Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information for:

Homoleptic Cerium Tris(dialkylamido)imidophosphorane Guanidinate Complexes

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General Considerations

Unless otherwise stated, all reagents were obtained from commercial suppliers, and the syntheses and manipulations were conducted under argon with exclusion of dioxygen (O_2) and H_2O using Schlenk techniques or in an inert atmosphere box (Vigor) under a dinitrogen (<0.1 ppm O_2/H_2O) atmosphere. All glassware was stored in an oven over-night (>8 h) at a temperature of ca. 160˚C prior to use. Celite and molecular sieves were dried under vacuum at a temperature >250 °C for a minimum of 24 h. d_8-THF was stored over 3 Å molecular sieves prior to use. Diethyl ether, *n*-pentane, *n*-hexane, benzene, toluene, and tetrahydrofuran (THF) were purged with UHP-grade argon (Airgas) and passed through columns containing Q-5 and molecular sieves in a solvent purification system (JC Meyer Solvent Systems). All solvents in the glovebox were stored in bottles over 3 Å molecular sieves. The reagents $CeCl_3(THF)_4$ and $K[NP(pip)_3]$ were prepared by published procedures.[1, 2] NMR spectra were obtained on a Bruker Avance III 400 MHz spectrometer at 298 K, unless otherwise noted. ^1H, $^{13}C\{^1H\}$, and $^{31}P\{^1H\}$ NMR chemical shifts are reported in δ, parts per million. All NMR samples were prepared in d_8-THF (unless otherwise noted) and ^1H NMR are references to the residual ^1H resonances of d_8-THF.[3] $^{13}C\{^1H\}$ NMR are referenced to the $^{13}C\{^1H\}$ resonance of the d_8-THF.[3] The peak position is listed, followed by the peak multiplicity, integration value, and proton assignment, where applicable. The multiplicity and shape are indicated by one or more of the following abbreviations: s (singlet); d (doublet); t (triplet); q (quartet); m (multiplet); br (broad). Elemental analyses were determined at Robertson Microlit Laboratories (Ledgewood, NJ) and University of California, Berkeley, Microanalytical Facility (Berkeley, CA). Infrared (IR) samples were taken on a Bruker ALPHA FTIR spectrometer from 400 to 4000 cm^{-1}. IR samples were prepared as Nujol mulls sandwiched between two KBr plates. The peaks are listed in wavenumber [cm^{-1}] and intensity by using the following abbreviations: vw (very weak); w (weak); m (medium); s (strong); vs (very strong); br (broad). UV/visible/NIR spectroscopy was performed in Teflon-valve sealed quartz cuvettes with a 1 cm path length on a Hitachi UH4150 UV-vis-NIR scanning spectrophotometer between 2400-200 nm.

Synthetic Procedures

Synthesis of $[K(THF)_2{}^{Cy}GNP(pip)_3]_2$ (1-K)

Inside a glovebox, 10 mL of THF was added to a 50 mL round-bottomed flask charged with N,N'-dicyclohexylcarbodiimide (0.699 g, 3.385 mmol, 1 equiv.) and a stir bar. A solution of $K[NP(pip)_3]$ (1.139 g, 3.385 mmol, 1 equiv.) in 15 mL of THF was then added to the flask and the reaction mixture was stirred for 24 hours. The mixture was filtered through a pipet packed with glass filter paper and Celite. The filtrate was reduced *in vacuo* to a residue and triturated three times with 4-6 mL of pentane. The residue was then extracted into approximately 20 mL of THF and filtered through pipet packed with glass filter paper and Celite. The filtrate was then concentrated *in vacuo* until saturated and placed in the freezer at −35 °C for 24 hours, during which time, colorless crystals formed. Decantation and removal of volatiles yielded the title compound in 89% yield (1.85 g). The product was recrystallized from THF at −35 °C to provide X-ray quality crystals. ^{1}H NMR (400.13 MHz, d_8-THF, 295 K): δ 3.62 (m, THF), 1.77 (m, THF), 3.21 (br, m, 2H, cyclohexyl methyne C-*H*, A), 3.16 (s, 12 H, piperidinyl methylene C-*H*, E), 1.62 (br, m, 8H, cyclohexyl methylene C-*H*, B), 1.54 (br, m, 6H, piperidinyl methylene C-*H*, G), 1.50 (br, m, 12H, piperidinyl methylene C-*H*, F), 1.33 (br, m, 12H cyclohexyl methylene C-*H*, C), 1.18 (br, m, 4H, cyclohexyl methylene C-*H*, D): the series of overlapped features from 1.62 ppm to 1.18 ppm integrates to 38 protons corresponding to methylenes of the ligand labeled B, C, D, F, and G as depicted in Figure S1. ^{31}P{^{1}H} NMR (161.98 MHz, d_8-THF, 295 K): δ -13.13 (br, s). ^{13}C{^{1}H} NMR (100.62 MHz, d_8-THF, 295 K): δ 55.41 (br, s, cyclohexyl methyne *C*-H, A), 47.07 (s, piperidinyl methylene *C*-H, E), 39.07 (br, s, cyclohexyl methylene *C*-H, D), 27.69 (d, piperidinyl methylene *C*-H, F), 27.18 (br, s, cyclohexyl methylene *C*-H, B; and cyclohexyl methylene *C*-H, C), 26.08 (s, piperidinyl methylene *C*-H, G). The N=*C*=N guanidinate carbon ^{13}C{^{1}H} peak is not observed. IR (cm^{-1}): ν 1582 (vw), 1337 (s), 1298 (w), 1259 (m), 1157 (s), 1123 (s), 1062 (vs), 1027(s), 988 (vw), 944 (vs), 885 (vw), 854 (vw), 835 (vw), 800 (w), 660 (vw). Elem. Anal. Found (calculated) for $C_{36}H_{68}N_6PO_2K$: C 58.49 (62.50), H 9.17 (9.84), N 13.28 (13.67). Multiple burns varied significantly from calculated (at both Berkeley and Microlit) – as evidenced by the SC-XRD analysis the ligated THF's are loosely bound and introduce significant variability. ^{1}H and ^{13}C NMR suggest one THF per potassium remains after isolation under reduced pressure. Combustion analyses consistently provided low carbon on multiple burns.

Synthesis of $[Ce(^{Cy}GNP(pip)_3)_3]$ (1-Ce)

Inside a glovebox, 5 mL of THF and a stir bar were added to a 20 mL scintillation vial charged with $CeCl_3(THF)_4$ (0.139 g, 0.259 mmol, 1 equiv.). A solution of $[K(THF)_2{}^{Cy}GNP(pip)_3]$ (0.479 g, 0.697 mmol, 2.7 equiv.) in 10 mL of THF was added and the mixture allowed to stir for 32 hours. The mixture was filtered through a pipet packed with glass filter paper and Celite. The filtrate was reduced *in vacuo* to a residue and triturated three times with 2-3 mL of pentane. The residue was then extracted into approximately 15 mL of pentane and filtered through pipet packed with glass filter paper and Celite. The filtrate was then concentrated *in vacuo* until saturated and placed in the freezer at −35 °C for 24 hours, during which time, yellow-green crystals formed. Decantation and removal of volatiles yielded the title compound in 84% yield (0.322 g). The product was recrystallized from pentane at −35 °C to provide X-ray quality crystals.

This compound appears to exhibit dissymmetry, and the cyclohexyl ring protons appear to be diastereotopic. Compounded by the paramagnetic broadening arising from the $4f^1$ Ce^{3+} center, these effects result in broadening of several low intensity peaks into the baseline. ^{1}H NMR (400.13 MHz, d_8-THF, 295 K): δ 5.85 (s, 36H, piperidinyl methylene C-*H*, E), 2.72 (s, 36H, piperidinyl methylene C-*H*, F), 2.41 (s, 16H, piperidinyl methylene C-*H*, G), 0.29 (br, s, 12H cyclohexyl methylene C-*H*, $H_F + H_G$). The peaks at 11.20 (br-s), -0.73 (br-s), -1.36 (br-s), -4.34 (br-s) correspond to unassigned cyclohexyl protons. A total of 30 cyclohexyl protons are paramagnetically broadened to the baseline. ^{31}P{^{1}H} NMR (161.97 MHz, d_8-THF, 295 K): δ 0.84 (s). ^{13}C{^{1}H} NMR (100.62 MHz, d_8-THF, 295 K): δ 49.58 (s, piperidinyl methylene *C*-H, E), 29.04 (d, piperidinyl methylene *C*-H, F), 26.97 (br, s, piperidinyl methylene *C*-H, G), 23.89 (br, m, cyclohexyl methylene *C*-H, $H_F + H_G$). The peaks at δ 56.89 (s), 50.03 (br-m) , 34.89 (br-s), 32.12 (br-m), 29.36 (br-s), 27.62 (br-s), 23.38 (s) correspond to unassiged cyclohexyl methylene, methyne, and guanidinate carbons. IR (cm^{-1}): ν 1353 (vw), 1338 (vw), 1267 (s), 1235 (vw), 1214 (vs), 1186 (vw), 1161 (s), 1120 (s), 1061 (vs), 1026 (m), 991 (vw), 948 (vs), 896 (w), 886 (w), 853 (w), 833 (vw), 785 (s), 661 (m). Elem. Anal. Found (calculated) for $C_{84}H_{156}N_{18}P_3Ce$: C 61.09 (61.10), H 9.81 (9.52), N 14.92 (15.27).

Synthesis of [Ce(^{Cy}GNP(pip)$_3$)$_3$]BPh$_4$, 2-Ce

Inside a glovebox, 5 mL of Et_2O and a stir bar were added to a 20 mL scintillation vial charged with $AgBPh_4$ (0.032 g, 0.077 mmol, 1 equiv.). A solution of [Ce(^{Cy}GNP(pip)$_3$)$_3$] (0.128 g, 0.077 mmol, 1 equiv.) in 10 mL of Et_2O was added and the reaction mixture allowed to stir for 32 hours. The reaction mixture was placed in in the freezer at −35 °C for 4 hours. The mixture was then filtered through a fine porosity sintered-glass frit. The solid residue was washed three times with 2-3 mL of pentane. The residue was then extracted into approximately 20 mL of Et_2O and filtered again through a fine porosity sintered-glass frit. The filtrate was then concentrated *in vacuo* until saturated and placed in the freezer at −35 °C for 24 hours, during which time, dark blue crystals formed. Decantation and removal of volatiles yielded the title compound in 81% yield (0.123 g). The product was recrystallized from Et_2O at −35 °C to provide X-ray quality crystals. ^{1}H NMR (400.13 MHz, d_8-THF, 295 K): δ 3.38 (q,4 H, Et_2O-C*H*$_2$), 1.12 (t, 6 H, Et_2O-C*H*$_3$), δ 7.26 (m, 8 H, phenyl C-*H*, X), 6.83 (t, 8H, phenyl C-*H*, Y), 6.68 (t, 4 H, phenyl C-*H*, Z), 4.05 (m, 6 H, cyclohexyl methyne C-*H*, A), 3.10 (br, m, 36 H, piperidinyl methylene C-*H*, E) 1.88 (br, m, 24 H, cyclohexyl methylene C-*H*, B), 1.67 (br, m, 12H, cyclohexyl methylene C-*H*, D) 1.59 (br, m, 18H, cyclohexyl methylene C-*H*, G), 1.54 (br, m, 36H, piperidinyl methylene C-*H*, F), 1.29 (br, m; 24H, cyclohexyl methylene C-*H*, C): The series of overlapped features from 1.70 ppm to 1.16 ppm integrated to 90 protons corresponding to methylenes of the ligand labeled C, D, F, and G as shown in Figure S7. ^{1}H NMR indicates one molecule of residual Et_2O. ^{31}P{^{1}H} NMR (161.97 MHz, d_8-THF, 295 K): δ -1.03 (s). ^{13}C{^{1}H} NMR (100.62 MHz, d_8-THF, 295 K): δ 163. 01 (d, B-*C*, [BPh4]$^{1-}$, K), 137.03 (s, phenyl *C*-H, X), 125.37 (s, phenyl *C*-H, Y), 121.43 (s, phenyl *C*-H, Z), 100.78 (s, N=*C*=N guanidinate carbon., J), 57.94 (s, cyclohexyl methyne *C*-H, A), 47.00 (s, piperidinyl methylene *C*-H, E), 39.83 (s, cyclohexyl methylene *C*-H, B), 38.04 (s, cyclohexyl methylene *C*-H, D), 27.15 (d, piperidinyl methylene *C*-H, F), 26.82 (d, cyclohexyl methylene *C*-H, C), 25.46 (s, piperidinyl methylene *C*-H, G). ^{11}B NMR (128.38 MHz, d_8-THF, 295 K): δ -8.68 (s, [*B*Ph4]$^{1-}$). IR (cm^{-1}): ν 1579 (vw), 1261 (w), 1209 (m),

1156 (m), 1111 (m), 1059 (m), 1024 (w), 947 (s), 896 (vw), 833 (vw), 800 (m), 768 (m), 701 (vw), 659 (vw). Elem. Anal. Found (calculated) for $C_{112}H_{186}N_{18}P_3BOCe$ (including one Et_2O): C 64.35 (65.75), H 9.18 (9.17), N 11.85 (12.33). Combustion analyses consistently provided low carbon on multiple burns (at both UC-Berkeley and Microlit).

NMR Spectra of Reported Compounds

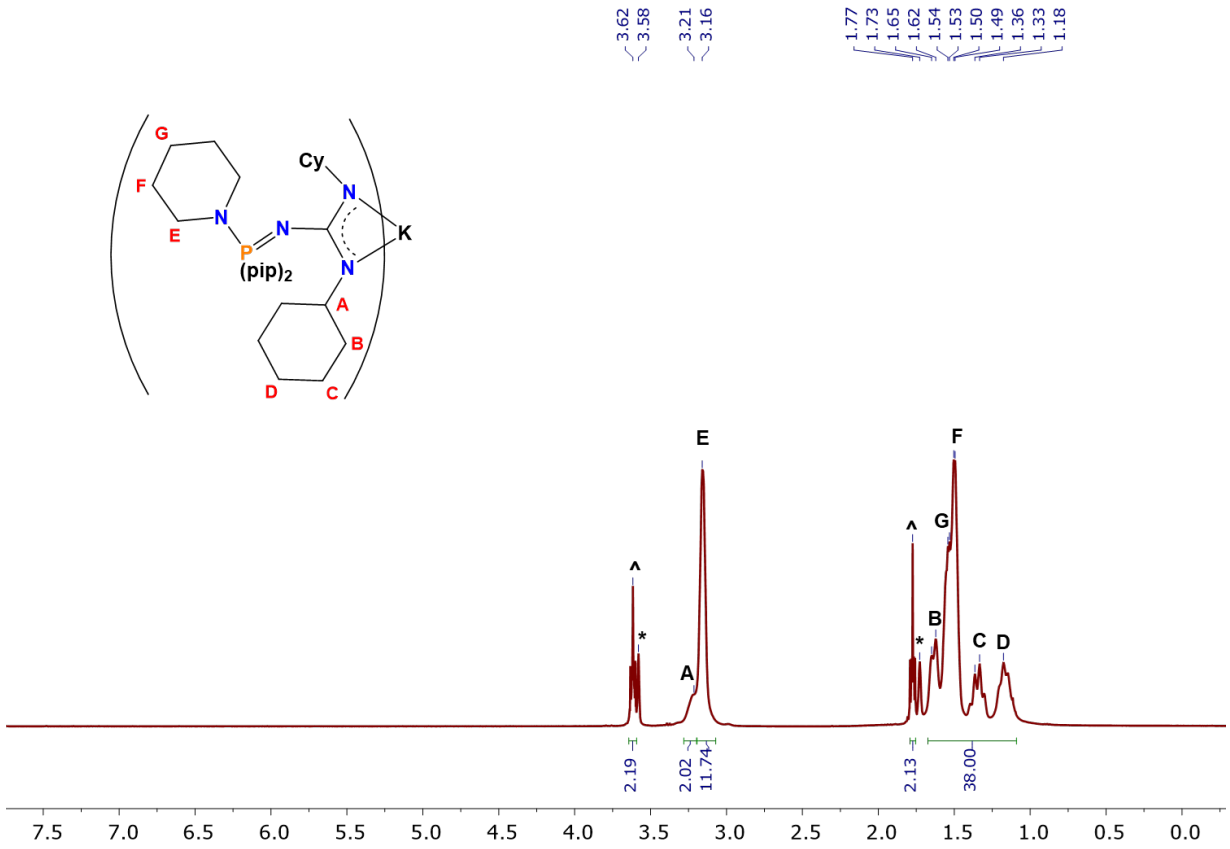

Figure S1. ^{1}H NMR of **1-K** (400.13 MHz, d_8-THF, 295 K). C_4D_7HO noted by *. Residual THF noted by ^.

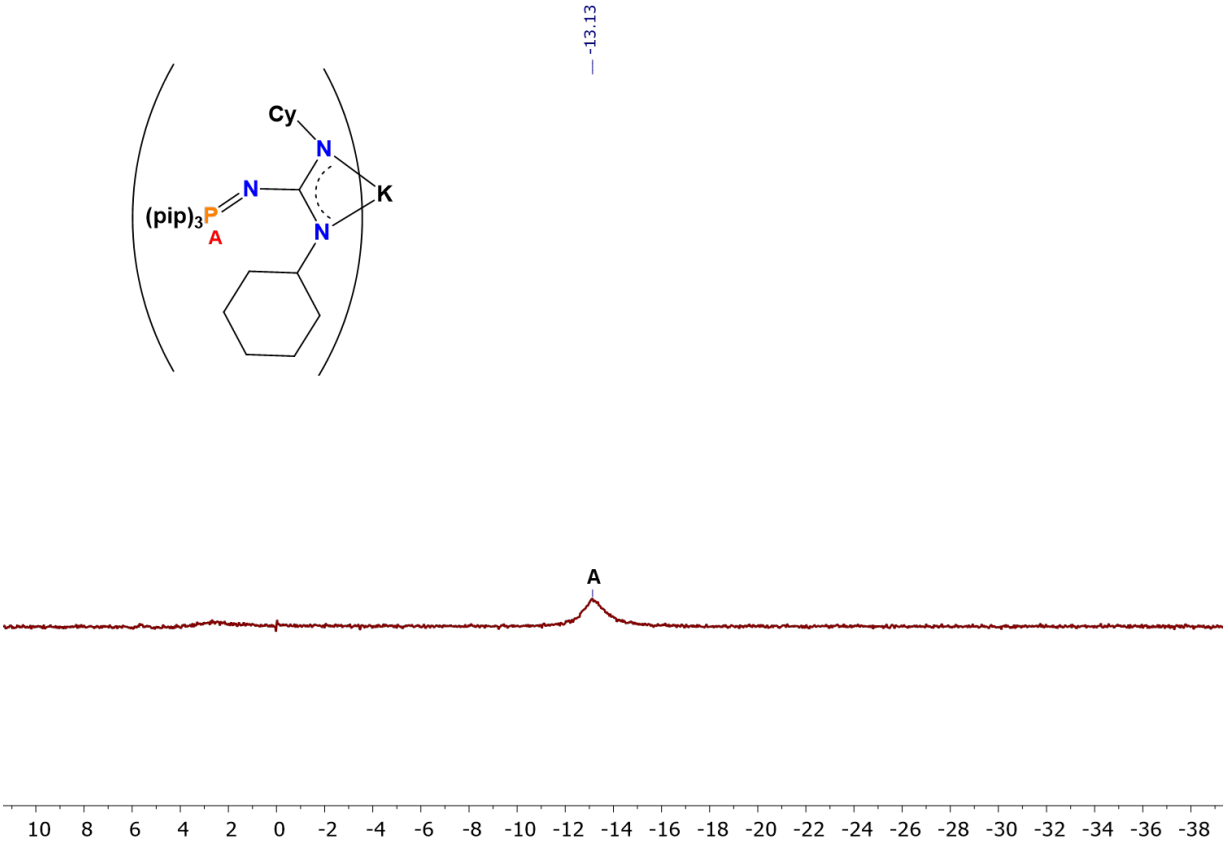

Figure S2. $^{31}P\{^{1}H\}$ NMR of **1-K** (161.98 MHz, d_8-THF, 295 K).

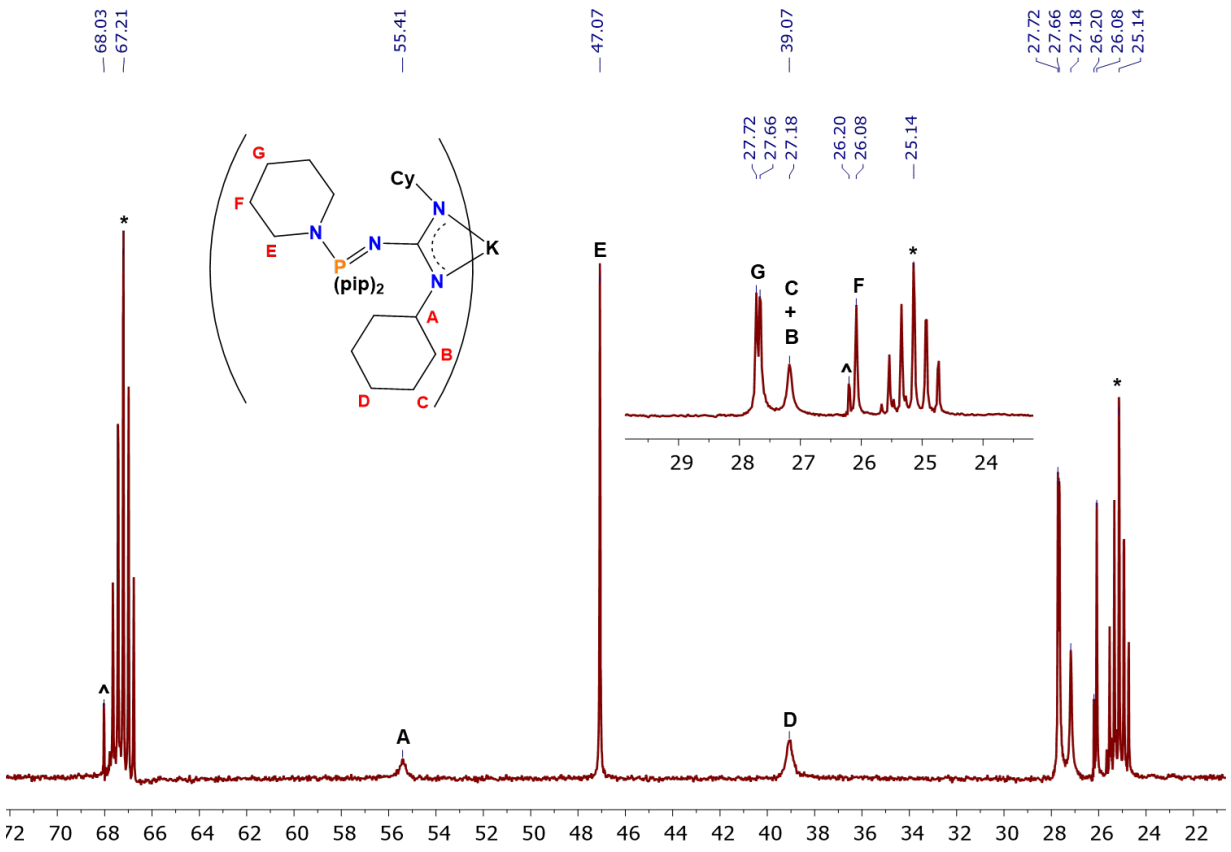

Figure S3. $^{13}C\{^{1}H\}$ NMR of **1-K** (100.62 MHz, d_8-THF, 295 K). C_4D_7HO noted by *. Residual THF noted by ^.

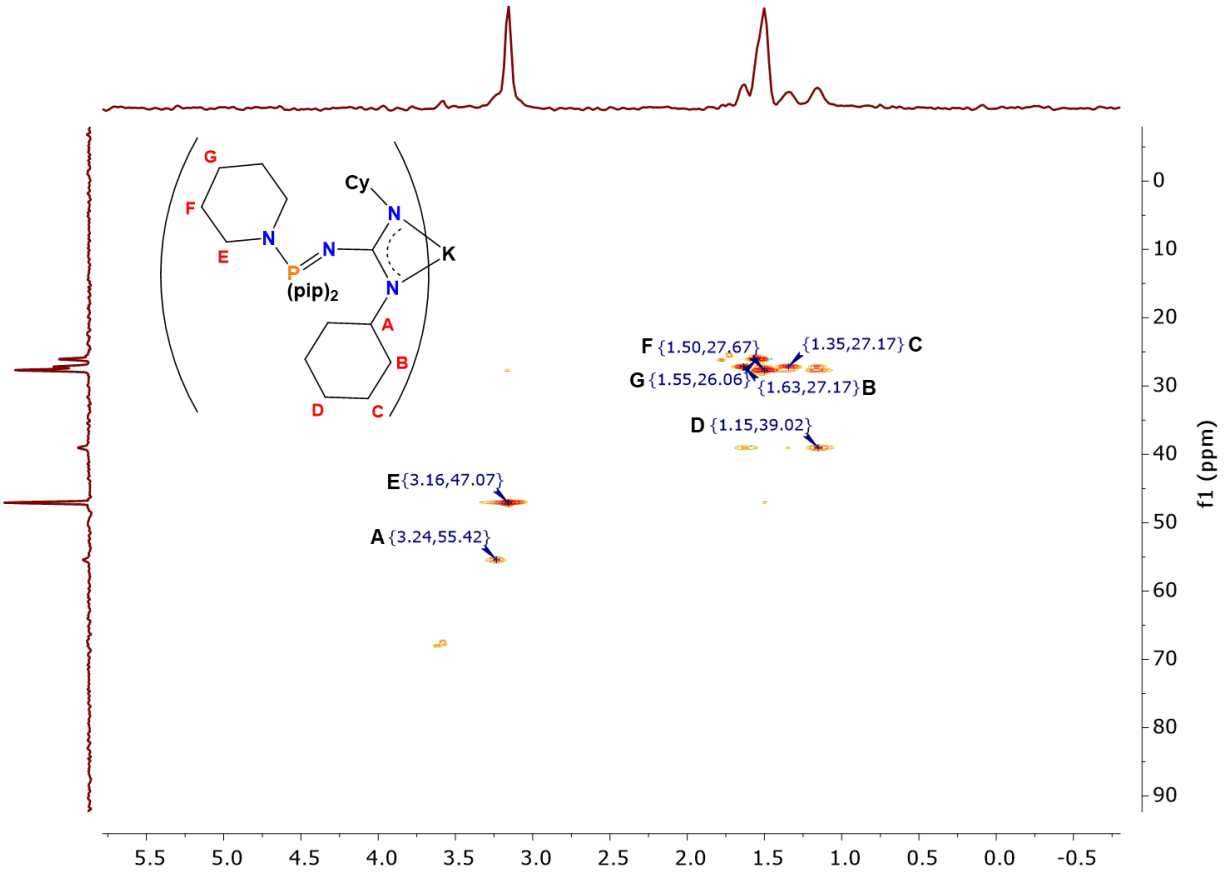

Figure S4. HSQC NMR contour plot of **1-K** (400.13 MHz, d_8-THF, 295 K). The X-axis (f2) corresponds to the ^{1}H NMR spectrum of **1-K** and the Y-axis (f1) corresponds to the ^{13}C{^{1}H} NMR spectrum of **1-K**.

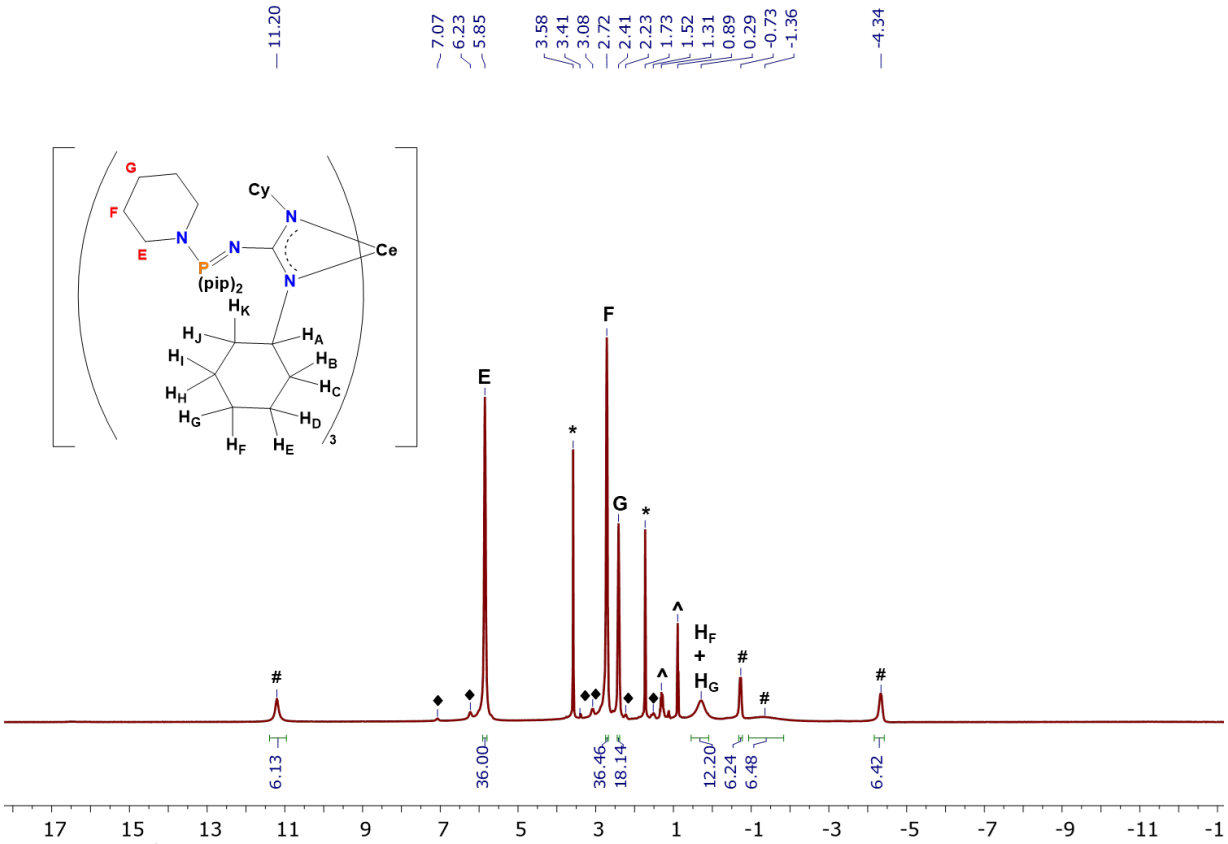

Figure S5. ^{1}H NMR of **1-Ce** in (400.13 MHz, d_8-THF, 295 K). C_4D_7HO noted by *. Residual n-pentane noted by ^. Unassigned cyclohexyl C-*H* signals noted by #. ♦ is unknown.

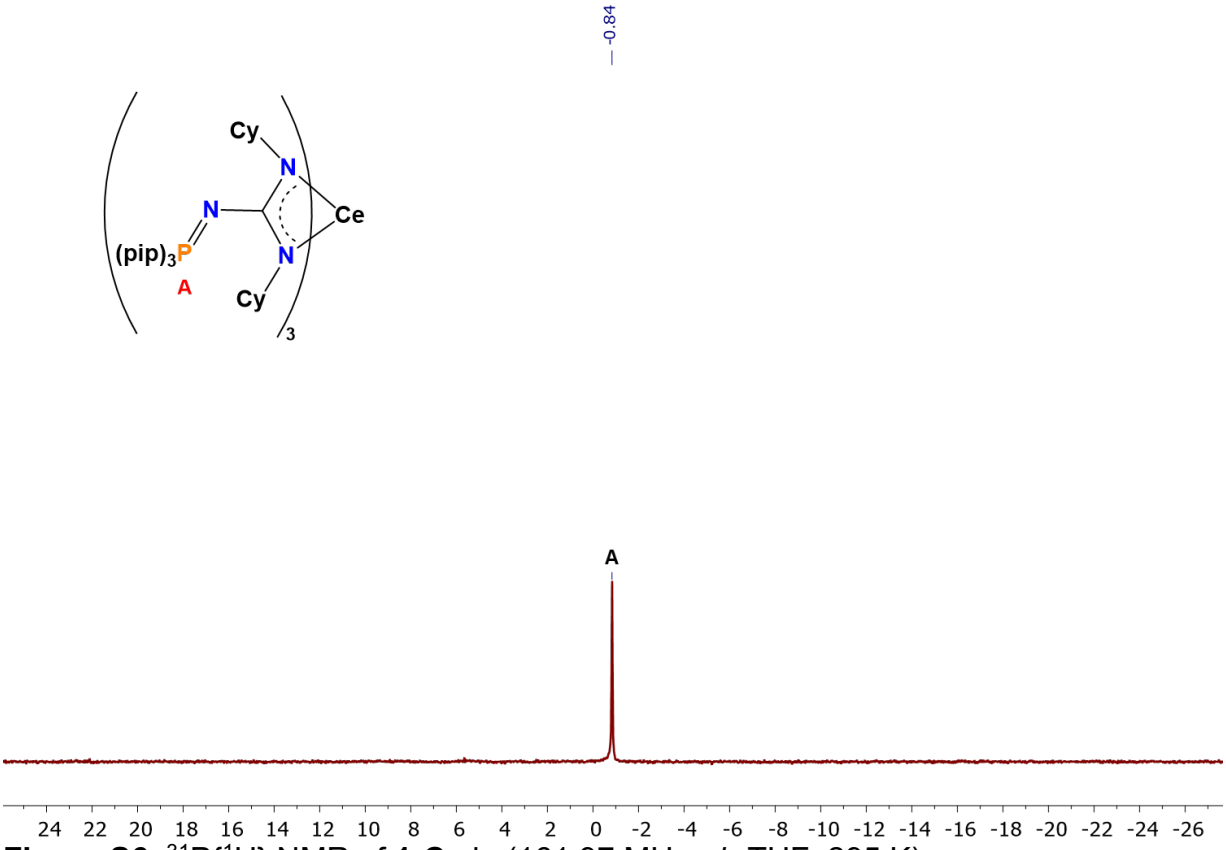

Figure S6. $^{31}P\{^{1}H\}$ NMR of **1-Ce** in (161.97 MHz, d_8-THF, 295 K).

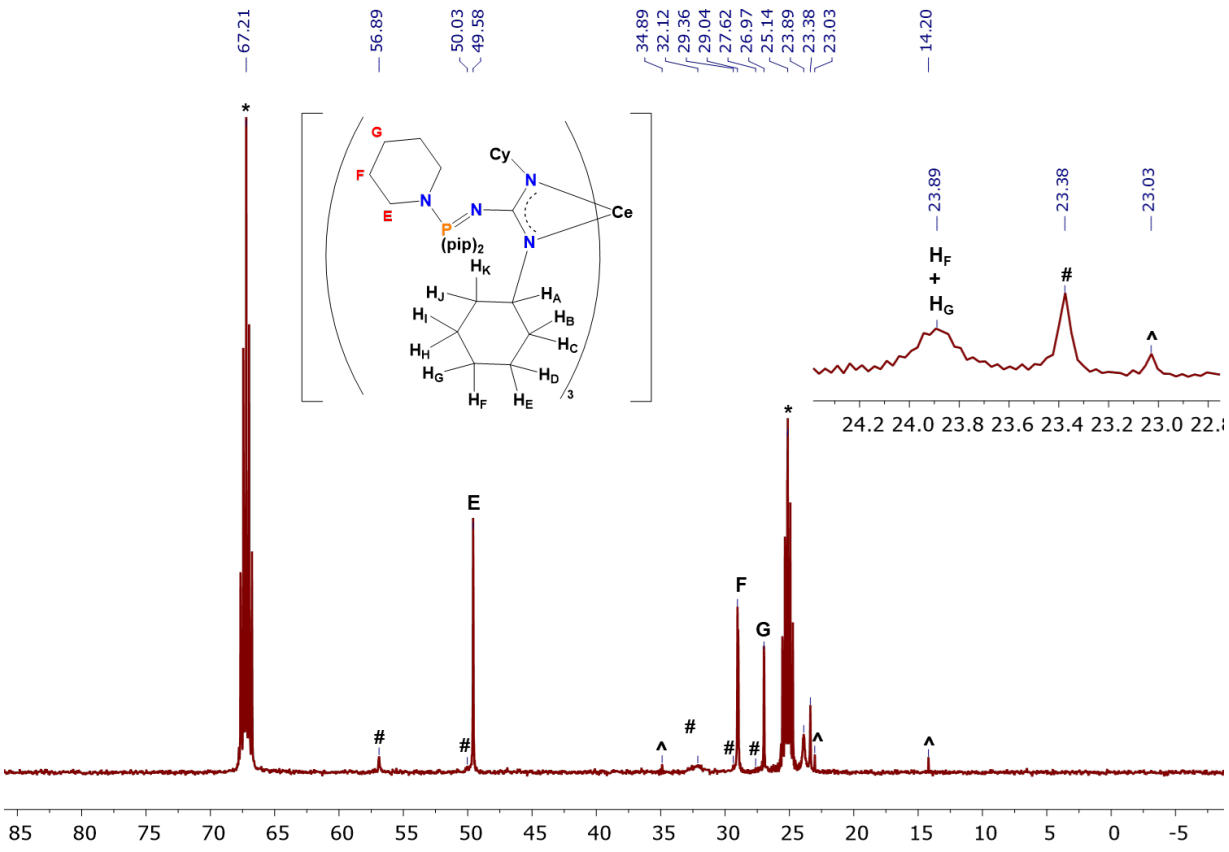

Figure S7. $^{13}C\{^{1}H\}$ NMR of **1-Ce** (100.62 MHz, d_8-THF, 295 K). C_4D_7HO noted by *. Residual n-pentane noted by ^. Unassigned cyclohexyl and guanidinate carbon signals noted by #.

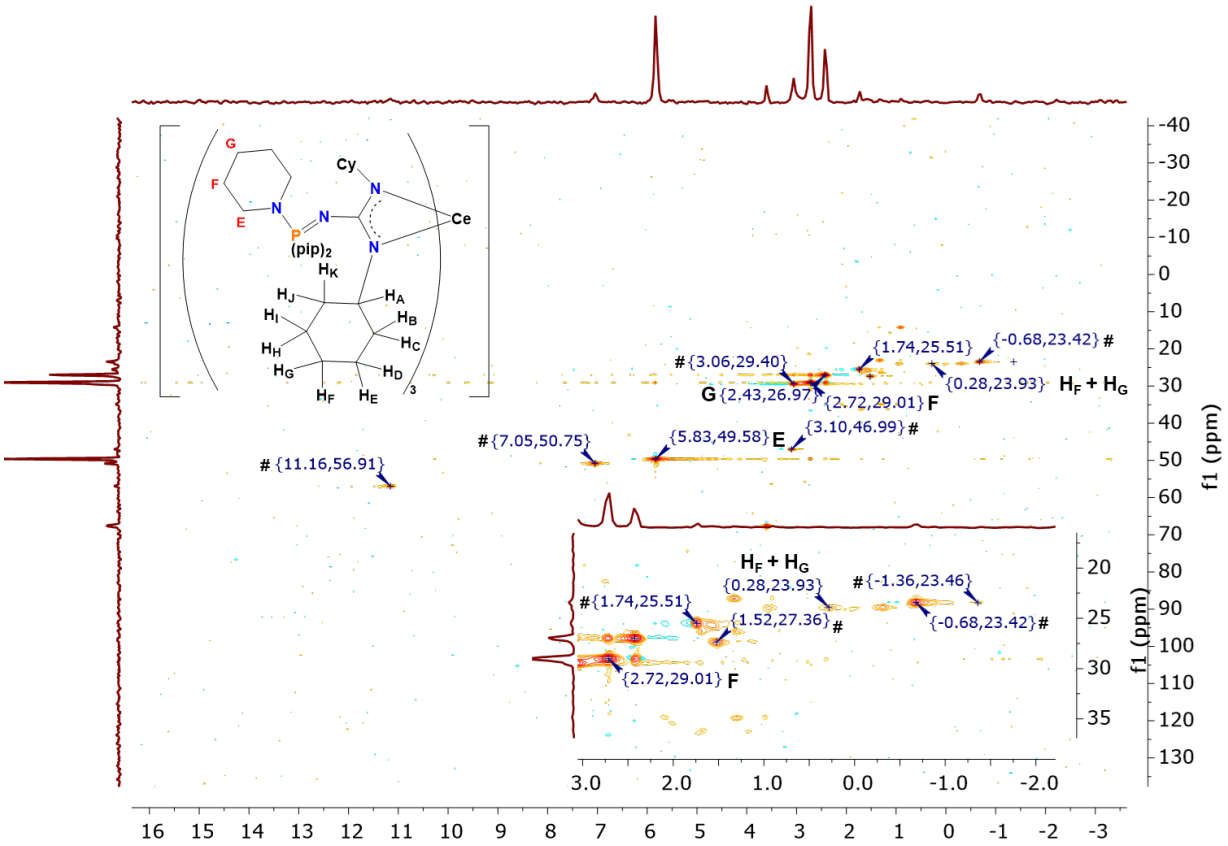

Figure S8. HSQC NMR Contour plot of **1-Ce** in (400.13 MHz, d_8-THF, 295 K). The X-axis (f2) corresponds to the ^{1}H NMR spectrum of **1-Ce** and the Y-axis (f1) corresponds to the $^{13}C\{^{1}H\}$ NMR spectrum of **1-Ce**. Unassigned cyclohexyl C-H signals noted by #.

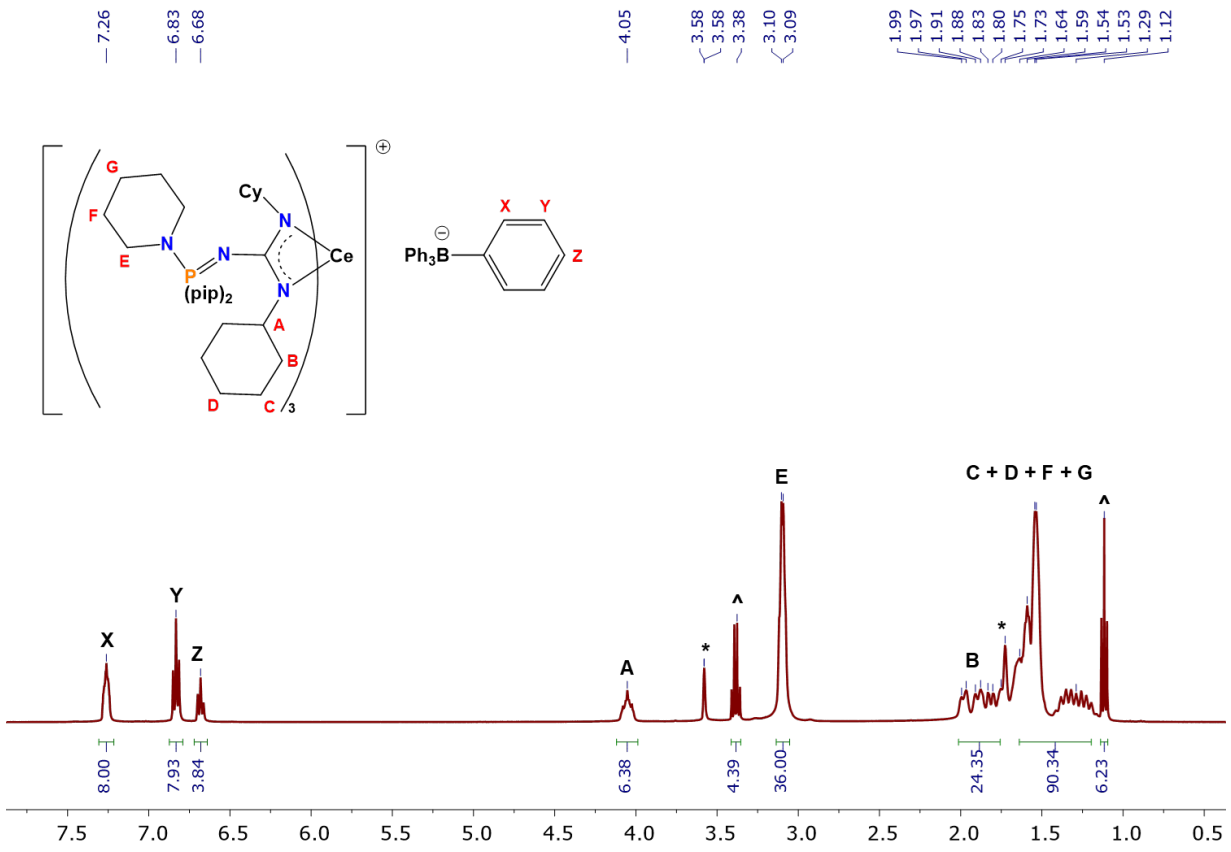

Figure S9. ^{1}H NMR of **2-Ce** (400.13 MHz, d_8-THF, 295 K). C_4D_7HO noted by *. Residual Et_2O noted by ^.

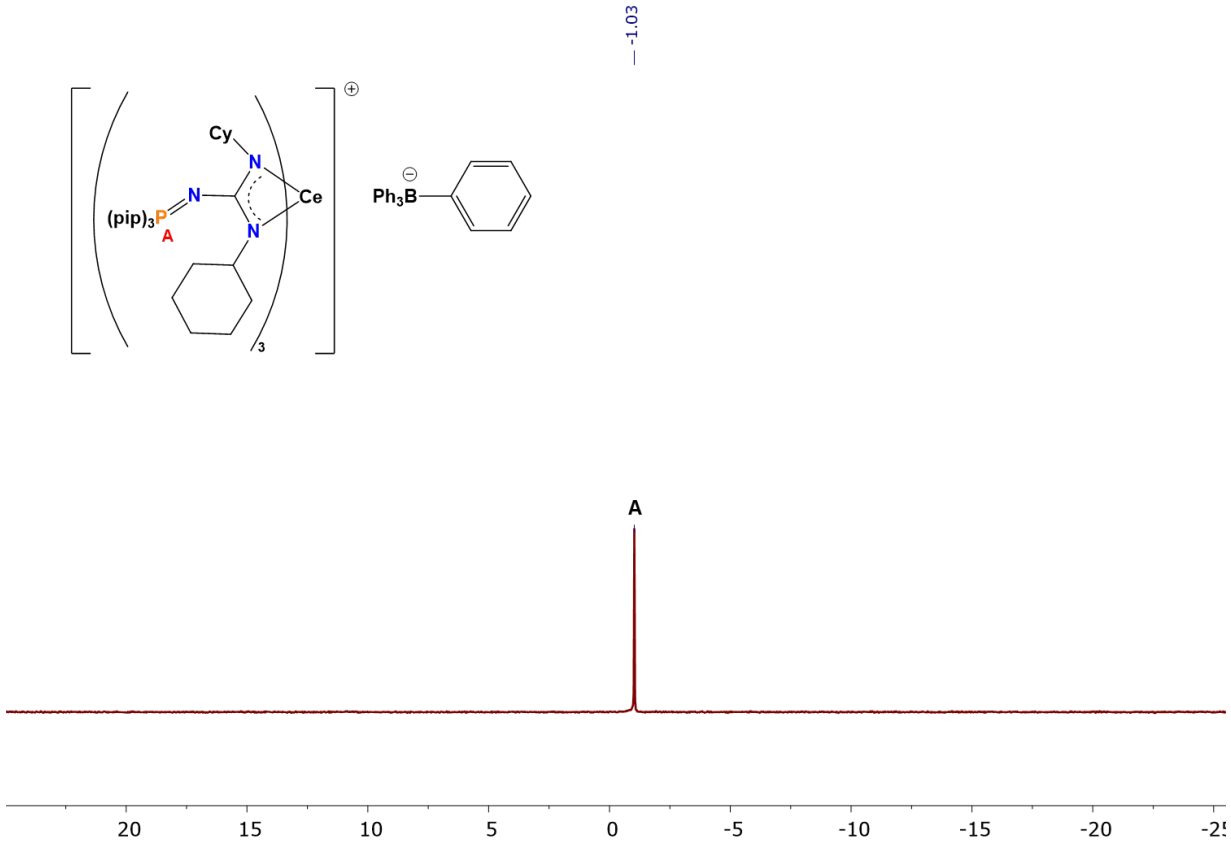

Figure S10. $^{31}P\{^{1}H\}$ NMR of **2-Ce** (161.97 MHz, d_8-THF, 295 K).

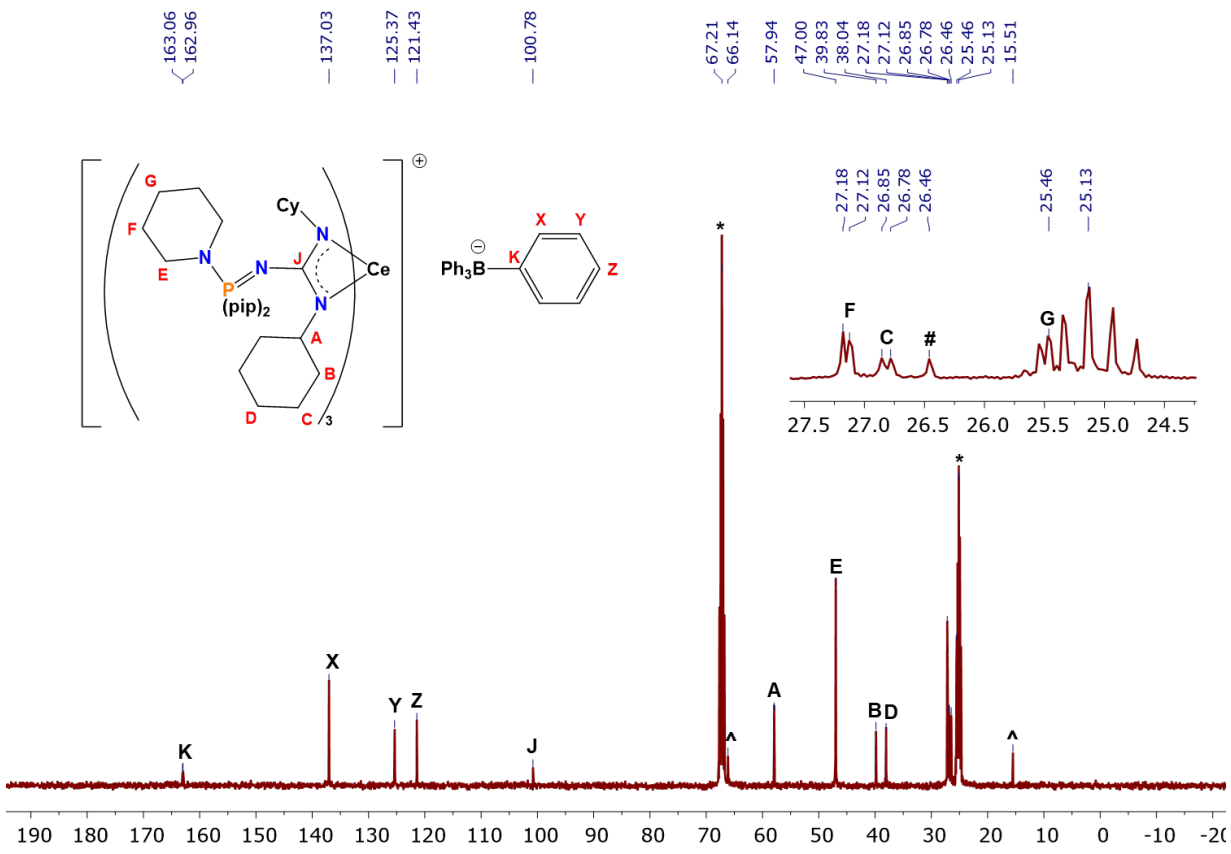

Figure S11. $^{13}C\{^{1}H\}$ NMR of **2-Ce** (100.62 MHz, d_8-THF, 295 K). C_4D_7HO noted by *. Residual Et_2O noted by ^. Unassigned signal noted by #.

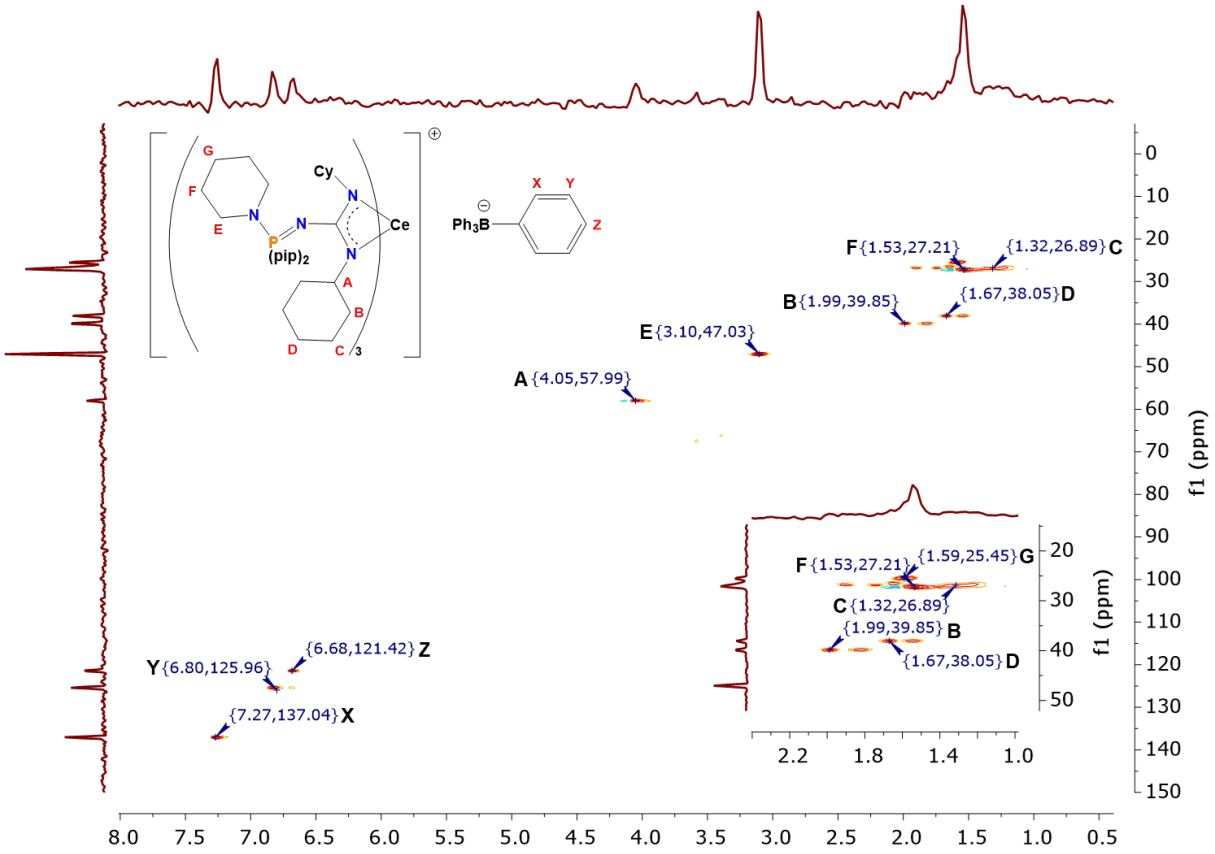

Figure S12. HSQC NMR contour plot of **2-Ce** (400.13 MHz, d_8-THF, 295 K). The X-axis (f2) corresponds to the ^{1}H NMR spectrum of **2-Ce** and the Y-axis (f1) corresponds to the ^{13}C{^{1}H} NMR spectrum of **2-Ce**.

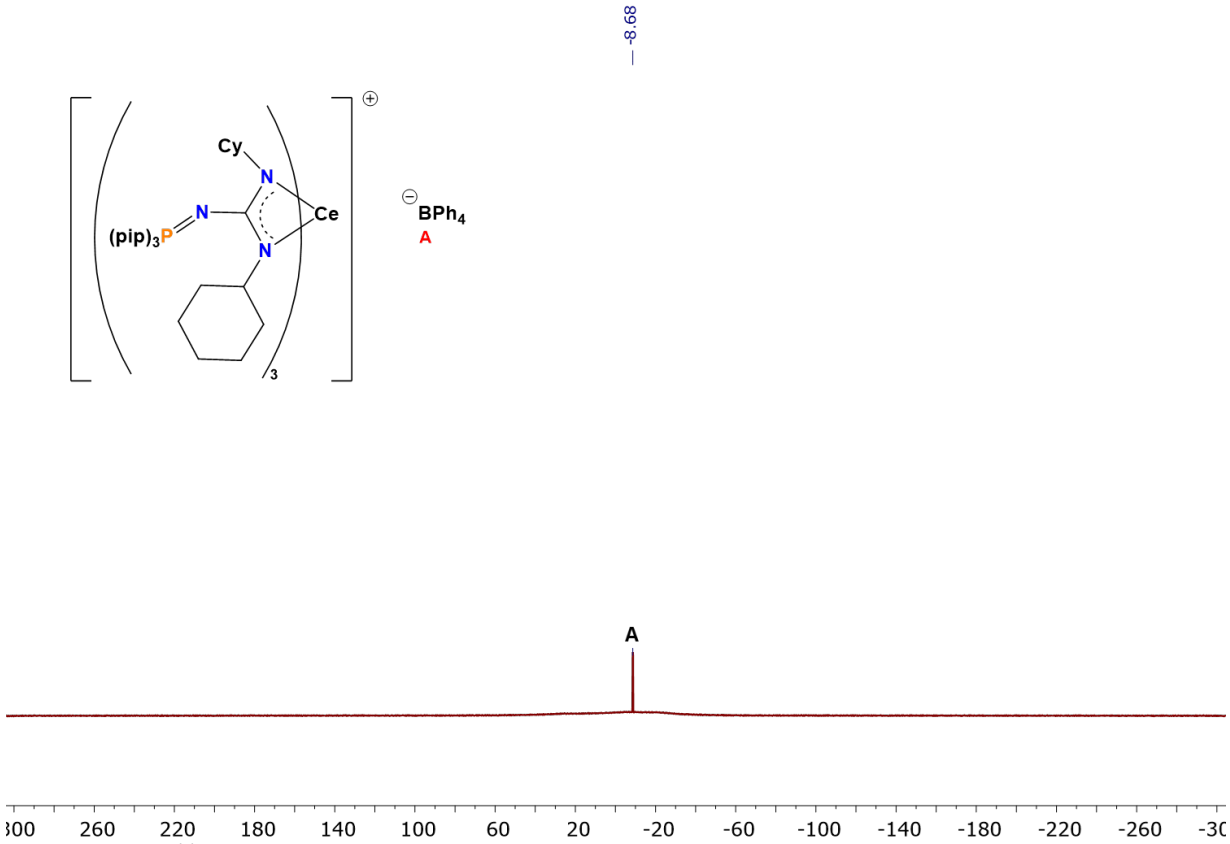

Figure S13. ^{11}B NMR of **2-Ce** (128.38 MHz, d_8-THF, 295 K).

UV-vis-NIR Spectroscopy

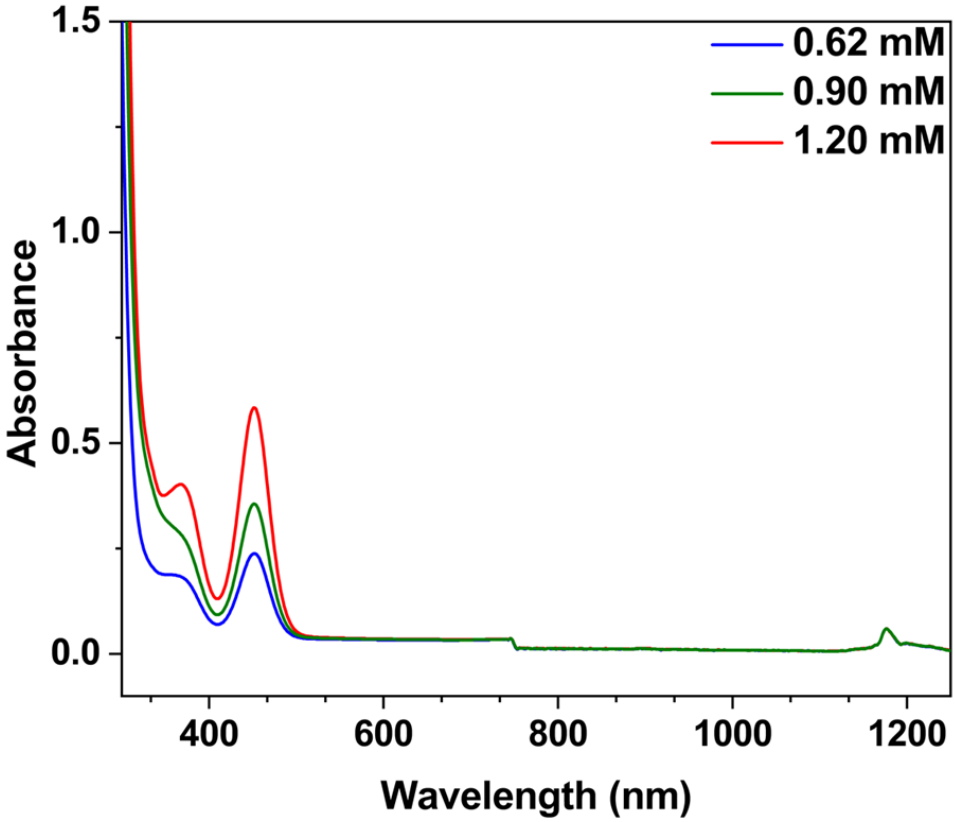

Figure S14. UV-Vis-NIR spectra of **1-Ce** in THF.

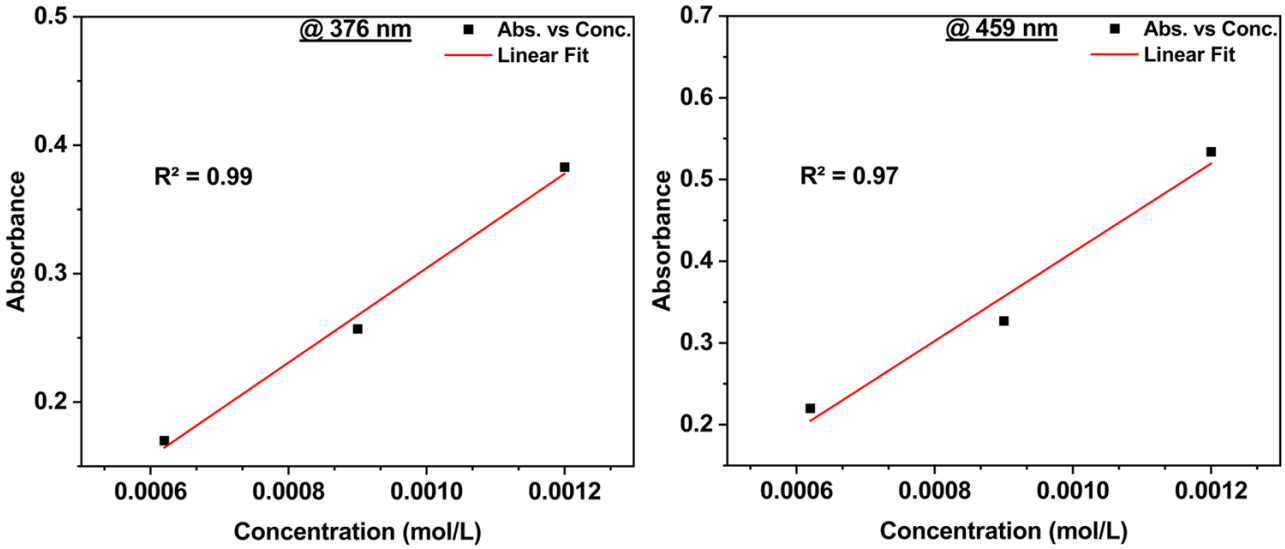

Figure S15. (Left) Linear regression of absorbance at 376 nm maximum where ε = 368 $cm^{-1}M^{-1}$. (Right) Linear regression of absorbance at 459 nm maximum where ε = 543 $cm^{-1}M^{-1}$.

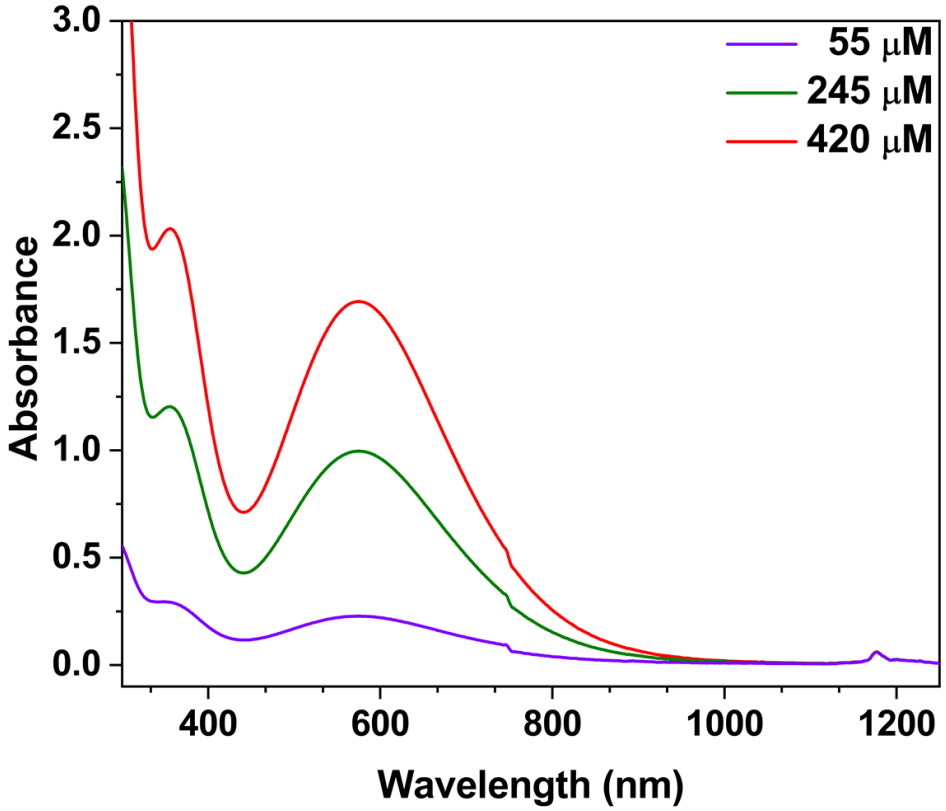

Figure S16. UV-Vis-NIR spectra of **2-Ce** in THF.

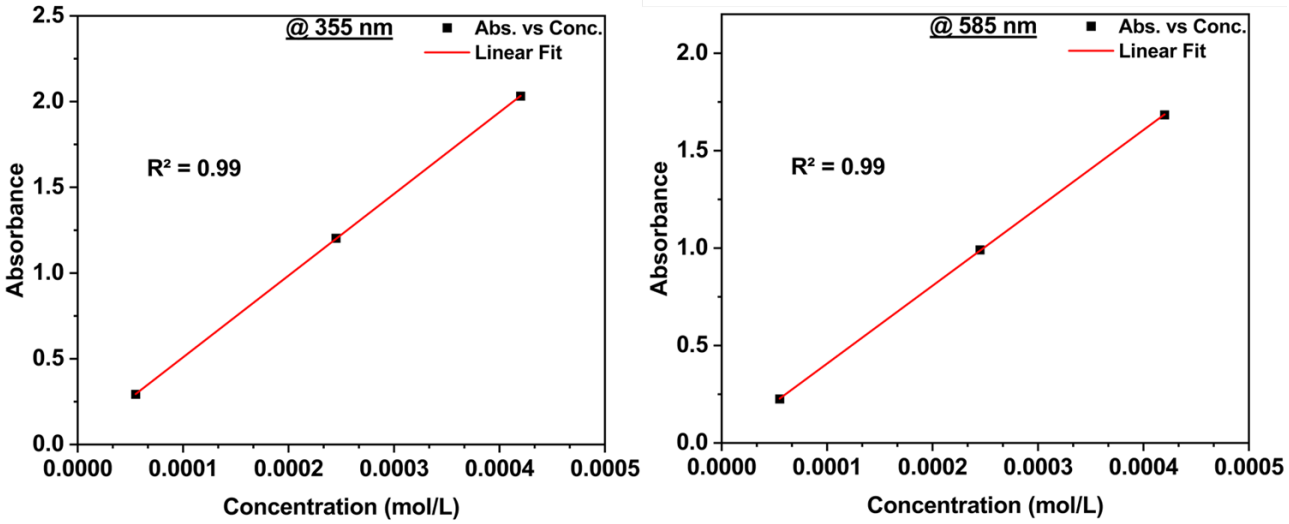

Figure S17. (Left) Linear regression of absorbance at 355 nm maximum where ε = 4765 $cm^{-1}M^{-1}$. (Right) Linear regression of absorbance at 585 nm maximum where ε = 3995 $cm^{-1}M^{-1}$.

Excitation and Emission Spectra

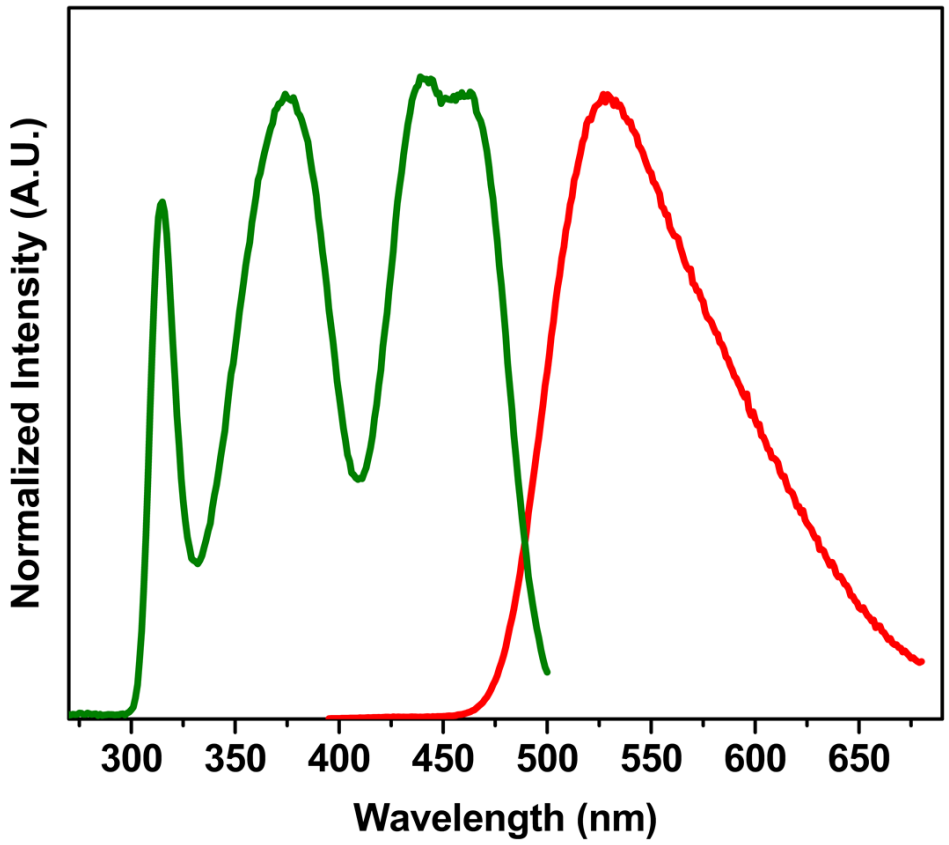

Figure S18. Co-plotted normalized excitation (green) and emission (red) spectra of **1-Ce** in THF.

Cyclic Voltammetry

Electrochemical measurements were performed on a Pine Wave Driver 20 Bipotentiostat/Galvanostat. Measurements were performed inside a N_2 atmosphere glovebox in a 20 mL electrochemical cell with a glassy carbon, a platinum wire counter electrode, and a Ag/AgCl pseudo reference electrode. Electrode were polished before each use. Measurements were performed in a positive feedback IR compensation mode and referenced versus Fc/Fc^+.

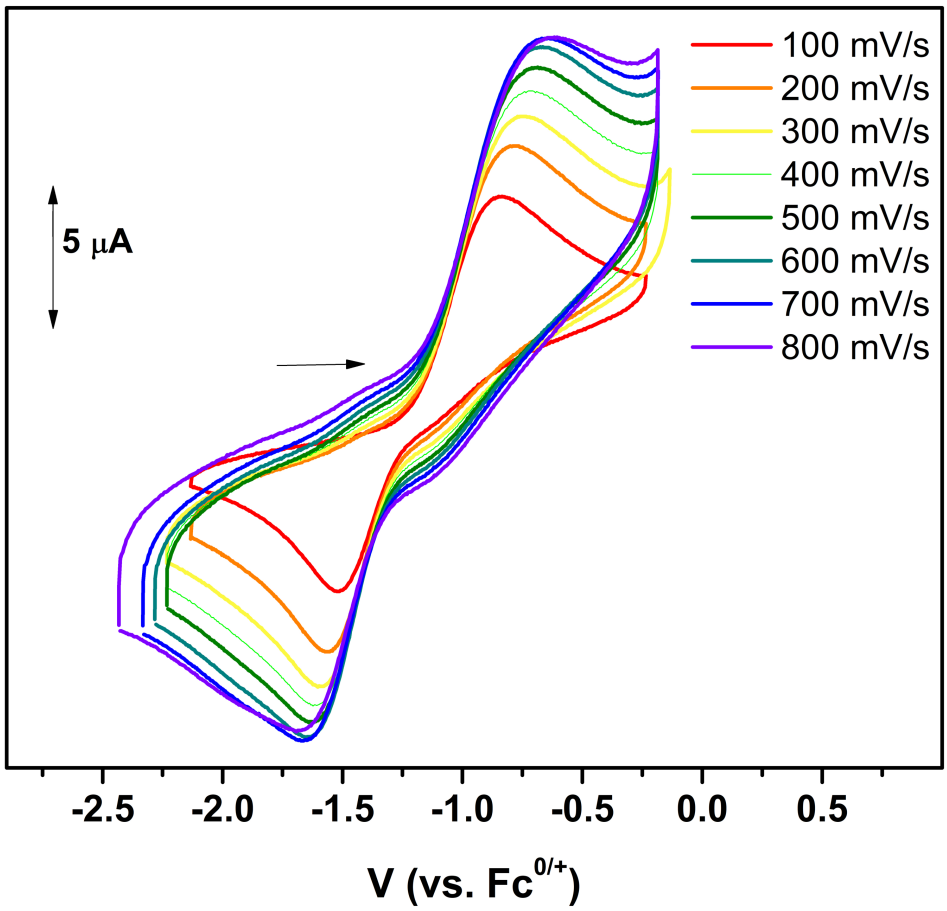

Figure S19. Scan rate dependence of **Ce(III)** in THF (0.1 M $[NBu_4][PF_6]$, 3mM analyte).

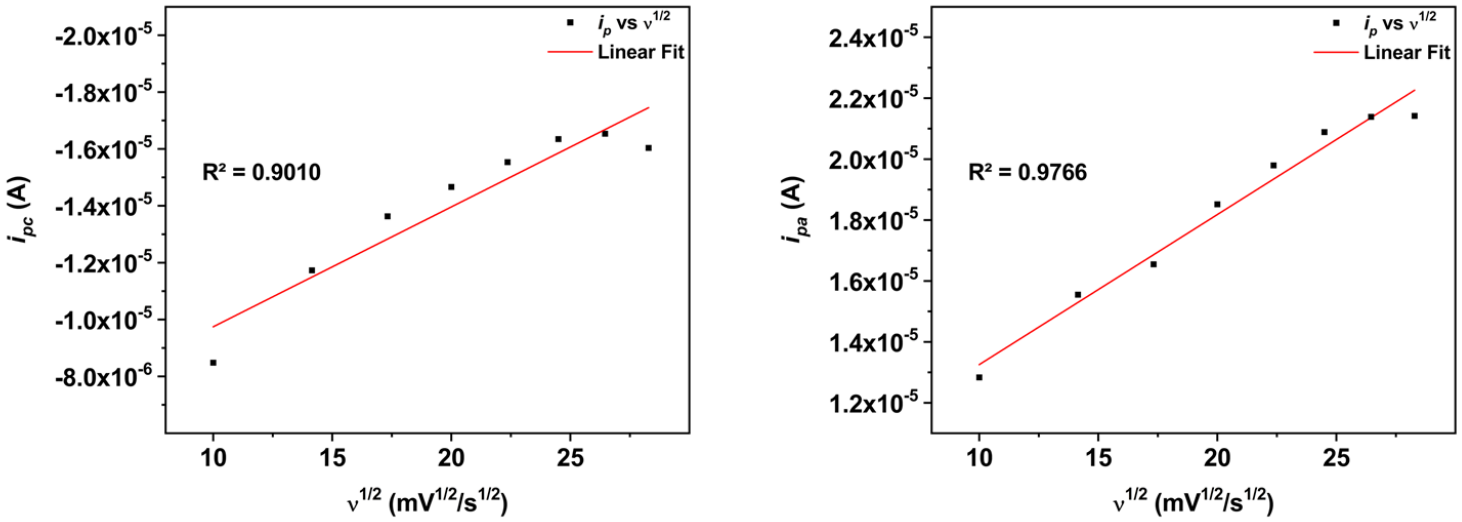

Figure S20. Randles-Sevcik Plots (left: cathodic wave, right: anodic wave) associated with Fig. S17.

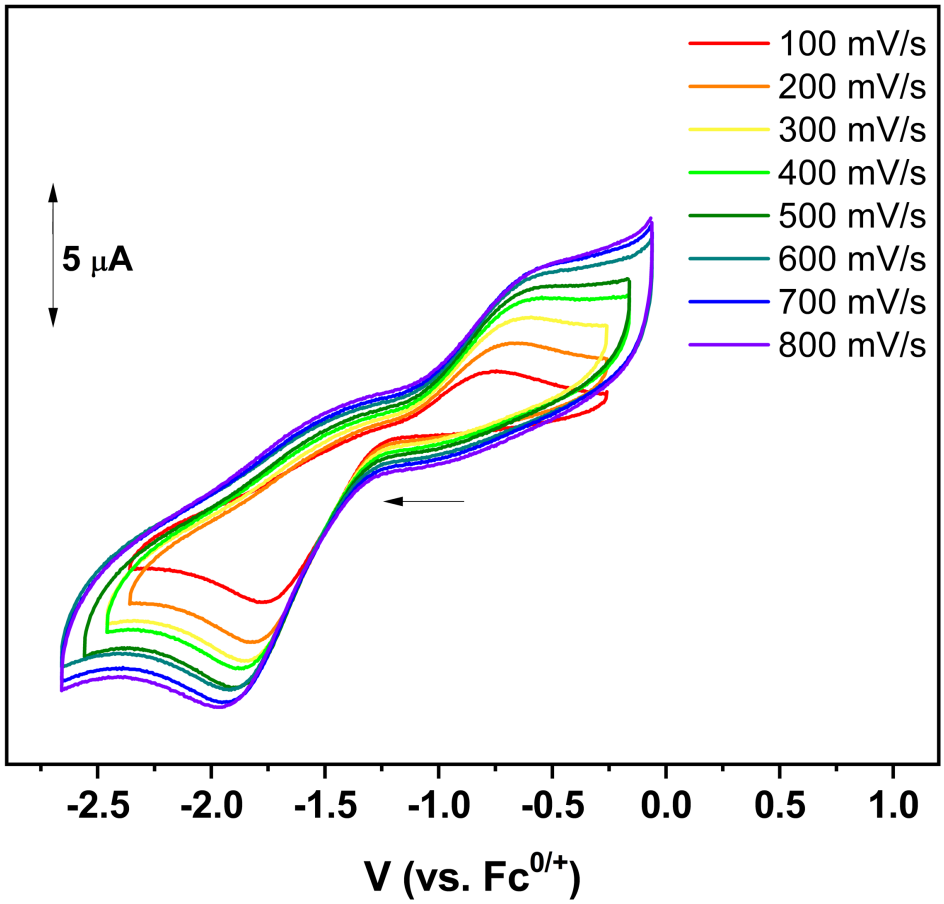

Figure S21. Scan rate dependence of **Ce(IV)** in THF (0.1 M $[NBu_4][PF_6]$, 3mM analyte).

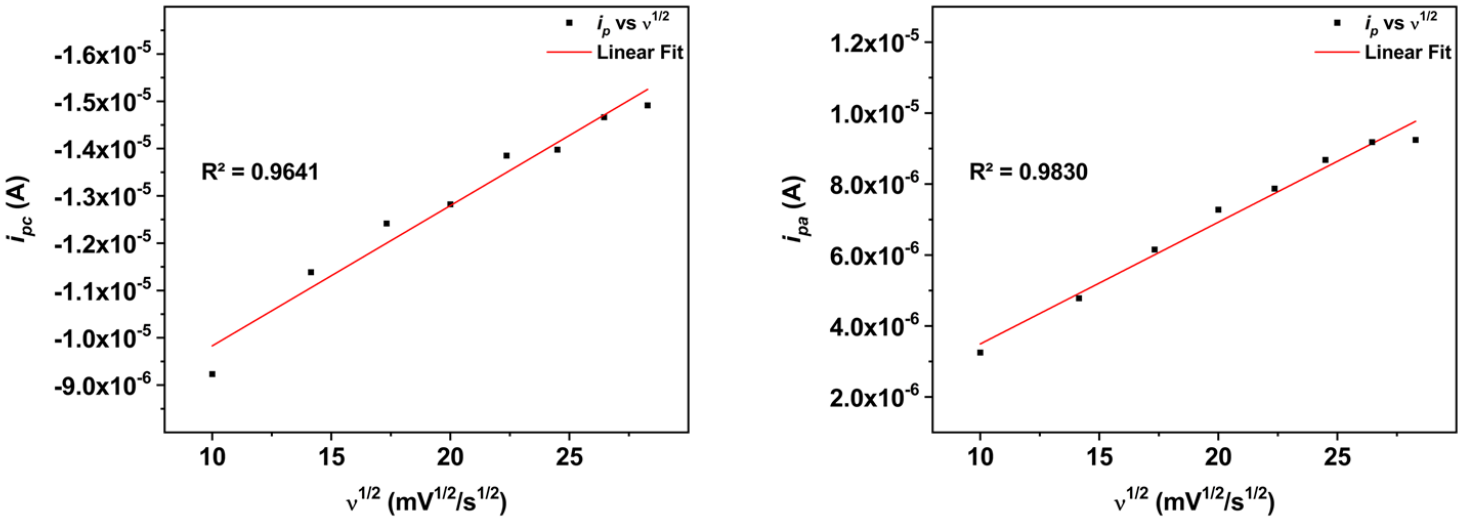

Figure S22. Randles-Sevcik Plots (left: cathodic wave, right: anodic wave) associated with Fig. S19.

Ce L_3-Edge XANES Spectroscopy

Cerium samples were prepared in an argon glovebox at Stanford Synchrotron Radiation Lightsource (SSRL) because both Ce^{4+} and Ce^{3+} complexes are air-sensitive. A mixture of the analyte and boron nitride (BN) was weighed, such that the edge jump for the absorbing atom was calculated to be at one absorption length in transmission (~8−12 mg for the cerium samples). The samples were diluted with BN (~10 mg), which had been dried at elevated temperature (250 °C) under vacuum (1×10^{-3} Torr) for 24 h prior to use. Samples were ground with a mortar and pestle. Solid-state sample holders for the cerium samples consisted of an aluminum plate with a 3 × 15 mm oval window and screw holes. One side of the plate was covered with 0.5 mm Kapton tape, and the sample was evenly loaded in the window. The powder was then secured by covering the sample with a second piece of 0.5 mm Kapton tape. A second layer of the compound was painted onto a third piece of Kapton tape, which was subsequently fixed to the backside of the sample holder. The sample holder was then loaded onto a sample rod, taken out of the glovebox, and transported to the beamline while submerged within a liquid-nitrogen cooling bath. Once at the beam, the rod with the sample was placed at 45° inside the Oxford liquid helium cryostat, which was precooled at 85 K and attached to the SSRL beamline 4-3 rail. When the cryostat was closed, the system was put under vacuum and flushed with helium three times. The valve was closed, and the measurements were performed in the cryostat at 4 K.

The solid-state cerium complexes were characterized by metal L_3- edge X-ray measurements. The XAS measurements were made at SSRL, under dedicated operating conditions (3.0 GeV, 5%, 500 mA using continuous top-off injections) on end station 11-2. With the use of a liquid-nitrogen-cooled double-crystal Si(220) (φ = 0) monochromator that employed collimating and focusing mirrors, a single energy was selected from the incident white beam. For cerium measurements, the beam was fully tuned at 6023 eV, and harmonic rejection was achieved with Rh-coated mirror. The horizontal slit sizes were 8 mm, and vertical slit sizes were 1 mm in all measurements. The cryostat was attached to the beamline 11-2 XAS rail (SSRL), which was equipped with three ionization chambers, through which nitrogen gas was continually flowed. One chamber was positioned before the helium beam pass and the cryostat (10 cm) to monitor the incident radiation (I0). The second chamber was positioned after the cryostat (30 cm) so that sample transmission (I1) could be evaluated against I0 and so that the absorption coefficient (μ) could be calculated as ln(I0/I1). The third chamber (I2; 30 cm) was positioned downstream from I1 so that the XANES of a calibration foil could be measured against I1. A potential of 1100 V was applied in series to the ionization chambers. A Lytle detector under argon was placed on one side of the cryostat (4 cm) to detect the fluorescence from the samples. The cerium samples were calibrated in situ to the energy of the first inflection point of the K-edge of chromium foil (5989 eV). Data were acquired in triplicate and averaged. Background subtraction and normalization (at 5800 eV) were performed in Athena.[4] Curve fitting was performed in IgorPro 7.0 using a modified version of EDG_FIT.[5] Derivative spectra were used as guides to determine the number and positions of the peaks, and edge features were modeled by pseudo-Voigt line shapes and an additional function consisting of arctangent and error function contributions, which was used to model the absorption threshold. Deconvoluted spectral models were performed

over several energy ranges. In the spectrum of **2−Ce**, five Voigts were employed to fit the spectrum: p_1 (the quadrupole-allowed $2p_{3/2} \rightarrow 4f$ transition), p_2, p_3, p_4, and p_5 to model the double-white line feature. In the spectrum of **1−Ce**, a single Voigt was employed to model the white-line feature. The area under the (defined as the intensity) was calculated with the formula ph × fwhm × 1 /4([π/ln(2)]$^{1/2}$ + π), where ph = peak height (normalized intensity), fwhm = full-width at half-maximum height (eV), and the value 1 /4([π/ln(2)]$^{1/2}$ + π) ≈ 1.318 is a constant associated with the pseudo-Voigt function. The fits are shown in Figure S21 and summarized in Table S6. Relative parameter error estimates are calculated from the covariance matrix assuming normally distributed variances in the data. The absolute error in n_f is about 0.02 or 5%.

Table S1. Summary of fit parameters for Ce L_3-edge XANES of **Ce(III)** and **Ce(IV)**. For **Ce(IV)** 5 Voigt functions were used.

Complex	Peak 1		Peak 2		Peak 3		Peak 4		Peak 5	
	Intensity	Energy (eV)	Intensity	Energy (eV)	Intensity	Energy (eV)	Intensity	Energy (eV)	Intensity	Energy (eV)
1-Ce	7.47(0)	5726.0(0)	-	-	-	-	-	-	-	-
2-Ce	0.11(0)	5719.5(0)	1.57(4)	5724.8(0)	7.23(7)	5729.0(0)	6.71(10)	5735.6(0)	1.99(6)	5739.3(6)
				n_f	0.50(2)					

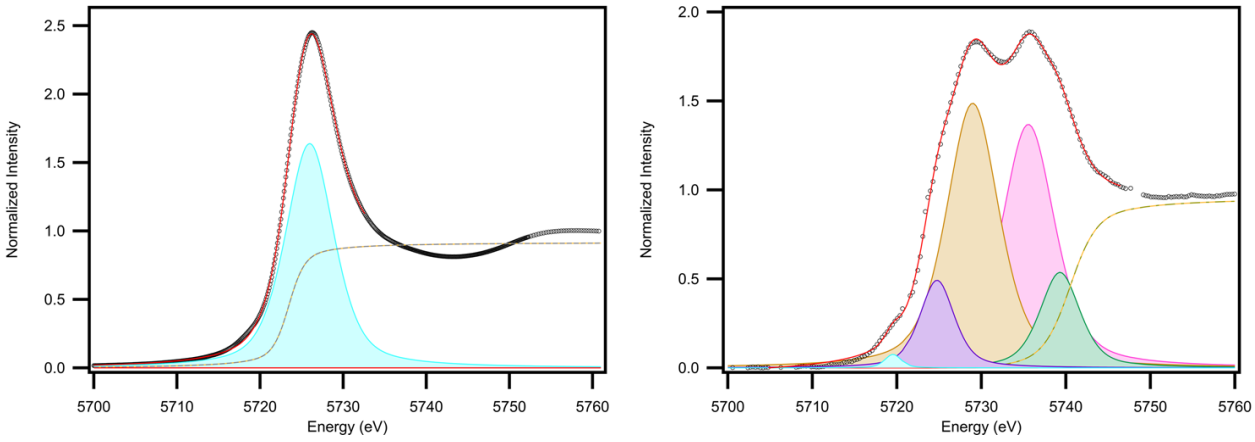

Figure S23. Ce L_3-edge XAS Experimental data (black) obtained for **Ce(III)** (right) and **Ce(IV)** (left) and the pseudo-Voigt [blue (p1), purple (p2), orange (p3), pink (p4), and green (p5)] and steplike functions (yellow/gray dashed line), which sum to generate the curve fit (red).

Table S2. Background subtracted and normalized spectrum of Ce L_3-edge XANES of **1-Ce** and **2-Ce**.

CeIII_Int	CeIII_eV	CeIV_Int	CeIV_eV
5.57E+03	-5.07E-01	5.52E+03	-2.45E-03
5.58E+03	-4.10E-01	5.53E+03	3.87E-03
5.58E+03	-3.15E-01	5.53E+03	3.14E-03
5.59E+03	-2.27E-01	5.53E+03	3.03E-03
5.59E+03	-1.54E-01	5.53E+03	2.67E-03
5.60E+03	-1.05E-01	5.54E+03	1.07E-03
5.60E+03	-6.65E-02	5.54E+03	1.67E-03
5.61E+03	-4.41E-02	5.54E+03	1.80E-03
5.61E+03	-1.32E-02	5.55E+03	1.59E-03
5.62E+03	2.27E-03	5.55E+03	1.39E-03
5.62E+03	1.91E-02	5.55E+03	1.30E-03
5.63E+03	2.67E-02	5.56E+03	1.12E-03
5.63E+03	3.84E-02	5.56E+03	1.42E-03
5.64E+03	3.60E-02	5.56E+03	1.07E-03
5.64E+03	3.10E-02	5.57E+03	8.26E-04
5.65E+03	2.93E-02	5.57E+03	1.18E-03
5.65E+03	2.34E-02	5.57E+03	1.42E-03
5.66E+03	1.64E-02	5.58E+03	8.68E-04
5.66E+03	1.02E-02	5.58E+03	1.10E-03
5.67E+03	-4.16E-03	5.58E+03	2.30E-03
5.67E+03	-1.28E-02	5.58E+03	1.56E-03
5.68E+03	-1.30E-02	5.59E+03	-3.29E-04
5.68E+03	-1.19E-02	5.59E+03	-1.14E-04
5.69E+03	-1.33E-02	5.59E+03	-6.79E-04
5.69E+03	-1.43E-02	5.60E+03	-5.94E-04
5.69E+03	-1.23E-02	5.60E+03	-7.76E-04
5.69E+03	-8.57E-03	5.60E+03	-7.54E-04
5.69E+03	-1.02E-02	5.61E+03	-1.12E-03
5.69E+03	-9.75E-03	5.61E+03	-8.03E-04
5.69E+03	-6.92E-03	5.61E+03	-1.38E-03
5.69E+03	-5.42E-04	5.62E+03	-1.30E-03
5.69E+03	3.12E-03	5.62E+03	-1.84E-03
5.70E+03	8.34E-03	5.62E+03	-1.39E-03
5.70E+03	8.29E-03	5.62E+03	-1.19E-03
5.70E+03	4.15E-03	5.63E+03	-1.13E-03
5.70E+03	5.11E-03	5.63E+03	-1.73E-03
5.70E+03	3.73E-03	5.63E+03	-1.57E-03
5.70E+03	3.91E-03	5.64E+03	-1.46E-03

5.70E+03	-2.77E-03	5.64E+03	-1.66E-03
5.70E+03	-5.96E-03	5.64E+03	-1.45E-03
5.70E+03	-8.58E-03	5.65E+03	-1.77E-03
5.70E+03	-6.43E-03	5.65E+03	-1.03E-03
5.70E+03	-3.98E-03	5.65E+03	-1.36E-03
5.70E+03	-4.21E-03	5.66E+03	-7.07E-04
5.70E+03	-2.77E-03	5.66E+03	-5.45E-04
5.70E+03	-3.48E-03	5.66E+03	8.11E-05
5.70E+03	-4.12E-03	5.66E+03	5.04E-04
5.70E+03	1.40E-03	5.67E+03	5.30E-04
5.70E+03	-4.37E-03	5.67E+03	7.63E-04
5.70E+03	-3.80E-03	5.67E+03	1.19E-03
5.70E+03	-3.66E-03	5.68E+03	2.18E-03
5.70E+03	-9.61E-04	5.68E+03	3.10E-03
5.70E+03	-1.67E-03	5.68E+03	4.03E-03
5.70E+03	4.43E-04	5.69E+03	1.45E-03
5.70E+03	2.99E-03	5.69E+03	6.33E-03
5.70E+03	5.17E-03	5.69E+03	8.43E-03
5.70E+03	2.72E-03	5.69E+03	8.31E-03
5.70E+03	5.02E-03	5.69E+03	8.36E-03
5.70E+03	5.51E-04	5.69E+03	8.28E-03
5.70E+03	1.11E-04	5.69E+03	8.22E-03
5.70E+03	2.94E-03	5.69E+03	8.46E-03
5.70E+03	1.83E-03	5.69E+03	8.52E-03
5.71E+03	-6.67E-04	5.69E+03	8.96E-03
5.71E+03	-3.56E-03	5.69E+03	8.59E-03
5.71E+03	-3.79E-03	5.69E+03	8.66E-03
5.71E+03	-7.93E-04	5.69E+03	9.04E-03
5.71E+03	2.30E-03	5.69E+03	8.94E-03
5.71E+03	-7.14E-05	5.69E+03	9.07E-03
5.71E+03	-1.45E-03	5.69E+03	9.36E-03
5.71E+03	-3.98E-03	5.69E+03	9.35E-03
5.71E+03	-6.98E-04	5.69E+03	9.48E-03
5.71E+03	-1.79E-03	5.69E+03	9.69E-03
5.71E+03	3.26E-03	5.69E+03	9.50E-03
5.71E+03	5.88E-03	5.69E+03	9.83E-03
5.71E+03	7.84E-03	5.69E+03	9.65E-03
5.71E+03	8.80E-03	5.69E+03	9.64E-03
5.71E+03	8.57E-03	5.69E+03	9.73E-03
5.71E+03	9.44E-03	5.69E+03	1.01E-02
5.71E+03	5.54E-03	5.69E+03	1.02E-02
5.71E+03	6.48E-03	5.70E+03	1.01E-02
5.71E+03	4.83E-03	5.70E+03	1.03E-02

5.71E+03	4.69E-03	5.70E+03	1.04E-02
5.71E+03	6.49E-03	5.70E+03	1.04E-02
5.71E+03	7.51E-03	5.70E+03	1.04E-02
5.71E+03	1.05E-02	5.70E+03	1.05E-02
5.71E+03	1.57E-02	5.70E+03	1.08E-02
5.71E+03	2.06E-02	5.70E+03	1.10E-02
5.71E+03	1.85E-02	5.70E+03	1.09E-02
5.71E+03	1.88E-02	5.70E+03	1.10E-02
5.71E+03	1.98E-02	5.70E+03	1.12E-02
5.71E+03	2.25E-02	5.70E+03	1.11E-02
5.71E+03	3.06E-02	5.70E+03	1.14E-02
5.71E+03	3.16E-02	5.70E+03	1.14E-02
5.71E+03	3.68E-02	5.70E+03	1.15E-02
5.71E+03	3.48E-02	5.70E+03	1.16E-02
5.71E+03	4.32E-02	5.70E+03	1.18E-02
5.72E+03	4.69E-02	5.70E+03	1.19E-02
5.72E+03	5.25E-02	5.70E+03	1.18E-02
5.72E+03	6.15E-02	5.70E+03	1.21E-02
5.72E+03	6.57E-02	5.70E+03	1.23E-02
5.72E+03	7.50E-02	5.70E+03	1.23E-02
5.72E+03	8.64E-02	5.70E+03	1.23E-02
5.72E+03	9.69E-02	5.70E+03	1.25E-02
5.72E+03	1.15E-01	5.70E+03	1.26E-02
5.72E+03	1.32E-01	5.70E+03	1.28E-02
5.72E+03	1.51E-01	5.70E+03	1.30E-02
5.72E+03	1.72E-01	5.70E+03	1.33E-02
5.72E+03	1.87E-01	5.70E+03	1.32E-02
5.72E+03	2.03E-01	5.70E+03	1.33E-02
5.72E+03	2.25E-01	5.70E+03	1.33E-02
5.72E+03	2.42E-01	5.70E+03	1.35E-02
5.72E+03	2.63E-01	5.70E+03	1.36E-02
5.72E+03	2.79E-01	5.70E+03	1.36E-02
5.72E+03	2.94E-01	5.70E+03	1.37E-02
5.72E+03	3.33E-01	5.70E+03	1.39E-02
5.72E+03	4.05E-01	5.70E+03	1.42E-02
5.72E+03	4.25E-01	5.70E+03	1.43E-02
5.72E+03	4.82E-01	5.70E+03	1.44E-02
5.72E+03	5.48E-01	5.70E+03	1.44E-02
5.72E+03	6.25E-01	5.70E+03	1.46E-02
5.72E+03	7.39E-01	5.70E+03	1.47E-02
5.72E+03	8.78E-01	5.70E+03	1.50E-02
5.72E+03	9.58E-01	5.70E+03	1.50E-02
5.72E+03	9.95E-01	5.70E+03	1.51E-02

5.72E+03	1.05E+00	5.70E+03	1.55E-02
5.72E+03	1.12E+00	5.70E+03	1.57E-02
5.72E+03	1.19E+00	5.70E+03	1.61E-02
5.73E+03	1.26E+00	5.70E+03	1.59E-02
5.73E+03	1.32E+00	5.70E+03	1.62E-02
5.73E+03	1.38E+00	5.70E+03	1.63E-02
5.73E+03	1.44E+00	5.70E+03	1.64E-02
5.73E+03	1.49E+00	5.70E+03	1.66E-02
5.73E+03	1.54E+00	5.70E+03	1.65E-02
5.73E+03	1.60E+00	5.70E+03	1.67E-02
5.73E+03	1.65E+00	5.70E+03	1.70E-02
5.73E+03	1.69E+00	5.70E+03	1.71E-02
5.73E+03	1.74E+00	5.70E+03	1.73E-02
5.73E+03	1.77E+00	5.70E+03	1.75E-02
5.73E+03	1.80E+00	5.70E+03	1.77E-02
5.73E+03	1.82E+00	5.70E+03	1.80E-02
5.73E+03	1.83E+00	5.70E+03	1.80E-02
5.73E+03	1.83E+00	5.70E+03	1.82E-02
5.73E+03	1.83E+00	5.70E+03	1.84E-02
5.73E+03	1.82E+00	5.70E+03	1.83E-02
5.73E+03	1.80E+00	5.70E+03	1.88E-02
5.73E+03	1.79E+00	5.70E+03	1.89E-02
5.73E+03	1.77E+00	5.70E+03	1.93E-02
5.73E+03	1.76E+00	5.70E+03	1.93E-02
5.73E+03	1.74E+00	5.70E+03	1.96E-02
5.73E+03	1.73E+00	5.70E+03	1.97E-02
5.73E+03	1.73E+00	5.70E+03	1.99E-02
5.73E+03	1.72E+00	5.70E+03	2.01E-02
5.73E+03	1.72E+00	5.70E+03	2.02E-02
5.73E+03	1.72E+00	5.70E+03	2.05E-02
5.73E+03	1.73E+00	5.70E+03	2.05E-02
5.73E+03	1.74E+00	5.70E+03	2.07E-02
5.73E+03	1.76E+00	5.70E+03	2.09E-02
5.73E+03	1.78E+00	5.70E+03	2.13E-02
5.73E+03	1.81E+00	5.70E+03	2.15E-02
5.73E+03	1.83E+00	5.70E+03	2.17E-02
5.74E+03	1.86E+00	5.70E+03	2.19E-02
5.74E+03	1.88E+00	5.70E+03	2.14E-02
5.74E+03	1.89E+00	5.70E+03	2.16E-02
5.74E+03	1.89E+00	5.70E+03	2.19E-02
5.74E+03	1.87E+00	5.70E+03	2.22E-02
5.74E+03	1.85E+00	5.70E+03	2.24E-02
5.74E+03	1.83E+00	5.70E+03	2.26E-02

5.74E+03	1.80E+00	5.70E+03	2.30E-02
5.74E+03	1.77E+00	5.70E+03	2.30E-02
5.74E+03	1.75E+00	5.70E+03	2.33E-02
5.74E+03	1.73E+00	5.70E+03	2.36E-02
5.74E+03	1.71E+00	5.70E+03	2.37E-02
5.74E+03	1.69E+00	5.70E+03	2.40E-02
5.74E+03	1.65E+00	5.70E+03	2.42E-02
5.74E+03	1.62E+00	5.70E+03	2.45E-02
5.74E+03	1.58E+00	5.70E+03	2.49E-02
5.74E+03	1.53E+00	5.70E+03	2.50E-02
5.74E+03	1.49E+00	5.70E+03	2.56E-02
5.74E+03	1.45E+00	5.70E+03	2.56E-02
5.74E+03	1.41E+00	5.71E+03	2.60E-02
5.74E+03	1.37E+00	5.71E+03	2.61E-02
5.74E+03	1.33E+00	5.71E+03	2.64E-02
5.74E+03	1.28E+00	5.71E+03	2.65E-02
5.74E+03	1.25E+00	5.71E+03	2.70E-02
5.74E+03	1.21E+00	5.71E+03	2.73E-02
5.74E+03	1.18E+00	5.71E+03	2.76E-02
5.74E+03	1.16E+00	5.71E+03	2.81E-02
5.74E+03	1.13E+00	5.71E+03	2.82E-02
5.74E+03	1.12E+00	5.71E+03	2.86E-02
5.74E+03	1.10E+00	5.71E+03	2.88E-02
5.74E+03	1.10E+00	5.71E+03	2.91E-02
5.74E+03	1.09E+00	5.71E+03	2.94E-02
5.74E+03	1.08E+00	5.71E+03	2.98E-02
5.74E+03	1.07E+00	5.71E+03	3.00E-02
5.75E+03	1.05E+00	5.71E+03	3.03E-02
5.75E+03	1.04E+00	5.71E+03	3.07E-02
5.75E+03	1.03E+00	5.71E+03	3.09E-02
5.75E+03	1.03E+00	5.71E+03	3.13E-02
5.75E+03	1.02E+00	5.71E+03	3.15E-02
5.75E+03	1.01E+00	5.71E+03	3.20E-02
5.75E+03	1.01E+00	5.71E+03	3.23E-02
5.75E+03	1.01E+00	5.71E+03	3.29E-02
5.75E+03	9.72E-01	5.71E+03	3.33E-02
5.75E+03	9.68E-01	5.71E+03	3.37E-02
5.75E+03	9.66E-01	5.71E+03	3.42E-02
5.75E+03	9.60E-01	5.71E+03	3.47E-02
5.75E+03	9.60E-01	5.71E+03	3.51E-02
5.75E+03	9.60E-01	5.71E+03	3.54E-02
5.75E+03	9.58E-01	5.71E+03	3.58E-02
5.75E+03	9.58E-01	5.71E+03	3.63E-02

5.75E+03	9.56E-01	5.71E+03	3.68E-02
5.75E+03	9.57E-01	5.71E+03	3.72E-02
5.75E+03	9.63E-01	5.71E+03	3.80E-02
5.75E+03	9.59E-01	5.71E+03	3.85E-02
5.75E+03	9.61E-01	5.71E+03	3.89E-02
5.75E+03	9.63E-01	5.71E+03	3.92E-02
5.75E+03	9.61E-01	5.71E+03	3.98E-02
5.75E+03	9.64E-01	5.71E+03	4.02E-02
5.75E+03	9.60E-01	5.71E+03	4.08E-02
5.75E+03	9.62E-01	5.71E+03	4.14E-02
5.75E+03	9.68E-01	5.71E+03	4.19E-02
5.75E+03	9.73E-01	5.71E+03	4.26E-02
5.76E+03	9.71E-01	5.71E+03	4.31E-02
5.76E+03	9.68E-01	5.71E+03	4.38E-02
5.76E+03	9.67E-01	5.71E+03	4.42E-02
5.76E+03	9.65E-01	5.71E+03	4.48E-02
5.76E+03	9.64E-01	5.71E+03	4.51E-02
5.76E+03	9.64E-01	5.71E+03	4.60E-02
5.76E+03	9.66E-01	5.71E+03	4.65E-02
5.76E+03	9.63E-01	5.71E+03	4.71E-02
5.76E+03	9.63E-01	5.71E+03	4.79E-02
5.76E+03	9.67E-01	5.71E+03	4.84E-02
5.76E+03	9.66E-01	5.71E+03	4.91E-02
5.76E+03	9.69E-01	5.71E+03	4.97E-02
5.76E+03	9.73E-01	5.71E+03	5.03E-02
5.76E+03	9.75E-01	5.71E+03	5.12E-02
5.76E+03	9.75E-01	5.71E+03	5.19E-02
5.76E+03	9.75E-01	5.71E+03	5.24E-02
5.76E+03	9.77E-01	5.71E+03	5.32E-02
5.76E+03	9.78E-01	5.71E+03	5.40E-02
5.76E+03	9.75E-01	5.71E+03	5.48E-02
5.76E+03	9.74E-01	5.71E+03	5.55E-02
5.76E+03	9.74E-01	5.71E+03	5.62E-02
5.76E+03	9.79E-01	5.71E+03	5.69E-02
5.76E+03	9.83E-01	5.71E+03	5.79E-02
5.76E+03	9.84E-01	5.71E+03	5.86E-02
5.76E+03	9.81E-01	5.71E+03	5.93E-02
5.76E+03	9.85E-01	5.71E+03	6.03E-02
5.76E+03	9.90E-01	5.71E+03	6.12E-02
5.76E+03	9.90E-01	5.71E+03	6.24E-02
5.76E+03	9.93E-01	5.71E+03	6.34E-02
5.76E+03	9.94E-01	5.71E+03	6.41E-02
5.76E+03	9.96E-01	5.71E+03	6.53E-02

5.76E+03	1.00E+00	5.71E+03	6.65E-02
5.76E+03	9.99E-01	5.71E+03	6.74E-02
5.77E+03	9.97E-01	5.71E+03	6.86E-02
5.77E+03	9.97E-01	5.71E+03	6.98E-02
5.77E+03	1.00E+00	5.71E+03	7.09E-02
5.77E+03	1.00E+00	5.71E+03	7.20E-02
5.77E+03	1.00E+00	5.71E+03	7.34E-02
5.77E+03	1.01E+00	5.71E+03	7.46E-02
5.77E+03	1.01E+00	5.71E+03	7.58E-02
5.77E+03	1.03E+00	5.71E+03	7.69E-02
5.77E+03	1.03E+00	5.71E+03	7.85E-02
5.77E+03	1.03E+00	5.71E+03	7.98E-02
5.77E+03	1.04E+00	5.71E+03	8.12E-02
5.77E+03	1.05E+00	5.71E+03	8.25E-02
5.77E+03	1.05E+00	5.71E+03	8.40E-02
5.77E+03	1.05E+00	5.71E+03	8.61E-02
5.77E+03	1.05E+00	5.71E+03	8.75E-02
5.77E+03	1.04E+00	5.71E+03	8.91E-02
5.77E+03	1.04E+00	5.71E+03	9.09E-02
5.77E+03	1.04E+00	5.71E+03	9.24E-02
5.77E+03	1.04E+00	5.71E+03	9.37E-02
5.77E+03	1.05E+00	5.71E+03	9.56E-02
5.77E+03	1.05E+00	5.71E+03	9.73E-02
5.77E+03	1.05E+00	5.71E+03	9.93E-02
5.77E+03	1.05E+00	5.71E+03	1.01E-01
5.77E+03	1.04E+00	5.71E+03	1.03E-01
5.77E+03	1.04E+00	5.72E+03	1.06E-01
5.77E+03	1.04E+00	5.72E+03	1.08E-01
5.77E+03	1.04E+00	5.72E+03	1.10E-01
5.77E+03	1.04E+00	5.72E+03	1.13E-01
5.78E+03	1.01E+00	5.72E+03	1.15E-01
5.79E+03	9.46E-01	5.72E+03	1.17E-01
5.80E+03	9.02E-01	5.72E+03	1.20E-01
5.81E+03	9.16E-01	5.72E+03	1.23E-01
5.82E+03	9.56E-01	5.72E+03	1.26E-01
5.84E+03	1.00E+00	5.72E+03	1.28E-01
5.85E+03	1.00E+00	5.72E+03	1.32E-01
5.86E+03	1.00E+00	5.72E+03	1.35E-01
5.87E+03	9.78E-01	5.72E+03	1.39E-01
5.88E+03	9.87E-01	5.72E+03	1.42E-01
5.89E+03	9.85E-01	5.72E+03	1.45E-01
5.90E+03	1.04E+00	5.72E+03	1.49E-01
5.92E+03	1.01E+00	5.72E+03	1.53E-01

5.93E+03	9.55E-01	5.72E+03	1.57E-01
5.94E+03	9.00E-01	5.72E+03	1.62E-01
5.95E+03	8.34E-01	5.72E+03	1.66E-01
5.96E+03	7.71E-01	5.72E+03	1.71E-01
5.96E+03	7.71E-01	5.72E+03	1.76E-01
5.96E+03	7.68E-01	5.72E+03	1.81E-01
5.96E+03	7.69E-01	5.72E+03	1.87E-01
5.96E+03	7.65E-01	5.72E+03	1.92E-01
5.96E+03	7.63E-01	5.72E+03	1.98E-01
5.96E+03	7.58E-01	5.72E+03	2.03E-01
5.96E+03	7.60E-01	5.72E+03	2.09E-01
5.96E+03	7.64E-01	5.72E+03	2.15E-01
5.96E+03	7.64E-01	5.72E+03	2.21E-01
5.96E+03	7.62E-01	5.72E+03	2.28E-01
5.96E+03	7.61E-01	5.72E+03	2.33E-01
5.96E+03	7.59E-01	5.72E+03	2.40E-01
5.96E+03	7.57E-01	5.72E+03	2.47E-01
5.96E+03	7.55E-01	5.72E+03	2.53E-01
5.96E+03	7.54E-01	5.72E+03	2.59E-01
5.96E+03	7.56E-01	5.72E+03	2.66E-01
5.96E+03	7.55E-01	5.72E+03	2.73E-01
5.96E+03	7.53E-01	5.72E+03	2.80E-01
5.96E+03	7.52E-01	5.72E+03	2.87E-01
5.96E+03	7.49E-01	5.72E+03	2.94E-01
5.96E+03	7.50E-01	5.72E+03	3.02E-01
5.96E+03	7.47E-01	5.72E+03	3.09E-01
5.96E+03	7.51E-01	5.72E+03	3.17E-01
5.97E+03	7.42E-01	5.72E+03	3.26E-01
5.97E+03	7.37E-01	5.72E+03	3.35E-01
5.97E+03	7.36E-01	5.72E+03	3.46E-01
5.97E+03	7.38E-01	5.72E+03	3.56E-01
5.97E+03	7.38E-01	5.72E+03	3.66E-01
5.97E+03	7.38E-01	5.72E+03	3.79E-01
5.97E+03	7.40E-01	5.72E+03	3.90E-01
5.97E+03	7.36E-01	5.72E+03	4.02E-01
5.97E+03	7.37E-01	5.72E+03	4.17E-01
5.97E+03	7.36E-01	5.72E+03	4.31E-01
5.97E+03	7.28E-01	5.72E+03	4.47E-01
5.97E+03	7.27E-01	5.72E+03	4.63E-01
5.97E+03	7.27E-01	5.72E+03	4.79E-01
5.97E+03	7.23E-01	5.72E+03	4.99E-01
5.97E+03	7.18E-01	5.72E+03	5.18E-01
5.97E+03	7.15E-01	5.72E+03	5.40E-01

5.97E+03	7.11E-01	5.72E+03	5.61E-01
5.97E+03	7.07E-01	5.72E+03	5.83E-01
5.97E+03	7.03E-01	5.72E+03	6.11E-01
5.97E+03	6.97E-01	5.72E+03	6.36E-01
5.97E+03	6.90E-01	5.72E+03	6.63E-01
5.97E+03	6.87E-01	5.72E+03	6.95E-01
5.97E+03	6.85E-01	5.72E+03	7.25E-01
5.97E+03	6.80E-01	5.72E+03	7.62E-01
5.97E+03	6.76E-01	5.72E+03	7.95E-01
5.97E+03	6.76E-01	5.72E+03	8.30E-01
5.97E+03	6.75E-01	5.72E+03	8.72E-01
5.97E+03	6.78E-01	5.72E+03	9.11E-01
5.97E+03	6.76E-01	5.72E+03	9.52E-01
5.97E+03	6.78E-01	5.72E+03	1.00E+00
5.97E+03	6.73E-01	5.72E+03	1.04E+00
5.97E+03	6.68E-01	5.72E+03	1.09E+00
5.97E+03	6.64E-01	5.72E+03	1.14E+00
5.98E+03	6.67E-01	5.72E+03	1.19E+00
5.98E+03	6.66E-01	5.72E+03	1.24E+00
5.98E+03	6.59E-01	5.72E+03	1.29E+00
5.98E+03	6.61E-01	5.72E+03	1.34E+00
5.98E+03	6.58E-01	5.72E+03	1.39E+00
5.98E+03	6.53E-01	5.72E+03	1.44E+00
5.98E+03	6.53E-01	5.72E+03	1.49E+00
5.98E+03	6.50E-01	5.72E+03	1.55E+00
5.98E+03	6.46E-01	5.72E+03	1.60E+00
5.98E+03	6.42E-01	5.72E+03	1.65E+00
5.98E+03	6.38E-01	5.72E+03	1.70E+00
5.98E+03	6.33E-01	5.72E+03	1.75E+00
5.98E+03	6.32E-01	5.72E+03	1.80E+00
5.98E+03	6.28E-01	5.72E+03	1.84E+00
5.98E+03	6.21E-01	5.72E+03	1.89E+00
5.98E+03	6.20E-01	5.72E+03	1.93E+00
5.98E+03	6.17E-01	5.72E+03	1.97E+00
5.98E+03	6.17E-01	5.72E+03	2.01E+00
5.98E+03	6.16E-01	5.72E+03	2.06E+00
5.98E+03	6.12E-01	5.72E+03	2.09E+00
5.98E+03	6.06E-01	5.72E+03	2.13E+00
5.98E+03	6.04E-01	5.72E+03	2.17E+00
5.98E+03	6.00E-01	5.72E+03	2.20E+00
5.98E+03	5.95E-01	5.73E+03	2.23E+00
5.98E+03	5.96E-01	5.73E+03	2.26E+00
5.98E+03	5.91E-01	5.73E+03	2.29E+00

5.98E+03	5.87E-01	5.73E+03	2.32E+00
5.98E+03	5.84E-01	5.73E+03	2.34E+00
5.98E+03	5.81E-01	5.73E+03	2.36E+00
5.98E+03	5.78E-01	5.73E+03	2.38E+00
5.98E+03	5.73E-01	5.73E+03	2.40E+00
5.98E+03	5.67E-01	5.73E+03	2.42E+00
5.98E+03	5.63E-01	5.73E+03	2.43E+00
5.98E+03	5.57E-01	5.73E+03	2.44E+00
5.99E+03	5.56E-01	5.73E+03	2.45E+00
5.99E+03	5.51E-01	5.73E+03	2.45E+00
5.99E+03	5.44E-01	5.73E+03	2.45E+00
5.99E+03	5.38E-01	5.73E+03	2.45E+00
5.99E+03	5.36E-01	5.73E+03	2.44E+00
5.99E+03	5.31E-01	5.73E+03	2.44E+00
5.99E+03	5.29E-01	5.73E+03	2.42E+00
5.99E+03	5.28E-01	5.73E+03	2.41E+00
5.99E+03	5.27E-01	5.73E+03	2.40E+00
5.99E+03	5.23E-01	5.73E+03	2.38E+00
5.99E+03	5.18E-01	5.73E+03	2.36E+00
5.99E+03	5.15E-01	5.73E+03	2.33E+00
5.99E+03	5.15E-01	5.73E+03	2.31E+00
5.99E+03	5.16E-01	5.73E+03	2.29E+00
5.99E+03	5.14E-01	5.73E+03	2.26E+00
5.99E+03	5.13E-01	5.73E+03	2.23E+00
5.99E+03	5.11E-01	5.73E+03	2.20E+00
5.99E+03	5.02E-01	5.73E+03	2.17E+00
5.99E+03	4.96E-01	5.73E+03	2.14E+00
5.99E+03	4.95E-01	5.73E+03	2.11E+00
5.99E+03	4.88E-01	5.73E+03	2.08E+00
5.99E+03	4.84E-01	5.73E+03	2.05E+00
5.99E+03	4.81E-01	5.73E+03	2.01E+00
5.99E+03	4.78E-01	5.73E+03	1.98E+00
5.99E+03	4.74E-01	5.73E+03	1.95E+00
5.99E+03	4.71E-01	5.73E+03	1.92E+00
5.99E+03	4.63E-01	5.73E+03	1.89E+00
5.99E+03	4.61E-01	5.73E+03	1.86E+00
5.99E+03	4.57E-01	5.73E+03	1.83E+00
5.99E+03	4.52E-01	5.73E+03	1.80E+00
5.99E+03	4.48E-01	5.73E+03	1.77E+00
5.99E+03	4.37E-01	5.73E+03	1.74E+00
5.99E+03	4.33E-01	5.73E+03	1.71E+00
6.00E+03	4.27E-01	5.73E+03	1.69E+00
6.00E+03	4.21E-01	5.73E+03	1.66E+00

6.00E+03	4.21E-01	5.73E+03	1.63E+00
6.00E+03	4.18E-01	5.73E+03	1.61E+00
6.00E+03	4.11E-01	5.73E+03	1.58E+00
6.00E+03	4.13E-01	5.73E+03	1.56E+00
6.00E+03	4.08E-01	5.73E+03	1.54E+00
6.00E+03	4.07E-01	5.73E+03	1.51E+00
6.00E+03	4.07E-01	5.73E+03	1.49E+00
6.00E+03	4.06E-01	5.73E+03	1.47E+00
6.00E+03	3.99E-01	5.73E+03	1.45E+00
6.00E+03	3.96E-01	5.73E+03	1.43E+00
6.00E+03	3.93E-01	5.73E+03	1.41E+00
6.00E+03	3.90E-01	5.73E+03	1.39E+00
6.00E+03	3.86E-01	5.73E+03	1.37E+00
6.00E+03	3.82E-01	5.73E+03	1.36E+00
6.00E+03	3.79E-01	5.73E+03	1.34E+00
6.00E+03	3.76E-01	5.73E+03	1.32E+00
6.00E+03	3.68E-01	5.73E+03	1.31E+00
6.00E+03	3.62E-01	5.73E+03	1.29E+00
6.00E+03	3.59E-01	5.73E+03	1.28E+00
6.00E+03	3.58E-01	5.73E+03	1.26E+00
6.00E+03	3.55E-01	5.73E+03	1.25E+00
6.00E+03	3.45E-01	5.73E+03	1.23E+00
6.00E+03	3.44E-01	5.73E+03	1.22E+00
6.00E+03	3.40E-01	5.73E+03	1.21E+00
6.00E+03	3.33E-01	5.73E+03	1.19E+00
6.00E+03	3.29E-01	5.73E+03	1.18E+00
6.00E+03	3.23E-01	5.73E+03	1.17E+00
6.00E+03	3.15E-01	5.73E+03	1.16E+00
6.00E+03	3.06E-01	5.73E+03	1.15E+00
6.00E+03	3.06E-01	5.73E+03	1.14E+00
6.00E+03	3.06E-01	5.73E+03	1.12E+00
6.00E+03	3.01E-01	5.73E+03	1.11E+00
6.01E+03	2.92E-01	5.73E+03	1.10E+00
6.01E+03	2.86E-01	5.73E+03	1.09E+00
6.01E+03	2.82E-01	5.73E+03	1.09E+00
6.01E+03	2.82E-01	5.73E+03	1.08E+00
6.01E+03	2.78E-01	5.73E+03	1.07E+00
6.01E+03	2.73E-01	5.73E+03	1.06E+00
6.01E+03	2.73E-01	5.73E+03	1.05E+00
6.01E+03	2.62E-01	5.73E+03	1.04E+00
6.01E+03	2.59E-01	5.73E+03	1.04E+00
6.01E+03	2.57E-01	5.73E+03	1.03E+00
6.01E+03	2.49E-01	5.73E+03	1.02E+00

6.01E+03	2.40E-01	5.73E+03	1.02E+00
6.01E+03	2.36E-01	5.73E+03	1.01E+00
6.01E+03	2.31E-01	5.73E+03	1.00E+00
6.01E+03	2.29E-01	5.73E+03	9.98E-01
6.01E+03	2.25E-01	5.73E+03	9.92E-01
6.01E+03	2.22E-01	5.73E+03	9.86E-01
6.01E+03	2.19E-01	5.73E+03	9.81E-01
6.01E+03	2.12E-01	5.73E+03	9.76E-01
6.01E+03	2.04E-01	5.73E+03	9.71E-01
6.01E+03	1.99E-01	5.73E+03	9.66E-01
6.01E+03	1.99E-01	5.73E+03	9.62E-01
6.01E+03	1.92E-01	5.74E+03	9.57E-01
6.01E+03	1.92E-01	5.74E+03	9.53E-01
6.01E+03	1.92E-01	5.74E+03	9.49E-01
6.01E+03	1.83E-01	5.74E+03	9.45E-01
6.01E+03	1.78E-01	5.74E+03	9.42E-01
6.01E+03	1.75E-01	5.74E+03	9.38E-01
6.01E+03	1.73E-01	5.74E+03	9.34E-01
6.01E+03	1.68E-01	5.74E+03	9.31E-01
6.01E+03	1.61E-01	5.74E+03	9.28E-01
6.01E+03	1.62E-01	5.74E+03	9.24E-01
6.01E+03	1.56E-01	5.74E+03	9.21E-01
6.02E+03	1.55E-01	5.74E+03	9.18E-01
6.02E+03	1.58E-01	5.74E+03	9.15E-01
6.02E+03	1.53E-01	5.74E+03	9.12E-01
6.02E+03	1.52E-01	5.74E+03	9.10E-01
6.02E+03	1.51E-01	5.74E+03	9.07E-01
6.02E+03	1.43E-01	5.74E+03	9.04E-01
6.02E+03	1.36E-01	5.74E+03	9.01E-01
6.02E+03	1.25E-01	5.74E+03	8.98E-01
6.02E+03	1.24E-01	5.74E+03	8.96E-01
6.02E+03	1.21E-01	5.74E+03	8.93E-01
6.02E+03	1.17E-01	5.74E+03	8.91E-01
6.02E+03	1.07E-01	5.74E+03	8.88E-01
6.02E+03	1.01E-01	5.74E+03	8.86E-01
6.02E+03	9.90E-02	5.74E+03	8.84E-01
6.02E+03	9.62E-02	5.74E+03	8.82E-01
6.02E+03	1.71E-02	5.74E+03	8.80E-01
6.03E+03	-6.70E-02	5.74E+03	8.77E-01
6.03E+03	-1.60E-01	5.74E+03	8.75E-01
6.04E+03	-2.62E-01	5.74E+03	8.74E-01
6.04E+03	-3.63E-01	5.74E+03	8.71E-01
		5.74E+03	8.69E-01

5.74E+03	8.67E-01
5.74E+03	8.65E-01
5.74E+03	8.63E-01
5.74E+03	8.61E-01
5.74E+03	8.59E-01
5.74E+03	8.57E-01
5.74E+03	8.56E-01
5.74E+03	8.54E-01
5.74E+03	8.52E-01
5.74E+03	8.50E-01
5.74E+03	8.48E-01
5.74E+03	8.47E-01
5.74E+03	8.45E-01
5.74E+03	8.43E-01
5.74E+03	8.42E-01
5.74E+03	8.40E-01
5.74E+03	8.38E-01
5.74E+03	8.37E-01
5.74E+03	8.36E-01
5.74E+03	8.34E-01
5.74E+03	8.33E-01
5.74E+03	8.31E-01
5.74E+03	8.30E-01
5.74E+03	8.29E-01
5.74E+03	8.27E-01
5.74E+03	8.26E-01
5.74E+03	8.25E-01
5.74E+03	8.24E-01
5.74E+03	8.23E-01
5.74E+03	8.22E-01
5.74E+03	8.21E-01
5.74E+03	8.20E-01
5.74E+03	8.19E-01
5.74E+03	8.19E-01
5.74E+03	8.18E-01
5.74E+03	8.17E-01
5.74E+03	8.16E-01
5.74E+03	8.16E-01
5.74E+03	8.15E-01
5.74E+03	8.15E-01
5.74E+03	8.14E-01
5.74E+03	8.14E-01
5.74E+03	8.13E-01

5.74E+03	8.13E-01
5.74E+03	8.13E-01
5.74E+03	8.12E-01
5.74E+03	8.12E-01
5.74E+03	8.12E-01
5.74E+03	8.12E-01
5.74E+03	8.12E-01
5.74E+03	8.12E-01
5.74E+03	8.12E-01
5.74E+03	8.12E-01
5.74E+03	8.12E-01
5.74E+03	8.12E-01
5.74E+03	8.12E-01
5.74E+03	8.12E-01
5.74E+03	8.12E-01
5.74E+03	8.13E-01
5.74E+03	8.13E-01
5.74E+03	8.13E-01
5.74E+03	8.14E-01
5.74E+03	8.14E-01
5.74E+03	8.15E-01
5.74E+03	8.15E-01
5.74E+03	8.16E-01
5.74E+03	8.17E-01
5.74E+03	8.17E-01
5.74E+03	8.18E-01
5.75E+03	8.19E-01
5.75E+03	8.19E-01
5.75E+03	8.20E-01
5.75E+03	8.21E-01
5.75E+03	8.22E-01
5.75E+03	8.23E-01
5.75E+03	8.24E-01
5.75E+03	8.25E-01
5.75E+03	8.26E-01
5.75E+03	8.27E-01
5.75E+03	8.28E-01
5.75E+03	8.29E-01
5.75E+03	8.31E-01
5.75E+03	8.32E-01
5.75E+03	8.33E-01
5.75E+03	8.35E-01
5.75E+03	8.36E-01
5.75E+03	8.37E-01

5.75E+03	8.39E-01
5.75E+03	8.41E-01
5.75E+03	8.42E-01
5.75E+03	8.44E-01
5.75E+03	8.45E-01
5.75E+03	8.47E-01
5.75E+03	8.49E-01
5.75E+03	8.51E-01
5.75E+03	8.53E-01
5.75E+03	8.54E-01
5.75E+03	8.56E-01
5.75E+03	8.58E-01
5.75E+03	8.60E-01
5.75E+03	8.62E-01
5.75E+03	8.64E-01
5.75E+03	8.66E-01
5.75E+03	8.68E-01
5.75E+03	8.70E-01
5.75E+03	8.72E-01
5.75E+03	8.74E-01
5.75E+03	8.77E-01
5.75E+03	8.79E-01
5.75E+03	8.81E-01
5.75E+03	8.83E-01
5.75E+03	8.86E-01
5.75E+03	8.88E-01
5.75E+03	8.90E-01
5.75E+03	8.93E-01
5.75E+03	8.95E-01
5.75E+03	8.97E-01
5.75E+03	9.00E-01
5.75E+03	9.02E-01
5.75E+03	9.04E-01
5.75E+03	9.07E-01
5.75E+03	9.10E-01
5.75E+03	9.12E-01
5.75E+03	9.14E-01
5.75E+03	9.17E-01
5.75E+03	9.19E-01
5.75E+03	9.22E-01
5.75E+03	9.24E-01
5.75E+03	9.26E-01
5.75E+03	9.29E-01

5.75E+03	9.31E-01
5.75E+03	9.33E-01
5.75E+03	9.36E-01
5.75E+03	9.38E-01
5.75E+03	9.40E-01
5.75E+03	9.42E-01
5.75E+03	9.44E-01
5.75E+03	9.47E-01
5.75E+03	9.49E-01
5.75E+03	9.51E-01
5.75E+03	9.53E-01
5.75E+03	9.55E-01
5.75E+03	9.57E-01
5.75E+03	9.62E-01
5.75E+03	9.68E-01
5.75E+03	9.73E-01
5.75E+03	9.78E-01
5.75E+03	9.82E-01
5.75E+03	9.85E-01
5.75E+03	9.89E-01
5.75E+03	9.92E-01
5.76E+03	9.94E-01
5.76E+03	9.96E-01
5.76E+03	9.98E-01
5.76E+03	9.99E-01
5.76E+03	1.00E+00
5.76E+03	1.00E+00
5.76E+03	1.00E+00
5.76E+03	1.00E+00
5.76E+03	1.00E+00
5.76E+03	1.00E+00
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5.76E+03	1.00E+00
5.76E+03	1.00E+00
5.76E+03	1.00E+00
5.76E+03	1.00E+00
5.76E+03	1.00E+00
5.76E+03	9.99E-01
5.76E+03	9.98E-01
5.76E+03	9.97E-01

5.76E+03	9.96E-01
5.76E+03	9.94E-01
5.76E+03	9.93E-01
5.76E+03	9.92E-01
5.76E+03	9.91E-01
5.76E+03	9.90E-01
5.76E+03	9.89E-01
5.76E+03	9.87E-01
5.76E+03	9.85E-01
5.76E+03	9.84E-01
5.76E+03	9.83E-01
5.76E+03	9.81E-01
5.77E+03	9.80E-01
5.77E+03	9.79E-01
5.77E+03	9.77E-01
5.77E+03	9.76E-01
5.77E+03	9.74E-01
5.77E+03	9.73E-01
5.77E+03	9.71E-01
5.77E+03	9.70E-01
5.77E+03	9.68E-01
5.77E+03	9.66E-01
5.77E+03	9.65E-01
5.77E+03	9.61E-01
5.77E+03	9.60E-01
5.77E+03	9.59E-01
5.77E+03	9.57E-01
5.77E+03	9.55E-01
5.77E+03	9.54E-01
5.77E+03	9.52E-01
5.77E+03	9.50E-01
5.77E+03	9.48E-01
5.77E+03	9.46E-01
5.77E+03	9.44E-01
5.77E+03	9.43E-01
5.77E+03	9.41E-01
5.77E+03	9.39E-01
5.77E+03	9.37E-01
5.77E+03	9.34E-01
5.77E+03	9.32E-01
5.77E+03	9.30E-01
5.77E+03	9.29E-01
5.77E+03	9.27E-01

5.77E+03	9.25E-01
5.77E+03	9.23E-01
5.78E+03	9.21E-01
5.78E+03	9.19E-01
5.78E+03	9.17E-01
5.78E+03	9.16E-01
5.78E+03	9.14E-01
5.78E+03	9.13E-01
5.78E+03	9.11E-01
5.78E+03	9.10E-01
5.78E+03	9.08E-01
5.78E+03	9.07E-01
5.78E+03	9.06E-01
5.78E+03	9.05E-01
5.78E+03	9.03E-01
5.78E+03	9.03E-01
5.78E+03	9.02E-01
5.78E+03	9.01E-01
5.78E+03	9.00E-01
5.78E+03	8.99E-01
5.78E+03	8.98E-01
5.78E+03	8.98E-01
5.78E+03	8.97E-01
5.78E+03	8.97E-01
5.78E+03	8.96E-01
5.78E+03	8.96E-01
5.78E+03	8.96E-01
5.78E+03	8.96E-01
5.78E+03	8.95E-01
5.78E+03	8.96E-01
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5.78E+03	8.96E-01
5.78E+03	8.96E-01
5.78E+03	8.96E-01
5.78E+03	8.97E-01
5.79E+03	8.97E-01
5.79E+03	8.98E-01
5.79E+03	8.98E-01
5.79E+03	8.98E-01
5.79E+03	8.99E-01
5.79E+03	9.00E-01
5.79E+03	9.01E-01
5.79E+03	9.01E-01

5.79E+03	9.02E-01
5.79E+03	9.03E-01
5.79E+03	9.03E-01
5.79E+03	9.04E-01
5.79E+03	9.05E-01
5.79E+03	9.06E-01
5.79E+03	9.07E-01
5.79E+03	9.08E-01
5.79E+03	9.09E-01
5.79E+03	9.10E-01
5.79E+03	9.11E-01
5.79E+03	9.12E-01
5.79E+03	9.13E-01
5.79E+03	9.14E-01
5.79E+03	9.15E-01
5.79E+03	9.17E-01
5.80E+03	9.31E-01
5.80E+03	9.44E-01
5.80E+03	9.56E-01
5.81E+03	9.67E-01
5.81E+03	9.73E-01
5.81E+03	9.74E-01
5.81E+03	9.73E-01
5.82E+03	9.69E-01
5.82E+03	9.64E-01
5.82E+03	9.62E-01
5.83E+03	9.61E-01
5.83E+03	9.60E-01
5.83E+03	9.59E-01
5.84E+03	9.57E-01
5.84E+03	9.57E-01
5.84E+03	9.59E-01
5.85E+03	9.66E-01
5.85E+03	9.73E-01
5.85E+03	9.77E-01
5.86E+03	9.80E-01
5.86E+03	9.82E-01
5.86E+03	9.83E-01
5.86E+03	9.84E-01
5.87E+03	9.87E-01
5.87E+03	9.89E-01
5.87E+03	9.92E-01
5.88E+03	9.94E-01

5.88E+03	9.96E-01
5.88E+03	9.98E-01
5.89E+03	9.99E-01
5.89E+03	9.98E-01
5.89E+03	9.98E-01
5.90E+03	9.98E-01
5.90E+03	9.98E-01
5.90E+03	9.98E-01
5.90E+03	9.99E-01
5.91E+03	9.99E-01
5.91E+03	1.00E+00
5.91E+03	1.00E+00
5.92E+03	1.00E+00
5.92E+03	1.00E+00
5.92E+03	1.01E+00
5.93E+03	1.01E+00
5.93E+03	1.01E+00
5.93E+03	1.02E+00
5.94E+03	1.01E+00
5.94E+03	1.02E+00
5.94E+03	1.02E+00
5.95E+03	1.03E+00
5.95E+03	1.03E+00
5.95E+03	1.04E+00
5.95E+03	1.04E+00
5.96E+03	1.05E+00
5.96E+03	1.05E+00
5.96E+03	1.05E+00
5.97E+03	1.06E+00
5.97E+03	1.06E+00
5.97E+03	1.06E+00
5.98E+03	1.07E+00
5.98E+03	1.07E+00
5.98E+03	1.07E+00
5.98E+03	1.07E+00
5.98E+03	1.07E+00
5.98E+03	1.07E+00
5.98E+03	1.07E+00
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5.98E+03	1.07E+00
5.98E+03	1.07E+00
5.98E+03	1.07E+00

5.98E+03	1.07E+00
5.98E+03	1.07E+00
5.98E+03	1.07E+00
5.98E+03	1.07E+00
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5.98E+03	1.07E+00
5.98E+03	1.07E+00
5.98E+03	1.08E+00
5.98E+03	1.08E+00
5.98E+03	1.08E+00
5.98E+03	1.08E+00
5.98E+03	1.08E+00
5.98E+03	1.08E+00
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5.98E+03	1.12E+00
5.98E+03	1.12E+00
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5.99E+03	1.12E+00
5.99E+03	1.12E+00
5.99E+03	1.13E+00
5.99E+03	1.13E+00
5.99E+03	1.13E+00
5.99E+03	1.13E+00
5.99E+03	1.13E+00
5.99E+03	1.14E+00
5.99E+03	1.14E+00
5.99E+03	1.14E+00
5.99E+03	1.14E+00
5.99E+03	1.15E+00
5.99E+03	1.15E+00

5.99E+03	1.15E+00
5.99E+03	1.16E+00
5.99E+03	1.16E+00
5.99E+03	1.16E+00
5.99E+03	1.17E+00
5.99E+03	1.17E+00
5.99E+03	1.18E+00
5.99E+03	1.18E+00
5.99E+03	1.19E+00
5.99E+03	1.20E+00
5.99E+03	1.21E+00
5.99E+03	1.21E+00
5.99E+03	1.22E+00
5.99E+03	1.23E+00
5.99E+03	1.25E+00
5.99E+03	1.26E+00
5.99E+03	1.28E+00
5.99E+03	1.30E+00
5.99E+03	1.32E+00
5.99E+03	1.35E+00
5.99E+03	1.38E+00
5.99E+03	1.42E+00
5.99E+03	1.46E+00
5.99E+03	1.50E+00
5.99E+03	1.56E+00
5.99E+03	1.61E+00
5.99E+03	1.67E+00
5.99E+03	1.73E+00
5.99E+03	1.78E+00
5.99E+03	1.83E+00
5.99E+03	1.88E+00
5.99E+03	1.91E+00
5.99E+03	1.95E+00
5.99E+03	1.98E+00
5.99E+03	2.01E+00
5.99E+03	2.04E+00
5.99E+03	2.07E+00
5.99E+03	2.10E+00
5.99E+03	2.12E+00
5.99E+03	2.15E+00
5.99E+03	2.18E+00
5.99E+03	2.20E+00
5.99E+03	2.23E+00

5.99E+03	2.25E+00
5.99E+03	2.27E+00
5.99E+03	2.30E+00
5.99E+03	2.32E+00
5.99E+03	2.34E+00
5.99E+03	2.36E+00
5.99E+03	2.38E+00
5.99E+03	2.40E+00
5.99E+03	2.42E+00
5.99E+03	2.44E+00
5.99E+03	2.46E+00
5.99E+03	2.48E+00
5.99E+03	2.50E+00
5.99E+03	2.52E+00
5.99E+03	2.53E+00
5.99E+03	2.55E+00
5.99E+03	2.57E+00
5.99E+03	2.58E+00
5.99E+03	2.60E+00
5.99E+03	2.62E+00
5.99E+03	2.63E+00
5.99E+03	2.64E+00
5.99E+03	2.66E+00
5.99E+03	2.67E+00
5.99E+03	2.68E+00
5.99E+03	2.69E+00
5.99E+03	2.70E+00
5.99E+03	2.71E+00
5.99E+03	2.72E+00
5.99E+03	2.73E+00
5.99E+03	2.73E+00
5.99E+03	2.74E+00
5.99E+03	2.75E+00
5.99E+03	2.75E+00
5.99E+03	2.75E+00
5.99E+03	2.76E+00
5.99E+03	2.76E+00
5.99E+03	2.76E+00
5.99E+03	2.76E+00
5.99E+03	2.76E+00
5.99E+03	2.76E+00
5.99E+03	2.76E+00
5.99E+03	2.76E+00

6.00E+03	2.76E+00
6.00E+03	2.76E+00
6.00E+03	2.75E+00
6.00E+03	2.75E+00
6.00E+03	2.75E+00
6.00E+03	2.75E+00
6.00E+03	2.75E+00
6.00E+03	2.75E+00
6.00E+03	2.75E+00
6.00E+03	2.75E+00
6.00E+03	2.76E+00
6.00E+03	2.76E+00
6.00E+03	2.77E+00
6.00E+03	2.78E+00
6.00E+03	2.79E+00
6.00E+03	2.80E+00
6.00E+03	2.81E+00
6.00E+03	2.83E+00
6.00E+03	2.84E+00
6.00E+03	2.86E+00
6.00E+03	2.88E+00
6.00E+03	2.91E+00
6.00E+03	2.93E+00
6.00E+03	2.96E+00
6.00E+03	2.98E+00
6.00E+03	3.01E+00
6.00E+03	3.04E+00
6.00E+03	3.06E+00
6.00E+03	3.09E+00
6.00E+03	3.12E+00
6.00E+03	3.15E+00
6.00E+03	3.18E+00
6.00E+03	3.20E+00
6.00E+03	3.23E+00
6.00E+03	3.26E+00
6.00E+03	3.28E+00
6.00E+03	3.31E+00
6.00E+03	3.34E+00
6.00E+03	3.36E+00
6.00E+03	3.39E+00
6.00E+03	3.41E+00
6.00E+03	3.44E+00
6.00E+03	3.46E+00

6.00E+03	3.49E+00
6.00E+03	3.51E+00
6.00E+03	3.53E+00
6.00E+03	3.55E+00
6.00E+03	3.57E+00
6.00E+03	3.59E+00
6.00E+03	3.61E+00
6.00E+03	3.63E+00
6.00E+03	3.65E+00
6.00E+03	3.67E+00
6.00E+03	3.69E+00
6.00E+03	3.70E+00
6.00E+03	3.72E+00
6.00E+03	3.73E+00
6.00E+03	3.75E+00
6.00E+03	3.76E+00
6.00E+03	3.77E+00
6.00E+03	3.79E+00
6.00E+03	3.80E+00
6.00E+03	3.81E+00
6.00E+03	3.83E+00
6.00E+03	3.84E+00
6.00E+03	3.85E+00
6.00E+03	3.86E+00
6.00E+03	3.88E+00
6.00E+03	3.89E+00
6.00E+03	3.90E+00
6.00E+03	3.91E+00
6.00E+03	3.92E+00
6.00E+03	3.93E+00
6.00E+03	3.94E+00
6.00E+03	3.95E+00
6.00E+03	3.96E+00
6.00E+03	3.97E+00
6.00E+03	3.98E+00
6.00E+03	3.99E+00
6.00E+03	4.00E+00
6.00E+03	4.01E+00
6.00E+03	4.02E+00
6.00E+03	4.03E+00
6.00E+03	4.04E+00
6.00E+03	4.05E+00
6.00E+03	4.06E+00

6.00E+03	4.07E+00
6.00E+03	4.08E+00
6.00E+03	4.09E+00
6.00E+03	4.09E+00
6.00E+03	4.10E+00
6.00E+03	4.11E+00
6.00E+03	4.12E+00
6.00E+03	4.13E+00
6.00E+03	4.14E+00
6.00E+03	4.14E+00
6.00E+03	4.15E+00
6.00E+03	4.16E+00
6.00E+03	4.17E+00
6.00E+03	4.18E+00
6.01E+03	4.19E+00
6.01E+03	4.20E+00
6.01E+03	4.21E+00
6.01E+03	4.21E+00
6.01E+03	4.22E+00
6.01E+03	4.23E+00
6.01E+03	4.24E+00
6.01E+03	4.25E+00
6.01E+03	4.26E+00
6.01E+03	4.27E+00
6.01E+03	4.28E+00
6.01E+03	4.29E+00
6.01E+03	4.29E+00
6.01E+03	4.30E+00
6.01E+03	4.31E+00
6.01E+03	4.32E+00
6.01E+03	4.33E+00
6.01E+03	4.34E+00
6.01E+03	4.34E+00
6.01E+03	4.35E+00
6.01E+03	4.36E+00
6.01E+03	4.37E+00
6.01E+03	4.38E+00
6.01E+03	4.39E+00
6.01E+03	4.40E+00
6.01E+03	4.40E+00
6.01E+03	4.41E+00
6.01E+03	4.42E+00
6.01E+03	4.43E+00

6.01E+03	4.44E+00
6.01E+03	4.45E+00
6.01E+03	4.46E+00
6.01E+03	4.47E+00
6.01E+03	4.48E+00
6.01E+03	4.48E+00
6.01E+03	4.49E+00
6.01E+03	4.50E+00
6.01E+03	4.50E+00
6.01E+03	4.51E+00
6.01E+03	4.51E+00
6.01E+03	4.52E+00
6.01E+03	4.52E+00
6.01E+03	4.52E+00
6.01E+03	4.52E+00
6.01E+03	4.52E+00
6.01E+03	4.51E+00
6.01E+03	4.51E+00
6.01E+03	4.51E+00
6.01E+03	4.50E+00
6.01E+03	4.49E+00
6.01E+03	4.49E+00
6.01E+03	4.48E+00
6.01E+03	4.47E+00
6.01E+03	4.46E+00
6.01E+03	4.45E+00

Crystallographic Analyses

Crystals suitable for X-ray diffraction were covered in paratone oil in a glove box and transferred to the diffractometer in a 20-mL capped vial. Crystals were mounted on a loop with paratone oil on a Bruker D8 VENTURE diffractometer. The crystals were cooled and kept at T = 100(2) K during data collections. The structures were solved with the ShelXT structure solution program using the Intrinsic Phasing solution method and by using Olex2 as the graphical interface.[6, 7] The model was refined with version 2014/7 of XL using Least Squares minimization.[8] Structures were visualized in Mercury and graphics were generated with POV-ray.[9, 10]

Further Refinement Details:
In order to obtain reasonable chemical constraints (1,2 and 1,3 distance constraints) for the disordered groups (piperidine) during the X-ray refinements for **1-K**, the molecular structure was optimized using Orca 4.2.1 using the PBE method and the def2-SVP basis and a multiplicity of 1. Normal or default parameters were used for optimization.[11]

Both complex **1-Ce** and **2-Ce** contained extensively disordered solvent in the crystal lattice. The solvent was too disordered to model reliably and therefore treated by solvent masking in Olex2. The treatment gave 72 electrons for each unit cell in **1-Ce** and 115 electrons for **2-Ce**. This corresponds to approximately 2 and 3 pentane molecules respectively or 1 and 1.5 molecules for each formula unit.

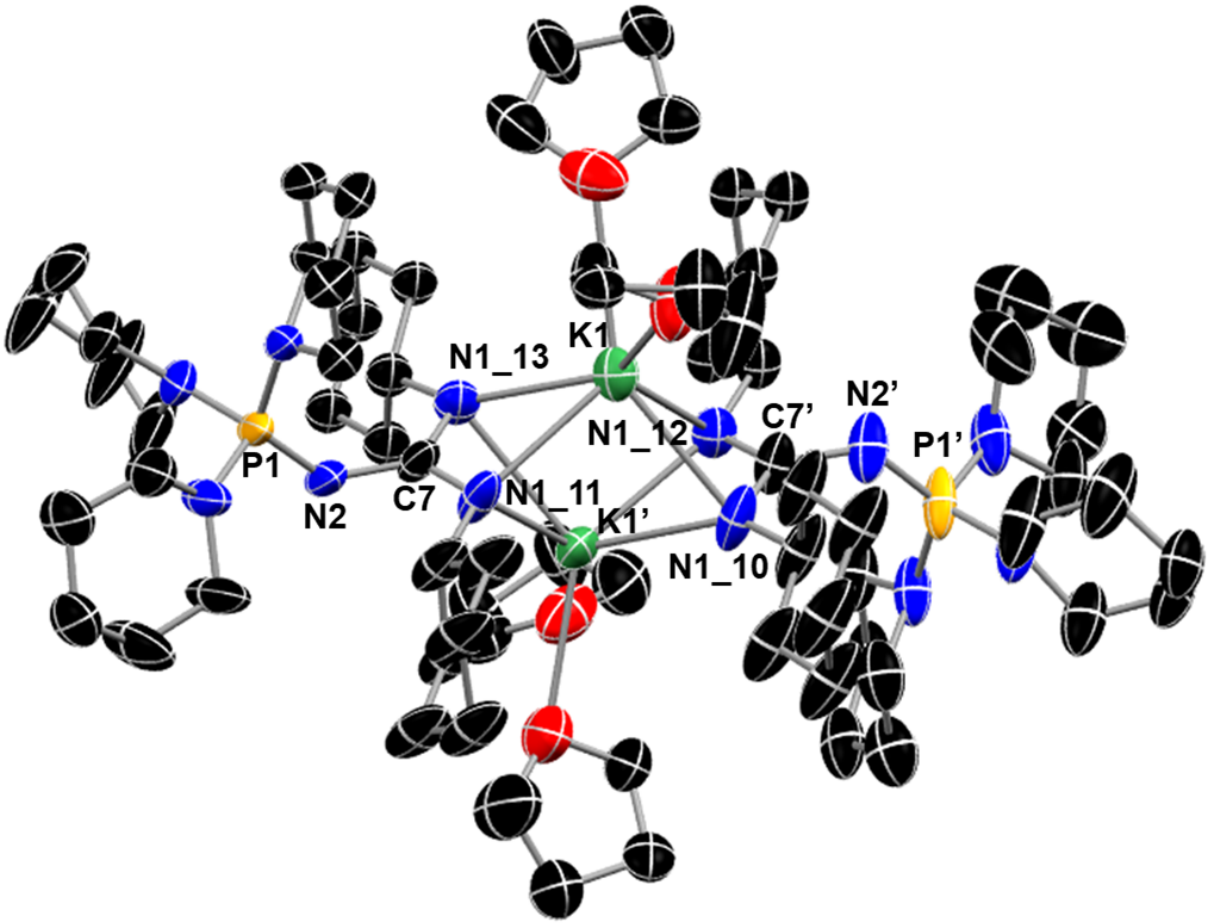

Figure S24. Molecular structure of **1-K** with thermal ellipsoids shown at 50% probability; H atoms are omitted for clarity.

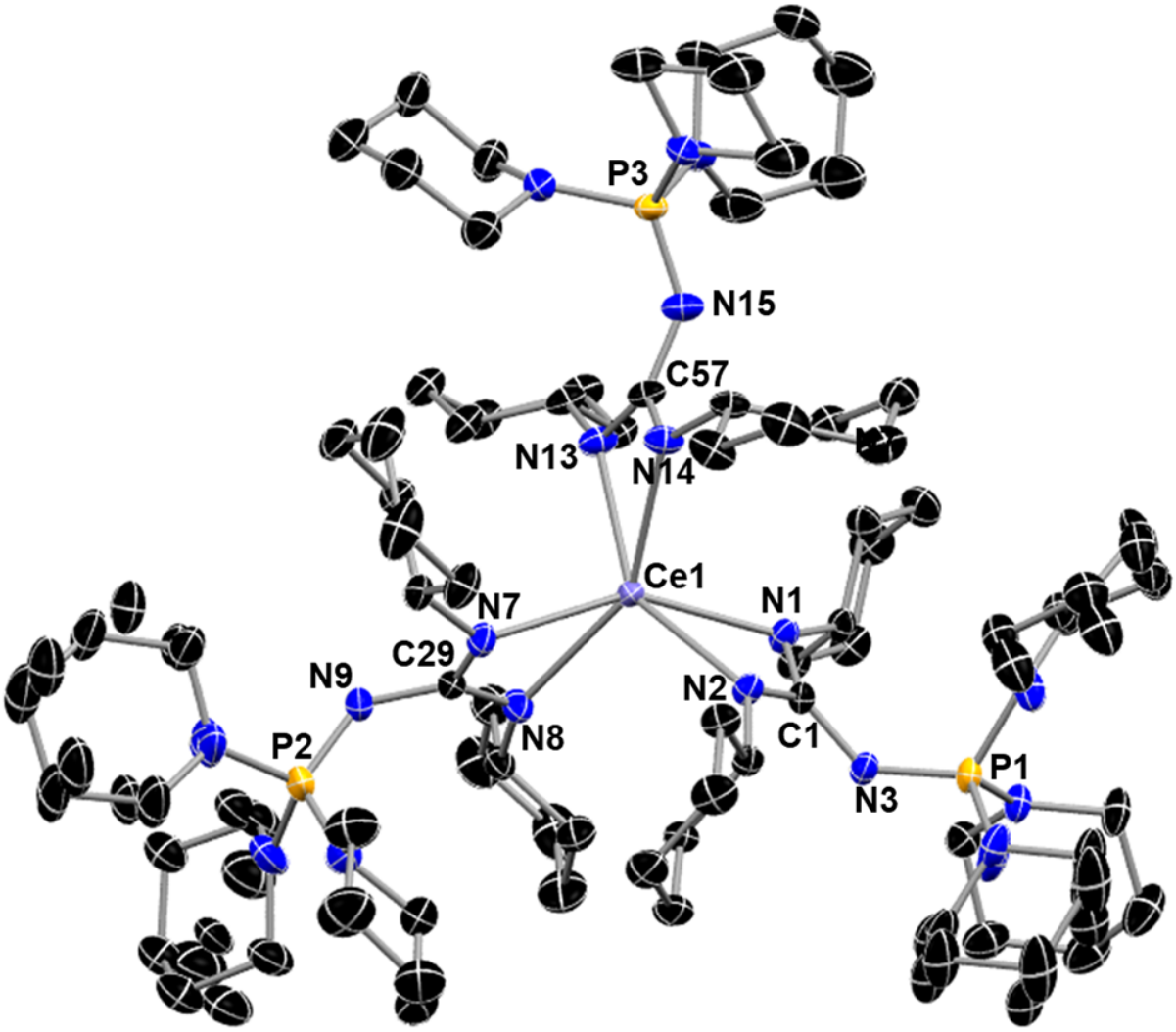

Figure S25. Molecular structure of **1-Ce** with thermal ellipsoids shown at 50% probability; H atoms are omitted for clarity.

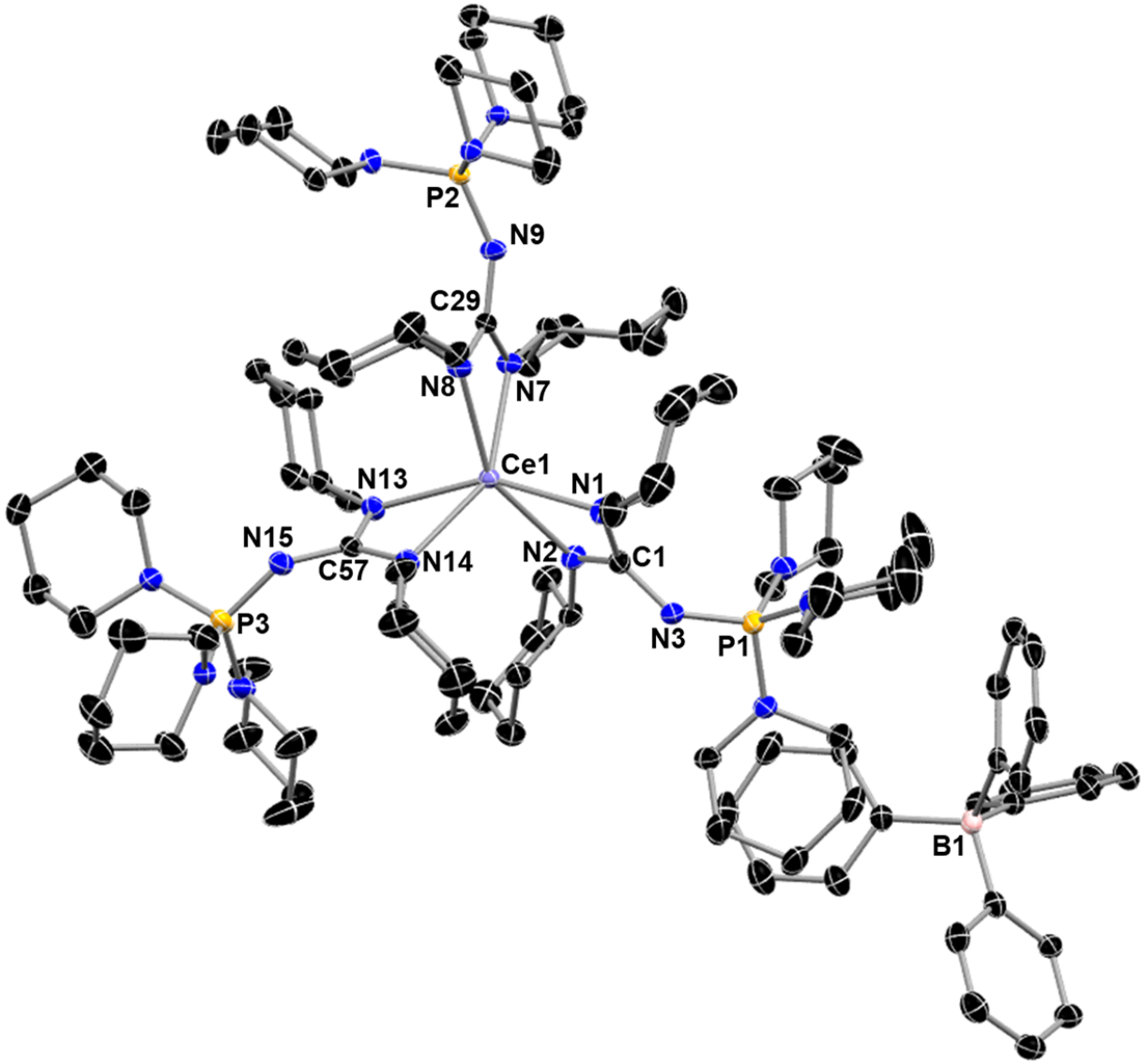

Figure S26. Molecular structure of **2-Ce** with thermal ellipsoids shown at 50% probability; H atoms are omitted for clarity.

Table S3. Crystallographic Data and Structure Refinement for **1-K**, **1-Ce**, and **2-Ce**

	1-K	1-Ce	2-Ce
Empirical Formula	$C_{72}H_{136}K_2N_{12}O_4P_2$	$C_{89}H_{168}CeN_{18}P_3$	$C_{123}H_{214}BCeN_{18}P_3$
Formula Weight	1347.06	1723.43	2188.95
Temperature (K)	100(2)	100(1)	100.0(2)
Crystal System	monoclinic	triclinic	triclinic
Space Group	*C*2/*c*	P-$\bar{1}$	P-$\bar{1}$
a/Å	16.8786(16)	16.104(2)	13.438(2)
b/Å	20.720(2)	16.452(2)	19.340(3)
c/Å	22.088(2)	20.980(3)	22.773(4)
α/°	90	81.638(5)	95.893(7)
β/°	92.938(4)	88.524(6)	99.060(7)
γ/°	90	61.054(4)	91.156(7)
Volume/Å3	7714.6(13)	4806.0(11)	5809.9(17)
Z	4	2	2
Z'	0.5	1	1
ρ(g/cm3)	1.183	1.191	1.251
μ(mm-1)	0.218	0.575	0.490
F(000)	3008.0	1862.0	2372
Crystal Size/mm3	0.341 x 0.189 x 0.137	0.591 x 0.351 x 0.342	0.34 x 0.167 x 0.133
Radiation	MoKα (λ=0.71073)	MoKα (λ=0.71073)	MoKα (λ=0.71073)
2θ range for data collection(°)	4.34 to 49.43	4.50 to 62.01	4.41 to 57.42
Index Ranges	-19 ≤ h ≤ 19, -24 ≤ k ≤24, -25 ≤ 1 ≤ 25	-22 ≤ h ≤ 23, -23 ≤ k ≤23, -30 ≤ 1 ≤ 28	-18 ≤ h ≤ 18, -25 ≤ k ≤26, -30 ≤ 1 ≤ 29
Reflections Collected	61569	148026	120674
Independent Reflections	6615 [Rint = 0.1348, Rsigma = 0.0602]]	30201 [Rint = 0.0431, Rsigma = 0.0390]]	29760 [Rint = 0.0534, Rsigma = 0.0524]]
Data/Restraints/ Parameters	6615/885/542	30201/1264/1137	29760/57/1205
Goodness-of-Fit on F2	2.808	1.024	1.032
Final R Indexes [I>=2σ (I)]	R1=0.1627, wR2=0.4009	R1=0.0409, wR2=0.0958	R1=0.0437, wR2=0.1005
Final R Indexes [all data]	R1=0.1964, wR2=0.4197	R1=0.0523, wR2=0.1015	R1=0.0574, wR2=0.1066
Largest Diff. Peak/Hole/ (e Å3)	1.17/-0.64	1.29/-0.72	1.15/-0.74
Flack Parameter	-	-	-
Completeness to 2θ	100	100	100

Table S4. Lengths for **1-KAtom**	**Atom**	**Length/ Å**	**Atom**	**Atom**	**Length/ Å**
K1	O1_5	2.814(14)	K1	O1_5	2.814(14)
K1	O1_6	2.999(14)	K1	O1_6	2.999(14)
K1	O1_8	2.811(15)	K1	O1_8	2.811(15)
K1	O1_9	2.998(15)	K1	O1_9	2.998(15)
K1	N1_10	2.855(10)	K1	N1_10	2.855(10)
K1	N1_11	2.900(10)	K1	N1_11	2.900(10)
K1	N1_12	2.854(10)	K1	N1_12	2.854(10)
K1	N1_13	2.895(10)	K1	N1_13	2.895(10)
K1	N1_10#1	2.765(10)	K1	N1_10#1	2.765(10)
K1	N1_11#1	2.745(12)	K1	N1_11#1	2.745(12)
K1	N1_12#1	2.882(11)	K1	N1_12#1	2.882(11)
K1	N1_13#1	2.711(9)	K1	N1_13#1	2.711(9)
P1	N2_3	1.659(10)	P1	N2_3	1.659(10)
P1	N2	1.550(7)	P1	N2	1.550(7)
P1	N3_4	1.645(9)	P1	N3_4	1.645(9)
P1	N4_7	1.669(10)	P1	N4_7	1.669(10)
O1_5	C1_5	1.40(2)	O1_5	C1_5	1.40(2)
O1_5	C4_5	1.44(3)	O1_5	C4_5	1.44(3)
O1_6	C1_6	1.40(2)	O1_6	C1_6	1.40(2)
O1_6	C4_6	1.44(2)	O1_6	C4_6	1.44(2)
O1_8	C1_8	1.40(3)	O1_8	C1_8	1.40(3)
O1_8	C4_8	1.44(2)	O1_8	C4_8	1.44(2)
O1_9	C1_9	1.40(2)	O1_9	C1_9	1.40(2)
O1_9	C4_9	1.44(3)	O1_9	C4_9	1.44(3)
N2_3	C2_3	1.416(18)	N2_3	C2_3	1.416(18)
N2_3	C6_3	1.478(13)	N2_3	C6_3	1.478(13)
N2	C7	1.411(13)	N2	C7	1.411(13)

Table S4. Lengths for **1-KAtom**	**Atom**	**Length/ Å**	**Atom**	**Atom**	**Length/ Å**
N3_4	C2_4	1.513(15)	N3_4	C2_4	1.513(15)
N3_4	C6_4	1.498(13)	N3_4	C6_4	1.498(13)
N4_7	C2_7	1.465(16)	N4_7	C2_7	1.465(16)
N4_7	C6_7	1.511(14)	N4_7	C6_7	1.511(14)
N1_10	C7	1.341(10)	N1_10	C7	1.341(10)
N1_10	C1_10	1.482(13)	N1_10	C1_10	1.482(13)
N1_11	C7	1.343(11)	N1_11	C7	1.343(11)
N1_11	C1_11	1.481(11)	N1_11	C1_11	1.481(11)
N1_12	C7	1.341(9)	N1_12	C7	1.341(9)
N1_12	C1_12	1.482(11)	N1_12	C1_12	1.482(11)
N1_13	C7	1.341(10)	N1_13	C7	1.341(10)
N1_13	C1_13	1.483(12)	N1_13	C1_13	1.483(12)
C1_3	C3_3	1.541(17)	C1_3	C3_3	1.541(17)
C1_3	C5_3	1.47(2)	C1_3	C5_3	1.47(2)
C2_3	C3_3	1.42(3)	C2_3	C3_3	1.42(3)
C5_3	C6_3	1.470(17)	C5_3	C6_3	1.470(17)
C1_4	C3_4	1.482(16)	C1_4	C3_4	1.482(16)
C1_4	C5_4	1.495(16)	C1_4	C5_4	1.495(16)
C2_4	C3_4	1.451(16)	C2_4	C3_4	1.451(16)
C5_4	C6_4	1.513(14)	C5_4	C6_4	1.513(14)
C1_5	C2_5	1.50(2)	C1_5	C2_5	1.50(2)
C2_5	C3_5	1.53(3)	C2_5	C3_5	1.53(3)
C3_5	C4_5	1.47(3)	C3_5	C4_5	1.47(3)
C1_6	C2_6	1.50(2)	C1_6	C2_6	1.50(2)
C2_6	C3_6	1.53(3)	C2_6	C3_6	1.53(3)

Table S5. Angles for **1-K**

Atom	Atom	Atom	Angle/˚
O1_5	K1	O1_6	65.8(4)
O1_5	K1	O1_8	16.5(4)
O1_5	K1	O1_9	69.4(4)
O1_5	K1	N1_10	104.8(3)
O1_5	K1	N1_11	105.5(4)
O1_5	K1	N1_12	128.7(4)
O1_5	K1	N1_13	131.4(3)
O1_5	K1	C7	109.6(3)
O1_5	K1	N1_10$^{\#1}$	110.1(3)
O1_5	K1	N1_11$^{\#1}$	109.2(4)
O1_5	K1	N1_12$^{\#1}$	139.5(3)
O1_5	K1	N1_13$^{\#1}$	137.4(4)
O1_6	K1	O1_8	68.6(4)
O1_6	K1	O1_9	10.2(4)
O1_6	K1	N1_10	146.1(4)
O1_6	K1	N1_11	146.5(4)
O1_6	K1	N1_12	111.6(3)
O1_6	K1	N1_13	115.1(3)
O1_6	K1	N1_10$^{\#1}$	124.2(3)
O1_6	K1	N1_11$^{\#1}$	123.3(4)
O1_6	K1	N1_12$^{\#1}$	97.5(3)
O1_6	K1	N1_13$^{\#1}$	95.9(3)
O1_8	K1	O1_9	74.9(4)
O1_8	K1	N1_10	112.0(4)
O1_8	K1	N1_11	112.7(4)
O1_8	K1	N1_12	144.4(4)
O1_8	K1	N1_13	146.6(4)
O1_8	K1	N1_10$^{\#1}$	94.8(4)
O1_8	K1	N1_11$^{\#1}$	93.8(4)
O1_8	K1	N1_12$^{\#1}$	124.1(4)
O1_8	K1	N1_13$^{\#1}$	122.2(4)
O1_9	K1	N1_10	136.9(3)
O1_9	K1	N1_11	137.2(4)
O1_9	K1	N1_12	101.8(3)
O1_9	K1	N1_13	105.3(3)
O1_9	K1	N1_10$^{\#1}$	133.2(3)
O1_9	K1	N1_11$^{\#1}$	132.3(3)
O1_9	K1	N1_12$^{\#1}$	100.9(3)

Atom	Atom	Atom	Angle/˚
O1_5	K1	O1_6	65.8(4)
O1_5	K1	O1_8	16.5(4)
O1_5	K1	O1_9	69.4(4)
O1_5	K1	N1_10	104.8(3)
O1_5	K1	N1_11	105.5(4)
O1_5	K1	N1_12	128.7(4)
O1_5	K1	N1_13	131.4(3)
O1_5	K1	C7	109.6(3)
O1_5	K1	N1_10$^{\#1}$	110.1(3)
O1_5	K1	N1_11$^{\#1}$	109.2(4)
O1_5	K1	N1_12$^{\#1}$	139.5(3)
O1_5	K1	N1_13$^{\#1}$	137.4(4)
O1_6	K1	O1_8	68.6(4)
O1_6	K1	O1_9	10.2(4)
O1_6	K1	N1_10	146.1(4)
O1_6	K1	N1_11	146.5(4)
O1_6	K1	N1_12	111.6(3)
O1_6	K1	N1_13	115.1(3)
O1_6	K1	N1_10$^{\#1}$	124.2(3)
O1_6	K1	N1_11$^{\#1}$	123.3(4)
O1_6	K1	N1_12$^{\#1}$	97.5(3)
O1_6	K1	N1_13$^{\#1}$	95.9(3)
O1_8	K1	O1_9	74.9(4)
O1_8	K1	N1_10	112.0(4)
O1_8	K1	N1_11	112.7(4)
O1_8	K1	N1_12	144.4(4)
O1_8	K1	N1_13	146.6(4)
O1_8	K1	N1_10$^{\#1}$	94.8(4)
O1_8	K1	N1_11$^{\#1}$	93.8(4)
O1_8	K1	N1_12$^{\#1}$	124.1(4)
O1_8	K1	N1_13$^{\#1}$	122.2(4)
O1_9	K1	N1_10	136.9(3)
O1_9	K1	N1_11	137.2(4)
O1_9	K1	N1_12	101.8(3)
O1_9	K1	N1_13	105.3(3)
O1_9	K1	N1_10$^{\#1}$	133.2(3)
O1_9	K1	N1_11$^{\#1}$	132.3(3)
O1_9	K1	N1_12$^{\#1}$	100.9(3)

Atom	Atom	Atom	Angle/˚
O1_9	K1	N1_13$^{\#1}$	99.5(3)
N1_10	K1	N1_12	47.1(2)
N1_10	K1	N1_13	45.2(2)
N1_10	K1	N1_10$^{\#1}$	89.7(3)
N1_10	K1	N1_11$^{\#1}$	90.6(3)
N1_10	K1	N1_12$^{\#1}$	107.7(3)
N1_10	K1	N1_13$^{\#1}$	109.8(3)
N1_11	K1	N1_12	46.8(2)
N1_11	K1	N1_13	44.8(2)
N1_10$^{\#1}$	K1	N1_11	89.3(3)
N1_11	K1	N1_11$^{\#1}$	90.2(3)
N1_11	K1	N1_12$^{\#1}$	107.0(3)
N1_11	K1	N1_13$^{\#1}$	109.1(3)
N1_12	K1	N1_13	4.0(3)
N1_10$^{\#1}$	K1	N1_12	111.0(3)
N1_11$^{\#1}$	K1	N1_12	112.1(3)
N1_12	K1	N1_12$^{\#1}$	91.4(3)
N1_12	K1	N1_13$^{\#1}$	93.4(3)
N1_10$^{\#1}$	K1	N1_13	107.1(3)
N1_11$^{\#1}$	K1	N1_13	108.2(3)
N1_12$^{\#1}$	K1	N1_13	89.0(3)
N1_13	K1	N1_13$^{\#1}$	91.1(3)
N1_10$^{\#1}$	K1	N1_11$^{\#1}$	1.2(3)
N1_10$^{\#1}$	K1	N1_12$^{\#1}$	47.6(2)
N1_10$^{\#1}$	K1	N1_13$^{\#1}$	47.6(2)
N1_11$^{\#1}$	K1	N1_12$^{\#1}$	47.8(2)
N1_11$^{\#1}$	K1	N1_13$^{\#1}$	47.8(2)
N1_12$^{\#1}$	K1	N1_13$^{\#1}$	2.2(3)
N2_3	P1	N2	110.1(5)
N2_3	P1	N3_4	101.0(4)
N2_3	P1	N4_7	109.4(5)
N2	P1	N3_4	121.7(4)
N2	P1	N4_7	111.6(5)
N3_4	P1	N4_7	102.1(4)
K1	O1_5	C1_5	102.5(10)
K1	O1_5	C4_5	139.8(11)
C1_5	O1_5	C4_5	108.0(13)
K1	O1_6	C1_6	119.3(11)
K1	O1_6	C4_6	125.0(10)

Atom	Atom	Atom	Angle/˚
O1_9	K1	N1_13$^{\#1}$	99.5(3)
N1_10	K1	N1_12	47.1(2)
N1_10	K1	N1_13	45.2(2)
N1_10	K1	N1_10$^{\#1}$	89.7(3)
N1_10	K1	N1_11$^{\#1}$	90.6(3)
N1_10	K1	N1_12$^{\#1}$	107.7(3)
N1_10	K1	N1_13$^{\#1}$	109.8(3)
N1_11	K1	N1_12	46.8(2)
N1_11	K1	N1_13	44.8(2)
N1_10$^{\#1}$	K1	N1_11	89.3(3)
N1_11	K1	N1_11$^{\#1}$	90.2(3)
N1_11	K1	N1_12$^{\#1}$	107.0(3)
N1_11	K1	N1_13$^{\#1}$	109.1(3)
N1_12	K1	N1_13	4.0(3)
N1_10$^{\#1}$	K1	N1_12	111.0(3)
N1_11$^{\#1}$	K1	N1_12	112.1(3)
N1_12	K1	N1_12$^{\#1}$	91.4(3)
N1_12	K1	N1_13$^{\#1}$	93.4(3)
N1_10$^{\#1}$	K1	N1_13	107.1(3)
N1_11$^{\#1}$	K1	N1_13	108.2(3)
N1_12$^{\#1}$	K1	N1_13	89.0(3)
N1_13	K1	N1_13$^{\#1}$	91.1(3)
N1_10$^{\#1}$	K1	N1_11$^{\#1}$	1.2(3)
N1_10$^{\#1}$	K1	N1_12$^{\#1}$	47.6(2)
N1_10$^{\#1}$	K1	N1_13$^{\#1}$	47.6(2)
N1_11$^{\#1}$	K1	N1_12$^{\#1}$	47.8(2)
N1_11$^{\#1}$	K1	N1_13$^{\#1}$	47.8(2)
N1_12$^{\#1}$	K1	N1_13$^{\#1}$	2.2(3)
N2_3	P1	N2	110.1(5)
N2_3	P1	N3_4	101.0(4)
N2_3	P1	N4_7	109.4(5)
N2	P1	N3_4	121.7(4)
N2	P1	N4_7	111.6(5)
N3_4	P1	N4_7	102.1(4)
K1	O1_5	C1_5	102.5(10)
K1	O1_5	C4_5	139.8(11)
C1_5	O1_5	C4_5	108.0(13)
K1	O1_6	C1_6	119.3(11)
K1	O1_6	C4_6	125.0(10)

Atom	Atom	Atom	Angle/˚
C1_6	O1_6	C4_6	107.7(13)
K1	O1_8	C1_8	134.9(10)
K1	O1_8	C4_8	112.6(13)
C1_8	O1_8	C4_8	107.9(14)
K1	O1_9	C1_9	99.0(11)
K1	O1_9	C4_9	144.4(12)
C1_9	O1_9	C4_9	107.9(14)
P1	N2_3	C2_3	119.0(9)
P1	N2_3	C6_3	118.7(8)
C2_3	N2_3	C6_3	112.3(10)
P1	N2	C7	127.8(7)
P1	N3_4	C2_4	119.6(7)
P1	N3_4	C6_4	117.9(6)
C2_4	N3_4	C6_4	109.3(8)
P1	N4_7	C2_7	124.1(8)
P1	N4_7	C6_7	127.3(7)
C2_7	N4_7	C6_7	108.4(9)
K1	N1_10	C7	87.0(5)

Atom	Atom	Atom	Angle/˚
C1_6	O1_6	C4_6	107.7(13)
K1	O1_8	C1_8	134.9(10)
K1	O1_8	C4_8	112.6(13)
C1_8	O1_8	C4_8	107.9(14)
K1	O1_9	C1_9	99.0(11)
K1	O1_9	C4_9	144.4(12)
C1_9	O1_9	C4_9	107.9(14)
P1	N2_3	C2_3	119.0(9)
P1	N2_3	C6_3	118.7(8)
C2_3	N2_3	C6_3	112.3(10)
P1	N2	C7	127.8(7)
P1	N3_4	C2_4	119.6(7)
P1	N3_4	C6_4	117.9(6)
C2_4	N3_4	C6_4	109.3(8)
P1	N4_7	C2_7	124.1(8)
P1	N4_7	C6_7	127.3(7)
C2_7	N4_7	C6_7	108.4(9)
K1	N1_10	C7	87.0(5)

Symmetry transformations used to generate equivalent atoms:
#1: -X, +Y, 0.5-Z;

Table S6. Lengths for **1-Ce**

Atom	Atom	Length/Å
Ce1	N1	2.4815(17)
Ce1	N2	2.5007(18)
Ce1	N7	2.5057(17)
Ce1	N8	2.5019(19)
Ce1	N13	2.508(2)
Ce1	N14	2.484(2)
P1	N5_1	1.6597(15)
P1	N5_2	1.671(5)
P1	N3	1.5378(17)
P1	N5	1.658(6)
P1	N5_3	1.656(7)
P1	N5_8	1.679(10)
P2	N9	1.540(2)
P2	N5_11	1.661(3)
P2	N5_13	1.663(2)
P2	N5_14	1.663(3)
P2	N5_9	1.682(5)
P2	N5_12	1.692(6)
P3	N5_4	1.6529(16)

Atom	Atom	Length/Å
Ce1	N1	2.4815(17)
Ce1	N2	2.5007(18)
Ce1	N7	2.5057(17)
Ce1	N8	2.5019(19)
Ce1	N13	2.508(2)
Ce1	N14	2.484(2)
P1	N5_1	1.6597(15)
P1	N5_2	1.671(5)
P1	N3	1.5378(17)
P1	N5	1.658(6)
P1	N5_3	1.656(7)
P1	N5_8	1.679(10)
P2	N9	1.540(2)
P2	N5_11	1.661(3)
P2	N5_13	1.663(2)
P2	N5_14	1.663(3)
P2	N5_9	1.682(5)
P2	N5_12	1.692(6)
P3	N5_4	1.6529(16)

Atom	Atom	Length/Å
P3	N5_7	1.6548(18)
P3	N5_10	1.6699(18)
P3	N15	1.535(2)
N1	C1	1.344(3)
N1	C2	1.449(2)
N5_1	C19_1	1.464(2)
N5_1	C23_1	1.463(2)
N2	C1	1.343(2)
N2	C8	1.450(3)
N5_2	C19_2	1.463(7)
N5_2	C23_2	1.466(6)
N3	C1	1.388(3)
N5_3	C23_3	1.467(9)
N5_3	C19_3	1.464(9)
N5_4	C23_4	1.461(3)
N5_4	C19_4	1.466(2)
N5	C23	1.495(9)
N5	C19	1.462(10)
N5_7	C19_7	1.465(3)
N5_7	C23_7	1.464(3)
N5_8	C19_8	1.466(14)
N5_8	C23_8	1.468(12)
N7	C30	1.454(3)
N7	C29	1.343(3)
N5_9	C19_9	1.467(9)
N5_9	C23_9	1.467(9)
N8	C29	1.337(3)
N8	C36	1.450(3)
N5_10	C19_10	1.465(2)
N5_10	C23_10	1.468(3)
N9	C29	1.396(2)
N5_11	C19_11	1.467(5)
N5_11	C23_11	1.467(4)

Atom	Atom	Length/Å
P3	N5_7	1.6548(18)
P3	N5_10	1.6699(18)
P3	N15	1.535(2)
N1	C1	1.344(3)
N1	C2	1.449(2)
N5_1	C19_1	1.464(2)
N5_1	C23_1	1.463(2)
N2	C1	1.343(2)
N2	C8	1.450(3)
N5_2	C19_2	1.463(7)
N5_2	C23_2	1.466(6)
N3	C1	1.388(3)
N5_3	C23_3	1.467(9)
N5_3	C19_3	1.464(9)
N5_4	C23_4	1.461(3)
N5_4	C19_4	1.466(2)
N5	C23	1.495(9)
N5	C19	1.462(10)
N5_7	C19_7	1.465(3)
N5_7	C23_7	1.464(3)
N5_8	C19_8	1.466(14)
N5_8	C23_8	1.468(12)
N7	C30	1.454(3)
N7	C29	1.343(3)
N5_9	C19_9	1.467(9)
N5_9	C23_9	1.467(9)
N8	C29	1.337(3)
N8	C36	1.450(3)
N5_10	C19_10	1.465(2)
N5_10	C23_10	1.468(3)
N9	C29	1.396(2)
N5_11	C19_11	1.467(5)
N5_11	C23_11	1.467(4)

Table S7. Angles for **1-Ce**

Atom	Atom	Atom	Angle/˚
N1	Ce1	N2	53.65(5)
N1	Ce1	N7	149.58(7)
N1	Ce1	N8	107.59(6)
N1	Ce1	N13	104.09(6)
N1	Ce1	N14	100.66(6)
N2	Ce1	N7	104.44(6)
N2	Ce1	N8	104.73(6)

Atom	Atom	Atom	Angle/˚
N1	Ce1	N2	53.65(5)
N1	Ce1	N7	149.58(7)
N1	Ce1	N8	107.59(6)
N1	Ce1	N13	104.09(6)
N1	Ce1	N14	100.66(6)
N2	Ce1	N7	104.44(6)
N2	Ce1	N8	104.73(6)

Atom	Atom	Atom	Angle/˚
N2	Ce1	N13	145.50(6)
N2	Ce1	N14	100.85(6)
N7	Ce1	N8	53.23(6)
N7	Ce1	N13	104.48(6)
N7	Ce1	N14	104.59(6)
N8	Ce1	N13	107.51(6)
N8	Ce1	N14	149.62(6)
N13	Ce1	N14	53.52(6)
N5_1	P1	N5_2	113.18(17)
N5_1	P1	N3	109.89(8)
N5_1	P1	N5	102.5(2)
N5_1	P1	N5_3	106.5(3)
N5_1	P1	N5_8	107.2(3)
N5_2	P1	N3	110.50(17)
N3	P1	N5	118.2(2)
N3	P1	N5_3	122.5(3)
N3	P1	N5_8	109.2(3)
N9	P2	N5_11	112.04(15)
N9	P2	N5_13	119.91(10)
N9	P2	N5_14	107.95(14)
N5_9	P2	N9	111.6(2)
N9	P2	N5_12	111.8(3)
N5_11	P2	N5_13	101.88(14)
N5_13	P2	N5_14	108.16(15)
N5_9	P2	N5_13	97.9(2)
N5_12	P2	N5_13	100.7(3)
N5_4	P3	N5_7	107.22(9)
N5_4	P3	N5_10	100.92(8)
N5_4	P3	N15	119.20(10)
N5_7	P3	N5_10	107.94(9)
N5_7	P3	N15	107.56(10)
N5_10	P3	N15	113.37(9)
Ce1	N1	C1	95.16(11)
Ce1	N1	C2	141.47(13)
C1	N1	C2	122.28(17)
P1	N5_1	C19_1	121.27(11)
P1	N5_1	C23_1	125.12(13)
C19_1	N5_1	C23_1	112.69(15)
Ce1	N2	C1	94.32(11)
Ce1	N2	C8	136.55(12)
C1	N2	C8	119.43(18)
P1	N5_2	C19_2	119.7(3)
P1	N5_2	C23_2	120.3(4)

Atom	Atom	Atom	Angle/˚
N2	Ce1	N13	145.50(6)
N2	Ce1	N14	100.85(6)
N7	Ce1	N8	53.23(6)
N7	Ce1	N13	104.48(6)
N7	Ce1	N14	104.59(6)
N8	Ce1	N13	107.51(6)
N8	Ce1	N14	149.62(6)
N13	Ce1	N14	53.52(6)
N5_1	P1	N5_2	113.18(17)
N5_1	P1	N3	109.89(8)
N5_1	P1	N5	102.5(2)
N5_1	P1	N5_3	106.5(3)
N5_1	P1	N5_8	107.2(3)
N5_2	P1	N3	110.50(17)
N3	P1	N5	118.2(2)
N3	P1	N5_3	122.5(3)
N3	P1	N5_8	109.2(3)
N9	P2	N5_11	112.04(15)
N9	P2	N5_13	119.91(10)
N9	P2	N5_14	107.95(14)
N5_9	P2	N9	111.6(2)
N9	P2	N5_12	111.8(3)
N5_11	P2	N5_13	101.88(14)
N5_13	P2	N5_14	108.16(15)
N5_9	P2	N5_13	97.9(2)
N5_12	P2	N5_13	100.7(3)
N5_4	P3	N5_7	107.22(9)
N5_4	P3	N5_10	100.92(8)
N5_4	P3	N15	119.20(10)
N5_7	P3	N5_10	107.94(9)
N5_7	P3	N15	107.56(10)
N5_10	P3	N15	113.37(9)
Ce1	N1	C1	95.16(11)
Ce1	N1	C2	141.47(13)
C1	N1	C2	122.28(17)
P1	N5_1	C19_1	121.27(11)
P1	N5_1	C23_1	125.12(13)
C19_1	N5_1	C23_1	112.69(15)
Ce1	N2	C1	94.32(11)
Ce1	N2	C8	136.55(12)
C1	N2	C8	119.43(18)
P1	N5_2	C19_2	119.7(3)
P1	N5_2	C23_2	120.3(4)

Atom	Atom	Atom	Angle/˚
C19_2	N5_2	C23_2	112.7(5)
P1	N3	C1	133.47(16)
P1	N5_3	C19_3	122.6(5)
P1	N5_3	C23_3	117.0(5)
C19_3	N5_3	C23_3	111.8(5)
P3	N5_4	C19_4	122.67(13)
P3	N5_4	C23_4	118.06(14)
C19_4	N5_4	C23_4	112.69(15)
C19	N5	C23	111.6(5)
P1	N5	C19	125.0(5)
P1	N5	C23	117.9(5)
P3	N5_7	C19_7	123.73(16)
P3	N5_7	C23_7	123.54(15)
C19_7	N5_7	C23_7	112.73(17)
C19_8	N5_8	C23_8	111.6(9)
P1	N5_8	C19_8	118.0(6)
P1	N5_8	C23_8	123.4(7)
Ce1	N7	C29	94.68(11)
C29	N7	C30	121.13(16)
Ce1	N7	C30	132.47(15)
P2	N5_9	C23_9	122.5(4)
P2	N5_9	C19_9	125.8(5)
C19_9	N5_9	C23_9	111.6(5)
Ce1	N8	C29	95.00(13)
C29	N8	C36	121.32(17)
Ce1	N8	C36	142.17(13)
P3	N5_10	C23_10	124.62(13)
C19_10	N5_10	C23_10	111.29(17)
P3	N5_10	C19_10	119.22(14)
P2	N9	C29	129.21(17)
C19_11	N5_11	C23_11	111.7(3)
P2	N5_11	C19_11	120.6(2)
P2	N5_11	C23_11	115.7(3)
P2	N5_12	C23_12	129.3(4)
P2	N5_12	C19_12	118.5(6)
C19_12	N5_12	C23_12	111.2(5)
C19_13	N5_13	C23_13	110.92(18)
P2	N5_13	C19_13	119.33(14)
P2	N5_13	C23_13	120.01(19)
P2	N5_14	C23_14	119.6(3)
C19_14	N5_14	C23_14	112.2(3)
P2	N5_14	C19_14	122.5(2)
Ce1	N13	C57	94.29(13)

Atom	Atom	Atom	Angle/˚
C19_2	N5_2	C23_2	112.7(5)
P1	N3	C1	133.47(16)
P1	N5_3	C19_3	122.6(5)
P1	N5_3	C23_3	117.0(5)
C19_3	N5_3	C23_3	111.8(5)
P3	N5_4	C19_4	122.67(13)
P3	N5_4	C23_4	118.06(14)
C19_4	N5_4	C23_4	112.69(15)
C19	N5	C23	111.6(5)
P1	N5	C19	125.0(5)
P1	N5	C23	117.9(5)
P3	N5_7	C19_7	123.73(16)
P3	N5_7	C23_7	123.54(15)
C19_7	N5_7	C23_7	112.73(17)
C19_8	N5_8	C23_8	111.6(9)
P1	N5_8	C19_8	118.0(6)
P1	N5_8	C23_8	123.4(7)
Ce1	N7	C29	94.68(11)
C29	N7	C30	121.13(16)
Ce1	N7	C30	132.47(15)
P2	N5_9	C23_9	122.5(4)
P2	N5_9	C19_9	125.8(5)
C19_9	N5_9	C23_9	111.6(5)
Ce1	N8	C29	95.00(13)
C29	N8	C36	121.32(17)
Ce1	N8	C36	142.17(13)
P3	N5_10	C23_10	124.62(13)
C19_10	N5_10	C23_10	111.29(17)
P3	N5_10	C19_10	119.22(14)
P2	N9	C29	129.21(17)
C19_11	N5_11	C23_11	111.7(3)
P2	N5_11	C19_11	120.6(2)
P2	N5_11	C23_11	115.7(3)
P2	N5_12	C23_12	129.3(4)
P2	N5_12	C19_12	118.5(6)
C19_12	N5_12	C23_12	111.2(5)
C19_13	N5_13	C23_13	110.92(18)
P2	N5_13	C19_13	119.33(14)
P2	N5_13	C23_13	120.01(19)
P2	N5_14	C23_14	119.6(3)
C19_14	N5_14	C23_14	112.2(3)
P2	N5_14	C19_14	122.5(2)
Ce1	N13	C57	94.29(13)

Atom	Atom	Atom	Angle/˚
Ce1	N13	C58	142.22(15)
C57	N13	C58	121.7(2)
Ce1	N14	C64	134.97(14)
C57	N14	C64	119.54(19)
Ce1	N14	C57	95.38(13)
P3	N15	C57	138.59(17)
N1	C1	N2	113.62(18)
N1	C1	N3	124.16(16)
N2	C1	N3	122.05(18)
N5_1	C19_1	C20_1	110.18(16)
C3	C2	C7	109.39(17)
N1	C2	C7	108.91(17)
N1	C2	C3	111.83(16)
C19_1	C20_1	C21_1	110.39(19)
C2	C3	C4	112.38(17)
C20_1	C21_1	C22_1	110.24(19)
C3	C4	C5	110.9(2)
C21_1	C22_1	C23_1	111.4(2)
C4	C5	C6	110.8(2)
N5_1	C23_1	C22_1	112.04(18)
C5	C6	C7	111.1(2)
N5_2	C19_2	C20_2	109.9(4)
C2	C7	C6	112.26(19)
C19_2	C20_2	C21_2	110.8(4)

Atom	Atom	Atom	Angle/˚
Ce1	N13	C58	142.22(15)
C57	N13	C58	121.7(2)
Ce1	N14	C64	134.97(14)
C57	N14	C64	119.54(19)
Ce1	N14	C57	95.38(13)
P3	N15	C57	138.59(17)
N1	C1	N2	113.62(18)
N1	C1	N3	124.16(16)
N2	C1	N3	122.05(18)
N5_1	C19_1	C20_1	110.18(16)
C3	C2	C7	109.39(17)
N1	C2	C7	108.91(17)
N1	C2	C3	111.83(16)
C19_1	C20_1	C21_1	110.39(19)
C2	C3	C4	112.38(17)
C20_1	C21_1	C22_1	110.24(19)
C3	C4	C5	110.9(2)
C21_1	C22_1	C23_1	111.4(2)
C4	C5	C6	110.8(2)
N5_1	C23_1	C22_1	112.04(18)
C5	C6	C7	111.1(2)
N5_2	C19_2	C20_2	109.9(4)
C2	C7	C6	112.26(19)
C19_2	C20_2	C21_2	110.8(4)

Table S8. Lengths for **2-Ce**

Atom	Atom	Length/Å
Ce1	N1	2.336(2)
Ce1	N2	2.3592(18)
Ce1	N7	2.3443(19)
Ce1	N8	2.359(2)
Ce1	N13	2.3664(19)
Ce1	N14	2.3668(19)
Ce1	C1	2.830(2)
Ce1	C29	2.839(2)
Ce1	C57	2.825(2)
P1	N3	1.555(2)
P1	N4	1.655(2)
P1	N5	1.663(2)
P1	N6	1.634(2)
P2	N9	1.543(2)
P2	N10	1.6498(19)
P2	N11	1.6753(19)
P2	N12	1.6533(19)
P3	N15	1.545(2)
P3	N16	1.658(2)
P3	N17	1.656(2)
P3	N18A	1.667(3)
P3	N18B	1.675(3)
N1	C1	1.353(3)
N1	C2	1.458(3)
N2	C1	1.349(3)
N2	C8	1.466(3)
N3	C1	1.352(3)
N4	C14	1.465(3)
N4	C18	1.465(3)
N5	C19	1.469(4)
N5	C23	1.481(4)
N6	C24	1.481(3)
N6	C28	1.452(3)
N7	C29	1.364(3)
N7	C30	1.458(3)
N8	C29	1.355(3)
N8	C36	1.457(3)
N9	C29	1.342(3)

Atom	Atom	Length/Å
Ce1	N1	2.336(2)
Ce1	N2	2.3592(18)
Ce1	N7	2.3443(19)
Ce1	N8	2.359(2)
Ce1	N13	2.3664(19)
Ce1	N14	2.3668(19)
Ce1	C1	2.830(2)
Ce1	C29	2.839(2)
Ce1	C57	2.825(2)
P1	N3	1.555(2)
P1	N4	1.655(2)
P1	N5	1.663(2)
P1	N6	1.634(2)
P2	N9	1.543(2)
P2	N10	1.6498(19)
P2	N11	1.6753(19)
P2	N12	1.6533(19)
P3	N15	1.545(2)
P3	N16	1.658(2)
P3	N17	1.656(2)
P3	N18A	1.667(3)
P3	N18B	1.675(3)
N1	C1	1.353(3)
N1	C2	1.458(3)
N2	C1	1.349(3)
N2	C8	1.466(3)
N3	C1	1.352(3)
N4	C14	1.465(3)
N4	C18	1.465(3)
N5	C19	1.469(4)
N5	C23	1.481(4)
N6	C24	1.481(3)
N6	C28	1.452(3)
N7	C29	1.364(3)
N7	C30	1.458(3)
N8	C29	1.355(3)
N8	C36	1.457(3)
N9	C29	1.342(3)

Atom	Atom	Length/Å
N10	C42	1.473(3)
N10	C46	1.476(3)
N11	C47	1.479(3)
N11	C51	1.480(3)
N12	C52	1.469(3)
N12	C56	1.475(3)
N13	C57	1.349(3)
N13	C58	1.462(3)
N14	C57	1.357(3)
N14	C64	1.463(3)
N15	C57	1.351(3)
N16	C70	1.473(4)
N16	C74	1.494(4)
N17	C75	1.471(4)
N17	C79	1.468(3)
N18A	C80A	1.461(6)
N18A	C84A	1.479(6)
N18B	C84B	1.484(6)
N18B	C80B	1.464(6)
C2	C3	1.521(4)
C2	C7	1.532(4)
C3	C4	1.536(4)
C4	C5	1.508(5)
C5	C6	1.510(5)
C6	C7	1.529(4)
C8	C9	1.532(3)
C8	C13	1.522(3)
C9	C10	1.529(4)
C10	C11	1.522(4)
C11	C12	1.511(4)
C12	C13	1.533(3)
C14	C15	1.531(4)
C15	C16	1.518(4)
C16	C17	1.526(4)
C17	C18	1.517(4)
C19	C20	1.499(4)
C20	C21	1.537(6)
C21	C22	1.518(6)
C22	C23	1.500(6)

Atom	Atom	Length/Å
N10	C42	1.473(3)
N10	C46	1.476(3)
N11	C47	1.479(3)
N11	C51	1.480(3)
N12	C52	1.469(3)
N12	C56	1.475(3)
N13	C57	1.349(3)
N13	C58	1.462(3)
N14	C57	1.357(3)
N14	C64	1.463(3)
N15	C57	1.351(3)
N16	C70	1.473(4)
N16	C74	1.494(4)
N17	C75	1.471(4)
N17	C79	1.468(3)
N18A	C80A	1.461(6)
N18A	C84A	1.479(6)
N18B	C84B	1.484(6)
N18B	C80B	1.464(6)
C2	C3	1.521(4)
C2	C7	1.532(4)
C3	C4	1.536(4)
C4	C5	1.508(5)
C5	C6	1.510(5)
C6	C7	1.529(4)
C8	C9	1.532(3)
C8	C13	1.522(3)
C9	C10	1.529(4)
C10	C11	1.522(4)
C11	C12	1.511(4)
C12	C13	1.533(3)
C14	C15	1.531(4)
C15	C16	1.518(4)
C16	C17	1.526(4)
C17	C18	1.517(4)
C19	C20	1.499(4)
C20	C21	1.537(6)
C21	C22	1.518(6)
C22	C23	1.500(6)

Atom	Atom	Length/Å
C24	C25	1.503(4)
C25	C26	1.514(4)

Atom	Atom	Length/Å
C24	C25	1.503(4)
C25	C26	1.514(4)

Table S9. Angles for **2-Ce**

Atom	Atom	Atom	Angle/˚
N1	Ce1	N2	56.27(6)
N1	Ce1	N7	104.73(7)
N1	Ce1	N8	104.01(7)
N1	Ce1	N13	151.73(7)
N1	Ce1	N14	102.66(7)
N1	Ce1	C1	28.36(6)
N1	Ce1	C29	105.16(7)
N1	Ce1	C57	130.40(7)
N2	Ce1	N7	105.06(7)
N2	Ce1	N8	151.52(7)
N2	Ce1	N13	106.15(6)
N2	Ce1	N14	102.49(7)
N2	Ce1	C1	28.32(6)
N2	Ce1	C29	129.77(7)
N2	Ce1	C57	110.23(7)
N7	Ce1	N8	56.82(6)
N7	Ce1	N13	101.25(7)
N7	Ce1	N14	148.76(7)
N7	Ce1	C1	110.49(7)
N7	Ce1	C29	28.53(6)
N7	Ce1	C57	124.47(7)
N8	Ce1	N13	99.41(7)
N8	Ce1	N14	101.99(6)
N8	Ce1	C1	131.13(7)
N8	Ce1	C29	28.34(6)
N8	Ce1	C57	98.22(6)
N13	Ce1	N14	56.50(6)
N13	Ce1	C1	129.11(6)
N13	Ce1	C29	102.99(6)
N13	Ce1	C57	28.40(6)
N14	Ce1	C1	100.75(6)
N14	Ce1	C29	127.72(6)
N14	Ce1	C57	28.60(6)
C1	Ce1	C29	123.86(6)
C1	Ce1	C57	121.02(6)
C29	Ce1	C57	114.80(6)
N3	P1	N4	117.28(10)
N3	P1	N5	112.30(11)

Atom	Atom	Atom	Angle/˚
N1	Ce1	N2	56.27(6)
N1	Ce1	N7	104.73(7)
N1	Ce1	N8	104.01(7)
N1	Ce1	N13	151.73(7)
N1	Ce1	N14	102.66(7)
N1	Ce1	C1	28.36(6)
N1	Ce1	C29	105.16(7)
N1	Ce1	C57	130.40(7)
N2	Ce1	N7	105.06(7)
N2	Ce1	N8	151.52(7)
N2	Ce1	N13	106.15(6)
N2	Ce1	N14	102.49(7)
N2	Ce1	C1	28.32(6)
N2	Ce1	C29	129.77(7)
N2	Ce1	C57	110.23(7)
N7	Ce1	N8	56.82(6)
N7	Ce1	N13	101.25(7)
N7	Ce1	N14	148.76(7)
N7	Ce1	C1	110.49(7)
N7	Ce1	C29	28.53(6)
N7	Ce1	C57	124.47(7)
N8	Ce1	N13	99.41(7)
N8	Ce1	N14	101.99(6)
N8	Ce1	C1	131.13(7)
N8	Ce1	C29	28.34(6)
N8	Ce1	C57	98.22(6)
N13	Ce1	N14	56.50(6)
N13	Ce1	C1	129.11(6)
N13	Ce1	C29	102.99(6)
N13	Ce1	C57	28.40(6)
N14	Ce1	C1	100.75(6)
N14	Ce1	C29	127.72(6)
N14	Ce1	C57	28.60(6)
C1	Ce1	C29	123.86(6)
C1	Ce1	C57	121.02(6)
C29	Ce1	C57	114.80(6)
N3	P1	N4	117.28(10)
N3	P1	N5	112.30(11)

Atom	Atom	Atom	Angle/˚
N3	P1	N6	108.04(11)
N4	P1	N5	101.87(11)
N4	P1	N6	108.16(11)
N5	P1	N6	108.85(11)
N9	P2	N10	119.60(10)
N9	P2	N11	111.70(10)
N9	P2	N12	106.62(10)
N10	P2	N11	104.08(9)
N10	P2	N12	102.74(9)
N11	P2	N12	111.85(9)
N15	P3	N16	108.88(11)
N15	P3	N17	119.56(11)
N15	P3	N18A	110.39(15)
N15	P3	N18B	109.57(16)
N16	P3	N17	103.96(11)
N16	P3	N18A	116.58(15)
N16	P3	N18B	106.5(2)
N17	P3	N18A	97.43(16)
N17	P3	N18B	107.56(17)
Ce1	N1	C1	96.54(13)
Ce1	N1	C2	141.68(14)
C1	N1	C2	121.77(19)
Ce1	N2	C1	95.61(13)
Ce1	N2	C8	136.61(14)
C1	N2	C8	121.53(18)
P1	N3	C1	136.09(18)
P1	N4	C14	118.77(17)
P1	N4	C18	119.37(17)
C14	N4	C18	111.9(2)
P1	N5	C19	117.33(18)
P1	N5	C23	123.3(2)
C19	N5	C23	112.6(2)
P1	N6	C24	120.93(17)
P1	N6	C28	125.90(16)
C24	N6	C28	112.9(2)
Ce1	N7	C29	96.32(12)
Ce1	N7	C30	141.90(14)
C29	N7	C30	120.07(17)
Ce1	N8	C29	95.91(13)
Ce1	N8	C36	140.82(13)
C29	N8	C36	122.35(18)
P2	N9	C29	148.54(17)
P2	N10	C42	123.08(14)

Atom	Atom	Atom	Angle/˚
N3	P1	N6	108.04(11)
N4	P1	N5	101.87(11)
N4	P1	N6	108.16(11)
N5	P1	N6	108.85(11)
N9	P2	N10	119.60(10)
N9	P2	N11	111.70(10)
N9	P2	N12	106.62(10)
N10	P2	N11	104.08(9)
N10	P2	N12	102.74(9)
N11	P2	N12	111.85(9)
N15	P3	N16	108.88(11)
N15	P3	N17	119.56(11)
N15	P3	N18A	110.39(15)
N15	P3	N18B	109.57(16)
N16	P3	N17	103.96(11)
N16	P3	N18A	116.58(15)
N16	P3	N18B	106.5(2)
N17	P3	N18A	97.43(16)
N17	P3	N18B	107.56(17)
Ce1	N1	C1	96.54(13)
Ce1	N1	C2	141.68(14)
C1	N1	C2	121.77(19)
Ce1	N2	C1	95.61(13)
Ce1	N2	C8	136.61(14)
C1	N2	C8	121.53(18)
P1	N3	C1	136.09(18)
P1	N4	C14	118.77(17)
P1	N4	C18	119.37(17)
C14	N4	C18	111.9(2)
P1	N5	C19	117.33(18)
P1	N5	C23	123.3(2)
C19	N5	C23	112.6(2)
P1	N6	C24	120.93(17)
P1	N6	C28	125.90(16)
C24	N6	C28	112.9(2)
Ce1	N7	C29	96.32(12)
Ce1	N7	C30	141.90(14)
C29	N7	C30	120.07(17)
Ce1	N8	C29	95.91(13)
Ce1	N8	C36	140.82(13)
C29	N8	C36	122.35(18)
P2	N9	C29	148.54(17)
P2	N10	C42	123.08(14)

Atom	Atom	Atom	Angle/˚
P2	N10	C46	117.13(15)
C42	N10	C46	111.26(17)
P2	N11	C47	114.02(14)
P2	N11	C51	117.70(14)
C47	N11	C51	111.12(17)
P2	N12	C52	122.23(14)
P2	N12	C56	123.04(15)
C52	N12	C56	112.27(17)
Ce1	N13	C57	95.05(13)
Ce1	N13	C58	139.68(14)
C57	N13	C58	121.73(18)
Ce1	N14	C57	94.80(13)
Ce1	N14	C64	144.44(14)
C57	N14	C64	120.61(18)
P3	N15	C57	140.28(17)
P3	N16	C70	119.75(17)
P3	N16	C74	117.90(17)
C70	N16	C74	111.9(2)
P3	N17	C75	117.79(17)
P3	N17	C79	118.17(17)
C75	N17	C79	111.2(2)
P3	N18A	C80A	117.5(3)
P3	N18A	C84A	126.8(3)
C80A	N18A	C84A	113.8(3)
P3	N18B	C84B	122.4(3)
C80B	N18B	C84B	111.9(4)
P3	N18B	C80B	121.0(3)
Ce1	C1	N1	55.10(11)
Ce1	C1	N2	56.07(11)
N2	C1	N3	125.0(2)
N1	C1	N3	124.8(2)
Ce1	C1	N3	166.61(16)
N1	C1	N2	110.06(19)
N1	C2	C7	108.6(2)
C3	C2	C7	110.5(2)
N1	C2	C3	110.3(2)

Atom	Atom	Atom	Angle/˚
P2	N10	C46	117.13(15)
C42	N10	C46	111.26(17)
P2	N11	C47	114.02(14)
P2	N11	C51	117.70(14)
C47	N11	C51	111.12(17)
P2	N12	C52	122.23(14)
P2	N12	C56	123.04(15)
C52	N12	C56	112.27(17)
Ce1	N13	C57	95.05(13)
Ce1	N13	C58	139.68(14)
C57	N13	C58	121.73(18)
Ce1	N14	C57	94.80(13)
Ce1	N14	C64	144.44(14)
C57	N14	C64	120.61(18)
P3	N15	C57	140.28(17)
P3	N16	C70	119.75(17)
P3	N16	C74	117.90(17)
C70	N16	C74	111.9(2)
P3	N17	C75	117.79(17)
P3	N17	C79	118.17(17)
C75	N17	C79	111.2(2)
P3	N18A	C80A	117.5(3)
P3	N18A	C84A	126.8(3)
C80A	N18A	C84A	113.8(3)
P3	N18B	C84B	122.4(3)
C80B	N18B	C84B	111.9(4)
P3	N18B	C80B	121.0(3)
Ce1	C1	N1	55.10(11)
Ce1	C1	N2	56.07(11)
N2	C1	N3	125.0(2)
N1	C1	N3	124.8(2)
Ce1	C1	N3	166.61(16)
N1	C1	N2	110.06(19)
N1	C2	C7	108.6(2)
C3	C2	C7	110.5(2)
N1	C2	C3	110.3(2)

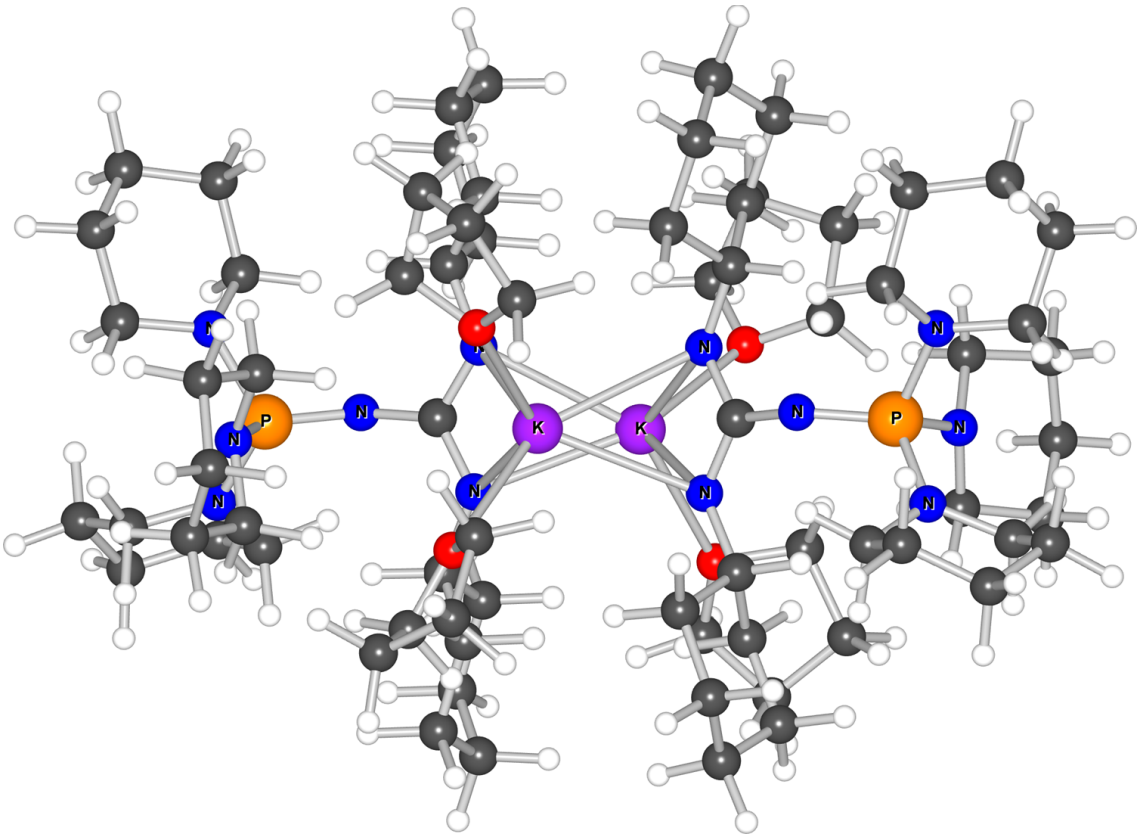

Figure S27. Representation of the molecular structure of **1-K** as its bis-THF adduct as determined by geometry optimization refined to match the crystal structure.

Table S10. Optimized atomic coordinates of **1-K**.

228			
Energy:	-5657.450393		
C	5.45969	11.58311	7.86654
N	4.24991	11.66563	7.10664
N	6.03709	10.41201	8.19702
N	6.11298	12.69851	8.25817
P	2.73245	11.51915	7.47349
C	10.17928	11.57375	10.71957
N	11.13932	11.66987	11.78188
N	9.66989	12.69031	10.15682
N	9.67929	10.39081	10.30777
P	12.69703	11.56247	11.89192
K	8.66834	11.39955	7.70622
K	7.04302	11.41213	10.67947
C	5.63551	14.00203	7.86555
H	4.51453	14.05135	7.87310
C	6.13835	15.07951	8.85052
H	7.25039	15.01938	8.90578

H	5.77301	14.85381	9.87569
C	5.71878	16.50098	8.45063
H	4.60566	16.56997	8.48201
H	6.09867	17.2408	9.18794
C	6.19686	16.85228	7.03406
H	5.87230	17.87873	6.75634
H	7.31198	16.86274	7.02579
C	5.69674	15.81494	6.01959
H	6.07861	16.0409	4.99956
H	4.58581	15.88019	5.95929
C	6.10066	14.39033	6.43488
H	5.71076	13.63783	5.71704
H	7.21515	14.30676	6.42564
C	5.54549	9.13475	7.74848
H	4.42629	9.11353	7.61179
C	6.17242	8.70183	6.39464
H	7.28088	8.74425	6.51714
H	5.91616	9.45597	5.62039
C	5.76852	7.28290	5.95423
H	4.67095	7.24691	5.76561
H	6.25497	7.02745	4.98635
C	6.10883	6.24522	7.03214
H	5.78424	5.22591	6.72963
H	7.21562	6.19573	7.15784
C	5.47258	6.63887	8.37365
H	5.73490	5.90285	9.16479
H	4.36191	6.60087	8.26578
C	5.87975	8.05650	8.80178
H	5.38666	8.31119	9.76096
H	6.97696	8.09818	8.99924
C	2.34767	13.85722	6.08237
H	3.44529	13.72692	5.99039
H	1.88367	13.57215	5.10184
C	1.99546	15.32213	6.38000
H	2.33783	15.9671	5.54275
H	2.55715	15.63796	7.28418
C	0.49829	15.50801	6.65106
H	0.27696	16.56301	6.91570
H	-0.08097	15.28748	5.72482
C	0.05366	14.54929	7.76144
H	-1.04528	14.59991	7.91835
H	0.54336	14.83006	8.72018
C	0.44277	13.10214	7.42125

H	0.17778	12.43564	8.26519
H	-0.16326	12.7829	6.53246
N	1.87600	12.98349	7.15865
C	2.39330	9.87872	9.64854
H	2.11280	9.14589	8.86912
H	3.46868	9.68554	9.89267
C	1.54356	9.70860	10.91124
H	1.70831	8.69328	11.3269
H	0.46747	9.77658	10.64021
C	1.86147	10.78661	11.95655
H	1.16984	10.70047	12.8203
H	2.89422	10.64756	12.35494
C	1.74528	12.18019	11.32542
H	2.05855	12.96837	12.04054
H	0.67948	12.37863	11.07328
C	2.59491	12.28397	10.05747
H	2.46050	13.26444	9.56037
H	3.67823	12.19728	10.31902
N	2.23421	11.23065	9.09274
C	10.10433	13.98407	10.62849
H	11.07802	13.88507	11.17355
C	10.32642	14.97462	9.47172
H	9.37633	15.07869	8.89497
H	11.07451	14.53432	8.77602
C	10.7934	16.35526	9.95600
H	11.79542	16.24741	10.42851
H	10.91793	17.05297	9.09955
C	9.82047	16.95525	10.98555
H	10.2064	17.92814	11.36171
H	8.85846	17.18873	10.47276
C	9.55631	15.9844	12.14573
H	8.79884	16.41742	12.83812
H	10.49062	15.87208	12.73757
C	9.11139	14.60126	11.64716
H	9.02533	13.87938	12.48707
H	8.11215	14.67854	11.16422
C	10.18735	9.14282	10.82261
H	11.19668	9.28542	11.28864
C	9.29690	8.54274	11.94651
H	8.25515	8.45185	11.56429
H	9.27930	9.27061	12.78685
C	9.77813	7.16592	12.43678
H	10.75564	7.27361	12.95953

H	9.07400	6.75442	13.19515
C	9.94910	6.16828	11.28525
H	10.34366	5.19765	11.65752
H	8.95312	5.94568	10.83791
C	10.86309	6.74124	10.19051
H	10.94294	6.02478	9.34434
H	11.89101	6.86197	10.60473
C	10.3518	8.10163	9.69535
H	11.04701	8.52350	8.93678
H	9.36947	7.96194	9.18374
C	12.27654	9.57889	13.76224
H	11.29571	10.08088	13.66097
H	12.12091	8.51752	13.45051
C	12.79877	9.58208	15.20592
H	12.07475	9.04725	15.85714
H	12.86062	10.62706	15.5825
C	14.18187	8.92069	15.27915
H	14.58483	8.96897	16.31275
H	14.08619	7.83923	15.03151
C	15.1469	9.60620	14.30447
H	16.12322	9.07774	14.26373
H	15.34616	10.6393	14.66055
C	14.56527	9.67497	12.88349
H	15.22047	10.28289	12.22956
H	14.55463	8.63930	12.45535
N	13.21154	10.22171	12.83973
C	12.538	13.68553	13.62314
H	11.46743	13.54219	13.3738
H	12.70084	13.22656	14.63475
C	12.92142	15.16765	13.70733
H	12.33524	15.64479	14.52092
H	12.62523	15.67603	12.76339
C	14.4264	15.34455	13.95667
H	14.70124	16.41951	13.92645
H	14.66065	14.98772	14.98458
C	15.24272	14.53599	12.94263
H	16.32949	14.57805	13.16717
H	15.1095	14.97262	11.92883
C	14.78071	13.0734	12.91388
H	15.33203	12.4878	12.15147
H	15.01584	12.60871	13.90767
N	13.34879	12.98856	12.6221
C	13.73181	10.16397	9.75840

H	13.58101	9.31549	10.44888
H	12.89396	10.13947	9.01618
C	15.06259	10.03226	9.00132
H	15.07419	9.08125	8.42732
H	15.89218	9.99512	9.74056
C	15.26789	11.23229	8.06371
H	16.23814	11.16462	7.52876
H	14.47207	11.21398	7.28424
C	15.15112	12.54686	8.85085
H	15.21813	13.41761	8.16563
H	15.98735	12.6186	9.58001
C	13.82258	12.59135	9.61883
H	13.7301	13.50835	10.22985
H	12.97579	12.60213	8.88739
N	13.70291	11.42582	10.50662
C	2.70045	9.54687	5.54103
H	3.72509	9.95933	5.48880
H	2.80499	8.46915	5.81567
C	1.99606	9.65010	4.18084
H	2.55289	9.03289	3.44426
H	2.04550	10.70258	3.81946
C	0.53432	9.19663	4.27925
H	0.00229	9.34234	3.31590
H	0.50369	8.10220	4.48532
C	-0.18518	9.95096	5.40289
H	-1.22051	9.57176	5.54313
H	-0.27235	11.02505	5.12715
C	0.57916	9.85589	6.73200
H	0.09498	10.48656	7.50114
H	0.52015	8.80063	7.10693
N	1.98136	10.24921	6.59841
C	4.93951	13.8276	12.7899
H	4.01422	13.34499	13.19453
H	4.82419	13.9142	11.69021
C	5.22625	15.15288	13.49285
H	5.92038	15.76126	12.87407
H	4.31388	15.75369	13.67725
C	5.91008	14.65878	14.77435
H	5.14181	14.33331	15.50606
H	6.54692	15.42016	15.26644
C	6.71549	13.44819	14.27239
H	7.76759	13.71086	14.03335
H	6.74406	12.62295	15.02059

O	6.08083	13.00255	13.05779
C	4.99365	8.24018	12.40598
H	5.68165	7.46697	11.98544
H	4.15680	8.37315	11.68785
C	4.52781	7.87028	13.81645
H	3.57936	8.39339	14.06136
H	4.36656	6.78068	13.93975
C	5.67942	8.41983	14.66696
H	6.52496	7.69935	14.66915
H	5.40974	8.61006	15.72414
C	6.04580	9.70463	13.91505
H	5.47172	10.57858	14.29496
H	7.12901	9.94199	13.98198
O	5.69054	9.48852	12.5367
C	9.81208	13.74472	4.87057
H	8.70438	13.70402	4.90774
H	10.13071	13.55321	3.81569
C	10.39383	15.05629	5.39851
H	10.38283	15.86971	4.64664
H	9.81942	15.38586	6.28909
C	11.80718	14.62241	5.81290
H	12.22866	15.26009	6.61532
H	12.51053	14.66019	4.95478
C	11.59146	13.16811	6.28194
H	12.40241	12.48921	5.93342
H	11.53377	13.0886	7.39217
O	10.32374	12.73692	5.75130
C	9.65157	8.16185	5.19345
H	9.78577	8.42850	4.11353
H	8.61296	7.80582	5.33695
C	10.74183	7.17936	5.63643
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H	10.97504	6.42611	4.85924
C	11.92632	8.12579	5.95151
H	12.69442	8.10586	5.15175
H	12.43568	7.85160	6.89600
C	11.26279	9.52402	6.03868
H	11.51331	10.07121	6.97107
H	11.55255	10.164	5.17123
O	9.84990	9.30690	6.02010

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