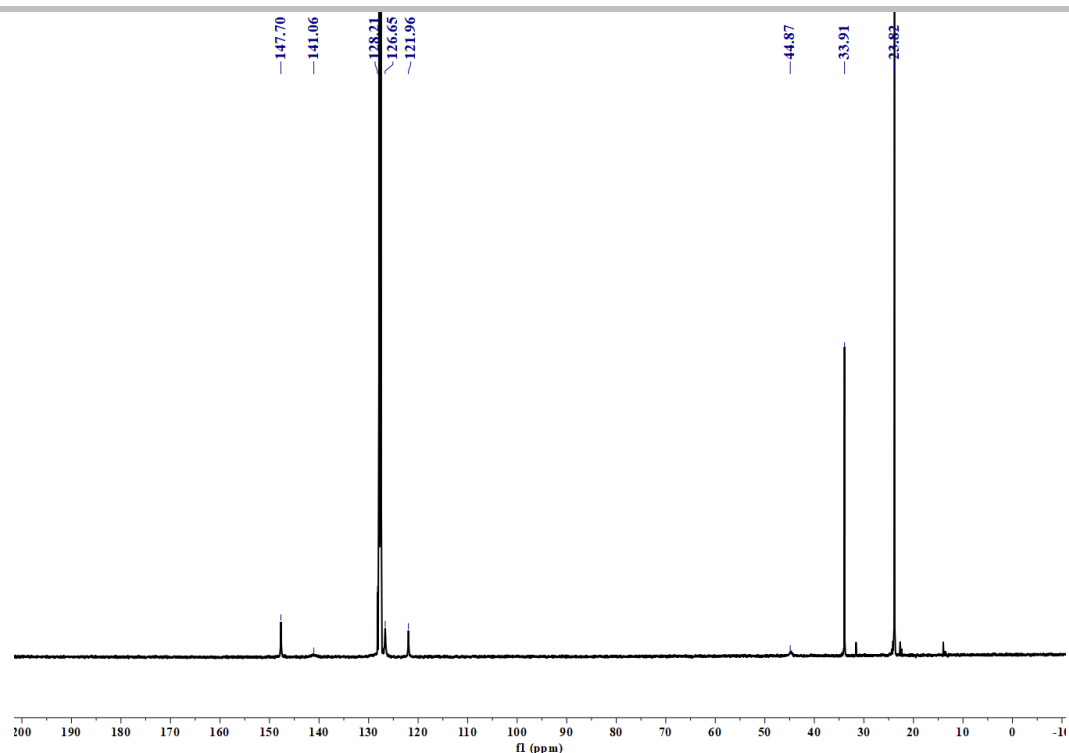


Figure S24. ^{13}C $\{^1\text{H}\}$ NMR spectrum (125 MHz) of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{III}}(\mu\text{-}\eta^2\text{:}\eta^1\text{-O}_2\text{CH})(\mu\text{-}\eta^2\text{:}\eta^2\text{-CO}_3)(\mu\text{-}\eta^1\text{:}\eta^1\text{-O}_2\text{CH})\text{Sm}^{\text{III}}(\text{Cp}^{\text{Ar5}})(\text{DABCO})]$ (**8**) in C_6D_6 at $25\text{ }^\circ\text{C}$.

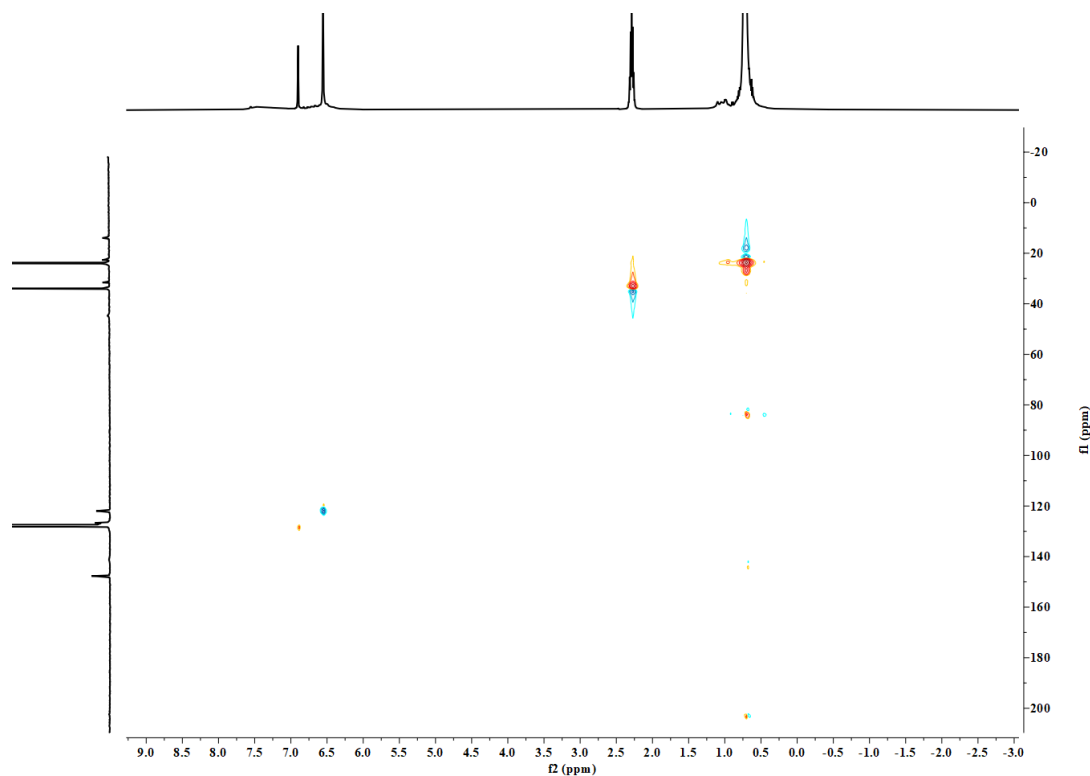


Figure S25. ^1H - ^{13}C HSQC NMR spectrum (500 MHz) of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{III}}(\mu\text{-}\eta^2\text{:}\eta^1\text{-O}_2\text{CH})(\mu\text{-}\eta^2\text{:}\eta^2\text{-CO}_3)(\mu\text{-}\eta^1\text{:}\eta^1\text{-O}_2\text{CH})\text{Sm}^{\text{III}}(\text{Cp}^{\text{Ar5}})(\text{DABCO})]$ (**8**) in C_6D_6 at $25\text{ }^\circ\text{C}$.

Synthesis of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{III}}(\mu\text{-}\eta^2\text{:}\eta^2\text{-CS}_3)(\text{DABCO})]_2$ (9**)**

To a stirring solution of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{II}}(\mu\text{-H})(\text{DABCO})]_2$ (**4**) (88 mg, 0.039 mmol) in toluene (5 mL) was added carbon disulfide (18 mg, 0.234 mmol) at -30 °C. Upon addition the solution immediately turned red-brown. The reaction mixture was warmed to room temperature and stirred for 30 minutes, then filtered. The filtrate was concentrated to 1 mL, layered with 3 mL hexane, and kept at -30 °C to give complex **9** (40 mg, 0.016 mmol, 41 % yield) as red-brown powder. Single crystals of complex **9**•(Benzene) suitable for X-ray analysis were grown from volatilization of a concentrated benzene/hexane solution at room temperature as red-brown crystals.

^1H NMR (500 MHz, C_6D_6 , 25 °C): δ = 1.08 (br, 60H, $\text{CH}(\text{CH}_3)_2$), 2.52, 2.72, 6.78 (br, 5H, aryl) ppm. ^{13}C $\{^1\text{H}\}$ NMR (125 MHz, C_6D_6 , 25 °C): δ = 24.25 (s, $\text{CH}(\text{CH}_3)_2$), 34.22 (s, $\text{CH}(\text{CH}_3)_2$), 121.13, 146.24, 156.72 ppm. Detailed identification of the signals could not be performed due to paramagnetism of samarium(III). Anal. calcd. for (**9**) $\text{C}_{144}\text{H}_{194}\text{N}_4\text{S}_6\text{Sm}_2$ (2474.08): C, 69.90; H, 7.90; N, 2.26; found: C, 69.79; H, 7.77; N, 2.32. IR: 3440 (br), 2956 (s), 2931 (s), 2871 (s), 1765 (w), 1595 (s), 1462 (s), 1379 (m), 1361 (m), 1302 (m), 1259 (s), 1101 (s), 943 (m), 872 (m), 711 (m), 643 (w), 593 (m) cm^{-1} .

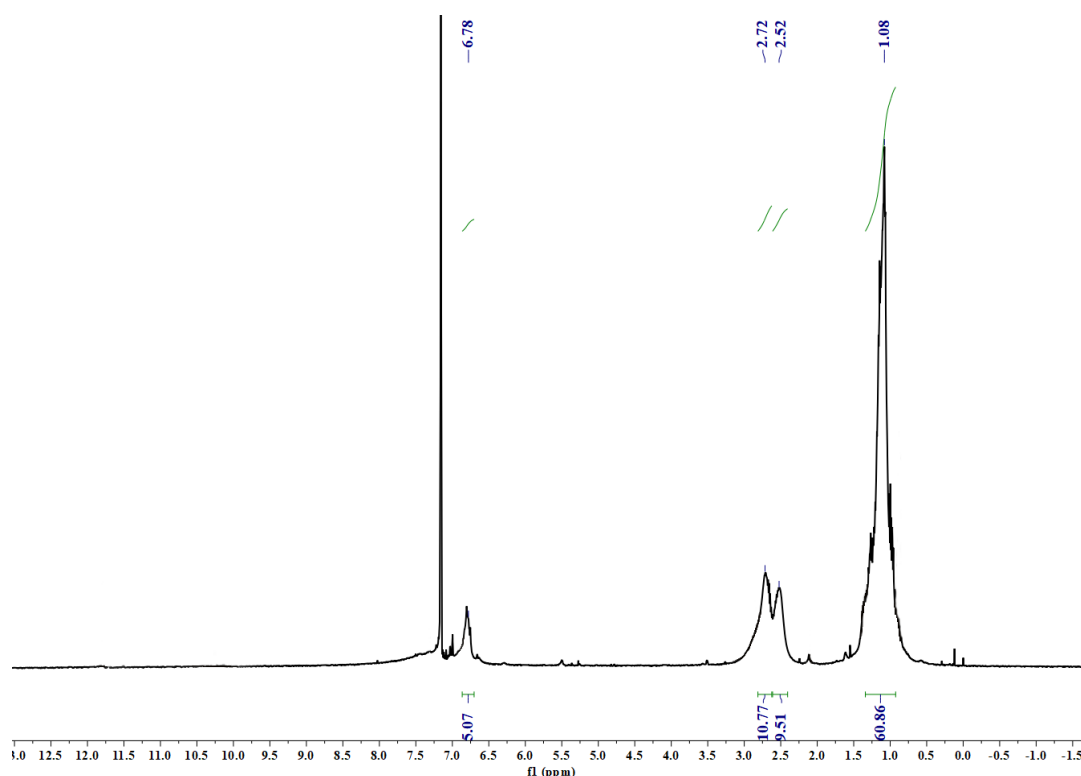


Figure S26. ^1H NMR spectrum (500 MHz) of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{III}}(\mu\text{-}\eta^2\text{:}\eta^2\text{-CS}_3)(\text{DABCO})]_2$ (**9**) in C_6D_6 at 25 °C.

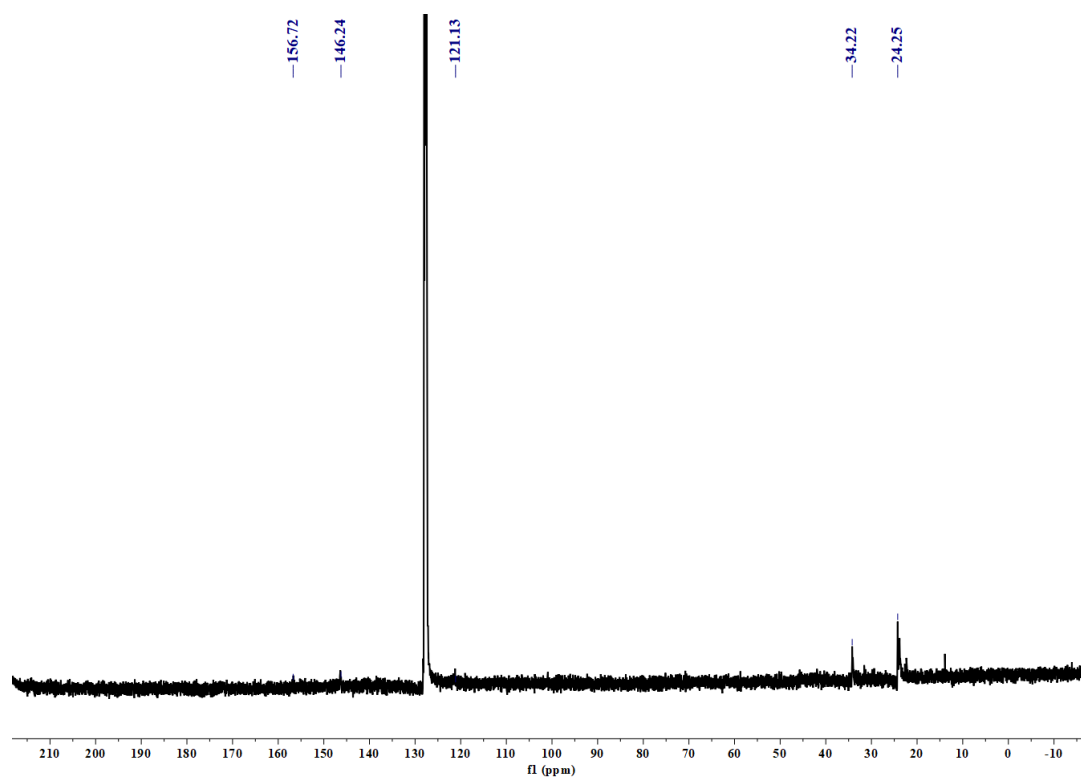


Figure S27. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (125 MHz) of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{III}}(\mu\text{-}\eta^2\text{:}\eta^2\text{-CS}_3)(\text{DABCO})]_2$ (**9**) in C_6D_6 at 25 °C.

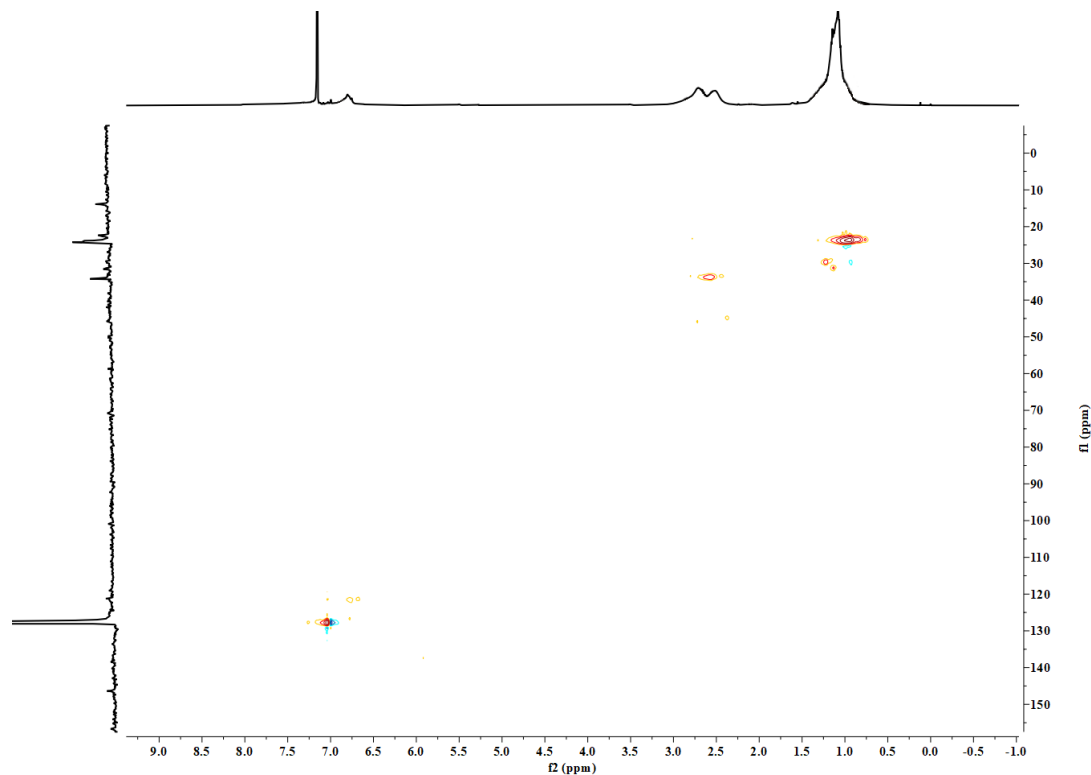


Figure S28. ^1H - ^{13}C HSQC NMR spectrum (500 MHz) of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{III}}(\mu\text{-}\eta^2\text{:}\eta^2\text{-CS}_3)(\text{DABCO})]_2$ (**9**) in C_6D_6 at 25 °C.

X-ray Crystallographic Studies

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

Refinement of **2**: The SQUEEZE^[11] routine of the program PLATON^[12] was implemented to remove the contributions of one disordered hexane to the observed structure factors. Five *i*Pr groups were disordered. C23~C25 and C23'~C25' disordered over two sites with occupancies 0.503:0.497. C35~C37 and C35'~C37' disordered over two sites with occupancies 0.544:0.456. C54~C56 and C54'~C56' disordered over two sites with occupancies 0.515:0.485. C59~C61 and C59'~C61' disordered over two sites with occupancies 0.495:0.505. C66~C68 and C66'~C68' disordered over two sites with occupancies 0.609:0.391.

Refinement of **4**: The SQUEEZE^[11] routine of the program PLATON^[12] was implemented to remove the contributions of one disordered DABCO to the observed structure factors. The terminal hydride (H1) was located by difference Fourier syntheses and refined. Two *i*Pr groups were disordered. C36~C38 and C36'~C38' disordered over two sites with occupancies 0.391:0.609. C55~C57 and C55'~C57' disordered over two sites with occupancies 0.570:0.430.

Refinement of **5**: Two *i*Pr groups were disordered. C23~C25 and C36'~C38' disordered over two sites with occupancies 0.451:0.549. C59~C61 and C59'~C61' disordered over two sites with occupancies 0.578:0.422.

Refinement of **6**: The SQUEEZE^[11] routine of the program PLATON^[12] was implemented to remove the contributions of half a disordered hexane to the observed structure factors. One *i*Pr groups were disordered. C45~C47 and C45'~C47' disordered over two sites with occupancies 0.593:0.407.

SUPPORTING INFORMATION

Refinement of **7**: Three i Pr groups were disordered. C28~C30 and C28'~C30' disordered over two sites with occupancies 0.431:0.569. C64~C66 and C64'~C66' disordered over two sites with occupancies 0.656:0.344. C76~C78 and C76'~C78' disordered over two sites with occupancies 0.422:0.578.

Refinement of **8**: The SQUEEZE^[11] routine of the program PLATON^[12] was implemented to remove the contributions of half a disordered benzene to the observed structure factors. The hydrogen atoms (H2 and H3) of formate ligands were located by difference Fourier syntheses and refined. C1, C2, O3 and C1', C2', O3' disordered over two sites with occupancies 0.631:0.369. Ten i Pr groups were disordered. C52~C54 and C52'~C54' disordered over two sites with occupancies 0.629:0.371. C57~C59 and C57'~C59' disordered over two sites with occupancies 0.464:0.536. C76~C78 and C76'~C78' disordered over two sites with occupancies 0.408:0.592. C81~C83 and C81'~C83' disordered over two sites with occupancies 0.348:0.652. C98~C100 and C198~C200 disordered over two sites with occupancies 0.588:0.412. C110~C112 and C210~C212 disordered over two sites with occupancies 0.678:0.322. C117~C119 and C217~C219 disordered over two sites with occupancies 0.685:0.315. C129~C131 and C229~C231 disordered over two sites with occupancies 0.331:0.669. C134~C136 and C234~C236 disordered over two sites with occupancies 0.516:0.484. C141~C143 and C241~C243 disordered over two sites with occupancies 0.547:0.453.

Refinement of **9**: The SQUEEZE^[11] routine of the program PLATON^[12] was implemented to remove the contributions of one disordered benzene to the observed structure factors. Three i Pr groups were disordered. C18~C20 and C18'~C20' disordered over two sites with occupancies 0.657:0.343. C30~C32 and C30'~C32' disordered over two sites with occupancies 0.432:0.568. C42~C44 and C42'~C44' disordered over two sites with occupancies 0.512:0.488.

Other hydrogen atoms were placed at the calculated positions and were included in the structure calculation without further refinement of the parameters. The residual electron densities were of no chemical significance. Crystal data and analysis results are listed in Table **S1-7**.

CCDC number 2104460 (**2**), 2104461 (**4**), 2104462 (**5**), 2104463 (**6**), 2104464 (**7**), 2104465 (**8**), 2104466 (**9**) contain the supplementary crystallographic data for this paper. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+44)1223-336-033; E-mail: deposit@ccdc.cam.ac.uk).

Table S1. Crystal data and structure refinement for complex **2**

Identification code	2
CCDC number	2104460
Empirical formula	C ₁₄₂ H ₁₉₄ I ₂ N ₄ Sm ₂ •(Hexane)
Formula weight	2511.50
Temperature	193(2) K
Wavelength	0.71073 Å
Crystal system, space group	Trigonal, P-3c1
a	31.3935(5) Å
b	31.3935(5) Å
c	27.5926(6) Å
α	90 °
β	90 °
γ	120 °
Volume	23550.6(9) Å ³
Z, Calculated density	6, 1.063 Mg/m ³
Absorption coefficient	1.174 mm ⁻¹
F(000)	7824
Crystal size	0.210 x 0.160 x 0.130 mm
Theta range for data collection	1.965 to 24.999 °
Limiting indices	-37<=h<=37, -37<=k<=37, -32<=l<=32
Reflections collected / unique	231000 / 13704 [R(int) = 0.0562]
Completeness to theta	(24.999) 98.9 %
Absorption correction	Empirical
Max. and min. transmission	0.858 and 0.798
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	13704 / 27 / 655
Goodness-of-fit on F ²	1.058
Final R indices [I>2sigma(I)]	R1 = 0.0597, wR2 = 0.1712
R indices (all data)	R1 = 0.0737, wR2 = 0.1884
Largest diff. peak and hole	2.030 and -4.314 e. Å ⁻³

Table S2. Crystal data and structure refinement for complex **4**

Identification code	4
CCDC number	2104461
Empirical formula	C ₁₄₂ H ₁₉₆ N ₄ Sm ₂ •(DABCO)
Formula weight	2259.72
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>n</i>
<i>a</i>	16.4155 (11) Å
<i>b</i>	25.5172 (16) Å
<i>c</i>	17.9798 (12) Å
α	90 °
β	116.305 (1) °
γ	90 °
Volume	6751.4(8) Å ³
Z, Calculated density	2, 1.112 Mg/m ³
Absorption coefficient	0.907 mm ⁻¹
F(000)	2400
Crystal size	0.230 x 0.150 x 0.130 mm
Theta range for data collection	1.494 to 24.999 °
Limiting indices	-19 ≤ <i>h</i> ≤ 16, -29 ≤ <i>k</i> ≤ 30, -17 ≤ <i>l</i> ≤ 21
Reflections collected / unique	34433 / 11837 [R(int) = 0.0727]
Completeness to theta	(24.999 °) 99.4 %
Absorption correction	Empirical
Max. and min. transmission	0.889 and 0.849
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	11837 / 12 / 673
Goodness-of-fit on F ²	0.973
Final R indices [<i>I</i> > 2σ(<i>I</i>)]	R1 = 0.0524, wR2 = 0.1117
R indices (all data)	R1 = 0.0924, wR2 = 0.1271
Largest diff. peak and hole	1.033 and -0.585 e. Å ⁻³

Table S3. Crystal data and structure refinement for complex **5**

Identification code	5
CCDC number	2104462
Empirical formula	C ₁₃₀ H ₁₇₀ Sm ₁
Formula weight	1883.00
Temperature	193(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/n
a	17.1221(9) Å
b	18.2035(10) Å
c	18.4974(11) Å
α	90 °
β	100.735(2) °
γ	90 °
Volume	5664.4(5) Å ³
Z, Calculated density	2, 1.104 Mg/m ³
Absorption coefficient	0.565 mm ⁻¹
F(000)	2024
Crystal size	0.180 x 0.140 x 0.110 mm
Theta range for data collection	1.862 to 25.000 °
Limiting indices	-20 ≤ h ≤ 20, -21 ≤ k ≤ 21, -21 ≤ l ≤ 21
Reflections collected / unique	206596 / 9902 [R(int) = 0.0943]
Completeness to theta	(25.000) 99.3 %
Absorption correction	Gaussian
Max. and min. transmission	0.940 and 0.909
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	9902 / 9 / 574
Goodness-of-fit on F ²	1.058
Final R indices [I > 2σ(I)]	R1 = 0.0632, wR2 = 0.1441
R indices (all data)	R1 = 0.0928, wR2 = 0.1688
Largest diff. peak and hole	1.239 and -2.194 e. Å ⁻³

Table S4. Crystal data and structure refinement for complex **6**

Identification code	6
CCDC number	2104463
Empirical formula	$C_{142}H_{194}N_4Se_2Sm_2 \cdot (0.5 \times \text{Hexane})$
Formula weight	2415.62
Temperature	193(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/n
a	25.4365(19) Å
b	17.2334(10) Å
c	30.027(2) Å
α	90 °
β	98.082(3) °
γ	90 °
Volume	13031.7(16) Å ³
Z, Calculated density	4, 1.231 Mg/m ³
Absorption coefficient	1.499 mm ⁻¹
F(000)	5064
Crystal size	0.180 x 0.120 x 0.080 mm
Theta range for data collection	2.003 to 25.000 °
Limiting indices	-30 ≤ h ≤ 30, -20 ≤ k ≤ 20, -35 ≤ l ≤ 35
Reflections collected / unique	263503 / 22885 [R(int) = 0.1189]
Completeness to theta	(25.000) 99.7 %
Absorption correction	Empirical
Max. and min. transmission	0.887 and 0.806
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	22885 / 6 / 1289
Goodness-of-fit on F ²	1.019
Final R indices [I > 2σ(I)]	R1 = 0.0507, wR2 = 0.1098
R indices (all data)	R1 = 0.0853, wR2 = 0.1292
Largest diff. peak and hole	2.524 and -0.986 e. Å ⁻³

Table S5. Crystal data and structure refinement for complex **7**

Identification code	7
CCDC number	2104464
Empirical formula	C ₇₇ H ₉₅ N ₂ Sm ₁
Formula weight	1198.89
Temperature	193(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
a	14.7083(8) Å
b	14.9791(8) Å
c	17.3833(10) Å
α	82.778(2)°
β	75.024(2) °
γ	62.966(2) °
Volume	3295.4(3) Å ³
Z, Calculated density	2, 1.208 Mg/m ³
Absorption coefficient	0.934 mm ⁻¹
F(000)	1266
Crystal size	0.190 x 0.140 x 0.110 mm
Theta range for data collection	2.214 to 24.999 °
Limiting indices	-17<=h<=17, -17<=k<=17, -20<=l<=20
Reflections collected / unique	90091 / 11551 [R(int) = 0.0563]
Completeness to theta	(24.999) 99.5 %
Absorption correction	Empirical
Max. and min. transmission	0.902 and 0.855
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	11551 / 15 / 715
Goodness-of-fit on F ²	1.045
Final R indices [I>2sigma(I)]	R1 = 0.0329, wR2 = 0.0748
R indices (all data)	R1 = 0.0397, wR2 = 0.0789
Largest diff. peak and hole	0.975 and -0.619 e. Å ⁻³

Table S6. Crystal data and structure refinement for complex **8**

Identification code	8
CCDC number	2104465
Empirical formula	C ₁₃₉ H ₁₈₄ N ₂ O ₇ Sm ₂ •(0.5 x Benzene)
Formula weight	2295.57
Temperature	193(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
a	14.4270(10) Å
b	14.7683(9) Å
c	34.5942(18) Å
α	88.821(2) °
β	79.946(2) °
γ	63.694(2) °
Volume	6492.5(7) Å ³
Z, Calculated density	2, 1.174 Mg/m ³
Absorption coefficient	0.948 mm ⁻¹
F(000)	2424
Crystal size	0.190 x 0.160 x 0.140 mm
Theta range for data collection	2.155 to 24.999 °
Limiting indices	-17<=h<=17, -17<=k<=17, -41<=l<=41
Reflections collected / unique	215230 / 22749 [R(int) = 0.0424]
Completeness to theta	(24.999) 99.4 %
Absorption correction	Empirical
Max. and min. transmission	0.876 and 0.835
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	22749 / 49 / 1344
Goodness-of-fit on F ²	1.038
Final R indices [I>2σ(I)]	R1 = 0.0377, wR2 = 0.0933
R indices (all data)	R1 = 0.0471, wR2 = 0.1008
Largest diff. peak and hole	0.823 and -0.836 e. Å ⁻³

Table S7. Crystal data and structure refinement for complex **9**

Identification code	9
CCDC number	2104466
Empirical formula	C ₁₄₄ H ₁₉₄ N ₄ S ₆ Sm ₂ •(Benzene)
Formula weight	2474.08
Temperature	193(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
a	14.0683(7) Å
b	14.6664(8) Å
c	19.7775(12) Å
α	96.913(2) °
β	99.970(2) °
γ	117.769(2) °
Volume	3460.3(3) Å ³
Z, Calculated density	2, 1.187 Mg/m ³
Absorption coefficient	0.978 mm ⁻¹
F(000)	1306
Crystal size	0.190 x 0.150 x 0.130 mm
Theta range for data collection	2.134 to 25.000 °
Limiting indices	-16<=h<=16, -17<=k<=17, -23<=l<=23
Reflections collected / unique	98619 / 12146 [R(int) = 0.0523]
Completeness to theta	(25.000) 99.5 %
Absorption correction	Empirical
Max. and min. transmission	0.881 and 0.839
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	12146 / 14 / 724
Goodness-of-fit on F ²	1.033
Final R indices [I>2σ(I)]	R1 = 0.0322, wR2 = 0.0737
R indices (all data)	R1 = 0.0404, wR2 = 0.0784
Largest diff. peak and hole	0.963 and -0.606 e. Å ⁻³

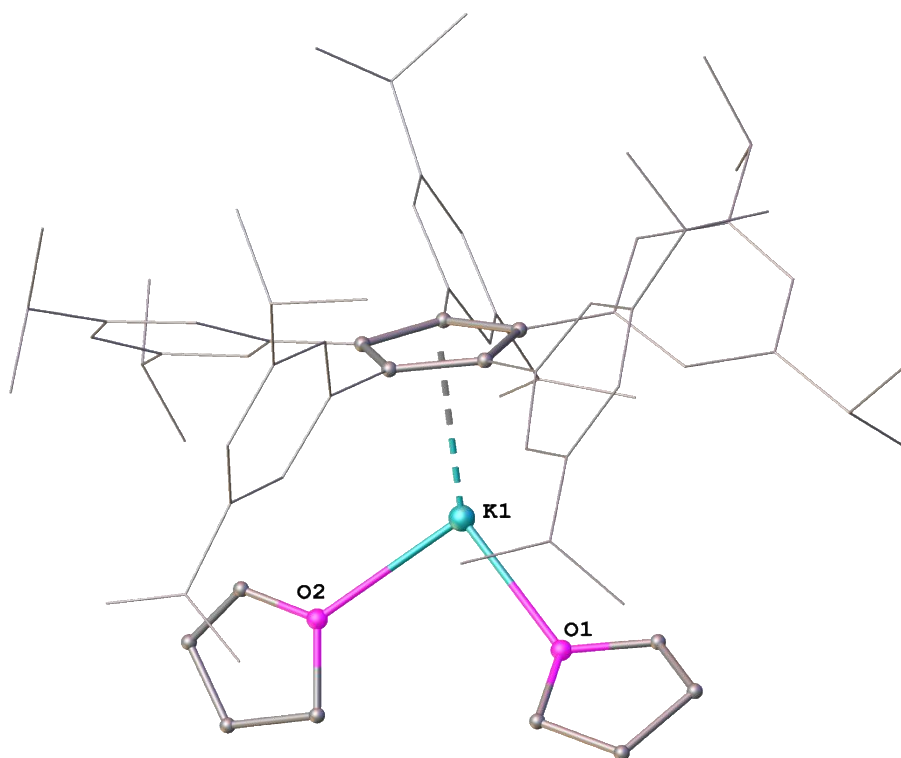


Figure S29. Molecular structure of $[(\text{Cp}^{\text{Ar}5})\text{K}(\text{THF})_2]$ (**1**).

*: Owing to the low-quality X-ray data set, the detailed discussion of bond lengths and angles is not warranted.

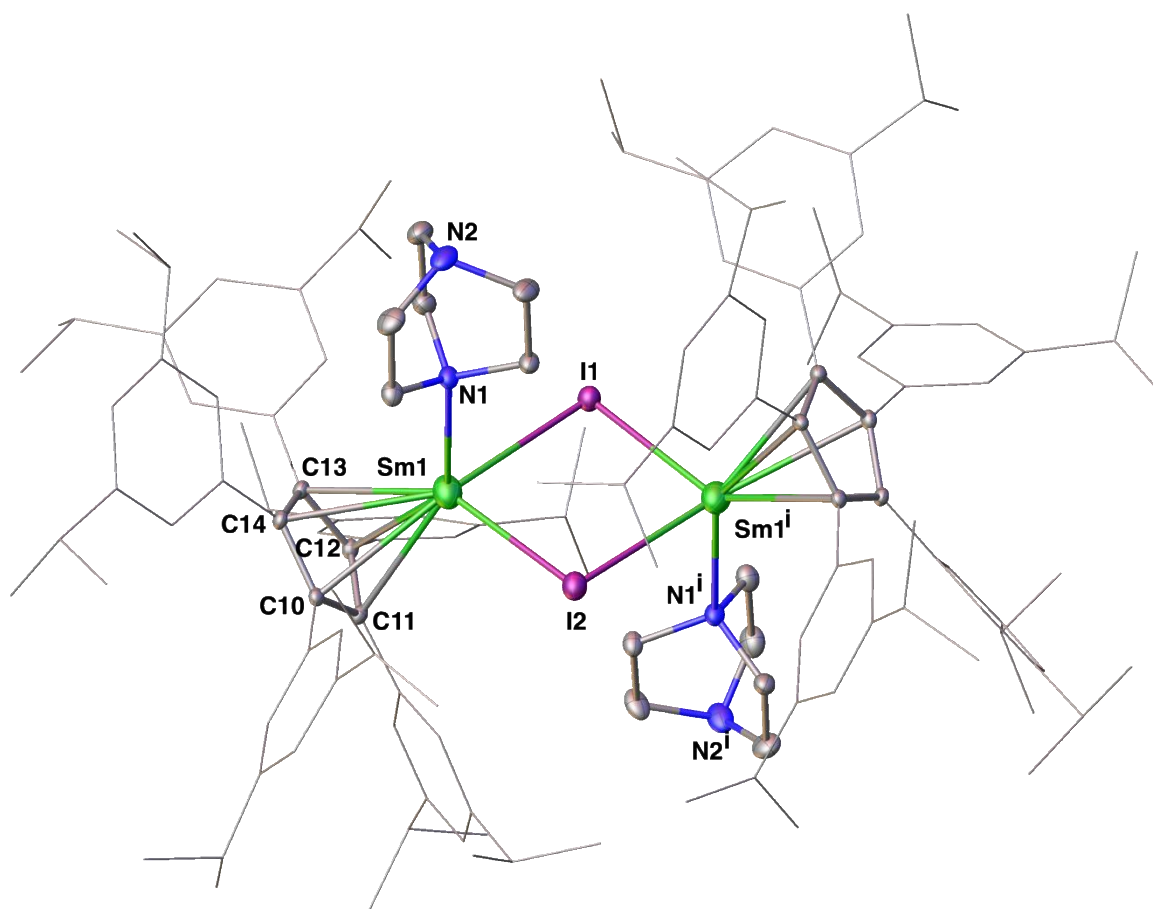


Figure S30. Molecular structure of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{II}}(\mu\text{-I})(\text{DABCO})]_2$ (**2**). All the hydrogen atoms are omitted for clarity. Selected interatomic distances [Å] and angles [deg]: Sm1–I1 3.2358(6), Sm1–I2 3.1523(7), Sm1–N1 2.664(5), Sm1–C10 2.802(5), Sm1–C11 2.818(5), Sm1–C12 2.849(5), Sm1–C13 2.858(5), Sm1–C14 2.834(5), Sm1–Cent1 2.557, Sm1---Sm1ⁱ 4.484(1), Sm1–I1–Sm1ⁱ 87.716(19), I1–Sm1–I2 90.803(16). Cent1: Centre of the Cp^{Ar5} ring (C10~C14).

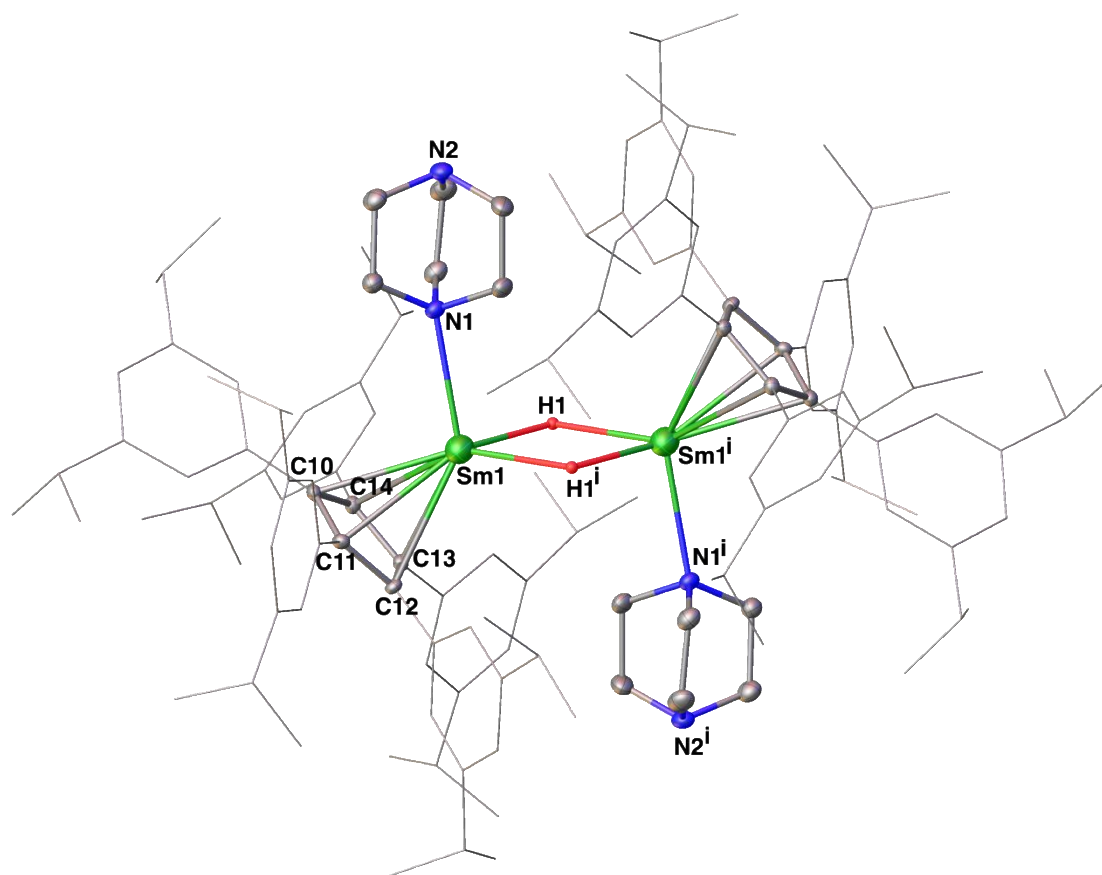


Figure S31. Molecular structure of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{II}}(\mu\text{-H})(\text{DABCO})]_2$ (**4**). Except the bridging hydride (H1 and H1ⁱ), all the hydrogen atoms are omitted for clarity. Selected interatomic distances [Å] and angles [deg]: Sm1–H1 2.26(6), Sm1–H1ⁱ 2.48(5), Sm1–N1 2.652 (4), Sm1–C11 2.800 (4), Sm1–C12 2.832 (4), Sm1–C13 2.885 (4), Sm1–C14 2.900 (4), Sm1–C15 2.887 (4), Sm1–Cent1 2.594, Sm1---Sm1ⁱ 3.7966 (5), Sm1–H1–Sm1ⁱ 106 (2), H1–Sm1–H1ⁱ 74 (2). Cent1: Centre of the Cp^{Ar5} ring (C11~C15).

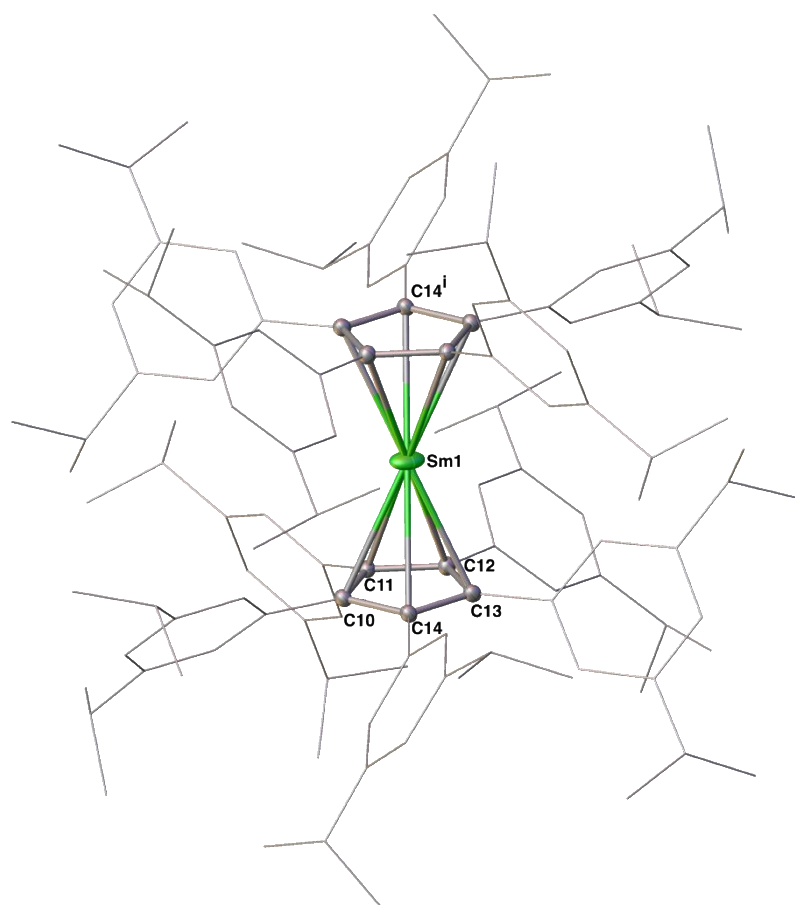


Figure S32. Molecular structure of $[(\text{Cp}^{\text{Ar5}})_2\text{Sm}^{\text{II}}]$ (**5**). All the hydrogen atoms are omitted for clarity. Selected interatomic distances [\AA]: Sm1–C10 2.790(3), Sm1–C11 2.807(3), Sm1–C12 2.761(4), Sm1–C13 2.722(4), Sm1–C14 2.749(3), Sm1–Cent1 2.486.

Cent1: Centre of the Cp^{Ar5} ring (C10~C14).

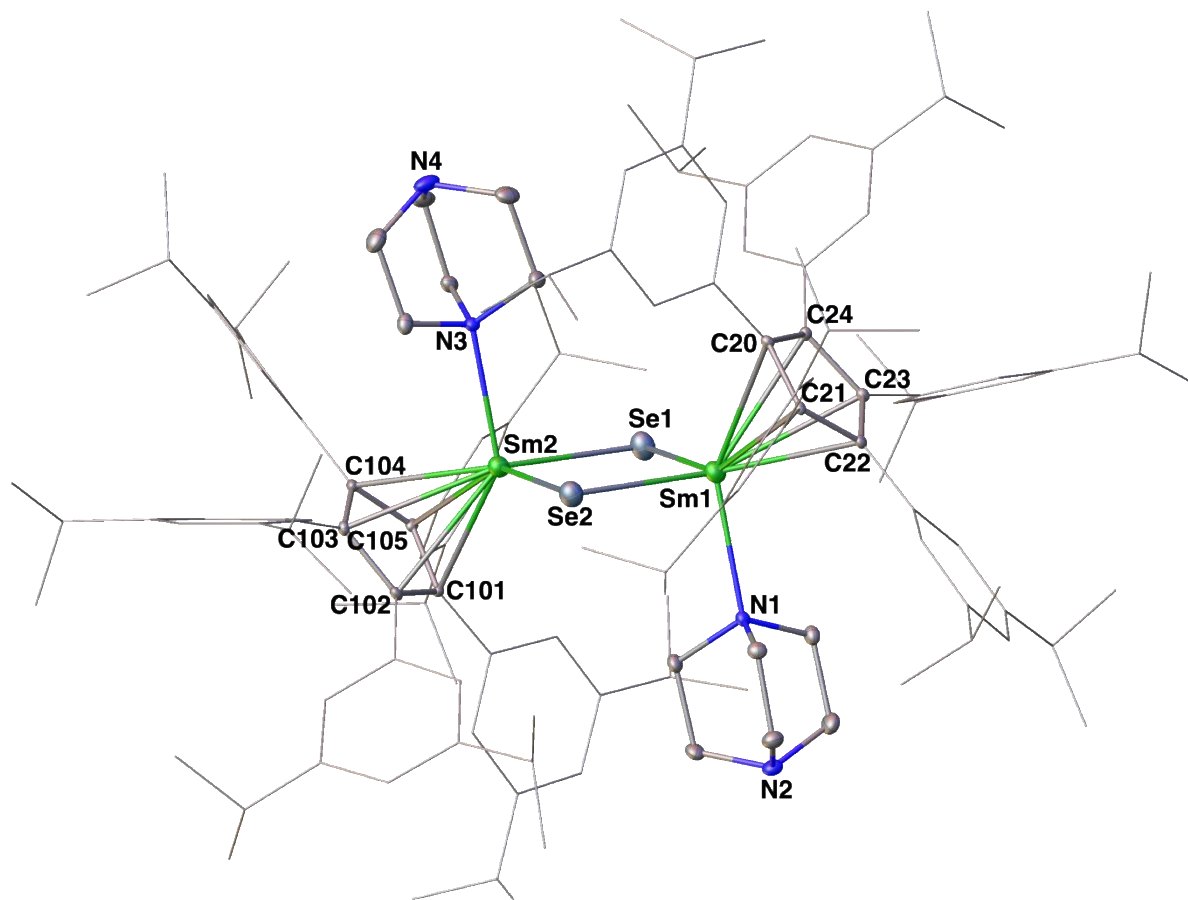


Figure S33. Molecular structure of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{III}}(\mu\text{-Se})(\text{DABCO})]_2$ (**6**). All the hydrogen atoms are omitted for clarity. Selected interatomic distances [Å] and angles [deg]: Sm1–Se1 2.7349(7), Sm1–Se2 2.7524(6), Sm1–N1 2.554(5), Sm1–C20 2.779(5), Sm1–C21 2.751(5), Sm1–C22 2.818(5), Sm1–C23 2.828(5), Sm1–C24 2.813(5), Sm1–Cent1 2.521, Sm2–Se1 2.7464(6), Sm2–Se2 2.7445(6), Sm2–N3 2.522(5), Sm2–C100 2.791(5), Sm2–C101 2.760(5), Sm2–C102 2.780(5), Sm2–C103 2.840(5), Sm2–C104 2.870(5), Sm2–Cent2 2.535, Sm1---Sm2 3.8699(4), Sm1–Se1–Sm2 89.83(2), Sm1–Se2–Sm2 89.50(2). Cent1: Centre of the Cp^{Ar5} ring (C20~C24).

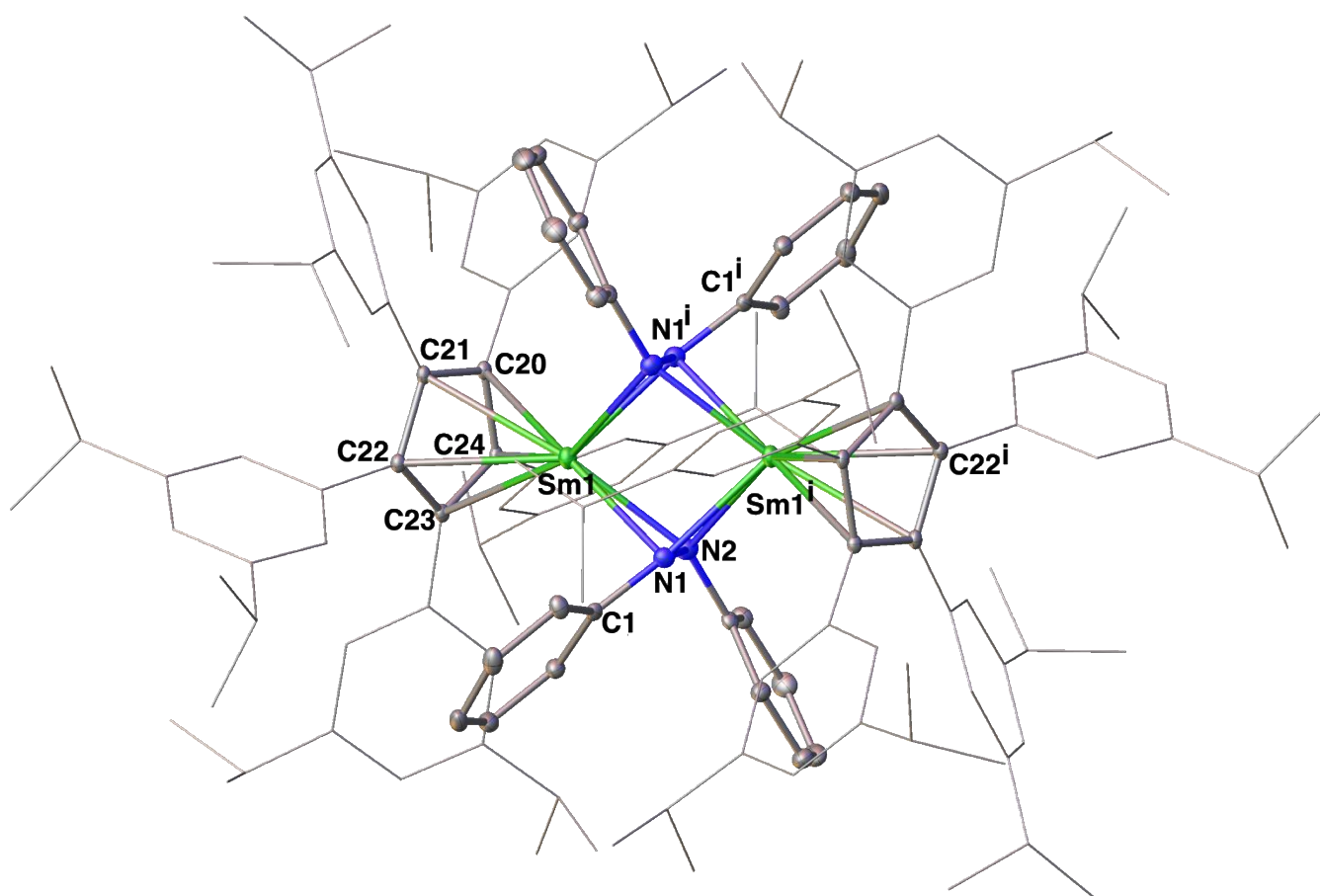


Figure S34. Molecular structure of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{III}}(\mu\text{-PhN-NPh})]_2$ (**7**). All the hydrogen atoms are omitted for clarity. Selected interatomic distances [\AA] and angles [deg]: Sm1–N1 2.458(2), Sm1–N2 2.337(2), Sm1–C1 2.846(3), Sm1–C20 2.788(3), Sm1–C21 2.759(3), Sm1–C22 2.754(3), Sm1–C23 2.809(3), Sm1–C24 2.811(3), Sm1–Cent1 2.506, Sm1---Sm1' 3.4535(3), N1–N2 1.462(3), C1–N1–N2 117.2(2).

Cent1: Centre of the Cp^{Ar5} ring (C20~C24).

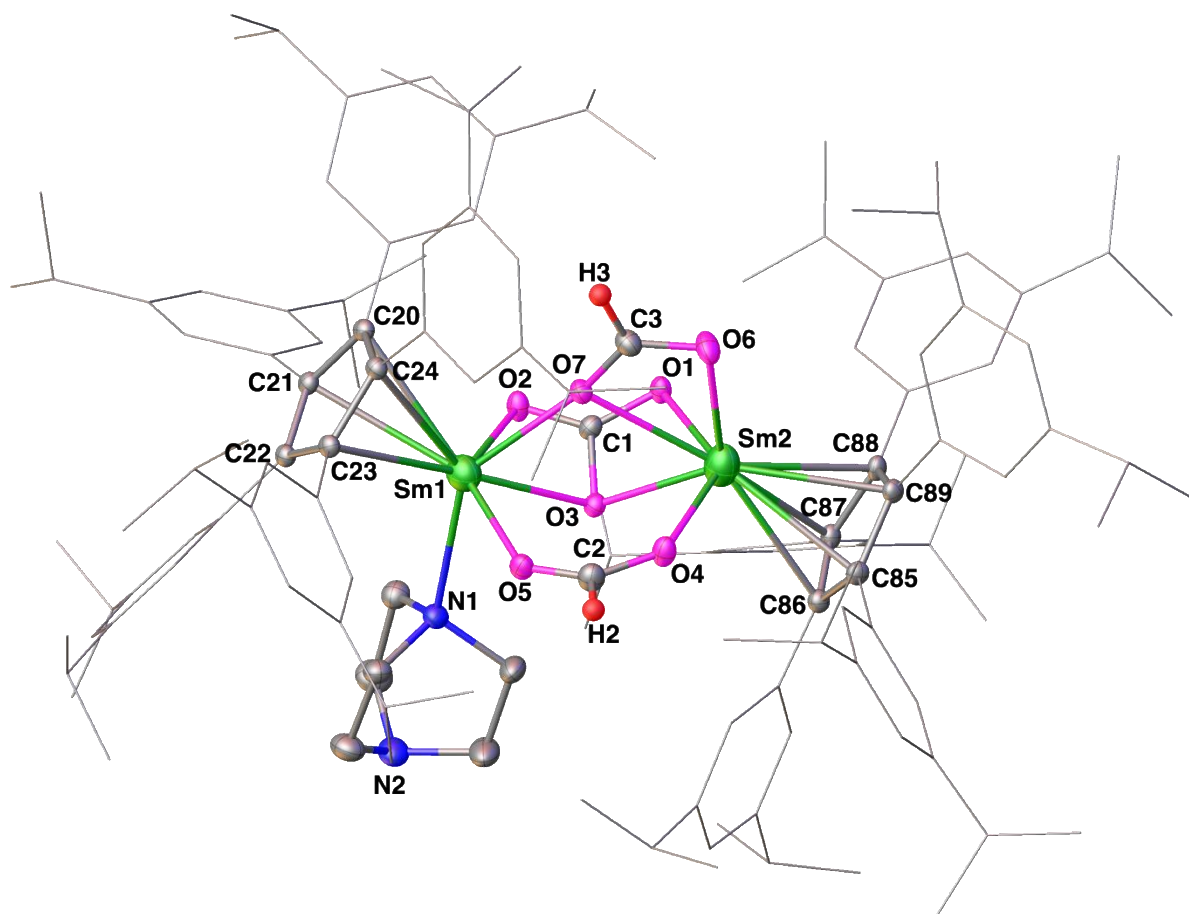


Figure S35. Molecular structure of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{III}}(\mu\text{-}\eta^2\text{:}\eta^1\text{-O}_2\text{CH})(\mu\text{-}\eta^2\text{:}\eta^2\text{-CO}_3)(\mu\text{-}\eta^1\text{:}\eta^1\text{-O}_2\text{CH})\text{Sm}^{\text{III}}(\text{Cp}^{\text{Ar5}})(\text{DABCO})]$ (**8**). All the hydrogen atoms, except H2 and H3, are omitted for clarity. Selected interatomic distances [\AA] and angles [deg]: Sm1–O2 2.354(2), Sm1–O3 2.397(3), Sm1–O5 2.338(2), Sm1–O7 2.426(2), Sm1–N1 2.605(3), Sm1–C20 2.773(3), Sm1–C21 2.829(3), Sm1–C22 2.856(3), Sm1–C23 2.785(3), Sm1–C24 2.755(3), Sm2–O1 2.373(3), Sm2–O3 2.398(3), Sm2–O4 2.346(2), Sm2–O6 2.406(3), Sm2–O7 2.644(2), Sm2–C85 2.738(3), Sm2–C86 2.752(3), Sm2–C87 2.746(3), Sm2–C88 2.722(3), Sm2–C89 2.717(3), C1–O1 1.251(6), C1–O2 1.204(6), C1–O3 1.349(8), C2–O4 1.248(7), C2–O5 1.206(7), C3–O6 1.249(5), C3–O7 1.271(4), Sm1–Cent1 2.523, Sm2–Cent2 2.453, O2–C1–O1 133.6(6), O2–C1–O3 112.1(5), O1–C1–O3 113.8(5), O5–C2–O4 133.1(7), O6–C3–O7 121.7(4).
Cent1: Centre of the Cp^{Ar5} ring (C20~C24),
Cent2: Centre of the Cp^{Ar5} ring (C85~C89).

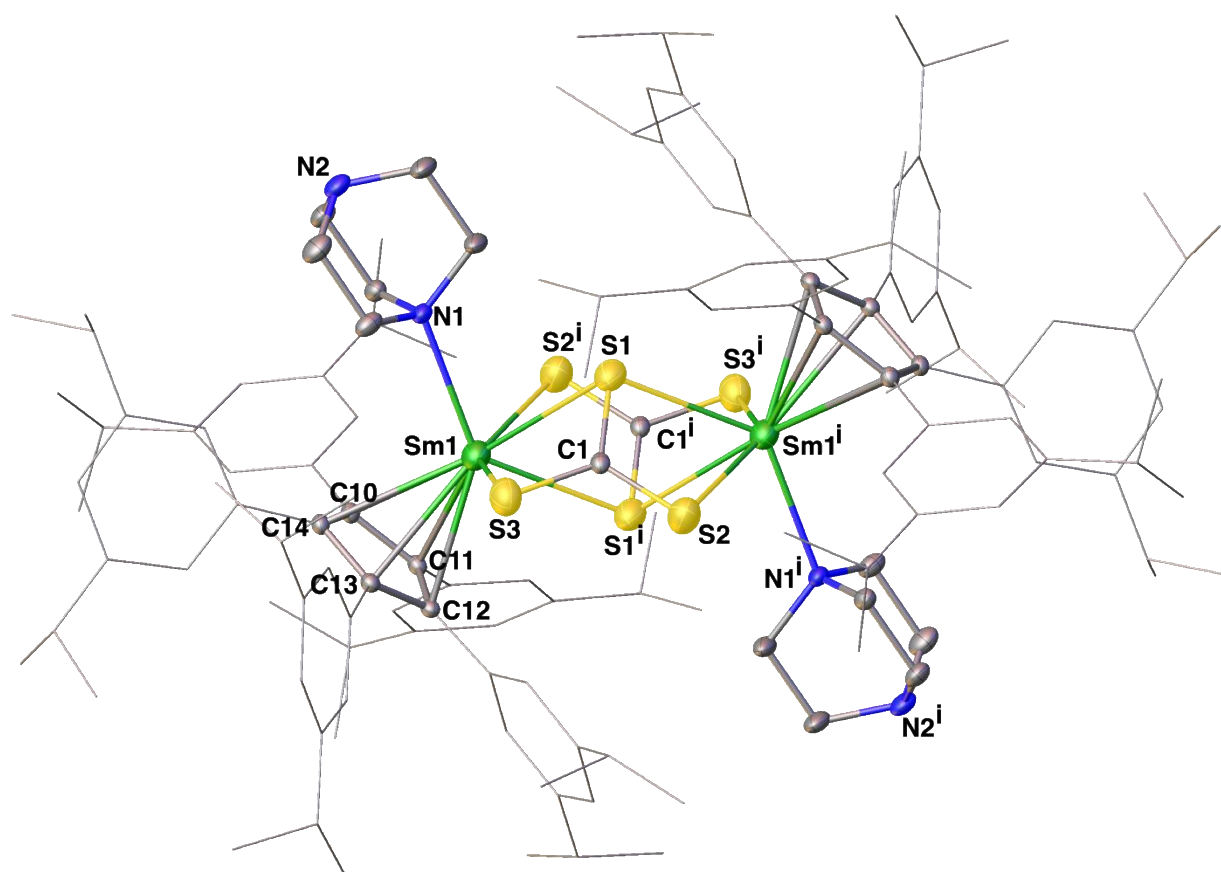


Figure S36. Molecular structure of $[(\text{Cp}^{\text{Ar5}})\text{Sm}^{\text{III}}(\mu\text{-}\eta^2:\eta^2\text{-CS}_3)(\text{DABCO})]_2$ (**9**). All the hydrogen atoms are omitted for clarity. Selected interatomic distances [\AA] and angles [deg]: Sm1–S1 2.9774(8), Sm1–S2 2.8243(8), Sm1–S3ⁱ 2.8393(8), C1–S1 1.726(3), C1–S2 1.698(3), C1–S3 1.705(3), Sm1–N1 2.581(3), Sm1–C10 2.834(3), Sm1–C11 2.784(3), Sm1–C12 2.741(3), Sm1–C13 2.771(3), Sm1–C14 2.847(3), Sm1–Cent1 2.518, S1–C1–S2 118.35(17), S1–C1–S3 119.28(17), S2–C1–S3 122.29(19).

Cent1: Centre of the Cp^{Ar5} ring (C10~C14).

Computational details

The optimization of reactants, transition states, IRC and products were carried out by employing DFT hybrid functional (B3PW91) along with small core pseudopotential Stuttgart basis set for samarium atom^[13] and People basis set^[14] (6-31G**) for the rest of the atoms. Frequency calculations were performed to locate saddle points for transition state structures, minima for rest of the structures and for obtaining thermal corrections over the energies. All the calculations were performed using Gaussian 09 suite of programs.^[15]

Optimized geometries

4

C	-0.077139000	9.844161000	14.694858000
H	0.814854000	10.480519000	14.706472000
H	-0.927051000	10.469116000	14.407196000
C	0.115864000	8.641198000	13.733938000
H	-0.710260000	8.569789000	13.018630000
H	1.037678000	8.756352000	13.157934000
C	0.938016000	8.643584000	16.500427000
H	0.776770000	8.266396000	17.515537000
H	1.754056000	9.374213000	16.537344000
C	1.245131000	7.494922000	15.495549000
H	2.186353000	7.681099000	14.969133000
H	1.334038000	6.532231000	16.011257000
C	-1.423589000	8.406402000	16.087644000
H	-2.307744000	8.943756000	15.726710000
H	-1.613915000	8.106362000	17.124083000
C	-1.096190000	7.186356000	15.179944000
H	-1.026231000	6.266416000	15.769805000
H	-1.876456000	7.033955000	14.425758000
C	-2.660543000	11.487731000	19.484938000
C	-1.982374000	12.733409000	19.689434000
C	-0.684813000	12.437368000	20.226655000
C	-0.569340000	11.019735000	20.336645000
C	-1.798178000	10.429027000	19.909116000
C	-4.063940000	11.326033000	19.038149000
C	-5.088648000	12.080872000	19.636642000
H	-4.816443000	12.794938000	20.406103000
C	-6.423986000	11.927829000	19.264050000
C	-7.556373000	12.712906000	19.912508000
H	-8.229324000	13.016535000	19.097176000
C	-7.107840000	13.984689000	20.633748000
H	-7.980590000	14.559323000	20.961201000
H	-6.519912000	13.751929000	21.528859000
H	-6.498459000	14.625255000	19.989583000
C	-8.368036000	11.817028000	20.862003000
H	-9.231249000	12.358434000	21.265313000
H	-8.736134000	10.920911000	20.353488000

SUPPORTING INFORMATION

H	-7.749755000	11.490271000	21.705224000
C	-6.736299000	10.994657000	18.264911000
H	-7.776280000	10.879374000	17.966251000
C	-5.750420000	10.220937000	17.649095000
C	-6.091601000	9.173409000	16.601178000
H	-5.164700000	8.962827000	16.049758000
C	-7.132880000	9.646575000	15.581509000
H	-7.256285000	8.901786000	14.787857000
H	-8.115764000	9.790218000	16.043344000
H	-6.840363000	10.594484000	15.119245000
C	-6.535360000	7.862410000	17.268012000
H	-6.722638000	7.084700000	16.518641000
H	-5.773387000	7.494627000	17.961807000
H	-7.460920000	8.012346000	17.835288000
C	-4.421315000	10.401450000	18.048194000
H	-3.647091000	9.787882000	17.591466000
C	-2.571617000	14.048650000	19.327503000
C	-3.216436000	14.220656000	18.090639000
H	-3.236084000	13.399941000	17.375706000
C	-3.881653000	15.402919000	17.745504000
C	-4.615877000	15.472560000	16.413794000
H	-4.021207000	14.886751000	15.698455000
C	-4.762103000	16.887037000	15.848996000
H	-5.199438000	16.848105000	14.846156000
H	-5.428436000	17.501914000	16.464193000
H	-3.799831000	17.403384000	15.777435000
C	-5.993811000	14.799708000	16.522138000
H	-5.912718000	13.773985000	16.892100000
H	-6.637392000	15.355095000	17.214051000
H	-6.491337000	14.775539000	15.545856000
C	-3.891362000	16.452502000	18.668247000
H	-4.412423000	17.375122000	18.427772000
C	-3.242087000	16.336389000	19.904963000
C	-3.285771000	17.464072000	20.925007000
H	-2.581068000	17.196551000	21.723742000
C	-4.679562000	17.578754000	21.560353000
H	-4.690920000	18.352326000	22.336419000
H	-5.431246000	17.847707000	20.809620000
H	-4.987677000	16.632784000	22.015905000

SUPPORTING INFORMATION

C	-2.838607000	18.814134000	20.349817000
H	-2.814837000	19.574058000	21.138689000
H	-1.840947000	18.758880000	19.903670000
H	-3.530624000	19.170988000	19.578821000
C	-2.593076000	15.139036000	20.215637000
H	-2.111596000	15.043046000	21.181655000
C	0.319174000	13.363455000	20.819571000
C	0.022215000	14.004881000	22.033684000
H	-0.947121000	13.826143000	22.493742000
C	0.944533000	14.821960000	22.686625000
C	0.585372000	15.503275000	23.996084000
H	-0.455101000	15.233395000	24.222495000
C	1.455397000	15.000966000	25.156445000
H	1.386105000	13.914134000	25.260973000
H	2.509727000	15.254169000	24.998833000
H	1.142476000	15.457183000	26.102315000
C	0.651425000	17.032358000	23.882018000
H	0.013798000	17.399279000	23.071761000
H	0.324971000	17.505320000	24.814890000
H	1.673320000	17.371807000	23.679477000
C	2.212959000	14.972796000	22.114480000
H	2.957032000	15.592760000	22.612015000
C	2.565453000	14.322930000	20.930491000
C	3.991598000	14.429104000	20.414340000
H	4.477196000	15.233624000	20.983658000
C	4.765881000	13.134269000	20.697280000
H	5.811375000	13.226132000	20.381782000
H	4.748094000	12.892917000	21.764379000
H	4.320433000	12.291396000	20.158782000
C	4.079275000	14.800577000	18.931549000
H	3.577374000	15.754047000	18.737051000
H	5.124938000	14.902934000	18.622844000
H	3.621769000	14.034353000	18.295423000
C	1.604044000	13.529052000	20.287364000
H	1.857103000	13.017789000	19.360158000
C	0.500800000	10.308830000	21.089954000
C	0.263746000	9.963400000	22.425473000
H	-0.692482000	10.234390000	22.865048000
C	1.218300000	9.284079000	23.188614000

SUPPORTING INFORMATION

C	0.962011000	8.938935000	24.646064000
H	1.826208000	8.356051000	24.993458000
C	0.880396000	10.202507000	25.513989000
H	1.786583000	10.808322000	25.416013000
H	0.028853000	10.826137000	25.220641000
H	0.754910000	9.941038000	26.570748000
C	-0.286097000	8.065986000	24.827129000
H	-0.217712000	7.149026000	24.234548000
H	-0.412272000	7.785622000	25.878900000
H	-1.192430000	8.594137000	24.513159000
C	2.430120000	8.942389000	22.583977000
H	3.173079000	8.406022000	23.171328000
C	2.711104000	9.275426000	21.254301000
C	4.025456000	8.871048000	20.605142000
H	4.093276000	9.415926000	19.653589000
C	5.249896000	9.253780000	21.445758000
H	6.173889000	9.032138000	20.900365000
H	5.247396000	10.318243000	21.695088000
H	5.284021000	8.689876000	22.384225000
C	4.045530000	7.369785000	20.281098000
H	3.212528000	7.091023000	19.628562000
H	4.978854000	7.089071000	19.779949000
H	3.963926000	6.773250000	21.196501000
C	1.735684000	9.962535000	20.523937000
H	1.942920000	10.235471000	19.489905000
C	-2.209049000	9.031946000	20.194814000
C	-1.366691000	7.930918000	19.978761000
H	-0.380312000	8.101683000	19.556371000
C	-1.752050000	6.630545000	20.334858000
C	-0.827992000	5.437854000	20.148929000
H	-1.406853000	4.544807000	20.421242000
C	-0.374175000	5.253912000	18.697111000
H	-1.232612000	5.169005000	18.022940000
H	0.238025000	6.098467000	18.362765000
H	0.231868000	4.347365000	18.590842000
C	0.375750000	5.513084000	21.097969000
H	0.048586000	5.552376000	22.141200000
H	1.024489000	4.637915000	20.976746000
H	0.974150000	6.409760000	20.908372000

SUPPORTING INFORMATION

C	-3.007097000	6.443235000	20.912327000
H	-3.317540000	5.435911000	21.188870000
C	-3.870212000	7.516078000	21.167227000
C	-5.181780000	7.246381000	21.890162000
H	-5.563193000	6.290336000	21.502671000
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H	-5.859986000	6.798416000	23.917224000
H	-4.198582000	6.271796000	23.587007000
H	-4.546547000	7.987067000	23.837207000
C	-6.261399000	8.303232000	21.654737000
H	-6.427439000	8.486239000	20.589438000
H	-7.208748000	7.980706000	22.099701000
H	-5.995155000	9.259170000	22.118628000
C	-3.457945000	8.796289000	20.802681000
H	-4.100703000	9.646166000	21.001553000
N	-0.288837000	9.358236000	16.080332000
N	0.180162000	7.389890000	14.494965000
Sm	-0.659287000	11.667019000	17.443560000
H	1.458894000	12.484053000	16.761180000
C	0.536697000	15.656437000	17.505598000
H	-0.353550000	15.017342000	17.494691000
H	1.388453000	15.032983000	17.791478000
C	0.343115000	16.857411000	18.468988000
H	1.168884000	16.926994000	19.184870000
H	-0.578998000	16.741129000	19.044215000
C	-0.481806000	16.860239000	15.704228000
H	-0.323355000	17.238215000	14.689051000
H	-1.298312000	16.129980000	15.668754000
C	-0.786667000	18.007908000	16.711047000
H	-1.727510000	17.822225000	17.238366000
H	-0.874922000	18.971396000	16.196681000
C	1.880488000	17.096624000	16.113556000
H	2.764877000	16.558235000	16.472104000
H	2.069558000	17.398157000	15.077525000
C	1.555090000	18.314434000	17.024870000
H	1.485382000	19.236101000	16.437692000
H	2.336173000	18.464172000	17.778772000
C	3.140937000	14.031875000	12.761568000
C	2.464460000	12.787214000	12.548903000

SUPPORTING INFORMATION

C	1.168204000	13.084456000	12.009412000
C	1.052201000	14.503224000	11.906548000
C	2.280460000	15.092279000	12.337723000
C	4.543458000	14.190628000	13.212288000
C	5.568591000	13.434562000	12.615983000
H	5.297510000	12.721346000	11.845316000
C	6.903162000	13.585447000	12.992236000
C	8.036171000	12.798732000	12.346847000
H	8.707272000	12.495458000	13.163839000
C	7.587946000	11.526456000	11.626303000
H	8.460766000	10.950424000	11.301483000
H	7.002168000	11.758655000	10.729632000
H	6.976458000	10.887495000	12.270066000
C	8.850523000	13.692715000	11.397896000
H	9.714184000	13.150152000	10.997078000
H	9.218186000	14.589183000	11.906097000
H	8.234267000	14.018907000	10.552975000
C	7.214282000	14.518183000	13.992140000
H	8.253688000	14.631917000	14.293352000
C	6.227903000	15.293277000	14.605422000
C	6.567366000	16.341250000	15.653507000
H	5.641272000	16.546321000	16.208312000
C	7.614951000	15.873253000	16.669032000
H	7.735554000	16.617329000	17.463774000
H	8.597477000	15.737588000	16.203990000
H	7.330724000	14.922366000	17.130399000
C	7.001733000	17.655323000	14.986434000
H	7.186816000	18.433494000	15.735882000
H	6.235786000	18.019371000	14.295064000
H	7.926493000	17.510916000	14.416413000
C	4.899476000	15.114313000	14.203336000
H	4.123957000	15.726979000	14.658463000
C	3.049519000	11.470828000	12.913497000
C	3.684363000	11.296468000	14.155228000
H	3.699948000	12.116681000	14.870875000
C	4.345959000	10.112976000	14.503553000
C	5.071253000	10.041033000	15.839905000
H	4.473394000	10.627900000	16.551671000
C	5.210218000	8.625776000	16.404563000

SUPPORTING INFORMATION

H	5.640271000	8.662830000	17.410565000
H	5.879526000	8.009818000	15.793684000
H	4.246184000	8.111698000	16.468592000
C	6.451492000	10.710570000	15.740377000
H	6.375211000	11.736646000	15.370367000
H	7.097941000	10.153910000	15.052174000
H	6.943019000	10.733043000	16.719723000
C	4.361453000	9.064623000	13.579567000
H	4.880116000	8.141358000	13.822699000
C	3.722016000	9.183107000	12.337928000
C	3.774201000	8.057967000	11.315414000
H	3.073521000	8.325894000	10.513270000
C	5.171991000	7.948741000	10.687836000
H	5.189869000	7.177379000	9.909697000
H	5.920002000	7.679665000	11.442190000
H	5.480232000	8.896788000	10.236749000
C	3.327503000	6.704913000	11.883785000
H	3.310574000	5.947502000	11.092337000
H	2.326936000	6.755602000	12.323959000
H	4.015986000	6.347373000	12.657609000
C	3.076502000	10.381460000	12.024145000
H	2.603220000	10.479479000	11.054346000
C	0.166728000	12.160768000	11.408605000
C	0.472408000	11.516405000	10.198088000
H	1.445938000	11.692413000	9.746021000
C	-0.446199000	10.700951000	9.538054000
C	-0.076870000	10.016442000	8.233085000
H	0.966467000	10.282879000	8.015984000
C	-0.934529000	10.519232000	7.063774000
H	-0.860847000	11.605609000	6.957672000
H	-1.991077000	10.269695000	7.212108000
H	-0.614314000	10.060088000	6.121775000
C	-0.148611000	8.487750000	8.349119000
H	0.479980000	8.120228000	9.166140000
H	0.185472000	8.012248000	7.420255000
H	-1.173481000	8.151767000	8.542188000
C	-1.720350000	10.554708000	10.098627000
H	-2.461646000	9.936276000	9.595113000
C	-2.081801000	11.207680000	11.278128000

SUPPORTING INFORMATION

C	-3.512346000	11.105480000	11.782869000
H	-3.999279000	10.311475000	11.200145000
C	-4.276235000	12.408827000	11.511530000
H	-5.324641000	12.319162000	11.817818000
H	-4.248652000	12.664407000	10.447978000
H	-3.830157000	13.241800000	12.064681000
C	-3.612403000	10.715328000	13.260268000
H	-3.118542000	9.755860000	13.445751000
H	-4.660837000	10.616263000	13.560753000
H	-3.153811000	11.470142000	13.909158000
C	-1.123843000	11.999751000	11.928653000
H	-1.386205000	12.513341000	12.852033000
C	-0.017239000	15.215073000	11.152808000
C	0.214806000	15.551242000	9.814113000
H	1.167499000	15.273168000	9.371300000
C	-0.740359000	16.230692000	9.051742000
C	-0.489287000	16.566567000	7.591206000
H	-1.353546000	17.149391000	7.243873000
C	-0.414026000	15.297825000	6.730328000
H	-1.321059000	14.694535000	6.835704000
H	0.437466000	14.674142000	7.023686000
H	-0.292471000	15.552946000	5.671569000
C	0.760119000	17.435573000	7.400114000
H	0.696446000	18.355891000	7.987974000
H	0.882516000	17.709898000	6.346302000
H	1.666469000	16.906864000	7.713113000
C	-1.947757000	16.581670000	9.660046000
H	-2.690847000	17.118152000	9.073023000
C	-2.223949000	16.257686000	10.992950000
C	-3.532859000	16.671520000	11.647216000
H	-3.600951000	16.126627000	12.598749000
C	-4.763837000	16.298869000	10.811716000
H	-5.683570000	16.526984000	11.361600000
H	-4.770694000	15.234679000	10.561283000
H	-4.798200000	16.864073000	9.874043000
C	-3.540172000	18.172620000	11.972511000
H	-2.701881000	18.444531000	12.621130000
H	-4.468893000	18.459755000	12.478520000
H	-3.458487000	18.769254000	11.057187000

SUPPORTING INFORMATION

C	-1.247865000	15.570476000	11.722321000
H	-1.451054000	15.305150000	12.759176000
C	2.694227000	16.488040000	12.050104000
C	1.852160000	17.591007000	12.257607000
H	0.863726000	17.423427000	12.676194000
C	2.240868000	18.889637000	11.898975000
C	1.317173000	20.083960000	12.076215000
H	1.900233000	20.976075000	11.809860000
C	0.848735000	20.268396000	13.523267000
H	1.700353000	20.350841000	14.206301000
H	0.230952000	19.425302000	13.851045000
H	0.243930000	21.176428000	13.623663000
C	0.123072000	20.010626000	11.114809000
H	0.461011000	19.970652000	10.075017000
H	-0.525583000	20.886825000	11.229086000
H	-0.478464000	19.114853000	11.298639000
C	3.498707000	19.073555000	11.326578000
H	3.811735000	20.079538000	11.048077000
C	4.361353000	17.998626000	11.079139000
C	5.676011000	18.263986000	10.360208000
H	6.057858000	19.220340000	10.746516000
C	5.432095000	18.445718000	8.852804000
H	6.362265000	18.705101000	8.334334000
H	4.700711000	19.235873000	8.657198000
H	5.046178000	17.519250000	8.412971000
C	6.752777000	17.205745000	10.602130000
H	6.914622000	17.025105000	11.668461000
H	7.702318000	17.525337000	10.159700000
H	6.486313000	16.249143000	10.139734000
C	3.946006000	16.720272000	11.446658000
H	4.588627000	15.869081000	11.253187000
N	0.745848000	16.144908000	16.120565000
N	0.279234000	18.110377000	17.710794000
Sm	1.104530000	13.815437000	14.791824000
H	-1.010571000	13.009334000	15.486459000

Int1

C	0.157456000	10.191702000	14.408160000
H	1.067390000	10.792737000	14.512653000

SUPPORTING INFORMATION

H	-0.664529000	10.873808000	14.177764000
C	0.334345000	9.107137000	13.314791000
H	-0.496103000	9.126702000	12.601189000
H	1.254400000	9.279126000	12.751022000
C	1.101331000	8.774143000	16.088366000
H	0.891965000	8.261668000	17.032977000
H	1.920863000	9.481636000	16.257967000
C	1.435388000	7.765154000	14.952139000
H	2.383249000	8.020344000	14.469610000
H	1.526541000	6.746572000	15.345415000
C	-1.243875000	8.626023000	15.580931000
H	-2.103321000	9.215308000	15.244166000
H	-1.481149000	8.218226000	16.568497000
C	-0.899800000	7.503664000	14.561992000
H	-0.842723000	6.527116000	15.055686000
H	-1.666696000	7.429718000	13.782564000
C	-3.014252000	10.639991000	18.990703000
C	-2.604024000	11.938322000	19.420107000
C	-1.317788000	11.807568000	20.056334000
C	-0.954037000	10.416462000	20.005380000
C	-2.013706000	9.695674000	19.376635000
C	-4.345630000	10.302503000	18.425314000
C	-5.523652000	10.738558000	19.056314000
H	-5.435925000	11.345107000	19.951407000
C	-6.787862000	10.408532000	18.560500000
C	-8.075648000	10.826687000	19.256064000
H	-8.823725000	10.976571000	18.464527000
C	-7.966480000	12.136977000	20.037718000
H	-8.954405000	12.446670000	20.395306000
H	-7.323823000	12.025385000	20.917959000
H	-7.553864000	12.942077000	19.423168000
C	-8.593053000	9.700137000	20.164773000
H	-9.552099000	9.973745000	20.619446000
H	-8.733402000	8.769094000	19.607313000
H	-7.880753000	9.500521000	20.972997000
C	-6.869216000	9.628683000	17.400696000
H	-7.852954000	9.377992000	17.006701000
C	-5.722994000	9.168435000	16.747225000
C	-5.818769000	8.310985000	15.495712000

SUPPORTING INFORMATION

H	-4.796456000	8.190581000	15.111596000
C	-6.648553000	8.977573000	14.391110000
H	-6.635404000	8.371146000	13.478638000
H	-7.695364000	9.094082000	14.691983000
H	-6.260803000	9.971129000	14.146481000
C	-6.355983000	6.908646000	15.813878000
H	-6.373701000	6.283787000	14.913570000
H	-5.735580000	6.411048000	16.564776000
H	-7.378042000	6.959205000	16.205545000
C	-4.476346000	9.509706000	17.277451000
H	-3.579235000	9.144844000	16.789646000
C	-3.482027000	13.123089000	19.226686000
C	-3.966104000	13.459937000	17.951728000
H	-3.658180000	12.861897000	17.094262000
C	-4.876914000	14.501946000	17.744248000
C	-5.433448000	14.752969000	16.351550000
H	-4.710333000	14.334571000	15.639132000
C	-5.604067000	16.236848000	16.012258000
H	-5.905103000	16.352443000	14.965622000
H	-6.383129000	16.706143000	16.623232000
H	-4.673550000	16.791634000	16.161201000
C	-6.758105000	13.995858000	16.165065000
H	-6.641169000	12.928833000	16.376192000
H	-7.524524000	14.388529000	16.843105000
H	-7.128738000	14.107149000	15.139561000
C	-5.297863000	15.244311000	18.851887000
H	-5.991564000	16.069199000	18.710579000
C	-4.862151000	14.931470000	20.143851000
C	-5.329456000	15.737275000	21.345321000
H	-4.896225000	15.264151000	22.237065000
C	-6.854289000	15.719938000	21.509832000
H	-7.150808000	16.262885000	22.414140000
H	-7.353213000	16.198331000	20.659960000
H	-7.233881000	14.697126000	21.586140000
C	-4.802555000	17.178476000	21.286047000
H	-5.089952000	17.735026000	22.185063000
H	-3.711427000	17.199756000	21.205412000
H	-5.210700000	17.711770000	20.420215000
C	-3.980624000	13.860523000	20.311813000

SUPPORTING INFORMATION

H	-3.712820000	13.558513000	21.320211000
C	-0.410498000	12.840493000	20.612626000
C	-0.848151000	13.931157000	21.381537000
H	-1.904232000	14.060813000	21.568991000
C	0.037687000	14.851309000	21.945575000
C	-0.492550000	15.991240000	22.800541000
H	-1.587244000	15.904163000	22.804938000
C	-0.017271000	15.877722000	24.255606000
H	-0.292081000	14.910268000	24.686657000
H	1.071682000	15.976125000	24.326434000
H	-0.462273000	16.666576000	24.872374000
C	-0.144355000	17.366349000	22.216162000
H	-0.520080000	17.469421000	21.193001000
H	-0.583469000	18.168564000	22.819702000
H	0.939195000	17.527579000	22.193793000
C	1.409236000	14.676363000	21.744047000
H	2.115518000	15.374143000	22.191461000
C	1.899119000	13.602785000	20.993039000
C	3.405179000	13.407548000	20.879357000
H	3.840966000	14.394649000	20.662454000
C	3.981285000	12.945085000	22.228755000
H	5.072406000	12.854399000	22.176452000
H	3.737507000	13.646167000	23.032562000
H	3.569185000	11.967967000	22.501952000
C	3.835995000	12.448799000	19.768422000
H	3.393494000	12.698564000	18.798362000
H	4.926461000	12.456312000	19.665574000
H	3.536978000	11.421479000	20.001878000
C	0.982369000	12.715901000	20.424570000
H	1.361215000	11.874748000	19.853214000
C	0.096633000	9.791198000	20.863671000
C	-0.123440000	9.754932000	22.245084000
H	-1.044735000	10.185897000	22.627487000
C	0.799810000	9.181734000	23.125588000
C	0.532679000	9.136768000	24.620533000
H	1.409521000	8.669221000	25.089359000
C	0.383537000	10.541963000	25.218707000
H	1.262620000	11.158331000	25.007459000
H	-0.489731000	11.058257000	24.805980000

SUPPORTING INFORMATION

H	0.255243000	10.487903000	26.305622000
C	-0.687014000	8.264526000	24.949243000
H	-0.565187000	7.249471000	24.558943000
H	-0.837129000	8.199907000	26.032875000
H	-1.599878000	8.680812000	24.509664000
C	1.975070000	8.643555000	22.598105000
H	2.699386000	8.200487000	23.279513000
C	2.243021000	8.664663000	21.224052000
C	3.540935000	8.089273000	20.676329000
H	3.558510000	8.303191000	19.598874000
C	4.779783000	8.747919000	21.299347000
H	5.694218000	8.360645000	20.836173000
H	4.767933000	9.833523000	21.172267000
H	4.842399000	8.539106000	22.372870000
C	3.613531000	6.566027000	20.849299000
H	2.776300000	6.064847000	20.357215000
H	4.543104000	6.171361000	20.423661000
H	3.589680000	6.289287000	21.909254000
C	1.288605000	9.233902000	20.373852000
H	1.489226000	9.262599000	19.303214000
C	-2.245167000	8.233973000	19.509660000
C	-1.282174000	7.262024000	19.184781000
H	-0.330542000	7.589109000	18.780419000
C	-1.517160000	5.899471000	19.391436000
C	-0.485751000	4.816883000	19.109800000
H	-1.036094000	3.958020000	18.698959000
C	0.576619000	5.204344000	18.082312000
H	0.121026000	5.529527000	17.141465000
H	1.217048000	6.014768000	18.447499000
H	1.226439000	4.350466000	17.863897000
C	0.165661000	4.353084000	20.423063000
H	-0.585819000	3.982604000	21.126690000
H	0.888572000	3.549115000	20.242547000
H	0.687413000	5.183927000	20.908819000
C	-2.743812000	5.509641000	19.938794000
H	-2.937298000	4.449787000	20.102714000
C	-3.717148000	6.440998000	20.297554000
C	-5.020737000	5.982736000	20.930489000
H	-4.922327000	4.904194000	21.116431000

SUPPORTING INFORMATION

C	-5.273241000	6.657944000	22.284650000
H	-6.177406000	6.254155000	22.753782000
H	-4.433508000	6.501205000	22.968827000
H	-5.414314000	7.738187000	22.171998000
C	-6.210764000	6.181003000	19.982784000
H	-6.067939000	5.624832000	19.051222000
H	-7.140471000	5.832505000	20.447318000
H	-6.336568000	7.236763000	19.722263000
C	-3.454476000	7.794398000	20.070437000
H	-4.194999000	8.536023000	20.351076000
N	-0.100916000	9.557668000	15.723603000
N	0.388425000	7.775603000	13.926016000
Sm	-0.498702000	11.708643000	17.385080000
H	1.741303000	12.271368000	16.808522000
C	2.372780000	15.647063000	17.956956000
H	1.403904000	15.157469000	18.089711000
H	3.141755000	14.888988000	18.132754000
C	2.533750000	16.860604000	18.914126000
H	3.464872000	16.792415000	19.487749000
H	1.711167000	16.897913000	19.634259000
C	1.392715000	17.049786000	16.250406000
H	1.581616000	17.455276000	15.252403000
H	0.442524000	16.507130000	16.208062000
C	1.361037000	18.176570000	17.319521000
H	0.487596000	18.082769000	17.974219000
H	1.309313000	19.162013000	16.844566000
C	3.767614000	16.830087000	16.404121000
H	4.568706000	16.156470000	16.723257000
H	3.922694000	17.060711000	15.346186000
C	3.740448000	18.110710000	17.284646000
H	3.709673000	19.013309000	16.664887000
H	4.637345000	18.177802000	17.910664000
C	3.937411000	13.919902000	13.021996000
C	3.119763000	12.787252000	12.705797000
C	1.872040000	13.282250000	12.197585000
C	1.924098000	14.707534000	12.224923000
C	3.213648000	15.112886000	12.699080000
C	5.369768000	13.806064000	13.410851000
C	6.274862000	13.208902000	12.522468000

SUPPORTING INFORMATION

H	5.898489000	12.851566000	11.567863000
C	7.631282000	13.070660000	12.836329000
C	8.607679000	12.447560000	11.851982000
H	9.584282000	12.405822000	12.353512000
C	8.217802000	11.011993000	11.478416000
H	8.966717000	10.570957000	10.811203000
H	7.253004000	10.983952000	10.961407000
H	8.133274000	10.378041000	12.365408000
C	8.772518000	13.314444000	10.596043000
H	9.520573000	12.882464000	9.921925000
H	9.090751000	14.329592000	10.852197000
H	7.830027000	13.388608000	10.042234000
C	8.077931000	13.532219000	14.078208000
H	9.130915000	13.420056000	14.330609000
C	7.205779000	14.128945000	14.997161000
C	7.697299000	14.595771000	16.357346000
H	6.842742000	15.066304000	16.863382000
C	8.151413000	13.415022000	17.227018000
H	8.447977000	13.757782000	18.224648000
H	9.012593000	12.906097000	16.780505000
H	7.352227000	12.676438000	17.341961000
C	8.803541000	15.652778000	16.247405000
H	9.093496000	16.013733000	17.240423000
H	8.475069000	16.510393000	15.653459000
H	9.700762000	15.242332000	15.771619000
C	5.862054000	14.262428000	14.640799000
H	5.174057000	14.727926000	15.340939000
C	3.585908000	11.391300000	12.922930000
C	4.211691000	11.038468000	14.133152000
H	4.289769000	11.776756000	14.928667000
C	4.796448000	9.786260000	14.341237000
C	5.546725000	9.502712000	15.633262000
H	5.269423000	10.292885000	16.343790000
C	5.178447000	8.159389000	16.272855000
H	5.705982000	8.033186000	17.224403000
H	5.457628000	7.315376000	15.632893000
H	4.104979000	8.087186000	16.470831000
C	7.063546000	9.594969000	15.407596000
H	7.341649000	10.568847000	14.994830000

SUPPORTING INFORMATION

H	7.399309000	8.821964000	14.706703000
H	7.607041000	9.451920000	16.348542000
C	4.727880000	8.841186000	13.312317000
H	5.187568000	7.865110000	13.450387000
C	4.083527000	9.131333000	12.104910000
C	4.010489000	8.101831000	10.988042000
H	3.386502000	8.535889000	10.195365000
C	5.395103000	7.825762000	10.384983000
H	5.321475000	7.116294000	9.553161000
H	6.071021000	7.394260000	11.131605000
H	5.856999000	8.744211000	10.010151000
C	3.340469000	6.796376000	11.438871000
H	3.229391000	6.112156000	10.590306000
H	2.349209000	6.973528000	11.867774000
H	3.942948000	6.280757000	12.195325000
C	3.529154000	10.402881000	11.925880000
H	3.059040000	10.632634000	10.977627000
C	0.772644000	12.546922000	11.513384000
C	1.022018000	11.935967000	10.273103000
H	2.023081000	11.995749000	9.852771000
C	0.017557000	11.301611000	9.541946000
C	0.329531000	10.640952000	8.209728000
H	1.408746000	10.756652000	8.040220000
C	-0.396642000	11.331329000	7.047046000
H	-0.158445000	12.398437000	7.009043000
H	-1.483614000	11.236142000	7.146873000
H	-0.111134000	10.882141000	6.089261000
C	0.023650000	9.137096000	8.232194000
H	0.558373000	8.633334000	9.043229000
H	0.316028000	8.667561000	7.286385000
H	-1.046777000	8.952847000	8.375579000
C	-1.283247000	11.316171000	10.057141000
H	-2.088610000	10.842121000	9.498364000
C	-1.587522000	11.953680000	11.261637000
C	-3.037598000	12.052617000	11.708933000
H	-3.606052000	11.324272000	11.114255000
C	-3.596464000	13.446235000	11.387904000
H	-4.657196000	13.514441000	11.655260000
H	-3.493695000	13.674834000	10.322725000

SUPPORTING INFORMATION

H	-3.052072000	14.215547000	11.944554000
C	-3.255392000	11.707043000	13.184568000
H	-2.931862000	10.683664000	13.400324000
H	-4.317119000	11.782160000	13.442744000
H	-2.706394000	12.387215000	13.845984000
C	-0.547123000	12.555068000	11.984445000
H	-0.762990000	13.052715000	12.927759000
C	0.919738000	15.583405000	11.557646000
C	1.145712000	15.983099000	10.235030000
H	2.051656000	15.641518000	9.741842000
C	0.237036000	16.794244000	9.549825000
C	0.461901000	17.178566000	8.096663000
H	-0.304081000	17.923556000	7.840791000
C	0.255181000	15.969583000	7.172063000
H	-0.738064000	15.531222000	7.309940000
H	0.995173000	15.189009000	7.380450000
H	0.359554000	16.260063000	6.120492000
C	1.831498000	17.824340000	7.856516000
H	1.975497000	18.699406000	8.496569000
H	1.927442000	18.143256000	6.812747000
H	2.647952000	17.124378000	8.063161000
C	-0.915613000	17.217025000	10.219700000
H	-1.622196000	17.850654000	9.688239000
C	-1.183342000	16.835441000	11.538424000
C	-2.421023000	17.316878000	12.281357000
H	-2.627807000	16.576400000	13.065681000
C	-3.669957000	17.417417000	11.399846000
H	-4.549914000	17.634663000	12.014502000
H	-3.855751000	16.486946000	10.855842000
H	-3.584482000	18.225804000	10.665303000
C	-2.151914000	18.657297000	12.982341000
H	-1.310723000	18.578857000	13.677556000
H	-3.030170000	18.985100000	13.549914000
H	-1.910161000	19.436694000	12.251134000
C	-0.255570000	16.012675000	12.188471000
H	-0.463106000	15.695263000	13.210302000
C	3.763138000	16.488005000	12.594849000
C	2.957253000	17.634629000	12.750145000
H	1.903611000	17.506904000	12.978571000

SUPPORTING INFORMATION

C	3.462762000	18.925303000	12.559010000
C	2.584101000	20.164072000	12.643941000
H	3.261255000	21.029165000	12.637098000
C	1.763060000	20.245988000	13.933554000
H	2.406868000	20.189605000	14.817312000
H	1.027748000	19.436530000	13.990629000
H	1.209542000	21.190200000	13.979564000
C	1.677352000	20.281081000	11.410304000
H	2.271827000	20.303224000	10.491847000
H	1.079685000	21.199183000	11.450977000
H	0.991977000	19.429873000	11.343244000
C	4.809605000	19.071758000	12.217003000
H	5.212933000	20.071692000	12.061822000
C	5.642212000	17.965278000	12.043339000
C	7.088474000	18.158282000	11.617653000
H	7.246688000	19.240118000	11.509191000
C	7.369094000	17.515209000	10.252912000
H	8.396018000	17.721845000	9.930724000
H	6.687756000	17.899135000	9.487232000
H	7.245761000	16.427978000	10.294758000
C	8.072043000	17.652507000	12.680241000
H	7.910339000	18.160407000	13.636655000
H	9.107347000	17.835324000	12.370521000
H	7.956274000	16.576742000	12.849066000
C	5.107771000	16.688951000	12.234453000
H	5.740465000	15.824048000	12.071701000
N	2.486817000	16.095055000	16.547093000
N	2.561173000	18.111226000	18.153231000
Sm	1.847290000	13.841822000	15.022651000
H	-0.454807000	13.345945000	15.517709000
O	-1.035611000	14.622444000	17.885080000
C	-1.569581000	15.151720000	16.984978000
O	-2.092315000	15.761309000	16.139520000

TS1

C	0.141791000	10.179883000	14.419735000
H	1.048777000	10.784299000	14.530675000
H	-0.683349000	10.860580000	14.195452000
C	0.323024000	9.106830000	13.316009000

SUPPORTING INFORMATION

H	-0.509286000	9.127941000	12.604759000
H	1.240444000	9.290426000	12.751649000
C	1.092674000	8.750521000	16.087251000
H	0.885079000	8.226237000	17.025576000
H	1.907926000	9.460975000	16.265476000
C	1.434728000	7.757214000	14.939867000
H	2.380216000	8.025791000	14.459978000
H	1.534673000	6.735335000	15.322253000
C	-1.252403000	8.593733000	15.576119000
H	-2.113770000	9.181100000	15.241225000
H	-1.490366000	8.177381000	16.559899000
C	-0.898631000	7.482245000	14.548628000
H	-0.832927000	6.502520000	15.034846000
H	-1.665230000	7.407765000	13.769050000
C	-3.017974000	10.632494000	18.988249000
C	-2.605254000	11.928664000	19.419464000
C	-1.316349000	11.795429000	20.050408000
C	-0.955023000	10.404046000	19.998530000
C	-2.015807000	9.685964000	19.367979000
C	-4.349247000	10.298910000	18.420581000
C	-5.527828000	10.736014000	19.049780000
H	-5.441066000	11.340093000	19.946625000
C	-6.791637000	10.410302000	18.549789000
C	-8.079926000	10.828917000	19.244123000
H	-8.829792000	10.970065000	18.452688000
C	-7.974309000	12.145547000	20.015617000
H	-8.962581000	12.453574000	20.373756000
H	-7.328589000	12.043396000	20.894683000
H	-7.567008000	12.947939000	19.394034000
C	-8.591607000	9.707127000	20.161864000
H	-9.550836000	9.980475000	20.616339000
H	-8.729510000	8.771710000	19.611142000
H	-7.877163000	9.515829000	20.970224000
C	-6.872154000	9.633468000	17.388039000
H	-7.855572000	9.386039000	16.991226000
C	-5.725434000	9.172107000	16.736226000
C	-5.820220000	8.317565000	15.482626000
H	-4.797697000	8.198970000	15.098385000
C	-6.650496000	8.985550000	14.379272000

SUPPORTING INFORMATION

H	-6.636363000	8.381109000	13.465491000
H	-7.697539000	9.100020000	14.680067000
H	-6.264048000	9.980143000	14.136896000
C	-6.356095000	6.913948000	15.797531000
H	-6.373442000	6.291143000	14.895777000
H	-5.735207000	6.415152000	16.547237000
H	-7.378116000	6.962807000	16.189497000
C	-4.479444000	9.509225000	17.270331000
H	-3.581919000	9.143568000	16.783818000
C	-3.483713000	13.115604000	19.237477000
C	-3.965998000	13.467714000	17.966208000
H	-3.658210000	12.878703000	17.102577000
C	-4.871820000	14.514933000	17.769587000
C	-5.419676000	14.795725000	16.379320000
H	-4.733518000	14.323209000	15.664345000
C	-5.480487000	16.287915000	16.036784000
H	-5.791712000	16.425204000	14.995590000
H	-6.206932000	16.818584000	16.662110000
H	-4.506020000	16.766864000	16.166205000
C	-6.796648000	14.136667000	16.203174000
H	-6.753213000	13.064230000	16.415431000
H	-7.529888000	14.583684000	16.884283000
H	-7.164540000	14.271539000	15.179586000
C	-5.295698000	15.243161000	18.885755000
H	-5.988070000	16.070725000	18.752156000
C	-4.864554000	14.913369000	20.174498000
C	-5.333051000	15.704533000	21.385194000
H	-4.906307000	15.216544000	22.272064000
C	-6.858600000	15.693875000	21.543069000
H	-7.155700000	16.224773000	22.454334000
H	-7.350944000	16.188431000	20.698629000
H	-7.244816000	14.672410000	21.601910000
C	-4.797861000	17.143464000	21.348303000
H	-5.085664000	17.689107000	22.253889000
H	-3.706380000	17.159572000	21.271662000
H	-5.199543000	17.690828000	20.488261000
C	-3.983772000	13.839567000	20.330573000
H	-3.717063000	13.525387000	21.335718000
C	-0.408936000	12.827741000	20.608369000

SUPPORTING INFORMATION

C	-0.848404000	13.917290000	21.377628000
H	-1.904877000	14.045789000	21.563479000
C	0.035753000	14.838549000	21.942640000
C	-0.496769000	15.976713000	22.798482000
H	-1.591240000	15.887248000	22.802960000
C	-0.021016000	15.863295000	24.253391000
H	-0.293832000	14.895030000	24.683885000
H	1.067772000	15.963766000	24.324065000
H	-0.467451000	16.650884000	24.870765000
C	-0.151737000	17.352925000	22.214916000
H	-0.526743000	17.454872000	21.191356000
H	-0.593620000	18.153902000	22.818085000
H	0.931465000	17.516924000	22.194112000
C	1.407431000	14.666523000	21.740326000
H	2.112809000	15.365415000	22.187523000
C	1.898847000	13.594454000	20.988156000
C	3.405251000	13.404775000	20.871166000
H	3.837307000	14.395414000	20.662982000
C	3.984573000	12.931607000	22.215389000
H	5.075956000	12.844927000	22.161270000
H	3.739222000	13.624642000	23.025692000
H	3.575781000	11.950781000	22.480149000
C	3.837415000	12.458503000	19.750079000
H	3.390730000	12.716046000	18.783917000
H	4.927539000	12.471527000	19.644174000
H	3.543286000	11.427659000	19.974081000
C	0.983943000	12.705346000	20.420402000
H	1.363660000	11.866618000	19.846222000
C	0.096460000	9.777650000	20.854824000
C	-0.121306000	9.741456000	22.236631000
H	-1.041935000	10.172572000	22.620436000
C	0.803382000	9.168539000	23.115811000
C	0.538729000	9.124283000	24.611215000
H	1.416075000	8.656400000	25.078768000
C	0.391462000	10.529873000	25.208948000
H	1.270587000	11.145582000	24.995977000
H	-0.482102000	11.046533000	24.797328000
H	0.264871000	10.476410000	26.296090000
C	-0.680948000	8.252957000	24.942380000

SUPPORTING INFORMATION

H	-0.560469000	7.237651000	24.552301000
H	-0.829197000	8.188884000	26.026297000
H	-1.594323000	8.669667000	24.504272000
C	1.977802000	8.630200000	22.586619000
H	2.703285000	8.187352000	23.266937000
C	2.243481000	8.651045000	21.212124000
C	3.540728000	8.076135000	20.662446000
H	3.553729000	8.284565000	19.583835000
C	4.779795000	8.741797000	21.277530000
H	5.693964000	8.354225000	20.814040000
H	4.764525000	9.826584000	21.143897000
H	4.846021000	8.539766000	22.352145000
C	3.618421000	6.554012000	20.842842000
H	2.780587000	6.047905000	20.356819000
H	4.547375000	6.159895000	20.415347000
H	3.599841000	6.282416000	21.904216000
C	1.287830000	9.220381000	20.363458000
H	1.487111000	9.248959000	19.292545000
C	-2.248527000	8.224141000	19.498453000
C	-1.284503000	7.252097000	19.176557000
H	-0.331035000	7.579304000	18.776636000
C	-1.520062000	5.889433000	19.381866000
C	-0.487088000	4.807227000	19.104670000
H	-1.035690000	3.946974000	18.694442000
C	0.577418000	5.193395000	18.078842000
H	0.123839000	5.516514000	17.136255000
H	1.216614000	6.004724000	18.444227000
H	1.228241000	4.339495000	17.863503000
C	0.161858000	4.346961000	20.420401000
H	-0.590938000	3.977773000	21.123293000
H	0.885626000	3.542961000	20.243444000
H	0.682028000	5.179347000	20.905238000
C	-2.748692000	5.499257000	19.924491000
H	-2.942686000	4.439342000	20.087389000
C	-3.723256000	6.430543000	20.280114000
C	-5.028859000	5.972342000	20.908933000
H	-4.932504000	4.893103000	21.091904000
C	-5.282664000	6.644068000	22.264618000
H	-6.188500000	6.240662000	22.730854000

SUPPORTING INFORMATION

H	-4.444525000	6.483697000	22.949906000
H	-5.421394000	7.724898000	22.154797000
C	-6.216796000	6.175372000	19.959658000
H	-6.073379000	5.621457000	19.026844000
H	-7.147925000	5.827301000	20.421641000
H	-6.340282000	7.232052000	19.701792000
C	-3.459795000	7.784072000	20.054638000
H	-4.201315000	8.525448000	20.333203000
N	-0.114500000	9.530517000	15.729159000
N	0.387140000	7.770163000	13.914668000
Sm	-0.507238000	11.671093000	17.373686000
H	1.729104000	12.277319000	16.788173000
C	2.335278000	15.696758000	17.981077000
H	1.355128000	15.233208000	18.122222000
H	3.086017000	14.919919000	18.154625000
C	2.533566000	16.909109000	18.933151000
H	3.465864000	16.818638000	19.501781000
H	1.716309000	16.970232000	19.657730000
C	1.374434000	17.117039000	16.280253000
H	1.557619000	17.509398000	15.275921000
H	0.410388000	16.599124000	16.258838000
C	1.385181000	18.251604000	17.341933000
H	0.513553000	18.187536000	18.002525000
H	1.359896000	19.235328000	16.861294000
C	3.746559000	16.840226000	16.413696000
H	4.532610000	16.146918000	16.728178000
H	3.898994000	17.064989000	15.353955000
C	3.761200000	18.122576000	17.291554000
H	3.750463000	19.024592000	16.670266000
H	4.664179000	18.166020000	17.910930000
C	3.931797000	13.924691000	13.032175000
C	3.112295000	12.791659000	12.723721000
C	1.863579000	13.284599000	12.214902000
C	1.916723000	14.710115000	12.236428000
C	3.207604000	15.116527000	12.706934000
C	5.364417000	13.812985000	13.420119000
C	6.268003000	13.206499000	12.536425000
H	5.889883000	12.838302000	11.586675000
C	7.625393000	13.073829000	12.848438000

SUPPORTING INFORMATION

C	8.600602000	12.441889000	11.868543000
H	9.578239000	12.406579000	12.368518000
C	8.211894000	11.002147000	11.510362000
H	8.960496000	10.555082000	10.846815000
H	7.246568000	10.967912000	10.994730000
H	8.129048000	10.377281000	12.403914000
C	8.761808000	13.295945000	10.603360000
H	9.509124000	12.857912000	9.932347000
H	9.079225000	14.314121000	10.848265000
H	7.818159000	13.363086000	10.050640000
C	8.074591000	13.550269000	14.083792000
H	9.128420000	13.442765000	14.334654000
C	7.204046000	14.156516000	14.997935000
C	7.698573000	14.641208000	16.350733000
H	6.844480000	15.115855000	16.853686000
C	8.158887000	13.472555000	17.233409000
H	8.457199000	13.828459000	18.225888000
H	9.020494000	12.961071000	16.790662000
H	7.362489000	12.732820000	17.359832000
C	8.801664000	15.699638000	16.224082000
H	9.094822000	16.072542000	17.211723000
H	8.468427000	16.549598000	15.621874000
H	9.697870000	15.286005000	15.749131000
C	5.859291000	14.284052000	14.643361000
H	5.172981000	14.758662000	15.338903000
C	3.579201000	11.396195000	12.944090000
C	4.199586000	11.044569000	14.157164000
H	4.271180000	11.782595000	14.953528000
C	4.785727000	9.793341000	14.368036000
C	5.528420000	9.511270000	15.664776000
H	5.231931000	10.291338000	16.378749000
C	5.176601000	8.157134000	16.290519000
H	5.693093000	8.034715000	17.248548000
H	5.481018000	7.322643000	15.649561000
H	4.102026000	8.062861000	16.472782000
C	7.045606000	9.629630000	15.453980000
H	7.311961000	10.610362000	15.049835000
H	7.400039000	8.866543000	14.751384000
H	7.582612000	9.489186000	16.399047000

SUPPORTING INFORMATION

C	4.725133000	8.848846000	13.338165000
H	5.186178000	7.873767000	13.478270000
C	4.086237000	9.137836000	12.127477000
C	4.020239000	8.107937000	11.010452000
H	3.403345000	8.542711000	10.212623000
C	5.408790000	7.828438000	10.418254000
H	5.339904000	7.118028000	9.586856000
H	6.078409000	7.396542000	11.170304000
H	5.875192000	8.745437000	10.045574000
C	3.344085000	6.804130000	11.456908000
H	3.240083000	6.118787000	10.608343000
H	2.349019000	6.983167000	11.876154000
H	3.938780000	6.288932000	12.219792000
C	3.529652000	10.408067000	11.946327000
H	3.063901000	10.637262000	10.995768000
C	0.765935000	12.546789000	11.530436000
C	1.018311000	11.933322000	10.291941000
H	2.020080000	11.993139000	9.873332000
C	0.015790000	11.296858000	9.559906000
C	0.331164000	10.633130000	8.230011000
H	1.410571000	10.749740000	8.062303000
C	-0.393532000	11.319356000	7.063973000
H	-0.156805000	12.386695000	7.023654000
H	-1.480579000	11.222816000	7.161625000
H	-0.105269000	10.868051000	6.108008000
C	0.027184000	9.128930000	8.255969000
H	0.561065000	8.628026000	9.069332000
H	0.321877000	8.657199000	7.311971000
H	-1.043277000	8.943723000	8.397886000
C	-1.286258000	11.312275000	10.071966000
H	-2.090232000	10.836991000	9.512230000
C	-1.593432000	11.952424000	11.274357000
C	-3.044486000	12.052806000	11.718038000
H	-3.612306000	11.324913000	11.122201000
C	-3.601123000	13.446998000	11.395499000
H	-4.662579000	13.516101000	11.659677000
H	-3.494965000	13.675460000	10.330623000
H	-3.057806000	14.215792000	11.953894000
C	-3.265948000	11.707917000	13.193303000

SUPPORTING INFORMATION

H	-2.944962000	10.683865000	13.409987000
H	-4.328000000	11.785125000	13.449459000
H	-2.717028000	12.387425000	13.855427000
C	-0.554834000	12.555241000	11.998574000
H	-0.772184000	13.054144000	12.940859000
C	0.916273000	15.584684000	11.561254000
C	1.148285000	15.975062000	10.236892000
H	2.055178000	15.628115000	9.749189000
C	0.244410000	16.784100000	9.542973000
C	0.476870000	17.159205000	8.088594000
H	-0.289256000	17.900688000	7.823197000
C	0.278682000	15.943812000	7.170609000
H	-0.714481000	15.504219000	7.305123000
H	1.019013000	15.166203000	7.388691000
H	0.389052000	16.227661000	6.117841000
C	1.846463000	17.806719000	7.852867000
H	1.984208000	18.686346000	8.488053000
H	1.948457000	18.118952000	6.807640000
H	2.663178000	17.110109000	8.069608000
C	-0.909806000	17.213870000	10.205555000
H	-1.612933000	17.845645000	9.667312000
C	-1.183226000	16.841812000	11.525827000
C	-2.422536000	17.331034000	12.260847000
H	-2.631065000	16.598697000	13.052181000
C	-3.669330000	17.422313000	11.375230000
H	-4.550710000	17.646689000	11.985297000
H	-3.854185000	16.485887000	10.841211000
H	-3.581833000	18.222431000	10.631922000
C	-2.154946000	18.678797000	12.948235000
H	-1.314211000	18.608210000	13.644896000
H	-3.033950000	19.011877000	13.511581000
H	-1.913078000	19.450897000	12.209339000
C	-0.259885000	16.021362000	12.185122000
H	-0.472078000	15.712460000	13.208446000
C	3.758360000	16.490551000	12.592570000
C	2.956311000	17.639373000	12.750597000
H	1.904932000	17.515062000	12.991340000
C	3.462302000	18.927827000	12.545495000
C	2.587654000	20.169463000	12.630380000

SUPPORTING INFORMATION

H	3.267221000	21.032492000	12.612249000
C	1.777849000	20.262608000	13.926241000
H	2.428679000	20.207417000	14.804922000
H	1.038414000	19.457728000	13.993880000
H	1.229910000	21.210082000	13.971664000
C	1.670911000	20.281322000	11.403658000
H	2.257607000	20.295418000	10.480078000
H	1.076625000	21.201652000	11.443374000
H	0.982239000	19.431993000	11.348005000
C	4.805642000	19.069213000	12.187865000
H	5.209011000	20.067358000	12.021697000
C	5.634333000	17.960190000	12.011880000
C	7.076025000	18.147599000	11.568612000
H	7.234331000	19.228232000	11.448870000
C	7.340952000	17.492205000	10.206588000
H	8.364135000	17.695789000	9.870903000
H	6.650940000	17.869408000	9.445355000
H	7.218129000	16.405372000	10.259425000
C	8.070717000	17.650127000	12.624779000
H	7.920394000	18.166949000	13.578242000
H	9.102722000	17.828801000	12.301906000
H	7.955525000	16.576087000	12.804685000
C	5.099344000	16.686240000	12.216459000
H	5.728065000	15.818799000	12.051444000
N	2.449317000	16.137715000	16.568851000
N	2.588649000	18.156576000	18.168426000
Sm	1.847016000	13.867633000	15.032460000
H	-0.470357000	13.341122000	15.488404000
O	-0.996658000	14.457091000	17.790724000
C	-1.471833000	14.942262000	16.827826000
O	-1.987840000	15.578955000	15.995822000

Int2

C	0.146106000	9.791669000	14.423111000
H	1.048435000	10.381395000	14.620395000
H	-0.653510000	10.482150000	14.140958000
C	0.403712000	8.724587000	13.324650000
H	-0.274911000	8.859389000	12.476778000
H	1.423714000	8.805873000	12.940242000

SUPPORTING INFORMATION

C	0.852490000	8.232466000	16.106162000
H	0.558945000	7.754809000	17.045565000
H	1.737051000	8.849550000	16.300566000
C	1.130140000	7.184022000	14.991042000
H	2.153459000	7.277324000	14.614148000
H	1.006093000	6.163191000	15.369947000
C	-1.459924000	8.314623000	15.447468000
H	-2.260978000	8.995332000	15.139169000
H	-1.756404000	7.853111000	16.395655000
C	-1.164536000	7.250424000	14.350930000
H	-1.303246000	6.235429000	14.739765000
H	-1.840260000	7.366126000	13.496345000
C	-2.767566000	10.886281000	19.292700000
C	-2.047200000	12.050794000	19.716502000
C	-0.801992000	11.611303000	20.267603000
C	-0.760306000	10.189332000	20.192364000
C	-1.977135000	9.732982000	19.591704000
C	-4.172418000	10.884847000	18.809226000
C	-5.180520000	11.412375000	19.632241000
H	-4.894395000	11.812431000	20.599570000
C	-6.517886000	11.434664000	19.230539000
C	-7.632966000	11.955776000	20.126006000
H	-8.363342000	12.444345000	19.464892000
C	-7.178089000	12.993110000	21.155231000
H	-8.046117000	13.423549000	21.665517000
H	-6.541786000	12.543519000	21.925735000
H	-6.615262000	13.808428000	20.691184000
C	-8.355867000	10.790474000	20.821020000
H	-9.203096000	11.153769000	21.413802000
H	-8.733792000	10.063787000	20.095335000
H	-7.673036000	10.263065000	21.496406000
C	-6.840354000	10.924383000	17.966934000
H	-7.878630000	10.957203000	17.639614000
C	-5.867285000	10.385266000	17.120607000
C	-6.227969000	9.873454000	15.735721000
H	-5.309575000	9.458965000	15.298446000
C	-6.697055000	11.017195000	14.825119000
H	-6.904494000	10.650536000	13.813395000
H	-7.616830000	11.473006000	15.208167000

SUPPORTING INFORMATION

H	-5.939493000	11.803744000	14.756507000
C	-7.267568000	8.746621000	15.777901000
H	-7.462994000	8.362615000	14.770395000
H	-6.925731000	7.914718000	16.400145000
H	-8.221134000	9.098817000	16.186359000
C	-4.541069000	10.363933000	17.563037000
H	-3.776835000	9.943968000	16.913295000
C	-2.567532000	13.437265000	19.667302000
C	-3.308104000	13.901798000	18.565602000
H	-3.456362000	13.247191000	17.710970000
C	-3.895760000	15.169811000	18.550770000
C	-4.760700000	15.591234000	17.372540000
H	-4.626348000	14.831303000	16.591191000
C	-4.349295000	16.942277000	16.777249000
H	-4.961079000	17.182229000	15.900612000
H	-4.476075000	17.757514000	17.497985000
H	-3.300631000	16.932880000	16.464223000
C	-6.248180000	15.592387000	17.753653000
H	-6.556725000	14.608794000	18.118859000
H	-6.450981000	16.325496000	18.542515000
H	-6.872497000	15.848171000	16.889892000
C	-3.720770000	16.004145000	19.660673000
H	-4.189021000	16.986120000	19.671237000
C	-2.973464000	15.587427000	20.768691000
C	-2.829867000	16.469489000	21.999198000
H	-2.131044000	15.959447000	22.675281000
C	-4.168477000	16.610559000	22.738788000
H	-4.046449000	17.194566000	23.657980000
H	-4.910691000	17.121424000	22.115061000
H	-4.577477000	15.631736000	23.007397000
C	-2.236316000	17.846377000	21.678041000
H	-2.098226000	18.429750000	22.595210000
H	-1.264340000	17.756603000	21.184333000
H	-2.893376000	18.424380000	21.018849000
C	-2.405520000	14.311132000	20.755222000
H	-1.849641000	13.974234000	21.624567000
C	0.177627000	12.406495000	21.059691000
C	0.119850000	12.317274000	22.458709000
H	-0.646203000	11.689621000	22.907787000

SUPPORTING INFORMATION

C	1.019035000	12.997648000	23.280847000
C	0.932226000	12.865725000	24.792018000
H	0.046463000	12.253794000	25.008188000
C	2.151526000	12.126914000	25.361352000
H	2.271336000	11.145996000	24.891841000
H	3.073113000	12.694694000	25.190208000
H	2.047794000	11.980647000	26.442452000
C	0.735871000	14.222140000	25.481417000
H	-0.152276000	14.736065000	25.100765000
H	0.617704000	14.093072000	26.562952000
H	1.596524000	14.880625000	25.319921000
C	2.006622000	13.781460000	22.675347000
H	2.722720000	14.310158000	23.301182000
C	2.101717000	13.893482000	21.285581000
C	3.212254000	14.713289000	20.650031000
H	3.026211000	14.723603000	19.567122000
C	3.218167000	16.168389000	21.136426000
H	3.976788000	16.752678000	20.603502000
H	2.245800000	16.647076000	20.984518000
H	3.450903000	16.230911000	22.204933000
C	4.583038000	14.059905000	20.875295000
H	4.600202000	13.035800000	20.490576000
H	5.375074000	14.627535000	20.375079000
H	4.825466000	14.017989000	21.942877000
C	1.177382000	13.203549000	20.491431000
H	1.259782000	13.266922000	19.406634000
C	0.244688000	9.365510000	20.909438000
C	-0.172256000	8.494738000	21.926139000
H	-1.236415000	8.404017000	22.125447000
C	0.744015000	7.766749000	22.691209000
C	0.278034000	6.849280000	23.810236000
H	1.180358000	6.438214000	24.283698000
C	-0.497668000	7.614950000	24.890849000
H	0.094102000	8.444564000	25.289995000
H	-1.429529000	8.030660000	24.492510000
H	-0.760159000	6.951241000	25.722268000
C	-0.543709000	5.667880000	23.277132000
H	0.036157000	5.072089000	22.565412000
H	-0.853508000	5.009453000	24.096759000

SUPPORTING INFORMATION

H	-1.446313000	6.012166000	22.761838000
C	2.106390000	7.914761000	22.417792000
H	2.823736000	7.355167000	23.015624000
C	2.563689000	8.769558000	21.408283000
C	4.049464000	8.944878000	21.145080000
H	4.143219000	9.564139000	20.242264000
C	4.732567000	9.700348000	22.294271000
H	5.791325000	9.876000000	22.071741000
H	4.252722000	10.667481000	22.470098000
H	4.678528000	9.126122000	23.226009000
C	4.757734000	7.612556000	20.868225000
H	4.281553000	7.070552000	20.045277000
H	5.808529000	7.779903000	20.606204000
H	4.741720000	6.959733000	21.747897000
C	1.621216000	9.485627000	20.666674000
H	1.967646000	10.172442000	19.896347000
C	-2.397402000	8.313676000	19.522198000
C	-1.474847000	7.291216000	19.220366000
H	-0.450492000	7.570368000	18.996040000
C	-1.824703000	5.941558000	19.279566000
C	-0.847732000	4.811527000	18.984413000
H	-1.063173000	4.022262000	19.718999000
C	-1.104761000	4.212654000	17.592961000
H	-2.144872000	3.892351000	17.479345000
H	-0.899270000	4.954172000	16.812511000
H	-0.458579000	3.346238000	17.412218000
C	0.625647000	5.188367000	19.145827000
H	0.822169000	5.662878000	20.111582000
H	1.254617000	4.295380000	19.066172000
H	0.954195000	5.880768000	18.362545000
C	-3.138979000	5.611341000	19.634155000
H	-3.422296000	4.561202000	19.699414000
C	-4.086360000	6.590492000	19.931972000
C	-5.493085000	6.192771000	20.346713000
H	-5.515878000	5.094930000	20.385048000
C	-5.847190000	6.706902000	21.748506000
H	-6.839026000	6.353072000	22.051377000
H	-5.120849000	6.363057000	22.491663000
H	-5.862749000	7.801533000	21.778568000

SUPPORTING INFORMATION

C	-6.535721000	6.640386000	19.314159000
H	-6.312776000	6.222423000	18.327221000
H	-7.539045000	6.308673000	19.604751000
H	-6.555786000	7.730973000	19.218305000
C	-3.702139000	7.934793000	19.870907000
H	-4.416940000	8.707134000	20.134498000
N	-0.247937000	9.131352000	15.692723000
N	0.211154000	7.377145000	13.868515000
Sm	-0.629790000	11.214868000	17.414350000
H	1.175712000	12.520393000	16.550879000
C	0.278520000	15.752709000	17.334508000
H	-0.637816000	15.206072000	17.089356000
H	0.960685000	15.044060000	17.814847000
C	-0.018814000	16.980633000	18.238951000
H	0.527461000	16.911500000	19.185167000
H	-1.084133000	17.036337000	18.482108000
C	-0.047545000	17.116171000	15.384003000
H	0.414417000	17.434886000	14.445008000
H	-0.944936000	16.540782000	15.135005000
C	-0.359024000	18.330576000	16.305807000
H	-1.427543000	18.389011000	16.537488000
H	-0.077907000	19.272367000	15.822927000
C	2.138585000	16.947807000	16.375112000
H	2.829012000	16.258846000	16.876100000
H	2.596156000	17.254319000	15.427804000
C	1.808844000	18.171794000	17.277577000
H	2.095336000	19.109262000	16.788097000
H	2.351161000	18.120306000	18.227968000
C	3.646660000	13.970249000	12.954546000
C	2.979025000	12.748523000	12.623272000
C	1.798595000	13.083935000	11.879816000
C	1.739908000	14.504383000	11.770544000
C	2.895246000	15.058419000	12.407022000
C	4.976340000	14.073500000	13.603880000
C	6.072310000	13.375530000	13.076142000
H	5.910311000	12.739787000	12.209970000
C	7.355314000	13.502651000	13.618970000
C	8.543771000	12.783387000	13.001615000
H	9.429200000	13.067859000	13.586562000

SUPPORTING INFORMATION

C	8.402556000	11.258726000	13.088511000
H	9.279727000	10.763324000	12.657290000
H	7.517900000	10.909549000	12.546181000
H	8.302581000	10.930888000	14.127053000
C	8.788613000	13.230467000	11.553682000
H	9.684522000	12.748580000	11.146582000
H	8.926536000	14.314220000	11.490346000
H	7.945780000	12.962444000	10.907205000
C	7.529178000	14.325896000	14.735000000
H	8.524934000	14.423301000	15.163956000
C	6.458756000	15.026723000	15.304027000
C	6.661504000	15.911551000	16.522902000
H	5.670189000	16.283349000	16.816970000
C	7.231779000	15.126999000	17.711737000
H	7.311551000	15.768742000	18.596387000
H	8.234872000	14.745455000	17.492421000
H	6.599729000	14.270360000	17.964708000
C	7.533769000	17.132946000	16.204814000
H	7.632198000	17.779408000	17.084180000
H	7.103382000	17.723363000	15.391314000
H	8.541287000	16.829452000	15.900013000
C	5.197515000	14.896568000	14.719344000
H	4.366741000	15.467496000	15.129220000
C	3.480144000	11.414312000	13.044413000
C	3.841757000	11.181647000	14.380489000
H	3.697135000	11.968364000	15.119297000
C	4.413938000	9.977012000	14.807903000
C	4.820040000	9.836863000	16.268608000
H	4.011871000	10.288887000	16.862522000
C	4.990676000	8.391306000	16.738630000
H	5.171550000	8.363782000	17.817294000
H	5.849207000	7.910646000	16.256161000
H	4.105312000	7.781643000	16.531117000
C	6.097876000	10.640418000	16.558929000
H	6.000082000	11.684398000	16.248802000
H	6.948423000	10.211616000	16.017970000
H	6.334149000	10.618753000	17.628884000
C	4.622290000	8.970282000	13.862866000
H	5.075231000	8.031196000	14.168668000

SUPPORTING INFORMATION

C	4.264966000	9.151196000	12.519237000
C	4.528123000	8.067631000	11.484889000
H	4.071576000	8.407231000	10.545637000
C	6.032506000	7.895290000	11.229928000
H	6.211669000	7.148660000	10.448166000
H	6.549751000	7.560657000	12.136089000
H	6.491896000	8.836667000	10.913216000
C	3.880591000	6.725798000	11.851098000
H	4.039718000	5.993553000	11.051791000
H	2.802065000	6.824481000	12.008028000
H	4.315491000	6.307158000	12.765753000
C	3.698587000	10.366896000	12.131332000
H	3.440896000	10.512344000	11.089199000
C	0.897468000	12.181313000	11.109728000
C	1.401952000	11.537606000	9.966623000
H	2.440364000	11.704669000	9.690110000
C	0.603400000	10.739119000	9.149447000
C	1.185472000	10.057863000	7.922533000
H	2.257784000	10.295810000	7.902316000
C	0.568735000	10.599143000	6.625404000
H	0.692807000	11.683566000	6.550646000
H	-0.504184000	10.382654000	6.577520000
H	1.039915000	10.138977000	5.749604000
C	1.052039000	8.530867000	7.998841000
H	1.512027000	8.135528000	8.909704000
H	1.534990000	8.056022000	7.137565000
H	0.000332000	8.223545000	7.998228000
C	-0.751518000	10.609976000	9.475436000
H	-1.401314000	10.006809000	8.843546000
C	-1.305719000	11.262276000	10.577442000
C	-2.801101000	11.159685000	10.835144000
H	-3.213235000	10.516328000	10.045837000
C	-3.483867000	12.527547000	10.712341000
H	-4.568327000	12.434877000	10.839366000
H	-3.288683000	12.973478000	9.732769000
H	-3.112994000	13.223715000	11.471792000
C	-3.135750000	10.497491000	12.176299000
H	-2.692125000	9.499038000	12.244000000
H	-4.219835000	10.392647000	12.294953000

SUPPORTING INFORMATION

H	-2.769388000	11.089240000	13.021474000
C	-0.466496000	12.037185000	11.393263000
H	-0.883189000	12.565410000	12.247166000
C	0.812390000	15.252191000	10.876627000
C	1.257380000	15.622432000	9.602564000
H	2.265082000	15.343356000	9.306660000
C	0.439987000	16.332571000	8.717945000
C	0.915428000	16.684512000	7.317860000
H	0.139569000	17.317318000	6.865075000
C	1.048240000	15.426404000	6.447152000
H	0.105736000	14.871455000	6.407625000
H	1.814561000	14.752991000	6.846647000
H	1.334242000	15.689636000	5.422466000
C	2.221147000	17.488617000	7.322586000
H	2.119951000	18.405327000	7.910333000
H	2.506286000	17.765473000	6.301445000
H	3.046312000	16.910748000	7.751877000
C	-0.844523000	16.686861000	9.139041000
H	-1.480054000	17.248150000	8.456572000
C	-1.329131000	16.330045000	10.402390000
C	-2.717274000	16.746969000	10.863038000
H	-2.943864000	16.159101000	11.762992000
C	-3.810932000	16.449076000	9.830410000
H	-4.799504000	16.679628000	10.242601000
H	-3.802947000	15.397245000	9.531932000
H	-3.687344000	17.054980000	8.926188000
C	-2.745101000	18.230121000	11.261817000
H	-2.009003000	18.445989000	12.042245000
H	-3.734076000	18.516555000	11.637732000
H	-2.514607000	18.869158000	10.402016000
C	-0.490400000	15.605317000	11.255985000
H	-0.862507000	15.305826000	12.234334000
C	3.380234000	16.447696000	12.208632000
C	2.528084000	17.565885000	12.268680000
H	1.479276000	17.409038000	12.503670000
C	2.986535000	18.854954000	11.975362000
C	2.073151000	20.071170000	11.961796000
H	2.726387000	20.952216000	12.029171000
C	1.106375000	20.136882000	13.145955000

SUPPORTING INFORMATION

H	1.638809000	20.050828000	14.098876000
H	0.358259000	19.338567000	13.096587000
H	0.563164000	21.088057000	13.145361000
C	1.310968000	20.166645000	10.631472000
H	2.005333000	20.215120000	9.787126000
H	0.680228000	21.062920000	10.605302000
H	0.669328000	19.291510000	10.485293000
C	4.326464000	19.019993000	11.612607000
H	4.690584000	20.018526000	11.373207000
C	5.201164000	17.936096000	11.521720000
C	6.634443000	18.144943000	11.060472000
H	6.734072000	19.208409000	10.802852000
C	6.950018000	17.336793000	9.794622000
H	7.961182000	17.559717000	9.435960000
H	6.244151000	17.568373000	8.990900000
H	6.896469000	16.259834000	9.986249000
C	7.645748000	17.843931000	12.173502000
H	7.470967000	18.482329000	13.045022000
H	8.670548000	18.019647000	11.826466000
H	7.574391000	16.802631000	12.504802000
C	4.716056000	16.663152000	11.829767000
H	5.376502000	15.806564000	11.744686000
N	0.898697000	16.199456000	16.063319000
N	0.376462000	18.219698000	17.566169000
Sm	1.316339000	13.928768000	14.605219000
H	-3.090922000	13.561543000	14.636409000
O	-1.980075000	12.253728000	15.691446000
C	-2.069119000	13.237290000	14.913817000
O	-1.116331000	13.889752000	14.410734000

TS2

C	0.189093000	-0.263140000	3.074375000
H	-0.248934000	-1.050912000	2.450828000
H	-0.090651000	0.703915000	2.643199000
C	-0.276113000	-0.394997000	4.550626000
H	-0.803115000	0.509865000	4.881150000
H	-0.967112000	-1.234407000	4.660433000
C	2.051295000	-1.704961000	3.539871000

SUPPORTING INFORMATION

H	3.136849000	-1.802180000	3.455358000
H	1.610414000	-2.475280000	2.899919000
C	1.568865000	-1.831594000	5.012483000
H	0.878209000	-2.673454000	5.128339000
H	2.412899000	-2.000247000	5.691618000
C	2.270681000	0.678167000	3.833613000
H	1.969070000	1.643481000	3.412252000
H	3.358523000	0.601370000	3.748023000
C	1.791230000	0.522714000	5.306382000
H	2.639121000	0.360588000	5.983674000
H	1.270294000	1.423897000	5.649461000
C	4.616090000	1.408338000	-0.272304000
C	4.177537000	0.760117000	-1.471656000
C	4.424349000	-0.643746000	-1.323859000
C	5.009090000	-0.854521000	-0.039478000
C	5.139105000	0.413623000	0.611532000
C	4.719159000	2.877595000	-0.079974000
C	5.494954000	3.633313000	-0.973660000
H	5.978404000	3.114837000	-1.794657000
C	5.647097000	5.013687000	-0.826181000
C	6.516291000	5.844543000	-1.755858000
H	5.999625000	6.806154000	-1.891523000
C	6.715457000	5.230766000	-3.141134000
H	7.231082000	5.940917000	-3.795796000
H	7.330015000	4.324694000	-3.096798000
H	5.764340000	4.964884000	-3.606137000
C	7.873523000	6.145048000	-1.103530000
H	8.476650000	6.798760000	-1.741643000
H	7.752727000	6.634745000	-0.134914000
H	8.435722000	5.219043000	-0.941409000
C	4.991697000	5.643926000	0.238930000
H	5.092899000	6.723367000	0.350927000
C	4.211321000	4.926107000	1.150339000
C	3.486858000	5.628860000	2.286896000

SUPPORTING INFORMATION

H	2.925250000	4.857962000	2.831805000
C	2.472719000	6.657290000	1.768916000
H	1.918583000	7.112260000	2.599056000
H	2.969450000	7.466822000	1.222320000
H	1.750592000	6.192896000	1.090956000
C	4.461265000	6.278037000	3.277161000
H	3.919666000	6.734361000	4.113966000
H	5.159986000	5.541014000	3.680882000
H	5.049503000	7.066420000	2.794270000
C	4.094144000	3.542509000	0.980684000
H	3.487995000	2.973785000	1.682040000
C	3.696439000	1.469603000	-2.678861000
C	2.828407000	2.569666000	-2.582370000
H	2.459045000	2.868454000	-1.603511000
C	2.465030000	3.328468000	-3.701675000
C	1.610254000	4.574411000	-3.507562000
H	1.032568000	4.423158000	-2.584676000
C	0.608767000	4.828228000	-4.636003000
H	-0.039790000	5.675834000	-4.385948000
H	1.107812000	5.075598000	-5.578581000
H	-0.023777000	3.953361000	-4.809502000
C	2.499880000	5.810874000	-3.286570000
H	3.172850000	5.664277000	-2.445018000
H	3.110968000	6.008128000	-4.173908000
H	1.889319000	6.706311000	-3.089350000
C	2.966976000	2.956977000	-4.954312000
H	2.709081000	3.543369000	-5.833707000
C	3.812182000	1.848588000	-5.097422000
C	4.399561000	1.471498000	-6.450383000
H	4.872481000	0.486638000	-6.331534000
C	5.498838000	2.461865000	-6.867180000
H	5.962262000	2.153430000	-7.812289000
H	5.085806000	3.470619000	-7.003797000
H	6.283252000	2.526562000	-6.111242000

SUPPORTING INFORMATION

C	3.338344000	1.340242000	-7.548354000
H	3.795859000	0.995362000	-8.484920000
H	2.556270000	0.622781000	-7.267836000
H	2.852494000	2.301421000	-7.755459000
C	4.166737000	1.121809000	-3.958405000
H	4.848282000	0.282831000	-4.057900000
C	4.319798000	-1.688938000	-2.373844000
C	5.477456000	-2.391644000	-2.743609000
H	6.412499000	-2.153607000	-2.245314000
C	5.462889000	-3.374393000	-3.734146000
C	6.745509000	-4.087084000	-4.125841000
H	7.542300000	-3.681473000	-3.488581000
C	6.670939000	-5.595319000	-3.861299000
H	6.450615000	-5.800450000	-2.808511000
H	5.888770000	-6.067851000	-4.466849000
H	7.620090000	-6.078833000	-4.111651000
C	7.129325000	-3.799303000	-5.583927000
H	7.214248000	-2.726215000	-5.763283000
H	8.092996000	-4.264653000	-5.831496000
H	6.378082000	-4.194284000	-6.279835000
C	4.250263000	-3.665302000	-4.364548000
H	4.221211000	-4.432186000	-5.135835000
C	3.074350000	-2.986468000	-4.030978000
C	1.768932000	-3.318961000	-4.732088000
H	1.000988000	-2.660815000	-4.309598000
C	1.845559000	-3.036486000	-6.240483000
H	0.878134000	-3.213097000	-6.724699000
H	2.143504000	-2.003542000	-6.439537000
H	2.575882000	-3.688355000	-6.725330000
C	1.328431000	-4.764925000	-4.464721000
H	1.232162000	-4.960762000	-3.395731000
H	0.363692000	-4.968340000	-4.935112000
H	2.051283000	-5.482177000	-4.870815000
C	3.127361000	-1.999052000	-3.041475000

SUPPORTING INFORMATION

H	2.218737000	-1.450160000	-2.794551000
C	5.606967000	-2.136004000	0.418840000
C	6.988235000	-2.208903000	0.645508000
H	7.582249000	-1.308707000	0.510628000
C	7.608077000	-3.404474000	1.025646000
C	9.113689000	-3.476813000	1.231101000
H	9.352948000	-4.518138000	1.490700000
C	9.881025000	-3.140021000	-0.054138000
H	9.577014000	-3.792712000	-0.879385000
H	9.700460000	-2.103269000	-0.361995000
H	10.960724000	-3.258393000	0.094480000
C	9.575341000	-2.588173000	2.394860000
H	9.086974000	-2.876094000	3.329919000
H	10.661454000	-2.672126000	2.538889000
H	9.341178000	-1.535798000	2.210080000
C	6.813538000	-4.542095000	1.197721000
H	7.290479000	-5.474813000	1.496887000
C	5.429701000	-4.507295000	0.988996000
C	4.575504000	-5.747049000	1.183422000
H	3.532723000	-5.445299000	1.013123000
C	4.911906000	-6.837069000	0.160281000
H	4.259652000	-7.707949000	0.290269000
H	4.791631000	-6.466998000	-0.865768000
H	5.944273000	-7.177483000	0.274906000
C	4.672556000	-6.288780000	2.615439000
H	4.404173000	-5.524300000	3.348442000
H	4.001915000	-7.141930000	2.752435000
H	5.689515000	-6.626968000	2.846749000
C	4.845711000	-3.301286000	0.592388000
H	3.776078000	-3.271407000	0.404113000
C	5.928314000	0.647842000	1.845799000
C	5.852788000	-0.225433000	2.948934000
H	5.157703000	-1.056955000	2.900072000
C	6.693538000	-0.089841000	4.054884000

SUPPORTING INFORMATION

C	6.658833000	-1.026086000	5.254694000
H	7.708077000	-1.191470000	5.538691000
C	5.969716000	-0.357662000	6.453671000
H	6.433330000	0.602233000	6.698555000
H	4.913020000	-0.167168000	6.232812000
H	6.016164000	-0.998360000	7.341397000
C	6.046580000	-2.399924000	4.973954000
H	6.491797000	-2.874508000	4.095131000
H	6.192800000	-3.063100000	5.833827000
H	4.968757000	-2.334362000	4.804728000
C	7.625725000	0.955286000	4.055124000
H	8.303766000	1.059678000	4.902191000
C	7.732218000	1.845513000	2.987065000
C	8.785604000	2.942722000	3.006980000
H	9.376971000	2.797755000	3.922962000
C	9.754089000	2.839535000	1.818542000
H	10.543011000	3.598948000	1.898959000
H	10.235114000	1.857517000	1.778908000
H	9.233644000	2.994120000	0.867009000
C	8.152689000	4.336502000	3.083893000
H	7.525391000	4.431433000	3.975331000
H	8.925160000	5.112087000	3.127405000
H	7.523412000	4.535698000	2.208829000
C	6.875976000	1.681272000	1.892280000
H	6.967917000	2.345345000	1.038742000
N	1.664767000	-0.384016000	2.994490000
N	0.876035000	-0.612138000	5.430805000
Sm	2.198623000	-0.009415000	0.365680000
H	-0.015957000	-0.777346000	-0.426416000
C	-0.521277000	0.263940000	-3.578782000
H	-0.027560000	1.093136000	-3.059648000
H	-0.135921000	-0.667522000	-3.150448000
C	-0.292782000	0.337721000	-5.114578000
H	0.196268000	-0.566835000	-5.485683000

SUPPORTING INFORMATION

H	0.352596000	1.183580000	-5.370913000
C	-2.497227000	1.616550000	-3.807548000
H	-3.570488000	1.657043000	-3.586949000
H	-2.008341000	2.429491000	-3.258403000
C	-2.232253000	1.704470000	-5.338765000
H	-1.592447000	2.557888000	-5.586304000
H	-3.170128000	1.828803000	-5.889344000
C	-2.654961000	-0.779084000	-3.985777000
H	-2.244648000	-1.717375000	-3.595554000
H	-3.722316000	-0.738444000	-3.732386000
C	-2.421987000	-0.661493000	-5.519280000
H	-3.372463000	-0.536718000	-6.051072000
H	-1.938438000	-1.561548000	-5.917046000
C	-4.649032000	-1.320913000	0.145986000
C	-4.067968000	-0.912116000	1.393363000
C	-4.242279000	0.505677000	1.506116000
C	-4.909163000	0.962330000	0.333460000
C	-5.185620000	-0.165251000	-0.506761000
C	-4.843944000	-2.737970000	-0.257487000
C	-5.569830000	-3.589999000	0.589340000
H	-5.963514000	-3.178529000	1.513334000
C	-5.779898000	-4.934441000	0.273022000
C	-6.602995000	-5.861687000	1.154350000
H	-6.151604000	-6.861005000	1.064748000
C	-6.593903000	-5.484650000	2.635619000
H	-7.080643000	-6.266774000	3.224048000
H	-7.145171000	-4.553134000	2.819826000
H	-5.576845000	-5.353546000	3.013562000
C	-8.043500000	-5.963779000	0.633930000
H	-8.619330000	-6.684298000	1.222983000
H	-8.071243000	-6.279215000	-0.412178000
H	-8.546258000	-4.993668000	0.702190000
C	-5.234507000	-5.430625000	-0.917332000
H	-5.377574000	-6.483371000	-1.159061000

SUPPORTING INFORMATION

C	-4.510152000	-4.613944000	-1.791568000
C	-3.888813000	-5.175446000	-3.059826000
H	-3.418839000	-4.334446000	-3.586955000
C	-2.782413000	-6.187949000	-2.733577000
H	-2.310294000	-6.550558000	-3.652319000
H	-3.188933000	-7.054287000	-2.202189000
H	-2.006512000	-5.742744000	-2.101839000
C	-4.934256000	-5.782270000	-4.004399000
H	-4.465330000	-6.123412000	-4.932405000
H	-5.708356000	-5.054428000	-4.261637000
H	-5.427640000	-6.646717000	-3.547873000
C	-4.336165000	-3.268151000	-1.449960000
H	-3.785720000	-2.624177000	-2.129981000
C	-3.454535000	-1.855280000	2.363692000
C	-2.665278000	-2.932317000	1.916305000
H	-2.466991000	-3.041463000	0.853144000
C	-2.180890000	-3.914965000	2.783652000
C	-1.425212000	-5.114561000	2.234574000
H	-1.185612000	-4.893938000	1.186557000
C	-0.107980000	-5.384637000	2.968619000
H	0.427929000	-6.217024000	2.498949000
H	-0.280616000	-5.655050000	4.015416000
H	0.549034000	-4.508396000	2.955081000
C	-2.316435000	-6.365116000	2.244881000
H	-3.228721000	-6.197056000	1.666094000
H	-2.604316000	-6.631152000	3.267620000
H	-1.790012000	-7.221546000	1.811168000
C	-2.472646000	-3.806525000	4.147102000
H	-2.119787000	-4.573692000	4.832025000
C	-3.226211000	-2.736826000	4.641573000
C	-3.592560000	-2.640538000	6.114748000
H	-4.002208000	-1.634294000	6.273775000
C	-4.698387000	-3.645682000	6.465904000
H	-5.009531000	-3.532269000	7.509272000

SUPPORTING INFORMATION

H	-4.345828000	-4.675427000	6.327500000
H	-5.579715000	-3.506761000	5.832300000
C	-2.388588000	-2.803087000	7.054130000
H	-2.699679000	-2.662370000	8.094703000
H	-1.598888000	-2.079342000	6.839568000
H	-1.952544000	-3.806970000	6.980515000
C	-3.703016000	-1.776578000	3.743935000
H	-4.306120000	-0.961586000	4.127284000
C	-4.088568000	1.372813000	2.710892000
C	-5.083789000	1.304987000	3.701460000
H	-5.896209000	0.591948000	3.575613000
C	-5.076679000	2.139730000	4.817764000
C	-6.172017000	2.042327000	5.866626000
H	-6.845941000	1.233625000	5.551531000
C	-7.001011000	3.330600000	5.940309000
H	-7.422405000	3.587614000	4.962029000
H	-6.390120000	4.176360000	6.273009000
H	-7.827430000	3.217877000	6.651174000
C	-5.614227000	1.668483000	7.248245000
H	-5.055518000	0.728999000	7.211545000
H	-6.425812000	1.555264000	7.976406000
H	-4.935628000	2.441481000	7.626395000
C	-4.051007000	3.086329000	4.926470000
H	-4.031256000	3.762489000	5.779471000
C	-3.061313000	3.209182000	3.952164000
C	-2.016299000	4.307300000	4.072397000
H	-2.227280000	4.843838000	5.007807000
C	-2.131444000	5.319918000	2.926726000
H	-1.413788000	6.137980000	3.057171000
H	-3.138159000	5.745924000	2.880492000
H	-1.930681000	4.847091000	1.959094000
C	-0.588519000	3.757347000	4.176448000
H	-0.493366000	3.069772000	5.020520000
H	0.129964000	4.571630000	4.322349000

SUPPORTING INFORMATION

H	-0.299676000	3.222785000	3.264504000
C	-3.086744000	2.337205000	2.851988000
H	-2.339687000	2.436312000	2.068996000
C	-5.489551000	2.324622000	0.185416000
C	-6.873649000	2.488203000	0.346112000
H	-7.471093000	1.607519000	0.561311000
C	-7.480545000	3.741099000	0.228315000
C	-8.970517000	3.953920000	0.453212000
H	-9.279782000	4.764221000	-0.221150000
C	-9.232042000	4.431885000	1.889121000
H	-8.661810000	5.335935000	2.120938000
H	-8.937565000	3.657973000	2.603695000
H	-10.296896000	4.650594000	2.042687000
C	-9.832249000	2.732267000	0.128801000
H	-9.622224000	2.343163000	-0.871623000
H	-10.893706000	2.994216000	0.180297000
H	-9.666252000	1.918803000	0.845054000
C	-6.672455000	4.845988000	-0.068149000
H	-7.144828000	5.821931000	-0.176945000
C	-5.288983000	4.725714000	-0.221603000
C	-4.422700000	5.922349000	-0.578509000
H	-3.383725000	5.639134000	-0.358667000
C	-4.744585000	7.172101000	0.247702000
H	-4.022247000	7.966861000	0.035260000
H	-4.714263000	6.962279000	1.320911000
H	-5.739573000	7.567193000	0.012081000
C	-4.508090000	6.232960000	-2.081068000
H	-4.226215000	5.364492000	-2.682849000
H	-3.844106000	7.061991000	-2.348541000
H	-5.529790000	6.514618000	-2.363093000
C	-4.709952000	3.456231000	-0.084607000
H	-3.631836000	3.349651000	-0.192731000
C	-6.109759000	-0.141921000	-1.669946000
C	-6.177533000	0.956247000	-2.551107000
H	-5.501979000	1.791547000	-2.392291000
C	-7.137317000	1.029329000	-3.567651000
C	-7.283744000	2.247891000	-4.466897000

SUPPORTING INFORMATION

H	-7.973206000	1.959214000	-5.271042000
C	-5.974901000	2.680569000	-5.131603000
H	-5.519442000	1.852713000	-5.682118000
H	-5.252540000	3.044043000	-4.390619000
H	-6.152575000	3.500963000	-5.837099000
C	-7.926096000	3.421942000	-3.712821000
H	-8.902118000	3.140709000	-3.307018000
H	-8.070762000	4.280320000	-4.378219000
H	-7.298441000	3.742907000	-2.877193000
C	-8.035254000	-0.030825000	-3.712918000
H	-8.791530000	0.017083000	-4.496105000
C	-8.004871000	-1.137428000	-2.861307000
C	-9.029526000	-2.247451000	-3.019169000
H	-9.701042000	-1.945587000	-3.831701000
C	-9.887649000	-2.412905000	-1.760299000
H	-10.663392000	-3.168648000	-1.916384000
H	-10.378820000	-1.472933000	-1.488445000
H	-9.278674000	-2.731062000	-0.907761000
C	-8.377572000	-3.576263000	-3.425822000
H	-7.817506000	-3.466325000	-4.359985000
H	-9.134876000	-4.355345000	-3.574117000
H	-7.682978000	-3.927663000	-2.660199000
C	-7.040852000	-1.178630000	-1.851535000
H	-7.027314000	-2.017629000	-1.164209000
N	-1.974083000	0.333661000	-3.281304000
N	-1.570539000	0.489330000	-5.816255000
Sm	-2.272475000	0.102412000	-0.572806000
H	0.058780000	3.792262000	0.063085000
O	0.900326000	2.033600000	0.557267000
C	-0.079474000	2.696945000	0.137902000
O	-1.210164000	2.250988000	-0.199095000
O	1.398985000	-2.605718000	0.143589000
C	0.404628000	-2.642595000	-0.513595000
O	-0.467191000	-3.059715000	-1.184646000

Int3

C	0.683114000	-0.307440000	3.297547000
H	0.253699000	-1.112297000	2.692384000
H	0.340445000	0.639864000	2.870566000

SUPPORTING INFORMATION

C	0.293826000	-0.448374000	4.796028000
H	-0.266083000	0.427053000	5.139693000
H	-0.343018000	-1.324166000	4.955112000
C	2.632224000	-1.652496000	3.697457000
H	3.717317000	-1.693216000	3.567846000
H	2.194301000	-2.453222000	3.091339000
C	2.233456000	-1.771878000	5.196704000
H	1.603260000	-2.650118000	5.371369000
H	3.119569000	-1.875471000	5.832752000
C	2.754227000	0.738143000	3.947090000
H	2.402767000	1.685294000	3.521738000
H	3.842060000	0.695268000	3.822312000
C	2.338305000	0.596563000	5.440030000
H	3.217798000	0.498684000	6.086016000
H	1.779177000	1.475069000	5.780083000
C	5.059234000	1.366580000	-0.244475000
C	4.533681000	0.844568000	-1.469408000
C	4.733520000	-0.572333000	-1.459001000
C	5.372816000	-0.918599000	-0.234261000
C	5.589115000	0.278745000	0.519580000
C	5.176230000	2.809720000	0.084503000
C	5.886190000	3.660993000	-0.777467000
H	6.327188000	3.232202000	-1.671375000
C	6.023676000	5.024981000	-0.510596000
C	6.828456000	5.958011000	-1.404616000
H	6.282185000	6.911972000	-1.434054000
C	6.978558000	5.470094000	-2.846858000
H	7.447701000	6.246656000	-3.460008000
H	7.617415000	4.581882000	-2.906700000
H	6.012047000	5.218726000	-3.293373000
C	8.206957000	6.241313000	-0.785753000
H	8.766954000	6.961576000	-1.392867000
H	8.116538000	6.647122000	0.226529000
H	8.797756000	5.320573000	-0.723620000
C	5.418956000	5.541570000	0.642694000
H	5.506017000	6.607980000	0.845796000
C	4.707302000	4.727136000	1.528105000
C	4.027936000	5.306692000	2.757873000
H	3.565989000	4.466036000	3.293737000

SUPPORTING INFORMATION

C	2.905669000	6.281084000	2.373079000
H	2.385608000	6.648755000	3.264834000
H	3.304396000	7.150600000	1.839056000
H	2.169484000	5.800798000	1.721105000
C	5.024618000	5.970200000	3.716646000
H	4.515366000	6.326867000	4.618940000
H	5.807988000	5.269865000	4.019770000
H	5.511533000	6.833355000	3.249682000
C	4.606575000	3.363283000	1.237733000
H	4.063316000	2.718267000	1.925365000
C	3.987194000	1.659966000	-2.578372000
C	3.118400000	2.736079000	-2.336678000
H	2.801345000	2.942220000	-1.317312000
C	2.670962000	3.572437000	-3.364861000
C	1.809468000	4.779071000	-3.022452000
H	1.311216000	4.552016000	-2.069713000
C	0.717351000	5.076395000	-4.053264000
H	0.065758000	5.882773000	-3.699945000
H	1.139077000	5.399322000	-5.011199000
H	0.095817000	4.195811000	-4.242971000
C	2.686237000	6.019903000	-2.792038000
H	3.431479000	5.835361000	-2.013099000
H	3.217837000	6.291494000	-3.711217000
H	2.076826000	6.879195000	-2.488748000
C	3.090454000	3.306633000	-4.671782000
H	2.760467000	3.951492000	-5.482743000
C	3.940112000	2.229427000	-4.957268000
C	4.414504000	1.962119000	-6.376613000
H	5.025924000	1.050827000	-6.341644000
C	5.306436000	3.098298000	-6.896550000
H	5.689297000	2.866180000	-7.896749000
H	4.748683000	4.039111000	-6.964405000
H	6.161218000	3.265193000	-6.233958000
C	3.248567000	1.698191000	-7.338398000
H	3.620107000	1.444189000	-8.337401000
H	2.624199000	0.870958000	-6.987606000
H	2.606169000	2.579902000	-7.440365000
C	4.377702000	1.421283000	-3.907061000
H	5.055840000	0.599539000	-4.118082000

SUPPORTING INFORMATION

C	4.537559000	-1.523600000	-2.584039000
C	5.664886000	-2.162609000	-3.122875000
H	6.641456000	-1.937978000	-2.702327000
C	5.566044000	-3.073685000	-4.175483000
C	6.811521000	-3.741508000	-4.733734000
H	7.668174000	-3.325669000	-4.187098000
C	6.800723000	-5.256446000	-4.487864000
H	6.700253000	-5.481029000	-3.421885000
H	5.966917000	-5.737274000	-5.011837000
H	7.727982000	-5.715543000	-4.849082000
C	7.015774000	-3.424715000	-6.221220000
H	7.056594000	-2.344885000	-6.394962000
H	7.950414000	-3.864535000	-6.586677000
H	6.199986000	-3.829484000	-6.830445000
C	4.298013000	-3.354472000	-4.693429000
H	4.202242000	-4.071242000	-5.506451000
C	3.150325000	-2.737420000	-4.187678000
C	1.777487000	-3.085121000	-4.738806000
H	1.057475000	-2.413376000	-4.251236000
C	1.676920000	-2.854018000	-6.251981000
H	0.658358000	-3.046016000	-6.608057000
H	1.945829000	-1.827430000	-6.518573000
H	2.345927000	-3.524006000	-6.802670000
C	1.379149000	-4.523622000	-4.378556000
H	1.411278000	-4.683900000	-3.296671000
H	0.365814000	-4.749183000	-4.729761000
H	2.060567000	-5.246054000	-4.841070000
C	3.287268000	-1.819191000	-3.141390000
H	2.396602000	-1.338994000	-2.741944000
C	5.864274000	-2.281215000	0.088621000
C	7.233754000	-2.516184000	0.265873000
H	7.917253000	-1.674522000	0.192899000
C	7.730295000	-3.801538000	0.508627000
C	9.224229000	-4.052563000	0.638369000
H	9.353831000	-5.127977000	0.822374000
C	9.963473000	-3.717560000	-0.665014000
H	9.545951000	-4.272548000	-1.510860000
H	9.890452000	-2.649446000	-0.897186000
H	11.027184000	-3.967948000	-0.583627000

SUPPORTING INFORMATION

C	9.841104000	-3.302291000	1.825871000
H	9.368343000	-3.594486000	2.768414000
H	10.912892000	-3.517171000	1.903927000
H	9.723737000	-2.218931000	1.718913000
C	6.822974000	-4.861451000	0.594163000
H	7.204881000	-5.863315000	0.784242000
C	5.446118000	-4.665554000	0.430217000
C	4.469523000	-5.826334000	0.517123000
H	3.463222000	-5.407504000	0.382078000
C	4.697205000	-6.846984000	-0.606419000
H	3.951394000	-7.648610000	-0.560090000
H	4.628423000	-6.372340000	-1.589666000
H	5.687123000	-7.309732000	-0.525710000
C	4.506343000	-6.506283000	1.892554000
H	4.309778000	-5.789248000	2.695807000
H	3.754971000	-7.301703000	1.952916000
H	5.484410000	-6.960550000	2.085651000
C	4.985887000	-3.372648000	0.172483000
H	3.920187000	-3.213360000	0.014045000
C	6.419756000	0.373204000	1.743967000
C	6.355907000	-0.600701000	2.760915000
H	5.653202000	-1.420024000	2.650184000
C	7.217820000	-0.576320000	3.858713000
C	7.186768000	-1.615443000	4.971540000
H	8.236401000	-1.820798000	5.226777000
C	6.522080000	-1.044837000	6.234123000
H	7.007550000	-0.119902000	6.559897000
H	5.467650000	-0.814823000	6.042716000
H	6.565673000	-1.763031000	7.060702000
C	6.548151000	-2.949433000	4.581944000
H	6.965979000	-3.348892000	3.653448000
H	6.704607000	-3.688240000	5.375071000
H	5.465238000	-2.855762000	4.443668000
C	8.162292000	0.454557000	3.939091000
H	8.854833000	0.474852000	4.780125000
C	8.258312000	1.440057000	2.957151000
C	9.321338000	2.521615000	3.058316000
H	9.929384000	2.288634000	3.943311000
C	10.259881000	2.521861000	1.844527000

SUPPORTING INFORMATION

H	11.060548000	3.258421000	1.975091000
H	10.720328000	1.539581000	1.699412000
H	9.722108000	2.777524000	0.925366000
C	8.699828000	3.907355000	3.276298000
H	8.086108000	3.922829000	4.182682000
H	9.478479000	4.671536000	3.380583000
H	8.059495000	4.190843000	2.434487000
C	7.379249000	1.388542000	1.870067000
H	7.459104000	2.129347000	1.081396000
N	2.158685000	-0.360830000	3.150915000
N	1.494283000	-0.584312000	5.624480000
Sm	2.691559000	-0.060371000	0.477051000
H	0.000205000	-3.448988000	-0.455933000
C	-0.658660000	0.371127000	-3.270807000
H	-0.171011000	1.109800000	-2.626871000
H	-0.348773000	-0.619955000	-2.925517000
C	-0.315119000	0.604633000	-4.768852000
H	0.203285000	-0.260959000	-5.193933000
H	0.345908000	1.468666000	-4.891421000
C	-2.557937000	1.822419000	-3.508924000
H	-3.633359000	1.908290000	-3.325188000
H	-2.052194000	2.559895000	-2.876115000
C	-2.217454000	2.017657000	-5.014914000
H	-1.565595000	2.884705000	-5.164820000
H	-3.123871000	2.186294000	-5.605213000
C	-2.794102000	-0.542245000	-3.905860000
H	-2.473941000	-1.528437000	-3.550183000
H	-3.874446000	-0.461872000	-3.741928000
C	-2.416589000	-0.326343000	-5.399836000
H	-3.309956000	-0.161378000	-6.012027000
H	-1.898594000	-1.200928000	-5.808571000
C	-4.946989000	-1.398028000	0.293685000
C	-4.456231000	-0.840039000	1.519198000
C	-4.704073000	0.569694000	1.481579000
C	-5.340349000	0.873101000	0.245753000
C	-5.511461000	-0.342444000	-0.491689000
C	-4.997321000	-2.849610000	-0.016598000
C	-5.678524000	-3.718148000	0.851837000
H	-6.147664000	-3.294322000	1.733793000

SUPPORTING INFORMATION

C	-5.752660000	-5.091007000	0.606562000
C	-6.527495000	-6.044454000	1.505843000
H	-5.943751000	-6.975350000	1.552033000
C	-6.710484000	-5.545609000	2.940669000
H	-7.156972000	-6.331988000	3.558213000
H	-7.382377000	-4.681174000	2.983718000
H	-5.758922000	-5.253707000	3.394582000
C	-7.887878000	-6.390791000	0.879278000
H	-8.422341000	-7.128023000	1.489039000
H	-7.772481000	-6.801585000	-0.128388000
H	-8.515649000	-5.495892000	0.804164000
C	-5.111355000	-5.598862000	-0.530691000
H	-5.149215000	-6.671167000	-0.717154000
C	-4.424979000	-4.768229000	-1.420948000
C	-3.705485000	-5.338133000	-2.632367000
H	-3.253586000	-4.489519000	-3.164269000
C	-2.567380000	-6.281963000	-2.219807000
H	-2.017151000	-6.636542000	-3.098425000
H	-2.954511000	-7.161355000	-1.693499000
H	-1.859425000	-5.781119000	-1.552261000
C	-4.666595000	-6.032070000	-3.606019000
H	-4.130075000	-6.388434000	-4.492522000
H	-5.456978000	-5.351473000	-3.934821000
H	-5.146680000	-6.899278000	-3.139452000
C	-4.389656000	-3.396240000	-1.153771000
H	-3.865332000	-2.740305000	-1.845781000
C	-3.843729000	-1.619662000	2.620808000
C	-2.958215000	-2.679716000	2.357379000
H	-2.677466000	-2.895096000	1.329816000
C	-2.454023000	-3.496163000	3.373707000
C	-1.581895000	-4.690710000	3.018465000
H	-1.254138000	-4.547562000	1.980073000
C	-0.324510000	-4.807887000	3.885466000
H	0.306137000	-5.634574000	3.540719000
H	-0.571177000	-5.003085000	4.934755000
H	0.269821000	-3.889901000	3.846848000
C	-2.395930000	-5.992418000	3.063570000
H	-3.255439000	-5.937479000	2.389657000
H	-2.770057000	-6.182961000	4.075870000

SUPPORTING INFORMATION

H	-1.780521000	-6.849180000	2.765654000
C	-2.826672000	-3.227279000	4.694943000
H	-2.457166000	-3.863533000	5.496239000
C	-3.683351000	-2.163389000	5.003263000
C	-4.116144000	-1.894549000	6.435833000
H	-4.740637000	-0.991668000	6.414631000
C	-4.978413000	-3.039705000	6.985737000
H	-5.337044000	-2.807134000	7.994791000
H	-4.406411000	-3.972608000	7.043479000
H	-5.848495000	-3.221848000	6.347489000
C	-2.927650000	-1.610312000	7.363099000
H	-3.275023000	-1.365466000	8.373041000
H	-2.329554000	-0.770543000	6.997291000
H	-2.266808000	-2.480367000	7.444999000
C	-4.179323000	-1.374589000	3.962991000
H	-4.864841000	-0.566733000	4.197783000
C	-4.613572000	1.557071000	2.597243000
C	-5.759696000	1.758798000	3.385085000
H	-6.645611000	1.164138000	3.172895000
C	-5.795673000	2.702777000	4.410100000
C	-7.052674000	2.898939000	5.240031000
H	-7.800572000	2.190077000	4.859990000
C	-7.628989000	4.311663000	5.072716000
H	-7.825488000	4.535903000	4.020094000
H	-6.934808000	5.070260000	5.451166000
H	-8.568068000	4.415602000	5.627613000
C	-6.817049000	2.572764000	6.721017000
H	-6.442149000	1.552440000	6.848370000
H	-7.747384000	2.668010000	7.292028000
H	-6.083832000	3.254632000	7.165980000
C	-4.647837000	3.471957000	4.638448000
H	-4.653247000	4.225479000	5.424478000
C	-3.494813000	3.313238000	3.870569000
C	-2.288860000	4.204123000	4.119962000
H	-2.554931000	4.878927000	4.944792000
C	-1.964600000	5.074406000	2.898461000
H	-1.116880000	5.737280000	3.105513000
H	-2.821717000	5.693951000	2.618689000
H	-1.706007000	4.456450000	2.031995000

SUPPORTING INFORMATION

C	-1.060425000	3.401907000	4.565792000
H	-1.280060000	2.810457000	5.460209000
H	-0.221204000	4.068997000	4.793535000
H	-0.735797000	2.714542000	3.776976000
C	-3.488572000	2.344259000	2.855328000
H	-2.603398000	2.226821000	2.234398000
C	-5.933063000	2.196564000	-0.071661000
C	-7.327948000	2.333102000	-0.137056000
H	-7.937972000	1.449919000	0.022149000
C	-7.929391000	3.564818000	-0.400607000
C	-9.439877000	3.754531000	-0.416241000
H	-9.662826000	4.438940000	-1.247689000
C	-9.907740000	4.440268000	0.878074000
H	-9.389625000	5.390519000	1.039747000
H	-9.707220000	3.800005000	1.744330000
H	-10.984803000	4.640731000	0.847288000
C	-10.233822000	2.468586000	-0.652879000
H	-9.888145000	1.935166000	-1.543024000
H	-11.296108000	2.700231000	-0.783152000
H	-10.154712000	1.784469000	0.199467000
C	-7.102577000	4.674616000	-0.617968000
H	-7.565460000	5.635696000	-0.838591000
C	-5.710357000	4.580939000	-0.550677000
C	-4.828382000	5.796058000	-0.785305000
H	-3.791339000	5.474591000	-0.619101000
C	-5.125426000	6.924227000	0.211385000
H	-4.424024000	7.755377000	0.077262000
H	-5.045632000	6.570377000	1.243555000
H	-6.137147000	7.321653000	0.073849000
C	-4.931469000	6.300775000	-2.231271000
H	-4.677993000	5.511826000	-2.946453000
H	-4.253400000	7.144967000	-2.399970000
H	-5.948172000	6.639714000	-2.458883000
C	-5.141284000	3.333815000	-0.271063000
H	-4.057890000	3.250509000	-0.198431000
C	-6.364437000	-0.487636000	-1.696988000
C	-6.407143000	0.490316000	-2.710474000
H	-5.763311000	1.360543000	-2.622302000
C	-7.295992000	0.397596000	-3.786732000

SUPPORTING INFORMATION

C	-7.41920000	1.48285000	-4.845742000
H	-7.941692000	1.028476000	-5.698849000
C	-6.076052000	2.001286000	-5.363288000
H	-5.441800000	1.180608000	-5.713384000
H	-5.533483000	2.549649000	-4.585722000
H	-6.227376000	2.692244000	-6.199701000
C	-8.286797000	2.645790000	-4.341551000
H	-9.281423000	2.295443000	-4.049407000
H	-8.410735000	3.407222000	-5.120510000
H	-7.829579000	3.122101000	-3.467679000
C	-8.151841000	-0.706238000	-3.851033000
H	-8.850872000	-0.786922000	-4.682728000
C	-8.147645000	-1.695008000	-2.865750000
C	-9.119354000	-2.860767000	-2.948180000
H	-9.764406000	-2.676649000	-3.818322000
C	-10.027145000	-2.940462000	-1.713762000
H	-10.763468000	-3.744246000	-1.825820000
H	-10.567952000	-2.001640000	-1.558592000
H	-9.448372000	-3.145761000	-0.806899000
C	-8.390846000	-4.189852000	-3.185368000
H	-7.795119000	-4.150937000	-4.103006000
H	-9.105774000	-5.015182000	-3.279651000
H	-7.713829000	-4.422540000	-2.356839000
C	-7.250754000	-1.573166000	-1.801799000
H	-7.254711000	-2.320462000	-1.015865000
N	-2.124082000	0.477945000	-3.065786000
N	-1.536839000	0.834239000	-5.542221000
Sm	-2.605832000	0.064737000	-0.402031000
H	0.144743000	3.475166000	0.289648000
O	1.016449000	1.665739000	0.442637000
C	-0.004625000	2.377304000	0.274326000
O	-1.183101000	1.975001000	0.094236000
O	1.250259000	-1.930755000	-0.033074000
C	0.103545000	-2.353676000	-0.324098000
O	-0.935786000	-1.664572000	-0.483184000

Int4

C	2.473636000	1.457022000	-3.378110000
H	3.480924000	1.433369000	-2.953848000

SUPPORTING INFORMATION

H	1.954943000	2.299076000	-2.912102000
C	2.498441000	1.571142000	-4.925629000
H	2.159921000	2.561262000	-5.251716000
H	3.511367000	1.427368000	-5.316724000
C	2.317107000	-0.952644000	-3.679866000
H	1.780434000	-1.835147000	-3.319785000
H	3.365375000	-1.056506000	-3.389158000
C	2.169565000	-0.769098000	-5.215601000
H	3.137383000	-0.879365000	-5.715999000
H	1.494375000	-1.518998000	-5.642431000
C	0.340959000	0.369255000	-3.414960000
H	-0.127230000	1.164899000	-2.829028000
H	-0.174667000	-0.566863000	-3.183342000
C	0.299189000	0.674729000	-4.939489000
H	-0.376601000	-0.013538000	-5.458636000
H	-0.064729000	1.690197000	-5.126990000
C	3.911323000	-1.141626000	1.454825000
C	4.284740000	0.225695000	1.258781000
C	4.826729000	0.346024000	-0.061367000
C	4.828572000	-0.950595000	-0.671962000
C	4.231951000	-1.861870000	0.260890000
C	3.403427000	-1.753645000	2.706157000
C	4.018660000	-1.464342000	3.933975000
H	4.856793000	-0.776728000	3.945420000
C	3.577937000	-2.047669000	5.124584000
C	4.258997000	-1.797310000	6.463275000
H	3.457069000	-1.676693000	7.206514000
C	5.122034000	-0.535298000	6.505825000
H	5.469375000	-0.350657000	7.527756000
H	6.011897000	-0.639682000	5.875026000
H	4.575449000	0.348923000	6.165501000
C	5.088384000	-3.022658000	6.882188000
H	5.528818000	-2.875571000	7.874912000
H	4.478910000	-3.930910000	6.911441000
H	5.905136000	-3.192408000	6.171668000
C	2.490884000	-2.927260000	5.072630000
H	2.132978000	-3.372044000	6.000161000
C	1.863773000	-3.254754000	3.866684000
C	0.687562000	-4.216913000	3.829848000

SUPPORTING INFORMATION

H	0.415738000	-4.352231000	2.775261000
C	-0.538720000	-3.642266000	4.552033000
H	-1.385879000	-4.333627000	4.487825000
H	-0.328006000	-3.468629000	5.613443000
H	-0.848707000	-2.690907000	4.109597000
C	1.050946000	-5.597171000	4.391564000
H	0.204925000	-6.286772000	4.297428000
H	1.902334000	-6.027930000	3.857644000
H	1.314974000	-5.540973000	5.453550000
C	2.336541000	-2.664461000	2.691663000
H	1.866208000	-2.919525000	1.744281000
C	4.405415000	1.285814000	2.301089000
C	3.321456000	1.798058000	3.023702000
H	2.324560000	1.428345000	2.810831000
C	3.496532000	2.771729000	4.012811000
C	2.297279000	3.313936000	4.774088000
H	1.402177000	2.869168000	4.319294000
C	2.170295000	4.837235000	4.641414000
H	1.261132000	5.194869000	5.137543000
H	3.019994000	5.352038000	5.103230000
H	2.129475000	5.140113000	3.590705000
C	2.322794000	2.893026000	6.249964000
H	2.356766000	1.803917000	6.349641000
H	3.200820000	3.302674000	6.761762000
H	1.431862000	3.255675000	6.775150000
C	4.788863000	3.227337000	4.287610000
H	4.935868000	3.980888000	5.058660000
C	5.898015000	2.734450000	3.592249000
C	7.301587000	3.235437000	3.891133000
H	7.987800000	2.658387000	3.257332000
C	7.706353000	2.990508000	5.350715000
H	8.744039000	3.298540000	5.520780000
H	7.076165000	3.561278000	6.041777000
H	7.616668000	1.932721000	5.615639000
C	7.463908000	4.714646000	3.515348000
H	8.492307000	5.049915000	3.691617000
H	7.225190000	4.880398000	2.460659000
H	6.800818000	5.349765000	4.113521000
C	5.688029000	1.770370000	2.604681000

SUPPORTING INFORMATION

H	6.541263000	1.378544000	2.058012000
C	5.499010000	1.575112000	-0.556316000
C	6.868432000	1.558601000	-0.850476000
H	7.414246000	0.622367000	-0.762089000
C	7.553064000	2.715168000	-1.239346000
C	9.054629000	2.638520000	-1.476031000
H	9.250435000	1.657271000	-1.930474000
C	9.595440000	3.704673000	-2.431760000
H	9.043684000	3.721814000	-3.376972000
H	9.542903000	4.707074000	-1.992079000
H	10.648551000	3.508930000	-2.658333000
C	9.813028000	2.681647000	-0.139520000
H	9.481752000	1.883778000	0.532083000
H	10.891316000	2.566403000	-0.297700000
H	9.645229000	3.637918000	0.368595000
C	6.833464000	3.908045000	-1.348111000
H	7.346129000	4.815812000	-1.655091000
C	5.461919000	3.962031000	-1.071962000
C	4.691362000	5.265862000	-1.196989000
H	3.640311000	5.036668000	-0.974950000
C	5.164716000	6.303356000	-0.169561000
H	4.571004000	7.222010000	-0.240041000
H	5.077902000	5.915987000	0.849912000
H	6.213163000	6.574427000	-0.336121000
C	4.751327000	5.833972000	-2.621369000
H	4.384337000	5.109086000	-3.354773000
H	4.143145000	6.741824000	-2.704720000
H	5.776508000	6.098907000	-2.901815000
C	4.811618000	2.792549000	-0.672336000
H	3.749074000	2.833883000	-0.439080000
C	5.638244000	-1.320645000	-1.864973000
C	6.452979000	-2.463560000	-1.828071000
H	6.423838000	-3.098604000	-0.949718000
C	7.325528000	-2.784998000	-2.873605000
C	8.234584000	-4.000564000	-2.791081000
H	8.854211000	-3.995638000	-3.698485000
C	9.184836000	-3.919668000	-1.588734000
H	9.772042000	-2.996060000	-1.608476000
H	8.633055000	-3.944787000	-0.643259000

SUPPORTING INFORMATION

H	9.880877000	-4.765928000	-1.589165000
C	7.440164000	-5.312673000	-2.782220000
H	6.818806000	-5.400672000	-3.678985000
H	8.116502000	-6.174627000	-2.753244000
H	6.778335000	-5.372905000	-1.912152000
C	7.371715000	-1.950826000	-3.991097000
H	8.051428000	-2.199032000	-4.804256000
C	6.581980000	-0.799586000	-4.071489000
C	6.674956000	0.126997000	-5.272535000
H	5.895727000	0.891929000	-5.150315000
C	8.025567000	0.855385000	-5.311935000
H	8.066080000	1.558085000	-6.151896000
H	8.195007000	1.415243000	-4.387983000
H	8.851409000	0.145145000	-5.430043000
C	6.410720000	-0.599488000	-6.597573000
H	5.447196000	-1.118361000	-6.587652000
H	6.407499000	0.109366000	-7.432809000
H	7.184813000	-1.346370000	-6.804089000
C	5.734929000	-0.498976000	-3.003191000
H	5.166121000	0.423910000	-3.041634000
C	4.186277000	-3.341004000	0.120223000
C	3.525958000	-3.967482000	-0.942233000
H	2.970798000	-3.357263000	-1.645708000
C	3.543161000	-5.357095000	-1.093564000
C	2.770596000	-6.032395000	-2.213768000
H	3.016481000	-7.102619000	-2.174218000
C	1.257319000	-5.892629000	-1.994475000
H	0.958116000	-6.332092000	-1.038202000
H	0.955424000	-4.840098000	-1.978653000
H	0.699727000	-6.398239000	-2.791139000
C	3.176967000	-5.520537000	-3.601005000
H	4.251760000	-5.635965000	-3.768618000
H	2.646071000	-6.071567000	-4.385236000
H	2.934524000	-4.459465000	-3.721740000
C	4.262217000	-6.117780000	-0.167439000
H	4.291561000	-7.200831000	-0.281240000
C	4.943045000	-5.528375000	0.903648000
C	5.731098000	-6.386560000	1.880324000
H	5.664455000	-7.422292000	1.519996000

SUPPORTING INFORMATION

C	7.217867000	-6.007531000	1.909585000
H	7.774421000	-6.676540000	2.575485000
H	7.664285000	-6.072653000	0.912557000
H	7.360962000	-4.984556000	2.274707000
C	5.128318000	-6.348570000	3.290157000
H	4.092389000	-6.699424000	3.283395000
H	5.698707000	-6.987356000	3.973987000
H	5.130807000	-5.332143000	3.697095000
C	4.883326000	-4.139111000	1.041538000
H	5.396903000	-3.651973000	1.866041000
N	1.750723000	0.224621000	-2.970143000
N	1.632514000	0.557098000	-5.527850000
Sm	1.981665000	-0.114408000	-0.285707000
H	-0.097656000	3.689263000	-0.342241000
C	0.431122000	6.659083000	0.857574000
H	0.034965000	6.176878000	1.758410000
H	1.489664000	6.384786000	0.780189000
C	0.239815000	8.204977000	0.904115000
H	1.199364000	8.730433000	0.831587000
H	-0.233786000	8.522640000	1.840439000
C	-1.705203000	6.417777000	-0.190051000
H	-2.218380000	5.986630000	-1.056507000
H	-2.100804000	5.914169000	0.698211000
C	-1.902200000	7.961752000	-0.116702000
H	-2.378021000	8.261069000	0.824416000
H	-2.538864000	8.324767000	-0.932005000
C	0.253446000	6.725765000	-1.524707000
H	1.316398000	6.470106000	-1.606492000
H	-0.257627000	6.278071000	-2.385218000
C	0.037408000	8.268334000	-1.470932000
H	-0.598278000	8.613385000	-2.294771000
H	0.987870000	8.809795000	-1.545338000
C	-4.559403000	0.499709000	-1.132090000
C	-4.544346000	-0.930281000	-1.113494000
C	-4.646347000	-1.363175000	0.246288000
C	-4.736415000	-0.202143000	1.070037000
C	-4.675361000	0.951322000	0.221414000
C	-4.679107000	1.333972000	-2.358673000
C	-5.770978000	1.114027000	-3.208718000

SUPPORTING INFORMATION

H	-6.474849000	0.326467000	-2.955406000
C	-5.975130000	1.886707000	-4.356362000
C	-7.180080000	1.655943000	-5.252668000
H	-7.128931000	2.402382000	-6.057197000
C	-7.144299000	0.267502000	-5.904646000
H	-8.008476000	0.125940000	-6.563380000
H	-7.160620000	-0.525947000	-5.150251000
H	-6.236660000	0.134043000	-6.500635000
C	-8.499615000	1.879675000	-4.501409000
H	-9.353771000	1.770623000	-5.178840000
H	-8.540446000	2.880551000	-4.060200000
H	-8.624247000	1.152356000	-3.691872000
C	-5.044548000	2.882541000	-4.658627000
H	-5.192525000	3.482651000	-5.554729000
C	-3.933309000	3.123900000	-3.842403000
C	-2.926523000	4.203166000	-4.207303000
H	-2.113499000	4.145079000	-3.470655000
C	-2.316164000	3.973585000	-5.596590000
H	-1.523223000	4.702402000	-5.798585000
H	-3.069323000	4.082464000	-6.384450000
H	-1.891834000	2.969499000	-5.686943000
C	-3.537336000	5.607938000	-4.117261000
H	-2.788263000	6.375310000	-4.344207000
H	-3.939375000	5.802343000	-3.119398000
H	-4.358394000	5.725651000	-4.833017000
C	-3.769958000	2.351530000	-2.688608000
H	-2.926129000	2.548284000	-2.030436000
C	-4.649740000	-1.811441000	-2.302654000
C	-3.719879000	-1.791260000	-3.348030000
H	-2.859899000	-1.129536000	-3.283615000
C	-3.863285000	-2.610151000	-4.471286000
C	-2.819415000	-2.592300000	-5.575476000
H	-2.042839000	-1.879248000	-5.266238000
C	-2.144380000	-3.960155000	-5.744419000
H	-1.351059000	-3.911310000	-6.498938000
H	-2.863674000	-4.719092000	-6.071132000
H	-1.703811000	-4.302918000	-4.803474000
C	-3.397966000	-2.093068000	-6.906060000
H	-3.835250000	-1.096082000	-6.796801000

SUPPORTING INFORMATION

H	-4.183124000	-2.763367000	-7.272557000
H	-2.619030000	-2.043365000	-7.675316000
C	-4.979635000	-3.448772000	-4.549111000
H	-5.103020000	-4.088586000	-5.420385000
C	-5.939811000	-3.484991000	-3.532533000
C	-7.152481000	-4.398098000	-3.618500000
H	-7.804245000	-4.140051000	-2.773213000
C	-7.959531000	-4.182227000	-4.904840000
H	-8.862927000	-4.802177000	-4.901656000
H	-7.379440000	-4.453552000	-5.793767000
H	-8.264941000	-3.136992000	-5.013423000
C	-6.755949000	-5.872330000	-3.457761000
H	-7.640264000	-6.519141000	-3.483509000
H	-6.240450000	-6.037126000	-2.507154000
H	-6.085647000	-6.190159000	-4.264330000
C	-5.754899000	-2.667707000	-2.415556000
H	-6.485949000	-2.691545000	-1.611563000
C	-4.817894000	-2.771482000	0.682463000
C	-5.932138000	-3.124645000	1.461015000
H	-6.626550000	-2.349413000	1.773437000
C	-6.178698000	-4.449152000	1.821645000
C	-7.414761000	-4.809645000	2.628762000
H	-7.915600000	-3.866234000	2.883613000
C	-7.063570000	-5.514607000	3.945132000
H	-6.386511000	-4.905135000	4.550939000
H	-6.574597000	-6.478167000	3.764586000
H	-7.967205000	-5.708285000	4.533874000
C	-8.400098000	-5.648566000	1.802647000
H	-8.688313000	-5.128664000	0.883664000
H	-9.310105000	-5.858814000	2.376010000
H	-7.957315000	-6.609073000	1.516100000
C	-5.276959000	-5.432526000	1.397052000
H	-5.451315000	-6.473593000	1.664642000
C	-4.151785000	-5.116742000	0.632654000
C	-3.173755000	-6.207511000	0.228911000
H	-3.647235000	-7.167535000	0.477791000
C	-1.875884000	-6.108915000	1.043082000
H	-1.201161000	-6.938382000	0.803012000
H	-2.081086000	-6.136028000	2.117971000

SUPPORTING INFORMATION

H	-1.350203000	-5.173605000	0.822780000
C	-2.874898000	-6.213935000	-1.274652000
H	-3.792062000	-6.304318000	-1.863713000
H	-2.220619000	-7.054769000	-1.530141000
H	-2.368400000	-5.294833000	-1.585942000
C	-3.934497000	-3.779696000	0.278364000
H	-3.070167000	-3.513677000	-0.323273000
C	-5.108289000	-0.182937000	2.510404000
C	-6.329159000	0.403546000	2.870815000
H	-6.940411000	0.849215000	2.090685000
C	-6.774353000	0.411726000	4.196359000
C	-8.125454000	1.000077000	4.569084000
H	-8.204883000	0.949839000	5.663765000
C	-9.275355000	0.165849000	3.986141000
H	-9.208230000	-0.878836000	4.305683000
H	-9.256939000	0.181752000	2.890792000
H	-10.245409000	0.560287000	4.309169000
C	-8.255557000	2.473087000	4.163209000
H	-7.465459000	3.080103000	4.614153000
H	-9.222921000	2.876659000	4.482763000
H	-8.185894000	2.594655000	3.077267000
C	-5.959818000	-0.167292000	5.172101000
H	-6.297709000	-0.159649000	6.207155000
C	-4.732712000	-0.759316000	4.850698000
C	-3.854564000	-1.370308000	5.929695000
H	-2.979975000	-1.800883000	5.425818000
C	-4.563171000	-2.508765000	6.675095000
H	-3.890069000	-2.970706000	7.405805000
H	-4.898342000	-3.285831000	5.981831000
H	-5.441513000	-2.144012000	7.219054000
C	-3.344961000	-0.306370000	6.912274000
H	-2.800812000	0.486808000	6.390149000
H	-2.671457000	-0.751913000	7.653050000
H	-4.174104000	0.160868000	7.455322000
C	-4.325141000	-0.768331000	3.514431000
H	-3.373728000	-1.222169000	3.253995000
C	-4.812494000	2.343872000	0.706403000
C	-4.099808000	2.772087000	1.839388000
H	-3.421625000	2.076319000	2.325401000

SUPPORTING INFORMATION

C	-4.264741000	4.052667000	2.366246000
C	-3.538484000	4.518434000	3.619130000
H	-3.383397000	5.601547000	3.509646000
C	-2.163884000	3.874855000	3.816828000
H	-1.536830000	3.978603000	2.925504000
H	-2.247742000	2.807325000	4.047161000
H	-1.643928000	4.346063000	4.657390000
C	-4.416454000	4.305602000	4.862821000
H	-5.373319000	4.827816000	4.765746000
H	-3.915426000	4.679095000	5.763276000
H	-4.628705000	3.240762000	5.006564000
C	-5.179087000	4.910717000	1.742558000
H	-5.331129000	5.908862000	2.152708000
C	-5.915168000	4.519211000	0.622023000
C	-6.933954000	5.464453000	0.006067000
H	-6.951575000	6.366598000	0.632949000
C	-8.348250000	4.869062000	0.021930000
H	-9.076542000	5.593046000	-0.360042000
H	-8.647985000	4.587282000	1.035983000
H	-8.410604000	3.974097000	-0.606362000
C	-6.534506000	5.894960000	-1.410470000
H	-5.560341000	6.393689000	-1.407059000
H	-7.269730000	6.592209000	-1.827812000
H	-6.466562000	5.033950000	-2.083622000
C	-5.709376000	3.235570000	0.103454000
H	-6.271012000	2.904992000	-0.765252000
N	-0.273832000	6.099255000	-0.304645000
N	-0.606913000	8.644255000	-0.209210000
Sm	-2.136577000	-0.091857000	0.075753000
H	0.181552000	-0.258665000	3.622656000
O	0.873820000	0.140982000	1.773538000
C	-0.065352000	-0.136668000	2.555637000
O	-1.278298000	-0.281889000	2.230497000
O	1.093275000	2.062384000	-0.540045000
C	-0.043769000	2.586703000	-0.407653000
O	-1.136090000	1.948423000	-0.364394000
C	-0.160289000	-1.470231000	-0.711023000
O	0.944491000	-2.077904000	-0.901821000
O	-1.306510000	-2.000685000	-0.889436000

SUPPORTING INFORMATION

Int5

Sm	-1.923988000	0.130553000	0.498219000
Sm	2.029710000	0.172343000	-0.320402000
C	0.305714000	-1.528712000	0.450904000
C	0.103180000	2.846573000	0.743741000
O	0.356818000	-0.459482000	1.243298000
C	0.131065000	1.210508000	-2.303686000
C	-0.606120000	1.005546000	3.721588000
H	-0.592775000	2.020012000	3.317510000
H	0.229836000	0.461127000	3.282513000
C	-0.555967000	1.008502000	5.274507000
H	0.360489000	0.529577000	5.635039000
H	-0.563437000	2.030530000	5.669529000
C	-1.872638000	-1.040074000	3.748916000
H	-1.058008000	-1.571323000	3.248836000
H	-2.814811000	-1.500031000	3.439251000
C	-1.724026000	-1.061965000	5.295899000
H	-2.551260000	-1.609948000	5.760488000
H	-0.794833000	-1.558552000	5.594754000
C	-2.992346000	1.104166000	3.870470000
H	-3.933053000	0.711983000	3.480108000
H	-2.900741000	2.145811000	3.550008000
C	-2.928089000	0.985344000	5.417521000
H	-2.950686000	1.973637000	5.890597000
H	-3.787191000	0.422663000	5.798132000
C	-3.874748000	-0.642652000	-1.479708000
C	-4.413879000	-1.121974000	-0.246425000
C	-4.798934000	0.011428000	0.552213000
C	-4.471451000	1.196393000	-0.194636000
C	-3.906748000	0.791434000	-1.445669000
C	-3.663078000	-1.466468000	-2.703004000
C	-4.703038000	-2.309220000	-3.119786000
H	-5.583297000	-2.401775000	-2.492117000
C	-4.644386000	-3.002204000	-4.333469000
C	-5.776037000	-3.908794000	-4.786989000
H	-5.544722000	-4.214440000	-5.816625000
C	-7.129439000	-3.187784000	-4.818335000
H	-7.088040000	-2.291836000	-5.445841000

SUPPORTING INFORMATION

H	-7.907686000	-3.847409000	-5.217767000
H	-7.442759000	-2.880621000	-3.815162000
C	-5.845433000	-5.181526000	-3.931846000
H	-4.901471000	-5.733663000	-3.973673000
H	-6.042034000	-4.940757000	-2.882013000
H	-6.643843000	-5.844271000	-4.285074000
C	-3.515488000	-2.834762000	-5.133239000
H	-3.465938000	-3.350916000	-6.091617000
C	-2.449255000	-2.011733000	-4.750662000
C	-1.265992000	-1.892689000	-5.700731000
H	-1.694499000	-1.793664000	-6.708675000
C	-0.387775000	-0.665142000	-5.465790000
H	-0.980242000	0.254984000	-5.446633000
H	0.164304000	-0.734642000	-4.522745000
H	0.355642000	-0.572456000	-6.263428000
C	-0.426895000	-3.180278000	-5.695958000
H	-1.033235000	-4.053238000	-5.955734000
H	0.397295000	-3.112711000	-6.414565000
H	-0.001515000	-3.366320000	-4.704737000
C	-2.533338000	-1.339421000	-3.528650000
H	-1.730533000	-0.684566000	-3.210419000
C	-4.764813000	-2.545247000	0.014417000
C	-6.109985000	-2.894062000	0.207845000
H	-6.861048000	-2.107570000	0.211827000
C	-6.506775000	-4.221664000	0.393125000
C	-7.988663000	-4.534324000	0.560964000
H	-8.397334000	-3.761058000	1.226936000
C	-8.729798000	-4.415704000	-0.780387000
H	-8.586628000	-3.429458000	-1.232016000
H	-8.365181000	-5.165656000	-1.490832000
H	-9.806143000	-4.572465000	-0.646213000
C	-8.276863000	-5.892620000	1.203682000
H	-7.748483000	-6.016486000	2.154168000
H	-9.349235000	-5.996594000	1.398361000
H	-7.986785000	-6.719375000	0.545490000
C	-5.516102000	-5.210316000	0.393257000
H	-5.790897000	-6.250723000	0.547316000
C	-4.165791000	-4.899176000	0.203737000
C	-3.118249000	-5.999752000	0.216710000

SUPPORTING INFORMATION

H	-3.646525000	-6.941208000	0.421860000
C	-2.426132000	-6.143263000	-1.145271000
H	-1.718040000	-6.979449000	-1.131127000
H	-3.154175000	-6.325702000	-1.941423000
H	-1.867360000	-5.238120000	-1.402349000
C	-2.088380000	-5.791665000	1.335588000
H	-2.575762000	-5.718959000	2.313428000
H	-1.382724000	-6.629179000	1.369159000
H	-1.512217000	-4.874808000	1.174063000
C	-3.801953000	-3.561912000	0.008130000
H	-2.758395000	-3.302484000	-0.147190000
C	-5.642769000	-0.075647000	1.771961000
C	-5.471322000	-1.105206000	2.716770000
H	-4.687161000	-1.840187000	2.559433000
C	-6.303214000	-1.241493000	3.829258000
C	-6.100109000	-2.397081000	4.796922000
H	-5.084043000	-2.780643000	4.629490000
C	-7.074172000	-3.542463000	4.484387000
H	-6.901355000	-4.394941000	5.151005000
H	-8.112281000	-3.216721000	4.615368000
H	-6.954155000	-3.883773000	3.452521000
C	-6.201435000	-1.984541000	6.269638000
H	-5.519114000	-1.162949000	6.509389000
H	-7.214900000	-1.661620000	6.531048000
H	-5.954393000	-2.830418000	6.919954000
C	-7.350855000	-0.327074000	3.989758000
H	-8.022729000	-0.418646000	4.840506000
C	-7.568235000	0.699132000	3.069056000
C	-8.740752000	1.649796000	3.245972000
H	-9.279380000	1.327838000	4.147752000
C	-9.723214000	1.564100000	2.070035000
H	-10.592828000	2.207048000	2.245512000
H	-9.252550000	1.888483000	1.135763000
H	-10.080253000	0.539656000	1.925138000
C	-8.278937000	3.094451000	3.475636000
H	-9.138454000	3.752002000	3.648088000
H	-7.618690000	3.162365000	4.345978000
H	-7.731033000	3.478879000	2.608926000
C	-6.705330000	0.817672000	1.973250000

SUPPORTING INFORMATION

H	-6.875847000	1.603776000	1.246366000
C	-4.912376000	2.595873000	0.076462000
C	-5.918759000	3.133263000	-0.744771000
H	-6.331475000	2.515203000	-1.538232000
C	-6.390459000	4.434046000	-0.575201000
C	-7.460734000	4.991639000	-1.498075000
H	-7.791395000	4.163548000	-2.138978000
C	-8.687709000	5.500461000	-0.730776000
H	-9.112270000	4.718234000	-0.094087000
H	-8.434825000	6.351916000	-0.089450000
H	-9.466259000	5.833019000	-1.425997000
C	-6.891056000	6.083337000	-2.415381000
H	-7.656118000	6.441877000	-3.113116000
H	-6.540766000	6.943930000	-1.834294000
H	-6.045924000	5.705013000	-2.997908000
C	-5.830686000	5.212814000	0.446369000
H	-6.176063000	6.234580000	0.593355000
C	-4.828132000	4.717922000	1.282316000
C	-4.244546000	5.600151000	2.374706000
H	-4.685269000	6.597922000	2.244680000
C	-4.637360000	5.108114000	3.774160000
H	-5.724081000	5.056638000	3.885818000
H	-4.238011000	4.106577000	3.966503000
H	-4.245145000	5.779197000	4.546505000
C	-2.723354000	5.753406000	2.251187000
H	-2.444861000	6.156922000	1.273122000
H	-2.340734000	6.431699000	3.021837000
H	-2.213612000	4.791403000	2.370411000
C	-4.380861000	3.403203000	1.084998000
H	-3.583443000	3.011962000	1.707827000
C	-3.683774000	1.715079000	-2.588580000
C	-4.300267000	1.448764000	-3.818755000
H	-4.871206000	0.532409000	-3.930920000
C	-4.226602000	2.352406000	-4.884067000
C	-4.929186000	2.074656000	-6.202834000
H	-4.795220000	2.967205000	-6.829200000
C	-6.438372000	1.866582000	-6.018176000
H	-6.897965000	2.721780000	-5.512779000
H	-6.931612000	1.738148000	-6.988005000

SUPPORTING INFORMATION

H	-6.647335000	0.972776000	-5.420591000
C	-4.296438000	0.889451000	-6.944519000
H	-3.233789000	1.067561000	-7.137185000
H	-4.378769000	-0.033451000	-6.360905000
H	-4.792970000	0.725457000	-7.907705000
C	-3.508700000	3.534774000	-4.701464000
H	-3.452257000	4.251775000	-5.520081000
C	-2.872142000	3.836674000	-3.491274000
C	-2.095233000	5.140697000	-3.381946000
H	-2.644847000	5.877357000	-3.985142000
C	-2.002357000	5.695663000	-1.959871000
H	-1.550647000	6.693152000	-1.972693000
H	-2.988591000	5.768609000	-1.492036000
H	-1.374237000	5.065228000	-1.321271000
C	-0.698455000	4.998368000	-4.007160000
H	-0.173151000	5.959725000	-4.011392000
H	-0.086591000	4.287113000	-3.441450000
H	-0.757833000	4.639361000	-5.039353000
C	-2.968940000	2.917021000	-2.443688000
H	-2.514567000	3.141853000	-1.483482000
C	4.605641000	1.138694000	0.197231000
C	4.256044000	0.433202000	1.397492000
C	4.219069000	-0.963587000	1.085088000
C	4.545715000	-1.124086000	-0.303016000
C	4.780084000	0.182032000	-0.850997000
C	4.957680000	2.577767000	0.091013000
C	4.392093000	3.414498000	-0.879722000
H	3.633814000	3.013840000	-1.547411000
C	4.786674000	4.750122000	-1.003031000
C	4.143605000	5.677948000	-2.020459000
H	4.766242000	6.582394000	-2.062870000
C	4.098577000	5.082557000	-3.432084000
H	3.711913000	5.818798000	-4.145438000
H	5.093843000	4.773385000	-3.764507000
H	3.445748000	4.204981000	-3.479522000
C	2.742850000	6.106567000	-1.558890000
H	2.778283000	6.576693000	-0.570818000
H	2.301209000	6.821927000	-2.261992000
H	2.075461000	5.240484000	-1.494417000

SUPPORTING INFORMATION

C	5.769347000	5.242271000	-0.137372000
H	6.074552000	6.281169000	-0.237998000
C	6.356938000	4.436747000	0.843306000
C	7.463008000	4.934506000	1.762865000
H	7.325203000	4.418412000	2.723063000
C	8.842705000	4.529934000	1.219393000
H	8.909163000	3.448248000	1.067829000
H	9.036149000	5.015075000	0.256016000
H	9.638568000	4.825732000	1.912480000
C	7.418438000	6.439182000	2.039933000
H	6.435570000	6.755866000	2.402189000
H	8.160790000	6.705258000	2.799683000
H	7.652691000	7.023973000	1.143328000
C	5.935626000	3.107987000	0.943966000
H	6.380588000	2.463866000	1.698414000
C	4.204314000	1.046069000	2.750928000
C	4.947891000	0.481354000	3.796109000
H	5.492242000	-0.439509000	3.613788000
C	5.025044000	1.093207000	5.051820000
C	5.856804000	0.490171000	6.171605000
H	5.801161000	1.185534000	7.020470000
C	5.292002000	-0.856756000	6.640196000
H	4.259279000	-0.749114000	6.986176000
H	5.295921000	-1.593485000	5.830045000
H	5.886192000	-1.260929000	7.467663000
C	7.335428000	0.363000000	5.780613000
H	7.749001000	1.328968000	5.474027000
H	7.927676000	-0.009247000	6.624042000
H	7.468812000	-0.336271000	4.948203000
C	4.338548000	2.291194000	5.248101000
H	4.397568000	2.782176000	6.219327000
C	3.590019000	2.891655000	4.228246000
C	2.956464000	4.248323000	4.498920000
H	2.640838000	4.246456000	5.552215000
C	4.003011000	5.362521000	4.334781000
H	4.871012000	5.189980000	4.978343000
H	4.355895000	5.401004000	3.298658000
H	3.578036000	6.340408000	4.589357000
C	1.723316000	4.554626000	3.649187000

SUPPORTING INFORMATION

H	1.267028000	5.497295000	3.969093000
H	1.984448000	4.660264000	2.590967000
H	0.969861000	3.765900000	3.736793000
C	3.523466000	2.253996000	2.987578000
H	2.957711000	2.697262000	2.174642000
C	4.135186000	-2.068638000	2.078035000
C	5.250115000	-2.898719000	2.255910000
H	6.125515000	-2.732354000	1.634164000
C	5.256758000	-3.920749000	3.211071000
C	6.470637000	-4.816083000	3.399647000
H	6.266179000	-5.450795000	4.272811000
C	7.743795000	-4.015691000	3.703098000
H	7.612395000	-3.376709000	4.581897000
H	8.585457000	-4.690051000	3.896047000
H	8.023473000	-3.374262000	2.860447000
C	6.678118000	-5.742661000	2.193195000
H	5.799480000	-6.372622000	2.024130000
H	6.853678000	-5.168181000	1.277771000
H	7.541777000	-6.398274000	2.352200000
C	4.109583000	-4.110967000	3.985837000
H	4.104673000	-4.909060000	4.726338000
C	2.973423000	-3.308249000	3.828551000
C	1.726589000	-3.553269000	4.660894000
H	0.992181000	-2.793786000	4.360962000
C	1.112014000	-4.928917000	4.367944000
H	0.885998000	-5.043250000	3.303903000
H	1.796431000	-5.735471000	4.653395000
H	0.183092000	-5.067933000	4.932370000
C	1.988812000	-3.377981000	6.162400000
H	2.389553000	-2.384188000	6.382074000
H	1.064856000	-3.510731000	6.736782000
H	2.711439000	-4.115619000	6.528268000
C	3.004679000	-2.285877000	2.876891000
H	2.131600000	-1.652435000	2.743136000
C	4.831875000	-2.424661000	-0.959259000
C	4.039335000	-3.565184000	-0.735730000
H	3.158923000	-3.476111000	-0.105849000
C	4.396292000	-4.814235000	-1.253518000
C	3.590524000	-6.083377000	-1.005529000

SUPPORTING INFORMATION

H	4.326875000	-6.864366000	-0.765184000
C	2.621024000	-5.995835000	0.173599000
H	3.122291000	-5.659308000	1.086166000
H	1.794447000	-5.307820000	-0.031986000
H	2.181165000	-6.979371000	0.369571000
C	2.857963000	-6.533538000	-2.279896000
H	3.547798000	-6.647462000	-3.121900000
H	2.358169000	-7.495421000	-2.119357000
H	2.095195000	-5.803254000	-2.566603000
C	5.561721000	-4.907673000	-2.023425000
H	5.851459000	-5.881763000	-2.414762000
C	6.365856000	-3.795564000	-2.280327000
C	7.647931000	-3.916664000	-3.087455000
H	8.054036000	-2.902216000	-3.194560000
C	7.395571000	-4.461733000	-4.499108000
H	6.668096000	-3.846173000	-5.036651000
H	8.324739000	-4.476301000	-5.079561000
H	7.009215000	-5.486626000	-4.470020000
C	8.697872000	-4.761012000	-2.351667000
H	8.914600000	-4.347861000	-1.361633000
H	8.350437000	-5.790949000	-2.213734000
H	9.635135000	-4.798386000	-2.918268000
C	5.989144000	-2.564287000	-1.739066000
H	6.625841000	-1.700485000	-1.901803000
C	5.335275000	0.494137000	-2.196514000
C	6.600939000	1.094758000	-2.276398000
H	7.113950000	1.346213000	-1.352582000
C	7.208630000	1.356058000	-3.506777000
C	8.582545000	1.999426000	-3.592264000
H	8.882573000	1.970609000	-4.648861000
C	8.535742000	3.473339000	-3.165722000
H	7.832080000	4.039626000	-3.783623000
H	8.213767000	3.572838000	-2.124028000
H	9.523767000	3.938112000	-3.261797000
C	9.641426000	1.227085000	-2.795244000
H	9.692614000	0.180727000	-3.112491000
H	10.631671000	1.674278000	-2.935923000
H	9.424532000	1.240853000	-1.721795000
C	6.514145000	1.018315000	-4.671936000

SUPPORTING INFORMATION

H	6.975156000	1.217475000	-5.638682000
C	5.245563000	0.434470000	-4.633989000
C	4.508562000	0.136052000	-5.928410000
H	5.234298000	0.263479000	-6.743485000
C	3.375695000	1.147928000	-6.156219000
H	3.759976000	2.172636000	-6.168393000
H	2.872115000	0.961676000	-7.111963000
H	2.628598000	1.084275000	-5.358163000
C	3.986960000	-1.303526000	-6.000137000
H	3.535734000	-1.499479000	-6.979183000
H	4.792949000	-2.027228000	-5.845935000
H	3.220802000	-1.491808000	-5.241182000
C	4.670586000	0.171865000	-3.385944000
H	3.688954000	-0.288827000	-3.337508000
N	-1.864235000	0.361603000	3.250354000
N	-1.706874000	0.297283000	5.834343000
O	0.684694000	-3.630606000	-2.014277000
O	-0.866146000	-2.035259000	0.363495000
O	1.190844000	2.283371000	0.471207000
O	-1.045212000	2.318132000	0.808677000
O	1.367201000	1.360326000	-2.420140000
O	-0.381461000	0.501761000	-1.369352000
H	0.147353000	3.928900000	0.953315000
H	-0.552861000	1.694501000	-3.015444000
C	1.227949000	-2.611323000	-2.114409000
O	1.790860000	-1.597326000	-2.326271000

TS3

Sm	-1.978489000	-0.040470000	0.362028000
Sm	2.136260000	0.078769000	-0.406145000
C	-0.059977000	-2.213182000	0.308044000
C	0.063747000	2.591332000	0.858649000
O	0.448009000	-1.119957000	0.784431000
C	0.130410000	1.079986000	-2.343512000
C	-0.357697000	0.110987000	3.535713000
H	-0.120411000	1.126738000	3.213615000
H	0.330280000	-0.563366000	3.025125000
C	-0.276010000	-0.034995000	5.080224000
H	0.449607000	-0.805341000	5.360756000

SUPPORTING INFORMATION

H	0.052182000	0.899627000	5.546559000
C	-2.054811000	-1.587592000	3.508109000
H	-1.335231000	-2.256981000	3.030348000
H	-3.043962000	-1.851728000	3.126851000
C	-1.996555000	-1.678091000	5.058476000
H	-2.976106000	-1.938755000	5.473692000
H	-1.289190000	-2.450967000	5.377955000
C	-2.665545000	0.751141000	3.726545000
H	-3.682614000	0.539702000	3.384823000
H	-2.391097000	1.753466000	3.384122000
C	-2.552322000	0.625771000	5.271629000
H	-2.238696000	1.573543000	5.722943000
H	-3.520108000	0.360160000	5.710067000
C	-3.999461000	-0.636260000	-1.510384000
C	-4.602803000	-1.043817000	-0.280169000
C	-4.872441000	0.131569000	0.502578000
C	-4.420717000	1.268306000	-0.251399000
C	-3.892304000	0.795862000	-1.497869000
C	-3.808508000	-1.516026000	-2.697610000
C	-4.922547000	-2.210194000	-3.189356000
H	-5.862851000	-2.134368000	-2.651873000
C	-4.850161000	-2.971428000	-4.360202000
C	-6.059319000	-3.717651000	-4.898408000
H	-5.771241000	-4.125842000	-5.876823000
C	-7.263845000	-2.795384000	-5.125550000
H	-7.008643000	-1.965278000	-5.791833000
H	-8.093848000	-3.350463000	-5.576481000
H	-7.626870000	-2.370298000	-4.183782000
C	-6.431631000	-4.901420000	-3.995303000
H	-5.595284000	-5.600324000	-3.898584000
H	-6.696302000	-4.561614000	-2.988827000
H	-7.287544000	-5.448725000	-4.406539000
C	-3.629238000	-3.029955000	-5.032112000
H	-3.559638000	-3.609801000	-5.952062000
C	-2.489922000	-2.361598000	-4.568409000
C	-1.199155000	-2.506020000	-5.359338000
H	-1.493149000	-2.543741000	-6.418233000
C	-0.229532000	-1.334931000	-5.198547000
H	-0.722939000	-0.375829000	-5.387538000

SUPPORTING INFORMATION

H	0.209333000	-1.308920000	-4.196106000
H	0.600825000	-1.433609000	-5.904694000
C	-0.507128000	-3.838729000	-5.031271000
H	-1.178474000	-4.686964000	-5.197869000
H	0.380816000	-3.977998000	-5.657873000
H	-0.187413000	-3.864840000	-3.984626000
C	-2.594808000	-1.606802000	-3.396502000
H	-1.731583000	-1.067170000	-3.021083000
C	-5.125155000	-2.414240000	-0.019797000
C	-6.505455000	-2.592534000	0.158854000
H	-7.155100000	-1.720451000	0.156090000
C	-7.065508000	-3.861048000	0.335642000
C	-8.575780000	-3.989100000	0.486553000
H	-8.898391000	-3.148796000	1.117492000
C	-9.276409000	-3.833731000	-0.872587000
H	-9.005464000	-2.890348000	-1.356182000
H	-8.994161000	-4.649105000	-1.547663000
H	-10.365802000	-3.854155000	-0.754823000
C	-9.030299000	-5.279848000	1.171752000
H	-8.527159000	-5.432604000	2.131762000
H	-10.108899000	-5.248811000	1.357385000
H	-8.835927000	-6.158444000	0.546314000
C	-6.206802000	-4.965969000	0.337112000
H	-6.611526000	-5.964889000	0.480144000
C	-4.826612000	-4.825484000	0.162381000
C	-3.923736000	-6.047156000	0.193422000
H	-4.578446000	-6.926126000	0.272865000
C	-3.098962000	-6.195725000	-1.091574000
H	-2.513053000	-7.121201000	-1.066098000
H	-3.743531000	-6.223821000	-1.975108000
H	-2.397706000	-5.364362000	-1.214835000
C	-3.011322000	-6.035748000	1.428431000
H	-3.594503000	-5.959668000	2.352225000
H	-2.413985000	-6.953081000	1.476694000
H	-2.318841000	-5.188339000	1.391005000
C	-4.297256000	-3.543051000	-0.019968000
H	-3.228765000	-3.415509000	-0.160067000
C	-5.752158000	0.152167000	1.701543000
C	-5.682834000	-0.851725000	2.684391000

SUPPORTING INFORMATION

H	-4.950150000	-1.645824000	2.577987000
C	-6.569080000	-0.901640000	3.761234000
C	-6.481869000	-2.026610000	4.779578000
H	-5.531346000	-2.548089000	4.601274000
C	-7.608415000	-3.047968000	4.567371000
H	-7.516835000	-3.881310000	5.272951000
H	-8.589787000	-2.584870000	4.719773000
H	-7.580713000	-3.453145000	3.552151000
C	-6.470224000	-1.521826000	6.227533000
H	-5.668661000	-0.795811000	6.396043000
H	-7.416165000	-1.037445000	6.492781000
H	-6.325161000	-2.355424000	6.923049000
C	-7.566507000	0.076224000	3.844976000
H	-8.281437000	0.050184000	4.665084000
C	-7.684835000	1.079813000	2.882472000
C	-8.807806000	2.099859000	2.975949000
H	-9.432905000	1.806160000	3.830357000
C	-9.701414000	2.086245000	1.728630000
H	-10.545797000	2.773075000	1.853219000
H	-9.147433000	2.401111000	0.837753000
H	-10.101408000	1.085671000	1.537015000
C	-8.275883000	3.511104000	3.257712000
H	-9.102726000	4.222824000	3.361054000
H	-7.692157000	3.532656000	4.183486000
H	-7.630081000	3.861088000	2.445432000
C	-6.767884000	1.111525000	1.825192000
H	-6.862222000	1.876753000	1.062964000
C	-4.731850000	2.697165000	0.032770000
C	-5.615459000	3.364392000	-0.833313000
H	-6.016371000	2.825986000	-1.688318000
C	-5.986307000	4.691809000	-0.624018000
C	-6.930278000	5.388116000	-1.589985000
H	-7.284533000	4.623908000	-2.294488000
C	-8.161147000	5.974126000	-0.886749000
H	-8.700859000	5.207599000	-0.322252000
H	-7.882717000	6.769668000	-0.186951000
H	-8.851617000	6.407822000	-1.618313000
C	-6.197895000	6.461815000	-2.407198000
H	-6.874441000	6.925452000	-3.133803000

SUPPORTING INFORMATION

H	-5.810257000	7.255676000	-1.758744000
H	-5.353211000	6.031152000	-2.953041000
C	-5.448913000	5.362674000	0.483136000
H	-5.718171000	6.401817000	0.664110000
C	-4.568338000	4.734763000	1.366068000
C	-3.986060000	5.503999000	2.540648000
H	-4.438712000	6.504610000	2.522074000
C	-4.340736000	4.866324000	3.889525000
H	-5.423271000	4.773497000	4.012731000
H	-3.909998000	3.863299000	3.980832000
H	-3.952316000	5.470568000	4.716827000
C	-2.468335000	5.682880000	2.400551000
H	-2.213211000	6.180406000	1.459995000
H	-2.070381000	6.285308000	3.224742000
H	-1.957581000	4.713958000	2.415255000
C	-4.221659000	3.397289000	1.128558000
H	-3.525494000	2.898638000	1.794594000
C	-3.545112000	1.675236000	-2.643735000
C	-4.063853000	1.399444000	-3.915885000
H	-4.657743000	0.502406000	-4.056892000
C	-3.861950000	2.271549000	-4.991978000
C	-4.456663000	1.982838000	-6.360274000
H	-4.206775000	2.838189000	-7.002900000
C	-5.987065000	1.880269000	-6.309778000
H	-6.432044000	2.784995000	-5.883585000
H	-6.397055000	1.740195000	-7.316086000
H	-6.309537000	1.029431000	-5.700114000
C	-3.839923000	0.730033000	-6.996269000
H	-2.754522000	0.831120000	-7.094515000
H	-4.037537000	-0.161599000	-6.392293000
H	-4.256273000	0.559478000	-7.995499000
C	-3.120769000	3.432505000	-4.774711000
H	-2.969576000	4.126100000	-5.601248000
C	-2.579913000	3.743812000	-3.520387000
C	-1.775908000	5.027771000	-3.373012000
H	-2.295852000	5.786747000	-3.975281000
C	-1.699989000	5.557695000	-1.940923000
H	-1.227317000	6.545153000	-1.928842000
H	-2.692176000	5.644557000	-1.488216000

SUPPORTING INFORMATION

H	-1.095486000	4.903995000	-1.302470000
C	-0.369579000	4.862715000	-3.970416000
H	0.181490000	5.808775000	-3.936415000
H	0.207800000	4.118351000	-3.411440000
H	-0.413487000	4.533415000	-5.013110000
C	-2.798409000	2.854658000	-2.466304000
H	-2.416077000	3.085977000	-1.476738000
C	4.542111000	1.201424000	0.409771000
C	4.200422000	0.344844000	1.512245000
C	4.329584000	-1.011408000	1.060563000
C	4.768890000	-0.993860000	-0.302154000
C	4.877499000	0.375748000	-0.710844000
C	4.778853000	2.667197000	0.460570000
C	4.196202000	3.553292000	-0.455524000
H	3.498220000	3.169368000	-1.194655000
C	4.513780000	4.914347000	-0.449159000
C	3.863690000	5.895438000	-1.411163000
H	4.509143000	6.784398000	-1.437136000
C	3.755073000	5.363360000	-2.843612000
H	3.394939000	6.149952000	-3.515548000
H	4.722547000	5.012433000	-3.213570000
H	3.051656000	4.527516000	-2.915056000
C	2.491355000	6.342976000	-0.885669000
H	2.569632000	6.765319000	0.121258000
H	2.049494000	7.102015000	-1.541157000
H	1.800748000	5.493613000	-0.841481000
C	5.434933000	5.383655000	0.494328000
H	5.683960000	6.442214000	0.492081000
C	6.036032000	4.530214000	1.424321000
C	7.088750000	5.004815000	2.415658000
H	6.937258000	4.423216000	3.335627000
C	8.499578000	4.682500000	1.896902000
H	8.610860000	3.615037000	1.683602000
H	8.705632000	5.231601000	0.971125000
H	9.260930000	4.963362000	2.633466000
C	6.980502000	6.485937000	2.785439000
H	5.974578000	6.746171000	3.129235000
H	7.685202000	6.726945000	3.588008000
H	7.225746000	7.134361000	1.936724000

SUPPORTING INFORMATION

C	5.690848000	3.175650000	1.394999000
H	6.151585000	2.491865000	2.103788000
C	3.984764000	0.799178000	2.911262000
C	4.594467000	0.114939000	3.973083000
H	5.173227000	-0.777035000	3.759308000
C	4.495873000	0.571086000	5.291993000
C	5.183498000	-0.161380000	6.432126000
H	4.970582000	0.405228000	7.349058000
C	4.626385000	-1.577266000	6.624769000
H	3.548070000	-1.551660000	6.811790000
H	4.796897000	-2.197299000	5.738582000
H	5.106143000	-2.070330000	7.477838000
C	6.707676000	-0.185780000	6.252377000
H	7.110224000	0.826839000	6.149174000
H	7.191922000	-0.659141000	7.113790000
H	6.993331000	-0.750744000	5.358679000
C	3.774140000	1.738557000	5.538598000
H	3.698825000	2.109431000	6.560569000
C	3.161405000	2.459664000	4.506693000
C	2.490902000	3.782319000	4.847520000
H	2.080098000	3.677993000	5.862000000
C	3.537401000	4.907959000	4.888946000
H	4.342325000	4.675378000	5.592747000
H	3.986624000	5.044829000	3.899429000
H	3.081086000	5.857028000	5.193331000
C	1.337693000	4.169142000	3.921611000
H	0.848478000	5.079037000	4.284423000
H	1.693576000	4.373892000	2.906576000
H	0.581224000	3.379530000	3.867514000
C	3.265068000	1.973879000	3.201571000
H	2.802918000	2.512853000	2.382264000
C	4.278684000	-2.239587000	1.900907000
C	5.462533000	-2.958915000	2.111033000
H	6.376012000	-2.601548000	1.643575000
C	5.485465000	-4.114213000	2.899677000
C	6.775495000	-4.884145000	3.129941000
H	6.535927000	-5.710322000	3.813548000
C	7.845521000	-4.021865000	3.812619000
H	7.479846000	-3.608960000	4.757977000

SUPPORTING INFORMATION

H	8.741916000	-4.615107000	4.024697000
H	8.148369000	-3.183716000	3.175466000
C	7.311723000	-5.500459000	1.830954000
H	6.572769000	-6.164252000	1.372811000
H	7.560772000	-4.728756000	1.095428000
H	8.218580000	-6.083800000	2.026669000
C	4.287486000	-4.550408000	3.472400000
H	4.297425000	-5.454732000	4.078240000
C	3.084640000	-3.860960000	3.280172000
C	1.782179000	-4.375477000	3.869194000
H	1.021328000	-3.606812000	3.675469000
C	1.325808000	-5.661009000	3.164374000
H	1.221735000	-5.504372000	2.087005000
H	2.049721000	-6.469210000	3.317534000
H	0.360003000	-5.999226000	3.556532000
C	1.859887000	-4.578097000	5.387438000
H	2.168328000	-3.661044000	5.898211000
H	0.886166000	-4.883260000	5.786841000
H	2.578721000	-5.361787000	5.649960000
C	3.099744000	-2.703028000	2.498381000
H	2.171853000	-2.162720000	2.331284000
C	5.294688000	-2.164088000	-1.050777000
C	4.636897000	-3.401177000	-1.092086000
H	3.685020000	-3.510889000	-0.585197000
C	5.193621000	-4.501284000	-1.752485000
C	4.471391000	-5.834831000	-1.870961000
H	5.251856000	-6.606466000	-1.937163000
C	3.583706000	-6.175975000	-0.671369000
H	4.124627000	-6.076910000	0.274627000
H	2.702333000	-5.528612000	-0.626365000
H	3.222382000	-7.206800000	-0.753025000
C	3.658828000	-5.887710000	-3.175246000
H	4.293237000	-5.699223000	-4.047263000
H	3.186926000	-6.869091000	-3.300461000
H	2.868895000	-5.128989000	-3.161571000
C	6.443770000	-4.351611000	-2.360292000
H	6.882263000	-5.209935000	-2.867454000
C	7.140759000	-3.140513000	-2.322345000
C	8.514242000	-2.997262000	-2.956883000

SUPPORTING INFORMATION

H	8.834917000	-1.960263000	-2.790743000
C	8.472297000	-3.227407000	-4.473441000
H	7.771904000	-2.539568000	-4.956366000
H	9.462302000	-3.073365000	-4.917506000
H	8.157201000	-4.249172000	-4.712401000
C	9.549208000	-3.913714000	-2.289968000
H	9.609963000	-3.725539000	-1.213461000
H	9.292694000	-4.969786000	-2.428968000
H	10.544358000	-3.754626000	-2.720482000
C	6.551281000	-2.058500000	-1.667576000
H	7.086673000	-1.114942000	-1.619905000
C	5.385218000	0.840362000	-2.028306000
C	6.504929000	1.681690000	-2.095724000
H	6.961438000	2.017787000	-1.169183000
C	7.052805000	2.062695000	-3.323936000
C	8.295263000	2.934994000	-3.398569000
H	8.568819000	3.008731000	-4.459992000
C	8.026366000	4.358255000	-2.891280000
H	7.236931000	4.842344000	-3.474495000
H	7.708704000	4.352852000	-1.843435000
H	8.929712000	4.974213000	-2.967890000
C	9.485060000	2.304695000	-2.662235000
H	9.696726000	1.299147000	-3.039022000
H	10.386381000	2.914106000	-2.791741000
H	9.292138000	2.225383000	-1.586974000
C	6.439848000	1.605028000	-4.494178000
H	6.857139000	1.896176000	-5.457548000
C	5.312775000	0.778440000	-4.467154000
C	4.655621000	0.344693000	-5.766563000
H	5.371598000	0.561730000	-6.571471000
C	3.391124000	1.174296000	-6.038023000
H	3.619250000	2.244536000	-6.066960000
H	2.941683000	0.894869000	-6.997870000
H	2.645153000	1.015126000	-5.252435000
C	4.348821000	-1.156270000	-5.814235000
H	3.959906000	-1.433551000	-6.800298000
H	5.244050000	-1.754526000	-5.620665000
H	3.595074000	-1.439543000	-5.072686000
C	4.802166000	0.396056000	-3.223377000

SUPPORTING INFORMATION

H	3.948903000	-0.276339000	-3.179430000
N	-1.736036000	-0.203649000	3.064524000
N	-1.578896000	-0.401701000	5.636810000
O	0.795929000	-3.465777000	-1.092211000
O	-1.311877000	-2.350136000	0.331083000
O	1.135457000	1.974998000	0.643130000
O	-1.090255000	2.084780000	0.955481000
O	1.356761000	1.323791000	-2.395197000
O	-0.386005000	0.402044000	-1.388440000
H	0.130410000	3.683665000	0.990306000
H	-0.535237000	1.453844000	-3.132720000
C	1.505437000	-2.876802000	-1.887133000
O	1.926806000	-1.710943000	-1.970232000

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Sm	-1.976961000	0.055345000	0.445686000
Sm	2.089746000	0.013087000	-0.285780000
C	0.115709000	-1.747874000	0.520175000
C	0.113288000	2.753080000	0.421833000
O	0.292743000	-0.602074000	1.178881000
C	0.204060000	0.258281000	-2.526811000
C	-0.626126000	0.764821000	3.651035000
H	-0.349532000	1.702024000	3.162906000
H	0.091652000	0.010391000	3.330558000
C	-0.681655000	0.904848000	5.196355000
H	0.086635000	0.285313000	5.670834000
H	-0.500266000	1.938921000	5.509040000
C	-2.297591000	-0.958216000	3.720042000
H	-1.573256000	-1.683736000	3.337611000
H	-3.284980000	-1.258440000	3.357786000
C	-2.267652000	-0.869618000	5.272553000
H	-3.225355000	-1.184651000	5.701348000
H	-1.493349000	-1.523716000	5.687445000
C	-2.943197000	1.381231000	3.592377000
H	-3.920527000	1.158113000	3.157589000
H	-2.609206000	2.346041000	3.197609000
C	-3.007416000	1.388846000	5.144510000
H	-2.846701000	2.397448000	5.541145000
H	-3.989842000	1.052740000	5.492535000

SUPPORTING INFORMATION

C	-3.914237000	-0.866115000	-1.382855000
C	-4.602201000	-0.987292000	-0.138062000
C	-4.895527000	0.332273000	0.348522000
C	-4.359221000	1.269543000	-0.597976000
C	-3.762801000	0.532315000	-1.673436000
C	-3.725274000	-1.999800000	-2.333528000
C	-4.883049000	-2.602502000	-2.846994000
H	-5.847862000	-2.249325000	-2.495857000
C	-4.813777000	-3.620537000	-3.801886000
C	-6.054743000	-4.309292000	-4.345555000
H	-5.766856000	-4.770276000	-5.300683000
C	-7.215773000	-3.352332000	-4.631854000
H	-6.909355000	-2.537595000	-5.295324000
H	-8.041018000	-3.888966000	-5.112066000
H	-7.611256000	-2.907798000	-3.712505000
C	-6.495414000	-5.440307000	-3.403023000
H	-5.692963000	-6.170965000	-3.262003000
H	-6.757951000	-5.042289000	-2.417320000
H	-7.369375000	-5.965535000	-3.805141000
C	-3.550190000	-4.034385000	-4.227442000
H	-3.479239000	-4.822134000	-4.977312000
C	-2.371863000	-3.478356000	-3.718114000
C	-1.043141000	-4.046997000	-4.191819000
H	-1.156368000	-4.246488000	-5.267342000
C	0.145886000	-3.102245000	-4.021160000
H	-0.037248000	-2.135632000	-4.501217000
H	0.374919000	-2.928977000	-2.964185000
H	1.040383000	-3.536318000	-4.479573000
C	-0.766511000	-5.393958000	-3.504825000
H	-1.595824000	-6.093538000	-3.647880000
H	0.141554000	-5.855676000	-3.906891000
H	-0.627484000	-5.254332000	-2.427573000
C	-2.475015000	-2.453871000	-2.771535000
H	-1.579342000	-2.003456000	-2.359954000
C	-5.132321000	-2.274373000	0.385505000
C	-6.515121000	-2.446146000	0.542649000
H	-7.178640000	-1.613212000	0.323111000
C	-7.060132000	-3.660697000	0.968987000
C	-8.573505000	-3.794707000	1.078908000

SUPPORTING INFORMATION

H	-8.942821000	-2.843373000	1.487280000
C	-9.208361000	-3.970937000	-0.309836000
H	-8.932540000	-3.153138000	-0.982377000
H	-8.876789000	-4.908608000	-0.769168000
H	-10.301665000	-3.997550000	-0.238577000
C	-9.038771000	-4.910172000	2.017893000
H	-8.579533000	-4.829882000	3.008166000
H	-10.125428000	-4.866999000	2.144875000
H	-8.800581000	-5.901200000	1.615443000
C	-6.184375000	-4.716183000	1.245690000
H	-6.578954000	-5.670031000	1.586879000
C	-4.800657000	-4.582545000	1.095882000
C	-3.882616000	-5.757045000	1.388511000
H	-4.518027000	-6.576968000	1.751004000
C	-3.173137000	-6.245216000	0.118251000
H	-2.552358000	-7.122053000	0.334019000
H	-3.895721000	-6.519232000	-0.656333000
H	-2.523662000	-5.466152000	-0.293501000
C	-2.868660000	-5.434094000	2.493790000
H	-3.371772000	-5.102843000	3.408372000
H	-2.268506000	-6.317817000	2.737208000
H	-2.180273000	-4.643727000	2.177067000
C	-4.286013000	-3.355956000	0.661503000
H	-3.214327000	-3.237658000	0.522105000
C	-5.884648000	0.625691000	1.419911000
C	-5.929067000	-0.109749000	2.617670000
H	-5.197350000	-0.894770000	2.783306000
C	-6.916933000	0.095891000	3.582307000
C	-6.936763000	-0.739011000	4.852456000
H	-5.960916000	-1.239870000	4.921503000
C	-8.008010000	-1.835794000	4.772999000
H	-7.994132000	-2.462215000	5.672059000
H	-9.008209000	-1.397120000	4.684081000
H	-7.843434000	-2.478517000	3.903837000
C	-7.114279000	0.104560000	6.120820000
H	-6.367905000	0.902663000	6.184543000
H	-8.103223000	0.573956000	6.157022000
H	-7.019717000	-0.522082000	7.014125000
C	-7.905766000	1.051497000	3.325235000

SUPPORTING INFORMATION

H	-8.697679000	1.219923000	4.052399000
C	-7.913306000	1.790577000	2.141144000
C	-9.023836000	2.793476000	1.874139000
H	-9.744546000	2.695266000	2.697575000
C	-9.774415000	2.489814000	0.570886000
H	-10.619300000	3.175775000	0.444844000
H	-9.122634000	2.604816000	-0.301740000
H	-10.162794000	1.466583000	0.565060000
C	-8.502791000	4.236665000	1.887881000
H	-9.323257000	4.946393000	1.732632000
H	-8.027371000	4.472512000	2.845253000
H	-7.762519000	4.398816000	1.097224000
C	-6.894315000	1.576352000	1.206467000
H	-6.898980000	2.135532000	0.277403000
C	-4.617993000	2.734741000	-0.617877000
C	-5.354606000	3.271942000	-1.687982000
H	-5.687344000	2.605751000	-2.479832000
C	-5.667008000	4.628926000	-1.756480000
C	-6.460583000	5.178712000	-2.929994000
H	-6.739224000	4.320481000	-3.555851000
C	-7.758623000	5.863774000	-2.482926000
H	-8.381273000	5.187661000	-1.889051000
H	-7.554878000	6.750973000	-1.873071000
H	-8.341798000	6.188689000	-3.351577000
C	-5.609597000	6.119704000	-3.793867000
H	-6.178320000	6.468585000	-4.662984000
H	-5.294935000	7.002419000	-3.225959000
H	-4.709498000	5.614225000	-4.155935000
C	-5.219797000	5.464958000	-0.723657000
H	-5.444482000	6.529556000	-0.758314000
C	-4.486449000	4.969613000	0.356052000
C	-4.000522000	5.909245000	1.447412000
H	-4.374171000	6.911064000	1.195861000
C	-4.567376000	5.541975000	2.824423000
H	-5.660823000	5.531372000	2.812550000
H	-4.231557000	4.548804000	3.142072000
H	-4.239645000	6.262096000	3.582398000
C	-2.468179000	5.986929000	1.485149000
H	-2.065039000	6.300494000	0.517326000

SUPPORTING INFORMATION

H	-2.133661000	6.704206000	2.242962000
H	-2.031515000	5.012187000	1.728480000
C	-4.196958000	3.598960000	0.396447000
H	-3.618850000	3.199988000	1.224150000
C	-3.249445000	1.133149000	-2.931043000
C	-3.575387000	0.566023000	-4.170163000
H	-4.170622000	-0.340208000	-4.192638000
C	-3.176667000	1.159435000	-5.374488000
C	-3.557649000	0.550154000	-6.713370000
H	-3.154079000	1.212762000	-7.491228000
C	-5.079859000	0.495570000	-6.901843000
H	-5.529205000	1.487964000	-6.795107000
H	-5.332367000	0.111395000	-7.896408000
H	-5.547195000	-0.164268000	-6.162983000
C	-2.926712000	-0.834426000	-6.910957000
H	-1.835878000	-0.785410000	-6.834165000
H	-3.282140000	-1.546117000	-6.158548000
H	-3.179174000	-1.235684000	-7.898922000
C	-2.441802000	2.342747000	-5.320606000
H	-2.140026000	2.821527000	-6.251677000
C	-2.093077000	2.942791000	-4.102931000
C	-1.276629000	4.226515000	-4.131809000
H	-1.680200000	4.830177000	-4.957835000
C	-1.382969000	5.067155000	-2.859048000
H	-0.878315000	6.028740000	-2.998302000
H	-2.424212000	5.261774000	-2.585573000
H	-0.902022000	4.570450000	-2.009226000
C	0.193071000	3.927756000	-4.466666000
H	0.768189000	4.854713000	-4.564970000
H	0.656136000	3.325904000	-3.676920000
H	0.286295000	3.370285000	-5.403635000
C	-2.498300000	2.324285000	-2.920025000
H	-2.252165000	2.776787000	-1.965208000
C	4.600908000	1.179640000	0.230705000
C	4.251313000	0.490910000	1.440806000
C	4.287903000	-0.916024000	1.168680000
C	4.666557000	-1.095015000	-0.201673000
C	4.851928000	0.200339000	-0.782941000
C	4.925144000	2.623781000	0.106308000

SUPPORTING INFORMATION

C	4.378917000	3.437517000	-0.893967000
H	3.645979000	3.015940000	-1.576473000
C	4.763275000	4.775179000	-1.031092000
C	4.143957000	5.677320000	-2.085766000
H	4.746266000	6.595949000	-2.109936000
C	4.180703000	5.067165000	-3.491097000
H	3.802745000	5.782527000	-4.229901000
H	5.198917000	4.787593000	-3.775571000
H	3.560805000	4.167282000	-3.557585000
C	2.714270000	6.078069000	-1.694062000
H	2.693734000	6.558493000	-0.710559000
H	2.289908000	6.776895000	-2.423971000
H	2.062364000	5.198915000	-1.651590000
C	5.716793000	5.293298000	-0.148588000
H	6.015354000	6.332954000	-0.260612000
C	6.285700000	4.511320000	0.861804000
C	7.368026000	5.035334000	1.794301000
H	7.235103000	4.512908000	2.751687000
C	8.762625000	4.668781000	1.261762000
H	8.859990000	3.589123000	1.112293000
H	8.949916000	5.157553000	0.298968000
H	9.544632000	4.987422000	1.960437000
C	7.279612000	6.537606000	2.074835000
H	6.285085000	6.825805000	2.428843000
H	8.007476000	6.821836000	2.842002000
H	7.505793000	7.131607000	1.182276000
C	5.874002000	3.181065000	0.975557000
H	6.306751000	2.554389000	1.751466000
C	4.105381000	1.136030000	2.770956000
C	4.798145000	0.619523000	3.874812000
H	5.378490000	-0.289154000	3.749980000
C	4.778215000	1.263727000	5.116481000
C	5.556155000	0.715103000	6.301059000
H	5.444561000	1.440085000	7.119103000
C	4.983752000	-0.622115000	6.788497000
H	3.932282000	-0.516251000	7.073639000
H	5.041869000	-1.388319000	6.008343000
H	5.536603000	-0.986399000	7.661761000
C	7.055499000	0.596058000	5.996959000

SUPPORTING INFORMATION

H	7.472533000	1.555982000	5.676450000
H	7.604402000	0.265265000	6.885673000
H	7.244594000	-0.132451000	5.201377000
C	4.043281000	2.442832000	5.240087000
H	4.027129000	2.958242000	6.200182000
C	3.343071000	2.995549000	4.160839000
C	2.659161000	4.341076000	4.352266000
H	2.290370000	4.365731000	5.387835000
C	3.682961000	5.478234000	4.201843000
H	4.520780000	5.350585000	4.893929000
H	4.087991000	5.491852000	3.184299000
H	3.220206000	6.451807000	4.400799000
C	1.462939000	4.583198000	3.431355000
H	0.967219000	5.524223000	3.691740000
H	1.773755000	4.658374000	2.383938000
H	0.724165000	3.779434000	3.510751000
C	3.374845000	2.327112000	2.935244000
H	2.851287000	2.738014000	2.078116000
C	4.169527000	-2.006848000	2.171758000
C	5.264534000	-2.852756000	2.390362000
H	6.160137000	-2.708003000	1.792925000
C	5.224242000	-3.864870000	3.355384000
C	6.414247000	-4.781306000	3.586928000
H	6.182099000	-5.387279000	4.473580000
C	7.701929000	-4.003868000	3.888002000
H	7.571616000	-3.333102000	4.743120000
H	8.522009000	-4.692990000	4.118035000
H	8.013726000	-3.397666000	3.030674000
C	6.614325000	-5.744358000	2.408041000
H	5.720492000	-6.353244000	2.241261000
H	6.818542000	-5.198650000	1.481110000
H	7.456687000	-6.419408000	2.597376000
C	4.051406000	-4.030529000	4.095767000
H	4.011866000	-4.823427000	4.840813000
C	2.933024000	-3.212137000	3.896688000
C	1.651801000	-3.437557000	4.681282000
H	0.950402000	-2.648001000	4.377897000
C	1.010014000	-4.786490000	4.327200000
H	0.820897000	-4.865341000	3.252729000

SUPPORTING INFORMATION

H	1.662989000	-5.618567000	4.613019000
H	0.057748000	-4.916190000	4.853801000
C	1.863985000	-3.311566000	6.195223000
H	2.294322000	-2.340573000	6.456537000
H	0.914622000	-3.422637000	6.731496000
H	2.542735000	-4.086445000	6.567856000
C	3.012280000	-2.199628000	2.938797000
H	2.151744000	-1.555851000	2.773726000
C	5.036668000	-2.392789000	-0.820950000
C	4.200217000	-3.516023000	-0.753939000
H	3.220939000	-3.414210000	-0.297801000
C	4.618459000	-4.756523000	-1.245719000
C	3.735828000	-5.995105000	-1.206152000
H	4.397897000	-6.842059000	-0.973745000
C	2.646169000	-5.953382000	-0.133253000
H	3.065169000	-5.747044000	0.856517000
H	1.897243000	-5.183324000	-0.345661000
H	2.124539000	-6.915501000	-0.089025000
C	3.126615000	-6.260939000	-2.591730000
H	3.901492000	-6.347829000	-3.359973000
H	2.541205000	-7.187497000	-2.590318000
H	2.461759000	-5.439857000	-2.878925000
C	5.892677000	-4.856120000	-1.814296000
H	6.223403000	-5.825018000	-2.186449000
C	6.747450000	-3.754055000	-1.908096000
C	8.136480000	-3.881691000	-2.511589000
H	8.590104000	-2.882061000	-2.483634000
C	8.085512000	-4.323118000	-3.980140000
H	7.487478000	-3.630380000	-4.579618000
H	9.093183000	-4.363062000	-4.408896000
H	7.642834000	-5.320347000	-4.080233000
C	9.030577000	-4.818716000	-1.687709000
H	9.099980000	-4.486600000	-0.647190000
H	8.636915000	-5.841304000	-1.685137000
H	10.044203000	-4.854102000	-2.102740000
C	6.303831000	-2.529061000	-1.406870000
H	6.962129000	-1.665933000	-1.452899000
C	5.407040000	0.461844000	-2.137186000
C	6.610876000	1.170726000	-2.264539000

SUPPORTING INFORMATION

H	7.085564000	1.556186000	-1.366491000
C	7.211509000	1.365548000	-3.511061000
C	8.534393000	2.102156000	-3.643938000
H	8.825877000	2.045340000	-4.701710000
C	8.397688000	3.586868000	-3.281893000
H	7.658515000	4.080619000	-3.920131000
H	8.076187000	3.714115000	-2.243039000
H	9.354538000	4.106856000	-3.405937000
C	9.648269000	1.435120000	-2.825907000
H	9.766646000	0.382642000	-3.102139000
H	10.606126000	1.940771000	-2.991466000
H	9.434076000	1.476715000	-1.752537000
C	6.570265000	0.854533000	-4.643615000
H	7.026547000	1.002953000	-5.621664000
C	5.362336000	0.157578000	-4.558566000
C	4.678272000	-0.348706000	-5.817167000
H	5.369105000	-0.163469000	-6.651315000
C	3.388794000	0.436125000	-6.100092000
H	3.592722000	1.507572000	-6.193339000
H	2.924256000	0.094679000	-7.032283000
H	2.664349000	0.303983000	-5.289896000
C	4.405433000	-1.857054000	-5.771495000
H	3.970745000	-2.197260000	-6.718045000
H	5.324772000	-2.423295000	-5.595127000
H	3.700701000	-2.112779000	-4.973595000
C	4.797020000	-0.038371000	-3.294630000
H	3.862651000	-0.585879000	-3.208465000
N	-1.962532000	0.364995000	3.128260000
N	-1.992490000	0.499248000	5.707380000
O	1.122336000	-2.208762000	-0.103817000
O	-1.086484000	-2.179953000	0.464964000
O	1.202124000	2.168723000	0.185458000
O	-1.011538000	2.223404000	0.637859000
O	1.456878000	0.256013000	-2.644940000
O	-0.358140000	0.143332000	-1.391761000
H	0.144422000	3.855223000	0.449909000
H	-0.427561000	0.366941000	-3.418371000

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