Isolation and Redox Reactivity of Cerium Complexes in Four Redox States

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Experimental Procedures

Materials and Methods

General Considerations Unless otherwise noted, all manipulations were carried out at ambient temperature under an inert argon or nitrogen atmosphere using Schlenk techniques and an MBraun glovebox equipped with a purifier unit. The water and oxygen levels were always kept at less than 0.1 ppm. Glassware was dried overnight at 140°C before use.

NMR experiments were carried out using NMR tubes adapted with J-Young valves. NMR spectra were recorded on a Bruker 400 MHz or 500 or 600 MHz spectrometers. NMR chemical shifts are reported in ppm with solvent as internal reference.

Elemental analyses were performed under nitrogen using a Thermo Scientific Flash 2000 Organic Elemental Analyzer at the Institute of Chemistry and Chemical Engineering at EPFL.

UV-Vis spectra were recorded with a Perkin Elmer 750 spectrometer and 1 mm cuvettes equipped with a J-Young valve.

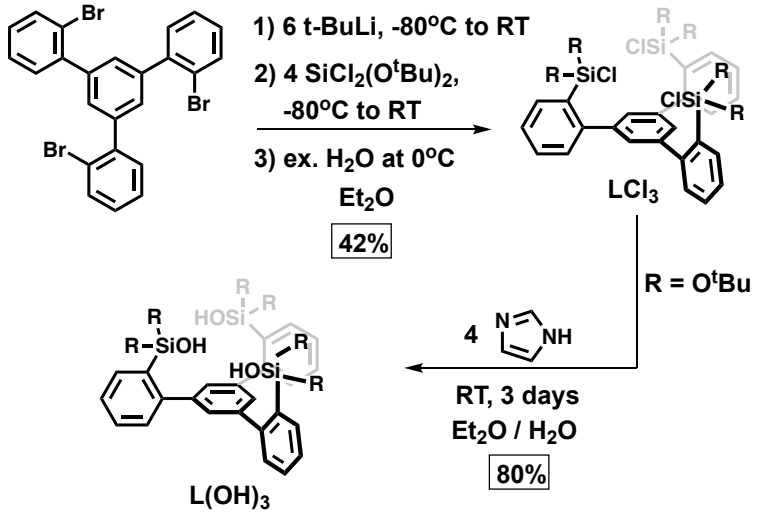
EPR analysis were performed on a Bruker Elexsys E500 spectrometer working at 9.4 GHz frequency with an Oxford ESR900 cryostat for 6-300 K operation.

Cyclic voltammetry data were carried out at room temperature in an argon-filled glovebox described above. Data were collected using a Biologic SP-300 potentiostat connected to a personal computer. All samples were saturated in complex with 0.1 M $[NBu_4][BPh_4]$ supporting electrolyte in THF solution. The experiments were carried out with a platinum disk (d = 5 mm) working electrode, a platinum wire counter electrode, and an Ag/AgCl reference electrode. Potential calibration was performed at the end of each data collection cycle using the ferrocene/ferrocenium $[Fe(C_5H_5)_2]^+/0$ couple as an internal standard.

Starting materials Unless otherwise noted, reagents were purchased from commercial suppliers and used without further purification. Anhydrous solvents were purchased from Aldrich and

further distilled from K/benzophenone (THF, toluene, diethyether), sodium sand/benzophenone (n-hexane). Deuterated solvents for NMR spectroscopy (THF-d_8, toluene-d_8) were purchased from Cortecnet, freeze-degassed and distilled over K/benzophenone. Precise amounts of gases are added to reaction flasks or NMR tubes equipped with a J-Young valve using a short connector of known volume adapted on a Schlenk line equipped with a pressure sensor. CO_2 (99.999%) was purchased from Carbagas, Switzerland. Potassium bis(trimethylsilyl)amide (KHMDS), cerium chloride, triethylphosphine oxide and sulfur (S_8) were purchased from Sigma-Aldrich and dried under high vacuum prior to use. *Tert*-butyllithium solution (1.7 M in pentane), imidazole, iodine were purchased from Sigma-Aldrich and used as received. KC_8[1], $[Ce(N(SiMe_3)_2)_3Cl]$[2], 1,3,5-tris-2'-bromophenylbenzene[3], $SiCl_2(O^tBu)_2$[4] were prepared according to the published procedure.

Synthesis and Reactivity



Scheme S1: Synthesis of 1,3,5-(2-HOSi(O^tBu)$_2$$C_6H_4$)$_3$$C_6H_3$, **L(OH)$_3$**

Synthesis of tripodal tris(ditert-butoxylchlorosilane) ligand, 1,3,5-(2-SiCl(O^tBu)$_2$$C_6H_4$)$_3$$C_6H_3$, LCl_3

A round-bottomed Schlenk flask was equipped with a glass-coated stir bar and charged with 1,3,5-tris-2'-bromophenylbenzene (2.06 g, 3.79 mmol, 1.0 equiv.) and Et_2O (15 mL). The resulting mixture was cooled to −80 °C for 15 mins. A solution of *tert*-butyllithium (1.7 M in heptane) (14.0 mL, 23.8 mmol, 6.0 equiv.) was added dropwise and the resulting in a black reaction mixture. The solution was allowed to warm to room temperature. After stirring at room temperature for 30

mins, the mixture was cooled to -80 °C and $SiCl_2(O^tBu)_2$ (3.99 g, 15.3 mmol, 4.0 equiv.) was added dropwise. The mixture was allowed to warm to room temperature and stirred overnight. The reaction was carefully quenched with water and extracted with $CHCl_3$ (3 x 30 mL). The combined organic solution were dried over $MgSO_4$, filtered and concentrated in vacuo, yielding a yellow oily residue. The yellow residue was recrystallized in concentrated hexane at -40 °C overnight affording light-yellow powder of **LCl_3**. (1.48 g, 42%). X-ray quality crystals were obtained by cooling a concentrated hexane solution to -40 °C (**Figure S78**). ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ 8.00 ppm (d, *J* = 6.9 Hz, 3H, arene), δ 7.78 ppm (s, 3H, arene), δ 7.53 ppm (d, *J* = 7.4 Hz, 3H, arene), δ 7.45 ppm (td, *J* = 7.5, 1.5 Hz, 3H, arene), δ 7.34 ppm (td, *J* = 7.4, 1.3 Hz, 3H, arene), δ 1.18 ppm (s, 54H, $OSi(O^tBu)_2$) (**Figure S2**). $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$, 298 K): δ 148.61 ppm (tripodal arene), δ 142.39 ppm (tripodal arene), δ 135.90 ppm (tripodal arene), δ 133.01 ppm (tripodal arene), δ 131.48 ppm (tripodal arene), δ 129.97 ppm (tripodal arene), δ 129.78 ppm (tripodal arene), δ 125.69 ppm (tripodal arene), δ 75.91 ppm ($OSi(O^tBu)_2$), δ 31.15 ppm ($OSi(O^tBu)_2$) (**Figure S3**). $^{29}Si\{^1H\}$ NMR (119 MHz, $CDCl_3$, 298 K): δ -57.06 ppm ($OSi(O^tBu)_2$) (**Figure S4**). *Anal. Calcd.* for $C_{48}H_{69}Cl_3O_6Si_3$: C: 61.81; H: 7.46; N: 0.00. *Found*: C: 61.53; H: 7.30; N: 0.00.

Synthesis of tripodal tris(ditert-butoxylsilanol) ligand, 1,3,5-(2-$HOSi(O^tBu)_2C_6H_4)_3C_6H_3$, $L(OH)_3$

A water solution (10 mL) of imidazole (270 mg, 3.97 mmol, 4.0 equiv.) was added to a solution of **LCl_3** (0.921 g, 0.987 mmol, 1.0 equiv.) in Et_2O (10 mL). The resulting mixture was stirred at room temperature for 3 days. The reaction mixture was extracted with DCM (3 x 30 mL) and acidic water (pH = 3). The combined organic solution were dried over $MgSO_4$, filtered and concentrated in vacuo, yielding a light-yellow residue. The light-yellow residue was recrystallized in concentrated THF/hexane at -40 °C overnight affording colorless powder of **$L(OH)_3$**. (0.692 g, 80%). X-ray quality crystals were obtained by slow evaporation of a concentrated hexane solution at room temperature (**Figure S79**). ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ 7.91 ppm (d, *J* = 7.4 Hz, 3H, arene), δ 7.74 ppm (s, 3H, arene), δ 7.49 – 7.34 ppm (m, 6H, arene), δ 7.32 ppm (ddd, *J* = 7.5, 5.4, 3.3 Hz, 3H, arene), δ 3.71 ppm (s, 3H, SiOH), δ 1.16 ppm (s, 54H, $OSi(O^tBu)_2$) (**Figure S6**). $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$, 298 K): δ 148.22 ppm (tripodal arene), δ 143.83 ppm (tripodal arene), δ 136.50 ppm (tripodal arene), δ 135.44 ppm (tripodal arene), δ 129.24 ppm (tripodal arene), δ

128.93 ppm (tripodal arene), δ 128.37 ppm (tripodal arene), δ 125.76 ppm (tripodal arene), δ 73.47 ppm (OSi(O^{t}Bu)$_2$), δ 31.57 ppm (OSi(O^{t}Bu)$_2$) (**Figure S7**). ^{29}Si{^{1}H} NMR (119 MHz, $CDCl_3$, 298 K): δ -66.17 ppm (OSi(O^{t}Bu)$_2$) (**Figure S8**). *Anal. Calcd.* for $C_{48}H_{72}O_9Si_3$: C: 65.71; H: 8.27; N: 0.00. *Found*: C: 65.66; H: 8.13; N: 0.00.

Synthesis of tripodal tris potassium(ditert-butoxylsilicate) ligand, 1,3,5-(2-KOSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$, L(OK)$_3$

A colorless solution of KHMDS (266.9 mg, 1.338 mmol, 3.0 equiv.) in THF (3.0 mL) was added to a stirring colorless solution of free ligand **L(OH)$_3$** (391.2 mg, 0.4459 mmol, 1.0 equiv.) in THF (2.0 mL). The reaction mixture was stirred for 3 h at room temperature, yielding a white suspension. The reaction mixture was filtered on a porosity 4 glass frit, yielding white powder. The resulting powder was washed by hexane (3.0 mL) affording analytically pure product **L(OK)$_3$** (408.7 mg, 92%). ^{1}H NMR (400 MHz, THF-d_8, 298 K): δ 8.15 ppm (s, 3H, arene), δ 8.12 ppm (d, 3H, arene), δ 7.24 – 7.07 ppm (m, 9H, arene), δ 1.24 ppm (s, 54H, OSi(O^{t}Bu)$_2$) (**Figure S10**). ^{13}C{^{1}H} NMR (151 MHz, THF-d_8, 298 K): δ 148.63 ppm (tripodal arene), δ 145.80 ppm (tripodal arene), δ 144.17 ppm (tripodal arene), δ 138.36 ppm (tripodal arene), δ 131.74 ppm (tripodal arene), δ 129.86 ppm (tripodal arene), δ 127.93 ppm (tripodal arene), δ 125.93 ppm (tripodal arene), δ 71.32 ppm (OSi(O^{t}Bu)$_2$), δ 32.60 ppm (OSi(O^{t}Bu)$_2$) (**Figure S11**). ^{29}Si{^{1}H} NMR (119 MHz, THF-d_8, 298 K): δ -69.14 ppm (OSi(O^{t}Bu)$_2$) (**Figure S12**). *Anal. Calcd.* for $C_{48}H_{69}K_3O_9Si_3(THF)_{2.8}$: C: 59.58; H: 7.72; N: 0.00. *Found*: C: 59.35; H: 7.64; N: 0.00.

Synthesis of [K(THF)$_3${1,3,5-(2-KOSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$}]$_2$, [(K(THF)$_3$)(L(OK)$_3$)]$_2$

A bronze suspension of KC_8 (4.1 mg, 0.030 mmol, 1.0 equiv.) in THF (1.0 mL) was added to a stirring white suspension of ligand **L(OK)$_3$** (28.8 mg, 0.0290 mmol, 1.0 equiv.) in THF (1.0 mL). The reaction mixture was stirred for 2 h at room temperature. The reaction mixture was filtered on a porosity 4 glass frit, yielding a dark blue-green solution. The volatiles were removed under vacuum and the residue was dissolved in THF (0.1 mL). The resulting solution was stored at -40 ^{o}C overnight affording dark crystals of **[(K(THF)$_3$)(L(OK)$_3$)]$_2$** (23.8 mg, 66%). X-ray quality crystals were obtained by cooling a concentrated THF solution to -40 ^{o}C (**Figure S80**). ^{1}H NMR (400 MHz, THF-d_8, 298 K): δ

1.19 ppm (br s) (**Figure S14**). ^{1}H NMR (400 MHz, THF-d_8, 233 K): δ 8.14 ppm (br s), δ 7.12 ppm (br s), δ 1.35 ppm (br s) (**Figure S14**). *Anal. Calcd.* for $C_{96}H_{138}K_8O_{18}Si_6(THF)_2$: C: 56.63; H: 7.04; N: 0.00. *Found*: C: 56.62; H: 6.98; N: 0.00.

Synthesis of [K(2.2.2-cryptand)]$_2$[{1,3,5-(2-KOSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$}]$_2$, [(K(crypt))(L(OK)$_3$)]$_2$

A colorless solution of 2.2.2-cryptand (3.1 mg, 0.0082 mmol, 2.0 equiv.) in THF (0.5 mL) was added to a dark blue-green solution of ligand **[(K(THF)$_3$)(L(OK)$_3$)]$_2$** (10.4 mg, 0.00417 mmol, 1.0 equiv.) in THF (0.5 mL). The reaction mixture was stirred for 30 min at room temperature. The volatiles were removed under vacuum, yielding an analytically pure dark blue-green powder. X-ray quality crystals were obtained by cooling a concentrated THF/hexane solution to -40 °C (**Figure S81**). ^{1}H NMR (400 MHz, THF-d_8, 298 K): δ 1.22 ppm (s), δ 2.53 ppm (s), δ 3.52 ppm (s) (**Figure S16**). ^{1}H NMR (400 MHz, THF-d_8, 233 K): δ 0.99–1.32 ppm (m), δ 2.51 ppm (br s), δ 6.99–7.10 ppm (m), δ 8.05–8.42 ppm (m) (**Figure S16**). *Anal. Calcd.* for $C_{132}H_{210}K_8N_4O_{30}Si_6$: C: 56.33; H: 7.52; N: 1.99. *Found*: C: 56.41; H: 7.82; N: 1.77.

Reaction of complex L(OK)$_3$ with 2 equiv. of KC$_8$

A bronze suspension of KC_8 (2.7 mg, 0.020 mmol, 2.0 equiv.) in THF-d_8 (0.25 mL) was added to a stirring white suspension of ligand **L(OK)$_3$** (9.6 mg, 0.0097 mmol, 1.0 equiv.) in THF-d_8 (0.25 mL). The reaction mixture was stirred for 2 h at room temperature. The reaction mixture was filtered on a porosity 4 glass frit, yielding a dark blue-green solution. The ^{1}H NMR spectrum of the resulting solution showed the appearance of **[(K(THF)$_3$)(L(OK)$_3$)]$_2$** and multiple resonances (**Figure S17**).

Synthesis of [(1,3,5-(2-OSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$)Ce(THF)], 1

A cold (-40 °C) yellow solution of [Ce(HMDS)$_3$] (180.2 mg, 0.2900 mmol, 1.0 equiv.) in THF (1.0 mL) was added to a cold (-40 °C) stirring colorless solution of free ligand **L(OH)$_3$** (254.5 mg, 0.2901 mmol, 1.0 equiv.) in THF (2.0 mL). The reaction mixture was then warmed to room temperature and stirred for 16 h, yielding a light-yellow solution. The volatiles were removed under vacuum and the residue was dissolved in toluene (1.0 mL). The resulting solution was stored at -40 °C

overnight affording light-yellow crystals of complex **1** (285.3 mg, 91%). X-ray quality crystals were obtained by cooling a concentrated toluene solution to -40 °C. ^{1}H NMR (400 MHz, THF-d_8, 298 K): δ 9.81 ppm (d, *J* = 7.5 Hz, 3H, arene), δ 7.69 ppm (t, *J* = 7.4 Hz, 3H, arene), δ 6.58 ppm (t, *J* = 7.3 Hz, 3H, arene), δ 3.40 ppm (s, 54H, OSi(O^{t}Bu)$_2$), δ 0.20 ppm (br s, 3H, arene) (**Figure S19**). One signal of the tripodal ligand is missing, possibly because of signal overlap. *Anal. Calcd.* for $C_{52}H_{77}O_{10}Si_3Ce$: C: 57.48; H: 7.14; N: 0.00. *Found*: C: 57.57; H: 7.24; N: 0.00.

Synthesis of [1,3,5-(2-OSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$)CeCl], 2

A cold (-40 °C) dark-purple solution of [CeCl(N(SiMe$_3$)$_2$)$_3$] (13.4 mg, 0.0204 mmol, 1.0 equiv.) in toluene (0.5 mL) was added to a cold (-40 °C) stirring colorless solution of free ligand **L(OH)$_3$** (17.9 mg, 0.0204 mmol, 1.0 equiv.) in toluene (0.5 mL). The reaction mixture was then warmed to room temperature and stirred for 3 h, yielding an orange solution. The volatiles were removed under vacuum and the residue was dissolved in toluene (1.0 mL). The resulting solution was stored at -40 °C overnight affording light-yellow crystals of complex **2** (20.4 mg, 95%). X-ray quality crystals were obtained by cooling a concentrated toluene solution to -40 °C. ^{1}H NMR (400 MHz, toluene-d_8, 298 K): δ 8.59 ppm (s, 3H, arene), δ 8.09–7.94 ppm (m, 3H, arene), δ 7.28–7.15 ppm (m, 6H, arene), δ 1.34 ppm (s, 54H, OSi(O^{t}Bu)$_2$) (**Figure S21**). One signal of the tripodal ligand is missing, possibly because of signal overlap with toluene. Complex **2** is stable in toluene solution at room temperature for up to 2 weeks (**Figure S22**), but begins to decompose in THF at room temperature immediately (**Figure S23**). *Anal. Calcd.* for $C_{48}H_{69}ClO_9Si_3Ce$: C: 54.91; H: 6.62; N: 0.00. *Found*: C: 54.79; H: 6.65; N: 0.00.

Reaction of complex 2 with 1 equiv. of KC$_8$

A bronze suspension of KC_8 (0.8 mg, 0.006 mmol, 1.0 equiv.) in toluene-d_8 (0.25 mL) was added to a stirring orange solution of **2** (5.5 mg, 0.0052 mmol, 1.0 equiv.) in toluene-d_8 (0.25 mL). The reaction mixture was stirred for 1 h at room temperature, resulting in a light-yellow suspension with concomitant formation of graphite and KCl. The reaction mixture was filtered on a porosity 4 glass frit, yielding a light-yellow solution. The ^{1}H NMR spectrum of the resulting solution showed one product assigned to complex **1** (**Figure S24**).

Reduction of complex 1

A bronze suspension of KC_8 (2.8 mg, 0.021 mmol, 1.0 equiv.) in THF (0.5 mL) was added to a stirring light-yellow solution of complex **1** (20.9 mg, 0.0192 mmol, 1.0 equiv.) in THF (1.0 mL). The reaction mixture was stirred for 16 h at -40 °C. The reaction mixture was filtered on a porosity 4 glass frit, yielding a dark-blue solution and ^{1}H NMR spectrum of the residue was recorded. ^{1}H NMR (400 MHz, THF-d_8, 298 K): δ 1.59 ppm (s, 54H, OSi(O^{t}Bu)$_2$) (**Figure S26**). ^{1}H NMR (400 MHz, THF-d_8, 233 K): δ 28.62 ppm (s, 3H, arene), δ 22.03 ppm (s, 3H, arene), δ 2.08 ppm (s, 27H, OSi(O^{t}Bu)$_2$), δ -0.63 ppm (s, 27H, OSi(O^{t}Bu)$_2$), δ -36.85 ppm (s, 3H, arene), δ -59.77 ppm (s, 3H, arene) (**Figure S27**). The volatiles were removed under vacuum and the residue was dissolved in THF (0.1 mL) and hexane (0.2 mL). The resulting solution was stored at -40 °C overnight affording dark-blue crystals (21.2 mg). X-ray crystallography proved unsuccessful after multiple trails, but elemental analysis of the product was consistent with the formula [{K(1,3,5-(2-OSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$)Ce(THF)}] *Anal. Calcd.* for $C_{52}H_{77}KO_{10}Si_3Ce$: C: 55.49; H: 6.90; N: 0.00. *Found*: C: 55.49; H: 7.03; N: 0.00. The ^{1}H NMR spectrum of a THF-d_8 solution of the residue after addition of 1 equiv. 2.2.2-cryptand showed the presence of complex **3** (**Figure S28**).

Synthesis of [K(2.2.2-cryptand)][(1,3,5-(2-OSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$)Ce(THF)], 3

A bronze suspension of KC_8 (7.7 mg, 0.057 mmol, 1.0 equiv.) in THF (1.0 mL) was added to a stirring light-yellow solution of complex **1** (61.0 mg, 0.0561 mmol, 1.0 equiv.) and 2.2.2-cryptand (21.2 mg, 0.0563 mmol, 1.0 equiv.) in THF (2.0 mL). The reaction mixture was stirred for 16 h at -40 °C. The reaction mixture was filtered on a porosity 4 glass frit, yielding a dark-blue solution. The volatiles were removed under vacuum and the residue was dissolved in Et_2O (0.1 mL) and hexane (0.2 mL). The resulting solution was stored at -40 °C overnight affording dark-blue crystals of complex **3** (77.9 mg, 92%). X-ray quality crystals were obtained by cooling a concentrated THF/Et_2O solution to -40 °C. ^{1}H NMR (400 MHz, THF-d_8, 298 K): δ 27.70 ppm (s, 3H. arene), δ 19.87 ppm (s, 3H. arene), δ 3.67 ppm (s, 12H, cryptand), δ 3.62 (t, J = 4.6 Hz, 12H, cryptand), δ 2.64 ppm (t, J = 4.6 Hz, 12H, cryptand), δ 1.58 ppm (br s, 54H, OSi(O^{t}Bu)$_2$), δ -31.44 ppm (s, 3H, arene), δ -50.00 ppm (s, 3H, arene) (**Figure S30**). ^{1}H NMR (400 MHz, THF-d_8, 233 K): δ 29.01 ppm (s, 3H, arene), δ 22.05 ppm (s, 3H, arene), δ 4.05 ppm (s, 12H, cryptand), δ 3.95 ppm (s, 12H, cryptand),

δ 2.94 ppm (s, 12H, cryptand), δ 2.10 ppm (s, 27H, OSi(O^{t}Bu)$_2$), δ -0.63 ppm (s, 27H, OSi(O^{t}Bu)$_2$), δ -37.37 ppm (s, 3H, arene), δ -60.51 ppm (s, 3H, arene) (**Figure S31**). One signal of the tripodal ligand is missing, possibly because of signal overlap or broadening. Complex **3** is stable in THF solution at room temperature at least for 1 week (**Figure S32**). *Anal. Calcd.* for $C_{70}H_{113}KN_2O_{16}Si_3Ce$: C: 55.97; H: 7.58; N: 1.86. *Found*: C: 55.70; H: 7.58; N: 1.72.

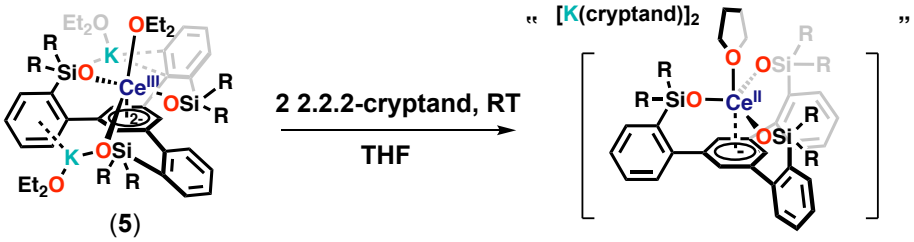
Synthesis of [K(2.2.2-cryptand)][(1,3,5-(2-OSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$)Ce(Et$_3$PO)], 4

A colorless solution of triethylphosphine oxide (1.8 mg, 0.013 mmol, 1.0 equiv.) in THF (0.5 mL) was added to a dark-blue solution of complex **3** (20.6 mg, 0.0137 mmol, 1.0 equiv.) in THF (0.5 mL). The reaction mixture was stirred for 30 mins at room temperature. The volatiles were removed under vacuum and the residue was dissolved in hexane (0.1 mL) and Et_2O (1 drop). The resulting solution was stored at -40 ^{o}C overnight affording dark-blue crystals of complex **4** (18.1 mg, 84%). X-ray quality crystals were obtained by cooling a concentrated Et_2O/THF solution to -40 ^{o}C. ^{1}H NMR (400 MHz, THF-d_8, 298 K): δ 27.68 ppm (s, 3H, arene), δ 19.87 ppm (s, 3H, arene), δ 3.74 ppm (s, 12H, cryptand), δ 3.68 ppm (t, J = 4.9 Hz, 12H, cryptand), δ 2.71 ppm (s, 12H, cryptand), δ 1.56 ppm (br s, 60H, OSi(O^{t}Bu)$_2$ and OPEt$_3$), δ 1.08 ppm (br s, 9H, OPEt$_3$), δ -31.39 ppm (s, 3H, arene), δ -49.90 ppm (s, 3H, arene) (**Figure S34**). One signal of the tripodal ligand is missing, possibly because of signal overlap or broadening.^{31}P{^{1}H} NMR (162 MHz, THF-d_8): δ -45.06 ppm (OPEt$_3$) (**Figure S35**). *Anal. Calcd.* for $C_{72}H_{120}KN_2O_{16}PSi_3Ce$: C: 55.29; H: 7.73; N: 1.79. *Found*: C: 55.13; H: 7.75; N: 1.67.

Synthesis of [K$_2${1,3,5-(2-OSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$)Ce(Et$_2$O)$_3$}], 5

A bronze suspension of KC_8 (21.5 mg, 0.159 mmol, 2.0 equiv.) in THF (1.5 mL) was added to a stirring light-yellow solution of complex **1** (85.4 mg, 0.0786 mmol, 1.0 equiv.) in THF (1.5 mL). The reaction mixture was stirred for 16 h at -40 ^{o}C. The reaction mixture was filtered on a porosity 4 glass frit, yielding a dark-purple solution. The volatiles were removed under vacuum and the residue was dissolved in Et_2O (0.1 mL) and hexane (0.2 mL). The resulting solution was stored at -40 ^{o}C overnight affording dark-purple crystals of complex **5** (62.1 mg, 60%). X-ray quality crystals were obtained by cooling a concentrated Et_2O/toluene solution to -40 ^{o}C. ^{1}H NMR (400 MHz, THF-

d_8, 298 K): NMR silent (**Figure S38**). ^{1}H NMR (400 MHz, THF-d_8, 233 K): δ 28.51 ppm (s), δ 22.12 ppm (s), δ 9.57 ppm (br s), δ 4.08 ppm (br s), δ 2.08 ppm (s), δ -0.70 ppm (s), δ -3.87 ppm (br s), δ -36.75 ppm (s), δ -59.63 ppm (s) (**Figure S39**). Complex **5** is stable in THF solution at room temperature for 3 days (**Figure S40**). *Anal. Calcd.* for $C_{48}H_{69}K_2O_9Si_3Ce$: C: 52.76; H: 6.38; N: 0.00. *Found*: C: 52.71; H: 6.61; N: 0.00.



Scheme S2: Addition of 2 equiv. of 2.2.2-cryptand to **5**.

Addition of 2 equiv. of 2.2.2-cryptand to a THF-d_8 solution of **5** resulted in a new ^{1}H NMR spectrum (**Figure S41-S42**). ^{1}H NMR (400 MHz, THF-d_8, 298 K): δ 3.05 ppm (s, 12H, cryptand), δ 3.01 ppm (s, 12H, cryptand), δ 2.02 ppm (s, 12H, cryptand) (**Figure S41**). ^{1}H NMR (400 MHz, THF-d_8, 233 K): δ 3.60 ppm (s, cryptand), δ 3.47 ppm (s, cryptand), δ 3.18 ppm (br s), δ 2.50 ppm (s, cryptand), δ 2.14 ppm (br s), δ 0.85 ppm (br s) (**Figure S43**).

Reaction of complex 1 with 1 equiv. of AgCl at room temperature and 70 °C

A white suspension of AgCl (1.5 mg, 0.010 mmol, 1.0 equiv.) in THF-d_8 (0.25 mL) was added to a light-yellow solution of complex **1** (10.1 mg, 0.00930 mmol, 1.0 equiv.) in THF-d_8 (0.25 mL). The reaction mixture was stirred at room temperature for 2 days. The ^{1}H NMR spectrum of the reaction mixture showed only one set of resonance assigned to unreacted **1** (**Figure S44**). The reaction mixture was then heated to 70 °C for 2 days. The ^{1}H NMR spectrum of the resulting solution showed only one product assigned to unreacted **1** (**Figure S44**).

Reaction of complex 1 with 1 equiv. of $AgBPh_4$ at room temperature and 70 °C

A white suspension of $AgBPh_4$ (4.8 mg, 0.011 mmol, 1.0 equiv.) in THF-d_8 (0.25 mL) was added to a light-yellow solution of complex **1** (12.1 mg, 0.0111 mmol, 1.0 equiv.) in THF-d_8 (0.25 mL). The reaction mixture was stirred at room temperature for 4 h. The ^{1}H NMR spectrum of the reaction mixture showed two set of resonance assigned to unreacted **1** and unknown species (**Figure S45**). The reaction mixture was then heated to 70 °C for 2 days. The ^{1}H NMR spectrum of the resulting solution showed unreacted **1** and unknown species (**Figure S45**).

Reaction of complex 3 with 1 equiv. of $AgBPh_4$

A white suspension of $AgBPh_4$ (2.1 mg, 0.0049 mmol, 1.0 equiv.) in THF-d_8 (0.25 mL) was added to a dark-blue solution of complex **3** (7.3 mg, 0.0049 mmol, 1.0 equiv.) in THF-d_8 (0.25 mL), yielding a light-yellow suspension with concomitant formation of [K(2.2.2-cryptand)][BPh_4] and Ag. The ^{1}H NMR spectrum of the reaction mixture showed one product assigned to complex **1** (**Figure S46**).

Synthesis of $[K(2.2.2\text{-cryptand})]_2[\{(1,3,5\text{-}(2\text{-}OSi(O^tBu)_2C_6H_4)_3C_6H_3)Ce)_2(\mu\text{-}C_2O_4)\}]$, 6

From complex 3 NMR scale:

A dark-blue solution of complex **3** (10.9 mg, 0.00726 mmol, 1.0 equiv.) in THF-d_8 (0.5 mL) was transferred in a J-Young adapted NMR tube and connected to a Schlenk line. The solution was degassed by three cycles of freeze-pump-thawing and 1 atm CO_2 was added to the reaction mixture, yielding a colorless solution immediately. The ^{1}H NMR spectrum of the resulting solution showed the appearance of a new set of resonance assigned to complex **6 (Figure S47)**. TMS_2O (3.0 µL) was added and used as internal standard to determine a conversion of 73% (**Figure S48**).

From complex 3 preparatory scale:

A dark-blue solution of complex **3** (24.4 mg, 0.0162 mmol, 1.0 equiv.) in THF (0.5 mL) was transferred in a J-Young adapted NMR tube and connected to a Schlenk line. The solution was degassed by three cycles of freeze-pump-thawing and 1 atm CO_2 was added to the reaction mixture, yielding a colorless solution immediately. The volatiles were removed under vacuum and the residue was dissolved in THF (0.1 mL). The resulting solution was stored at room temperature

overnight affording colorless crystals of complex **6**. (12.5 mg, 52%). X-ray quality crystals of **6** could be isolated from concentrated THF solution of **6** at room temperature. ^{1}H NMR (400 MHz, THF-d_8, 298 K): δ 8.97 ppm (d, *J* = 7.7 Hz, 3H, arene), δ 6.88 ppm (t, *J* = 7.5 Hz, 3H, arene), δ 5.83 ppm (t, *J* = 7.3 Hz, 3H, arene), δ 3.42 ppm (s, 12H, cryptand), δ 3.38 ppm (t, *J* = 4.3 Hz, 12H, cryptand), δ 3.20 ppm (s, 54H, OSi(O^{t}Bu)$_2$), δ 2.91 ppm (d, *J* = 7.2 Hz, 3H, arene), δ 2.39 ppm (t, *J* = 4.6 Hz, 12H, cryptand), δ -1.34 ppm (s, 3H, arene) (**Figure S49**). *Anal. Calcd.* for $C_{134}H_{210}K_2N_4O_{34}Si_6Ce_2$: C: 54.59; H: 7.18; N: 1.90. *Found*: C: 54.52; H: 7.01; N: 1.99.

Reaction of complex 5 with 2 equiv. of $AgBPh_4$

A white suspension of $AgBPh_4$ (5.2 mg, 0.012 mmol, 1.0 equiv.) in THF-d_8 (0.25 mL) was added to a dark-purple solution of complex **5** (8.0 mg, 0.0061 mmol, 1.0 equiv.) in THF-d_8 (0.25 mL), yielding a light-yellow suspension with concomitant formation of $KBPh_4$ and Ag. The ^{1}H NMR spectrum of the reaction mixture showed one product assigned to complex **1** (**Figure S50**).

Reaction of complex 5 with 1 equiv. of I_2

An orange solution of I_2 (1.8 mg, 0.0071 mmol, 1.0 equiv.) in THF-d_8 (0.25 mL) was added to a dark-purple solution of complex **5** (9.3 mg, 0.0071 mmol, 1.0 equiv.) in THF-d_8 (0.25 mL), yielding a light-yellow suspension with concomitant formation of KI. The ^{1}H NMR spectrum of the reaction mixture showed only one product assigned to complex **1** (**Figure S51**). TMS_2O (2.0 µL) was added and used as internal standard to determine a conversion of 99% (**Figure S52**).

Reaction of complex 5 with 1 equiv. of S_8

A dark-purple solution of complex **5** (7.3 mg, 0.0056 mmol, 1.0 equiv.) in THF-d_8 (0.25 mL) was added to a yellow suspension of S_8 (1.4 mg, 0.0055 mmol, 1.0 equiv.) in THF-d_8 (0.25 mL), yielding a light-yellow solution immediately. The ^{1}H NMR spectrum of the reaction mixture showed two set of resonance assigned to complex **1** and unknown species (**Figure S53**).

Reaction of complex 5 with 2 equiv. of 2.2.2-cryptand and 1 equiv. of S_8

A dark-purple solution of complex **5** (6.3 mg, 0.0048 mmol, 1.0 equiv.) and 2.2.2-cryptand (3.7 mg, 0.0098 mmol, 2.0 equiv.) in THF-d_8 (0.3 mL) was added to a yellow suspension of S_8 (1.2 mg, 0.0047 mmol, 1.0 equiv.) in THF-d_8 (0.2 mL), yielding a dark-red solution immediately. The ^{1}H NMR spectrum of the resulting solution showed the appearance of multiple new resonances (**Figure S54**). A few X-ray quality crystals of one of the products, [K(2.2.2-cryptand]$_2$[S_{10}] could be isolated from concentrated THF solution at room temperature.

NMR spectroscopic data

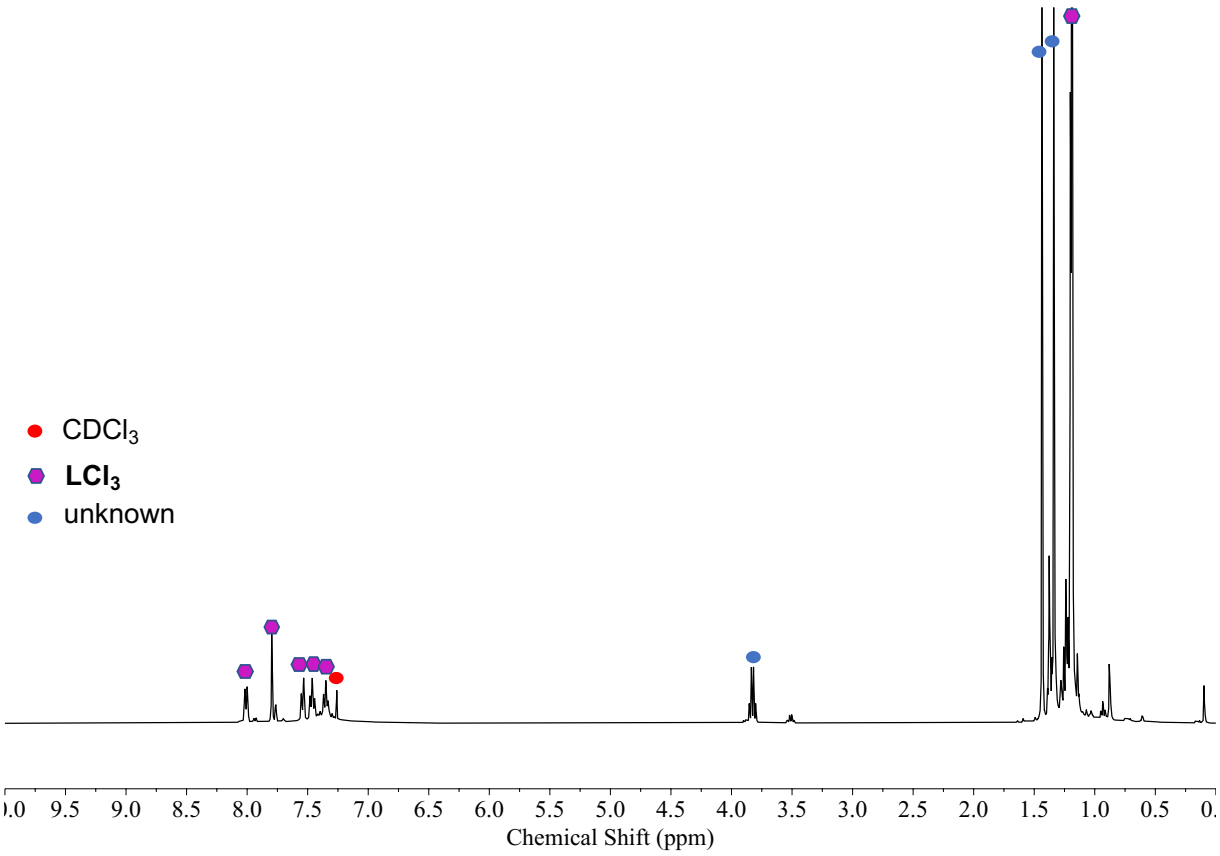


Figure S1: ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of the reaction mixture of 1,3,5-(2-$SiCl(O^tBu)_2C_6H_4)_3C_6H_3$, **$LCl_3$**.

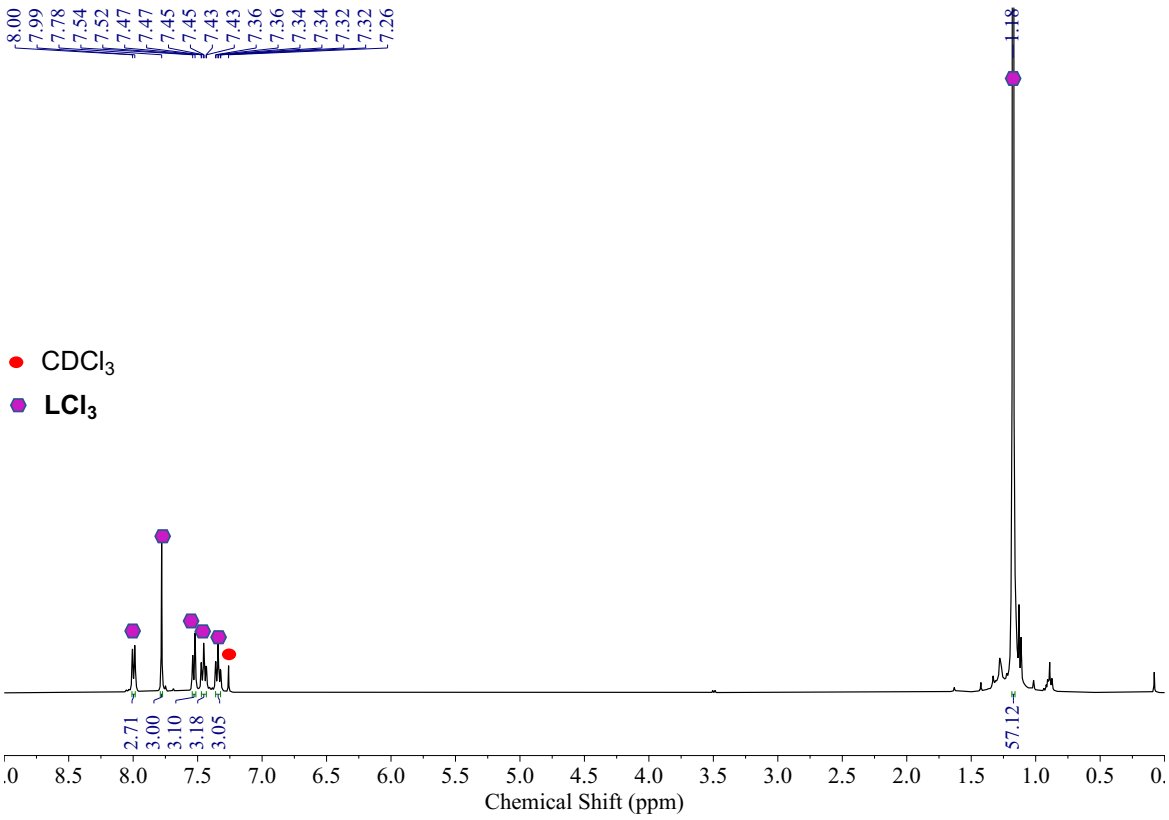


Figure S2: ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of isolated 1,3,5-(2-SiCl(O^tBu)$_2C_6H_4$)$_3C_6H_3$, **LCl_3**.

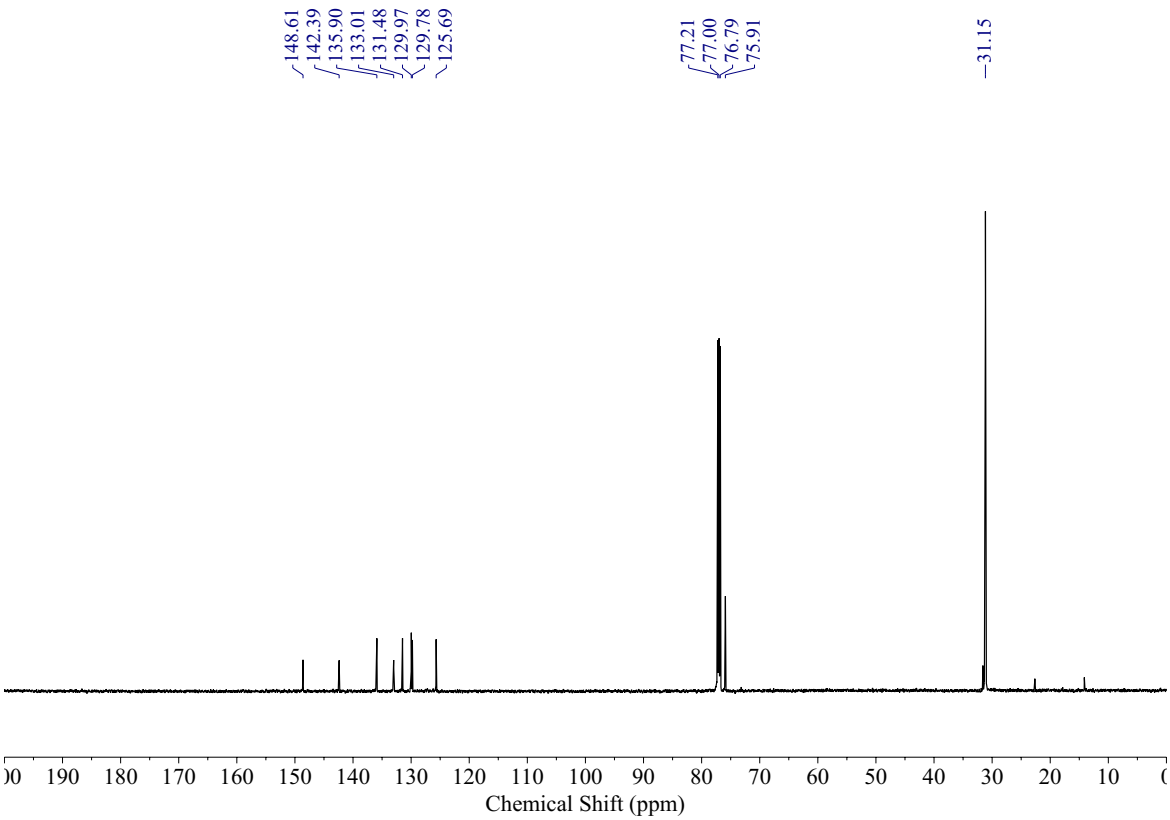


Figure S3: ^{13}C NMR spectrum (151 MHz, $CDCl_3$, 298 K) of isolated 1,3,5-(2-SiCl(O^tBu)$_2C_6H_4$)$_3C_6H_3$, **LCl_3**.

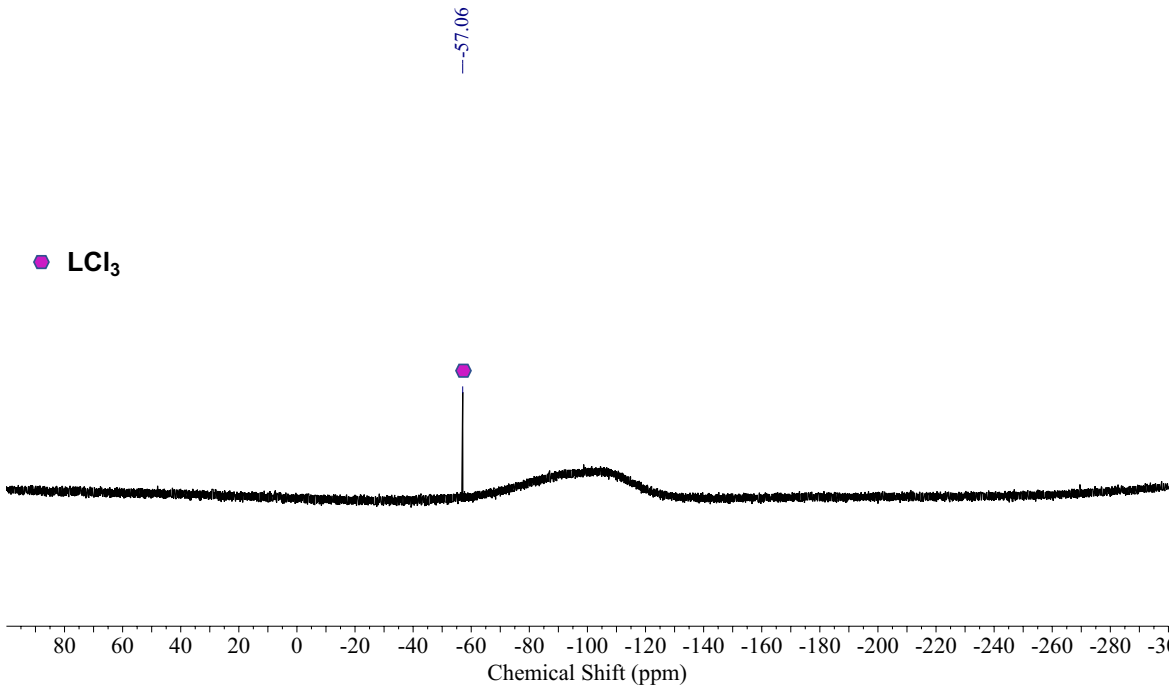


Figure S4: ^{29}Si NMR spectrum (119 MHz, $CDCl_3$, 298 K) of 1,3,5-(2-SiCl(O^tBu)$_2C_6H_4$)$_3C_6H_3$, **LCl_3**.

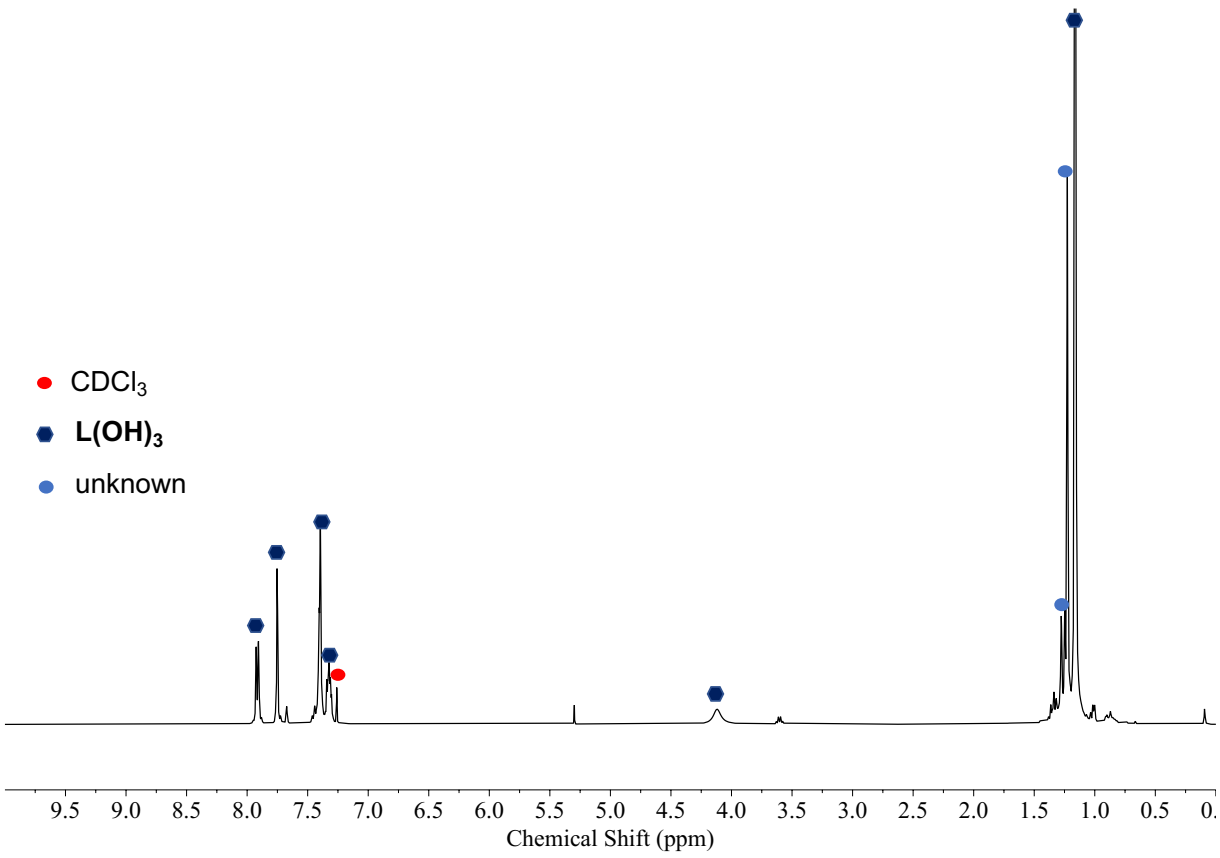


Figure S5: ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of the reaction mixture obtained after hydrolysis of **L(OH)$_3$** at 298 K for 3 days.

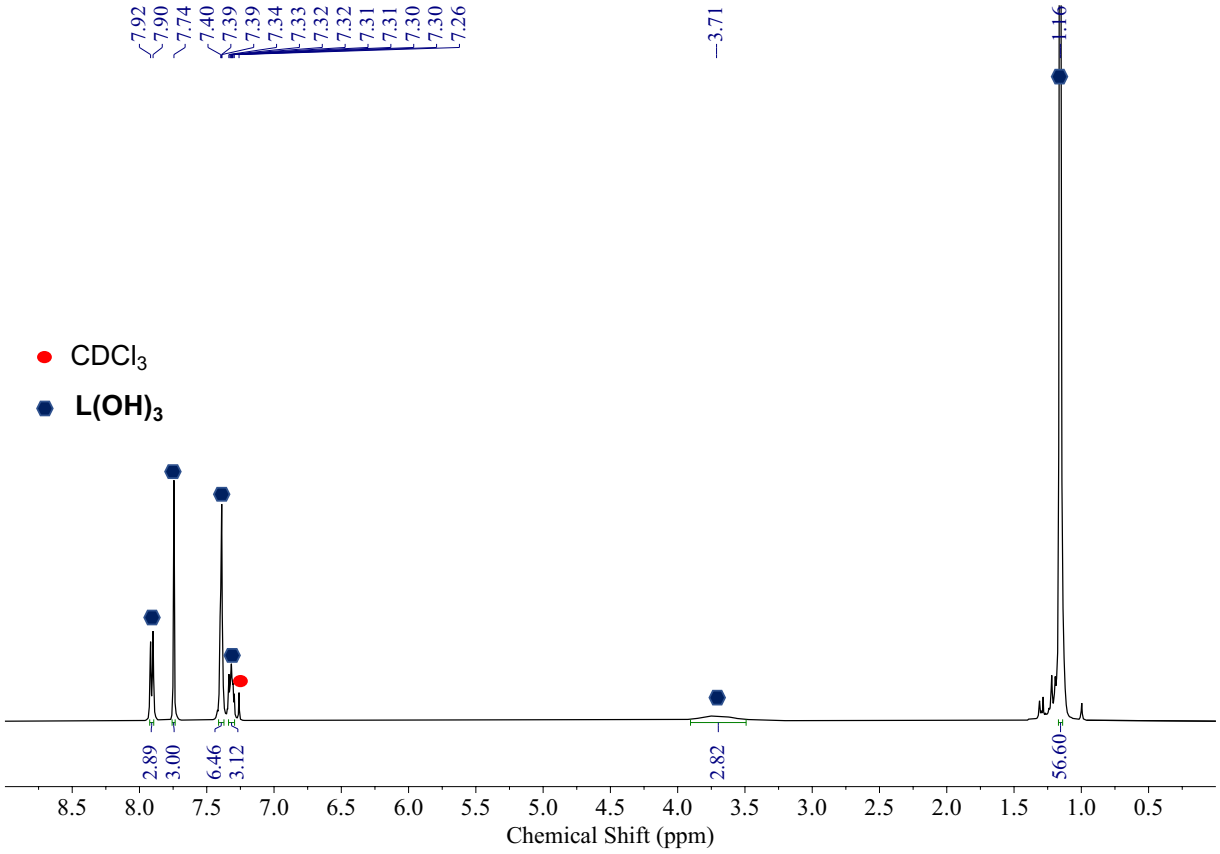


Figure S6: ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of isolated 1,3,5-(2-HOSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$, **L(OH)$_3$**.

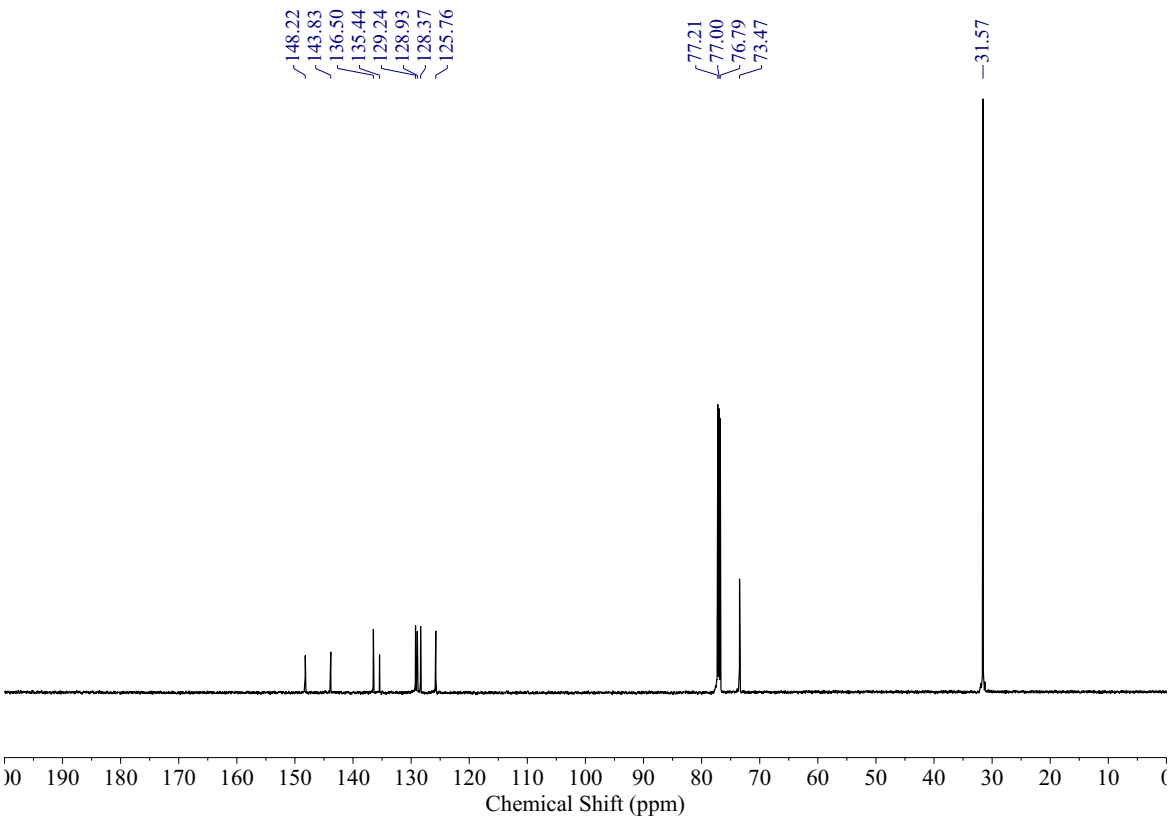


Figure S7: ^{13}C NMR spectrum (151 MHz, $CDCl_3$, 298 K) of isolated 1,3,5-(2-$HOSi(O^tBu)_2C_6H_4)_3C_6H_3$, **L(OH)$_3$**.

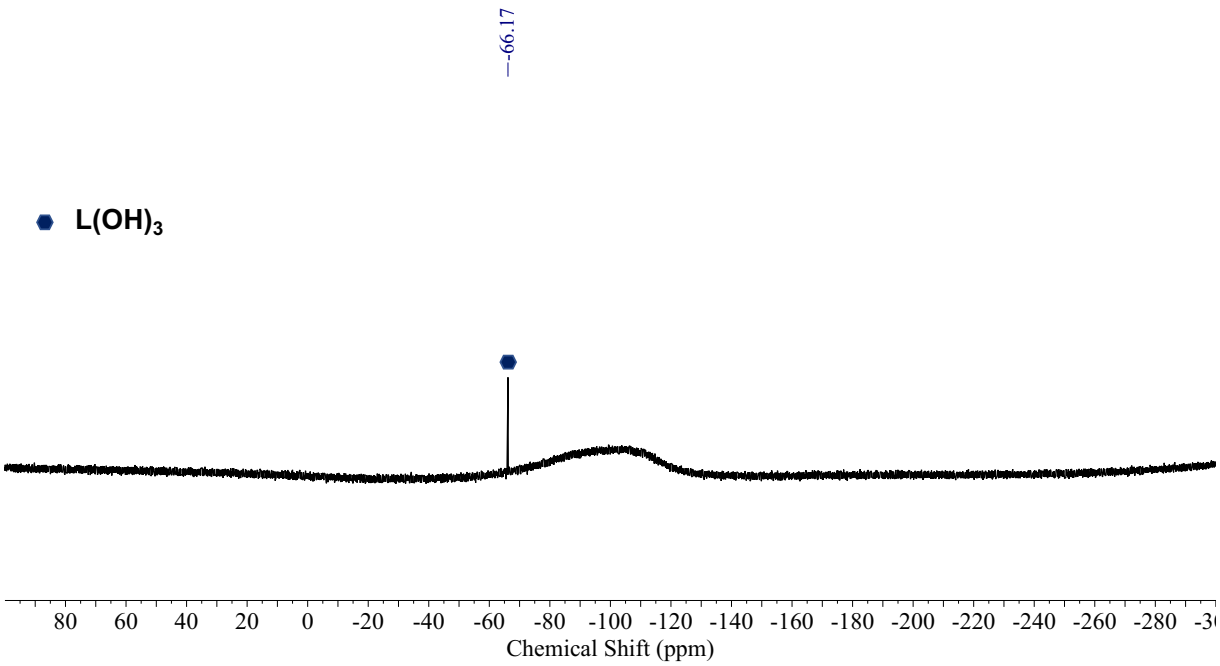


Figure S8: ^{29}Si NMR spectrum (119 MHz, $CDCl_3$, 298 K) of 1,3,5-(2-HOSi(O^tBu)$_2C_6H_4$)$_3C_6H_3$, **L(OH)$_3$**.

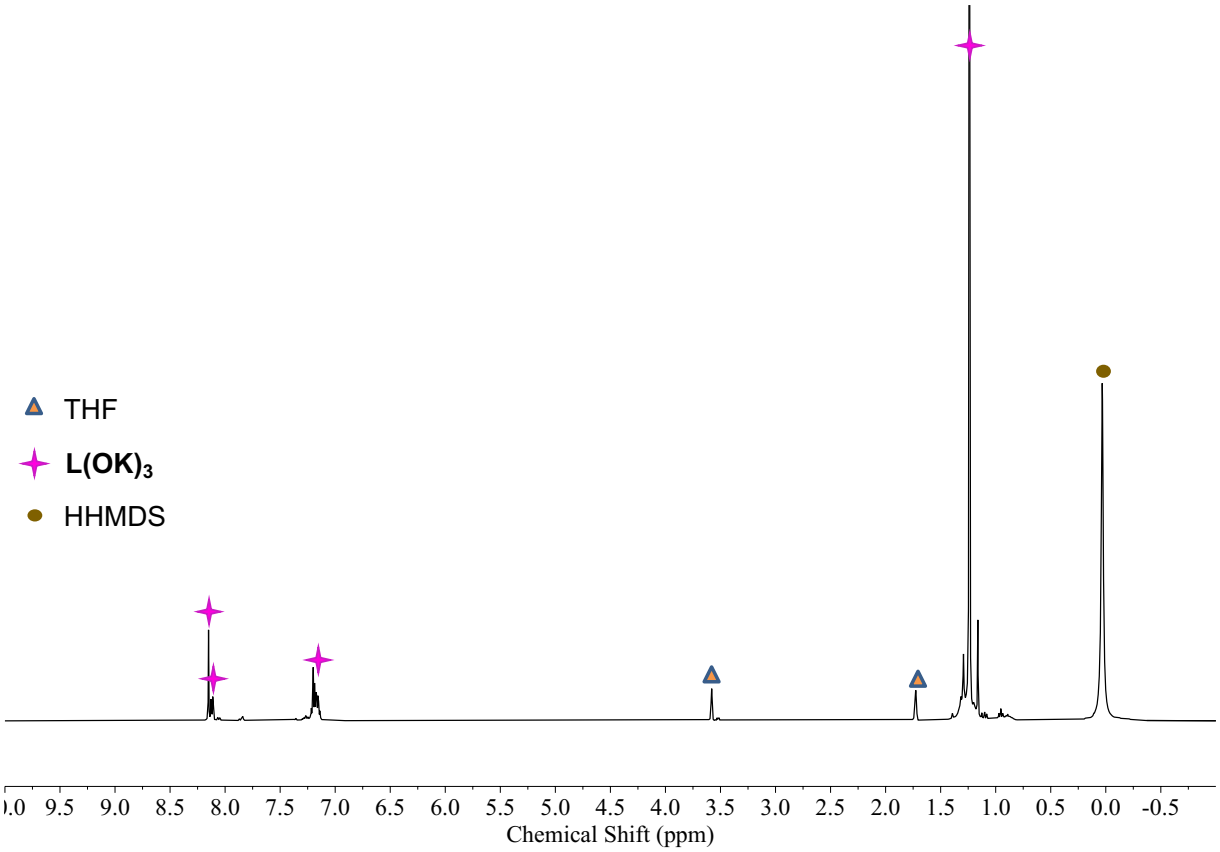


Figure S9: ^{1}H NMR spectrum (400 MHz, THF-d_8, 298 K) of the reaction mixture obtained after addition of 3 equiv. of KHMDS to **L(OH)$_3$** at 298 K for 3 h.

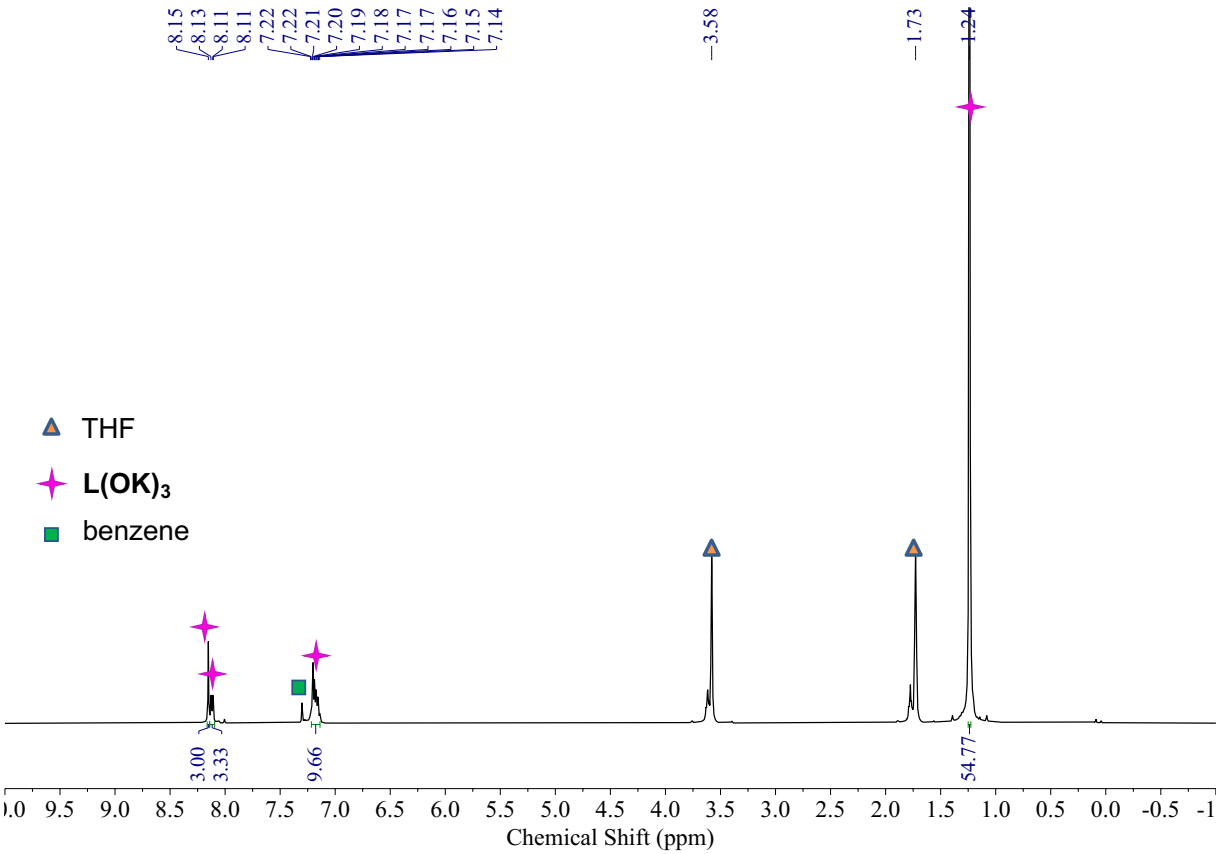


Figure S10: ^{1}H NMR spectrum (400 MHz, THF-d_8, 298 K) of isolated 1,3,5-(2-KOSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$, **L(OK)$_3$**.

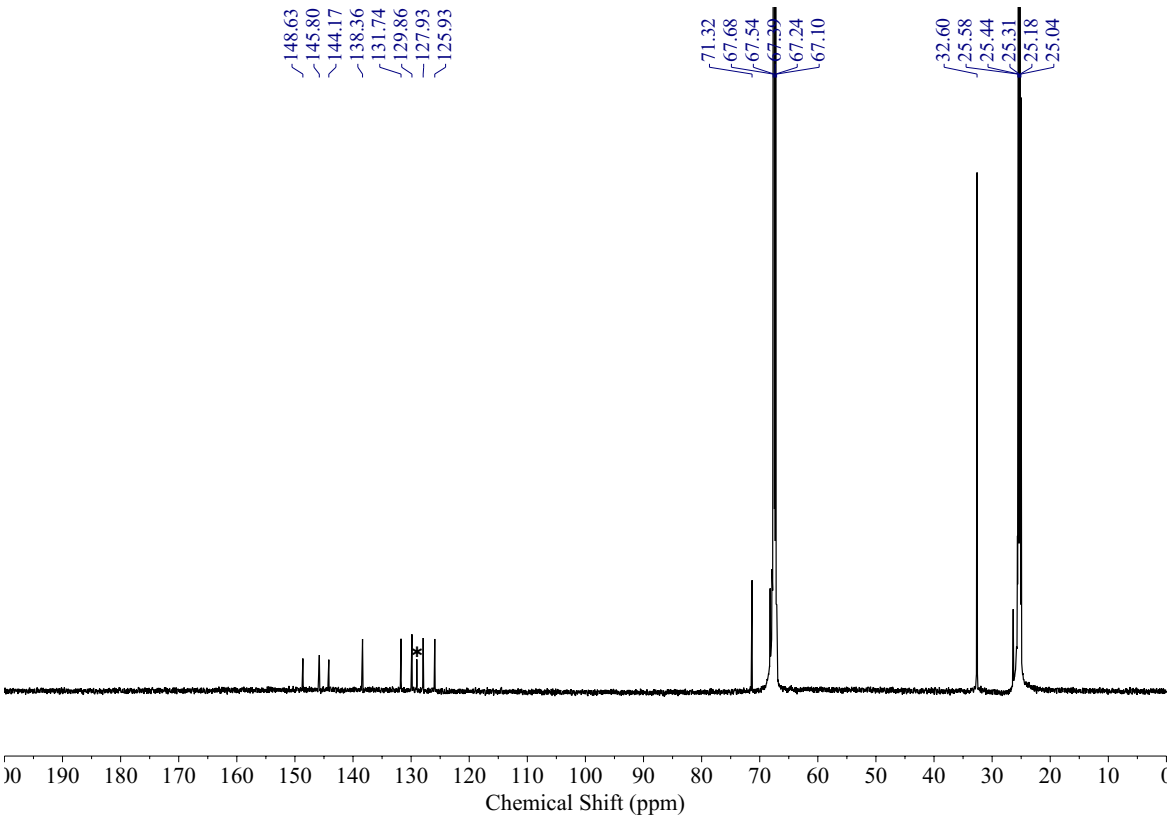


Figure S11: ^{13}C NMR spectrum (151 MHz, THF-d_8, 298 K) of isolated 1,3,5-(2-KOSi(O^tBu)$_2C_6H_4$)$_3C_6H_3$, **L(OK)$_3$**. (∗benzene)

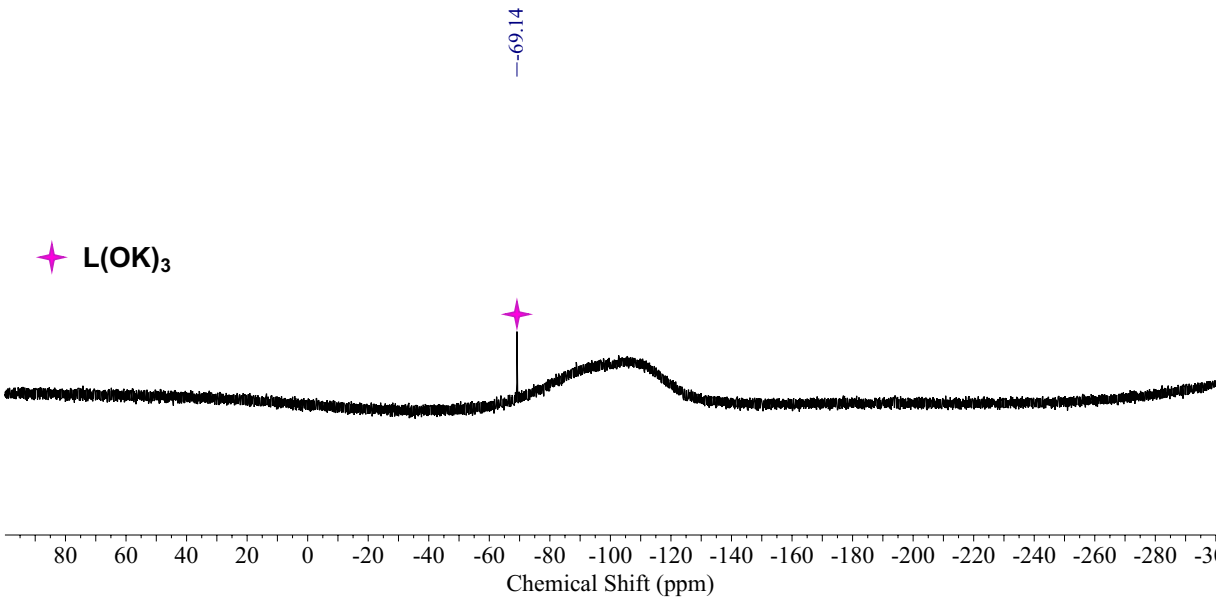


Figure S12: ^{29}Si NMR spectrum (119 MHz, $CDCl_3$, 298 K) of 1,3,5-(2-KOSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$, **L(OK)$_3$**.

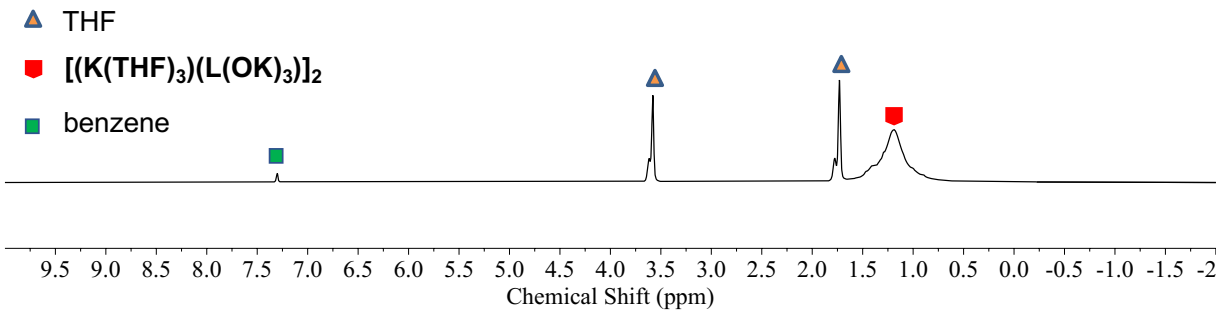


Figure S13: ^{1}H NMR spectrum (400 MHz, THF-d_8, 298 K) of the reaction mixture obtained after addition of 1 equiv. of KC_8 to **L(OK)$_3$** at 298 K for 2 h.

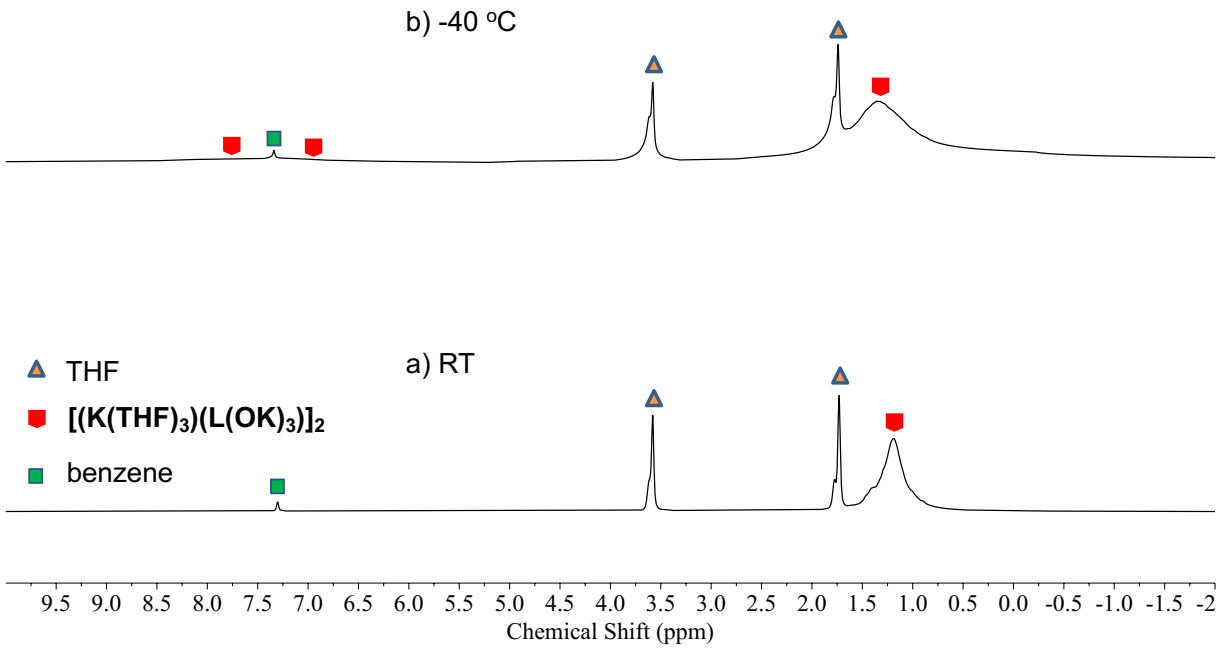


Figure S14: ^{1}H NMR spectrum (400 MHz, THF-d_8) of isolated [K(THF)$_3${1,3,5-(2-KOSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$}]$_2$, **[(K(THF)$_3$)(L(OK)$_3$)]$_2$** at different temperature a) RT b) -40 °C.

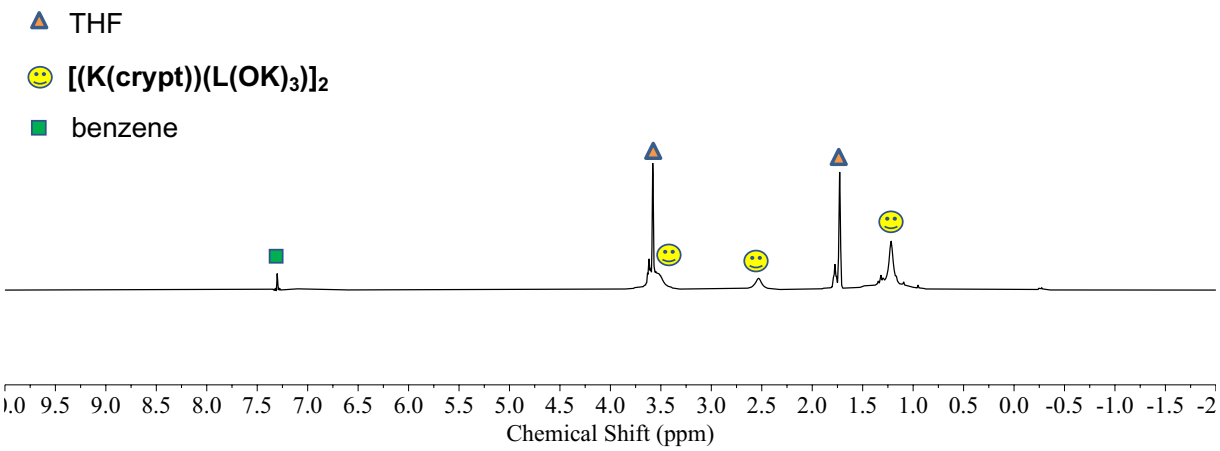


Figure S15: ^{1}H NMR spectrum (400 MHz, THF-d_8, 298 K) of the reaction mixture obtained after addition of 2 equiv. of 2.2.2-cryptand to **[(K(THF)$_3$)(L(OK)$_3$)]$_2$** at 298 K for 30 min.

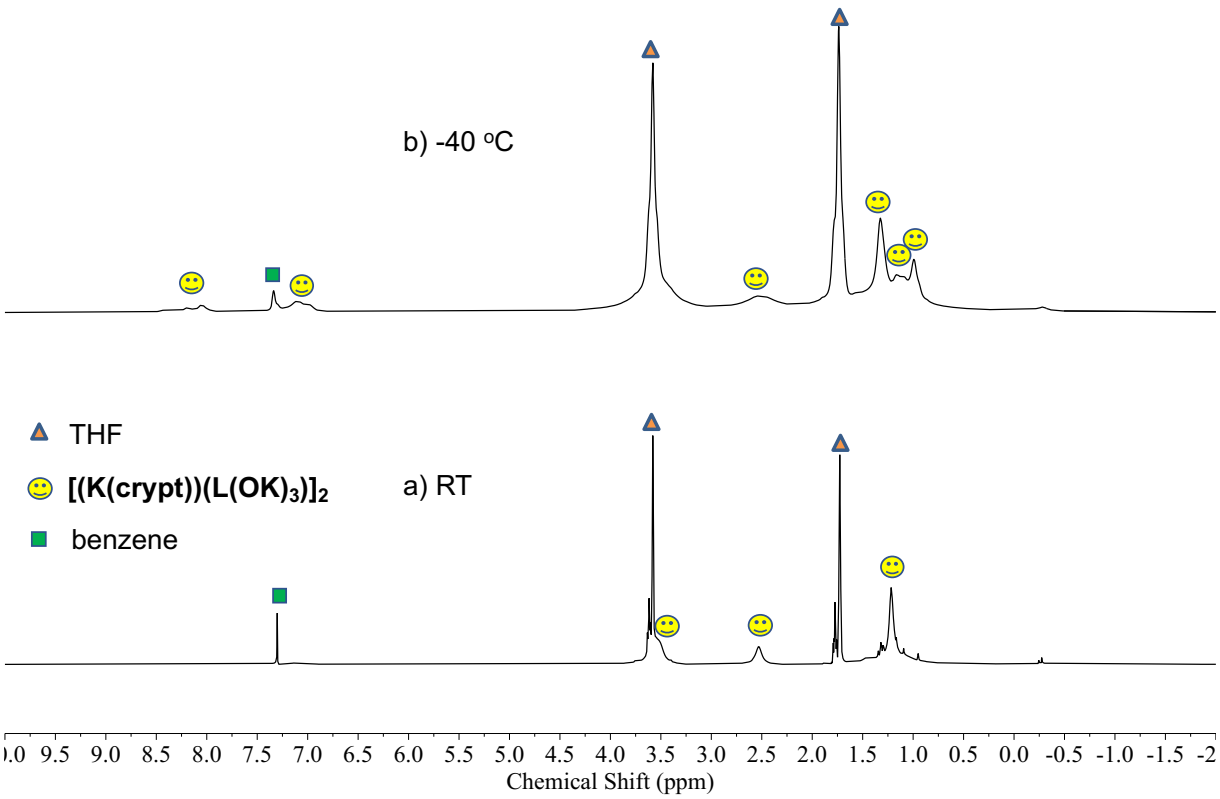


Figure S16: ^{1}H NMR spectrum (400 MHz, THF-d_8) of isolated [K(2.2.2-cryptand)]$_2$[{1,3,5-(2-KOSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$}]$_2$, **[(K(crypt))(L(OK)$_3$)]$_2$** at different temperature a) RT b) -40 °C.

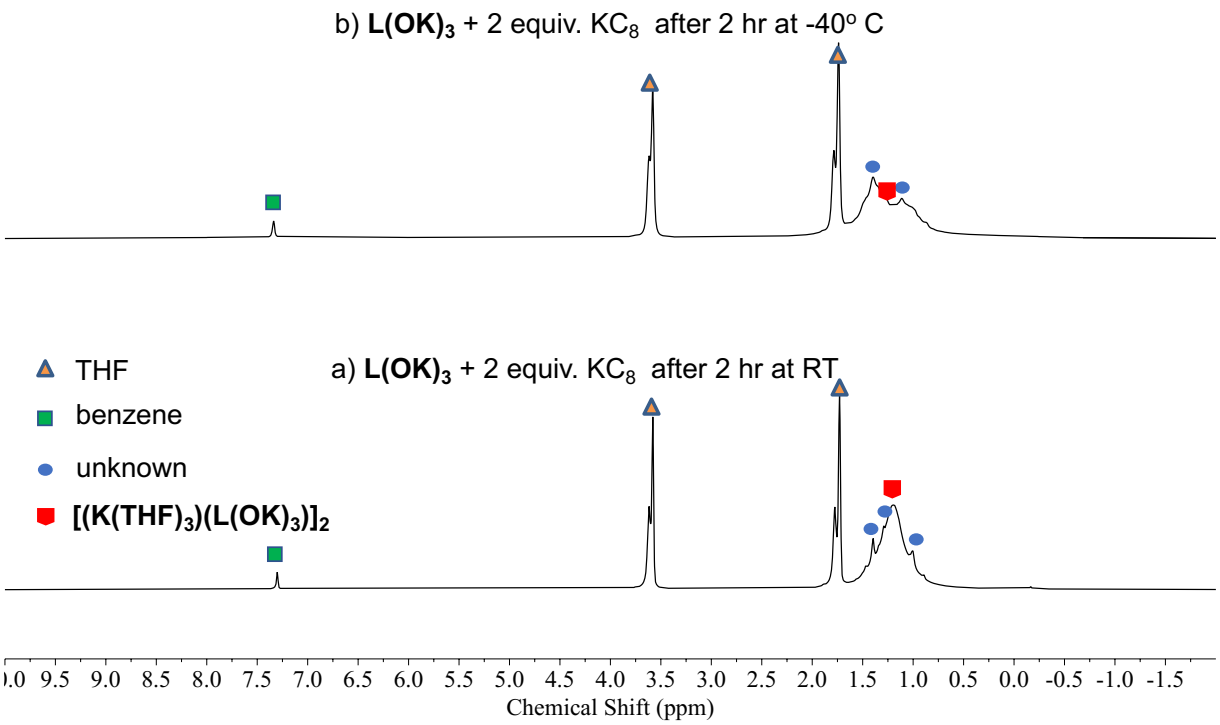


Figure S17: ^{1}H NMR spectrum (400 MHz, THF-d_8) of the reaction mixture obtained after addition of 2 equiv. of KC_8 to **L(OK)$_3$** at different temperature a) RT b) -40 °C.

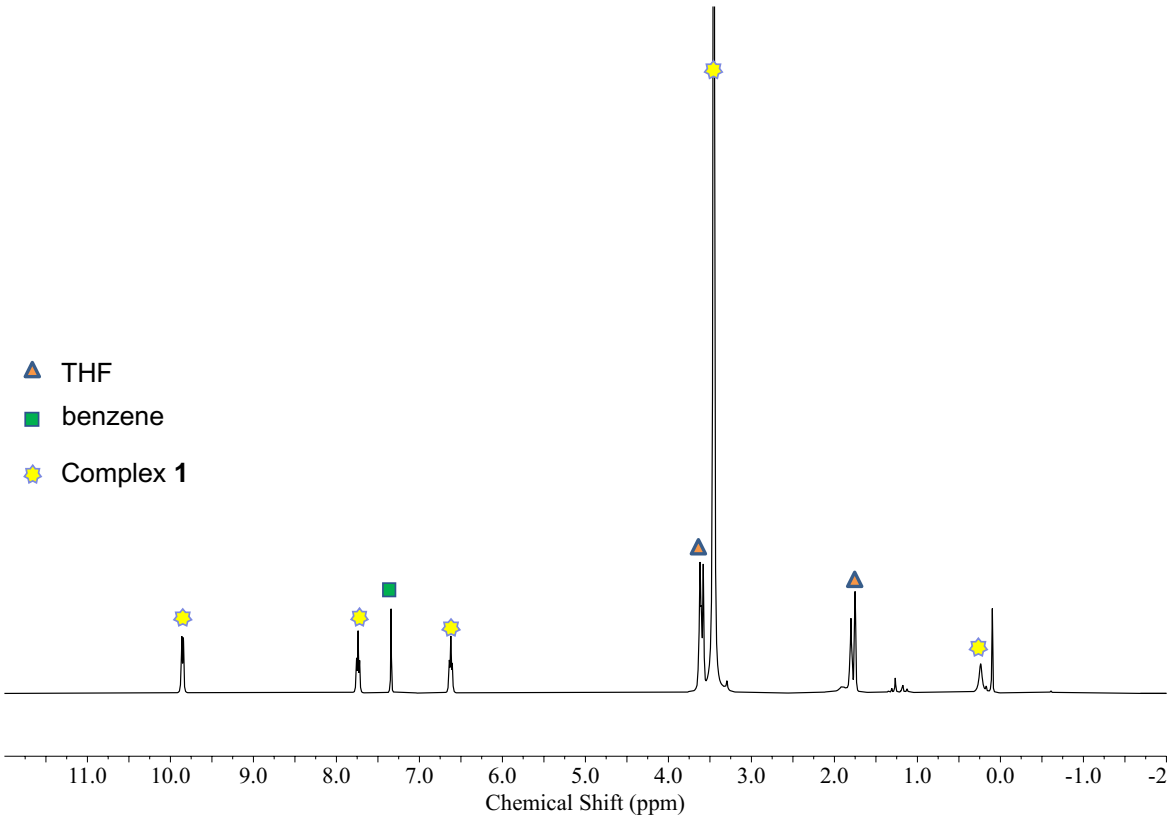


Figure S18: ^{1}H NMR spectrum (400 MHz, THF-d_8, 298 K) of the reaction mixture obtained after addition of 1 equiv. of [Ce(N(SiMe$_3$)$_2$)$_3$] to **L(OH)$_3$** after 16 h.

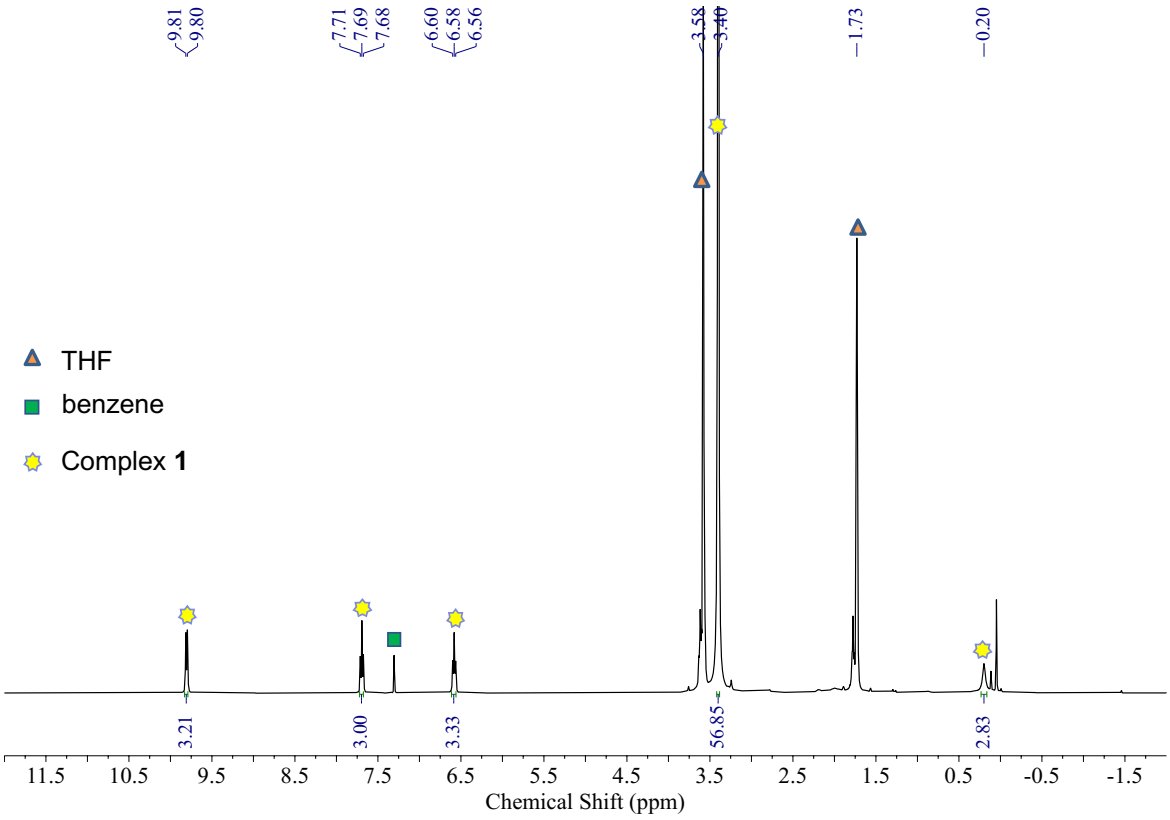


Figure S19: ^{1}H NMR spectrum (400 MHz, THF-d_8, 298 K) of isolated [(1,3,5-(2-OSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$)Ce(THF)], **1**

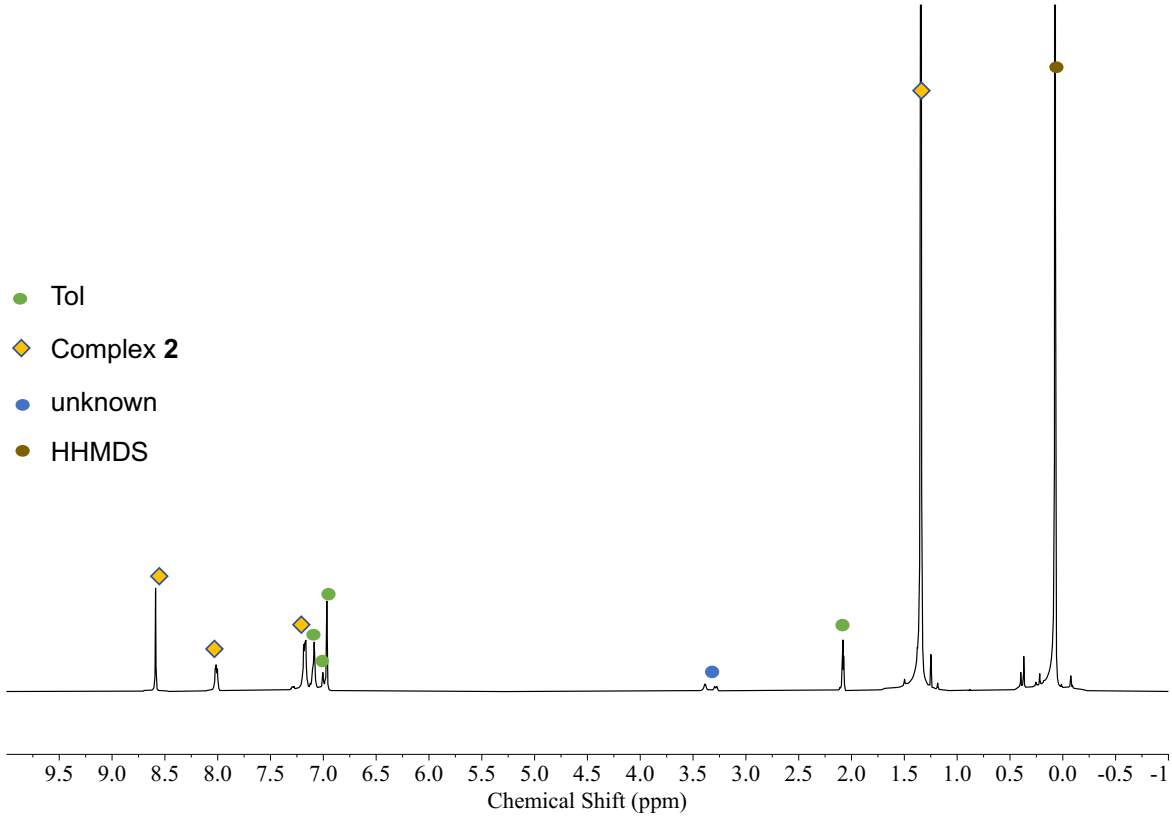


Figure S20: ^{1}H NMR spectrum (400 MHz, toluene-d_8, 298 K) of the reaction mixture obtained after addition of 1 equiv. of [CeCl(N(SiMe$_3$)$_2$)$_3$] to **L(OH)$_3$** after 3 h.

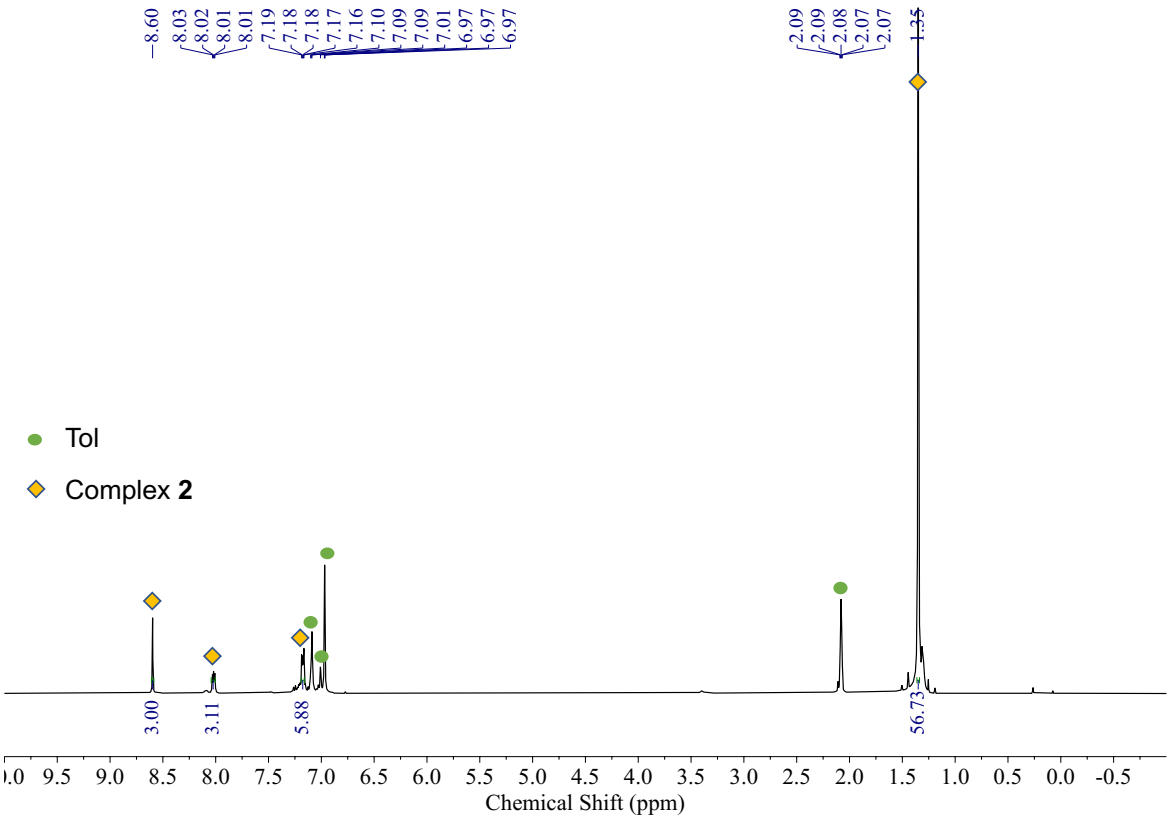


Figure S21: ^{1}H NMR spectrum (400 MHz, toluene-d_8, 298 K) of isolated [1,3,5-(2-OSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$)CeCl], **2**.

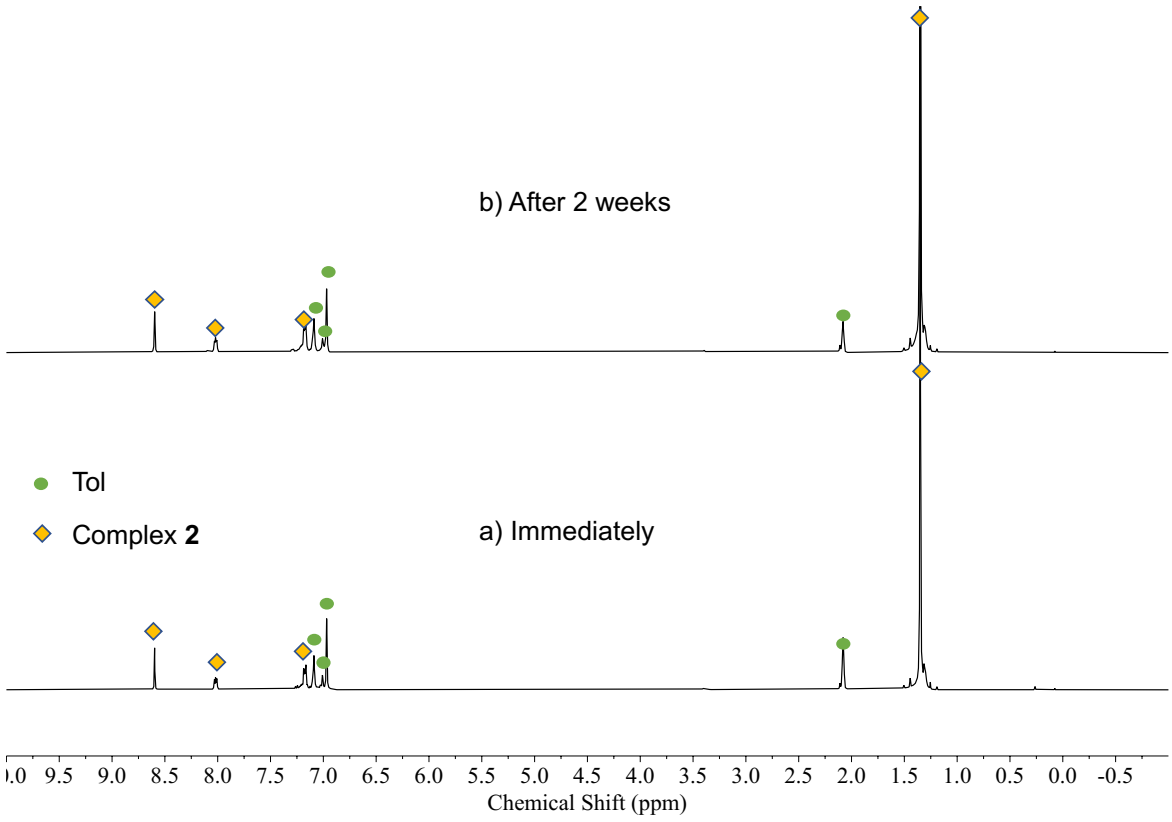


Figure S22: ^{1}H NMR spectra (400 MHz, toluene-d_8, 298 K) of isolated [1,3,5-(2-OSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$)CeCl], **2** at RT a) immediately b) after 2 weeks.

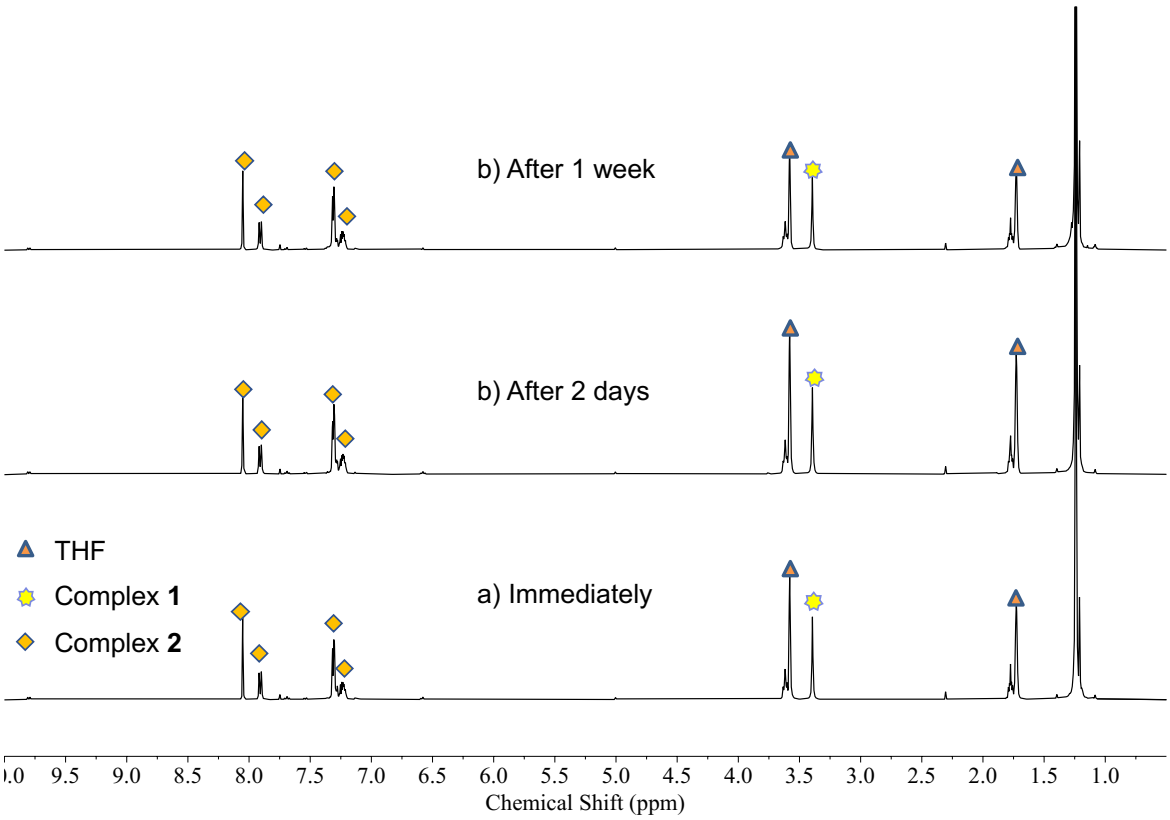


Figure S23: ^{1}H NMR spectra (400 MHz, THF-d_8, 298 K) of isolated [1,3,5-(2-OSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$)CeCl], **2** at RT a) immediately b) after 2 days c) after 1 week.

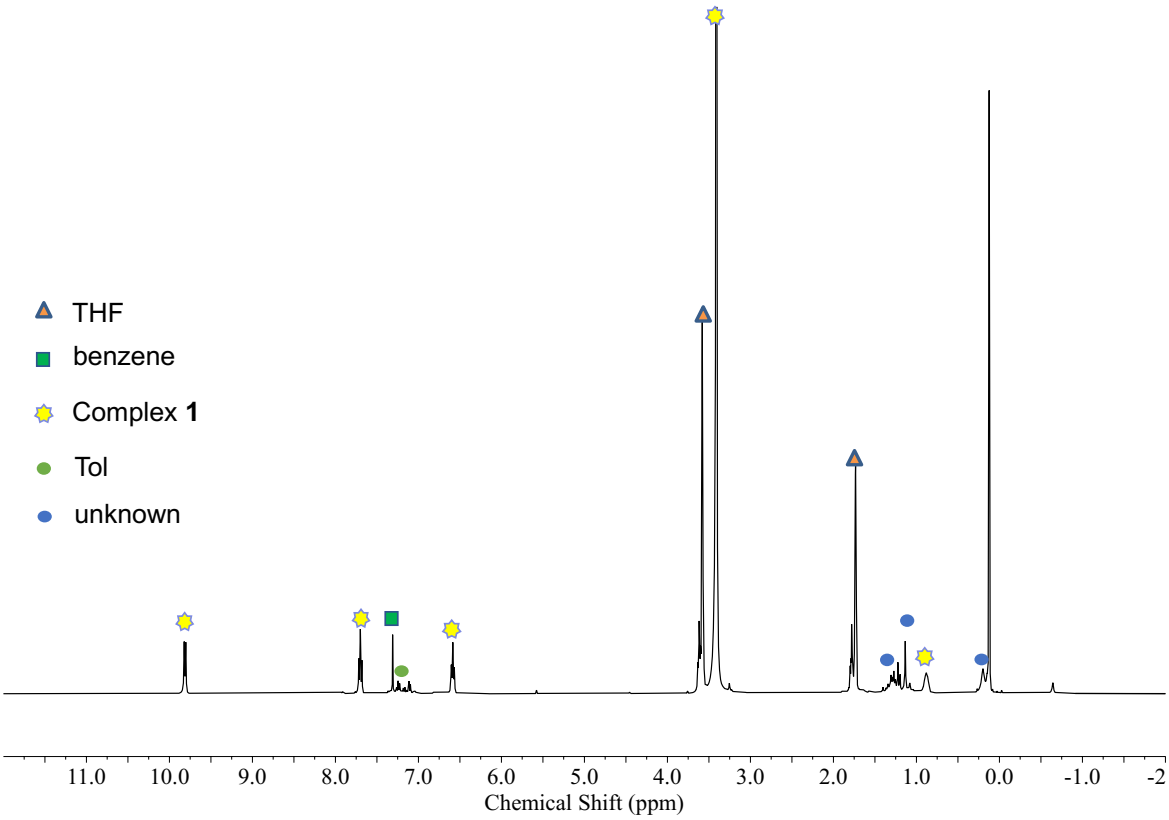


Figure S24: ^{1}H NMR spectrum (400 MHz, THF-d_8, 298 K) of the reaction mixture obtained after addition of 1 equiv. of KC_8 to **2** in toluene after 1 h.

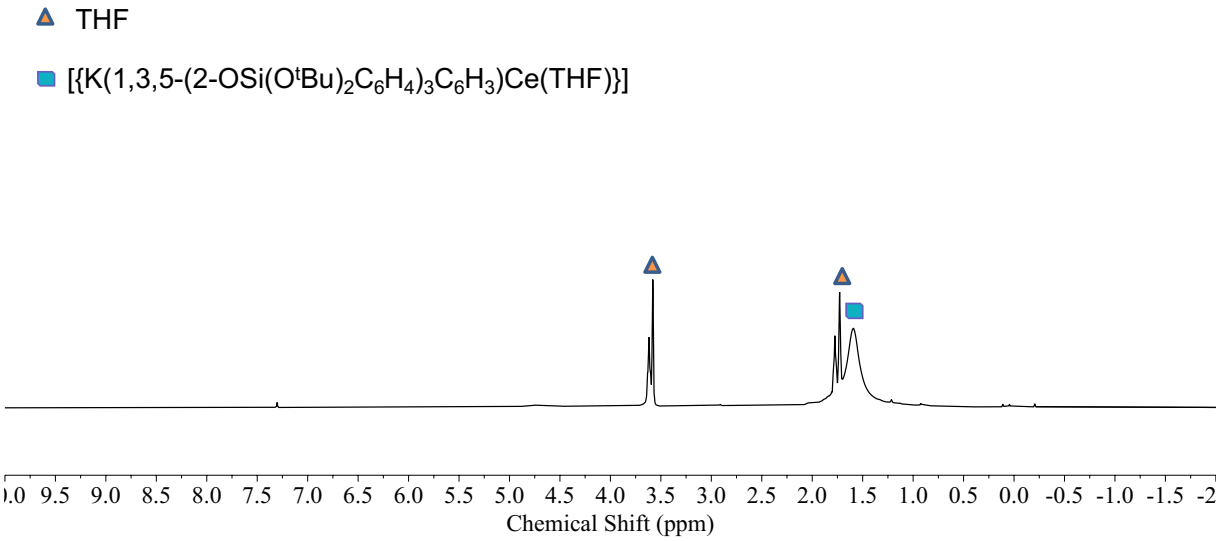


Figure S25: ^{1}H NMR spectrum (400 MHz, THF-d_8, 298 K) of the reaction mixture obtained after addition of 1 equiv. of KC_8 to **1** at 233 K for 16 h.

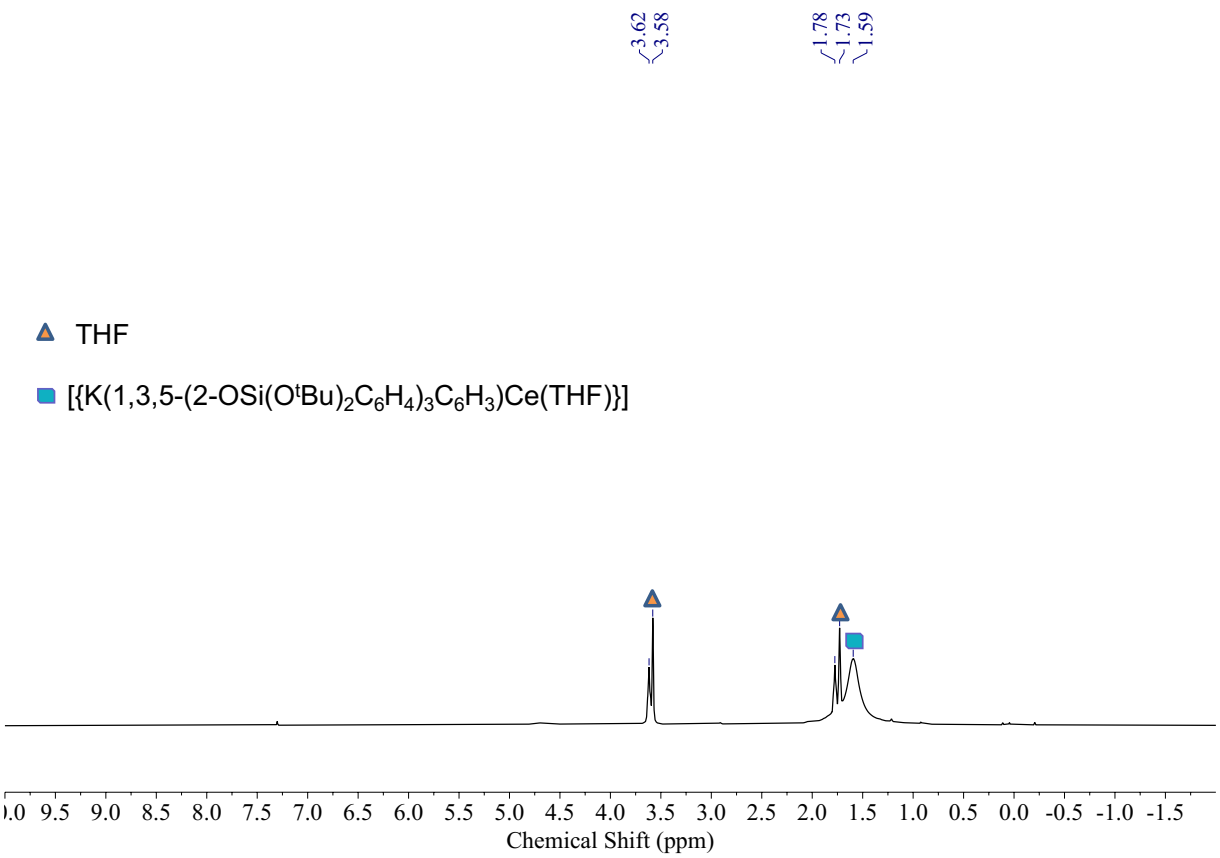


Figure S26: ^{1}H NMR spectrum (400 MHz, THF-d_8, 298 K) of isolated [{K(1,3,5-(2-OSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$)Ce(THF)}].

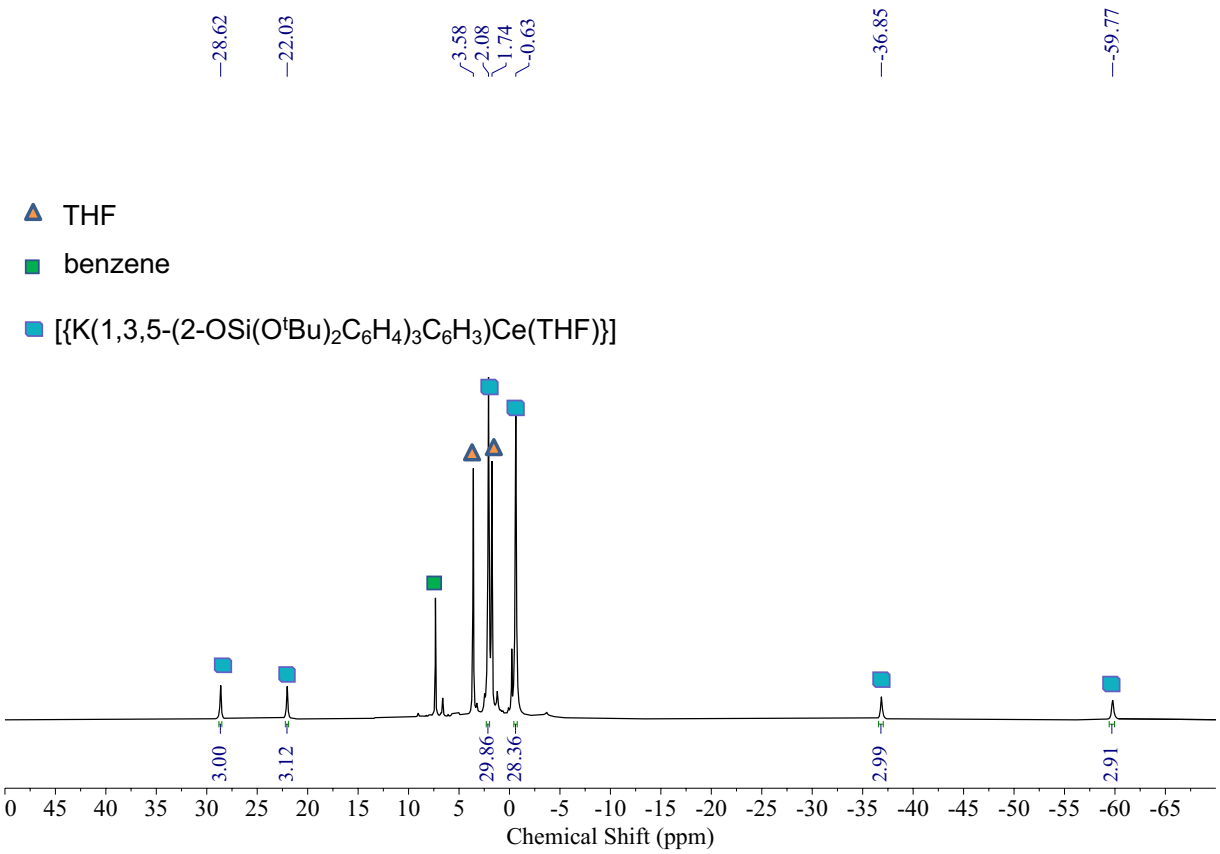


Figure S27: ^{1}H NMR spectrum (400 MHz, THF-d_8, 233 K) of isolated [{K(1,3,5-(2-OSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$)Ce(THF)}].

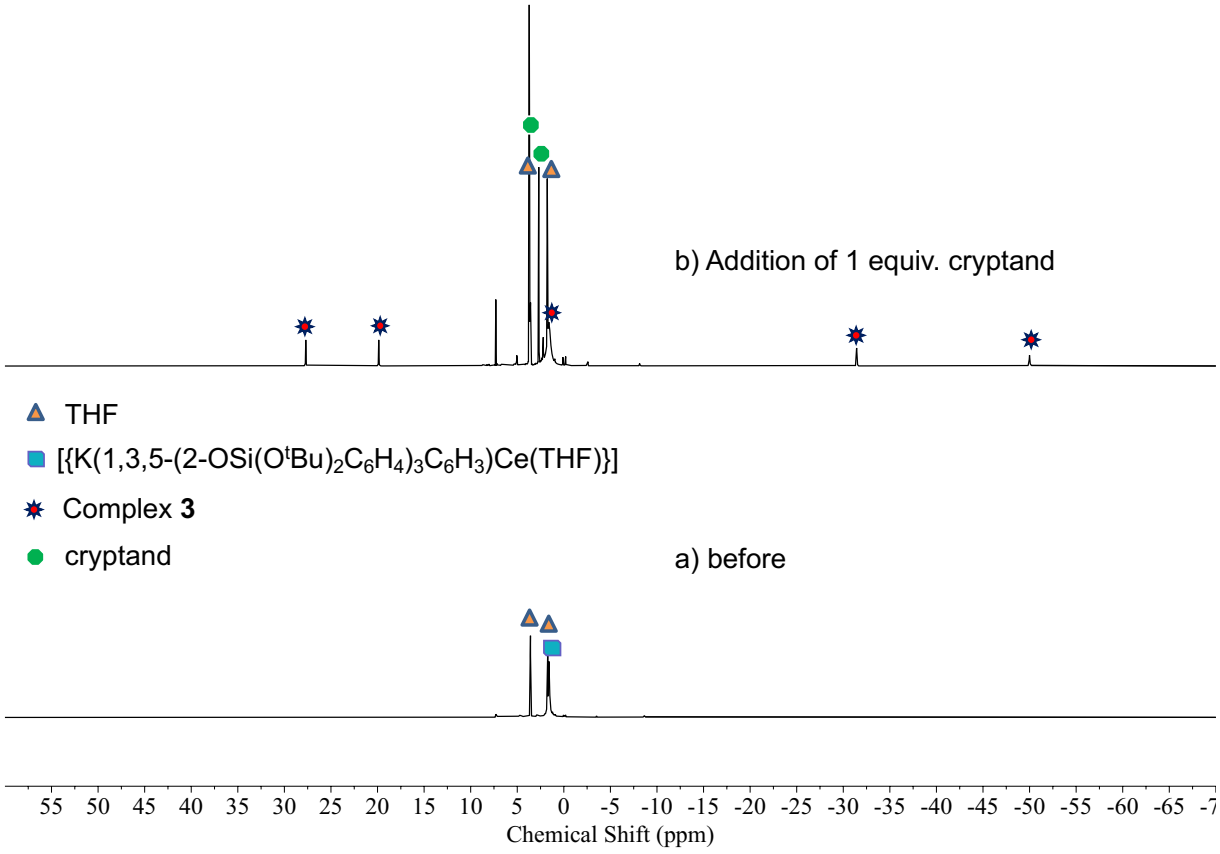


Figure S28: ^{1}H NMR spectra (400 MHz, THF-d_8, 298 K) of the reaction mixture obtained after addition of 1 equiv. of 2.2.2-cryptand to [{K(1,3,5-(2-OSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$)Ce(THF)}] a) before b) [{K(1,3,5-(2-OSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$)Ce(THF)}] + 1 equiv. of 2.2.2-cryptand immediately.

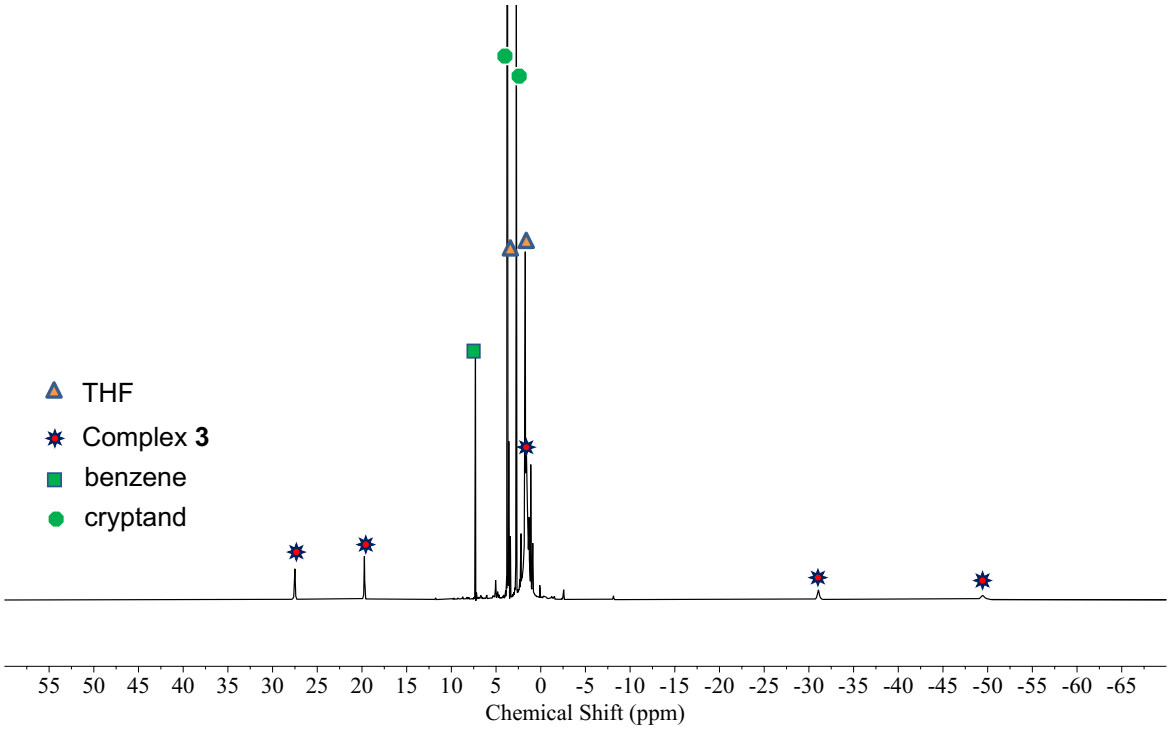


Figure S29: ^{1}H NMR spectrum (400 MHz, THF-d_8, 298 K) of the reaction mixture obtained after addition of 1 equiv. of KC_8 and 1 equiv. 2.2.2-cryptand to **1** at 233 K for 16 h.

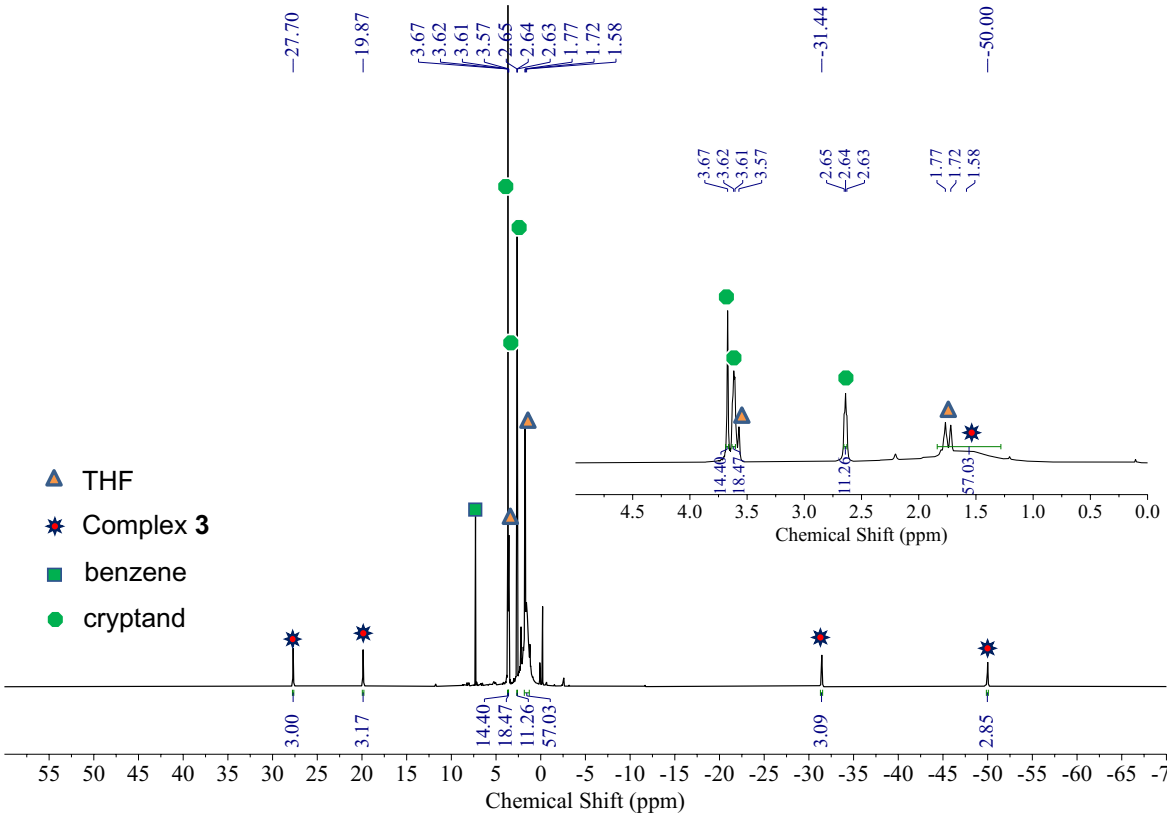


Figure S30: ^{1}H NMR spectrum (400 MHz, THF-d_8, 298 K) of isolated [K(2.2.2-cryptand)][(1,3,5-(2-OSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$)Ce(THF)], **3**.

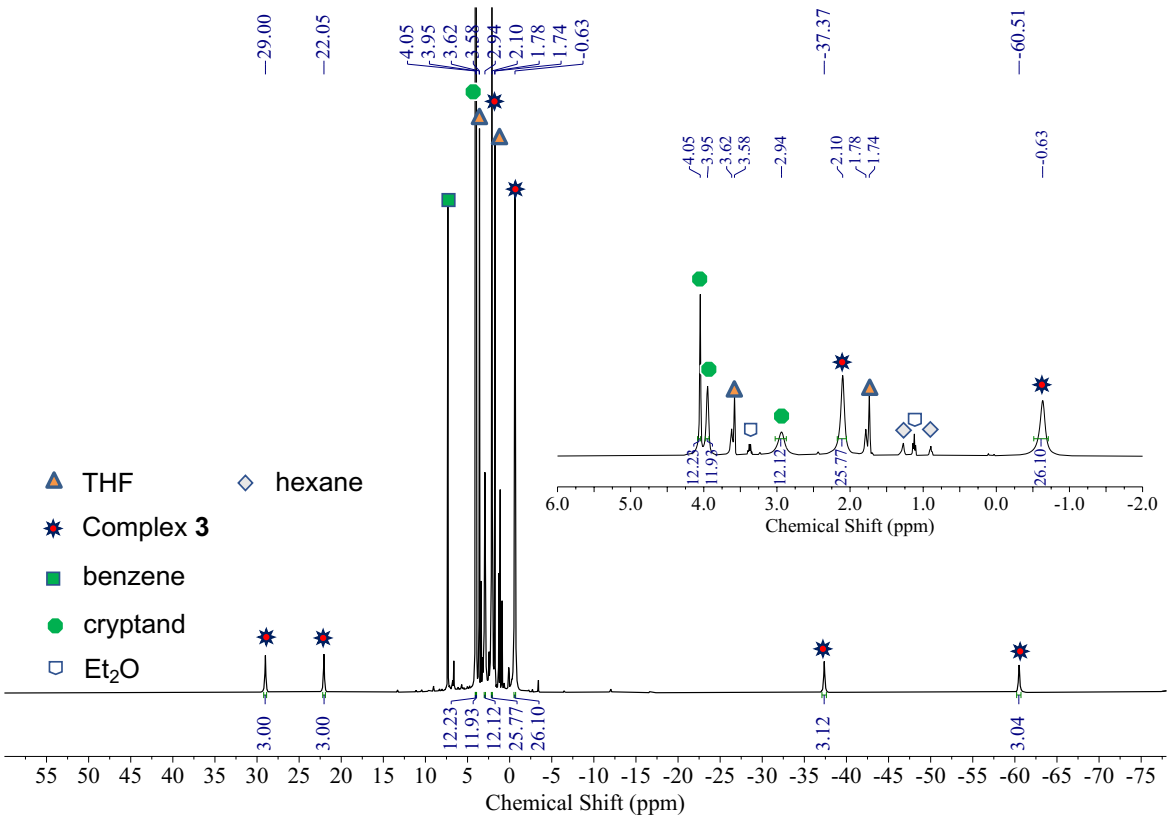


Figure S31: ^{1}H NMR spectrum (400 MHz, THF-d_8, 233 K) of isolated [K(2.2.2-cryptand)][(1,3,5-(2-OSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$)Ce(THF)], **3**.

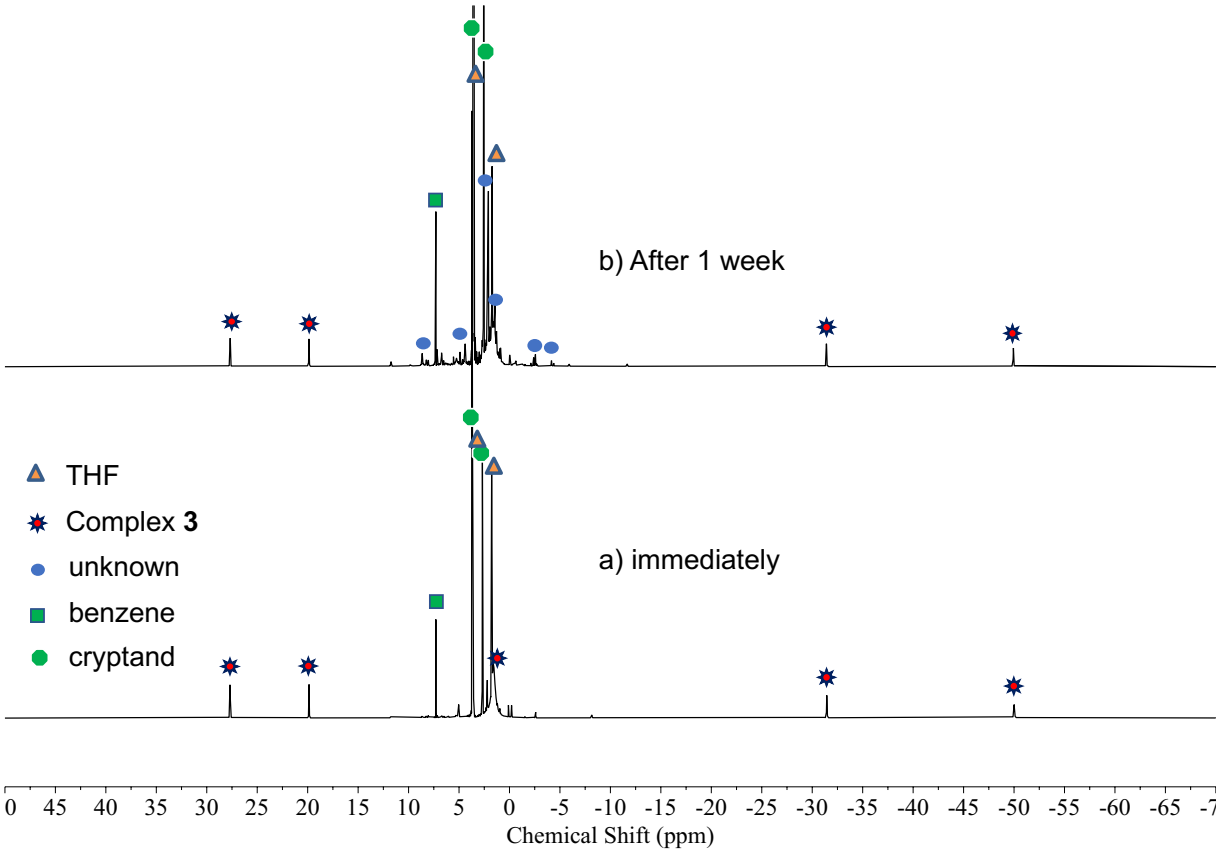


Figure S32: ^{1}H NMR spectra (400 MHz, THF-d_8, 298 K) of isolated [K(2.2.2-cryptand)][(1,3,5-(2-OSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$)Ce(THF)], **3** at RT a) immediately b) after 1 week.

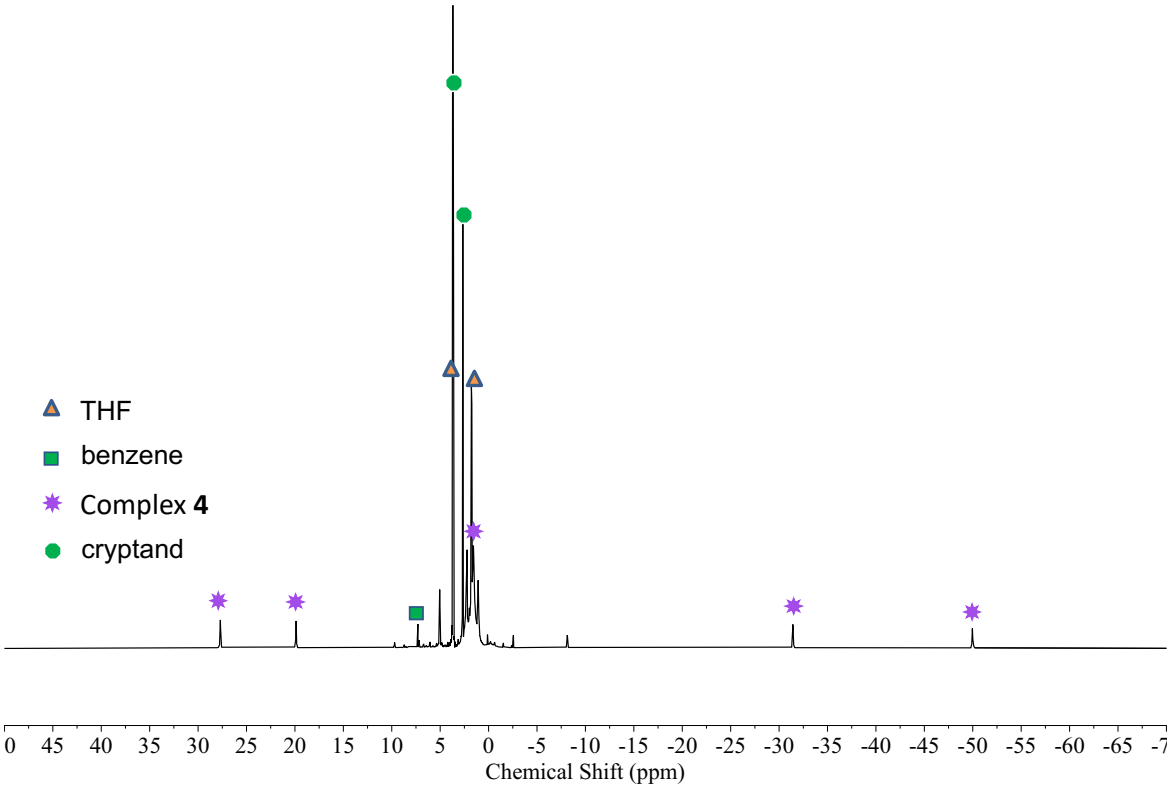


Figure S33: ^{1}H NMR spectrum (400 MHz, THF-d_8, 298 K) of the reaction mixture obtained after addition of 1 equiv. of $OPEt_3$ to **3** at 298 K for 30 mins.

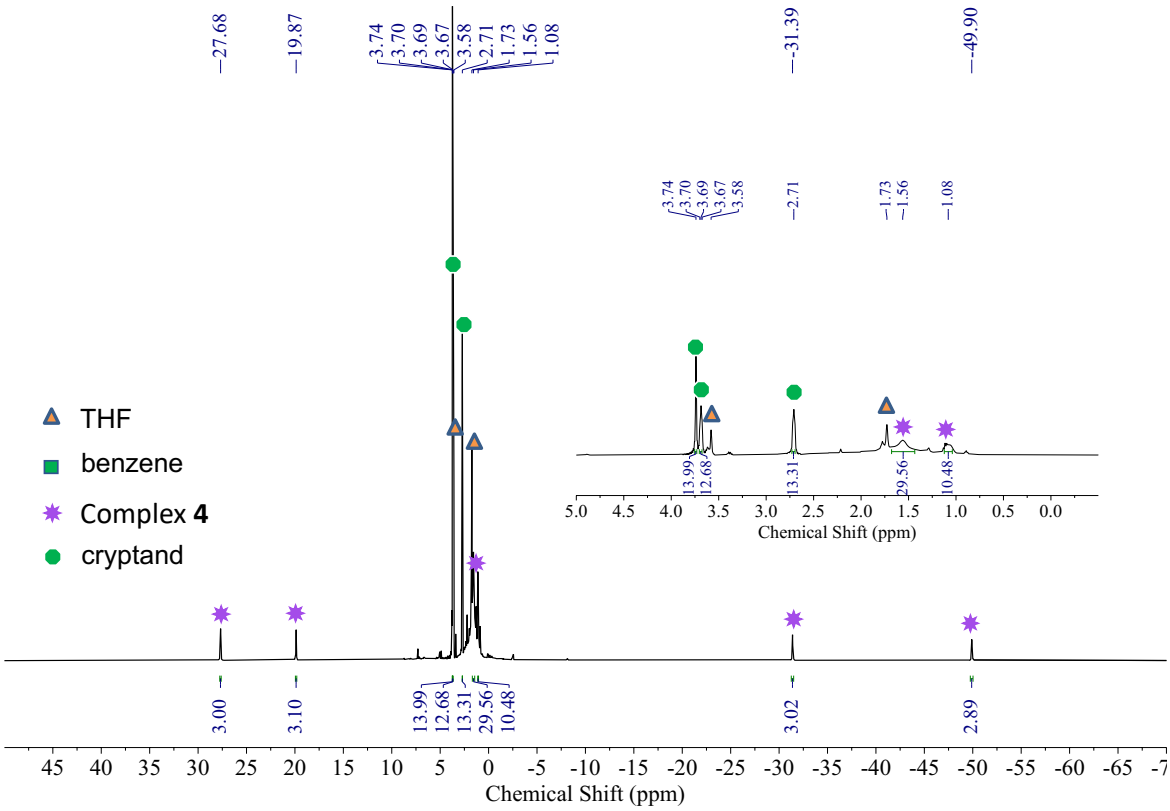


Figure S34: ^{1}H NMR spectrum (400 MHz, THF-d_8, 298 K) of isolated [K(2.2.2-cryptand)][(1,3,5-(2-OSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$)Ce(Et$_3$PO)], **4**.

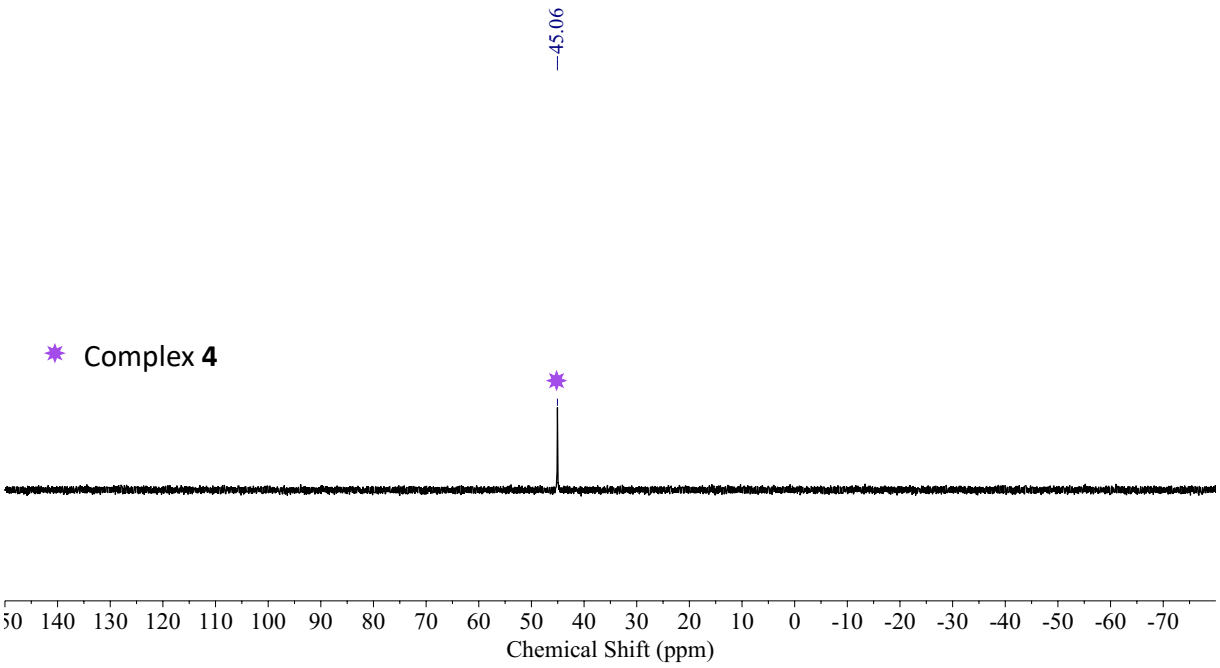


Figure S35: ^{31}P NMR spectrum (162 MHz, THF-d_8, 298 K) of isolated [K(2.2.2-cryptand)][(1,3,5-(2-OSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$)Ce(Et$_3$PO)], **4**.

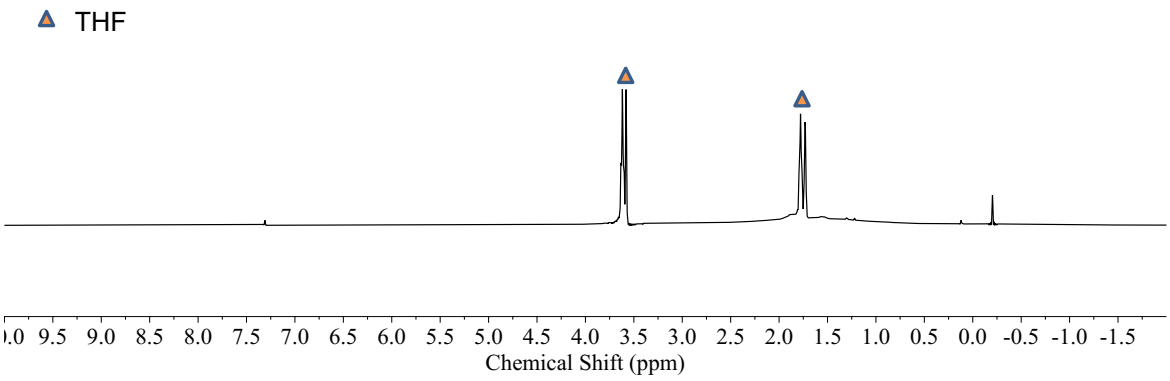


Figure S36: ^{1}H NMR spectrum (400 MHz, THF-d_8, 298 K) of the reaction mixture obtained after addition of 2 equiv. of KC_8 to **1** at 233 K for 16 h.

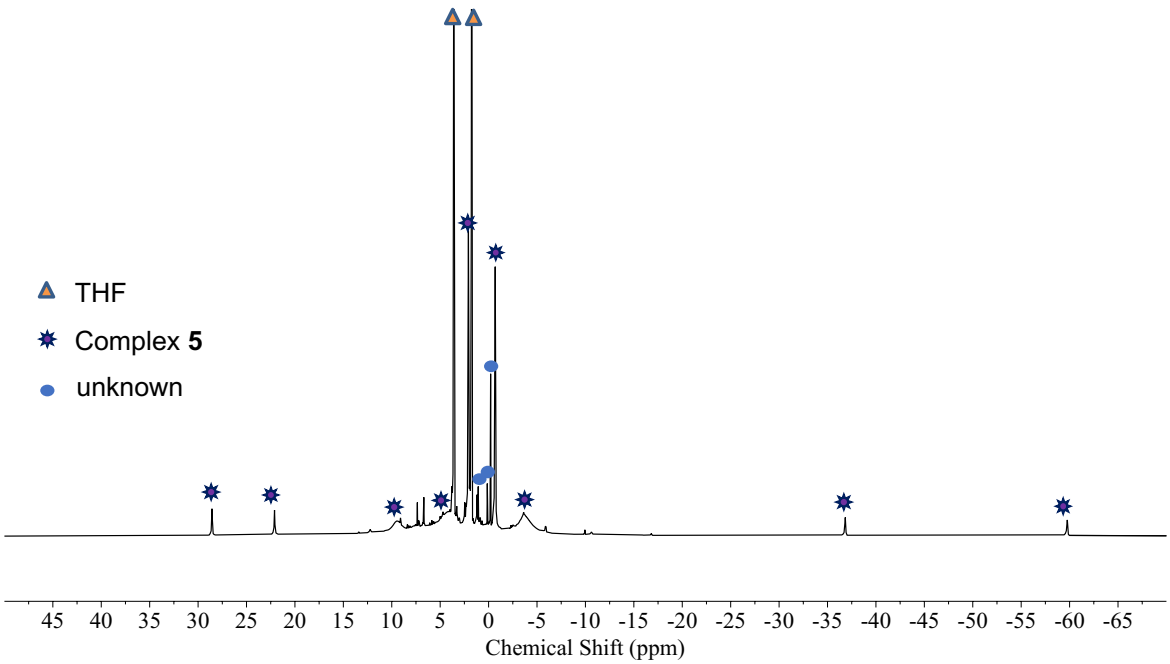


Figure S37: ^{1}H NMR spectrum (400 MHz, THF-d_8, 233 K) of the reaction mixture obtained after addition of 2 equiv. of KC_8 to **1** at 233 K for 16 h.

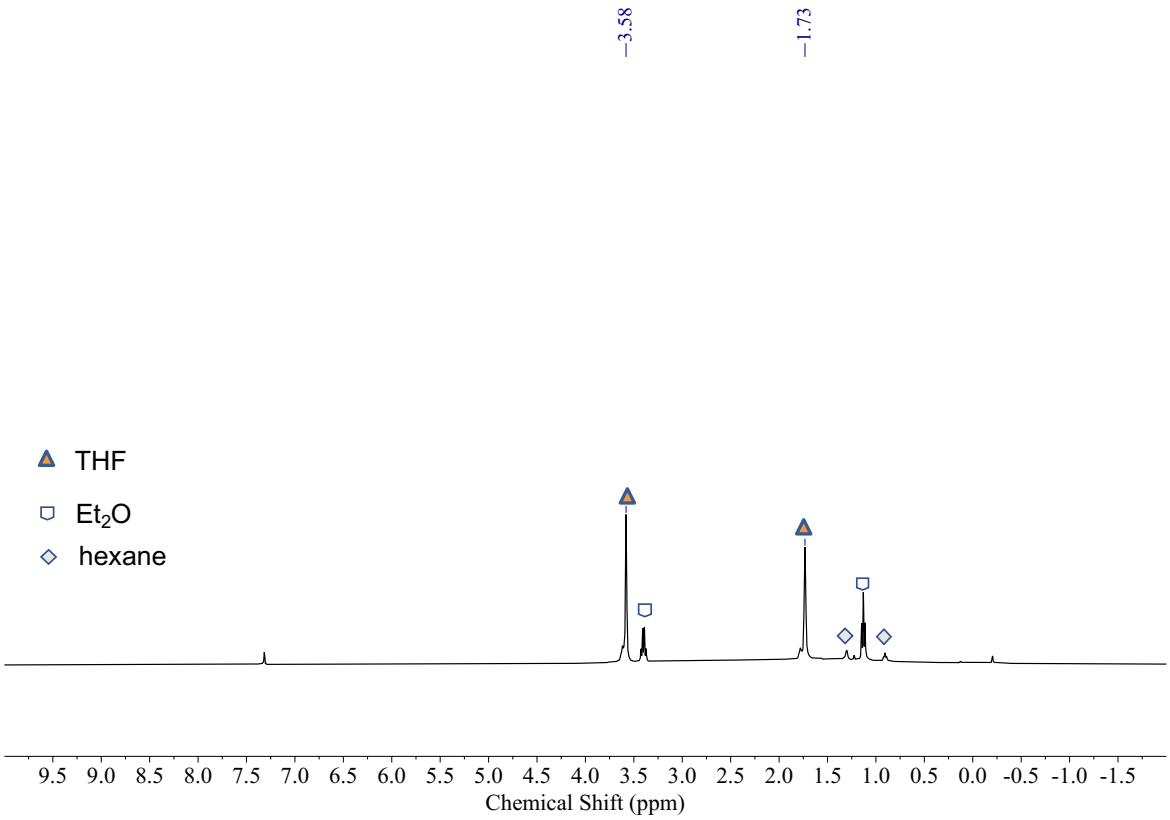


Figure S38: ^{1}H NMR spectrum (400 MHz, THF-d_8, 298 K) of isolated [K_2{1,3,5-(2-OSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$)Ce(Et$_2$O)$_3$}], **5**.

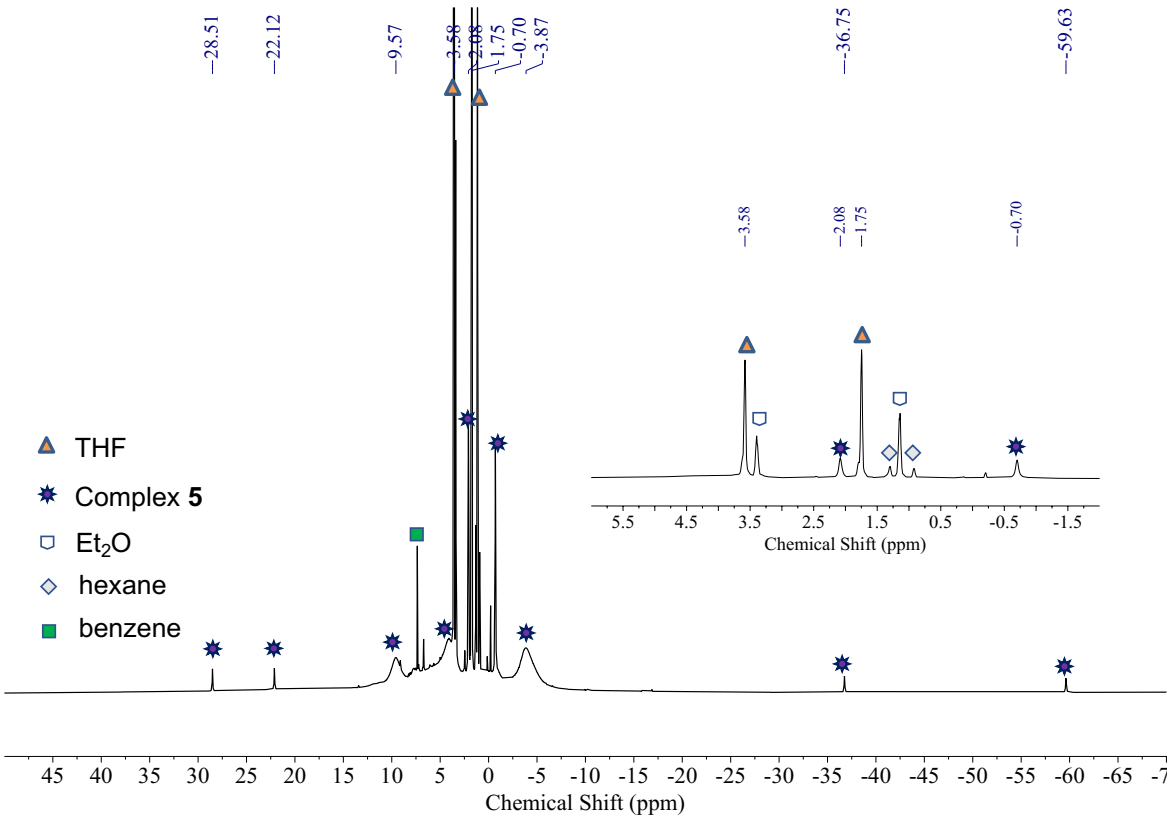


Figure S39: ^{1}H NMR spectrum (400 MHz, THF-d_8, 233 K) of isolated [K_2{1,3,5-(2-OSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$)Ce(Et$_2$O)$_3$}], **5**.

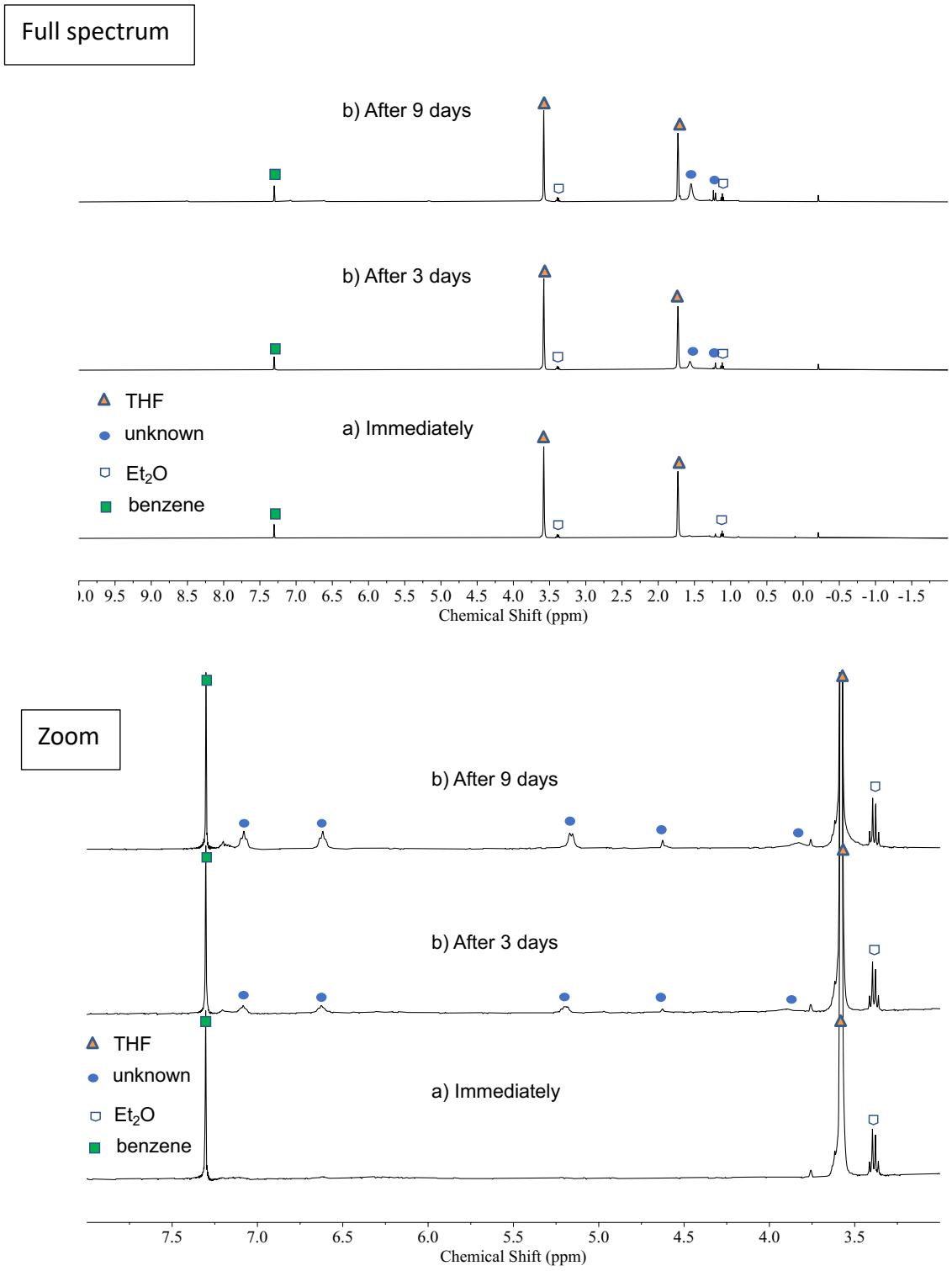


Figure S40: ^{1}H NMR spectra (400 MHz, THF-d_8, 298 K) of isolated [K_2{1,3,5-(2-OSi(O^tBu)$_2C_6H_4$)$_3C_6H_3$)Ce(Et_2O)$_3$}], **5** at RT top) full spectrum a) immediately b) after 3 days c) after 9 days; bottom) Zoom of the 3-8 ppm region.

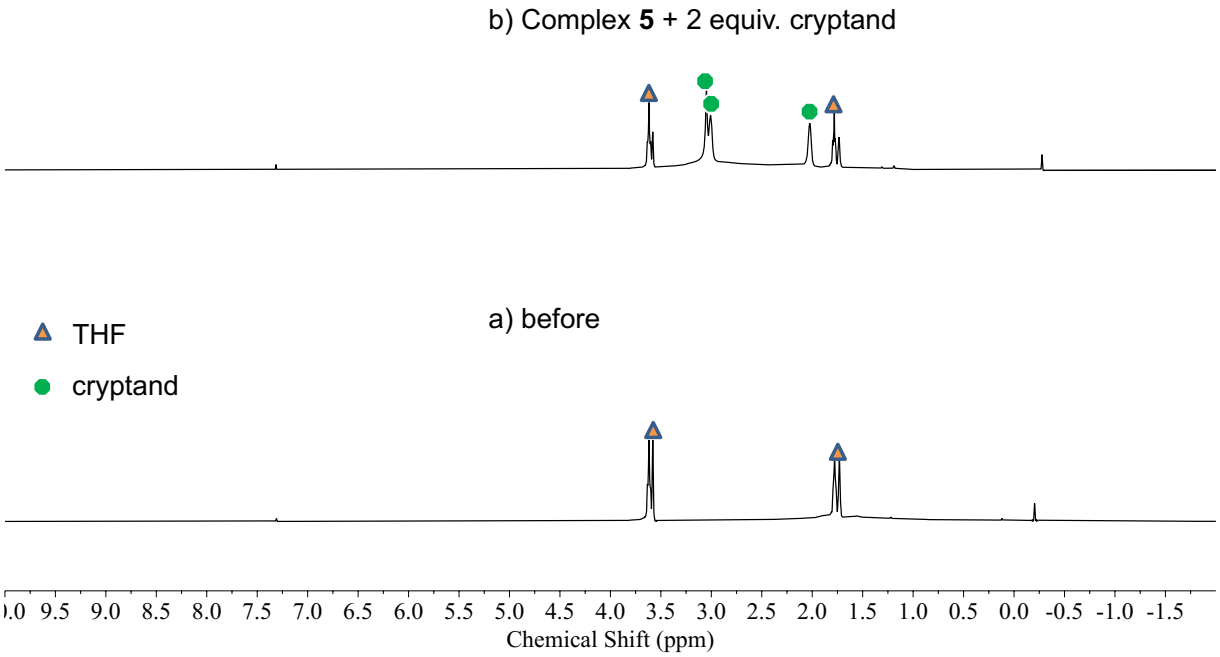


Figure S41: ^{1}H NMR spectra (400 MHz, THF-d_8, 298 K) of the reaction mixture obtained after addition of 2 equiv. of 2.2.2-cryptand to complex **5** at RT a) before b) **5** + 2 equiv. of 2.2.2-cryptand immediately.

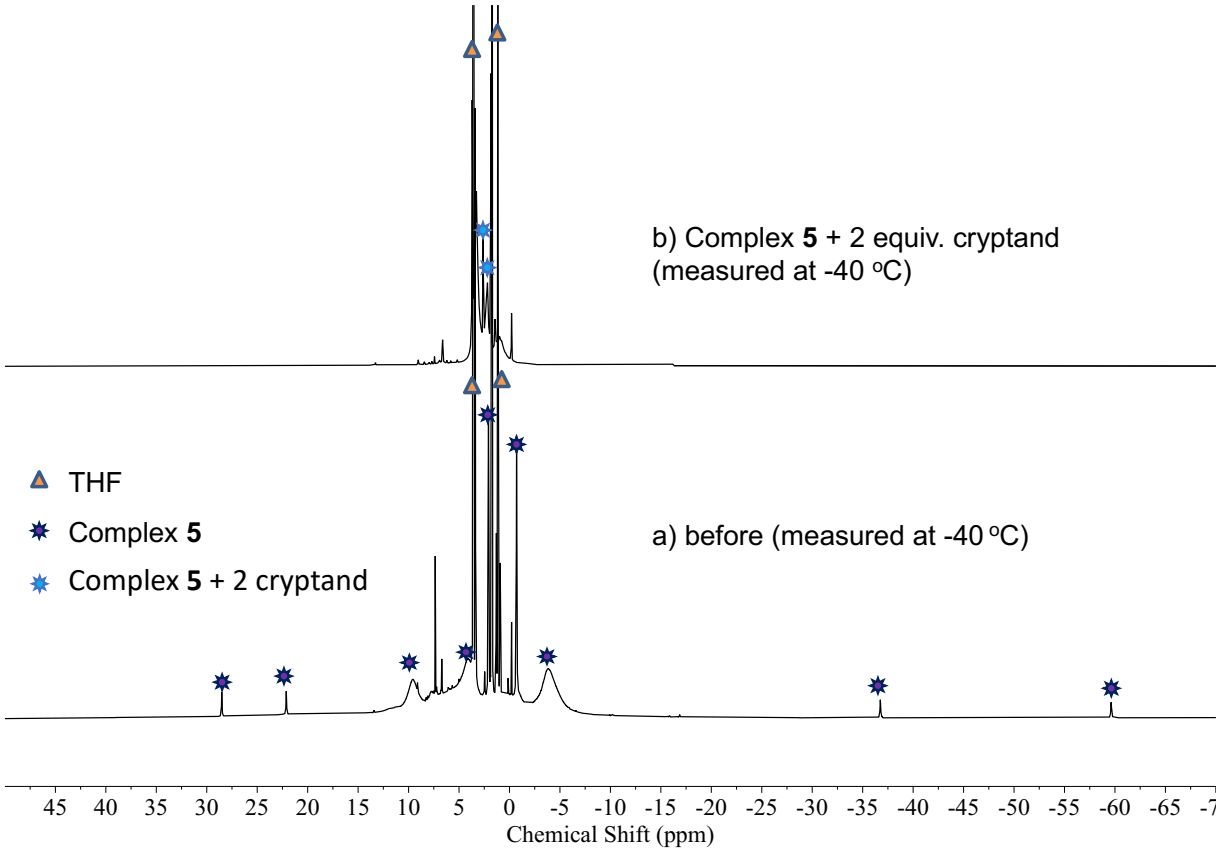


Figure S42: ^{1}H NMR spectra (400 MHz, THF-d_8, 233 K) of the reaction mixture obtained after addition of 2 equiv. of 2.2.2-cryptand to complex **5** at RT a) before (measured at -40 °C) b) **5** + 2 equiv. of 2.2.2-cryptand immediately (measured at -40 °C).

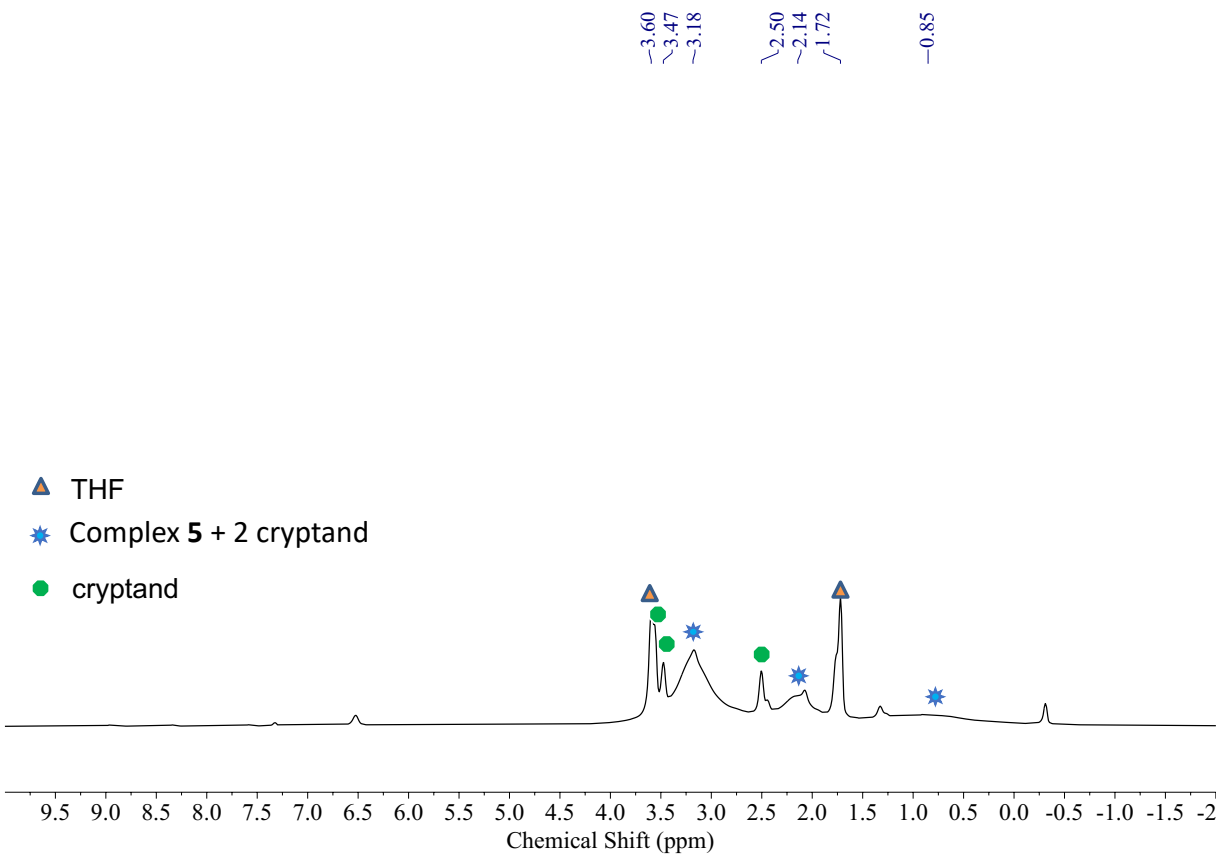


Figure S43: ^{1}H NMR spectrum (400 MHz, THF-d_8, 233 K) of the reaction mixture obtained after addition of 2 equiv. of 2.2.2-cryptand to complex **5** at RT (measured at -40 °C). Zoom of the -2-10 ppm region.

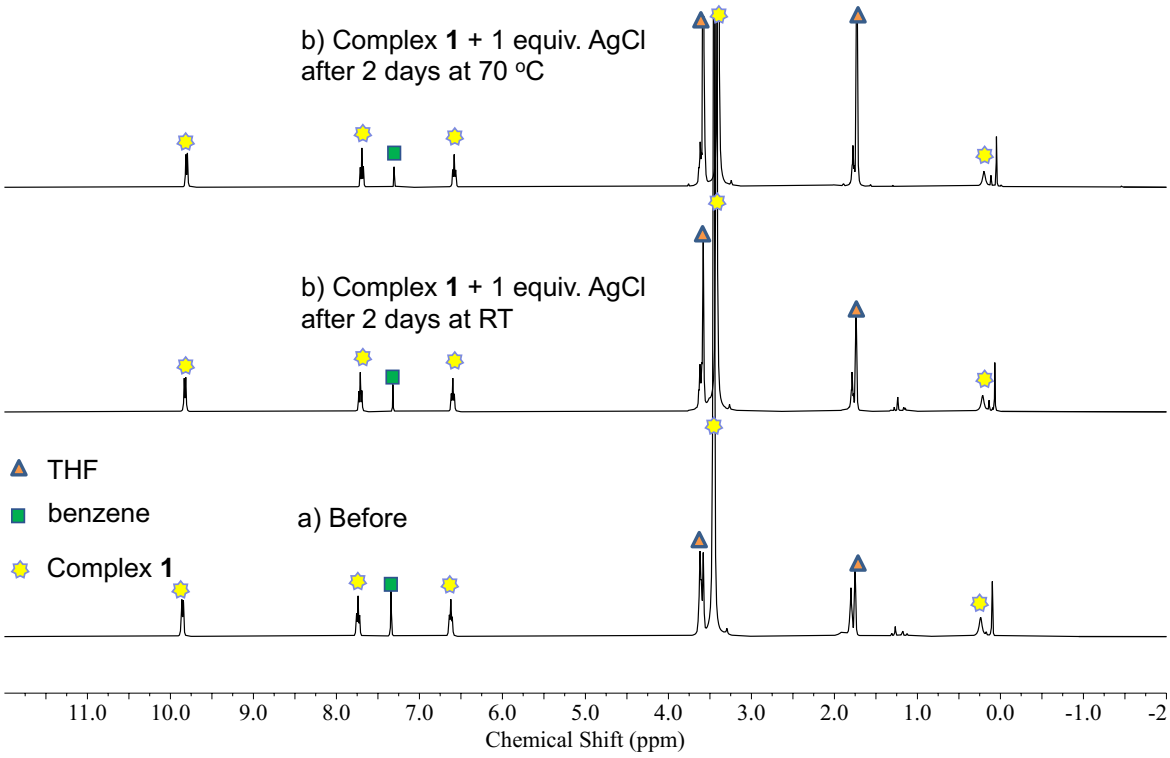


Figure S44: ^{1}H NMR spectra (400 MHz, THF-d_8, 298 K) of the reaction mixture obtained after addition of 1 equiv. of AgCl to complex **1** a) before b) **1** + 1 equiv. of AgCl at RT after 2 days, c) **1** + 1 equiv. of AgCl at 70 °C after 2 days.

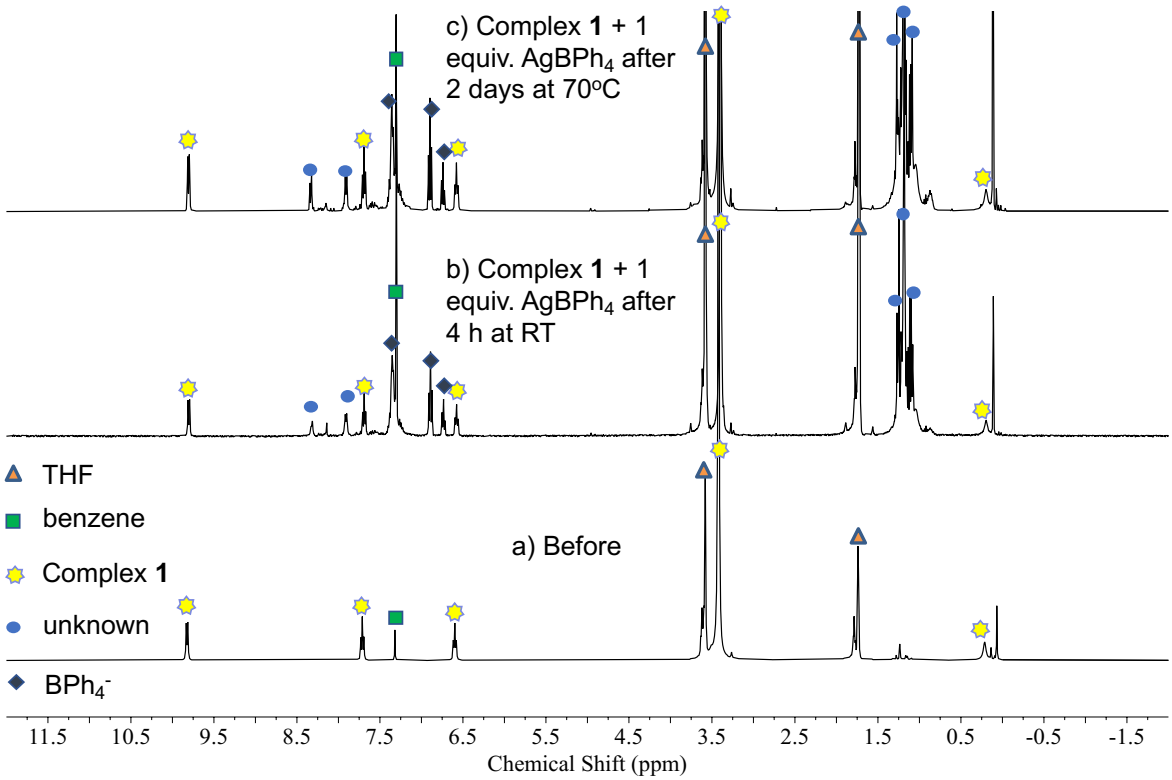


Figure S45: ^{1}H NMR spectra (400 MHz, THF-d_8, 298 K) of the reaction mixture obtained after addition of 1 equiv. of $AgBPh_4$ to complex **1** a) before b) **1** + 1 equiv. of $AgBPh_4$ at RT after 4 h, c) **1** + 1 equiv. of $AgBPh_4$ at 70 °C after 2 days.

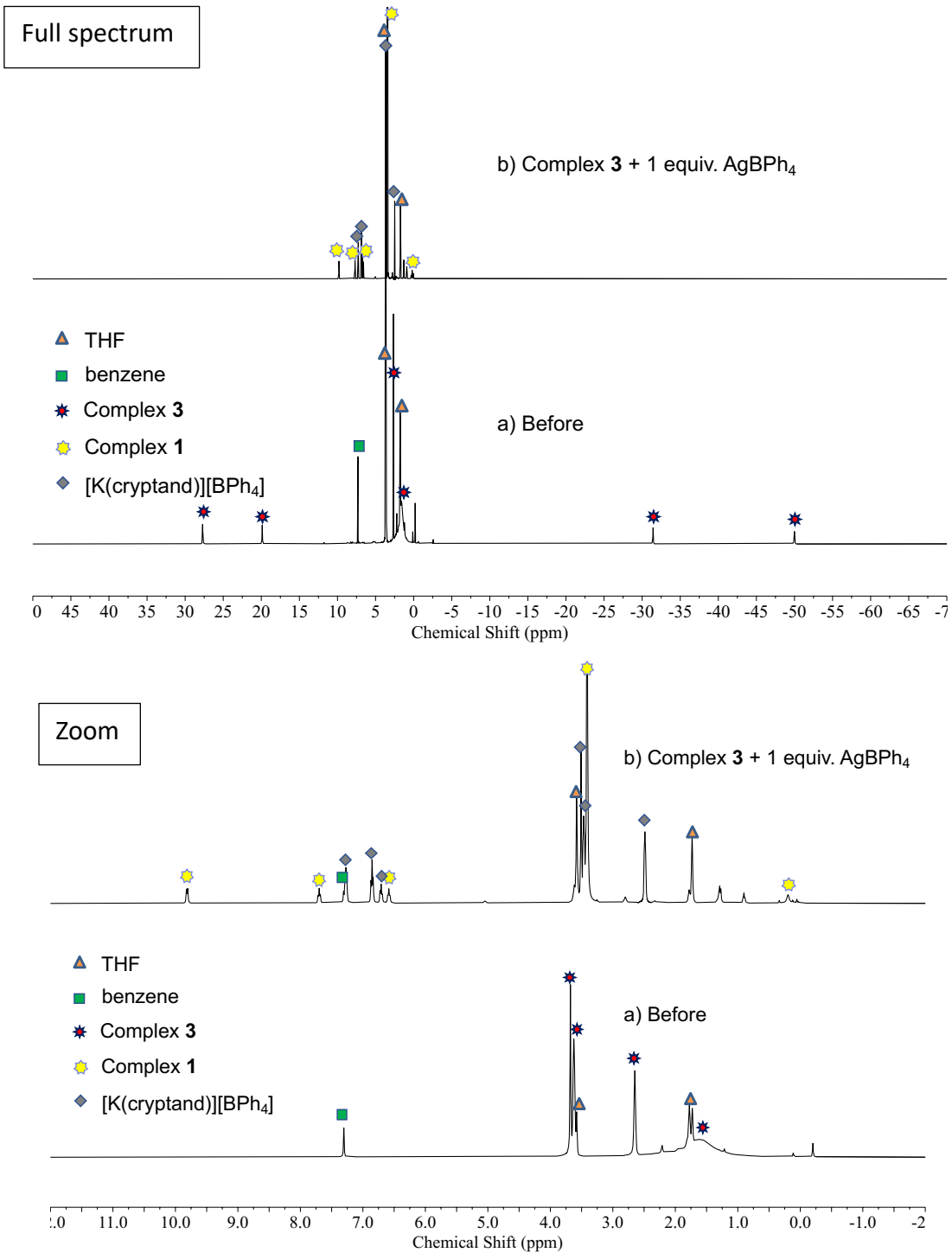


Figure S46: ^{1}H NMR spectra (400 MHz, THF-d_8, 298 K) of the reaction mixture obtained after addition of 1 equiv. of $AgBPh_4$ to complex **3** top) full spectrum a) before b) **3** + 1 equiv. of $AgBPh_4$ immediately; bottom) Zoom of the -2-12 ppm region a) before b) **3** + 1 equiv. of $AgBPh_4$ immediately.

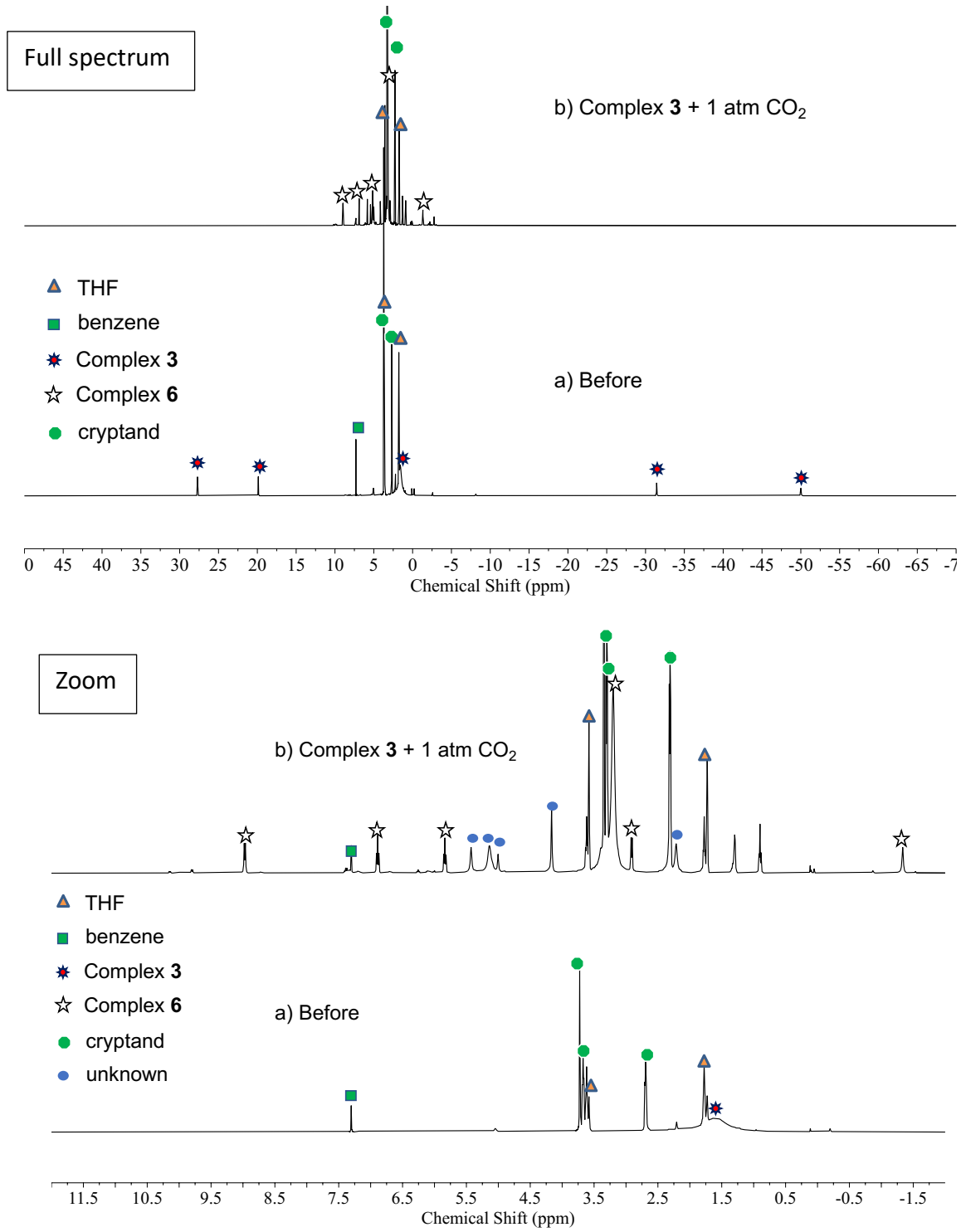


Figure S47: ^{1}H NMR spectra (400 MHz, THF-d_8, 298 K) of the reaction mixture obtained after addition of 1 atm of CO_2 to complex **3** top) full spectrum a) before b) **3** + 1 atm of CO_2 immediately; bottom) Zoom of the -2-12 ppm region a) before b) **3** + 1 atm of CO_2 immediately.

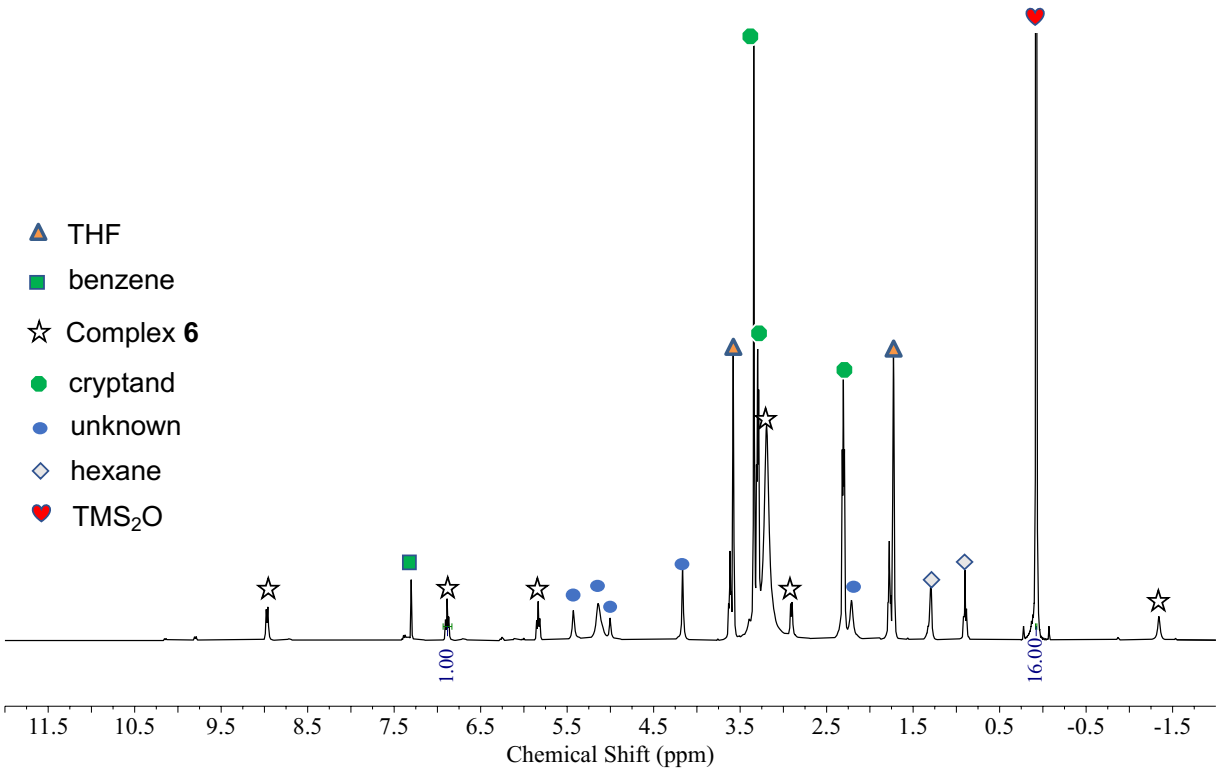


Figure S48: Quantitative ^{1}H NMR spectrum (400 MHz, THF-d_8, 298 K) of the reaction mixture obtained after addition of 1 atm of CO_2 to complex **3**. (TMS_2O was added as the internal standard.)

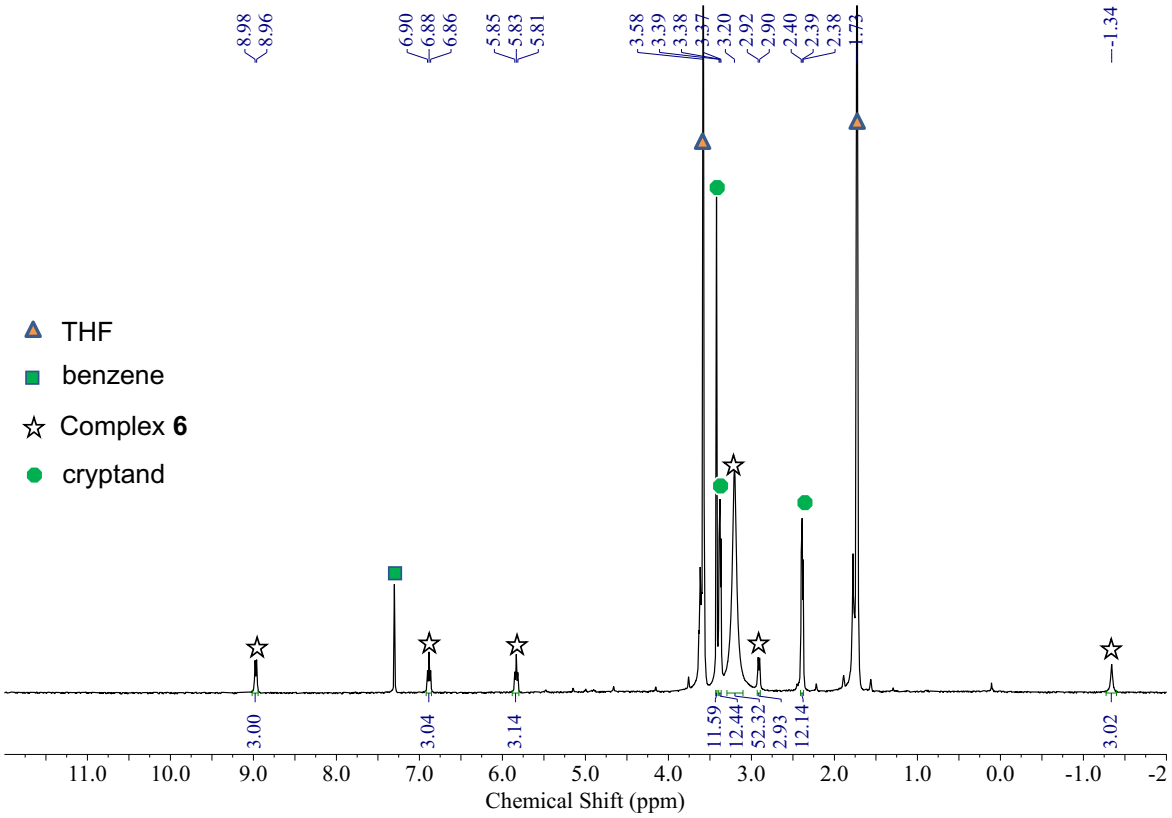


Figure S49: ^{1}H NMR spectrum (400 MHz, THF-d_8) of isolated [K(2.2.2-cryptand)]$_2$[{(1,3,5-(2-OSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$)Ce)$_2$(μ-C$_2$O$_4$) }], **6**.

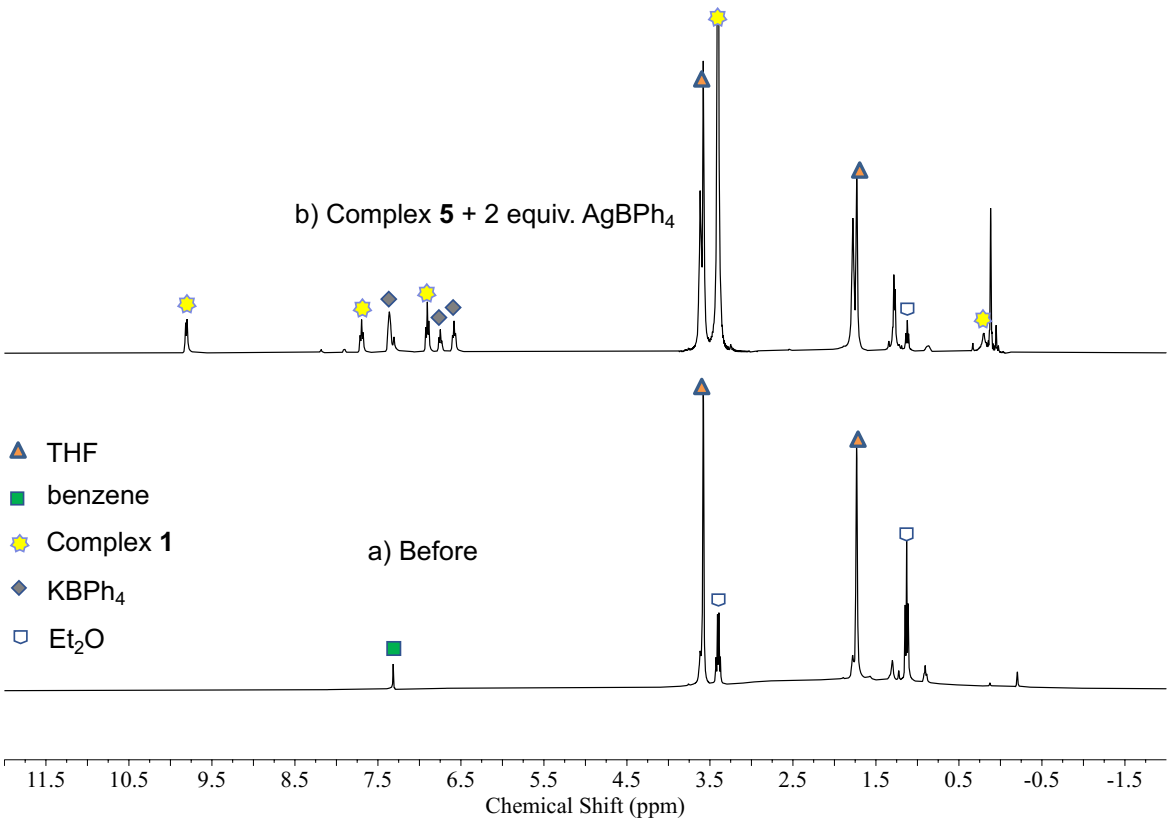


Figure S50: ^{1}H NMR spectra (400 MHz, THF-d_8, 298 K) of the reaction mixture obtained after addition of 2 equiv. of $AgBPh_4$ to complex **5** a) before b) **5** + 2 equiv. of $AgBPh_4$ immediately.

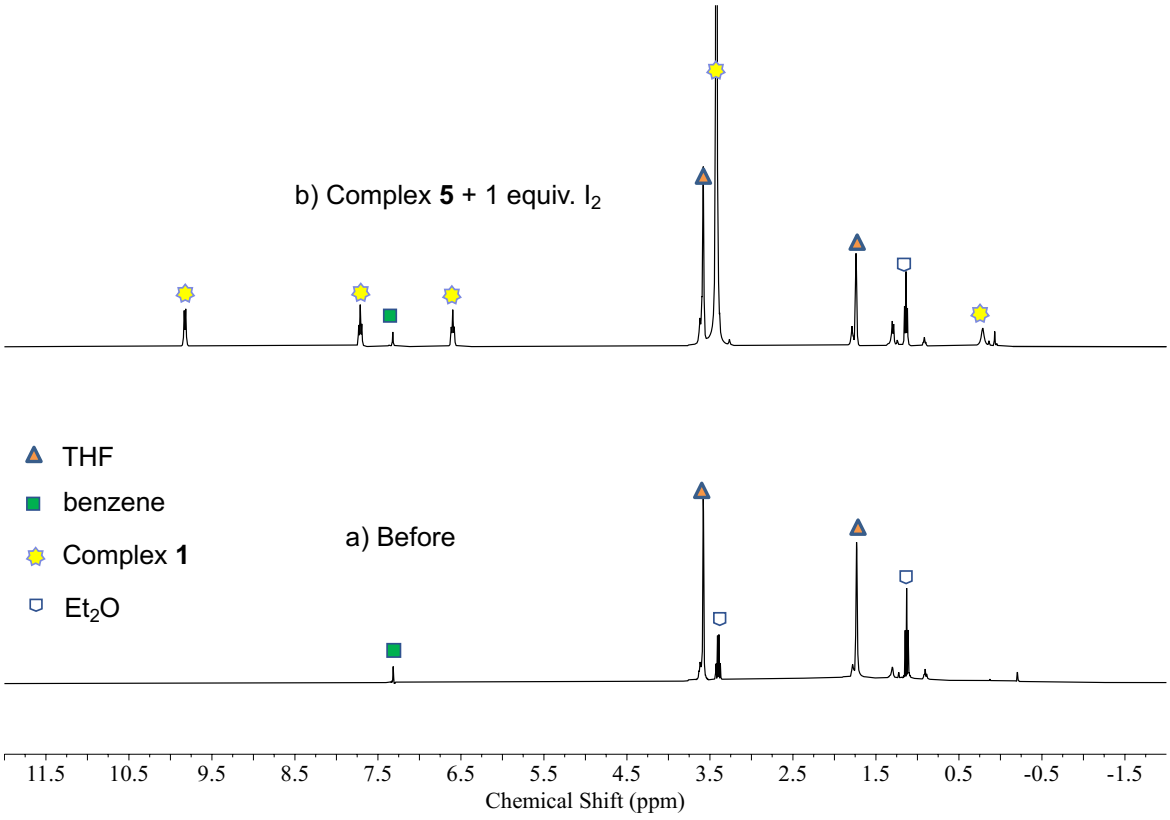


Figure S51: ^{1}H NMR spectra (400 MHz, THF-d_8, 298 K) of the reaction mixture obtained after addition of 1 equiv. of I_2 to complex **5** a) before b) **5** + 1 equiv. of I_2 immediately.

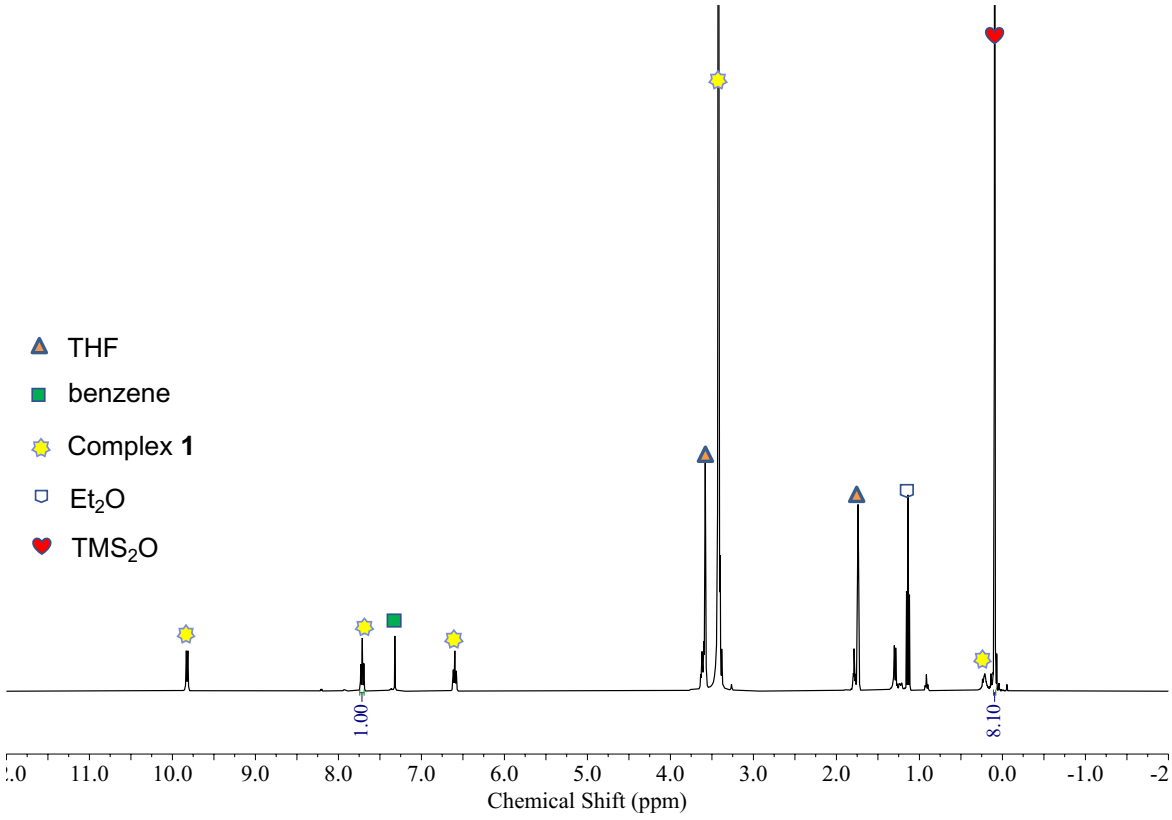


Figure S52: Quantitative ^{1}H NMR spectrum (400 MHz, THF-d_8, 298 K) of the reaction mixture obtained after addition of 1 equiv. of I_2 to complex **5**. (TMS_2O was added as the internal standard.)

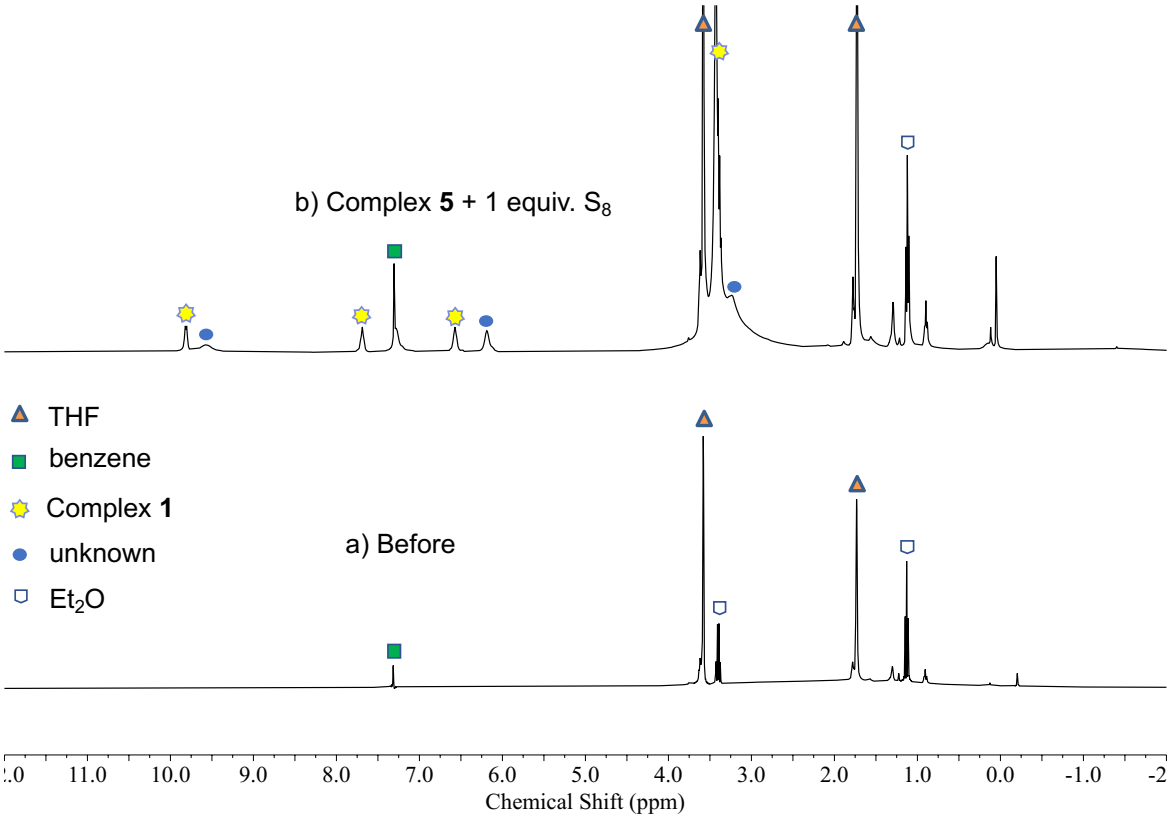


Figure S53: ^{1}H NMR spectra (400 MHz, THF-d_8, 298 K) of the reaction mixture obtained after addition of 1 equiv. of S_8 to complex **5** a) before b) **5** + 1 equiv. of S_8 immediately.

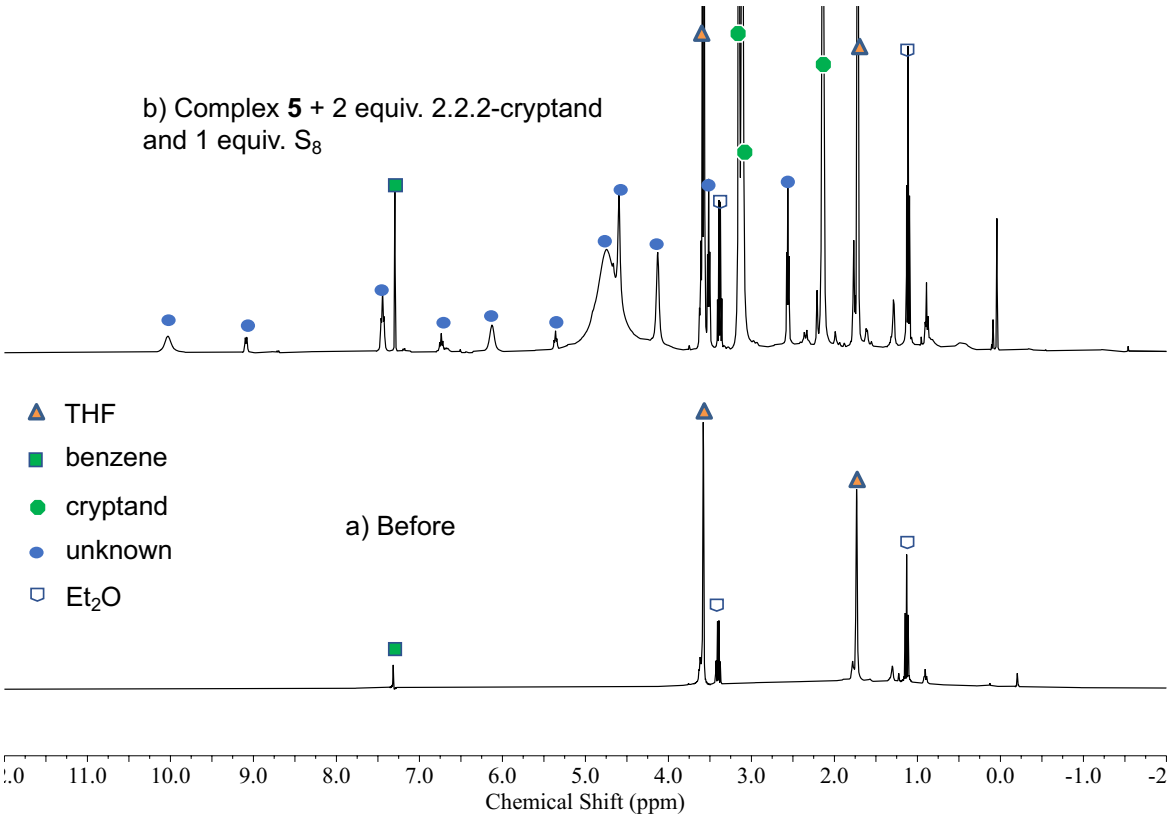


Figure S54: ^{1}H NMR spectra (400 MHz, THF-d_8, 298 K) of the reaction mixture obtained after addition of 2 equiv. of 2.2.2-cryptand and 1 equiv. of S_8 to complex **5** a) before b) **5** + 2 equiv. of 2.2.2-cryptand and 1 equiv. of S_8 immediately.

UV-Vis Spectra

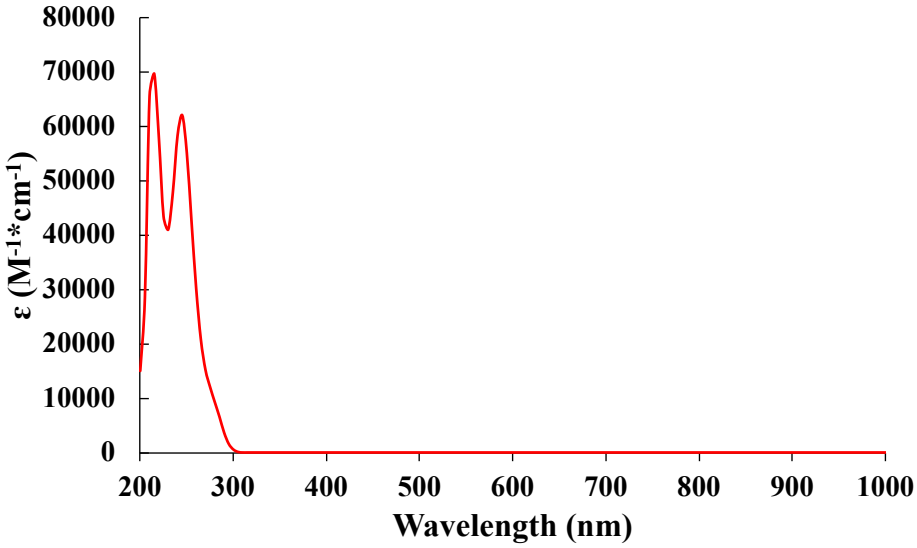


Figure S55: UV-Vis spectrum of a 0.4 mM solution of **L(OH)$_3$** in THF at room temperature.

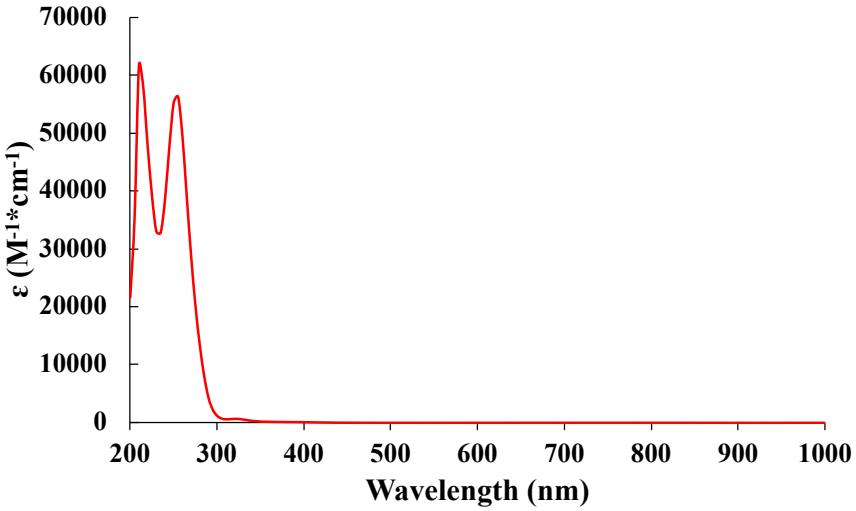


Figure S56: UV-Vis spectrum of a 0.4 mM solution of complex **1** in THF at room temperature.

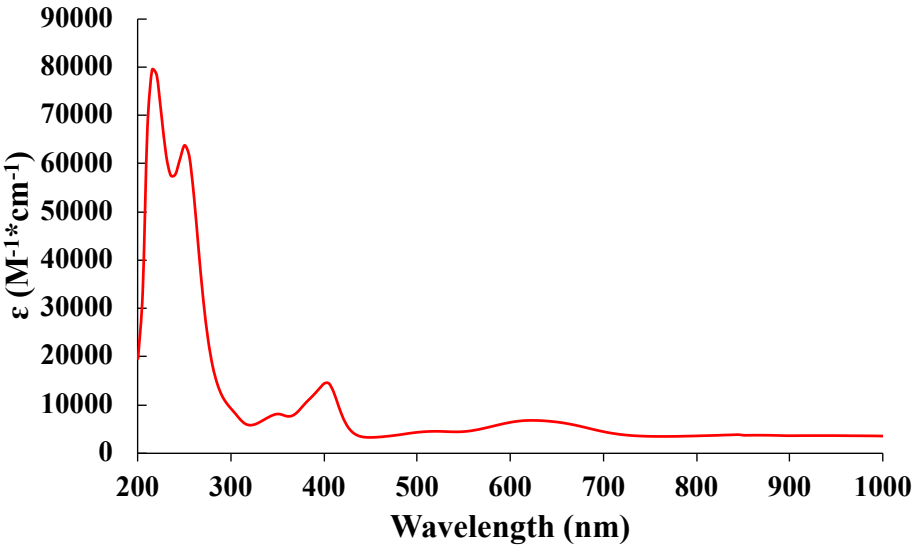


Figure S57: UV-Vis spectrum of a 0.4 mM solution of **$[(K(crypt))(L(OK)_3)]_2$** in THF at room temperature.

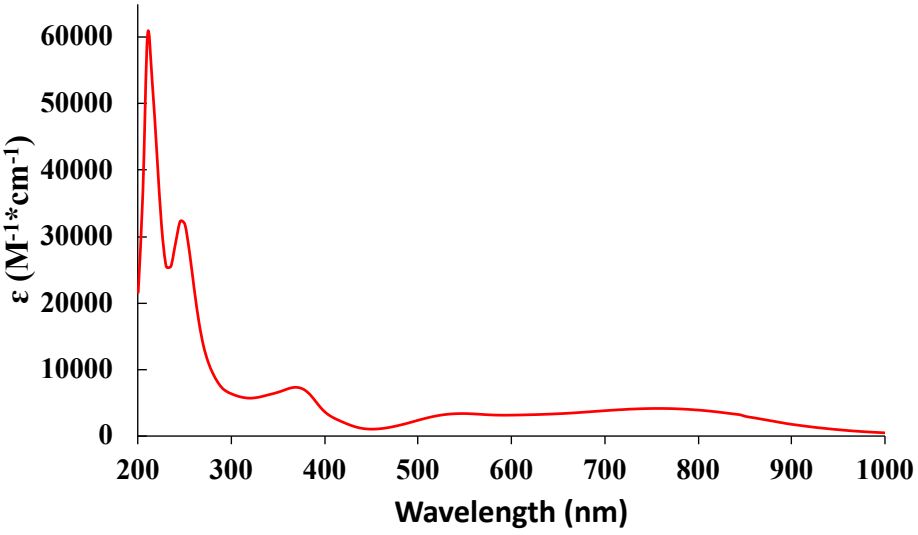


Figure S58: UV-Vis spectrum of a 0.4 mM solution of complex **3** in THF at room temperature.

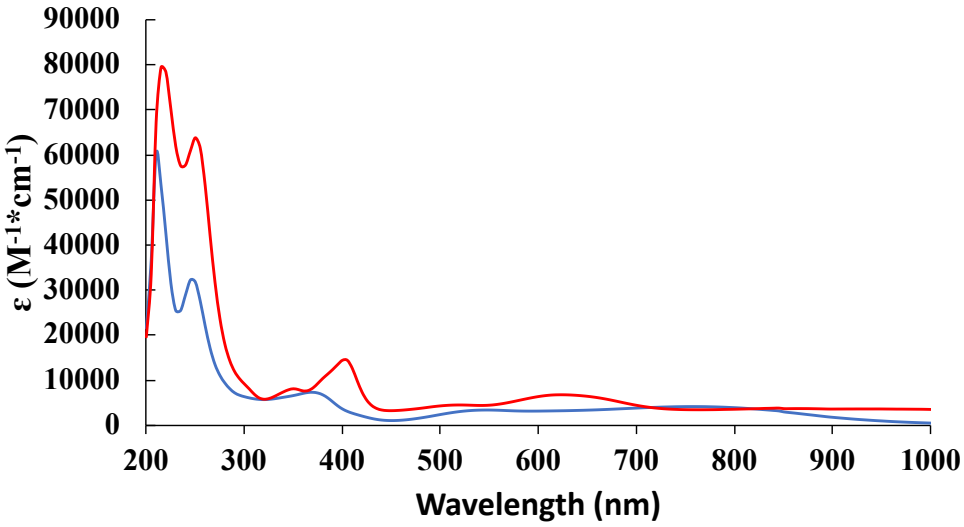


Figure S59: UV-Vis spectrum of a 0.4 mM solution of complex **3** (blue) and **[(K(crypt))(L(OK)$_3$)]$_2$** (red) in THF at room temperature.

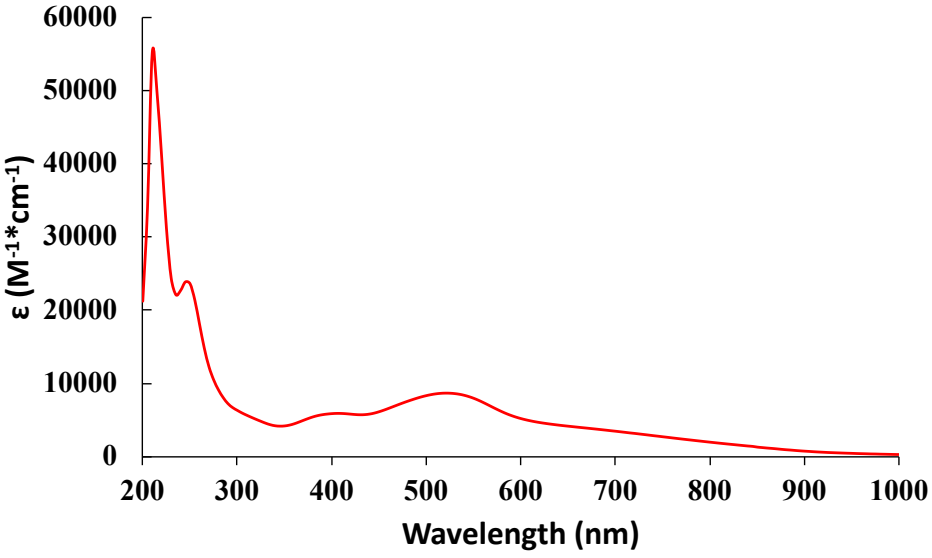


Figure S60: UV-Vis spectrum of a 0.4 mM solution of complex **5** in THF at room temperature.

EPR

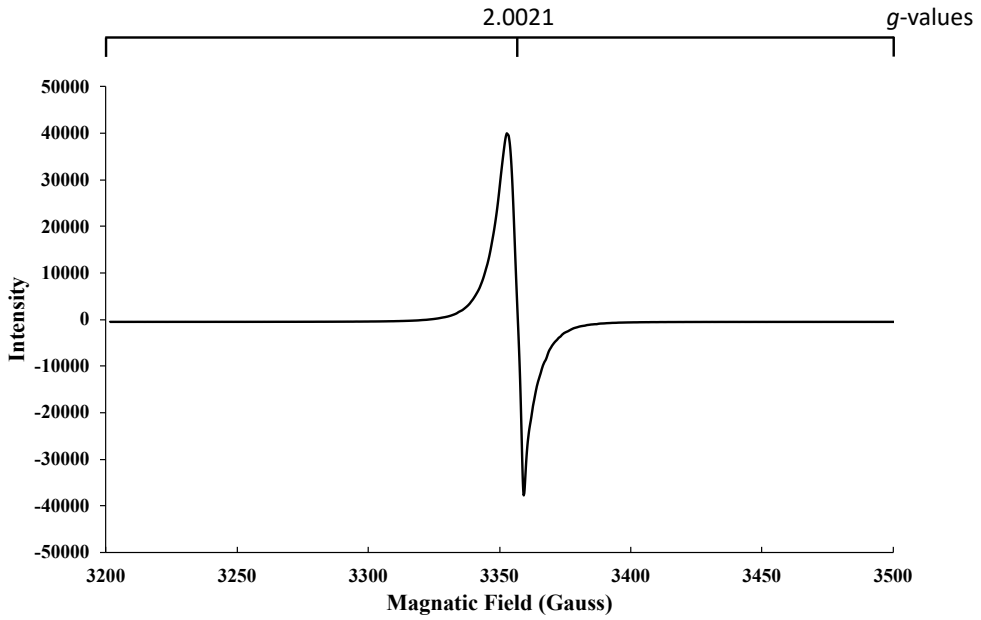


Figure S61: X-band (9.40 GHz) EPR spectrum of **$[(K(crypt))(L(OK)_3)]_2$** in solid-state (6 K).

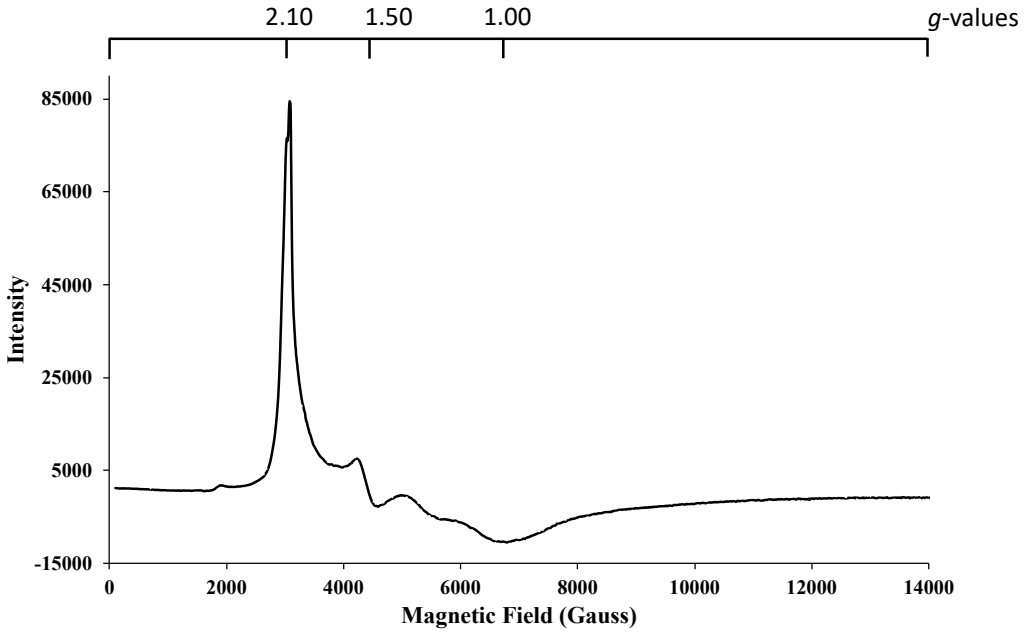


Figure S62: X-band (9.40 GHz) EPR spectrum of **1** in solid-state (6 K).

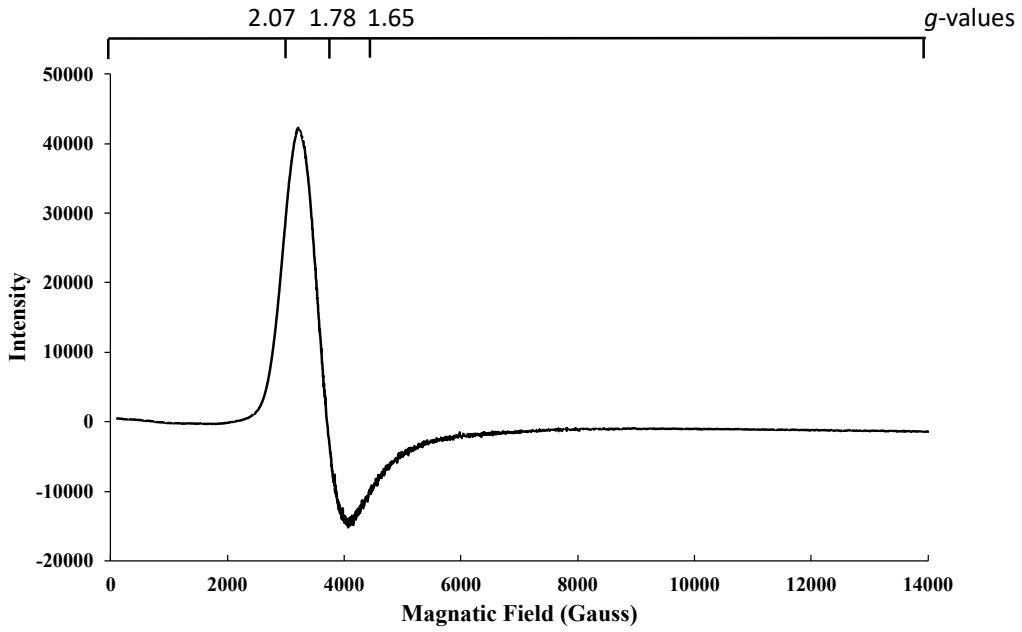


Figure S63: X-band (9.40 GHz) EPR spectrum of **1** in frozen-solution state (6 K).

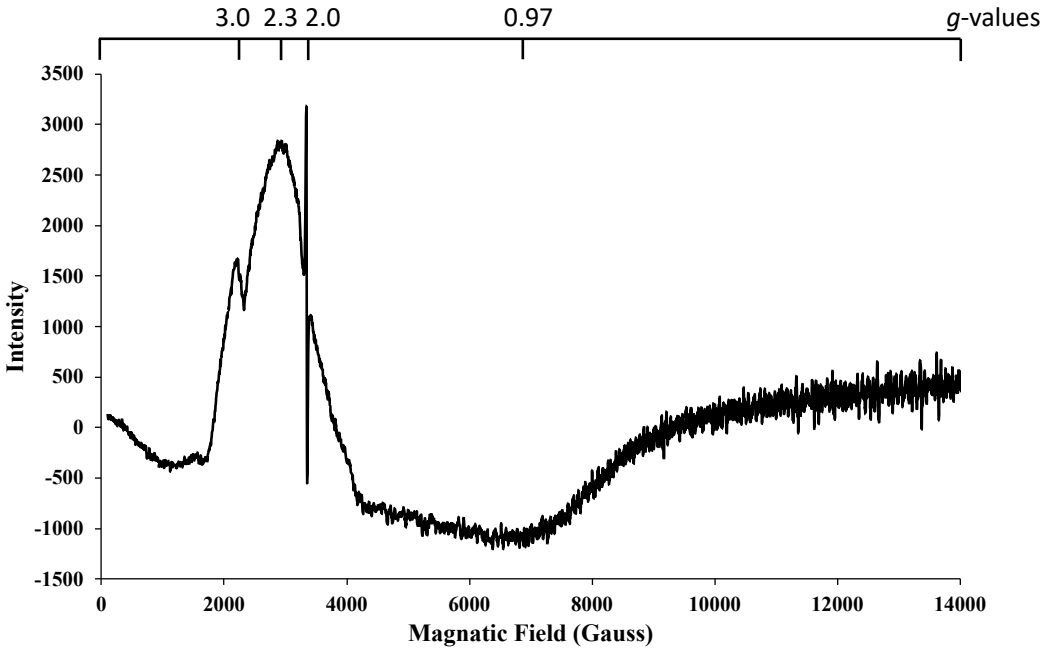


Figure S64: X-band (9.40 GHz) EPR spectrum of **3** in solid-state (6 K).

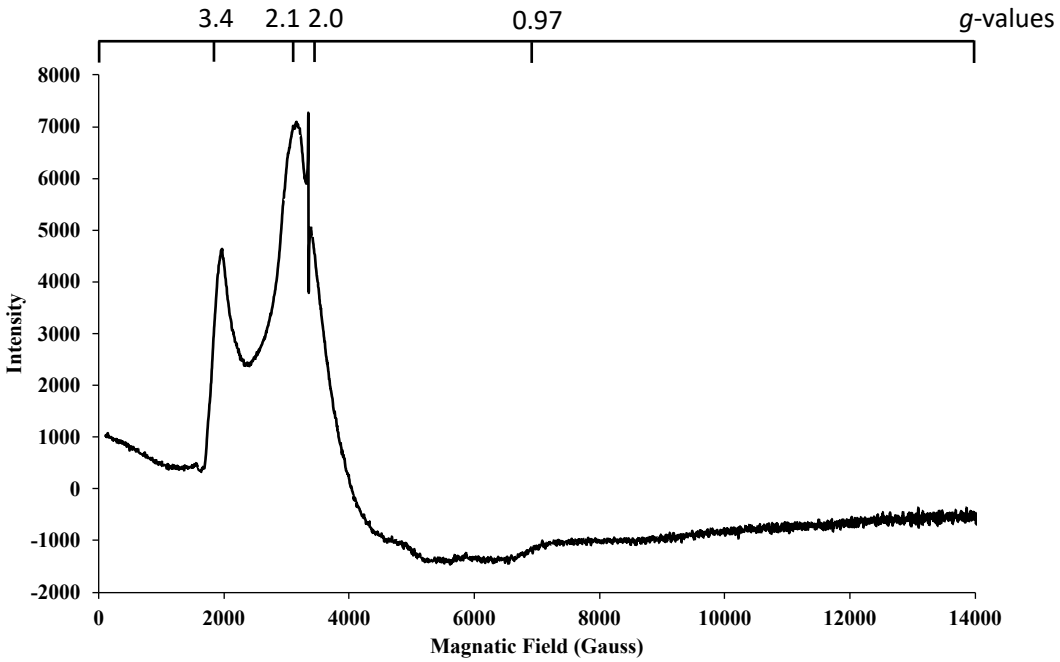


Figure S65: X-band (9.40 GHz) EPR spectrum of [{K(1,3,5-(2-OSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$)Ce(THF)}] in solid-state (6 K).

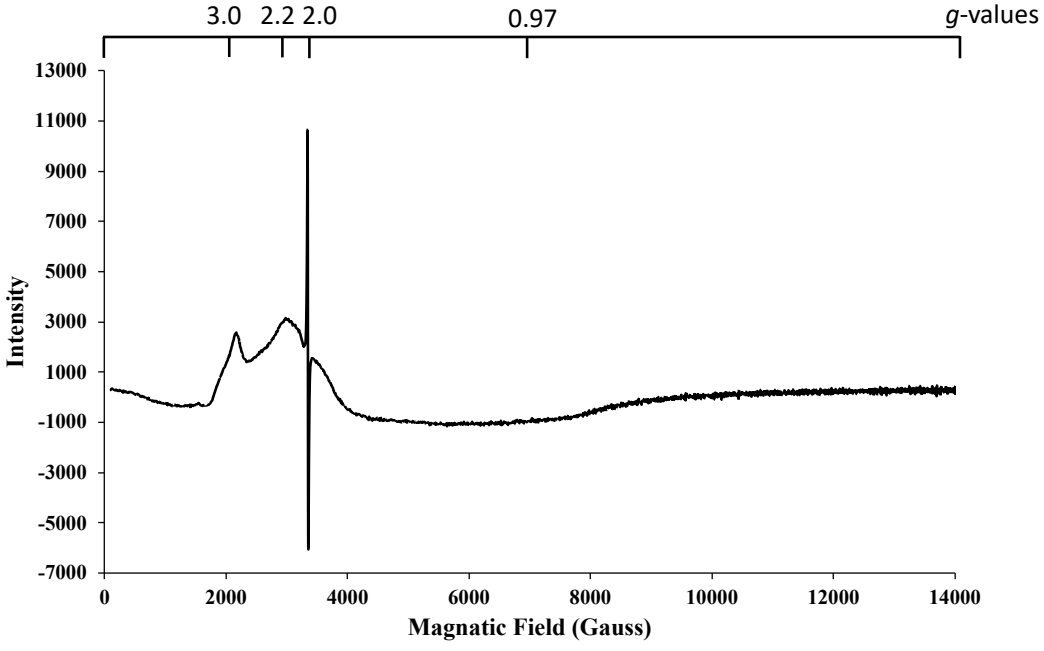


Figure S66: X-band (9.40 GHz) EPR spectrum of **4** in solid-state (6 K).

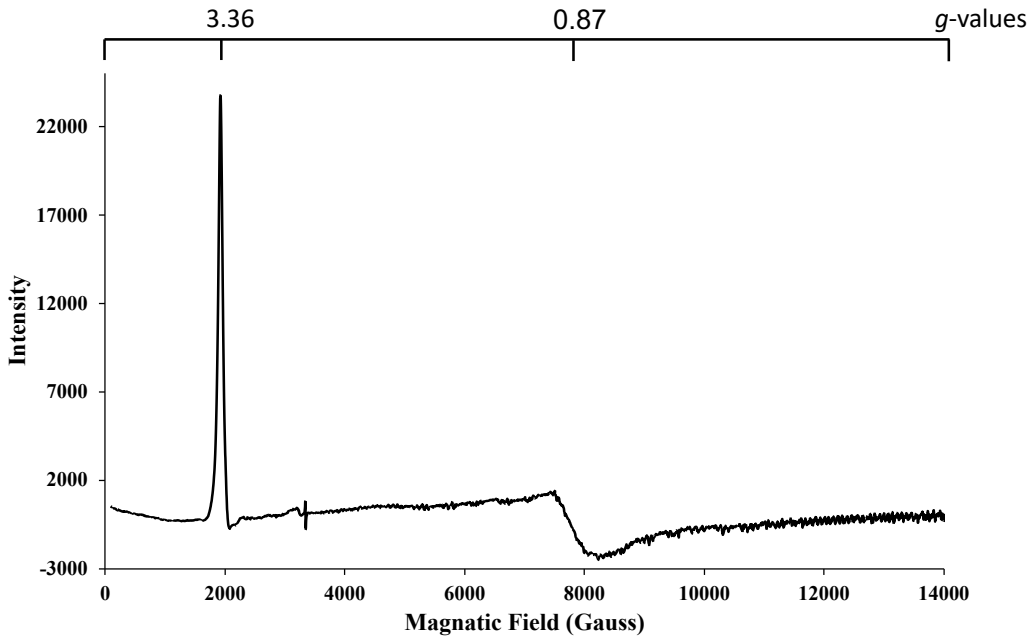


Figure S67: X-band (9.40 GHz) EPR spectrum of **5** in solid-state (6 K).

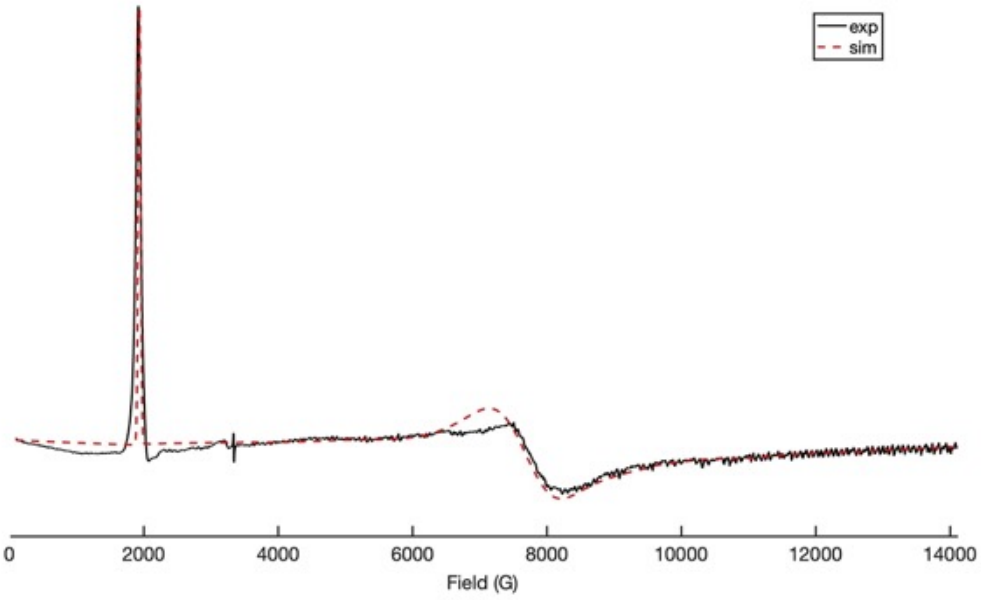


Figure S68: X-band (9.40 GHz) EPR spectrum of **5** in solid-state (6 K) (red dashed line, simulation; black line, experiment). The plot was fit to an axial set of g-values (g_y = 3.360; g_z = 0.870; g_x < 0.5).

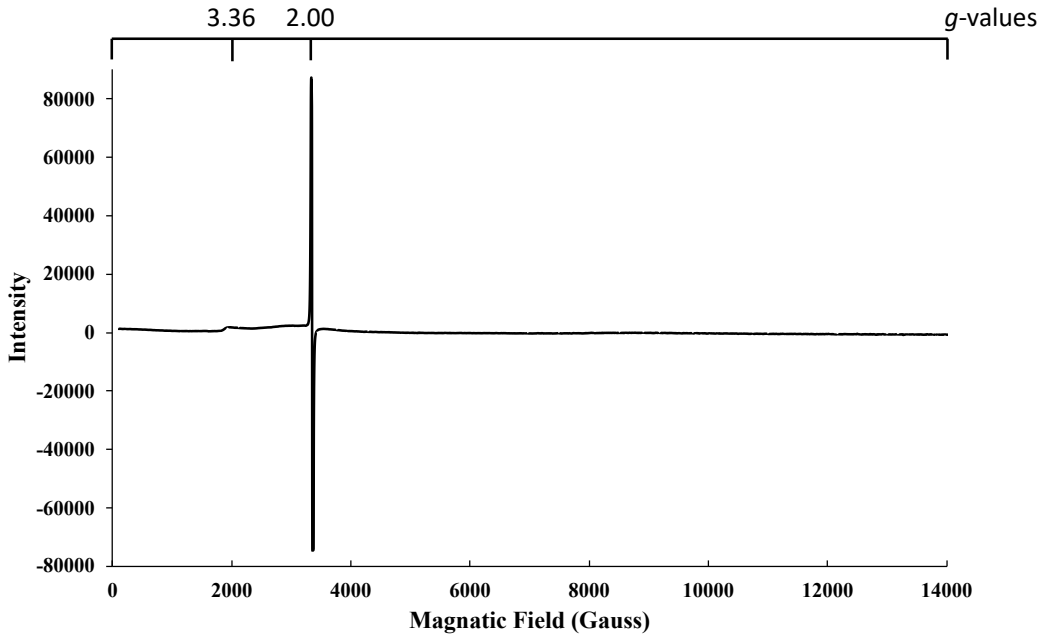


Figure S69: X-band (9.40 GHz) EPR spectrum of **5** + cryptands in solid-state (6 K).

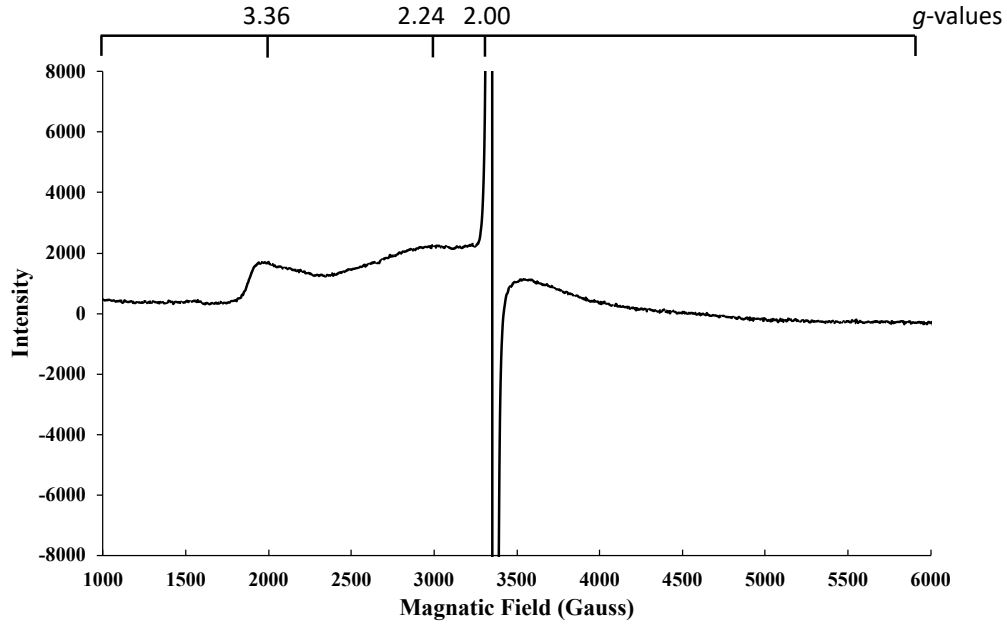


Figure S70: X-band (9.40 GHz) EPR spectrum of **5** + cryptands in solid-state (6 K) (Zoom in).

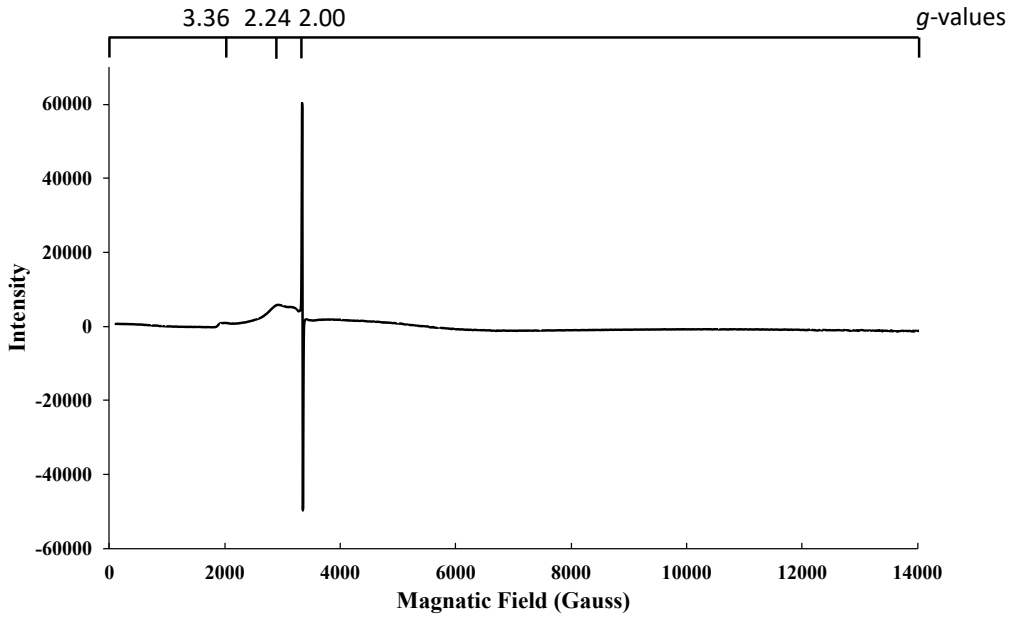


Figure S71: X-band (9.40 GHz) EPR spectrum of **5** + cryptands in frozen-solution state (6 K).

Electrochemistry

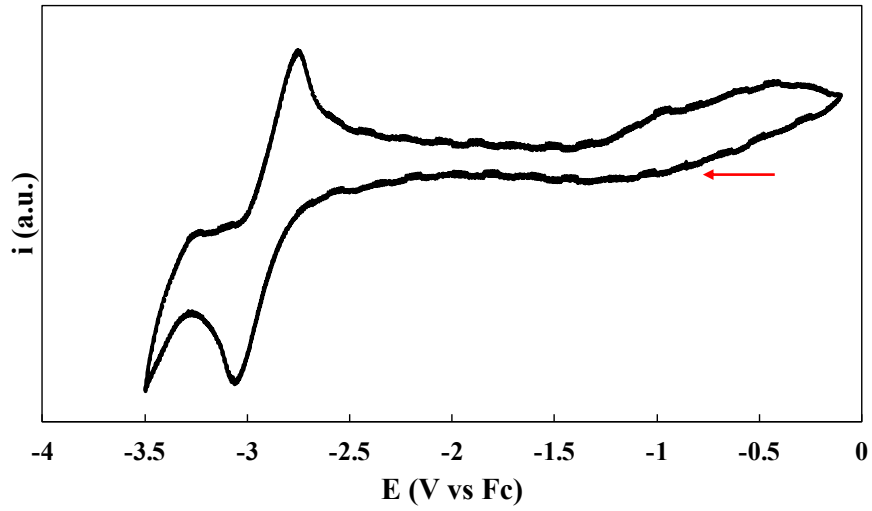


Figure S72: Cyclic voltammogram of complex **1** recorded in 0.1 M $[NBu_4][BPh_4]$ in 3.0 mM THF solution at 25°C, at a scan rate of 100 mV/sec, referenced against $[Fe(C_5H_5)_2]^+$/ $[Fe(C_5H_5)_2]$.

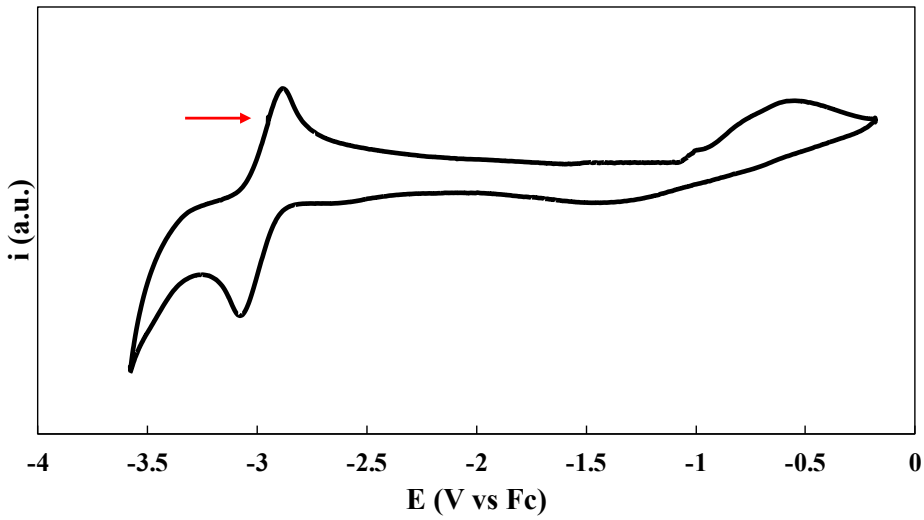


Figure S73: Cyclic voltammogram of complex **3** recorded in 0.1 M $[NBu_4][BPh_4]$ in 3.0 mM THF solution at 25°C, at a scan rate of 100 mV/sec, referenced against $[Fe(C_5H_5)_2]^+$/ $[Fe(C_5H_5)_2]$.

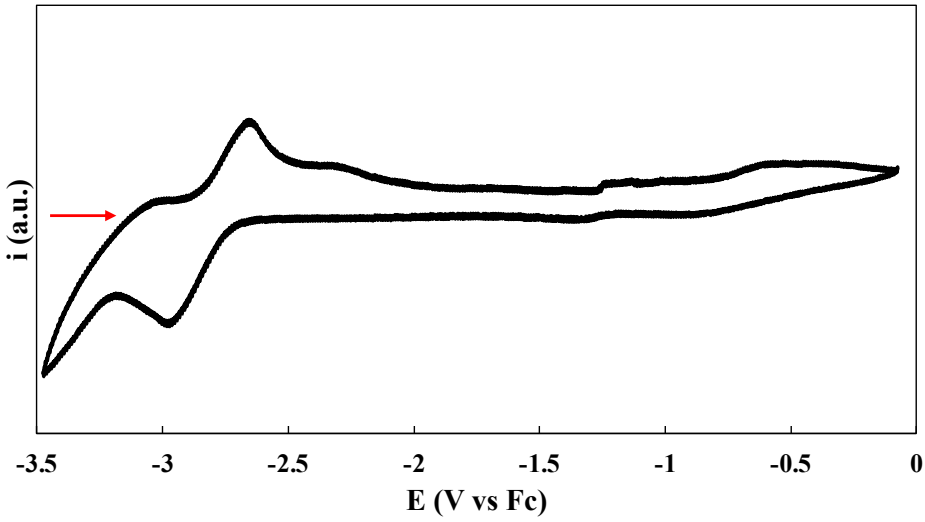


Figure S74: Cyclic voltammogram of complex **5** recorded in 0.1 M $[NBu_4][BPh_4]$ in 3.0 mM THF solution at 25°C, at a scan rate of 100 mV/sec, referenced against $[Fe(C_5H_5)_2]^+$/ $[Fe(C_5H_5)_2]$.

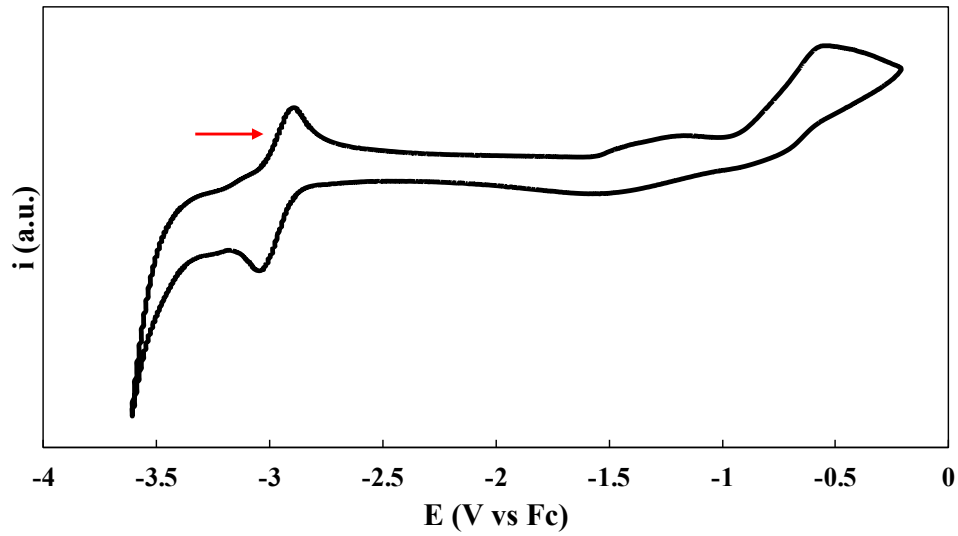


Figure S75: Cyclic voltammogram of complex **5** + cryptands recorded in 0.1 M $[NBu_4][BPh_4]$ in 3.0 mM THF solution at 25°C, at a scan rate of 100 mV/sec, referenced against $[Fe(C_5H_5)_2]^+/[Fe(C_5H_5)_2]$.

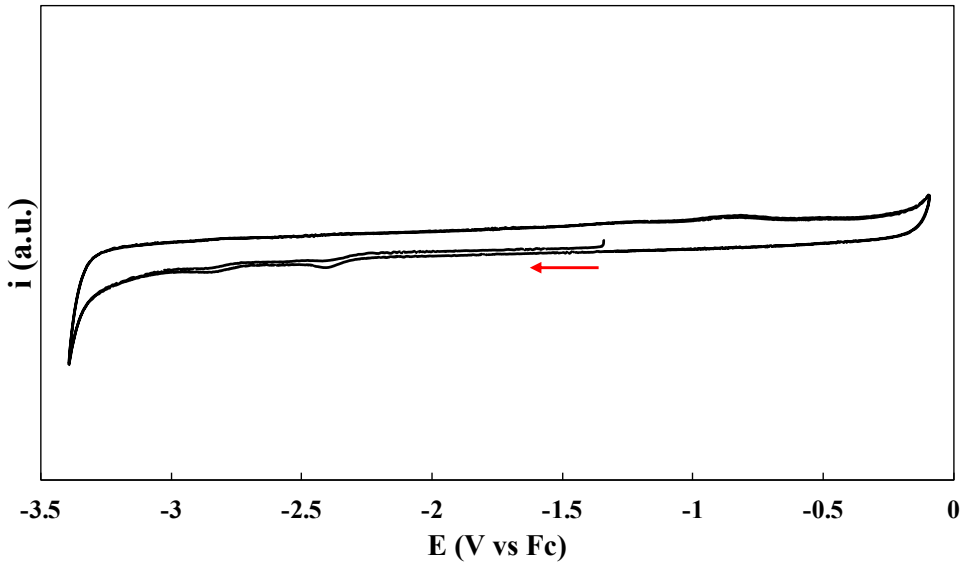


Figure S76: Cyclic voltammogram of **L(OK)$_3$** recorded in 0.1 M $[NBu_4][BPh_4]$ in 3.0 mM THF solution at 25°C, at a scan rate of 100 mV/sec, referenced against $[Fe(C_5H_5)_2]^+/[Fe(C_5H_5)_2]$.

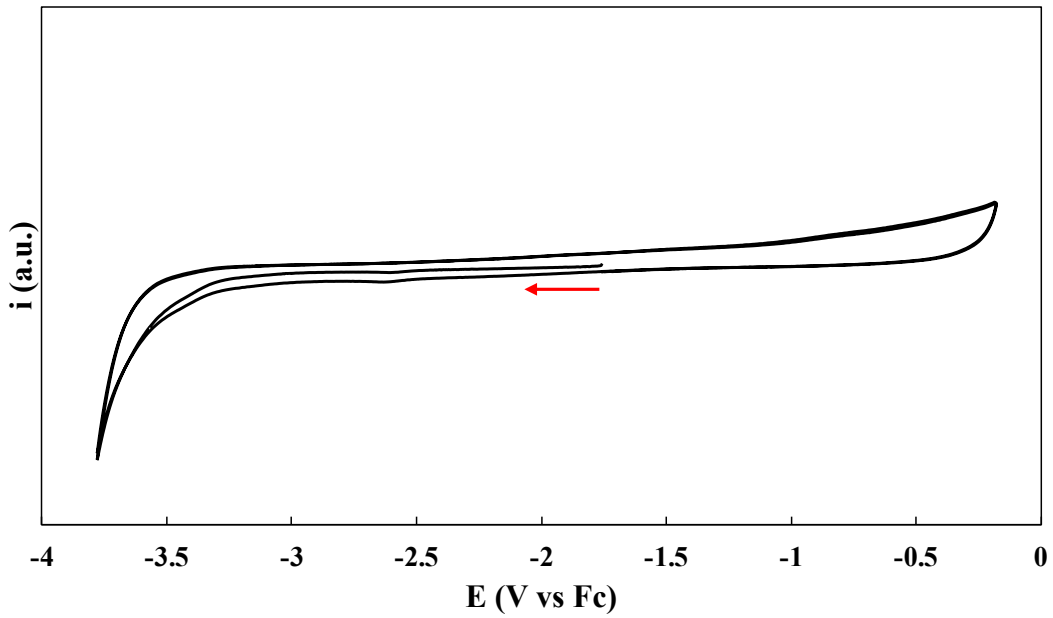


Figure S77: Cyclic voltammogram of **L(OK)$_3$** + cryptand recorded in 0.1 M [NBu$_4$][BPh$_4$] in 3.0 mM THF solution at 25°C, at a scan rate of 100 mV/sec, referenced against [Fe(C$_5$H$_5$)$_2$]$^+$/ [Fe(C$_5$H$_5$)$_2$].

X-ray Crystal Structure Determination Details

Suitable crystals were selected and mounted on various Rigaku diffractometers (XtaLAB Synergy R, DW system, HyPix-Arc 150 detector or SuperNova, Dual, Cu at home/near, AtlasS type detectors). The crystals were kept at a steady *T* = 140.00(10) K during data collection. Data were measured using ω scans with Cu K$_\alpha$ radiation. The diffraction patterns were indexed and the total number of runs and images were based on the strategy calculation from the program CrysAlisPro 1.171.42.72a (Rigaku OD, 2022)[5]. The unit cells were refined using CrysAlisPro 1.171.42.72a (Rigaku OD, 2022)[5]. Data reduction, scaling and absorption corrections were performed using CrysAlisPro 1.171.42.72a (Rigaku OD, 2022)[5]. The structures were solved with the **ShelXT** (Sheldrick, 2015)[8] solution program using dual methods and by using **Olex2** 1.5 (Dolomanov et al., 2009)[6] as the graphical interface. The models were refined with **ShelXL** 2018/3 (Sheldrick, 2015)[7] using full matrix least squares minimization on F^2. All non-hydrogen atoms were refined anisotropically. The positions of the hydrogen atom were calculated geometrically and refined using the riding model. Several structures displayed problems dealing with disorder (disordered ligands or solvent) or twinning. The major employed technique was the split model combined with a series of restraints and constraints. The restraints and constraints are used in order to get acceptable bond lengths and angles and/or anisotropic behavior. In some cases, the twinning treatment has been used for real twins or for multi-crystals, in order to properly separate the different domains. Finally, in some structures the solvent molecules were difficult to handle and the mask algorithm (by Olex2) was used to squeeze them completely from the final model.

Table S1. Crystal data and structural refinement parameters for complexes 1,3,5-(2-SiCl(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$, **LCl$_3$** (CCDC: 2239278), 1,3,5-(2-HOSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$, **L(OH)$_3$** (CCDC: 2239279), and [K(THF)$_3${1,3,5-(2-KOSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$}]$_2$, **[(K(THF)$_3$)(L(OK)$_3$)]$_2$** (CCDC: 2239283).

	LCl$_3$	**L(OH)$_3$**	**[(K(THF)$_3$)(L(OK)$_3$)]$_2$**
Formula	$C_{48}H_{69}Cl_3O_6Si_3$	$C_{48}H_{72}O_9Si_3$	$C_{120}H_{186}K_8O_{24}Si_6$
Crystal size (mm)	0.17×0.07×0.06	0.11×0.07×0.03	0.45×0.24×0.21
Crystal System	triclinic	triclinic	monoclinic
Space Group	*P*-1	*P*-1	*C*2/*c*
Volume (Å^3)	2568.28(17)	5077.3(6)	15536.37(19)
a (Å)	13.7393(4)	13.5317(9)	29.21058(19)
b (Å)	13.7546(5)	19.7750(16)	18.42416(15)
c (Å)	14.7849(6)	20.4919(12)	29.16367(18)
α (°)	112.760(4)	67.818(6)	90
β (°)	91.008(3)	89.464(5)	98.1608(7)
γ (°)	93.713(3)	89.905(6)	90
Z	2	4	4
Formula Weight	932.65	877.32	2494.02
Density (g cm^{-3})	1.206	1.148	1.066
μ (mm^{-1})	2.633	1.261	2.864
F(000)	996	1896	5336
Temperature (K)	140.00(11)	140.00(10)	140.00(10)
Total Reflections	23460	33428	50880
Unique Reflections	9934	17891	16032
R_{int}	0.0270	0.1103	0.0241
R Indices [I > 2σ(I)]	R_1 = 0.0362 wR_2 = 0.0908	R_1 = 0.0634 wR_2 = 0.0994	R_1 = 0.0301 wR_2 = 0.0817
Largest Diff. Peak and Hole (e.A^{-3})	0.462 and -0.336	0.254 and -0.364	0.260 and -0.293
GOF	1.026	0.854	1.035

F(000), structure factor evaluated in the zeroth-order case, h=k=l= 0; R(int) =∑|Fo2−Fo2(mean)| /∑[Fo2]; I, measured intensities; 'Largest diff. peak and hole', maximum and minimum electron density found in the final Fourier difference map; GOF, goodness of fit (= {∑ [w(Fo2−Fc2)2]/(n−p)} 1/2, where n is the number of reflections and p is the total number of parameters refined).

Table S2. Crystal data and structural refinement parameters for complexes [K(2.2.2-cryptand)]$_2$[{1,3,5-(2-KOSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$}]$_2$, **[(K(crypt))(L(OK)$_3$)]$_2$** (CCDC: 2239280), [(1,3,5-(2-OSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$)Ce(THF)], **1** (CCDC: 2239281), and [1,3,5-(2-OSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$)CeCl], **2** (CCDC: 2239284).

	[(K(crypt))(L(OK)$_3$)]$_2$	**1**	**2**
Formula	$C_{132}H_{210}K_8N_4O_{30}Si_6$	$C_{59}H_{85}CeO_{10}Si_3$	$C_{48}H_{69}CeClO_9Si_3$
Crystal size (mm)	0.38×0.23×0.20	0.23×0.15×0.14	0.25×0.14×0.11
Crystal System	triclinic	triclinic	triclinic
Space Group	*P*-1	*P*-1	*P*-1
Volume (Å^3)	4749.9(2)	3065.73(15)	3021.68(19)
a (Å)	15.5349(4)	14.0331(3)	13.2982(5)
b (Å)	16.9728(5)	15.4209(4)	13.6413(4)
c (Å)	21.2514(6)	16.9380(4)	17.7827(6)
α (°)	112.666(3)	109.329(2)	86.910(3)
β (°)	95.795(2)	108.864(2)	69.976(3)
γ (°)	108.276(2)	101.873(2)	85.916(3)
Z	1	2	2
Formula Weight	2814.37	1178.66	1049.87
Density (g cm^{-3})	0.984	1.277	1.154
μ (mm^{-1})	2.418	0.854	7.145
F(000)	1506	1238	1092
Temperature (K)	140.00(10)	139.99(10)	140.00(10)
Total Reflections	41088	41898	22630
Unique Reflections	18336	18696	11626
R_{int}	0.0297	0.0330	0.0448
R Indices [I > 2σ(I)]	R_1 = 0.0410 wR_2 = 0.1096	R_1 = 0.0421 wR_2 = 0.0994	R_1 = 0.0584 wR_2 = 0.1513
Largest Diff. Peak and Hole (e.A^{-3})	0.692 and -0.271	1.845 and -1.099	2.585 and -0.807
GOF	1.041	1.080	1.022

F(000), structure factor evaluated in the zeroth-order case, h=k=l= 0; R(int) =∑|Fo2−Fo2(mean)| /∑[Fo2]; I, measured intensities; 'Largest diff. peak and hole', maximum and minimum electron density found in the final Fourier difference map; GOF, goodness of fit (= {∑ [w(Fo2−Fc2)2]/(n−p)} 1/2, where n is the number of reflections and p is the total number of parameters refined).

Table S3. Crystal data and structural refinement parameters for complexes [K(2.2.2-cryptand)][(1,3,5-(2-OSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$)Ce(THF)], **3** (CCDC: 2239286), [K(2.2.2-cryptand)][(1,3,5-(2-OSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$)Ce(Et$_3$PO)], **4** (CCDC: 2239282), and [K$_2${1,3,5-(2-OSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$)Ce(Et$_2$O)$_3$}], **5** (CCDC: 2239285).

	3	**4**	**5**
Formula	$C_{78}H_{133}CeKN_2O_{18}Si_3$	$C_{76}H_{130}CeKN_2O_{17}PSi_3$	$C_{60}H_{99}CeK_2O_{12}Si_3$
Crystal size (mm)	0.48×0.24×0.07	0.45×0.15×0.10	0.29×0.05×0.05
Crystal System	monoclinic	monoclinic	monoclinic
Space Group	$P2_1/c$	$P2_1/n$	$P2_1/n$
Volume (Å^3)	8692.2(3)	9507.90(14)	6966.3(6)
a (Å)	20.1856(4)	13.77347(11)	25.2554(11)
b (Å)	20.8622(4)	45.4297(4)	11.0935(6)
c (Å)	21.3727(4)	15.21804(13)	25.7721(14)
α (°)	90	90	90
β (°)	105.036(2)	93.1526(7)	105.250(5)
γ (°)	90	90	90
Z	4	4	4
Formula Weight	1650.35	1638.27	1314.98
Density (g cm^{-3})	1.261	1.144	1.254
μ (mm^{-1})	5.381	5.062	7.035
F(000)	3512	3480	2772
Temperature (K)	140.00(10)	140.00(10)	140.00(10)
Total Reflections	46797	62211	35961
Unique Reflections	16810	19779	13487
R_{int}	0.0641	0.0356	0.1266
R Indices [I > 2σ(I)]	R_1 = 0.0560 wR_2 = 0.1406	R_1 = 0.0554 wR_2 = 0.1199	R_1 = 0.0762 wR_2 = 0.1703
Largest Diff. Peak and Hole (e.A^{-3})	1.003 and -1.048	1.375 and -1.458	1.351 and -0.655
GOF	1.056	1.148	1.017

F(000), structure factor evaluated in the zeroth-order case, h=k=l= 0; R(int) =∑|Fo2−Fo2(mean)| /∑[Fo2]; I, measured intensities; 'Largest diff. peak and hole', maximum and minimum electron density found in the final Fourier difference map; GOF, goodness of fit (= {∑ [w(Fo2−Fc2)2]/(n−p)} 1/2, where n is the number of reflections and p is the total number of parameters refined).

Table S4. Crystal data and structural refinement parameters for complexes [K(2.2.2-cryptand)]$_2$[{(1,3,5-(2-OSi(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$)Ce)$_2$(μ-C$_2$O$_4$) }], **6** (CCDC: 2240543).

	6
Formula	$C_{134}H_{210}Ce_2K_2N_4O_{34}Si_6$
Crystal size (mm)	0.44×0.36×0.22
Crystal System	monoclinic
Space Group	$P2_1/n$
Volume (Å^3)	9236.15(11)
a (Å)	13.54182(9)
b (Å)	33.4467(2)
c (Å)	20.39623(15)
α (°)	90
β (°)	91.1616(6)
γ (°)	90
Z	2
Formula Weight	2948.03
Density (g cm^{-3})	1.060
μ (mm^{-1})	5.007
F(000)	3104
Temperature (K)	140.00(10)
Total Reflections	73474
Unique Reflections	18064
R_{int}	0.0312
R Indices [I > 2σ(I)]	R_1 = 0.0315 wR_2 = 0.0817
Largest Diff. Peak and Hole (e.A^{-3})	0.761 and -0.312
GOF	1.043

F(000), structure factor evaluated in the zeroth-order case, h=k=l= 0; R(int) =∑|Fo2−Fo2(mean)| /∑[Fo2]; I, measured intensities; 'Largest diff. peak and hole', maximum and minimum electron density found in the final Fourier difference map; GOF, goodness of fit (= {∑ [w(Fo2−Fc2)2]/(n−p)}1/2, where n is the number of reflections and p is the total number of parameters refined).

Solid-state structure of LCl_3

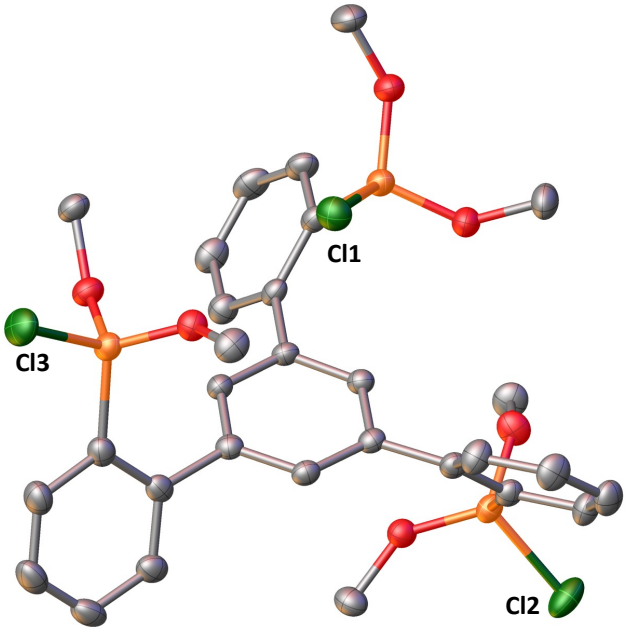


Figure S78: Molecular structure of 1,3,5-(2-SiCl(O^{t}Bu)$_2$C$_6$H$_4$)$_3$C$_6$H$_3$, **LCl_3** with thermal ellipsoids drawn at the 50% probability level. Hydrogen atoms and methyl groups on the –OSi(O^{t}Bu)$_2$ ligands have been omitted for clarity.

Solid-state structure of $L(OH)_3$

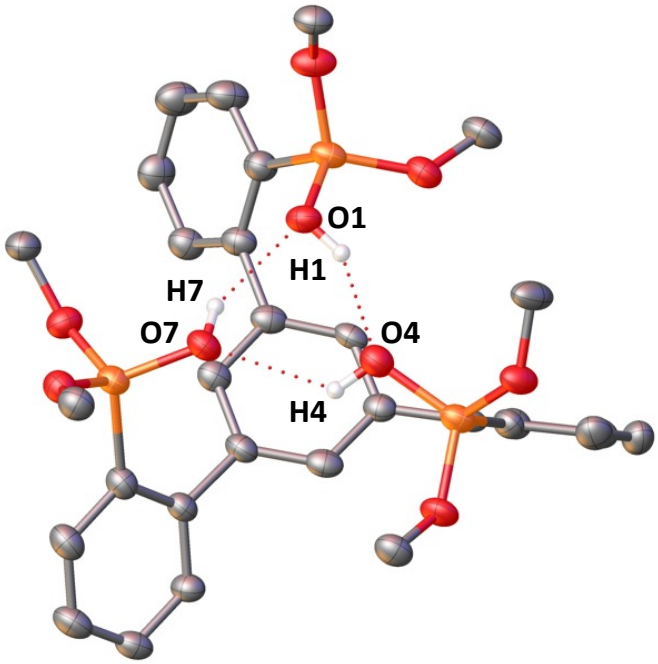


Figure S79: Molecular structure of 1,3,5-(2-HOSi(O^tBu)$_2$$C_6H_4$)$_3$$C_6H_3$, **$L(OH)_3$**, with thermal ellipsoids drawn at the 50% probability level. Hydrogen atoms and methyl groups on the −OSi(O^tBu)$_2$ ligands have been omitted for clarity.

Solid-state structure of $[(K(THF)_3)(L(OK)_3)]_2$

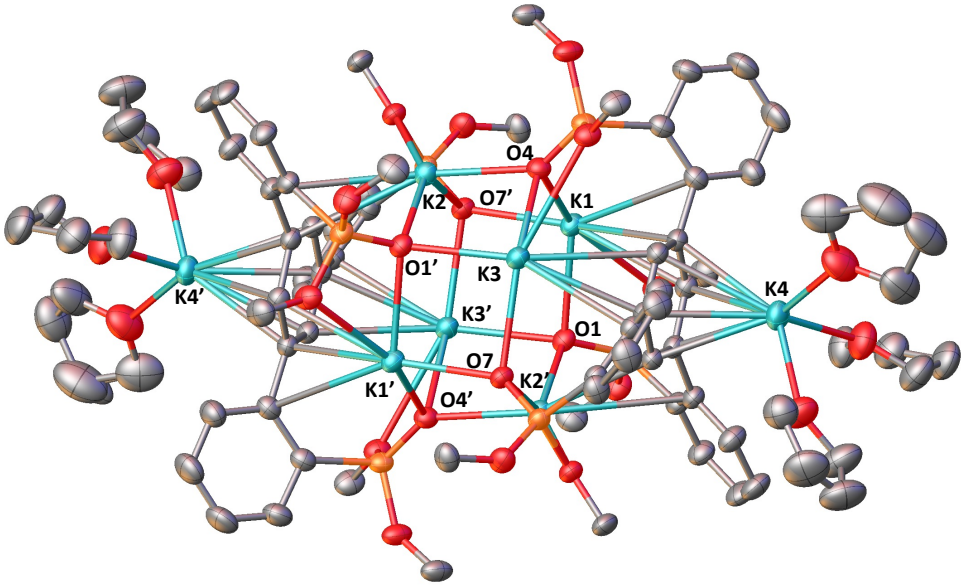


Figure S80: Molecular structure of $[K(THF)_3\{1,3,5\text{-}(2\text{-}KOSi(O^tBu)_2C_6H_4)_3C_6H_3\}]_2$, **$[(K(THF)_3)(L(OK)_3)]_2$** with thermal ellipsoids drawn at the 50% probability level. Hydrogen atoms and methyl groups on the $-OSi(O^tBu)_2$ ligands have been omitted for clarity.

Solid-state structure of $[(K(crypt))(L(OK)_3)]_2$

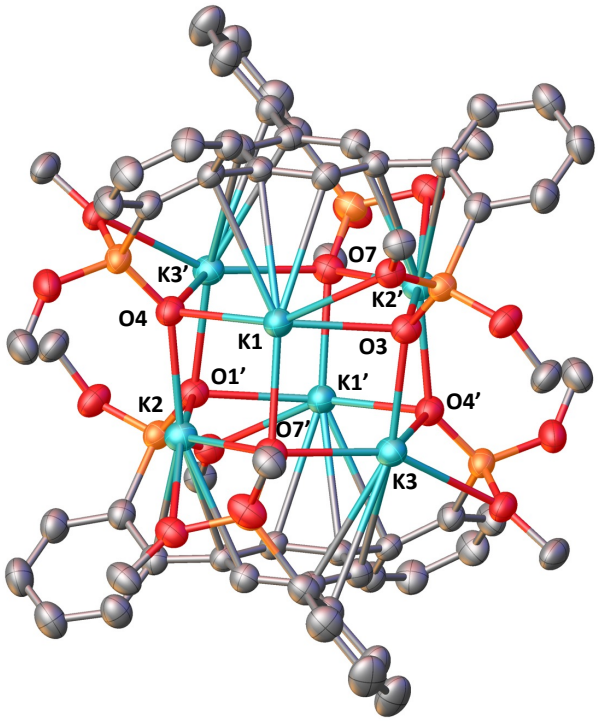


Figure S81: Molecular structure of $[K(2.2.2\text{-cryptand})]_2[\{1,3,5\text{-}(2\text{-}KOSi(O^tBu)_2C_6H_4)_3C_6H_3\}]_2$, **$[(K(crypt))(L(OK)_3)]_2$** with thermal ellipsoids drawn at the 50% probability level. Hydrogen atoms, [K(2.2.2-cryptand)] and methyl groups on the $-OSi(O^tBu)_2$ ligands have been omitted for clarity.

Computational Details

The optimization of different spin state for thorium and cerium complexes were carried out by employing DFT hybrid functional (B3PW91)[9] along with small core pseudopotential Stuttgart basis set[10] for thorium, cerium and silicon atoms (polarization functions[11] were added for silicon atoms). Pople basis set[12] (6-31G**) were employed for the rest of the atoms. Frequency calculations were performed to confirm the minima for optimized structures and for obtaining thermal corrections over the energies. Dispersion corrections were included in our calculations by employing D3 version of Grimme's dispersion with Becke-Johnson damping.[13] All the calculations were performed using Gaussian 16 suite of programs.[14] NBO analysis were carried out using NBO 6.0 version as implemented in the Gaussian program.[15]

Table S5. Selected structural parameters of Complex **1** for s=1/2

Atom Label	Bond distance (Å)	
	DFT	X-ray
Ce1-O5	2.23	2.24
Ce1-O8	2.20	2.23
Ce1-O11	2.21	2.24
Ce1-O14	2.52	2.52

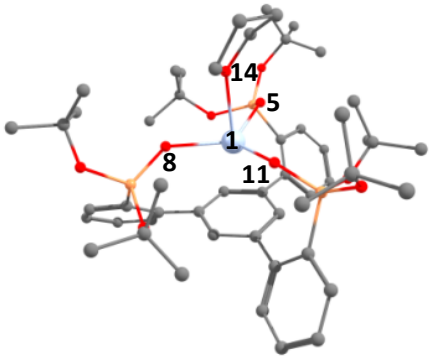


Table S6. Computed Natural charges for complex **1**

Atom Label	Natural charges
Ce1	1.88934
O5	-1.28568
O8	-1.28521
O11	-1.28264
O14	-0.62691

Table S7. Computed Wiberg bond index for complex **1**

Atom Label	Wiberg bond index
Ce1	0.0000
O5	0.4658
O8	0.4910
O11	0.4851
O14	0.1738

Table S8. Bonding orbitals from NBO analysis for complex **1**

(0.98989) BD (1)Ce 1- O 8
(5.39%) 0.2322*Ce 1 s(1.23%)p 0.45(0.55%)d63.03(77.45%) f16.70(20.52%)g 0.21(0.26%)
(94.61%) 0.9727* O 8 s(55.86%)p 0.79(44.12%)d 0.00(0.02%)
(0.98923) BD (1)Ce 1- O 11
(5.24%) 0.2290*Ce 1 s(1.40%)p 0.32(0.45%)d54.87(76.64%) f15.20(21.23%)g 0.21(0.29%)
(94.76%) 0.9734* O 11 s(56.15%)p 0.78(43.82%)d 0.00(0.03%)

Table S9. Second order perturbation analysis for complex **1**

Donor NBO	Acceptor NBO	E(2) kcal/mol
(0.94360) LP (1) O 5 s(57.67%)p 0.73(42.30%)d 0.00(0.03%)	(0.08822) LV (1)Ce 1 s(0.03%)p 9.66(0.25%)d99.99(94.47%) f99.99(5.22%)g 1.62(0.04%)	27.38
(0.91629) LP (2) O 5 s(2.90%)p33.51(97.05%)d 0.02(0.05%)	(0.08257) LV (2)Ce 1 s(0.04%)p 4.35(0.16%)d99.99(95.62%)f99.99(4.07%)g 3.25(0.12%)	6.39
(0.91309) LP (1) O 8 s(0.26%)p99.99(99.69%)d 0.20(0.05%)	(0.08822) LV (1)Ce 1 s(0.03%)p 9.66(0.25%)d99.99(94.47%) f99.99(5.22%)g 1.62(0.04%)	6.53
(0.90730) LP (2) O 11 s(1.27%)p77.50(98.66%)d 0.05(0.07%)	(0.08257) LV (2)Ce 1 s(0.04%)p 4.35(0.16%)d99.99(95.62%)f99.99(4.07%)g 3.25(0.12%)	8.79
(0.95328) LP (2) O 14 s(28.97%)p 2.45(71.02%)d 0.00(0.01%)	(0.08822) LV (1)Ce 1 s(0.03%)p 9.66(0.25%)d99.99(94.47%) f99.99(5.22%)g 1.62(0.04%)	6.00

Table S10. DFT computed MO's for **1**. Left (HOMO) and Right (LUMO)

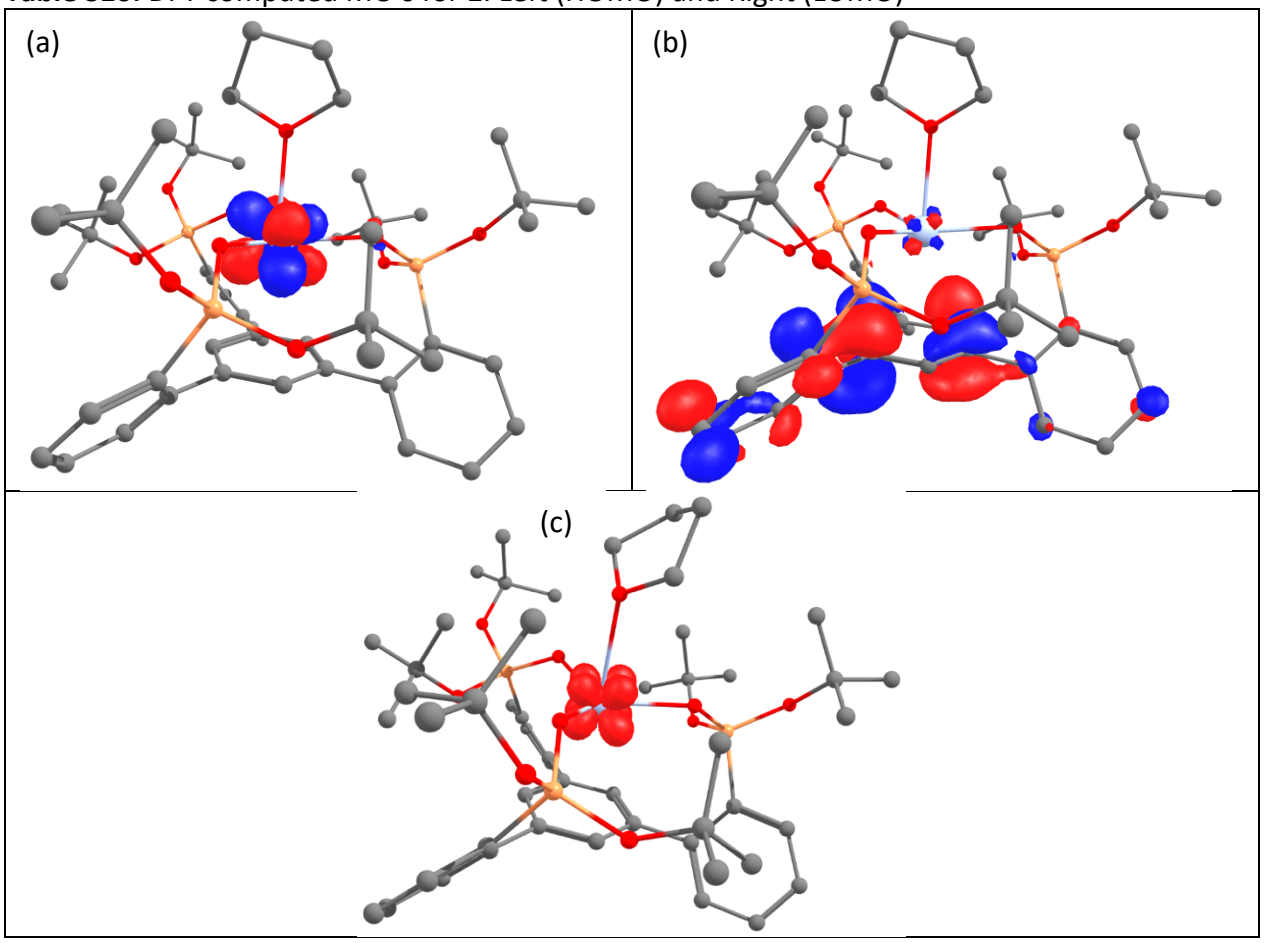


Table S11 Selected structural parameters of Complex **2** for s=0

Atom Label	Bond distance (Å)	
	DFT	X-ray
Ce1-Cl4	2.56	2.57
Ce1-O7	2.08	2.10
Ce1-O8	2.08	2.10
Ce1-O9	2.08	2.11

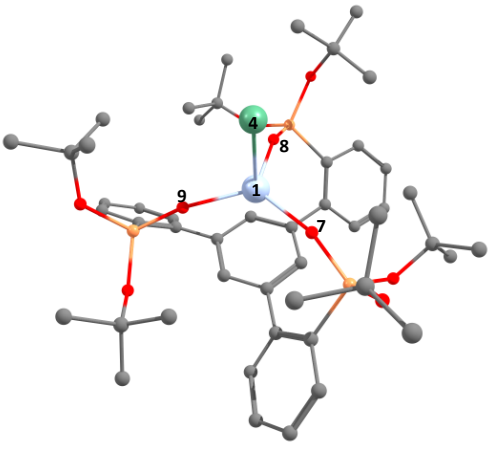


Table S12. Computed Natural charges for complex **2**

Atom Label	Natural charges
Ce1	1.91158
Cl4	-0.44945
O7	-1.17357
O8	-1.17419
O9	-1.17269

Table S13. Computed Wiberg bond index for complex **2**

Atom Label	Wiberg bond index
Ce1	0.0000
Cl4	0.9267
O7	0.7949
O8	0.7927
O9	0.7965

Table S14. Bonding orbitals from NBO analysis for complex **2**

(0.98213) BD (1)Ce 1-Cl 4
(11.80%) 0.3435*Ce 1 s(5.34%)p 0.14(0.72%)d13.46(71.87%) f 4.05(21.60%)g 0.09(0.47%)
(88.20%) 0.9392*Cl 4 s(27.24%)p 2.67(72.70%)d 0.00(0.06%)
(0.98522) BD (1)Ce 1- O 7
(7.47%) 0.2734*Ce 1 s(2.02%)p 0.25(0.50%)d17.65(35.67%)
(92.53%) 0.9619* O 7 s(51.96%)p 0.92(48.03%)d 0.00(0.01%)
(0.96645) BD (2)Ce 1- O 7
(7.12%) 0.2668*Ce 1 s(1.87%)p 0.25(0.46%)d25.49(47.65%) f26.52(49.57%)g 0.24(0.45%)
(92.88%) 0.9637* O 7 s(0.00%)p 1.00(99.98%)d 0.00(0.02%)
(0.96190) BD (3)Ce 1- O 7
(6.44%) 0.2537*Ce 1 s(0.23%)p 1.34(0.30%)d99.99(36.10%) f99.99(62.81%)g 2.47(0.56%)
(93.56%) 0.9673* O 7 s(0.08%)p99.99(99.90%)d 0.19(0.02%)
(0.98520) BD (1)Ce 1- O 8
(7.45%) 0.2730*Ce 1 s(2.00%)p 0.25(0.49%)d17.84(35.74%) f30.58(61.29%)g 0.24(0.47%)
(92.55%) 0.9620* O 8 s(51.95%)p 0.92(48.03%)d 0.00(0.01%)
(0.96641) BD (2)Ce 1- O 8
(7.09%) 0.2663*Ce 1 s(1.87%)p 0.25(0.47%)d25.23(47.19%) f26.74(50.02%)g 0.24(0.44%)
(92.91%) 0.9639* O 8 s(0.00%)p 1.00(99.98%)d 0.00(0.02%)
(0.96172) BD (3)Ce 1- O 8
(6.43%) 0.2535*Ce 1 s(0.23%)p 1.37(0.31%)d99.99(36.20%) f99.99(62.70%)g 2.47(0.56%)
(93.57%) 0.9673* O 8 s(0.09%)p99.99(99.89%)d 0.18(0.02%)
(0.98524) BD (1)Ce 1- O 9
(7.49%) 0.2736*Ce 1 s(2.06%)p 0.24(0.50%)d17.39(35.80%) f29.71(61.16%)g 0.23(0.48%)
(92.51%) 0.9618* O 9 s(52.04%)p 0.92(47.94%)d 0.00(0.01%)
(0.96651) BD (2)Ce 1- O 9
(7.13%) 0.2671*Ce 1 s(1.88%)p 0.24(0.46%)d25.40(47.66%) f26.42(49.57%)g 0.24(0.44%)
(92.87%) 0.9637* O 9 s(0.00%)p 1.00(99.98%)d 0.00(0.02%)

(0.96195) BD (3)Ce 1- O 9
(6.45%) 0.2540*Ce 1 s(0.22%)p 1.37(0.31%)d99.99(36.18%) f99.99(62.74%)g 2.46(0.55%)
(93.55%) 0.9672* O 9 s(0.06%)p99.99(99.92%)d 0.26(0.02%)

Table S15. Second order perturbation analysis for complex **2**

Donor NBO	Acceptor NBO	E(2) kcal/mol
(0.93405) LP (2)Cl 4 s(0.00%)p 1.00(99.98%)d 0.00(0.02%)	(0.03037) LV (2)Ce 1 s(0.00%)p 1.00(0.41%)d83.67(34.50%) f99.99(64.23%)g 2.08(0.86%)	6.02
(0.93382) LP (3)Cl 4 s(0.00%)p 1.00(99.98%)d 0.00(0.02%)	(0.03139) LV (1)Ce 1 s(0.00%)p 1.00(0.38%)d92.75(35.13%) f99.99(63.66%)g 2.21(0.84%)	6.17

Table S16. DFT computed MO's for **2**. Left (HOMO) and Right (LUMO)

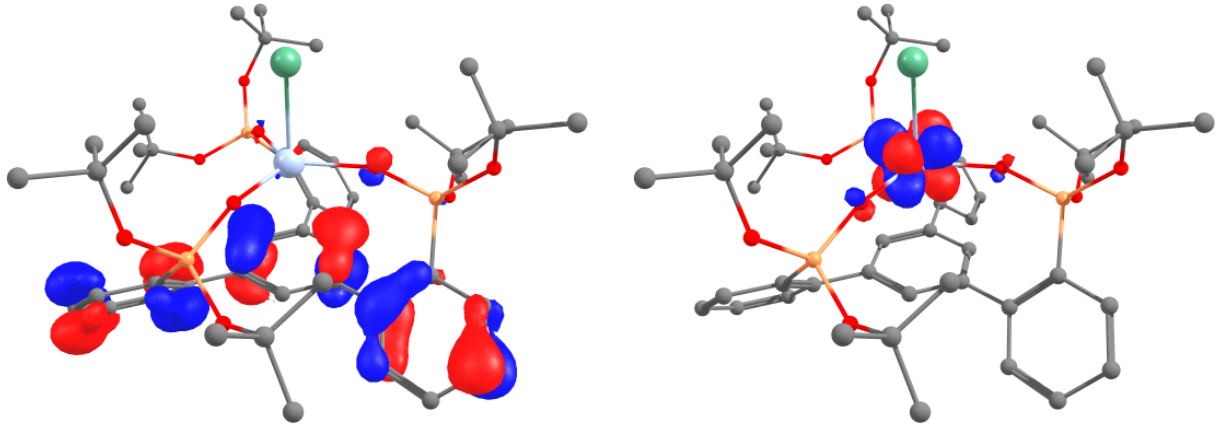


Table S17. Selected structural parameters of Complex **3**

Atom Label	Bond distance (Å)		
	DFT(disp)		X-ray
	s=0	s=1	
Ce1-O5	2.26	2.24	2.26
Ce1-O8	2.27	2.25	2.26
Ce1-O11	2.23	2.28	2.25
Ce1-O14	2.62	2.61	2.58
Ce1-C15	2.79	2.93	2.93
Ce1-C16	2.62	2.96	2.89
Ce1-C18	2.75	2.92	2.97
Ce1-C19	2.80	2.91	2.97
Ce1-C21	2.72	2.92	2.92
Ce1-C22	2.78	2.86	2.92

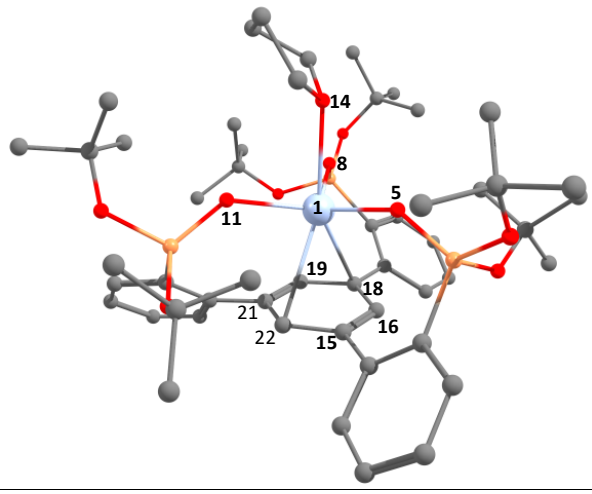


Table S18. Energetics of different spin states for complex **3**

Spin states	ΔH (kcal/mol)
s=0	17.1
s=1	0.0

Table S19. Computed Natural charges for complex **3** (s=1)

Atom Label	Natural charges
Ce1	1.79612
O5	-1.27888
O8	-1.28479
O11	-1.28386
O14	-0.60415
C15	-0.08969
C16	-0.25891
C18	-0.16428
C19	-0.28334
C21	-0.08656
C22	-0.39358

Table S20. Computed Wiberg bond index for complex **3** (s=1)

Atom Label	Wiberg bond index
Ce1	0.0000
O5	0.4621
O8	0.4568
O11	0.4253
O14	0.1496
C15	0.0814
C16	0.0903
C18	0.0937
C19	0.1015
C21	0.0799
C22	0.1423

Table S21. Bonding orbitals from NBO analysis for complex **3** (s=1)

(0.98935) BD (1)Ce 1- O 5
(5.38%) 0.2320*Ce 1 s(1.89%)p 0.26(0.49%)d40.79(77.00%) f10.78(20.36%)g 0.14(0.26%)
(94.62%) 0.9727* O 5 s(58.39%)p 0.71(41.59%)d 0.00(0.02%)
(0.98795) BD (1)Ce 1- O 8
(5.24%) 0.2290*Ce 1 s(2.23%)p 0.18(0.39%)d36.53(81.52%)f 6.99(15.59%)g 0.12(0.26%)
(94.76%) 0.9734* O 8 s(58.53%)p 0.71(41.45%)d 0.00(0.02%)

Table S22. Second order perturbation analysis for complex **3** (s=1)

Donor NBO	Acceptor NBO	E(2) kcal/mol
(0.94175) LP (1) O 11 s(60.33%)p 0.66(39.65%)d 0.00(0.03%)	(0.09452) LV (1)Ce 1 s(0.43%)p 0.29(0.12%)d99.99(86.87%) f29.37(12.54%)g 0.07(0.03%)	22.19
(0.51851) LP (1) C 21 s(0.92%)p99.99(99.05%)d 0.03(0.03%)	(0.09452) LV (1)Ce 1 s(0.43%)p 0.29(0.12%)d99.99(86.87%) f29.37(12.54%)g 0.07(0.03%)	3.65
(0.73062) LP (1) C 22 s(1.23%)p80.01(98.75%)d 0.01(0.01%)	(0.09452) LV (1)Ce 1 s(0.43%)p 0.29(0.12%)d99.99(86.87%) f29.37(12.54%)g 0.07(0.03%)	8.11
(0.98028) BD (1) C 21- C 22 (51.16%) 0.7153* C 21 s(33.26%)p 2.01(66.69%)d 0.00(0.05%) (48.84%) 0.6988* C 22 s(33.67%)p 1.97(66.27%)d 0.00(0.06%)	(0.09452) LV (1)Ce 1 s(0.43%)p 0.29(0.12%)d99.99(86.87%) f29.37(12.54%)g 0.07(0.03%)	3.25

Table S23. DFT computed MO's for **3** (s=1). Left (SOMO-1) and Right (SOMO)

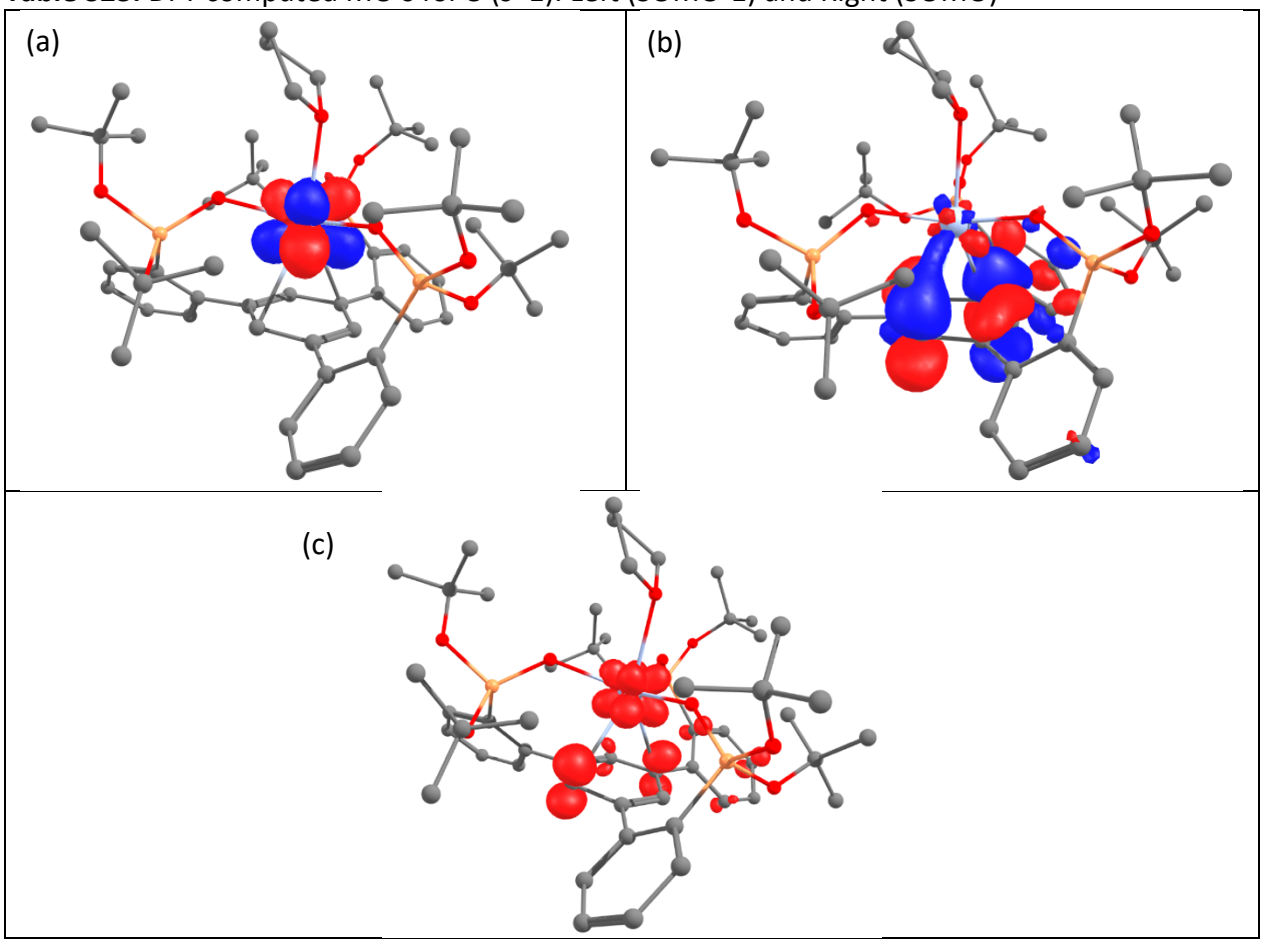


Table S24. Selected structural parameters for complex **4**

Atom Label	Bond distance (Å)		
	DFT(disp)		X-ray
	s=0	s=1	
Ce1-O8	2.27	2.25	2.28
Ce1-O9	2.30	2.28	2.27
Ce1-O12	2.52	2.42	2.44
Ce1-O15	2.28	2.26	2.28
Ce1-C16	2.82	3.03	2.99
Ce1-C17	2.80	3.00	2.92
Ce1-C20	2.79	3.08	3.00
Ce1-C22	2.67	2.95	2.93
Ce1-C91	2.82	3.04	3.03
Ce1-C94	2.72	3.08	3.06
Ce1-X (center of the arene ring)	2.38	2.68	2.63

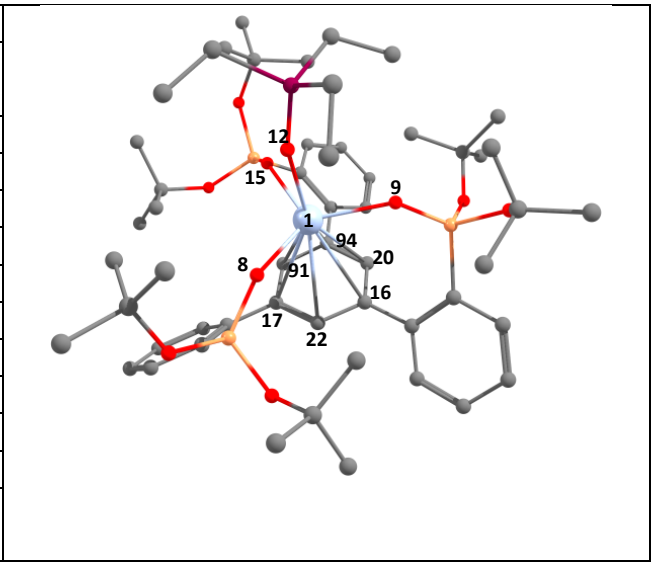


Table S25. Energetics of different spin states for complex **4**

Spin states	ΔH (kcal/mol)
s=1	0.0
s=0	18.0

Table S26. Computed Natural charges for complex **4** (s=1)

Atom Label	Natural charges
Ce1	1.86398
O8	-1.29167
O9	-1.29230
O12	-1.13802
O15	-1.29543
C16	-0.07925
C17	-0.11134
C20	-0.29105
C22	-0.38776
C91	-0.24478
C94	-0.15109

Table S27. Computed Wiberg bond index for complex **4** (s=1)

Atom Label	Wiberg bond index
Ce1	0.0000
O8	0.4297
O9	0.4061
O12	0.2413
O15	0.4270
C16	0.0586

C17	0.0655
C20	0.0761
C22	0.1147
C91	0.0684
C94	0.0627

Table S28. Second order perturbation analysis for complex **4** (s=1)

Donor NBO	Acceptor NBO	E(2) kcal/mol
(0.95628) LP (1) O 12 s(61.38%)p 0.63(38.60%)d 0.00(0.01%)	(0.09147) LV (3)Ce 1 s(0.60%)p 0.04(0.02%)d99.99(89.12%)f17.08(10.23%)g 0.04(0.03%)	27.54
(0.95628) LP (1) O 12 s(61.38%)p 0.63(38.60%)d 0.00(0.01%)	(0.01563) LV (9)Ce 1 s(2.78%)p 0.21(0.59%)d 2.24(6.23%)f32.20(89.46%)g 0.34(0.94%)	5.50
(0.94712) LP (1) O 8 s(42.23%)p 1.37(57.72%)d 0.00(0.04%)	(0.09724) LV (2)Ce 1 s(0.01%)p76.90(0.93%)d99.99(95.99%)f99.99(3.02%)g 4.30(0.05%)	12.89
(0.94712) LP (1) O 8 s(42.23%)p 1.37(57.72%)d 0.00(0.04%)	(0.09147) LV (3)Ce 1 s(0.60%)p 0.04(0.02%)d99.99(89.12%)f17.08(10.23%)g 0.04(0.03%)	9.94
(0.94712) LP (1) O 8 s(42.23%)p 1.37(57.72%)d 0.00(0.04%)	(0.08154) LV (4)Ce 1 s(0.06%)p 2.40(0.15%)d99.99(96.48%)f53.49(3.26%)g 0.77(0.05%)	5.61
(0.94666) LP (1) O 9 s(44.86%)p 1.23(55.10%)d 0.00(0.04%)	(0.12262) LV (1)Ce 1 s(0.01%)p 1.00(0.71%)d99.99(94.03%f 7.38(5.22%)g 0.05(0.04%)	13.34
(0.94666) LP (1) O 9 s(44.86%)p 1.23(55.10%)d 0.00(0.04%)	(0.08154) LV (4)Ce 1 s(0.06%)p 2.40(0.15%)d99.99(96.48%)f53.49(3.26%)g 0.77(0.05%)	5.07
(0.94666) LP (1) O 9 s(44.86%)p 1.23(55.10%)d 0.00(0.04%)	(0.07732) LV (5)Ce 1 s(0.06%)p 0.78(0.05%)d99.99(97.27%)f41.56(2.58%)g 0.66(0.04%)	7.93
(0.94658) LP (1) O 15 s(42.37%)p 1.36(57.59%)d 0.00(0.04%)	(0.12262) LV (1)Ce 1 s(0.01%)p 1.00(0.71%)d99.99(94.03%f 7.38(5.22%)g 0.05(0.04%)	5.36
(0.94658) LP (1) O 15 s(42.37%)p 1.36(57.59%)d 0.00(0.04%)	(0.09724) LV (2)Ce 1 s(0.01%)p76.90(0.93%)d99.99(95.99%)f99.99(3.02%)g 4.30(0.05%)	11.87
(0.94658) LP (1) O 15 s(42.37%)p 1.36(57.59%)d 0.00(0.04%)	(0.09147) LV (3)Ce 1 s(0.60%)p 0.04(0.02%)d99.99(89.12%)f17.08(10.23%)g 0.04(0.03%)	6.99
(0.72510) LP (1) C 22 s(0.71%)p99.99(99.27%)d 0.02(0.01%)	(0.12262) LV (1)Ce 1 s(0.01%)p 1.00(0.71%)d99.99(94.03%f 7.38(5.22%)g 0.05(0.04%)	6.17
(0.64858) LP (1) C 94 s(0.07%)p99.99(99.92%)d 0.05(0.00%)	(0.08154) LV (4)Ce 1	4.76

	s(0.06%)p 2.40(0.15%)d99.99(96.48%)f53.49(3.26%)g 0.77(0.05%)	
(0.90825) BD (2) C 16- C 20 (43.64%) 0.6606* C 16 s(0.09%)p99.99(99.83%)d 0.94(0.08%) (56.36%) 0.7507* C 20 s(0.06%)p99.99(99.89%)d 0.95(0.05%)	(0.07732) LV (5)Ce 1 s(0.06%)p 0.78(0.05%)d99.99(97.27%)f41.56(2.58%)g 0.66(0.04%)	3.78
(0.89298) BD (2) C 17- C 91 (54.37%) 0.7374* C 17 s(0.41%)p99.99(99.54%)d 0.12(0.05%) (45.63%) 0.6755* C 91 s(0.16%)p99.99(99.76%)d 0.47(0.08%)	(0.07732) LV (5)Ce 1 s(0.06%)p 0.78(0.05%)d99.99(97.27%)f41.56(2.58%)g 0.66(0.04%)	4.43

Table S29. DFT computed MOs for **4** (s=1) (a)HOMO-1 (b)HOMO

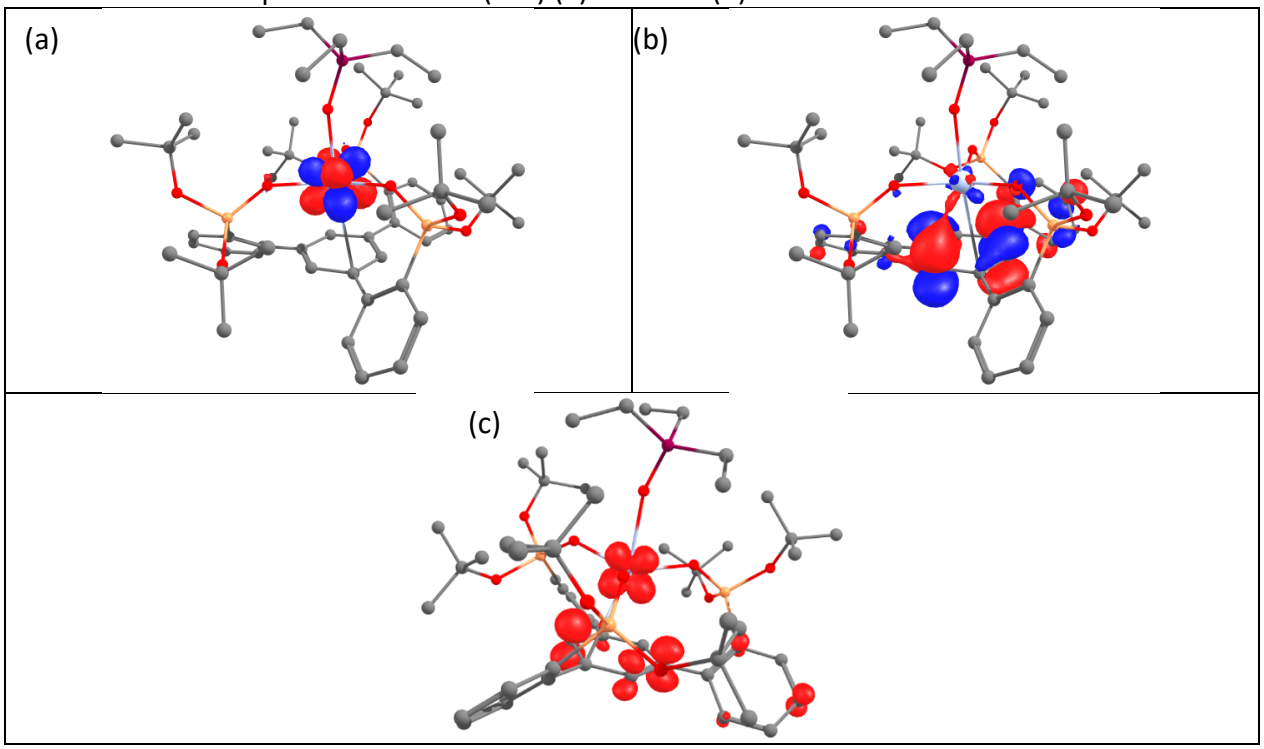


Table S30. Selected structural parameters for complex **5**

Atom Label	Bond distance (Å)		
	DFT(disp)		X-ray
	s=1/2	s=3/2	
Ce1-O67	2.35	2.35	2.37
Ce1-O68	2.36	2.34	2.33
Ce1-O69	2.68	2.69	2.74
Ce1-O71	2.36	2.34	2.33
Ce1-C23	2.77	2.82	2.85
Ce1-C70	2.74	2.79	2.79

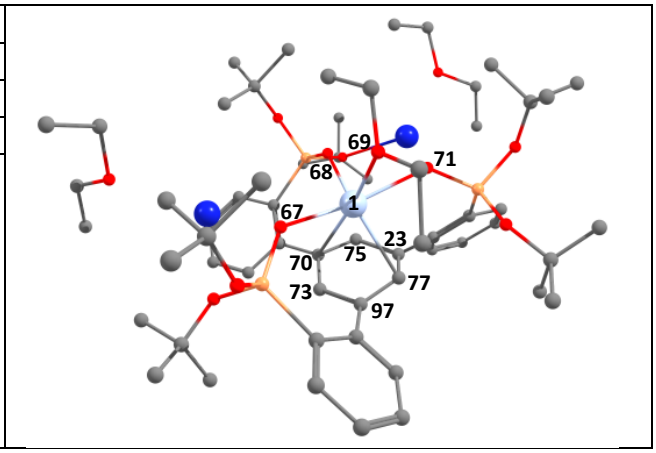
Ce1-C73	2.81	2.77	2.87	
Ce1-C75	2.77	2.78	2.87	
Ce1-C77	2.55	2.73	2.60	
Ce1-C97	2.71	2.72	2.86	
Ce1-X (center of the arene ring)	2.33	2.37	2.39	

Table S31. Energetics of different spin states for complex **5**

Spin states	ΔH (kcal/mol)
s=1/2	0.0
s=3/2	5.3

Table S32. Computed Natural charges for complex **5** (s=1/2)

Atom Label	Natural charges
Ce1	1.47559
O67	-1.29202
O68	-1.28062
O69	-0.58117
O71	-1.29102
C23	-0.06530
C70	-0.25167
C73	-0.22967
C75	-0.30891
C77	-0.55264
C97	-0.10594

Table S33. Computed Wiberg bond index for complex **5** (s=1/2)

Atom Label	Wiberg bond index
Ce1	0.0000
O67	0.4120
O68	0.4171
O69	0.1559
O71	0.4014
C23	0.1137

C70	0.1707
C73	0.1312
C75	0.1728
C77	0.3544
C97	0.1400

Table S34. Bonding orbitals from NBO analysis for complex **5** (s=1/2)

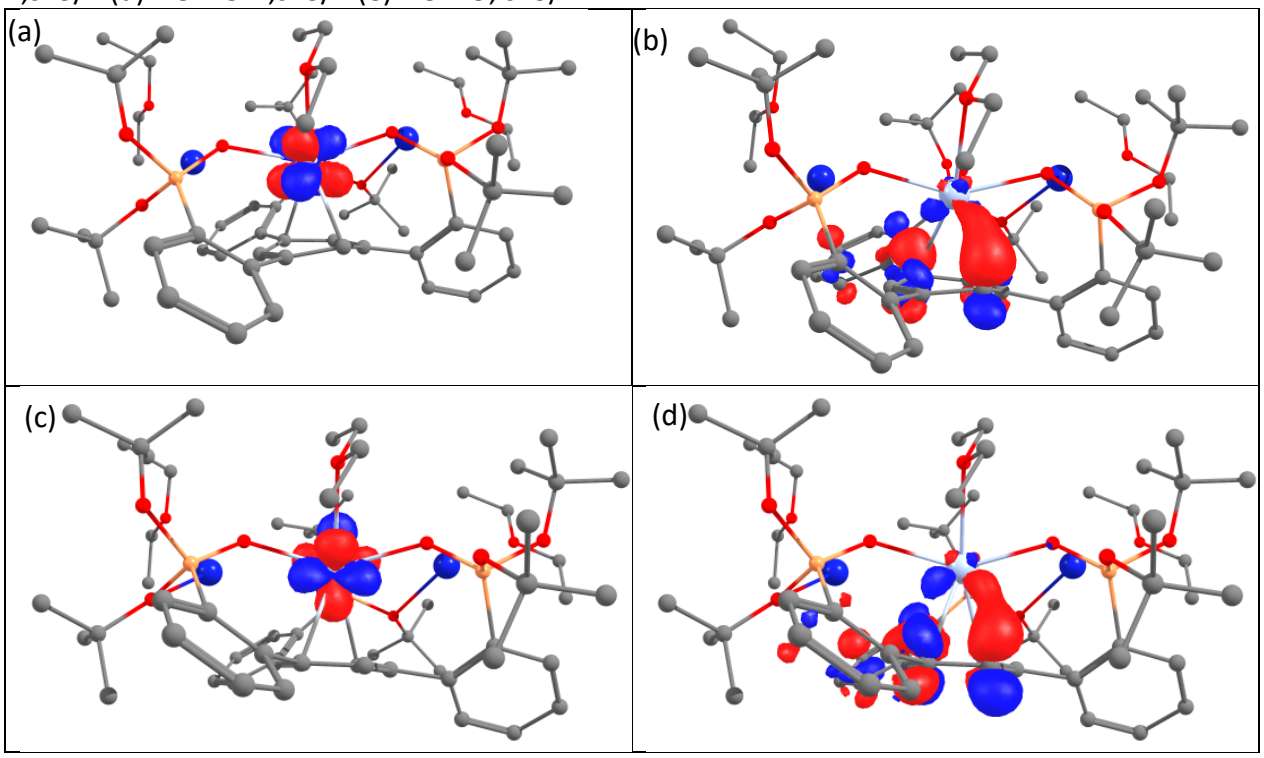
(0.98425) BD (1)Ce 1- O 67
(5.48%) 0.2341*Ce 1 s(10.08%)p 0.01(0.07%)d 7.39(74.47%)f 1.50(15.14%)g 0.02(0.25%)
(94.52%) 0.9722* O 67 s(59.87%)p 0.67(40.11%)d 0.00(0.02%)
(0.98319) BD (1)Ce 1- O 68
(5.61%) 0.2368*Ce 1 s(15.59%)p 0.01(0.09%)d 4.71(73.43%)f 0.69(10.68%)g 0.01(0.20%)
(94.39%) 0.9715* O 68 s(60.11%)p 0.66(39.88%)d 0.00(0.01%)
(0.98514) BD (1)Ce 1- O 71
(5.40%) 0.2325*Ce 1 s(9.96%)p 0.01(0.06%)d 7.77(77.37%)f 1.24(12.39%)g 0.02(0.22%)
(94.60%) 0.9726* O 71 s(60.14%)p 0.66(39.84%)d 0.00(0.02%)

Table S35. Second order perturbation analysis for complex **5** (s=1/2)

Donor NBO	Acceptor NBO	E(2) kcal/mol
(0.51576) LP (1) C 23 s(1.63%)p60.42(98.35%)d 0.02(0.03%)	(0.06988) LV (3)Ce 1 s(6.70%)p 0.05(0.31%)d 7.24(48.47%)f 6.61(44.26%)g 0.04(0.26%)	5.00
(0.51576) LP (1) C 23 s(1.63%)p60.42(98.35%)d 0.02(0.03%)	(0.04570) BD*(1)Ce 1- O 67 (94.52%) 0.9722*Ce 1 s(10.08%)p 0.01(0.07%)d 7.39(74.47%)f 1.50(15.14%)g 0.02(0.25%) (5.48%) -0.2341* O 67 s(59.87%)p 0.67(40.11%)d 0.00(0.02%)	3.74
(0.61950) LP (1) C 70 s(0.87%)p99.99(99.13%)d 0.00(0.00%)	(0.08525) LV (2)Ce 1 s(42.51%)p 0.01(0.26%)d 1.16(49.25%)f 0.19(7.88%)g 0.00(0.10%)	6.84
(0.51445) LP (1) C 73 s(0.76%)p99.99(99.19%)d 0.06(0.04%)	(0.05105) BD*(1)Ce 1- O 71 (94.60%) 0.9726*Ce 1 s(9.96%)p 0.01(0.06%)d 7.77(77.37%)f 1.24(12.39%)g 0.02(0.22%) (5.40%) -0.2325* O 71 s(60.14%)p 0.66(39.84%)d 0.00(0.02%)	4.71
(0.54123) LP (1) C 75 s(1.97%)p49.86(97.99%)d 0.02(0.05%)	(0.13313) LV (1)Ce 1 s(0.71%)p 0.38(0.27%)d86.48(61.77%)f51.88(37.06%)g 0.26(0.19%)	4.91
(0.54123) LP (1) C 75 s(1.97%)p49.86(97.99%)d 0.02(0.05%)	(0.08525) LV (2)Ce 1 s(42.51%)p 0.01(0.26%)d 1.16(49.25%)f 0.19(7.88%)g 0.00(0.10%)	5.43
(0.68907) LP (1) C 77 s(7.62%)p12.12(92.36%)d 0.00(0.02%)	(0.13313) LV (1)Ce 1	31.70

	s(0.71%)p 0.38(0.27%)d86.48(61.77%)f51.88(37.06%)g 0.26(0.19%)	
(0.68907) LP (1) C 77 s(7.62%)p12.12(92.36%)d 0.00(0.02%)	(0.03881) BD*(1)Ce 1- O 68 (94.39%) 0.9715*Ce 1 s(15.59%)p 0.01(0.09%)d 4.71(73.43%)f 0.69(10.68%)g 0.01(0.20%) (5.61%) -0.2368* O 68 s(60.11%)p 0.66(39.88%)d 0.00(0.01%)	5.42
(0.68907) LP (1) C 77 s(7.62%)p12.12(92.36%)d 0.00(0.02%)	(0.05105) BD*(1)Ce 1- O 71 (94.60%) 0.9726*Ce 1 s(9.96%)p 0.01(0.06%)d 7.77(77.37%)f 1.24(12.39%)g 0.02(0.22%) (5.40%) -0.2325* O 71 s(60.14%)p 0.66(39.84%)d 0.00(0.02%)	4.82
(0.53112) LP (1) C 97 s(0.84%)p99.99(99.13%)d 0.04(0.03%)	(0.06988) LV (3)Ce 1 s(6.70%)p 0.05(0.31%)d 7.24(48.47%)f 6.61(44.26%)g 0.04(0.26%)	5.09
(0.53112) LP (1) C 97 s(0.84%)p99.99(99.13%)d 0.04(0.03%)	(0.03881) BD*(1)Ce 1- O 68 (94.39%) 0.9715*Ce 1 s(15.59%)p 0.01(0.09%)d 4.71(73.43%)f 0.69(10.68%)g 0.01(0.20%) (5.61%) -0.2368* O 68 s(60.11%)p 0.66(39.88%)d 0.00(0.01%)	3.90

Table S36. DFT computed MO's for **5** (s=1/2). (a) SOMO,s=1/2 (b) HOMO-1,s=1/2 (c) HOMO-2,s=3/2 (d) HOMO-1,s=3/2 (e) HOMO, s=3/2



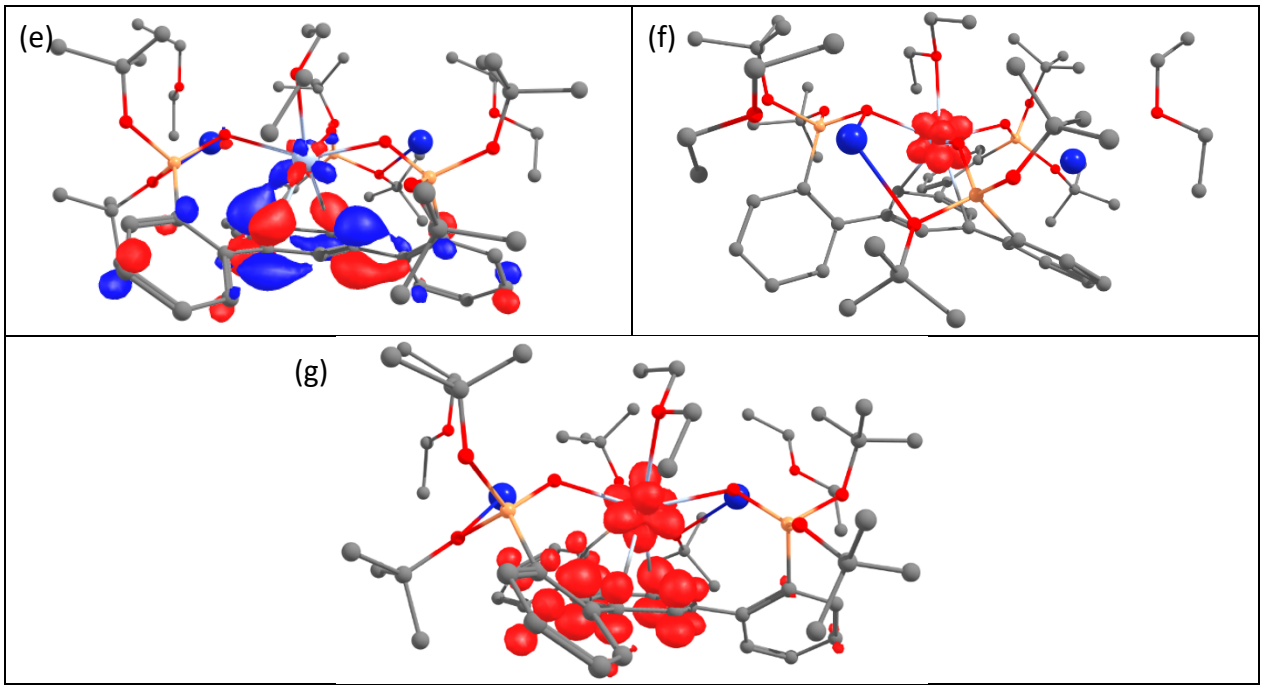


Table S37. Energetics of different spin states for complex $\mathbf{5}^{2-}$

Spin states	ΔH (kcal/mol)
s=1/2	3.4
s=3/2	0.0

Table S38. Selected structural parameters of $\mathbf{5}^{2-}$

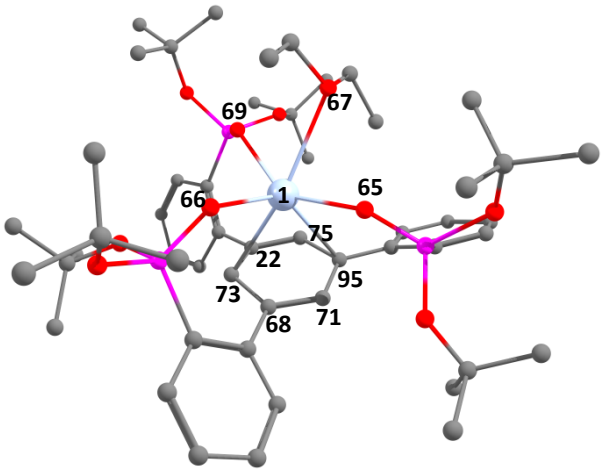
Atom Label	Bond distance (Å)		
	DFT(disp)		
	s=1/2	s=3/2	
Ce1-O65	2.30	2.30	
Ce1-O66	2.29	2.27	
Ce1-O67	2.74	2.77	
Ce1-O69	2.35	2.31	
Ce1-C22	2.81	2.89	
Ce1-C68	2.79	2.81	
Ce1-C71	2.81	2.78	
Ce1-C73	2.67	2.85	
Ce1-C75	2.78	2.78	
Ce1-C95	2.73	2.77	
Ce1-X(center of the arene)	2.37	2.43	

Table S39. Computed Natural charges for complex $\mathbf{5}^{2-}$ (s=3/2)

Atom Label	Natural charges
Ce1	1.66592
O65	-1.26994
O66	-1.26241
O67	-0.57464
O69	-1.27513
C22	-0.12809
C68	-0.14518
C71	-0.34051
C73	-0.34662
C75	-0.36262
C95	-0.14641

Table S40. Computed Wiberg bond index for complex $\mathbf{5}^{2-}$ (s=3/2)

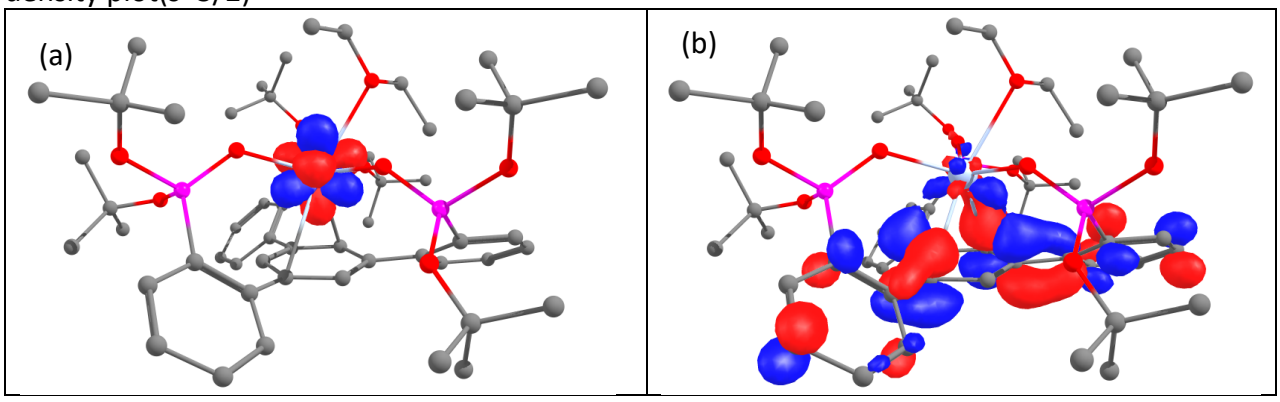
Atom Label	Wiberg bond index
Ce1	0.0000
O65	0.4280
O66	0.4584
O67	0.1171
O69	0.3968
C22	0.0948
C68	0.1075
C71	0.1489
C73	0.1430
C75	0.1569
C95	0.1075

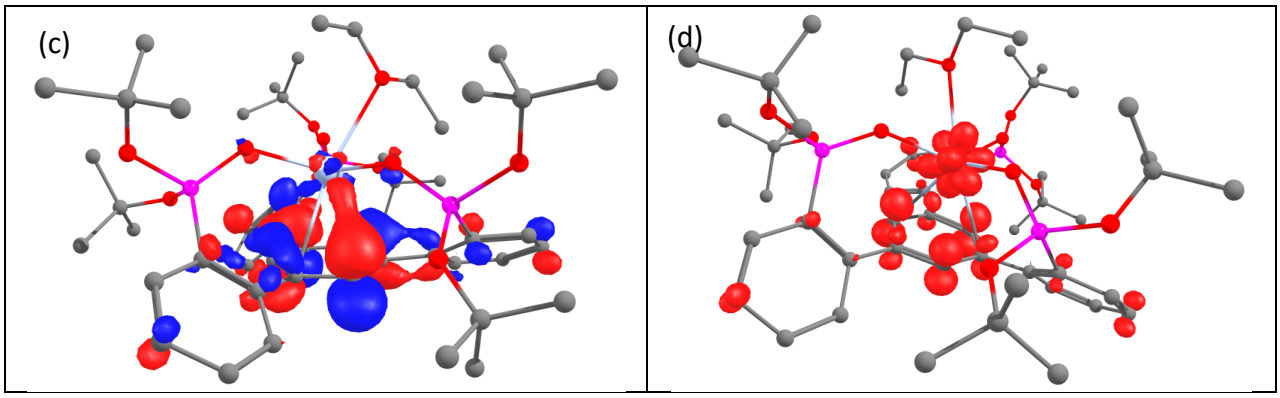
Table S41. Second order perturbation analysis for complex $\mathbf{5}^{2-}$ (s=3/2)

Donor NBO	Acceptor NBO	E(2) kcal/mol
(0.94493) LP (1) O 65 s(40.19%)p 1.49(59.76%)d 0.00(0.06%)	(0.12387) LV (2)Ce 1 s(0.26%)p 1.43(0.37%)d99.99(94.73%)f17.52(4.55%)g 0.33(0.08%)	11.61
(0.94493) LP (1) O 65 s(40.19%)p 1.49(59.76%)d 0.00(0.06%)	(0.09574) LV (3)Ce 1 s(0.10%)p 1.09(0.10%)d99.99(93.31%)f67.81(6.46%)g 0.25(0.02%)	9.37
(0.94493) LP (1) O 65 s(40.19%)p 1.49(59.76%)d 0.00(0.06%)	(0.04982) LV (5)Ce 1 s(81.81%)p 0.00(0.21%)d 0.04(2.89%)f 0.18(14.98%)g 0.00(0.11%)	7.69
(0.94283) LP (1) O 66 s(43.00%)p 1.32(56.95%)d 0.00(0.05%)	(0.09574) LV (3)Ce 1 s(0.10%)p 1.09(0.10%)d99.99(93.31%)f67.81(6.46%)g 0.25(0.02%)	24.35
(0.94283) LP (1) O 66	(0.04982) LV (5)Ce 1	5.01

s(43.00%)p 1.32(56.95%)d 0.00(0.05%)	s(81.81%)p 0.00(0.21%)d 0.04(2.89%)f 0.18(14.98%)g 0.00(0.11%)	
(0.94582) LP (1) O 69 s(41.72%)p 1.40(58.23%)d 0.00(0.05%)	(0.08684) LV (4)Ce 1 s(0.41%)p 0.69(0.28%)d99.99(88.14%)f27.02(10.97%)g 0.49(0.20%)	13.77
(0.94582) LP (1) O 69 s(41.72%)p 1.40(58.23%)d 0.00(0.05%)	(0.04644) LV (6)Ce 1 s(0.03%)p 9.83(0.28%)d99.99(25.63%)f99.99(73.91%)g 5.56(0.16%)	5.28
(0.98107) BD (1) C 22- C 73 (50.84%) 0.7130* C 22 s(32.56%)p 2.07(67.39%)d 0.00(0.05%) (49.16%) 0.7011* C 73 s(34.05%)p 1.94(65.89%)d 0.00(0.06%)	(0.08684) LV (4)Ce 1 s(0.41%)p 0.69(0.28%)d99.99(88.14%)f27.02(10.97%)g 0.49(0.20%)	2.79
(0.97982) BD (1) C 22- C 75 (50.74%) 0.7123* C 22 s(33.56%)p 1.98(66.39%)d 0.00(0.05%) (49.26%) 0.7018* C 75 s(33.75%)p 1.96(66.19%)d 0.00(0.06%)	(0.08684) LV (4)Ce 1 s(0.41%)p 0.69(0.28%)d99.99(88.14%)f27.02(10.97%)g 0.49(0.20%)	4.28
(0.97851) BD (1) C 68- C 73 (50.97%) 0.7139* C 68 s(33.01%)p 2.03(66.94%)d 0.00(0.05%) (49.03%) 0.7002* C 73 s(33.93%)p 1.95(66.01%)d 0.00(0.06%)	(0.12387) LV (2)Ce 1 s(0.26%)p 1.43(0.37%)d99.99(94.73%)f17.52(4.55%)g 0.33(0.08%)	2.48
(0.98100) BD (1) C 75- C 95 (49.27%) 0.7019* C 75 s(33.99%)p 1.94(65.96%)d 0.00(0.06%) (50.73%) 0.7122* C 95 s(32.25%)p 2.10(67.70%)d 0.00(0.05%)	(0.08684) LV (4)Ce 1 s(0.41%)p 0.69(0.28%)d99.99(88.14%)f27.02(10.97%)g 0.49(0.20%)	3.08
(0.59001) LP (1) C 22 s(1.09%)p90.70(98.91%)d 0.00(0.00%)	(0.08684) LV (4)Ce 1 s(0.41%)p 0.69(0.28%)d99.99(88.14%)f27.02(10.97%)g 0.49(0.20%)	5.70

Table S42. DFT computed MO's for $\mathbf{5}^{2-}$ (s=3/2) (a) HOMO-2 (b) HOMO-1 (c) HOMO (d) spin density plot(s=3/2)





TDDFT Caculations

Complex **3**

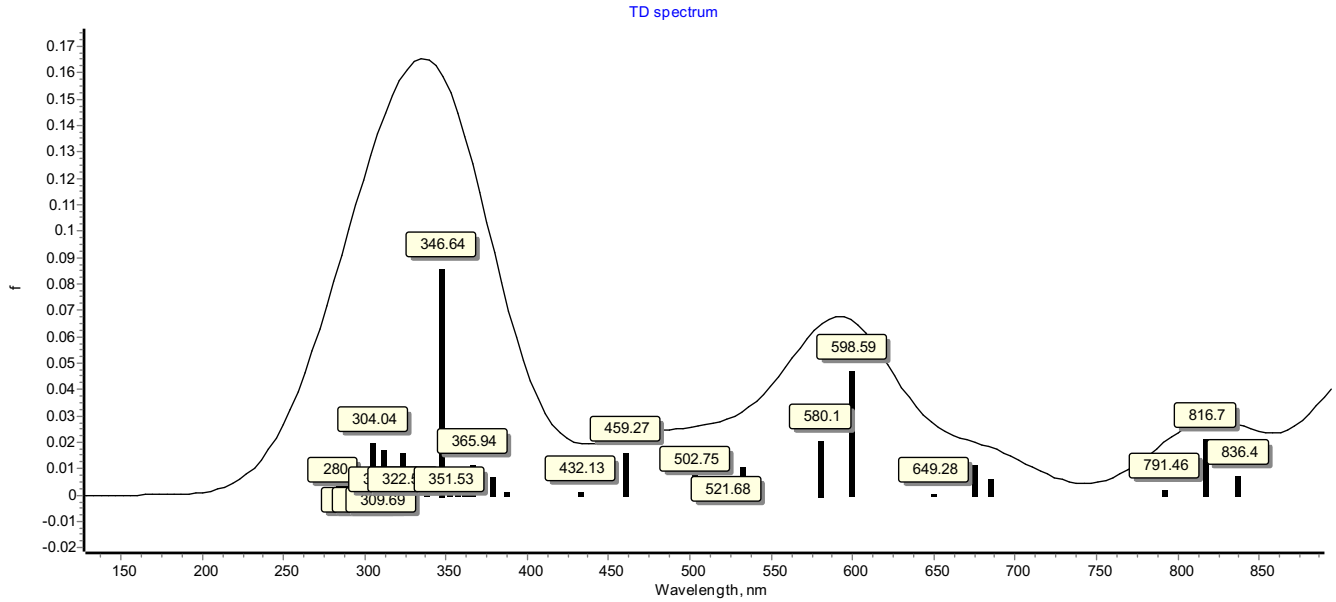
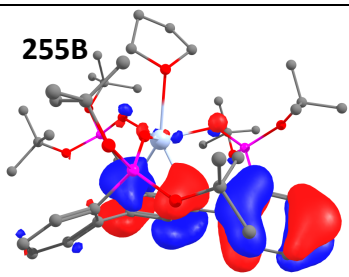
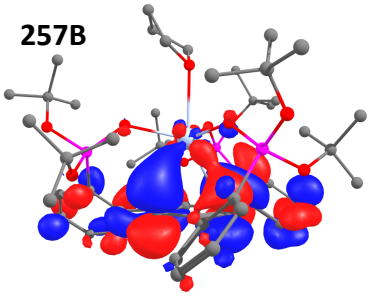
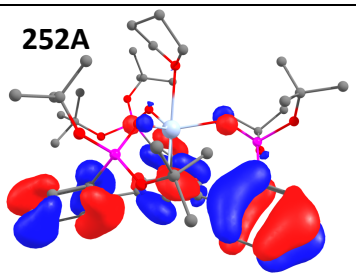
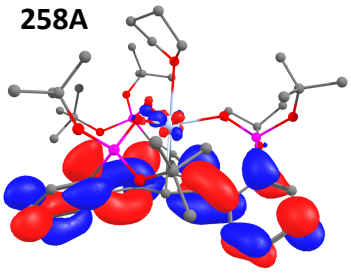
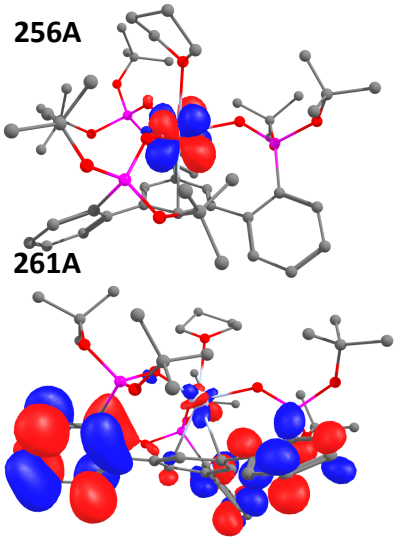
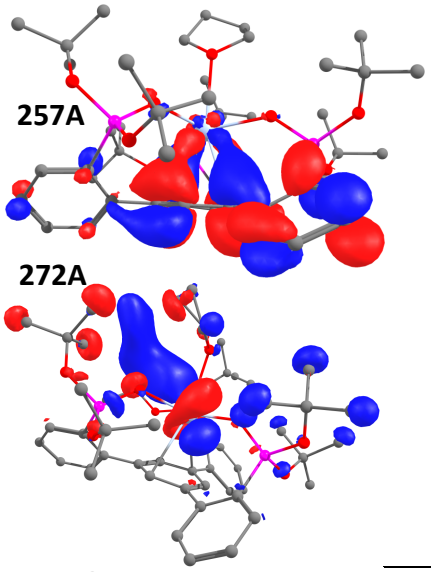
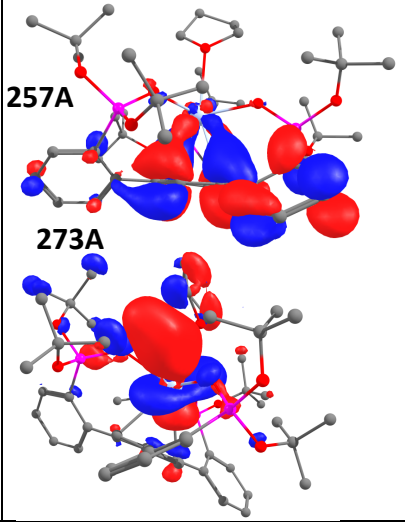
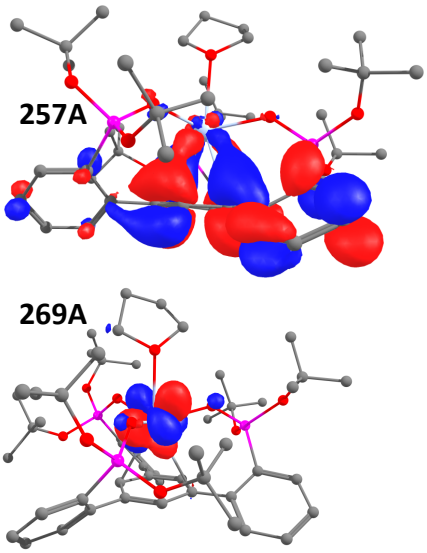
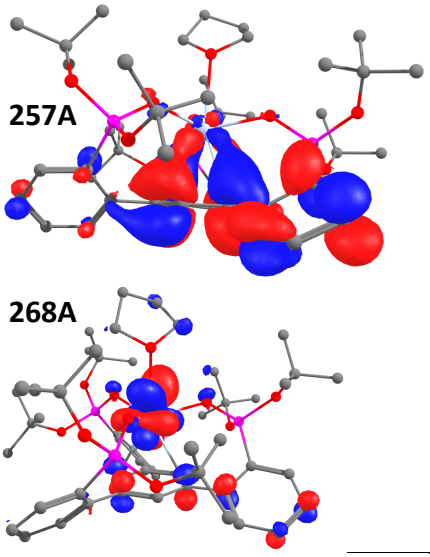
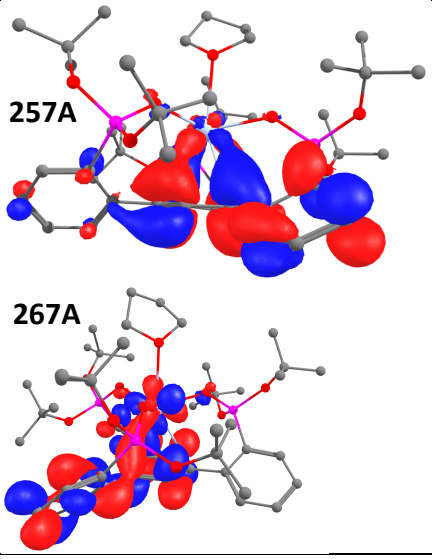


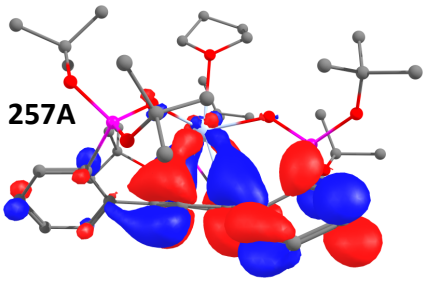
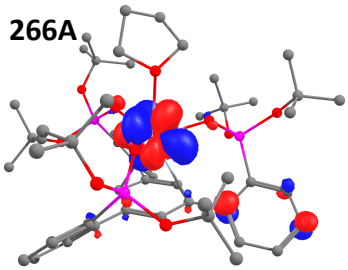
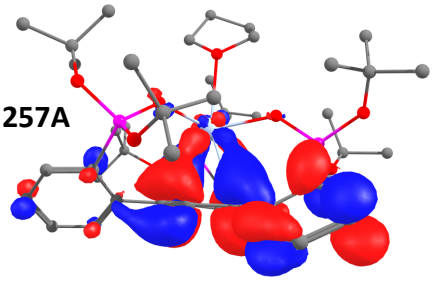
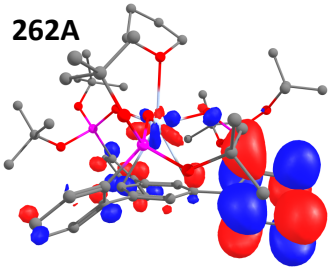
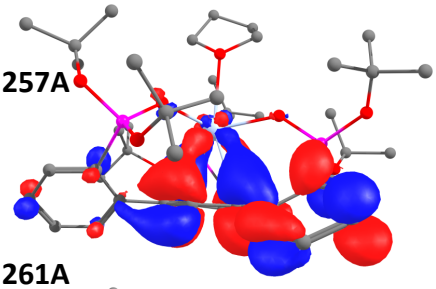
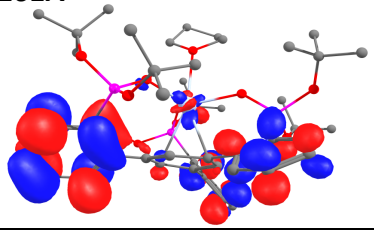
Figure S82. Simulated UV−Vis spectrum of complex **3**

Table S43. TDDFT caculations of complex **3**

Excited State 29: 3.697-?Sym 3.5768 eV **346.64 nm f=0.0858** <S**2>=3.166 253A -> 262A -0.23948 254A -> 258A -0.16437 255A -> 259A -0.18474 255A -> 261A -0.12856 255A -> 264A -0.10154 252B -> 257B 0.13879 252B -> 261B -0.12738 252B -> 263B -0.10115 253B -> 257B -0.16012 253B -> 261B -0.26169 254B -> 256B -0.17658 **255B(HOMO) -> 257B(LUMO+1) 0.57436** 255B -> 258B -0.17226 255B -> 260B -0.17539	**255B**  **257B** 
Excited State 28: 3.964-?Sym 3.5270 eV **351.53 nm f=0.0078** <S**2>=3.678 250A -> 260A 0.20416 251A -> 259A 0.12367 251A -> 261A -0.15368 **252A(HOMO-5) -> 258A(LUMO) 0.32620** 252A -> 267A -0.10650 254A -> 259A 0.22010 254A -> 261A 0.11715 255A -> 258A 0.14498 **256A(HOMO-1) -> 261A(LUMO+3) -0.30358** 250B -> 258B 0.11341 250B -> 259B -0.16831 251B -> 258B -0.12797 251B -> 259B -0.15991 252B -> 256B 0.27384 252B -> 262B 0.10748 253B -> 256B -0.15434 254B -> 257B -0.15951 254B -> 258B -0.15250 254B -> 260B -0.18054 255B -> 256B -0.27697	**252A**  **258A** 

	
Excited State 24: 3.372-?Sym 3.3881 eV **365.94 nm f=0.0112** <S**2>=2.592 252A -> 259A -0.11005 254A -> 258A -0.25536 256A -> 260A 0.25289 **257A(HOMO) -> 272A(LUMO+14) 0.54683** 257A -> 273A -0.12025 257A -> 275A -0.45887 257A -> 276A -0.11603 257A -> 277A 0.10354 254B -> 256B -0.28184 255B -> 257B -0.24744	
Excited State 23: 3.094-?Sym 3.2796 eV **378.04 nm f=0.0065** <S**2>=2.143 254A -> 258A 0.13364 257A -> 272A 0.49962 **257A(HOMO) -> 273A(LUMO+15) 0.74043** 257A -> 274A -0.19779 257A -> 276A -0.10763 257A -> 280A 0.10233 254B -> 256B 0.14671 255B -> 257B 0.14409	

Excited State 18: 3.008-?Sym 2.3766 eV **521.68 nm f=0.0014** <S**2>=2.012 256A -> 258A 0.16370 257A -> 268A 0.29052 **257A(HOMO) -> 269A(LUMO+11) 0.81593** 257A -> 270A -0.44987	
Excited State 17: 3.009-?Sym 2.3327 eV **531.50 nm f=0.0107** <S**2>=2.014 256A -> 258A -0.24654 257A -> 263A 0.10312 257A -> 267A 0.10347 **257A(HOMO) -> 268A(LUMO+10) 0.81401** 257A -> 269A -0.37981 257A -> 270A -0.20627 257A -> 271A -0.20361	
Excited State 16: 3.012-?Sym 2.1373 eV **580.10 nm f=0.0204** <S**2>=2.018 257A -> 258A -0.14685 257A -> 265A 0.17518 257A -> 266A 0.17927 **257A(HOMO) -> 267A(LUMO+9) 0.93015** 257A -> 268A -0.11310 257A -> 270A 0.11032	

Excited State 15: 3.012-?Sym 2.0713 eV **598.59 nm f=0.0468** <S**2>=2.019 256A -> 258A 0.17556 257A -> 263A 0.40771 257A -> 264A 0.45759 257A -> 265A -0.40814 **257A(HOMO) -> 266A(LUMO+8)** **0.60973** 257A -> 271A -0.10704	**257A**  **266A** 
Excited State 11: 3.014-?Sym 1.5665 eV **791.46 nm f=0.0018** <S**2>=2.021 257A -> 260A 0.16879 257A -> 261A 0.14465 **257A(HOMO)-> 262A(LUMO+4)** **0.92337** 257A -> 263A 0.22579 257A -> 264A -0.18549	**257A**  **262A** 
Excited State 10: 3.011-?Sym 1.5181 eV **816.70 nm f=0.0209** <S**2>=2.016 257A -> 260A -0.12019 **257A(HOMO)-> 261A(LUMO+3) 0.93850** 257A -> 262A -0.19721 257A -> 263A 0.15334 257A -> 264A -0.18207	**257A**  **261A** 

Ligand

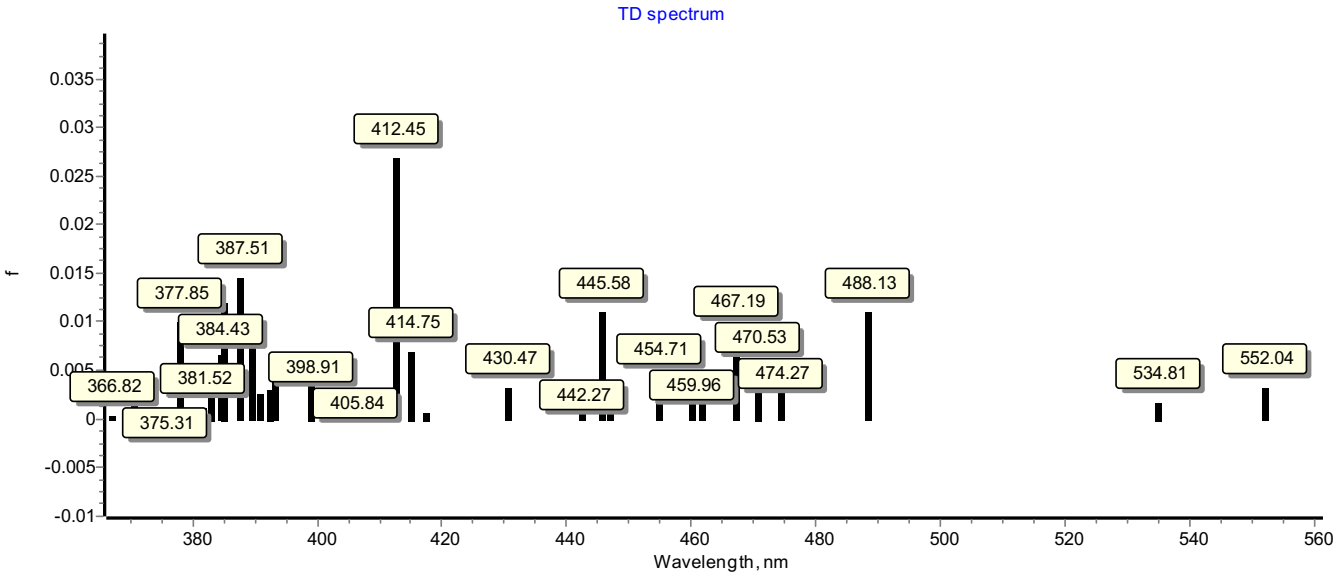
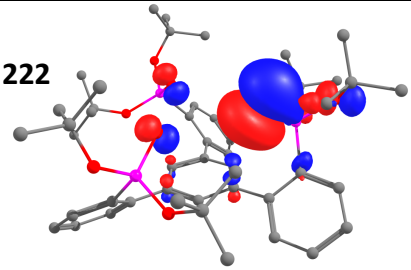
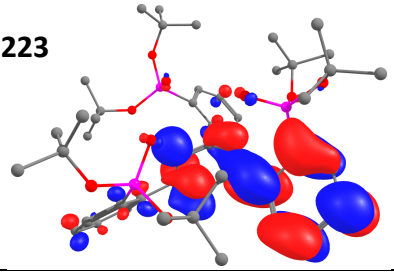
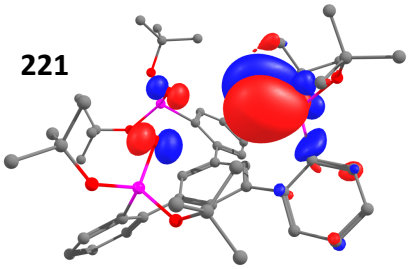
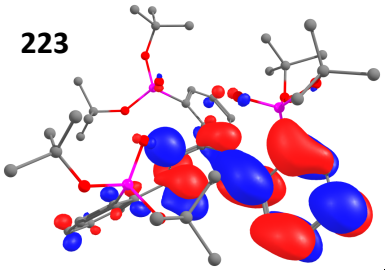
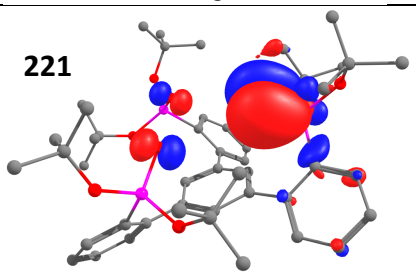
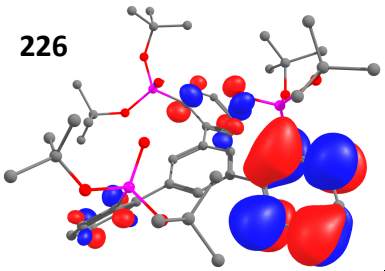
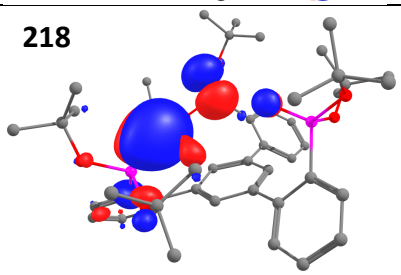
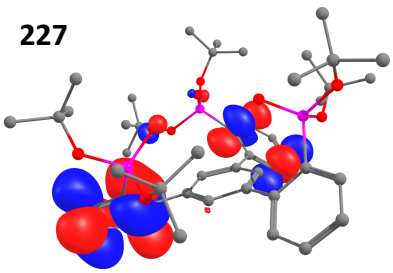
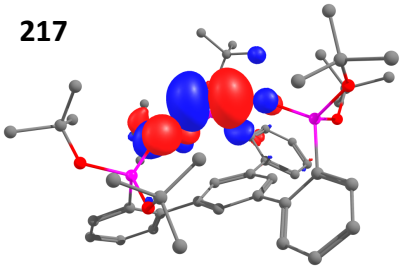
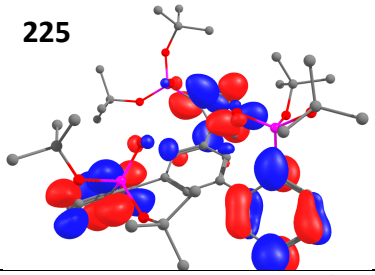
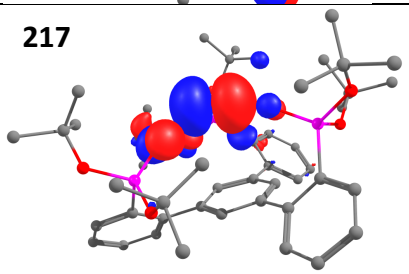
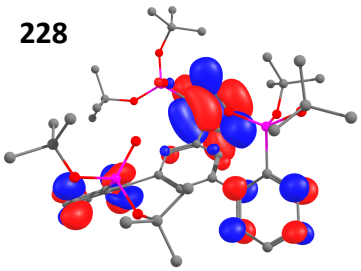


Figure S83. Simulated UV−Vis spectrum of ligand

Table S44. TDDFT caculations of ligand

Excited State 1: Singlet-?Sym 2.2459 eV **552.04 nm f=0.0031** <S**2>=0.000 221 -> 223 0.15538 **222(HOMO)** -> **223(LUMO)** **0.67527**	**222**  **223** 

Excited State 2: Singlet-?Sym 2.3183 eV **534.81 nm f=0.0016** <S**2>=0.000 **221 -> 223 0.67880** 222 -> 223 -0.15529	**221**  **223** 
Excited State 16: Singlet-?Sym 3.0061 eV **412.45 nm f=0.0268** <S**2>=0.000 221 -> 225 -0.23895 **221 -> 226 0.60854** 222 -> 224 -0.12296	**221**  **226** 
Excited State 24: Singlet-?Sym 3.1995 eV **387.51 nm f=0.0144** <S**2>=0.000 218 -> 225 -0.24229 218 -> 226 -0.11160 **218 -> 227 0.33791** 219 -> 225 -0.28079 219 -> 226 0.10054 219 -> 228 -0.24975 220 -> 226 -0.10927 220 -> 227 -0.10860 220 -> 228 0.18549 221 -> 228 0.26304	**218**  **227** 

Excited State 25: Singlet-?Sym 3.2215 eV **384.87 nm f=0.0120** <S**2>=0.000 217 -> 224 -0.13096 **217 -> 225 0.49210** 217 -> 226 0.17075 217 -> 227 0.14687 218 -> 225 0.31361 218 -> 227 0.14760 219 -> 226 0.11495 220 -> 226 0.12435	**217**  **225** 
Excited State 29: Singlet-?Sym 3.2813 eV **377.85 nm f=0.0099** <S**2>=0.000 217 -> 225 0.25852 217 -> 226 -0.14652 217 -> 227 -0.40321 **217 -> 228 0.41978** 218 -> 228 0.15190 221 -> 228 -0.11532	**217**  **228** 

Optimized geometries

1(s=1/2)

Ce	5.686968000	1.228280000	4.098728000
Si	5.562747000	4.345454000	2.551581000
Si	3.202202000	-1.215610000	3.354976000
Si	8.815482000	-0.041329000	4.979575000
O	5.933116000	3.432911000	3.854176000
O	5.309299000	5.964378000	2.898728000
O	4.187636000	3.789226000	1.773156000
O	3.764474000	0.169972000	4.008931000
O	1.746402000	-1.694831000	4.036688000
O	4.250787000	-2.509062000	3.504385000

O	7.218735000	0.153794000	5.269081000
O	9.694084000	-0.388768000	6.365289000
O	9.508243000	1.313531000	4.284411000
O	4.860587000	1.925676000	6.371216000
C	7.049290000	1.716113000	1.231435000
C	5.729301000	1.368603000	0.892444000
H	5.076902000	2.118537000	0.460155000
C	5.240204000	0.069783000	1.120077000
C	6.092224000	-0.885594000	1.701570000
H	5.718640000	-1.885302000	1.894199000
C	7.414113000	-0.560516000	2.051335000
C	7.881926000	0.743991000	1.813933000
H	8.896149000	1.004904000	2.093695000
C	7.591372000	3.058348000	0.900312000
C	8.773295000	3.104630000	0.150528000
H	9.248527000	2.172970000	-0.143994000
C	9.327510000	4.320434000	-0.236903000
H	10.244135000	4.336114000	-0.819492000
C	8.693306000	5.508789000	0.113793000
H	9.108896000	6.464087000	-0.194245000
C	7.525719000	5.466835000	0.871910000
H	7.039792000	6.392561000	1.164243000
C	6.958254000	4.257114000	1.293755000
C	5.829633000	6.755754000	3.973086000
C	7.241064000	6.314410000	4.358958000
H	7.237770000	5.272243000	4.684925000
H	7.627356000	6.938772000	5.170891000
H	7.920649000	6.401077000	3.506675000
C	5.839898000	8.193886000	3.461975000
H	6.517254000	8.290831000	2.608293000
H	6.170909000	8.884040000	4.244330000
H	4.837052000	8.485752000	3.137596000
C	4.878185000	6.618672000	5.159726000
H	3.869475000	6.929722000	4.872252000
H	5.205256000	7.232988000	6.004961000
H	4.838415000	5.576017000	5.479979000
C	2.812055000	3.888275000	2.173424000
C	2.304024000	5.279197000	1.801314000
H	2.871309000	6.042644000	2.338360000
H	1.240889000	5.382597000	2.041917000
H	2.436374000	5.446754000	0.728546000
C	2.655873000	3.636106000	3.672810000
H	2.979045000	2.623874000	3.934191000
H	1.603976000	3.727929000	3.961510000

H	3.232864000	4.358066000	4.255769000
C	2.081146000	2.807026000	1.383927000
H	2.223377000	2.959671000	0.310522000
H	1.008434000	2.824576000	1.598855000
H	2.468862000	1.818463000	1.641082000
C	3.875593000	-0.306844000	0.671682000
C	3.520915000	0.009451000	-0.645983000
H	4.238840000	0.525969000	-1.277102000
C	2.278282000	-0.349901000	-1.157580000
H	2.022116000	-0.097891000	-2.182648000
C	1.376555000	-1.043233000	-0.354875000
H	0.408068000	-1.339347000	-0.747970000
C	1.719988000	-1.347305000	0.960196000
H	1.009840000	-1.867445000	1.596290000
C	2.956863000	-0.980807000	1.505826000
C	0.753060000	-0.847814000	4.632679000
C	1.255557000	-0.372455000	5.996013000
H	1.486510000	-1.231327000	6.634029000
H	0.497961000	0.237211000	6.499282000
H	2.159675000	0.225714000	5.857564000
C	0.455569000	0.356368000	3.740858000
H	1.355307000	0.962726000	3.617731000
H	-0.321233000	0.982376000	4.191567000
H	0.112800000	0.039071000	2.752953000
C	-0.485686000	-1.724443000	4.786390000
H	-0.822266000	-2.078285000	3.807360000
H	-1.302904000	-1.167552000	5.255385000
H	-0.256633000	-2.597324000	5.404713000
C	4.593017000	-3.268193000	4.673065000
C	4.635877000	-2.373716000	5.908866000
H	3.662455000	-1.911994000	6.090103000
H	5.383708000	-1.588593000	5.772881000
H	4.910874000	-2.958612000	6.792439000
C	3.555674000	-4.375999000	4.836045000
H	3.798541000	-5.015963000	5.690795000
H	3.527040000	-4.994427000	3.934219000
H	2.565407000	-3.938450000	4.984503000
C	5.982401000	-3.839764000	4.405698000
H	6.712544000	-3.033272000	4.299968000
H	5.982272000	-4.426160000	3.482691000
H	6.300563000	-4.486886000	5.228966000
C	8.324679000	-1.609390000	2.576679000
C	8.433983000	-2.792258000	1.834996000
H	7.843778000	-2.903431000	0.929654000

C	9.297485000	-3.807705000	2.232568000
H	9.369820000	-4.717930000	1.644339000
C	10.073481000	-3.642901000	3.376438000
H	10.761271000	-4.423393000	3.689369000
C	9.957251000	-2.473728000	4.124308000
H	10.548882000	-2.352108000	5.026752000
C	9.079602000	-1.444515000	3.757900000
C	9.223021000	-1.027926000	7.559074000
C	8.307182000	-2.206947000	7.231578000
H	8.827306000	-2.945899000	6.616838000
H	7.427725000	-1.862875000	6.683448000
H	7.974093000	-2.698304000	8.151331000
C	10.473915000	-1.506984000	8.288858000
H	10.213794000	-1.975183000	9.243400000
H	11.143893000	-0.664369000	8.482480000
H	11.012228000	-2.238617000	7.679090000
C	8.473995000	0.009607000	8.394143000
H	7.632589000	0.393140000	7.812987000
H	9.136721000	0.843217000	8.645872000
H	8.097591000	-0.427701000	9.324779000
C	9.853749000	2.570791000	4.884740000
C	8.822585000	2.978097000	5.935832000
H	7.839965000	3.100288000	5.472334000
H	9.102278000	3.934776000	6.388647000
H	8.760122000	2.228177000	6.727401000
C	9.853821000	3.584883000	3.745775000
H	10.544569000	3.274333000	2.957122000
H	10.157012000	4.572950000	4.105302000
H	8.853306000	3.666966000	3.314749000
C	11.238307000	2.427937000	5.511023000
H	11.215730000	1.662378000	6.290617000
H	11.570528000	3.376182000	5.946325000
H	11.961116000	2.122009000	4.749202000
C	4.782672000	0.922529000	7.413995000
H	5.548900000	0.173873000	7.197652000
H	3.797997000	0.452817000	7.366797000
C	5.046936000	1.660538000	8.725868000
H	5.617818000	1.047913000	9.427340000
H	4.104439000	1.940864000	9.207446000
C	5.802778000	2.910964000	8.269972000
H	6.858653000	2.683093000	8.098409000
H	5.736239000	3.738345000	8.980637000
C	5.120108000	3.218316000	6.950752000
H	4.163317000	3.736457000	7.096462000

H	5.723052000	3.774104000	6.232787000

2(s=0)

Ce	9.811011000	8.474658000	12.802594000
Si	8.593906000	5.036715000	12.956660000
Si	13.383948000	8.829187000	12.125174000
Cl	9.610170000	9.265177000	15.230813000
Si	7.643347000	10.817094000	11.020381000
O	9.805542000	3.965831000	12.575165000
O	11.848008000	8.876830000	12.751215000
O	8.445992000	9.898985000	12.145771000
O	9.167663000	6.560384000	13.281293000
O	7.746050000	4.428693000	14.246993000
O	13.635123000	9.988987000	10.962251000
O	6.349598000	10.022271000	10.343677000
O	14.523393000	9.024604000	13.315161000
C	7.479361000	5.099991000	11.451466000
C	7.704995000	5.893422000	10.305364000
O	7.097608000	12.234168000	11.689986000
C	8.909461000	6.745202000	10.141692000
C	13.649920000	7.181557000	11.272890000
C	11.163451000	8.383885000	9.792014000
H	12.034350000	9.022344000	9.679803000
C	10.199906000	6.249843000	10.401693000
H	10.316209000	5.233154000	10.764107000
C	8.766281000	8.069580000	9.702430000
H	7.773121000	8.469327000	9.522019000
C	6.294033000	4.355299000	11.520374000
H	6.108287000	3.759825000	12.409428000
C	9.886735000	8.901298000	9.527558000
C	8.800787000	11.199781000	9.597354000
C	12.974690000	5.231852000	9.986969000
H	12.229308000	4.722233000	9.383027000
C	11.333092000	7.059152000	10.232995000
C	9.744797000	10.300786000	9.053777000
C	8.769061000	12.510216000	9.101764000
H	8.059419000	13.209821000	9.533792000
C	12.680616000	6.499816000	10.504936000
C	6.755142000	5.908213000	9.275637000
H	6.945504000	6.508734000	8.390677000
C	10.606478000	10.733906000	8.037517000
H	11.317230000	10.031095000	7.612088000
C	14.880924000	6.551464000	11.500109000
H	15.618887000	7.063908000	12.110356000

C	10.550958000	12.038403000	7.556852000
H	11.227228000	12.350949000	6.766663000
C	5.353553000	4.376408000	10.493690000
H	4.443827000	3.788910000	10.575663000
C	5.588474000	5.155578000	9.364675000
H	4.867242000	5.180331000	8.553102000
C	7.047038000	5.140440000	15.286164000
C	10.933816000	3.534358000	13.360950000
C	13.570076000	11.424797000	11.063845000
C	9.630140000	12.933854000	8.092712000
H	9.582284000	13.955890000	7.728496000
C	15.165848000	5.290480000	10.982546000
H	16.129020000	4.827065000	11.175065000
C	6.161572000	4.094229000	15.955135000
H	5.441793000	3.688064000	15.237936000
H	5.609793000	4.532732000	16.791940000
H	6.772714000	3.269517000	16.332318000
C	5.151170000	9.520942000	10.967743000
C	14.207236000	4.629828000	10.219856000
H	14.414327000	3.647308000	9.806086000
C	5.517991000	8.548571000	12.085779000
H	6.133641000	7.731877000	11.698465000
H	4.614992000	8.112122000	12.522606000
H	6.069441000	9.057953000	12.880606000
C	8.068682000	5.701706000	16.271560000
H	8.677979000	4.892655000	16.685601000
H	7.565736000	6.211054000	17.099433000
H	8.722627000	6.423402000	15.777696000
C	6.198035000	6.259984000	14.689521000
H	6.832888000	7.019247000	14.227753000
H	5.605962000	6.748250000	15.469335000
H	5.516396000	5.865989000	13.930700000
C	13.798552000	11.932497000	9.644161000
H	14.763209000	11.579635000	9.268778000
H	13.790801000	13.026400000	9.620036000
H	13.009025000	11.570394000	8.981719000
C	15.851355000	8.768231000	15.241088000
H	16.446722000	7.992026000	14.750830000
H	15.876759000	8.596290000	16.321322000
H	16.310383000	9.738050000	15.029740000
C	12.192320000	11.846394000	11.568075000
H	11.405605000	11.448600000	10.920787000
H	12.105678000	12.936826000	11.571834000
H	12.023715000	11.487233000	12.586816000

C	13.788279000	7.370614000	14.948290000
H	14.354531000	6.595750000	14.423913000
H	12.758281000	7.357693000	14.585528000
H	13.770943000	7.127128000	16.014777000
C	11.738121000	2.629599000	12.433799000
H	11.122029000	1.790845000	12.097819000
H	12.619249000	2.235369000	12.948949000
H	12.075306000	3.190758000	11.559286000
C	10.445441000	2.754903000	14.578328000
H	9.857086000	3.394133000	15.238949000
H	11.297683000	2.357280000	15.138565000
H	9.812076000	1.921194000	14.263587000
C	13.580130000	9.835890000	15.384871000
H	13.519908000	9.672877000	16.465400000
H	12.563497000	9.837235000	14.986227000
H	14.032944000	10.816724000	15.211071000
C	11.765563000	4.743209000	13.782253000
H	12.085565000	5.316381000	12.907675000
H	12.662625000	4.419458000	14.317966000
H	11.191982000	5.399752000	14.441883000
C	4.399056000	8.797584000	9.855863000
H	4.189467000	9.487217000	9.033480000
H	3.451975000	8.396328000	10.229086000
H	4.996908000	7.966366000	9.475355000
C	14.671724000	11.926125000	11.993250000
H	14.520678000	11.559611000	13.010025000
H	14.682431000	13.020557000	12.010277000
H	15.646343000	11.570778000	11.647989000
C	4.323025000	10.686565000	11.501002000
H	4.859582000	11.218179000	12.288561000
H	3.372664000	10.322405000	11.903898000
H	4.113736000	11.397936000	10.697412000
C	14.416722000	8.743288000	14.724282000
C	7.600632000	12.938173000	12.842480000
C	6.957243000	14.319281000	12.772490000
H	7.263528000	14.836775000	11.858398000
H	5.867629000	14.226473000	12.766406000
H	7.252360000	14.927610000	13.632688000
C	7.164940000	12.197831000	14.104336000
H	6.074479000	12.113126000	14.136192000
H	7.601130000	11.197237000	14.134710000
H	7.493068000	12.737059000	14.998369000
C	9.121381000	13.050814000	12.777255000
H	9.583109000	12.063247000	12.840792000

H	9.433777000	13.523912000	11.841994000
H	9.496643000	13.649866000	13.612361000

3(s=1)

Ce	11.823673000	10.904007000	6.225883000
Si	14.144790000	9.880424000	3.689984000
Si	11.848000000	9.366656000	9.477394000
Si	10.238483000	14.118972000	6.055871000
O	12.686132000	9.948404000	4.398195000
O	14.034078000	9.211205000	2.138537000
O	15.304706000	8.957575000	4.475830000
O	11.344840000	9.524860000	7.935908000
O	11.186370000	7.999334000	10.230823000
O	11.335527000	10.622594000	10.470674000
O	10.234012000	12.503299000	5.869629000
O	8.671282000	14.761225000	5.981824000
O	11.089828000	14.994770000	4.903995000
O	9.863460000	9.465620000	5.290105000
C	14.329417000	12.378556000	5.835769000
C	14.734304000	11.289794000	6.598713000
H	15.422539000	10.572807000	6.162474000
C	14.208527000	11.048878000	7.909815000
C	13.318215000	12.039257000	8.448329000
H	12.938621000	11.913844000	9.456947000
C	12.936763000	13.155354000	7.716960000
C	13.374330000	13.305343000	6.367683000
H	13.058131000	14.161804000	5.786710000
C	14.859689000	12.601117000	4.472593000
C	15.282399000	13.899841000	4.143666000
H	15.222422000	14.673427000	4.904133000
C	15.781773000	14.199526000	2.881776000
H	16.106164000	15.212335000	2.655850000
C	15.865275000	13.198595000	1.914578000
H	16.249851000	13.421905000	0.922587000
C	15.433340000	11.911936000	2.226604000
H	15.463790000	11.134075000	1.468627000
C	14.915768000	11.584856000	3.487984000
C	12.861490000	9.171485000	1.327665000
C	12.188117000	10.543109000	1.272993000
H	12.894807000	11.303531000	0.928478000
H	11.842647000	10.823074000	2.269988000
H	11.329197000	10.529885000	0.592789000
C	13.341152000	8.758792000	-0.062487000
H	12.498730000	8.658202000	-0.755408000

H	13.868176000	7.801570000	-0.006315000
H	14.033165000	9.507775000	-0.460175000
C	11.889556000	8.131848000	1.892123000
H	11.642188000	8.395434000	2.923616000
H	12.347129000	7.137513000	1.882488000
H	10.970832000	8.089650000	1.295214000
C	15.213533000	7.608627000	4.944658000
C	15.039841000	6.656741000	3.761062000
H	15.837762000	6.814849000	3.029950000
H	14.087248000	6.834363000	3.259304000
H	15.069713000	5.615555000	4.101321000
C	16.541810000	7.334069000	5.646099000
H	16.580488000	6.303136000	6.013379000
H	16.658717000	8.004337000	6.500364000
H	17.372641000	7.494282000	4.951962000
C	14.055923000	7.460824000	5.931004000
H	13.103471000	7.681093000	5.442787000
H	14.177740000	8.143407000	6.776232000
H	14.020620000	6.440435000	6.325859000
C	14.612131000	9.905733000	8.708938000
C	15.951289000	9.454533000	8.644178000
H	16.640924000	9.964268000	7.976648000
C	16.413102000	8.427045000	9.450639000
H	17.453927000	8.118412000	9.381680000
C	15.554728000	7.812341000	10.369225000
H	15.913514000	7.019252000	11.019710000
C	14.222884000	8.221357000	10.418239000
H	13.535146000	7.717065000	11.091822000
C	13.713969000	9.231561000	9.592905000
C	10.984996000	6.694302000	9.695268000
C	9.511003000	6.571781000	9.305486000
H	8.874633000	6.807358000	10.164391000
H	9.273529000	5.559304000	8.960296000
H	9.280665000	7.273318000	8.501480000
C	11.875245000	6.418630000	8.483339000
H	11.678075000	7.149844000	7.696075000
H	11.685734000	5.412737000	8.092729000
H	12.931094000	6.492098000	8.756194000
C	11.308771000	5.713150000	10.822724000
H	12.365668000	5.785165000	11.094428000
H	11.100335000	4.681414000	10.518980000
H	10.709080000	5.947440000	11.707750000
C	9.994389000	10.954511000	10.833259000
C	8.976457000	10.465318000	9.801451000

H	9.212618000	10.867057000	8.814577000
H	7.969968000	10.794781000	10.080739000
H	8.982996000	9.374559000	9.742033000
C	9.715883000	10.310737000	12.191842000
H	9.818744000	9.225845000	12.105447000
H	8.707405000	10.552555000	12.546882000
H	10.442195000	10.668779000	12.927926000
C	9.942516000	12.477305000	10.920603000
H	10.703820000	12.841859000	11.615402000
H	8.960082000	12.817731000	11.265314000
H	10.142743000	12.922780000	9.943009000
C	12.073534000	14.179912000	8.344966000
C	12.426861000	14.634281000	9.624369000
H	13.311377000	14.218212000	10.097568000
C	11.675492000	15.603543000	10.278595000
H	11.968420000	15.936373000	11.271175000
C	10.555360000	16.146075000	9.653633000
H	9.962308000	16.909584000	10.150842000
C	10.198358000	15.699027000	8.383361000
H	9.317260000	16.105677000	7.895783000
C	10.933350000	14.715770000	7.705353000
C	7.476349000	14.103053000	6.389950000
C	7.035997000	13.173251000	5.258968000
H	7.841105000	12.460986000	5.068529000
H	6.853979000	13.749547000	4.346480000
H	6.122017000	12.626542000	5.517310000
C	7.686342000	13.305398000	7.678431000
H	6.757899000	12.813032000	7.987290000
H	8.021009000	13.957354000	8.489646000
H	8.451945000	12.542498000	7.519390000
C	6.444878000	15.207209000	6.612434000
H	6.336288000	15.805842000	5.702995000
H	6.768810000	15.869162000	7.421543000
H	5.468950000	14.786225000	6.877482000
C	11.065267000	14.885467000	3.481311000
C	9.661568000	15.192079000	2.957847000
H	9.322675000	16.161980000	3.331907000
H	8.949372000	14.436517000	3.298376000
H	9.655617000	15.209209000	1.862231000
C	12.061755000	15.929127000	2.979938000
H	12.099351000	15.938629000	1.885466000
H	13.061845000	15.697273000	3.356085000
H	11.774659000	16.923912000	3.334068000
C	11.508702000	13.491644000	3.042686000

H	10.826099000	12.736867000	3.438696000
H	12.514238000	13.270663000	3.407802000
H	11.520868000	13.417718000	1.950981000
C	9.167751000	9.991033000	4.142224000
H	9.573076000	9.521673000	3.241855000
H	9.365283000	11.066853000	4.111496000
C	7.684273000	9.689297000	4.372174000
H	7.040630000	10.488421000	3.996779000
H	7.397853000	8.757476000	3.871308000
C	7.609330000	9.514222000	5.891167000
H	6.746561000	8.927648000	6.218907000
H	7.580912000	10.487713000	6.389249000
C	8.932892000	8.829279000	6.177290000
H	9.328575000	8.961996000	7.184658000
H	8.889080000	7.755786000	5.941667000

3(s=0)

Ce	11.923844000	11.036055000	6.386748000
Si	13.949159000	9.972331000	3.683855000
Si	11.815378000	9.346487000	9.458575000
Si	10.371714000	14.281978000	6.038064000
O	12.495282000	10.151534000	4.386129000
O	13.817025000	9.339060000	2.116293000
O	15.044788000	8.939006000	4.427927000
O	11.303704000	9.484475000	7.922218000
O	11.170710000	7.991766000	10.250783000
O	11.372159000	10.627008000	10.449909000
O	10.499008000	12.671222000	5.875359000
O	8.749241000	14.776916000	6.017627000
O	11.072577000	15.157061000	4.789313000
O	9.715067000	9.937504000	5.516889000
C	14.320776000	12.368994000	5.877235000
C	14.533699000	11.136223000	6.585881000
H	15.190015000	10.384874000	6.167665000
C	14.169565000	11.072089000	7.979643000
C	13.393083000	12.077414000	8.528603000
H	13.063065000	11.985726000	9.558370000
C	12.921472000	13.174729000	7.740986000
C	13.495699000	13.333288000	6.426414000
H	13.255686000	14.228172000	5.860003000
C	14.929818000	12.578168000	4.544618000
C	15.558941000	13.805482000	4.294910000
H	15.597192000	14.542229000	5.092337000
C	16.129922000	14.083347000	3.056694000

H	16.609059000	15.044087000	2.885173000
C	16.085142000	13.126665000	2.046001000
H	16.526755000	13.332086000	1.073977000
C	15.466514000	11.901865000	2.289798000
H	15.414033000	11.156635000	1.500961000
C	14.883518000	11.599016000	3.526932000
C	12.669403000	9.383693000	1.275682000
C	12.080129000	10.793586000	1.232845000
H	12.832777000	11.505955000	0.882892000
H	11.766274000	11.100542000	2.232234000
H	11.216215000	10.839717000	0.560771000
C	13.157641000	8.975014000	-0.112998000
H	12.327394000	8.936870000	-0.826662000
H	13.629394000	7.988812000	-0.067720000
H	13.898904000	9.692799000	-0.477859000
C	11.637175000	8.379217000	1.794996000
H	11.422809000	8.602912000	2.842186000
H	12.033772000	7.360842000	1.730570000
H	10.708046000	8.425421000	1.215903000
C	14.866265000	7.597839000	4.878206000
C	14.764121000	6.665744000	3.670428000
H	15.645564000	6.783226000	3.033469000
H	13.886138000	6.913764000	3.071022000
H	14.694262000	5.620358000	3.991521000
C	16.114793000	7.272610000	5.696450000
H	16.088300000	6.237386000	6.053082000
H	16.177600000	7.932598000	6.565758000
H	17.010729000	7.412386000	5.083788000
C	13.625943000	7.478127000	5.762071000
H	12.721918000	7.738129000	5.205999000
H	13.702076000	8.147956000	6.623274000
H	13.526321000	6.455549000	6.139159000
C	14.596989000	9.925191000	8.801464000
C	15.954325000	9.566065000	8.786926000
H	16.634549000	10.129617000	8.154178000
C	16.431609000	8.531610000	9.582893000
H	17.488462000	8.277203000	9.562469000
C	15.553250000	7.832458000	10.411437000
H	15.917223000	7.026168000	11.043294000
C	14.200515000	8.162166000	10.404650000
H	13.505867000	7.599831000	11.022090000
C	13.687869000	9.185017000	9.593685000
C	10.856593000	6.718392000	9.693490000
C	9.398446000	6.747197000	9.235764000

H	8.743018000	6.991749000	10.077722000
H	9.089786000	5.780957000	8.821291000
H	9.281007000	7.514094000	8.468411000
C	11.767501000	6.373291000	8.515914000
H	11.655891000	7.124190000	7.730595000
H	11.513520000	5.388662000	8.108359000
H	12.815773000	6.360722000	8.827012000
C	11.038527000	5.706060000	10.823706000
H	12.084611000	5.679358000	11.143357000
H	10.749537000	4.699886000	10.501072000
H	10.424155000	5.989771000	11.683701000
C	10.057058000	10.979010000	10.885900000
C	8.987295000	10.532675000	9.888312000
H	9.193352000	10.937393000	8.895771000
H	8.001497000	10.884914000	10.209856000
H	8.961930000	9.443159000	9.817375000
C	9.824829000	10.310514000	12.241223000
H	9.895145000	9.225505000	12.129020000
H	8.840261000	10.570627000	12.646425000
H	10.592186000	10.634736000	12.950894000
C	10.050032000	12.499143000	11.013087000
H	10.840042000	12.824028000	11.695809000
H	9.087662000	12.857777000	11.393421000
H	10.237706000	12.967001000	10.044420000
C	12.139258000	14.258060000	8.341070000
C	12.437653000	14.673590000	9.654693000
H	13.230679000	14.166295000	10.196992000
C	11.765673000	15.730523000	10.251976000
H	12.025204000	16.028297000	11.265469000
C	10.776514000	16.419665000	9.547595000
H	10.252525000	17.255508000	10.003995000
C	10.458309000	16.006515000	8.255881000
H	9.653663000	16.500833000	7.717098000
C	11.104869000	14.928197000	7.637894000
C	7.664586000	14.082465000	6.628062000
C	7.317939000	12.846075000	5.795683000
H	8.163597000	12.155559000	5.815685000
H	7.121023000	13.134477000	4.758333000
H	6.429573000	12.342615000	6.194561000
C	8.005914000	13.652923000	8.055295000
H	7.164996000	13.116197000	8.507394000
H	8.254809000	14.512421000	8.681750000
H	8.868167000	12.982201000	8.044048000
C	6.500676000	15.071784000	6.636071000

H	6.272311000	15.389069000	5.613834000
H	6.768864000	15.959200000	7.217660000
H	5.602925000	14.622716000	7.074756000
C	11.004937000	14.836054000	3.396344000
C	9.688962000	14.143082000	3.038660000
H	8.836943000	14.764764000	3.325023000
H	9.616159000	13.191836000	3.572095000
H	9.646443000	13.944780000	1.961957000
C	11.117352000	16.170942000	2.662707000
H	11.123513000	16.024121000	1.577053000
H	12.043146000	16.676778000	2.952718000
H	10.274794000	16.816994000	2.927715000
C	12.184755000	13.933239000	3.052742000
H	12.130511000	13.002653000	3.622866000
H	13.129621000	14.422132000	3.299056000
H	12.196060000	13.685930000	1.986904000
C	9.317970000	10.154882000	4.153994000
H	10.227130000	10.253090000	3.560549000
H	8.751123000	11.089947000	4.100853000
C	8.458068000	8.951598000	3.794214000
H	7.740312000	9.174052000	2.999889000
H	9.087927000	8.117971000	3.464999000
C	7.805303000	8.626991000	5.139343000
H	7.417879000	7.606493000	5.207032000
H	6.982397000	9.323128000	5.336864000
C	8.954120000	8.879617000	6.107342000
H	8.640298000	9.201686000	7.101810000
H	9.598524000	8.000115000	6.218800000

4(s=1)

Ce	2.220859000	18.017301000	5.468588000
P	1.905152000	21.707454000	4.273438000
Si	4.252062000	18.833830000	8.411962000
Si	-1.340062000	17.496697000	5.888098000
Si	3.895128000	16.227281000	2.795145000
O	-1.693684000	17.485829000	7.529410000
O	2.895333000	15.015562000	2.193595000
O	3.169148000	17.496145000	3.495965000
O	-0.034114000	18.361702000	5.456168000
O	-2.748074000	18.115818000	5.166595000
O	4.785171000	16.719396000	1.437111000
O	2.237083000	20.211513000	4.438932000
O	5.736399000	18.049594000	8.289091000
O	4.650273000	20.309732000	9.160743000

O	3.482345000	19.096391000	7.002489000
C	1.102007000	15.259745000	6.043520000
C	3.564876000	15.373740000	5.977713000
C	-0.178198000	14.838626000	5.431352000
C	-1.316146000	15.674586000	5.396582000
C	1.105664000	15.817290000	7.318425000
H	0.161843000	15.989515000	7.824500000
C	2.314358000	15.076999000	5.330440000
H	2.305126000	14.629077000	4.345087000
C	3.225558000	17.869530000	9.645188000
C	-2.503558000	15.147258000	4.865108000
H	-3.382696000	15.784817000	4.844224000
C	1.393841000	16.368587000	10.234371000
H	0.711561000	15.568379000	9.960412000
C	2.337149000	16.814017000	9.275871000
C	-0.247562000	13.548985000	4.882020000
H	0.643168000	12.927596000	4.907409000
C	-1.429968000	13.059988000	4.339420000
H	-1.460498000	12.055503000	3.924718000
C	1.348246000	16.899101000	11.512938000
H	0.616688000	16.521528000	12.224276000
C	7.871504000	17.254131000	7.714639000
H	8.133147000	17.221992000	8.776877000
H	8.783107000	17.415952000	7.129371000
H	7.445424000	16.290996000	7.427156000
C	-1.733324000	18.584593000	8.441120000
C	6.351886000	15.025499000	3.414359000
H	6.534067000	15.237053000	2.364120000
C	-2.687189000	19.662367000	7.924296000
H	-3.673784000	19.233696000	7.729284000
H	-2.320050000	20.084555000	6.986215000
H	-2.784850000	20.471364000	8.657123000
C	2.247773000	17.902484000	11.892159000
H	2.221389000	18.321957000	12.894400000
C	-2.251267000	18.001565000	9.754321000
H	-2.315213000	18.776178000	10.525923000
H	-1.568749000	17.222687000	10.104834000
H	-3.242945000	17.562146000	9.608385000
C	7.370176000	14.482534000	4.195528000
H	8.336520000	14.250279000	3.755285000
C	-2.848535000	18.670656000	3.859466000
C	-0.329503000	19.152234000	8.644973000
H	0.095264000	19.458105000	7.688223000
H	0.332064000	18.405514000	9.085757000

H	-0.355352000	20.019222000	9.313228000
C	7.448825000	19.715068000	7.872112000
H	6.736040000	20.520508000	7.689471000
H	8.366359000	19.917180000	7.307620000
H	7.681417000	19.713502000	8.940726000
C	3.952117000	21.534008000	8.997847000
C	-2.050179000	17.863192000	2.836096000
H	-2.140992000	18.307413000	1.838791000
H	-2.396810000	16.828269000	2.791580000
H	-0.993817000	17.855208000	3.114575000
C	2.439123000	21.328175000	9.097580000
H	2.102992000	20.664107000	8.297862000
H	1.907309000	22.284188000	9.020801000
H	2.179109000	20.860115000	10.050447000
C	5.316506000	18.022760000	1.220806000
C	-2.319148000	20.103980000	3.893665000
H	-1.264783000	20.068842000	4.173623000
H	-2.864507000	20.690101000	4.639962000
H	-2.423485000	20.590460000	2.916606000
C	4.319549000	22.127459000	7.633497000
H	5.398028000	22.305253000	7.577642000
H	3.808750000	23.083263000	7.462205000
H	4.043716000	21.404836000	6.859203000
C	-4.336168000	18.651337000	3.513715000
H	-4.519613000	19.100075000	2.531271000
H	-4.902602000	19.207157000	4.267122000
H	-4.705385000	17.621286000	3.499752000
C	4.436936000	22.445196000	10.124253000
H	4.177565000	22.010362000	11.094269000
H	3.981971000	23.439497000	10.053463000
H	5.525058000	22.550195000	10.076547000
C	4.852406000	15.088803000	5.317306000
C	3.546007000	15.939679000	7.252175000
H	4.488970000	16.204789000	7.721998000
C	1.764980000	15.129809000	1.331113000
C	2.337730000	16.206693000	7.955442000
C	5.887528000	14.536242000	6.094157000
H	5.692963000	14.322186000	7.141178000
C	-2.572681000	13.859068000	4.342624000
H	-3.506789000	13.485628000	3.930180000
C	7.130198000	14.241418000	5.547723000
H	7.907011000	13.814098000	6.177299000
C	3.164886000	18.370802000	10.951502000
H	3.834840000	19.184578000	11.217972000

C	6.855958000	18.366531000	7.461321000
C	5.090993000	15.337256000	3.940071000
C	6.448450000	18.384573000	5.988352000
H	6.016212000	17.424059000	5.698429000
H	7.319291000	18.571975000	5.351430000
H	5.702577000	19.162656000	5.807933000
C	3.432377000	22.679982000	3.958948000
H	3.139302000	23.715271000	3.748199000
H	3.978421000	22.675050000	4.907502000
C	4.274171000	22.071328000	2.843689000
H	3.760081000	22.117140000	1.879132000
H	4.485766000	21.022228000	3.058775000
H	5.225526000	22.602194000	2.742955000
C	0.749926000	21.959262000	2.854315000
H	-0.255043000	22.039353000	3.278470000
H	0.989742000	22.921099000	2.387123000
C	0.815225000	20.798624000	1.864777000
H	0.626333000	19.852250000	2.374668000
H	1.796525000	20.719203000	1.392040000
H	0.063364000	20.927636000	1.080386000
C	1.153349000	22.452760000	5.769575000
H	1.882430000	22.256625000	6.559341000
H	1.106439000	23.538728000	5.622870000
C	-0.199788000	21.849041000	6.125130000
H	-0.179078000	20.758879000	6.037924000
H	-0.994651000	22.222425000	5.474433000
H	-0.466091000	22.096569000	7.155955000
C	2.225373000	15.529944000	-0.070900000
H	2.961538000	14.811070000	-0.442133000
H	1.376037000	15.558836000	-0.762958000
H	2.702305000	16.511514000	-0.049493000
C	1.133066000	13.739009000	1.304255000
H	1.867290000	13.001142000	0.966657000
H	0.793706000	13.463916000	2.306103000
H	0.270096000	13.714296000	0.630122000
C	0.764130000	16.143006000	1.883920000
H	-0.127374000	16.185502000	1.249898000
H	0.452573000	15.854512000	2.891353000
H	1.211579000	17.138620000	1.937224000
C	4.172845000	18.978147000	0.870744000
H	3.634457000	18.613606000	-0.010095000
H	3.480816000	19.025083000	1.715507000
H	4.554379000	19.981369000	0.649256000
C	6.061822000	18.524468000	2.458214000

H	5.366135000	18.617085000	3.295374000
H	6.848020000	17.820467000	2.744531000
H	6.519551000	19.501878000	2.268520000
C	6.278016000	17.881547000	0.041885000
H	7.084427000	17.186691000	0.296156000
H	5.746629000	17.484004000	-0.828260000
H	6.720025000	18.847656000	-0.225529000

4(s=0)

Ce	2.126087000	17.861751000	5.556600000
P	1.619308000	21.639503000	4.587759000
Si	4.363026000	18.865900000	8.235412000
Si	-1.399529000	17.331479000	5.729312000
Si	3.852571000	16.437783000	2.768089000
O	-1.602673000	17.462529000	7.393856000
O	2.829299000	15.269791000	2.127806000
O	3.173192000	17.695562000	3.549846000
O	-0.116030000	18.085040000	5.090951000
O	-2.875672000	17.898562000	5.109943000
O	4.740412000	16.921406000	1.403940000
O	1.577449000	20.318950000	5.376482000
O	5.831400000	18.042132000	8.259309000
O	4.754883000	20.370391000	8.918747000
O	3.667497000	19.007860000	6.780661000
C	1.092491000	15.272495000	5.977617000
C	3.548859000	15.472704000	5.870428000
C	-0.165553000	14.734229000	5.412882000
C	-1.358706000	15.488216000	5.363241000
C	1.102957000	15.869535000	7.227278000
H	0.168679000	15.990734000	7.762773000
C	2.286879000	15.221245000	5.207498000
H	2.279674000	14.748334000	4.234482000
C	3.277639000	17.988319000	9.490408000
C	-2.510033000	14.874482000	4.851052000
H	-3.425599000	15.457827000	4.803168000
C	1.429190000	16.533137000	10.114377000
H	0.729175000	15.742657000	9.859255000
C	2.354744000	16.965035000	9.139914000
C	-0.151006000	13.424099000	4.913156000
H	0.780476000	12.865588000	4.943074000
C	-1.305515000	12.839313000	4.403277000
H	-1.274192000	11.820103000	4.026198000
C	1.418493000	17.069936000	11.394322000
H	0.692852000	16.709573000	12.120313000

C	7.949273000	17.123884000	7.820879000
H	8.142472000	17.097261000	8.897778000
H	8.902556000	17.229915000	7.291868000
H	7.493487000	16.176949000	7.522009000
C	-1.603959000	18.633762000	8.209595000
C	6.284680000	15.103372000	3.276446000
H	6.457978000	15.337752000	2.229821000
C	-2.678495000	19.615005000	7.740960000
H	-3.646590000	19.113162000	7.665645000
H	-2.429881000	20.013633000	6.756009000
H	-2.760578000	20.451930000	8.443825000
C	2.343728000	18.051936000	11.751861000
H	2.345388000	18.473701000	12.753605000
C	-1.919899000	18.143986000	9.621101000
H	-1.949474000	18.981217000	10.326554000
H	-1.149048000	17.444977000	9.953001000
H	-2.888979000	17.635455000	9.633318000
C	7.289307000	14.492571000	4.024255000
H	8.238791000	14.236558000	3.560816000
C	-3.061830000	18.571326000	3.870787000
C	-0.231463000	19.302510000	8.174867000
H	0.013878000	19.622552000	7.158596000
H	0.544538000	18.618912000	8.528157000
H	-0.214762000	20.180673000	8.828679000
C	7.637176000	19.610803000	7.900267000
H	6.959664000	20.437583000	7.677754000
H	8.583794000	19.770621000	7.371247000
H	7.827036000	19.617654000	8.977581000
C	4.008989000	21.577225000	8.837196000
C	-2.346837000	17.832423000	2.741835000
H	-2.513291000	18.326809000	1.778243000
H	-2.703613000	16.800856000	2.673553000
H	-1.275864000	17.809583000	2.946569000
C	2.506315000	21.326515000	8.701480000
H	2.288177000	20.814153000	7.761003000
H	1.959275000	22.276867000	8.723931000
H	2.147584000	20.705493000	9.526161000
C	5.438102000	18.149000000	1.236436000
C	-2.518327000	19.997813000	3.992919000
H	-1.478645000	19.941999000	4.325766000
H	-3.097723000	20.564413000	4.728600000
H	-2.569511000	20.523787000	3.032396000
C	4.515376000	22.357367000	7.623803000
H	5.587044000	22.558846000	7.717867000

H	3.990722000	23.314592000	7.512925000
H	4.354430000	21.750758000	6.731681000
C	-4.569649000	18.590445000	3.628944000
H	-4.814686000	19.133694000	2.709545000
H	-5.077133000	19.072947000	4.469802000
H	-4.949604000	17.567851000	3.540979000
C	4.302960000	22.341130000	10.128120000
H	3.924231000	21.781372000	10.988561000
H	3.829225000	23.329142000	10.120275000
H	5.383130000	22.467754000	10.249356000
C	4.823406000	15.155631000	5.200645000
C	3.543924000	16.015855000	7.142714000
H	4.489282000	16.249163000	7.623648000
C	1.685024000	15.423509000	1.292012000
C	2.331881000	16.361170000	7.810318000
C	5.838457000	14.535256000	5.946241000
H	5.647032000	14.293101000	6.987721000
C	-2.496505000	13.564134000	4.379477000
H	-3.403967000	13.116042000	3.981988000
C	7.063367000	14.215775000	5.370894000
H	7.834155000	13.740020000	5.972219000
C	3.257639000	18.493562000	10.795547000
H	3.960586000	19.282929000	11.049197000
C	7.007663000	18.279595000	7.486354000
C	5.049983000	15.454387000	3.837786000
C	6.687672000	18.279289000	5.992535000
H	6.214580000	17.340252000	5.699271000
H	7.604097000	18.401135000	5.405174000
H	5.999876000	19.090406000	5.747750000
C	3.335803000	22.147255000	4.132466000
H	3.296978000	22.634776000	3.152023000
H	3.647898000	22.899104000	4.864705000
C	4.272880000	20.945773000	4.147460000
H	3.971695000	20.193972000	3.419008000
H	4.254527000	20.446300000	5.120717000
H	5.297017000	21.254949000	3.919715000
C	0.624636000	21.545620000	3.039804000
H	-0.411761000	21.757651000	3.318736000
H	0.960704000	22.347988000	2.372847000
C	0.731093000	20.162958000	2.406274000
H	0.417173000	19.399959000	3.122930000
H	1.753896000	19.931184000	2.102271000
H	0.088811000	20.092990000	1.523553000
C	0.927494000	23.026229000	5.577463000

H	1.667300000	23.224422000	6.360037000
H	0.882115000	23.909983000	4.929115000
C	-0.425542000	22.680417000	6.189094000
H	-0.340641000	21.789841000	6.813867000
H	-1.180851000	22.476879000	5.424510000
H	-0.791102000	23.504395000	6.809585000
C	2.127761000	15.848593000	-0.108601000
H	2.841044000	15.124273000	-0.512571000
H	1.266307000	15.913764000	-0.783032000
H	2.626054000	16.819750000	-0.070856000
C	1.024720000	14.046488000	1.250065000
H	1.737054000	13.300550000	0.884200000
H	0.698314000	13.757428000	2.252696000
H	0.149338000	14.052448000	0.591826000
C	0.719693000	16.443949000	1.885663000
H	-0.188037000	16.507191000	1.277722000
H	0.436428000	16.160176000	2.902750000
H	1.183815000	17.431149000	1.933072000
C	4.415094000	19.227314000	0.872814000
H	3.934196000	18.982751000	-0.079843000
H	3.647622000	19.246229000	1.648377000
H	4.875545000	20.218111000	0.790586000
C	6.205420000	18.520415000	2.505295000
H	5.521079000	18.588171000	3.352952000
H	6.950428000	17.755368000	2.737833000
H	6.716474000	19.482054000	2.388479000
C	6.410021000	17.926288000	0.079045000
H	7.131051000	17.145060000	0.338685000
H	5.863370000	17.605151000	-0.812730000
H	6.959961000	18.844499000	-0.154934000

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Ce	6.764110000	9.543181000	22.019623000
K	8.129413000	7.531060000	19.102107000
Si	6.087585000	11.851294000	24.670591000
Si	8.710653000	10.800276000	19.181179000
Si	5.595683000	6.315158000	20.987640000
O	10.333804000	11.045155000	18.746399000
O	8.154765000	9.845382000	17.880214000
C	11.943516000	9.763332000	19.972846000
H	12.250278000	9.239775000	19.063194000
H	12.798633000	9.798390000	20.656618000
H	11.133781000	9.203135000	20.447527000
C	3.635434000	10.739299000	23.486872000

C	2.348399000	10.195217000	23.640795000
H	1.869199000	9.747355000	22.775101000
C	1.676564000	10.253882000	24.853961000
H	0.673453000	9.843522000	24.937037000
C	2.292606000	10.839377000	25.960518000
H	1.783090000	10.878362000	26.919253000
C	3.583342000	11.344106000	25.833759000
H	4.086848000	11.735191000	26.712609000
C	4.284594000	11.305645000	24.616372000
O	6.415496000	11.747743000	26.318697000
C	4.776825000	9.396006000	20.093632000
C	3.434698000	5.339178000	22.542547000
C	11.447139000	11.167012000	19.624688000
C	7.511629000	11.970256000	28.390026000
H	8.415641000	11.766242000	28.972931000
H	7.317416000	13.046829000	28.410521000
H	6.667478000	11.462322000	28.865107000
C	5.455794000	8.055629000	24.795647000
H	4.722953000	7.490810000	25.376865000
H	5.609051000	9.016399000	25.289215000
H	5.005065000	8.211607000	23.808134000
O	9.241495000	5.754376000	17.373414000
C	8.496780000	11.510997000	16.116406000
H	8.529575000	11.635622000	15.029269000
H	7.684064000	12.122319000	16.515691000
H	9.440092000	11.872744000	16.533793000
C	2.332293000	6.387042000	22.403780000
H	1.348658000	5.946182000	22.596600000
H	2.493333000	7.201585000	23.115572000
H	2.330656000	6.802175000	21.391597000
C	5.621255000	14.671752000	24.613935000
C	4.450720000	8.292660000	19.161994000
C	4.621075000	6.921984000	19.483175000
C	4.236621000	5.970101000	18.522726000
H	4.403894000	4.919591000	18.739175000
C	3.701312000	6.331689000	17.288949000
H	3.409842000	5.565687000	16.575373000
C	3.562477000	7.681636000	16.974214000
H	3.157430000	7.984646000	16.012322000
C	3.932041000	8.646087000	17.905551000
H	3.804576000	9.701162000	17.682933000
O	6.193464000	4.855522000	20.334877000
C	6.488907000	15.823566000	24.106024000
H	7.479788000	15.783238000	24.572363000

H	6.038328000	16.792861000	24.340232000
C	5.494580000	14.736713000	26.134017000
H	5.044642000	15.688236000	26.435330000
H	4.868678000	13.924617000	26.509755000
H	6.477285000	14.647370000	26.604294000
C	8.288683000	10.040979000	16.467941000
C	6.743295000	7.275644000	24.689631000
H	7.123274000	6.992173000	25.682254000
H	6.583368000	6.370424000	24.093365000
O	6.306387000	13.484023000	24.206598000
O	7.176731000	11.073067000	23.755874000
O	8.547610000	9.856619000	20.501788000
O	7.725243000	8.096470000	24.055076000
C	5.822604000	11.616195000	20.495840000
O	6.835978000	7.276485000	21.379782000
O	4.699918000	5.977373000	22.362564000
C	4.999051000	11.703449000	21.676772000
H	5.034166000	12.608899000	22.272631000
C	5.590445000	10.426895000	19.676407000
H	6.025498000	10.390824000	18.683928000
C	4.282759000	9.353640000	21.452610000
H	3.538735000	8.613966000	21.709436000
C	12.510691000	11.942732000	18.851431000
H	12.735203000	11.431310000	17.910872000
H	12.146303000	12.947081000	18.614793000
H	13.435779000	12.033012000	19.430226000
C	8.572811000	4.582164000	20.642999000
H	9.355717000	3.919788000	21.027049000
H	8.747465000	4.728359000	19.572526000
H	8.643844000	5.544299000	21.158480000
C	6.687080000	12.676372000	20.088377000
C	7.907389000	12.469081000	19.332989000
C	8.660338000	13.584639000	18.935085000
H	9.578778000	13.407299000	18.379707000
C	8.312213000	14.896876000	19.257657000
H	8.907415000	15.735125000	18.908922000
C	7.152591000	15.101009000	20.033652000
H	6.843777000	16.111561000	20.295094000
C	6.376580000	14.032578000	20.441017000
H	5.456689000	14.227905000	20.983553000
C	4.285530000	10.636729000	22.170283000
C	8.954063000	7.423638000	23.837047000
H	9.304354000	7.003216000	24.791749000
H	8.790056000	6.595938000	23.134007000

C	8.806109000	12.232377000	26.257283000
H	8.927927000	11.836352000	25.246070000
H	8.588840000	13.303186000	26.198405000
H	9.743307000	12.095019000	26.806123000
C	9.959405000	8.417618000	23.291430000
H	10.936684000	7.939000000	23.174750000
H	9.662142000	8.807426000	22.311411000
H	10.065726000	9.262240000	23.978892000
C	7.665205000	11.485300000	26.950467000
C	6.975250000	3.754160000	22.376668000
H	7.732027000	3.062807000	22.761603000
H	7.054096000	4.695047000	22.925621000
H	5.988281000	3.331091000	22.574195000
C	4.241217000	14.722290000	23.959763000
H	4.333918000	14.711785000	22.870326000
H	3.639558000	13.861726000	24.261092000
H	3.711747000	15.636095000	24.248179000
C	3.214172000	4.210562000	21.535993000
H	2.279376000	3.686485000	21.758893000
H	3.144154000	4.604838000	20.519993000
H	4.033591000	3.489151000	21.568412000
C	7.929222000	9.980649000	26.905909000
H	7.986590000	9.646456000	25.866781000
H	8.865471000	9.729239000	27.417100000
H	7.112215000	9.445635000	27.399681000
C	3.458272000	4.778950000	23.963526000
H	2.512866000	4.283642000	24.205658000
H	4.270542000	4.054844000	24.073261000
H	3.620392000	5.587063000	24.681256000
C	7.038132000	2.669122000	20.118279000
H	7.775261000	1.933305000	20.455441000
H	6.036603000	2.255678000	20.267969000
H	7.179335000	2.837454000	19.046198000
C	7.182017000	3.985224000	20.880291000
O	10.752017000	14.104592000	23.474596000
C	11.640586000	13.296902000	24.235322000
H	11.116559000	12.348884000	24.388521000
H	12.542618000	13.084254000	23.641330000
C	11.371300000	15.232826000	22.871643000
H	11.829640000	15.869080000	23.640744000
H	12.174096000	14.889185000	22.200126000
C	10.326200000	16.012065000	22.103748000
H	10.772412000	16.914029000	21.674451000
H	9.903187000	15.431342000	21.277283000

H	9.511699000	16.322649000	22.765849000
K	8.387720000	13.125904000	22.592382000
C	12.009795000	13.908693000	25.576355000
H	12.607131000	13.198462000	26.156836000
H	12.599991000	14.822580000	25.464853000
H	11.107477000	14.144726000	26.146063000
C	10.639763000	5.569259000	17.235983000
H	10.896608000	4.521357000	17.456285000
H	10.939483000	5.774291000	16.196612000
C	11.344669000	6.507845000	18.191012000
H	12.429399000	6.405646000	18.097514000
H	11.086077000	7.547574000	17.973869000
H	11.076223000	6.284820000	19.228836000
C	7.008895000	5.133220000	16.821447000
H	6.392277000	4.447236000	16.234026000
H	6.749716000	4.993700000	17.875126000
H	6.734371000	6.150660000	16.527825000
C	8.475371000	4.863351000	16.574352000
H	8.735469000	5.006793000	15.514219000
H	8.731356000	3.825934000	16.841892000
C	6.989641000	9.527930000	15.850201000
H	7.028927000	9.572146000	14.757127000
H	6.803076000	8.490998000	16.146856000
H	6.143074000	10.126976000	16.195496000
C	9.482963000	9.209306000	15.997709000
H	9.640823000	9.319594000	14.919661000
H	10.381787000	9.544073000	16.522931000
H	9.318916000	8.147285000	16.210593000
H	6.606603000	15.753183000	23.019331000
C	11.080902000	11.919332000	20.905318000
H	10.344464000	11.337814000	21.468544000
H	11.966003000	12.062278000	21.531878000
H	10.665954000	12.899715000	20.656080000

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Ce	6.770871000	9.544636000	21.969417000
K	7.983855000	7.530593000	19.049839000
Si	6.175191000	11.808996000	24.644425000
Si	8.730460000	10.806540000	19.190921000
Si	5.468944000	6.315492000	20.970904000
O	10.351089000	11.107150000	18.792973000
O	8.202897000	9.872845000	17.869067000
C	11.928302000	9.756557000	19.993236000
H	12.235332000	9.257331000	19.070025000

H	12.777567000	9.756470000	20.684941000
H	11.105283000	9.194775000	20.441798000
C	3.719415000	10.643639000	23.503225000
C	2.459824000	10.039256000	23.718104000
H	1.930698000	9.632810000	22.861533000
C	1.868682000	9.998168000	24.969757000
H	0.891736000	9.535597000	25.087320000
C	2.517037000	10.568240000	26.069206000
H	2.064110000	10.543427000	27.055993000
C	3.765158000	11.156371000	25.882209000
H	4.299474000	11.541692000	26.745466000
C	4.395204000	11.212621000	24.627951000
O	6.567265000	11.725763000	26.280934000
C	4.725342000	9.416593000	20.038679000
C	3.303023000	5.386564000	22.536330000
C	11.459356000	11.178186000	19.684462000
C	7.735818000	11.939561000	28.312248000
H	8.653114000	11.717902000	28.867443000
H	7.568692000	13.020801000	28.329170000
H	6.895398000	11.457059000	28.819287000
C	5.437935000	7.998894000	24.852072000
H	4.728710000	7.409103000	25.437267000
H	5.611034000	8.939136000	25.376835000
H	4.949753000	8.203165000	23.894413000
O	9.183433000	5.726644000	17.433252000
C	8.591318000	11.545583000	16.123393000
H	8.672036000	11.674530000	15.039457000
H	7.744575000	12.135195000	16.483187000
H	9.504721000	11.929024000	16.584812000
C	2.207926000	6.439886000	22.387413000
H	1.220067000	6.007901000	22.578746000
H	2.373091000	7.254735000	23.097905000
H	2.212896000	6.849524000	21.372734000
C	5.622540000	14.609419000	24.614420000
C	4.445469000	8.311993000	19.114173000
C	4.526114000	6.929751000	19.462077000
C	4.154118000	5.981097000	18.491700000
H	4.249742000	4.926950000	18.735494000
C	3.742552000	6.340017000	17.212039000
H	3.460481000	5.576711000	16.492293000
C	3.735394000	7.693377000	16.856423000
H	3.437720000	7.997286000	15.856016000
C	4.085745000	8.654478000	17.792281000
H	4.043807000	9.708190000	17.531713000

O	6.068979000	4.846550000	20.349614000
C	6.436728000	15.800205000	24.107606000
H	7.435506000	15.793767000	24.558698000
H	5.952279000	16.748003000	24.361163000
C	5.512083000	14.655677000	26.136319000
H	5.030877000	15.587048000	26.452153000
H	4.919904000	13.817562000	26.509779000
H	6.503057000	14.596652000	26.594055000
C	8.402480000	10.070180000	16.462232000
C	6.717670000	7.226096000	24.662009000
H	7.133731000	6.902019000	25.627537000
H	6.535816000	6.346346000	24.035382000
O	6.351694000	13.453429000	24.189269000
O	7.260354000	11.053396000	23.697485000
O	8.572985000	9.848082000	20.501100000
O	7.679147000	8.070262000	24.026706000
C	5.759640000	11.640469000	20.429202000
O	6.706406000	7.285104000	21.376100000
O	4.571860000	6.021815000	22.357794000
C	5.068952000	11.706271000	21.673985000
H	5.198381000	12.575270000	22.304876000
C	5.593595000	10.470366000	19.631855000
H	6.074441000	10.413848000	18.663096000
C	4.124332000	9.472542000	21.322840000
H	3.521462000	8.639535000	21.659797000
C	12.542735000	11.958388000	18.944285000
H	12.769013000	11.470576000	17.991809000
H	12.198304000	12.975464000	18.732888000
H	13.462724000	12.016271000	19.534973000
C	8.445218000	4.590988000	20.680120000
H	9.230327000	3.939375000	21.077931000
H	8.631171000	4.733413000	19.611180000
H	8.497858000	5.557809000	21.189013000
C	6.656273000	12.703192000	20.023300000
C	7.905738000	12.479351000	19.338264000
C	8.665098000	13.596606000	18.951657000
H	9.611138000	13.421099000	18.445757000
C	8.278688000	14.909171000	19.225048000
H	8.884265000	15.745769000	18.889380000
C	7.083182000	15.123605000	19.940809000
H	6.754988000	16.135539000	20.167217000
C	6.305389000	14.049028000	20.333597000
H	5.362948000	14.226723000	20.842779000
C	4.276915000	10.622732000	22.154066000

C	8.924480000	7.422857000	23.826901000
H	9.268210000	7.012569000	24.788518000
H	8.789272000	6.586099000	23.127797000
C	8.961002000	12.158785000	26.135313000
H	9.042243000	11.749865000	25.124958000
H	8.754209000	13.231926000	26.073519000
H	9.913689000	12.014835000	26.655387000
C	9.923652000	8.429645000	23.294120000
H	10.911920000	7.966932000	23.209364000
H	9.646515000	8.801700000	22.301973000
H	9.995919000	9.284354000	23.973068000
C	7.829520000	11.439167000	26.872691000
C	6.834888000	3.741925000	22.393861000
H	7.585953000	3.046995000	22.783500000
H	6.909930000	4.679219000	22.948837000
H	5.844939000	3.319386000	22.577619000
C	4.234066000	14.611040000	23.976317000
H	4.313792000	14.597517000	22.885829000
H	3.665629000	13.731371000	24.286496000
H	3.678347000	15.507851000	24.269047000
C	3.082215000	4.254447000	21.534020000
H	2.141285000	3.739473000	21.752331000
H	3.022984000	4.644427000	20.515582000
H	3.894982000	3.526043000	21.576522000
C	8.058698000	9.929018000	26.832789000
H	8.054185000	9.584407000	25.795738000
H	9.013691000	9.661646000	27.299342000
H	7.255889000	9.417058000	27.372144000
C	3.317730000	4.834275000	23.960197000
H	2.372423000	4.336090000	24.196955000
H	4.132179000	4.114201000	24.079925000
H	3.469766000	5.646936000	24.674902000
C	6.930701000	2.667914000	20.131890000
H	7.671473000	1.936813000	20.471373000
H	5.931565000	2.245239000	20.271458000
H	7.078440000	2.843152000	19.061844000
C	7.057508000	3.981401000	20.901499000
O	10.722713000	14.284023000	23.441327000
C	11.670730000	13.527251000	24.183660000
H	11.218522000	12.539991000	24.315422000
H	12.584248000	13.396660000	23.583418000
C	11.254644000	15.471461000	22.870447000
H	11.650753000	16.127013000	23.657627000
H	12.090533000	15.208992000	22.202746000

C	10.157491000	16.178034000	22.105155000
H	10.533139000	17.118772000	21.692113000
H	9.790475000	15.574854000	21.268591000
H	9.315664000	16.412472000	22.763955000
K	8.401658000	13.180997000	22.574719000
C	11.998608000	14.133298000	25.537875000
H	12.650013000	13.455663000	26.098794000
H	12.518632000	15.091066000	25.447768000
H	11.084296000	14.286342000	26.116628000
C	10.582520000	5.504849000	17.389495000
H	10.798250000	4.460327000	17.663077000
H	10.950779000	5.663779000	16.364200000
C	11.250616000	6.460848000	18.353963000
H	12.336542000	6.334913000	18.327714000
H	11.027137000	7.497814000	18.090084000
H	10.917310000	6.277371000	19.380576000
C	6.968612000	5.097499000	16.816971000
H	6.371382000	4.399659000	16.223732000
H	6.665001000	4.985648000	17.862039000
H	6.709115000	6.107599000	16.486336000
C	8.442077000	4.812148000	16.636261000
H	8.745065000	4.915276000	15.582896000
H	8.679797000	3.783882000	16.951367000
C	7.146907000	9.529104000	15.782926000
H	7.232334000	9.594564000	14.693688000
H	6.979309000	8.481090000	16.050183000
H	6.268616000	10.095976000	16.101515000
C	9.635751000	9.265568000	16.051370000
H	9.840411000	9.378294000	14.981556000
H	10.501949000	9.618681000	16.617249000
H	9.482810000	8.200657000	16.257363000
H	6.538788000	15.750131000	23.017825000
C	11.089393000	11.900583000	20.980943000
H	10.332617000	11.319239000	21.516796000
H	11.966513000	12.008178000	21.625322000
H	10.701848000	12.897456000	20.752322000

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Ce	6.817696000	9.505182000	22.033401000
Si	6.142181000	11.755945000	24.713821000
Si	8.691866000	10.758108000	19.322996000
Si	5.252163000	6.347642000	21.213317000
O	10.305934000	11.114006000	18.877739000
O	8.147436000	9.779444000	18.059191000

C	11.849856000	9.834943000	20.191905000
H	12.166543000	9.275335000	19.305089000
H	12.685962000	9.874657000	20.900639000
H	11.011118000	9.308332000	20.651585000
C	3.727945000	10.522673000	23.599395000
C	2.517302000	9.816878000	23.837241000
H	2.017513000	9.356858000	22.989362000
C	1.934915000	9.744472000	25.088826000
H	0.994908000	9.207477000	25.209808000
C	2.540796000	10.370048000	26.190188000
H	2.097263000	10.311699000	27.181449000
C	3.751399000	11.035785000	25.988759000
H	4.274668000	11.451123000	26.846786000
C	4.370130000	11.133784000	24.735486000
O	6.552435000	11.774828000	26.373728000
C	4.690411000	9.391010000	20.084515000
C	2.884449000	5.580284000	22.591223000
C	11.389428000	11.238570000	19.790265000
C	7.840749000	12.087064000	28.314702000
H	8.808202000	11.933426000	28.807687000
H	7.604812000	13.156147000	28.329892000
H	7.068443000	11.559433000	28.883998000
C	5.612337000	7.835280000	24.967904000
H	4.925504000	7.177402000	25.507329000
H	5.751276000	8.750807000	25.545073000
H	5.117274000	8.080365000	24.025391000
C	8.721339000	11.153336000	16.133107000
H	8.904916000	11.117211000	15.052265000
H	7.833813000	11.764922000	16.319986000
H	9.575928000	11.631044000	16.619395000
C	1.875562000	6.175754000	21.604521000
H	0.887176000	5.722576000	21.748252000
H	1.787528000	7.254702000	21.758066000
H	2.193868000	6.011635000	20.572567000
C	5.565950000	14.524630000	24.591682000
C	4.470474000	8.270600000	19.177948000
C	4.489301000	6.904046000	19.592239000
C	4.166193000	5.914712000	18.651768000
H	4.206250000	4.874541000	18.968937000
C	3.861404000	6.208766000	17.323901000
H	3.617888000	5.414170000	16.621974000
C	3.914796000	7.547451000	16.905498000
H	3.705298000	7.807804000	15.869232000
C	4.216227000	8.547017000	17.814124000

H	4.221990000	9.585968000	17.495144000
O	5.717693000	4.727218000	20.931260000
C	6.351975000	15.700761000	24.007153000
H	7.349495000	15.740785000	24.456703000
H	5.842264000	16.654609000	24.189918000
C	5.477434000	14.657310000	26.115438000
H	4.989988000	15.601497000	26.388741000
H	4.906563000	13.829855000	26.543550000
H	6.477650000	14.633333000	26.556388000
C	8.514081000	9.743413000	16.693958000
C	6.924879000	7.125577000	24.730286000
H	7.353742000	6.766056000	25.681534000
H	6.786093000	6.273646000	24.053638000
O	6.295027000	13.374742000	24.210667000
O	7.174505000	10.859006000	23.862091000
O	8.623311000	9.929435000	20.713102000
O	7.847590000	8.040700000	24.149659000
C	5.714731000	11.602826000	20.516188000
O	6.495606000	7.240033000	21.712921000
O	4.143027000	6.216819000	22.483993000
C	5.053160000	11.642709000	21.779103000
H	5.236199000	12.489513000	22.425608000
C	5.521497000	10.467971000	19.682192000
H	6.017562000	10.420358000	18.720697000
C	4.117017000	9.413943000	21.390013000
H	3.567474000	8.549202000	21.739404000
C	12.492815000	11.964623000	19.018856000
H	12.739363000	11.409734000	18.107392000
H	12.151264000	12.963923000	18.730294000
H	13.400010000	12.066562000	19.625745000
C	7.466413000	5.267095000	19.293702000
H	8.445872000	4.938681000	18.925905000
H	6.753813000	5.247325000	18.465182000
H	7.555031000	6.299763000	19.642071000
C	6.611764000	12.672226000	20.101563000
C	7.835974000	12.434660000	19.395390000
C	8.570250000	13.542182000	18.948710000
H	9.506399000	13.357967000	18.426786000
C	8.181331000	14.858122000	19.197959000
H	8.783056000	15.690305000	18.839012000
C	7.021916000	15.082163000	19.954352000
H	6.702512000	16.097696000	20.183874000
C	6.263763000	14.011913000	20.395977000
H	5.345749000	14.191964000	20.947792000

C	4.265352000	10.552443000	22.249245000
C	9.153244000	7.519902000	24.024348000
H	9.488777000	7.155971000	25.011144000
H	9.153220000	6.660628000	23.337148000
C	8.901036000	12.349302000	26.053748000
H	8.899816000	11.981616000	25.024194000
H	8.651331000	13.414542000	26.035618000
H	9.903516000	12.228223000	26.482594000
C	10.068512000	8.618683000	23.523539000
H	11.100334000	8.254973000	23.469854000
H	9.780591000	8.958563000	22.523927000
H	10.028588000	9.480348000	24.194953000
C	7.864920000	11.573334000	26.873635000
C	8.000903000	4.423993000	21.592058000
H	9.002694000	4.107465000	21.276935000
H	8.036111000	5.456733000	21.946990000
H	7.667195000	3.780965000	22.413788000
C	4.153492000	14.490053000	23.997112000
H	4.200251000	14.419768000	22.907183000
H	3.606089000	13.619055000	24.366396000
H	3.598882000	15.398212000	24.263724000
C	3.030161000	4.074817000	22.352362000
H	2.072561000	3.561748000	22.504657000
H	3.384115000	3.880682000	21.337009000
H	3.771178000	3.659983000	23.041834000
C	8.183479000	10.076607000	26.842950000
H	8.112065000	9.717664000	25.813417000
H	9.188149000	9.873578000	27.235632000
H	7.454855000	9.529267000	27.450964000
C	2.423150000	5.848304000	24.025387000
H	1.433206000	5.415022000	24.211997000
H	3.136799000	5.412154000	24.731565000
H	2.383424000	6.926252000	24.207159000
C	6.845427000	2.921489000	19.934086000
H	7.799715000	2.522654000	19.570791000
H	6.479172000	2.280785000	20.743135000
H	6.118807000	2.889569000	19.115591000
C	6.999748000	4.357710000	20.436168000
C	7.354031000	9.053868000	15.975386000
H	7.578597000	8.902911000	14.912443000
H	7.146531000	8.087401000	16.441505000
H	6.446142000	9.656717000	16.062905000
C	9.797372000	8.918907000	16.555118000
H	10.099032000	8.821573000	15.504574000

H	10.596670000	9.405400000	17.119031000
H	9.636012000	7.919330000	16.970312000
H	6.476118000	15.555397000	22.930499000
C	10.996543000	12.047831000	21.029820000
H	10.201932000	11.535534000	21.577285000
H	11.860402000	12.175020000	21.692962000
H	10.624165000	13.034077000	20.739985000

5^{2-} (s=1/2)

Ce	6.696050000	9.531552000	22.081152000
Si	6.134444000	11.949544000	24.697411000
Si	8.668981000	10.756059000	19.488486000
Si	5.566511000	6.370199000	20.848412000
O	10.271909000	11.113164000	18.997619000
O	8.168511000	9.638810000	18.329525000
C	11.816586000	9.882250000	20.358543000
H	12.078359000	9.257789000	19.497622000
H	12.684264000	9.946126000	21.026758000
H	10.986558000	9.410413000	20.888256000
C	3.701100000	10.739091000	23.660672000
C	2.505079000	10.017844000	23.962686000
H	2.003864000	9.483316000	23.160559000
C	1.924096000	10.040549000	25.216446000
H	0.994498000	9.494725000	25.380068000
C	2.508809000	10.762450000	26.267947000
H	2.065397000	10.768400000	27.260985000
C	3.718362000	11.416312000	26.018104000
H	4.243262000	11.888244000	26.846265000
C	4.340580000	11.419945000	24.764642000
O	6.593931000	12.020651000	26.342476000
C	4.608640000	9.468016000	20.195341000
C	3.333075000	5.259316000	22.227971000
C	11.373225000	11.268193000	19.882506000
C	7.920143000	12.173978000	28.273624000
H	8.863954000	11.904647000	28.762631000
H	7.824904000	13.264853000	28.269265000
H	7.090863000	11.761746000	28.857929000
C	5.282769000	7.982144000	24.685014000
H	4.507982000	7.462925000	25.255473000
H	5.440724000	8.961745000	25.141948000
H	4.871845000	8.112573000	23.677572000
C	8.330136000	11.002195000	16.319964000
H	8.387018000	10.949620000	15.225851000
H	7.413098000	11.526943000	16.602232000

H	9.180681000	11.583978000	16.686763000
C	2.209048000	6.279962000	22.036553000
H	1.223614000	5.808929000	22.136994000
H	2.298831000	7.071242000	22.786698000
H	2.280061000	6.734988000	21.044702000
C	5.717732000	14.735456000	24.471561000
C	4.243432000	8.404431000	19.229741000
C	4.580761000	7.043766000	19.390686000
C	4.223415000	6.153011000	18.357343000
H	4.532873000	5.115602000	18.444573000
C	3.537182000	6.571689000	17.224348000
H	3.285100000	5.856019000	16.443993000
C	3.197063000	7.920288000	17.083612000
H	2.663766000	8.267051000	16.200889000
C	3.563863000	8.822261000	18.076070000
H	3.335838000	9.880070000	17.976307000
O	6.119727000	4.904917000	20.165701000
C	6.556686000	15.847746000	23.837748000
H	7.563309000	15.844396000	24.268296000
H	6.104322000	16.833827000	24.001070000
C	5.661957000	14.921529000	25.991265000
H	5.237608000	15.902483000	26.239838000
H	5.047196000	14.145306000	26.453458000
H	6.665389000	14.847219000	26.418657000
C	8.347174000	9.598424000	16.929931000
C	6.555706000	7.167734000	24.652005000
H	6.836783000	6.818673000	25.659908000
H	6.422495000	6.299294000	23.996062000
O	6.371593000	13.534015000	24.115741000
O	7.077250000	10.954447000	23.852865000
O	8.610439000	10.080699000	20.954646000
O	7.608013000	7.988518000	24.156502000
C	5.696598000	11.647645000	20.567495000
O	6.738580000	7.264856000	21.475934000
O	4.577928000	5.922351000	22.158515000
C	5.003692000	11.748815000	21.768048000
H	5.149775000	12.645195000	22.360380000
C	5.592861000	10.399081000	19.805896000
H	6.037463000	10.324235000	18.824860000
C	3.995856000	9.525408000	21.438368000
H	3.259170000	8.778167000	21.696385000
C	12.476913000	11.927290000	19.053089000
H	12.709126000	11.310208000	18.178450000
H	12.143629000	12.909022000	18.700970000

H	13.391235000	12.059586000	19.643361000
C	8.524390000	5.048561000	20.113613000
H	9.460015000	4.542186000	20.381079000
H	8.506859000	5.204934000	19.030338000
H	8.480181000	6.028719000	20.595150000
C	6.573257000	12.712753000	20.100837000
C	7.806819000	12.439661000	19.432186000
C	8.555885000	13.525791000	18.958604000
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C	8.156227000	14.850973000	19.126890000
H	8.763032000	15.664883000	18.735626000
C	6.970806000	15.111424000	19.822824000
H	6.636472000	16.136028000	19.978452000
C	6.197460000	14.060701000	20.289987000
H	5.251072000	14.264886000	20.782454000
C	4.239191000	10.687148000	22.330947000
C	8.803630000	7.275122000	23.903109000
H	9.073565000	6.693921000	24.801797000
H	8.633588000	6.575708000	23.074207000
C	8.992664000	12.247666000	26.003510000
H	8.929170000	11.867790000	24.980441000
H	8.893262000	13.337355000	25.972893000
H	9.973020000	11.993926000	26.425821000
C	9.892211000	8.269440000	23.556451000
H	10.834631000	7.743418000	23.368801000
H	9.637255000	8.836279000	22.655054000
H	10.038884000	8.980095000	24.374639000
C	7.864362000	11.637672000	26.841227000
C	7.325101000	3.969424000	22.045416000
H	8.218982000	3.407488000	22.341393000
H	7.317918000	4.924598000	22.573719000
H	6.436094000	3.407261000	22.347938000
C	4.295448000	14.760492000	23.899994000
H	4.324602000	14.682105000	22.809802000
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H	2.287675000	3.573150000	21.346832000
H	3.200115000	4.549052000	20.179290000
H	4.066870000	3.458285000	21.265454000
C	7.970184000	10.110080000	26.837962000
H	7.894039000	9.741684000	25.812244000
H	8.920258000	9.776265000	27.274959000
H	7.147954000	9.682607000	27.422188000

C	3.267486000	4.666667000	23.638288000
H	2.315323000	4.151994000	23.812898000
H	4.086253000	3.953791000	23.780127000
H	3.377853000	5.465110000	24.377021000
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H	8.167469000	2.297253000	19.987142000
H	6.388287000	2.315455000	20.073929000
H	7.214573000	3.081171000	18.703876000
C	7.305051000	4.223854000	20.536113000
C	7.179353000	8.768170000	16.391920000
H	7.263798000	8.613074000	15.309318000
H	7.154914000	7.796167000	16.892084000
H	6.228626000	9.264690000	16.605233000
C	9.683265000	8.910251000	16.633051000
H	9.852534000	8.811087000	15.553279000
H	10.492801000	9.495257000	17.076823000
H	9.688709000	7.913330000	17.084573000
H	6.650594000	15.664904000	22.763735000
C	11.015191000	12.153060000	21.080684000
H	10.210979000	11.690083000	21.657913000
H	11.888391000	12.291421000	21.729504000
H	10.668622000	13.133539000	20.742258000

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