Electronic Supplementary Information for

Structural distortion by alkali metal cations modulates the redox and electronic properties of Ce^{3+} imidophosphorane complexes

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Table of Contents

General Considerations

Unless otherwise noted, all reagents were obtained from commercial suppliers and used as received. All manipulations were performed with rigorous exclusion of oxygen and water using Schlenk techniques under UHP argon, or in a glovebox (Vigor) under a dinitrogen atmosphere (<0.1 ppm O_2/H_2O). The glovebox is equipped with two -35 °C freezers and a cold well. All glassware and cannulas/needles were stored in an oven overnight (>8h) at ca. 160 °C prior to use.

Materials: Celite and molecular sieves were dried under vacuum at a temperature >250 °C for a minimum of 24 h. C_6D_6 (Cambridge Isotope Laboratories or Sigma-Aldrich) was pre-dried over 3 Å molecular sieves then vacuum-transferred from purple sodium/benzophenone and stored over 3 Å molecular sieves prior to use. THF-*d*$_8$ (Cambridge) was degassed by 3 freeze-pump-thaw cycles and dried over sodium metal, then vacuum transferred stored over 3 Å molecular sieves prior to use. *n*-Pentane, hexanes, diethyl ether, toluene, and tetrahydrofuran (THF) were purged with UHP-grade argon (Airgas) and passed through columns containing Q-5/alumina and molecular sieves in a commercial solvent purification system (JC Meyer Solvent Systems, Pure Process Technology). All solvents in the glovebox were stored in media bottles over 10% v/v 3 Å molecular sieves. Fluorobenzene was distilled from P_2O_5 and stored over 3 Å molecular sieves inside the glovebox. Methanol was dried by refluxing over magnesium turnings activated with iodine overnight under argon and then distilled and stored over 3 Å molecular sieves. Supporting electrolytes for electrochemical analysis were purified as follows: [^{n}Bu$_4$N][BPh$_4$] (Sigma-Aldrich, 99% or electrochemical grade >99%)$^{\phi}$ was recrystallized twice from 10:90 water:acetone followed by a final recrystallization from 30:70 diethyl ether:acetone, then dried under vacuum at 100°C for a minimum of 24 h prior to use. [^{n}Bu$_4$N][PF$_6$] (Oakwood) was recrystallized three times from absolute ethanol, then dried under vacuum at 85°C for a minimum of 24 h prior to use. Ferrocene and decamethylferrocene were sublimed prior to use. [K][NP(N,N'-di-*tert*-butylethylenediamide)(diethylamide)][1] (**KNP***), $CeI_3(THF)_4$[2], KC_8[3], and benzyl potassium[4] were prepared according to the published procedures. RbC_8 and CsC_8 were prepared analogously to KC_8. Graphite was flame dried in a Schlenk flask several times under vacuum on a Schlenk line prior to use. Potassium *tert*-butoxide was sublimed prior to use in the synthesis of benzyl potassium. Immersion oils (Paratone-N, Cargille Type NVH) were degassed on a Schlenk line by stirring under active vacuum with gentle heating (to facilitate stirring, ca. 40°C) overnight prior to use.

Analytical: NMR spectra were obtained on a Bruker Avance III 400 or 500 MHz spectrometer at 298 K, unless otherwise noted. ^{1}H, ^{13}C{^{1}H}, and ^{31}P{^{1}H} NMR chemical shifts are reported in δ, parts per million. ^{1}H NMR are referenced to the residual ^{1}H resonances of the solvent. ^{13}C{^{1}H} NMR are referenced to the resonance of the deuterated solvent. ^{13}C DEPT-135 NMR spectra are referenced to the standard ^{13}C{^{1}H} spectra. Peak position is listed, followed by peak multiplicity, integration value, and proton assignment, where applicable. Multiplicity and shape are indicated by one or more of the following abbreviations: s (singlet); d (doublet); t (triplet); q (quartet);dd (doublet of doublets); td (triplet of doublets); m (multiplet); br (broad). UV-visible-NIR spectroscopy was performed in small-volume screw-cap quartz cuvettes (Starna Scientific) with a 1 cm path length on a Hitachi UH4150 UV-vis-NIR scanning spectrophotometer from 1100 to 280 nm. ATR infrared measurements were performed on a Bruker ALPHA FTIR spectrometer from 400 to 4000 cm^{-1} inside a dinitrogen glovebox. Elemental analyses were determined at the University of California Berkeley Microanalytical Facility (Berkeley, CA). X-ray structural determinations were performed at the Georgia Institute of Technology X-ray Crystallography Facility on a Bruker D8 Venture diffractometer. Crystals for X-ray analysis were coated in either Paratone N or Cargille Type NVH immersion oil inside a glovebox and brought out in a capped 20 mL scintillation vial.

$^{\phi}$Standard and electrochemical grade [^{n}Bu$_4$N][BPh$_4$] were examined for use in cyclic voltammetry experiments. Even electrochemical grade displayed a small impurity in the background scan and required recrystallization. There was no observable difference between the standard or electrochemical grades after 3x recrystallization.

[Ce(NP(N,N'-di-*tert*-butylethylenediamide)(diethylamide))$_4$], **1-Ce:** This a modification of a previously reported procedure.[4] Inside a glovebox, **KNP*** (1.55 g, 4.7 mmol, 4 eq.) was transferred to a scintillation vial and dissolved in 18 mL of diethyl ether. This solution was then transferred to a scintillation vial charged with a glass-coated stir bar and $CeI_3(THF)_4$ (0.962 g, 1.2 mmol, 1 eq.). The reaction mixture was allowed to stir at room temperature for 2 h, then AgI (0.293 g, 1.2 mmol, 1.05 eq.) was added as a solid. Any remaining AgI was suspended in 1 mL diethyl ether and transferred to the reaction vial via pipette. The reaction mixture was stirred overnight (14 h) at room temperature. The precipitates were removed via filtration through a fine frit packed with Celite. The filter cake was washed with diethyl ether until the filtrate ran clear (about 80 mL), then the bright-red filtrate was brought to an orange solid *in vacuo*. The crude product was extracted with 25 mL of n-pentane and filtered through a pipette packed with a glass fiber filter and Celite. The volume of the filtrate was concentrated *in vacuo* to a volume of 15 mL, after which red crystals started to form. The solution was placed in a -35°C freezer overnight during which time red crystals formed. The supernatant was then decanted off, and residual volatiles were removed *in vacuo* to give the title compound as a bright-red crystalline solid (1.31 g, 85%). All spectroscopic data are consistent with the previously reported data (Figures S1-S3)

[LiCe(NP(N,N'-di-*tert*-butylethylenediamide)(diethylamide))$_4$], **2-Ce^{Li}**. **1-Ce** (425 mg, 0.2 mmol, 1.0 equiv.) was dissolved in 15 mL of diethyl ether and transferred to a 50 mL Schlenk flask equipped with a glass-coated stir bar and a glass stopper. The vessel was removed from the glovebox and connected to a Schlenk line. The red solution was sparged with argon for 3 min and, under a flow of argon, coarsely divided lithium wire (ca. 140 mg, 20 mmol, excess, approximately a 3 cm piece) was added. The reaction mixture was stirred vigorously at room temperature for 14 h. The resulting pale-yellow solution was then decanted via cannula and the volatiles were removed *in vacuo*. The vessel was transferred to a glovebox, and the pale-yellow solid was taken up in 5 mL of diethyl ether and filtered through a pipette packed with a glass-fiber filter. The solution was concentrated to 2 mL volume, then placed in a -35°C freezer overnight during which time yellow crystals grew (suitable for XRD analysis). The mother liquor was decanted off and the volatiles were removed *in vacuo* to give the title compound as a bright yellow solid (250 mg). The supernatant was concentrated to <1 mL and placed in a -35°C freezer overnight to yield a second crop of crystals (344 mg combined mass, 81% total isolated yield).
^{1}H NMR (400 MHz, toluene-d$_8$) T = 80°C δ 4.45 (s, 8H, FWHM = 16 Hz), 3.85 (s, 8H, FWHM = 22 Hz), 1.49 (s, 72H), 0.66 (br, 16H, FWHM = 220 Hz), -1.00 (br, 24H, FWHM = 56 Hz). ^{13}C{^{1}H} NMR (101 MHz, toluene-d$_8$) T = 80°C δ 53.65, 43.17, 37.57, 29.40, 12.11. ^{31}P{^{1}H} NMR (162 MHz, toluene-d$_8$) T = 80°C δ 74.17 (br). IR (ATR): ν [cm^{-1}] = 2965 (m), 1474 (vw), 1460 (vw), 1376 (w), 1355 (w), 1265 (w), 1249 (w), 1194 (m), 1144 (s), 1094 (m), 1050 (m), 1022 (s), 973 (m), 925 (m), 867 (w), 794 (m), 692 (s), 628 (m), 593 (vw), 498 (s), 447 (w). Elemental analysis, $C_{56}H_{128}CeLiN_{16}P_4$, found(calculated): C 52.14(51.87), H 9.95(9.95), N 17.08(17.28).

[NaCe(NP(N,N'-di-*tert*-butylethylenediamide)(diethylamide))$_4$], **2-Ce^{Na}**: **1-Ce** (228 mg, 0.18 mmol, 1.0 equiv.) was dissolved in 10 mL of diethyl ether and transferred to a 20 mL scintillation vial charged with a glass-coated stir bar and a smear of Na metal (51.1 mg, 2.2 mmol, excess). After stirring at room temperature for 3 h, the pale-yellow solution was filtered through a pipette packed with a glass fiber filter and Celite. The volume of the filtrate as concentrated *in vacuo* to 2 mL and the solution was placed in a -35°C freezer. Yellow crystals grew overnight, and the supernatant was decanted off. The residual volatiles were removed *in vacuo* to give the title compound as a pale-yellow solid (135 mg, 59%). Crystals suitable for XRD analysis were grown via slow evaporation of a concentrated *n*-pentane solution at -35°C over several days.
^{1}H NMR (400 MHz, C_6D_6) δ 5.29 (s, 8H, FWHM = 15 Hz), 4.28 (d, *J* = 9.3 Hz, 8H, FWHM = 19 Hz), 1.62 (s, 72H), 0.06 (br, 16H, FWHM = 120 Hz), -1.43 (s, 24H, FWHM = 55 Hz) ^{13}C{^{1}H} NMR (101 MHz, C_6D_6) δ 53.58, 43.65, 36.08, 28.74, 11.27. ^{31}P{^{1}H} NMR (162 MHz, C_6D_6) δ 111.53. IR (ATR): ν [cm^{-1}] = 2966 (m), 1477 (vw), 1375 (w), 1355 (w), 1248 (m), 1195 (m), 1148 (s), 1092 (m), 1051 (m), 1023 (m), 971 (m), 925 (m), 865 (m), 793 (m), 691 (m), 628 (w), 519 (m), 497 (m), 468 (w), 452 (w). Elemental analysis, $C_{56}H_{128}CeNaN_{16}P_4$, found(calculated): C 51.32(51.24), H 9.92(9.83), N 16.78(17.07).

[KCe(NP(N,N'-di-*tert*-butylethylenediamide)(diethylamide))$_4$], **2-Ce^K**: **1-Ce** (122 mg, 0.095 mmol, 1.0 equiv.) was added as a solid to a vial charged with 7 mL hexanes, KC_8 (13.4 mg, 0.010 mmol, 1.05 equiv.), and a glass-coated stir bar. The bronze suspension rapidly turned black, concomitant with the bleaching of the bright red color of the supernatant to a pale yellow. The reaction mixture was allowed to stir at room temperature for 20 min and was then filtered through a pipette packed with a glass-fiber filter and Celite. The filtrate was concentrated to 2 mL *in vacuo* and placed in a -35°C freezer. Yellow crystals grew overnight, and the supernatant was decanted off. The residual volatiles were removed *in vacuo* to give the title compound as a pale-yellow solid (87 mg, 69%). All spectroscopic data are consistent with the previously reported data (Figures S13-S15).

[K(18-crown-6)$_2$][Ce(NP(N,N'-di-*tert*-butylethylenediamide)(diethylamide))$_4$], **2-Ce^{K18c6}**: **1-Ce** (271 mg, 0.2 mmol, 1.0 equiv.) and 18-crown-6 (111 mg, 0.4 mmol, 2.0 equiv.) were dissolved in 15 mL of diethyl ether. The solution was then transferred to a 20 mL scintillation vial charged with KC_8 (29.8 mg, 0.22 mmol, 1.05 equiv.) and a glass-coated stir bar. The bronze suspension rapidly turned black, concomitant with the bleaching of the bright red color of the supernatant to a pale yellow. The reaction was allowed to stir at room temperature for 15 min, then the mixture was filtered through a pipette packed with a glass-fiber filter and Celite. The solution was concentrated to 3 mL *in vacuo* and placed in a -35°C freezer. Overnight, nearly colorless crystals grew, and the supernatant was decanted off. The volatiles were removed *in vacuo* to give the product as a pale-yellow solid (313 mg, 80%).
^{1}H NMR (400 MHz, THF-*d*$_8$) δ 3.75 (s, 16H, FWHM = 20 Hz), 3.60 (s, 48H), 2.84 (d, *J* = 12.1 Hz, 8H, FWHM = 19 Hz), 2.48 (s, 8H, FWHM = 11 Hz), 1.06 (s, 96H, FWHM = 6.6 Hz). ^{13}C{^{1}H} NMR (101 MHz, THF-*d*$_8$) δ 71.56, 52.52, 41.61 (d, *J* = 8.1 Hz), 40.63, 28.36, 15.26. ^{31}P{^{1}H} NMR (162 MHz, THF-*d*$_8$) δ 107.28. IR (ATR): ν [cm^{-1}] = 2957 (m), 2895 (m), 1456 (w), 1382 (w), 1295 (vw), 1251 (m), 1210 (m), 1195 (m), 1175 (s), 1147 (m), 1107 (s), 1049 (m), 1025 (m), 969 (m), 914 (m), 861 (w), 838 (w), 791 (m), 686 (m), 623 (m), 592 (w), 569 (vw), 518 (m), 495 (m), 469 (m), 449 (w). Elemental analysis, $C_{80}H_{176}CeKN_{16}O_{12}P_4$, found(calculated): C 51.47(51.73), H 9.60(9.55), N 12.34(12.07).

[K([2.2.2]-cryptand)][Ce(NP(N,N'-di-*tert*-butylethylenediamide)(diethylamide))$_4$] **2-Ce^{K222}**: **1-Ce** (179 mg, 0.14 mmol, 1.0 equiv.) and [2.2.2]-cryptand (52.2 mg, 0.14 mmol, 1.0 equiv.) were dissolved in 10 mL of diethyl ether and transferred to a 20 mL scintillation vial charged with KC_8 (19.7 mg, 0.15 mmol, 1.05 equiv.) and a glass-coated stir bar. The bronze suspension rapidly turned black, concomitant with the bleaching of the bright red color of the supernatant to a pale yellow. The reaction mixture was stirred for 15 min at room temperature, then filtered through a glass pipette packed with Celite and a glass fiber filter. The volatiles were removed *in vacuo* to give the crude product as a pale-yellow powder. The powder was taken up in 2 mL of fluorobenzene and filtered through a glass pipette packed with a glass fiber filter into a 4 mL shell vial. The solution was layered with 2 mL of *n*-pentane and placed in a -35°C freezer. Overnight, a pale-yellow powder precipitated out, which was collected on a fine-porosity frit and washed with 1 mL pentane. Residual volatiles were removed *in vacuo* to give the title compound as a pale-yellow powder (210 mg, 89%). Growth of crystals suitable for XRD analysis was not readily achievable.
^{1}H NMR (400 MHz, THF-*d*$_8$) δ 3.76 (br, 16H, FWHM = 22 Hz), 3.60 (s, 12H), 3.56 (t, *J* = 4.4 Hz, 12H), 2.84 (d, *J* = 12.0 Hz, 8H, FWHM = 21 Hz), 2.58 (t, *J* = 4.7 Hz, 12H), 2.47 (s, 8H, FWHM = 10 Hz), 1.06 (s, 96H, FWHM = 6.0 Hz). ^{13}C{^{1}H} NMR (101 MHz, THF-*d*$_8$) δ 71.51, 68.67, 54.95, 52.54, 41.62 (d, *J* = 8.8 Hz), 40.64, 28.37, 15.27. ^{31}P{^{1}H} NMR (162 MHz, THF-*d*$_8$) δ 107.78. IR (ATR): ν [cm^{-1}] = 2959 (m), 2890 (m), 2822 (m), 1477 (w), 1458 (w), 1382 (w), 1354 (m), 1298 (vw), 1251 (m), 1210 (m), 1195 (m), 1174 (s), 1149 (m), 1134 (m), 1105 (m), 1079 (m), 1046 (m), 1026 (m), 970 (m), 951 (m), 916 (m), 862 (w), 833 (vw), 791 (m), 754 (vw), 687 (m), 623 (m), 592 (vw), 572 (vw), 520 (m), 495 (m), 470 (w), 450 (w). Since isolation of this compound in crystalline form was not readily achievable, elemental analysis was not performed, however, NMR spectra are free of impurities and no insoluble solids are observed upon compound dissolution in organic solvents.

[RbCe(NP(N,N'-di-*tert*-butylethylenediamide)(diethylamide))$_4$], **2-Ce^{Rb}**: **1-Ce** (168 mg, 0.13 mmol, 1 equiv.) was added as a solid to a 20 mL scintillation vial charged with RbC_8 (26.0 mg, 0.14 mmol, 1.05 equiv.), 8 mL of hexanes, and a glass-coated stir bar. Any remaining **1-Ce** was dissolved in 2 mL hexanes and transferred to the reaction vial. The bronze suspension rapidly turned black, concomitant with the bleaching of the bright red color of the supernatant to a pale yellow. After stirring at room temperature for 20 min, the reaction mixture was filtered through a pipette packed with a glass fiber filter and Celite. The pale-yellow filtrate was concentrated to 5 mL *in vacuo* and placed in a -35°C freezer. Nearly colorless, pale-yellow crystals grew overnight. The supernatant was decanted off and the residual volatiles were removed *in vacuo* to give the title compound as a nearly colorless, pale-yellow solid (145 mg, 81%). Crystals suitable for XRD analysis were grown from a concentrated hexanes solution with 1 drop of diethyl ether at -35°C.

^{1}H NMR (400 MHz, C_6D_6) δ 4.76 (s, 8H, FWHM = 14 Hz), 3.98 (d, J = 8.5 Hz, 8H,FWHM = 17 Hz), 1.69 (s, 72H), -1.17 (s, 24H, FWHM = 36 Hz), -1.63 (br, 16H, FWHM = 230 Hz). ^{13}C{^{1}H} NMR (101 MHz, C_6D_6) δ 53.07, 43.01, 33.92, 28.86, 11.36. ^{31}P{^{1}H} NMR (162 MHz, C_6D_6) δ 109.08. IR (ATR): ν [cm^{-1}] = 2967 (m), 1476 (vw), 1374 (w), 1355 (w), 1249 (m), 1207 (m), 1194 (m), 1145 (s), 1093 (m), 1051 (m), 1022 (m), 973 (m), 918 (m), 864 (m), 794 (m), 687 (m), 623 (w), 517 (m), 497 (m), 468 (m), 449 (m). Elemental analysis, $C_{56}H_{128}CeN_{16}P_4Rb$, found(calculated): C 48.95(48.91), H 9.41(9.38), N 16.14(16.30).

[CsCe(NP(N,N'-di-*tert*-butylethylenediamide)(diethylamide))$_4$], **2-Ce^{Cs}**: **1-Ce** (123 mg, 0.095 mmol, 1.0 equiv.) was dissolved in 6 mL of diethyl ether and transferred to a 20 mL scintillation vial charged with a glass-coated stir bar and CsC_8 (22.9 mg, 0.10 mmol, 1.05 equiv.). The bronze suspension rapidly turned black, concomitant with the bleaching of the bright red color of the supernatant to a pale yellow. After stirring at room temperature for 15 min, the reaction mixture was filtered through a pipette packed with a glass fiber filter and Celite. The volume of the yellow supernatant was concentrated to 4 mL *in vacuo* and the solution was placed in a -35°C freezer. Overnight, nearly colorless, XRD-quality crystals grew. The supernatant was decanted off, and the residual volatiles were removed *in vacuo* to give the title compound as a nearly colorless, pale-yellow solid (98.6 mg, 73%).

^{1}H NMR (500 MHz, C_6D_6) δ 4.30 (s, 8H, FWHM = 15 Hz), 3.78 (d, J = 8.3 Hz, 8H, FWHM = 18 Hz), 1.62 (s, 72H), -0.93 (s, 24H, FWHM = 46 Hz), -1.28 (br, 16H, FWHM = 540 Hz). ^{13}C{^{1}H} NMR (101 MHz, C_6D_6) δ 52.88, 42.48, 34.18, 28.82, 11.62. ^{31}P{^{1}H} NMR (162 MHz, C_6D_6) δ 107.26. IR (ATR): ν [cm^{-1}] = 2967 (m), 1477 (vw), 1375 (w), 1355 (w), 1250 (m), 1208 (m), 1193 (m), 1145 (s), 1095 (m), 1050 (m), 1021 (m), 974 (m), 918 (m), 864 (m), 794 (m), 686 (m), 623 (w), 516 (m), 496 (m), 467 (m), 448 (m). Elemental analysis, $C_{56}H_{128}CeCsN_{16}P_4$, found(calculated): C 47.16(47.28), H 8.94(9.07), N 15.49(15.75).

Nuclear Magnetic Resonance (NMR) Spectra

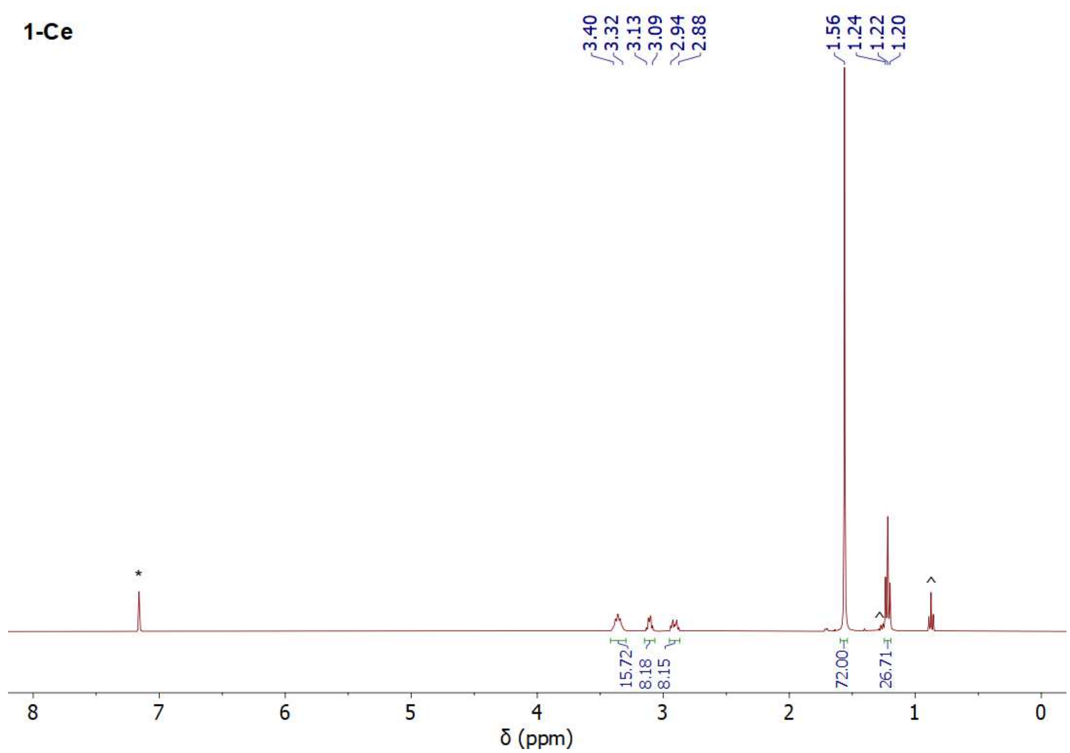


Figure S1. ^{1}H NMR of **1-Ce** in C_6D_6. * = C_6D_5H, ^ = *n*-pentane.

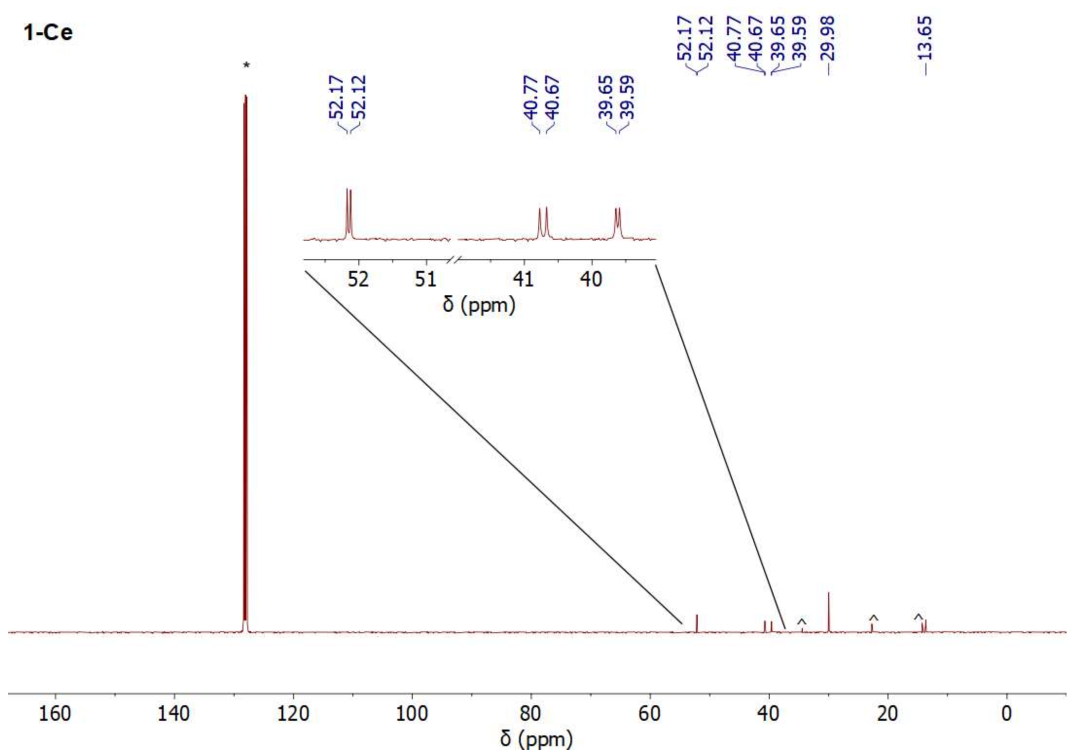


Figure S2. $^{13}C\{^{1}H\}$ NMR of **1-Ce** in C_6D_6. * = C_6D_6, ^ = *n*-pentane.

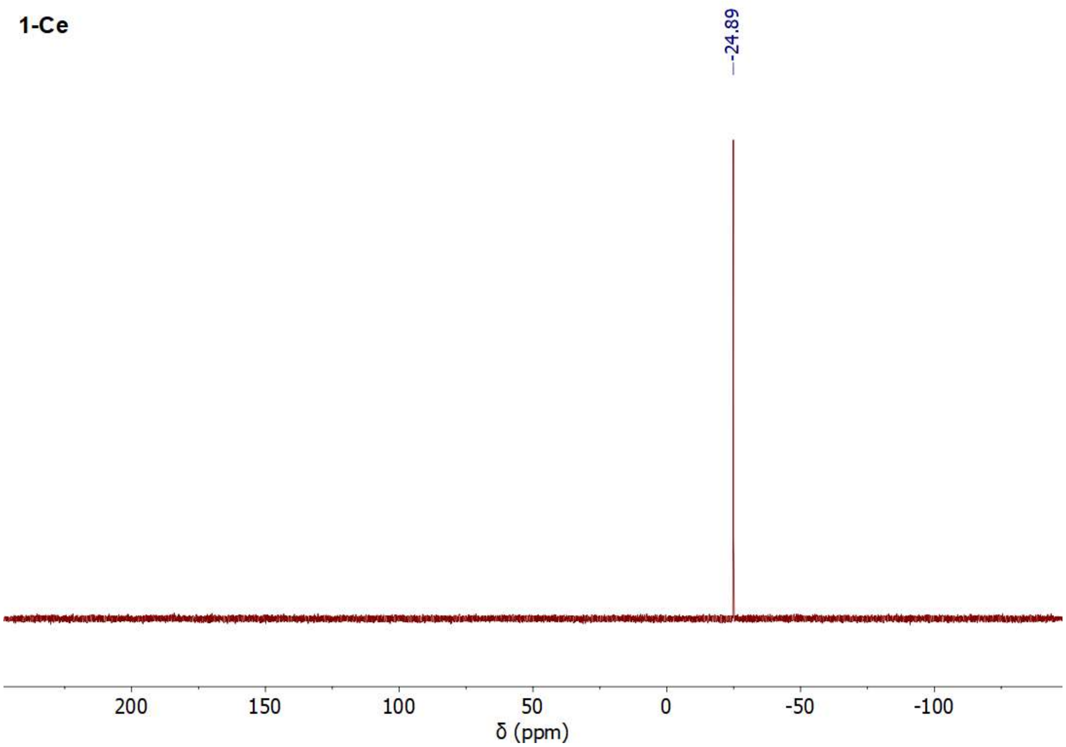


Figure S3. $^{31}P\{^{1}H\}$ NMR of **1-Ce** in C_6D_6.

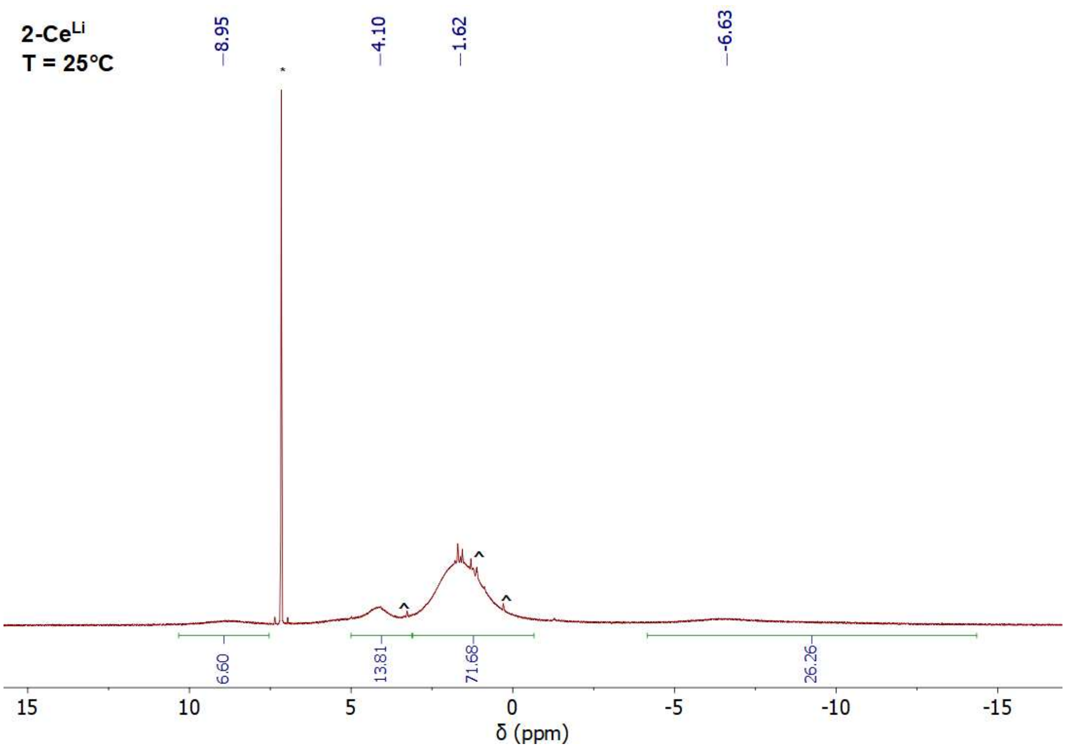


Figure S4. ^{1}H NMR of **2-Ce^{Li}** in C_6D_6, T = +25°C . * = C_6D_5H, ^ = *n*-pentane, Et_2O.

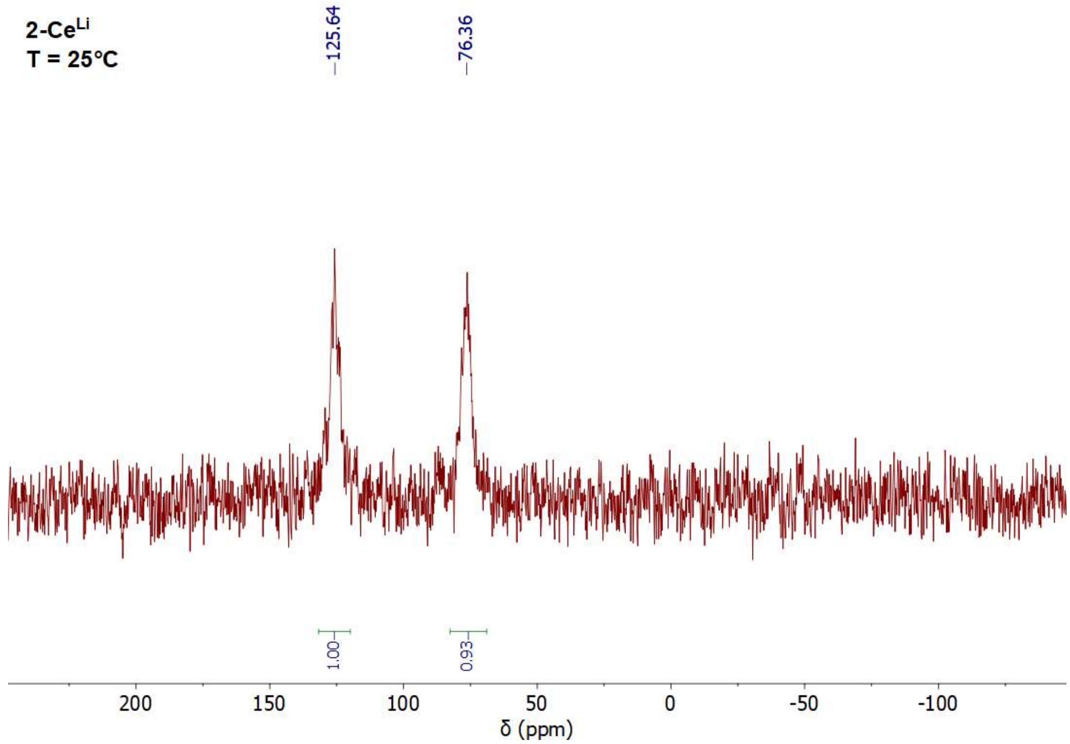


Figure S5. $^{31}P\{^1H\}$ NMR of **2-Ce^{Li}** in C_6D_6, T = +25°C.

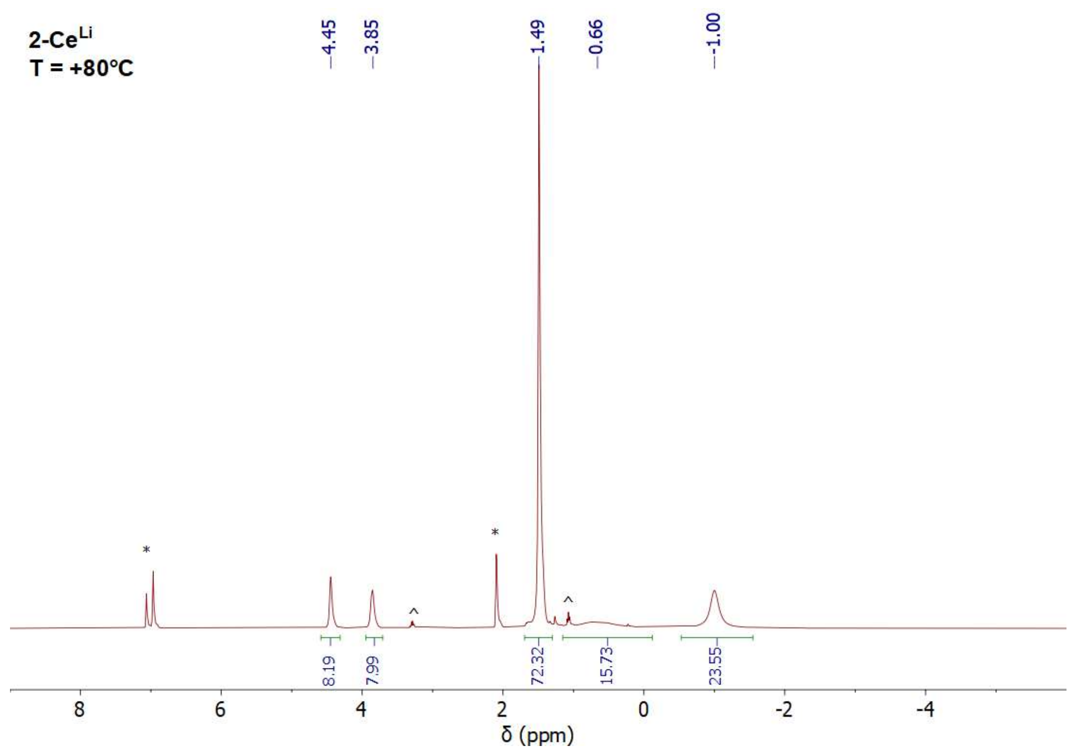


Figure S6. ^1H NMR of **2-Ce^{Li}** in tol-d_8, T = +80°C. *=tol-d_7, ^=Et_2O.

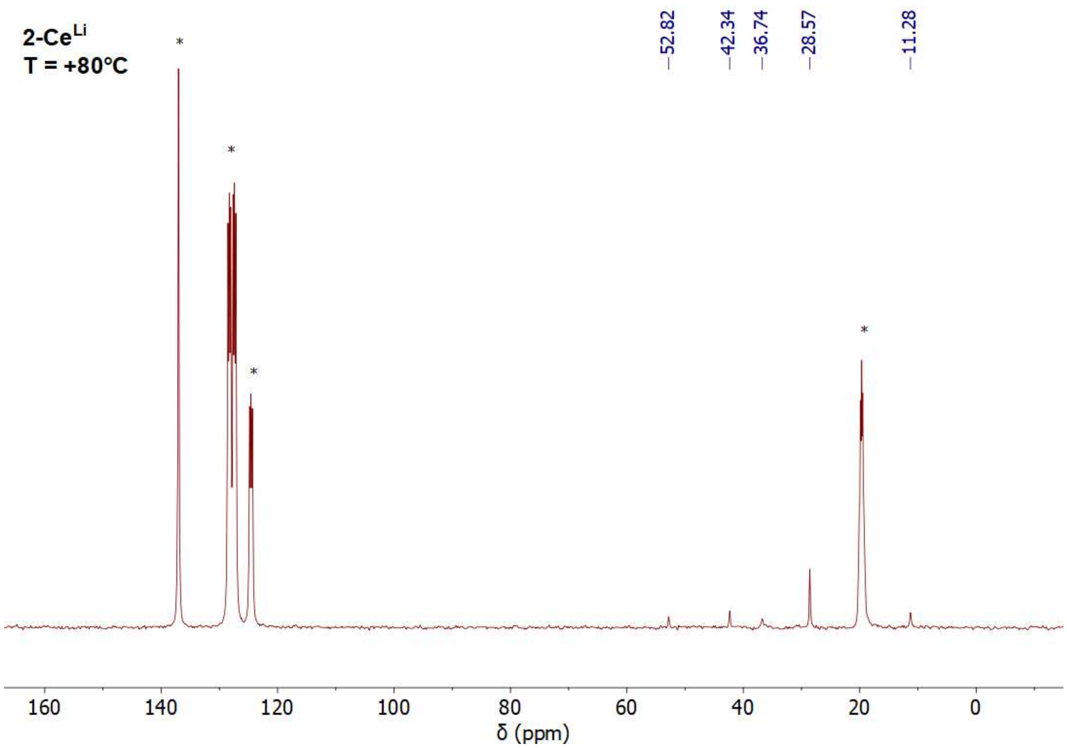


Figure S7. $^{13}C\{^1H\}$ NMR of **2-Ce^{Li}** in tol-d_8, T = +80°C. * = tol-d_8.

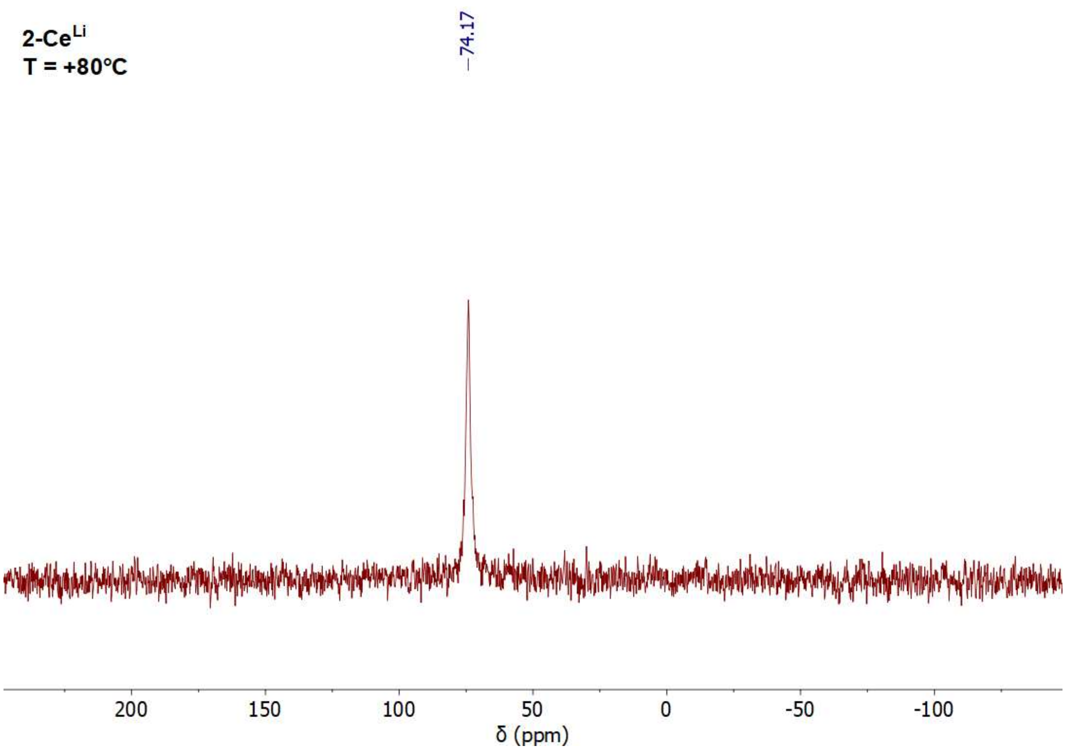


Figure S8. $^{31}P\{^1H\}$ NMR of **2-Ce^{Li}** in tol-d_8, T = +80°C.

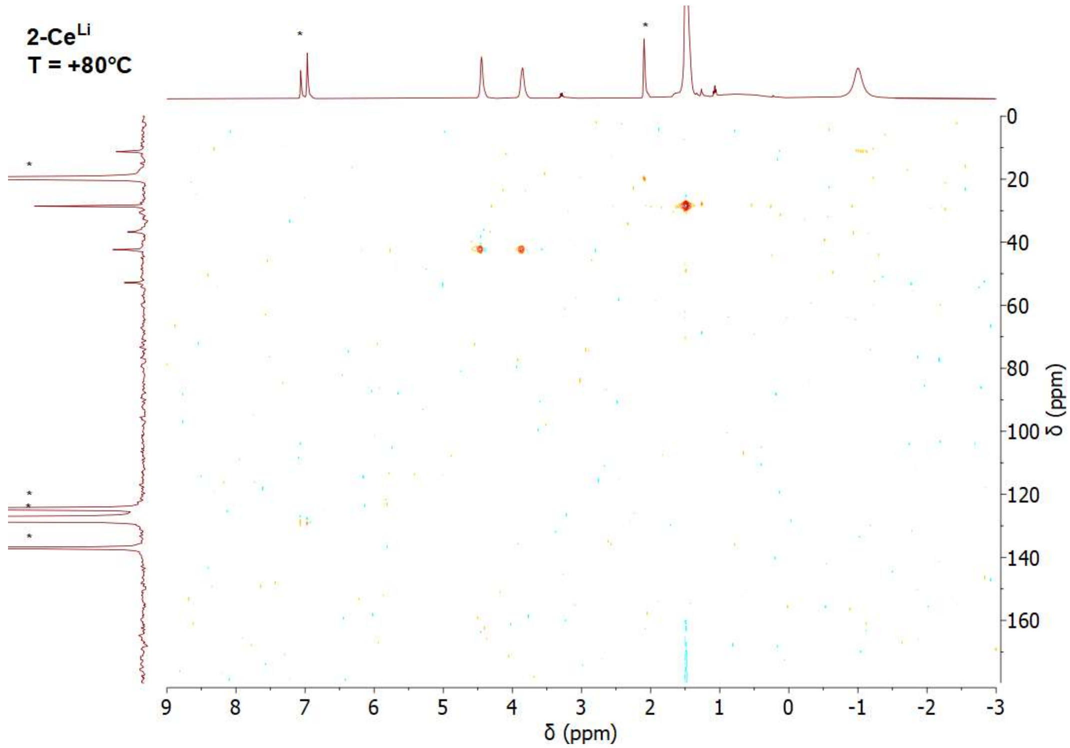


Figure S9. ^{1}H-^{13}C HSQC NMR of **2-Ce^{Li}** in tol-d_8, T = +80°C. * = tol-d_8.

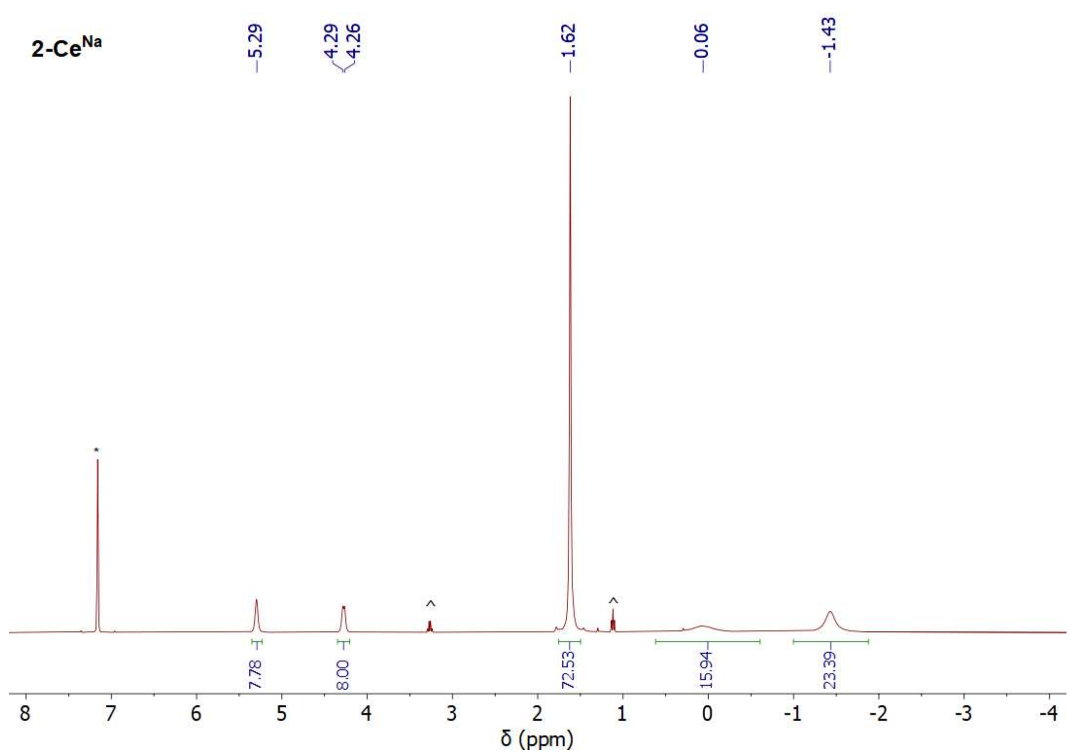


Figure S10. ^{1}H NMR of **2-Ce^{Na}** in C_6D_6, * = C_6D_5H, ^ = Et_2O.

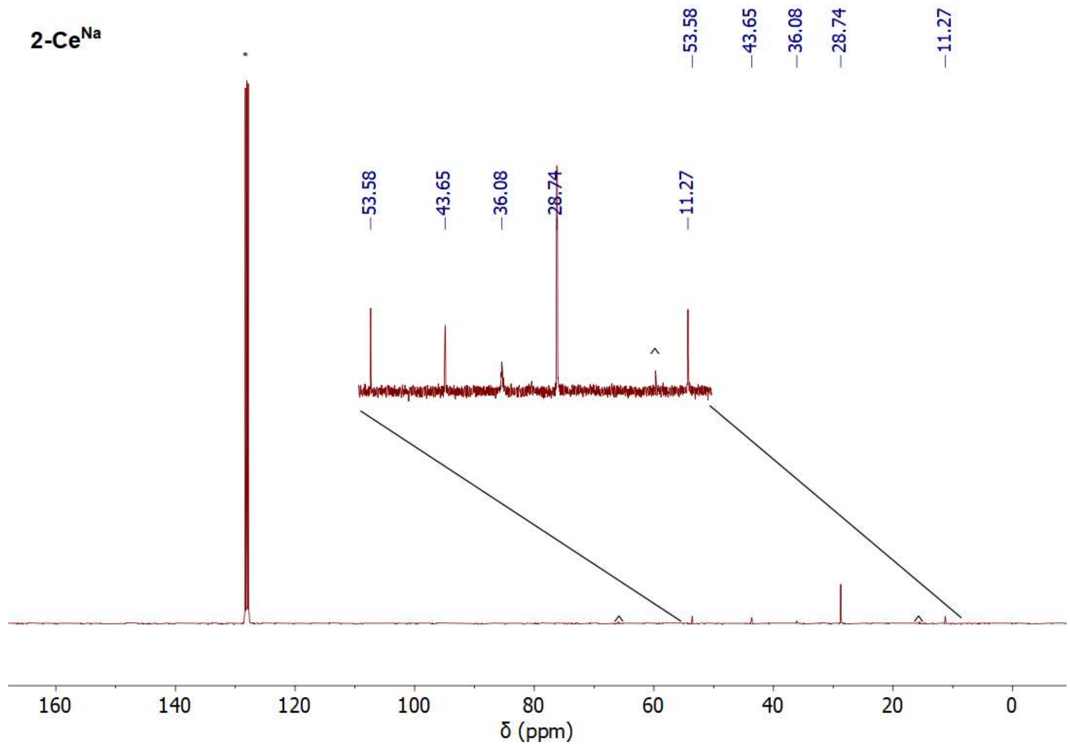


Figure S11. $^{13}C\{^1H\}$ NMR of 2-Ce^{Na} in C_6D_6, * = C_6D_6, ^ = Et_2O.

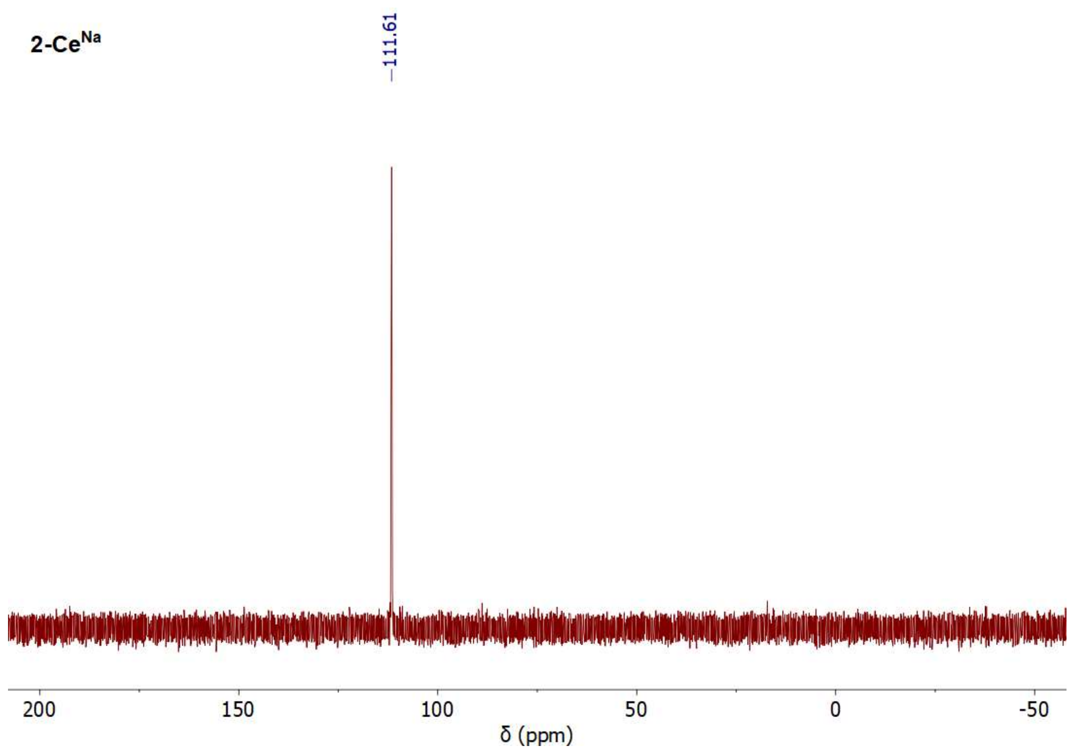


Figure S12. $^{31}P\{^1H\}$ NMR of 2-Ce^{Na} in C_6D_6.

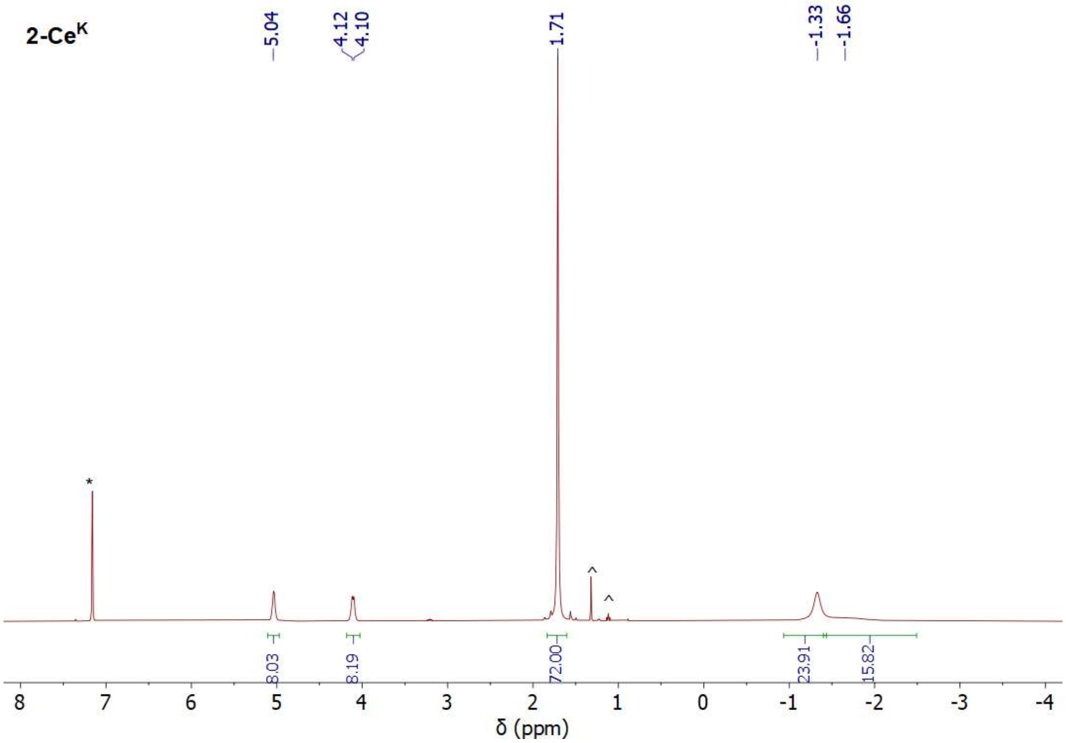


Figure S13. ^{1}H NMR of **2-Ce^{K}** in C_6D_6. * = C_6D_5H, ^ = hexane.

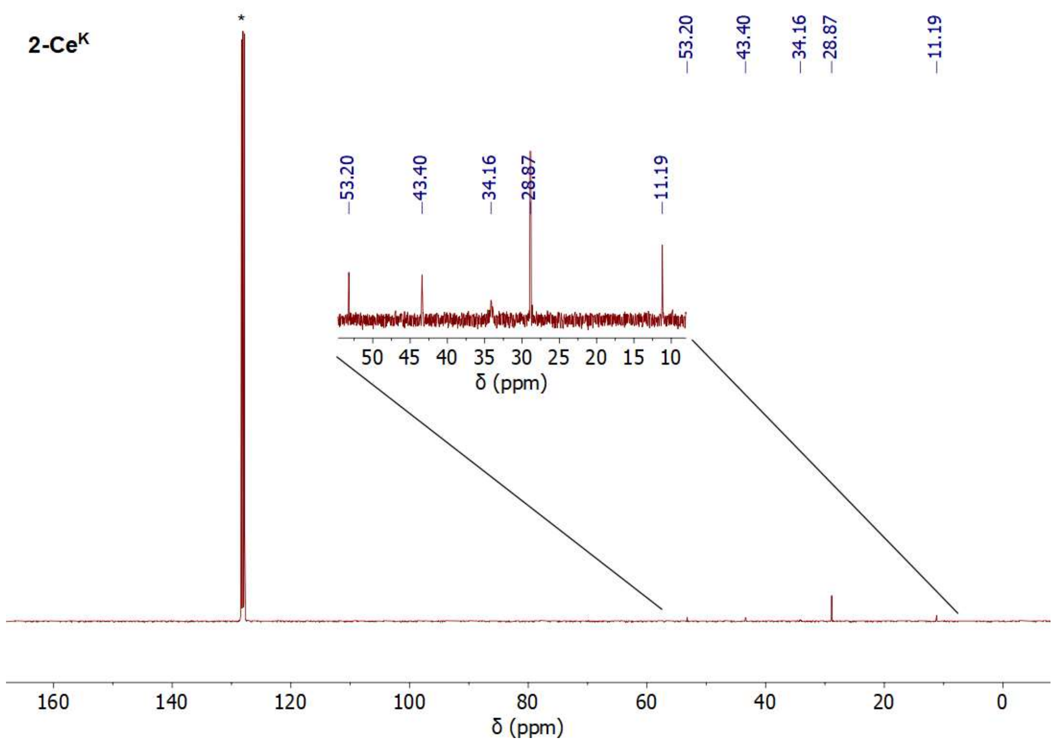


Figure S14. $^{13}C\{^{1}H\}$ NMR of **2-Ce^{K}** in C_6D_6.

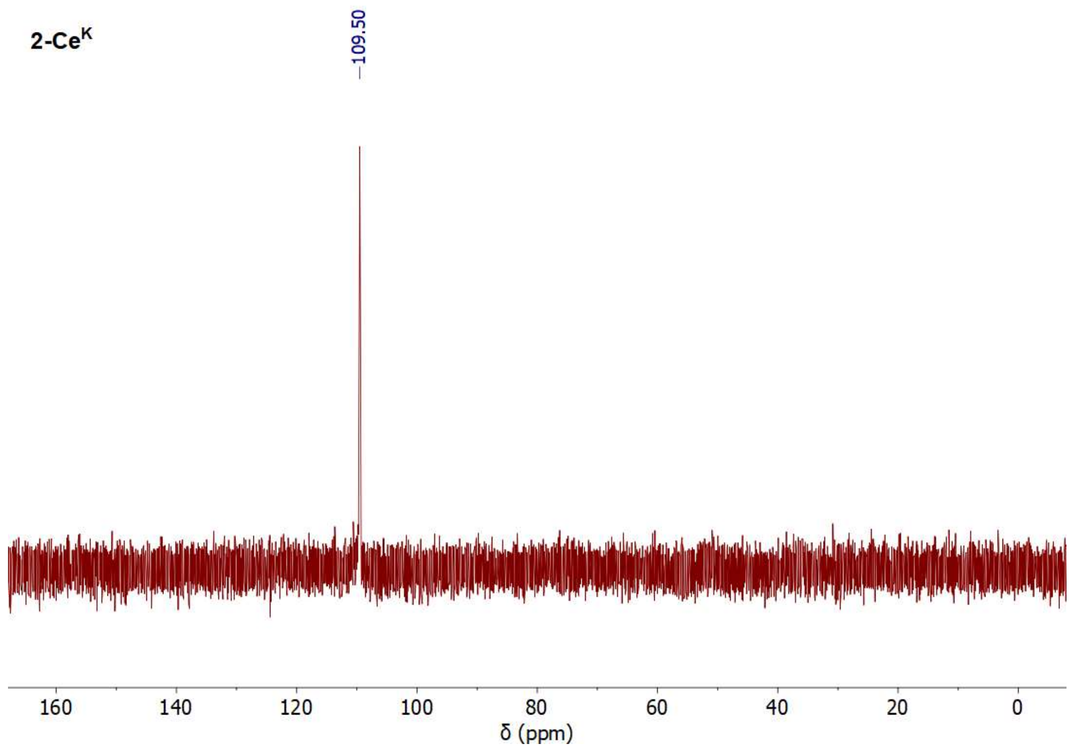


Figure S15. $^{31}P\{^{1}H\}$ NMR of **2-Ce^{K}** in C_6D_6.

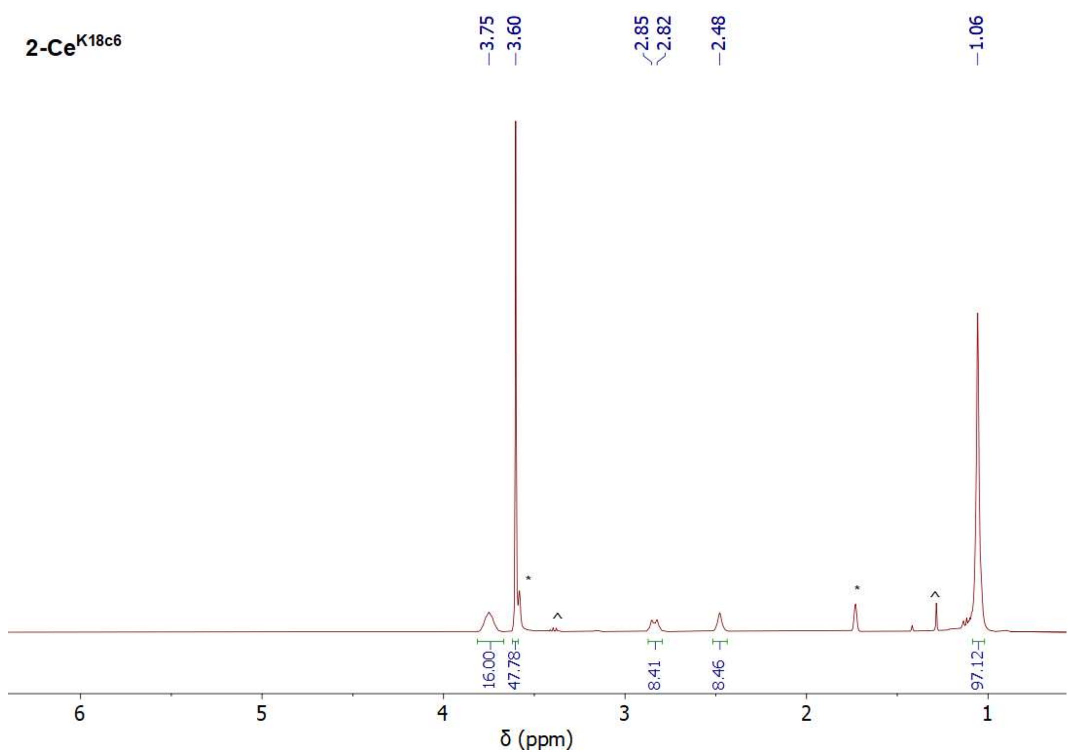


Figure S16. ^{1}H NMR of **2-Ce^{K18c6}** in THF-d_8. * = THF-d_7, ^ = Et_2O.

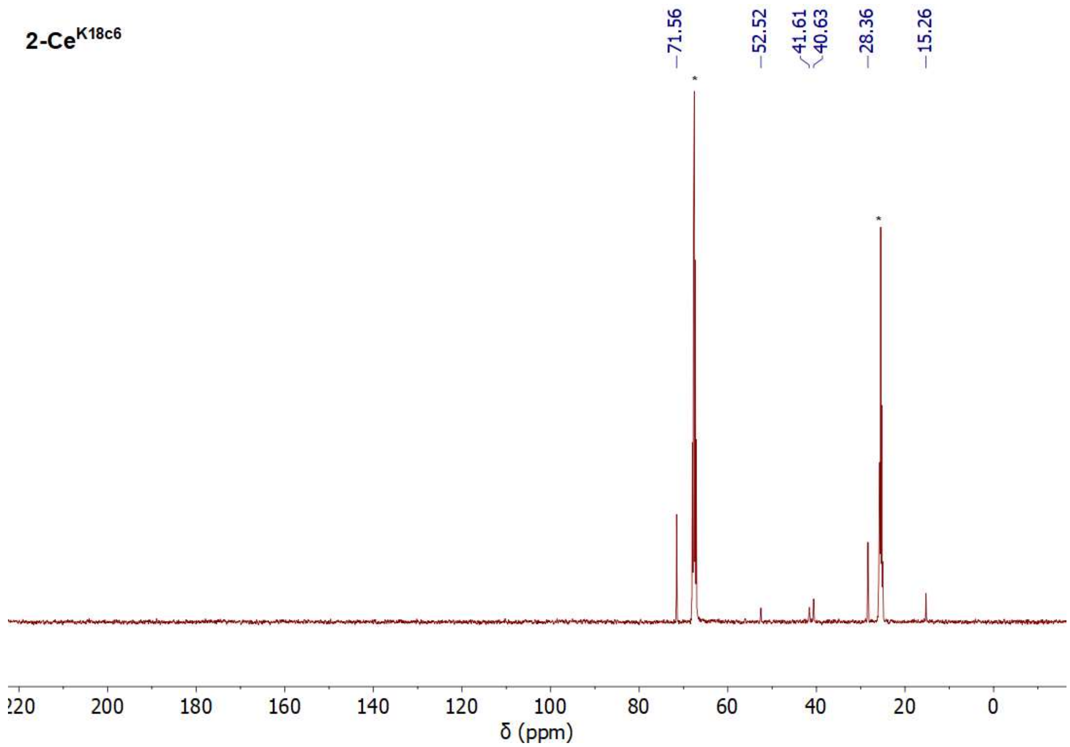


Figure S17. $^{13}C\{^{1}H\}$ NMR of 2-Ce^{K18c6} in THF-d_8. * = THF-d_8.

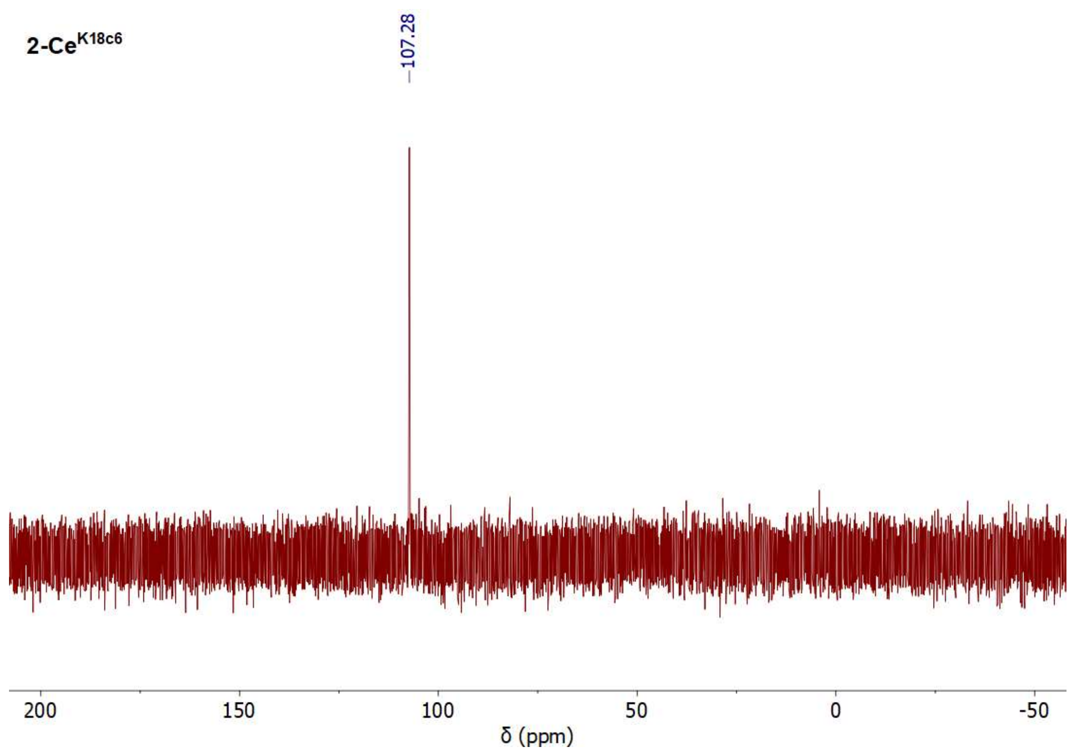


Figure S18. $^{31}P\{^{1}H\}$ NMR of 2-Ce^{K18c6} in THF-d_8.

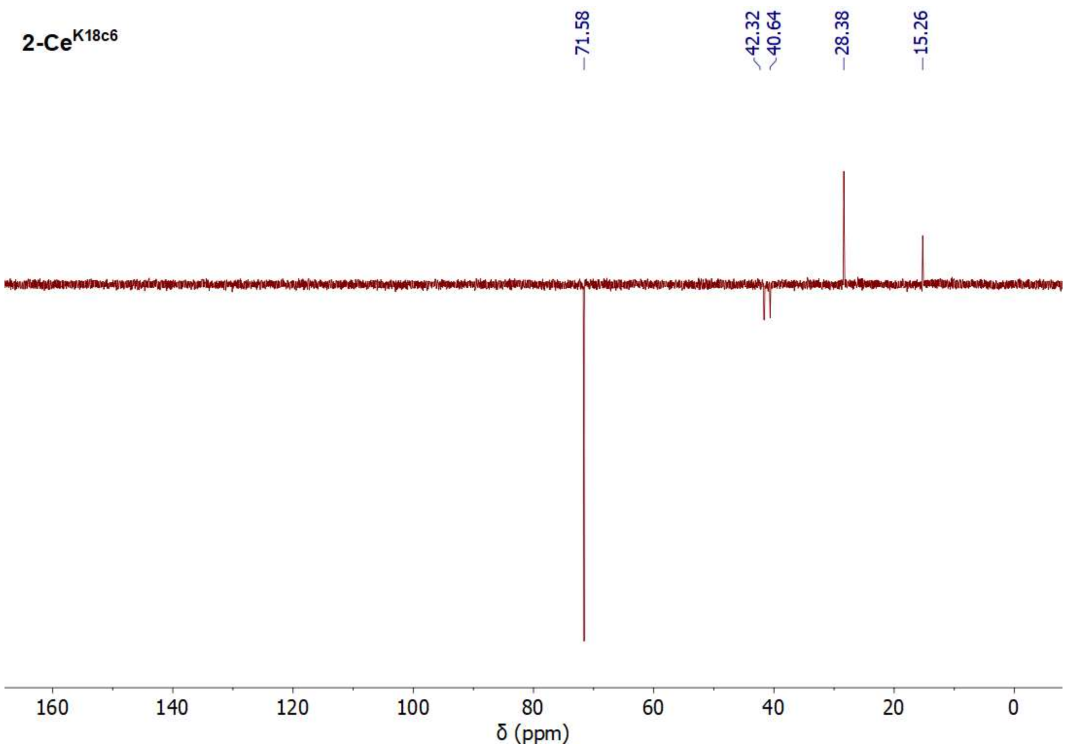


Figure S19. ^{13}C DEPT-135 NMR of **2-Ce^{K18c6}** in THF-d_8.

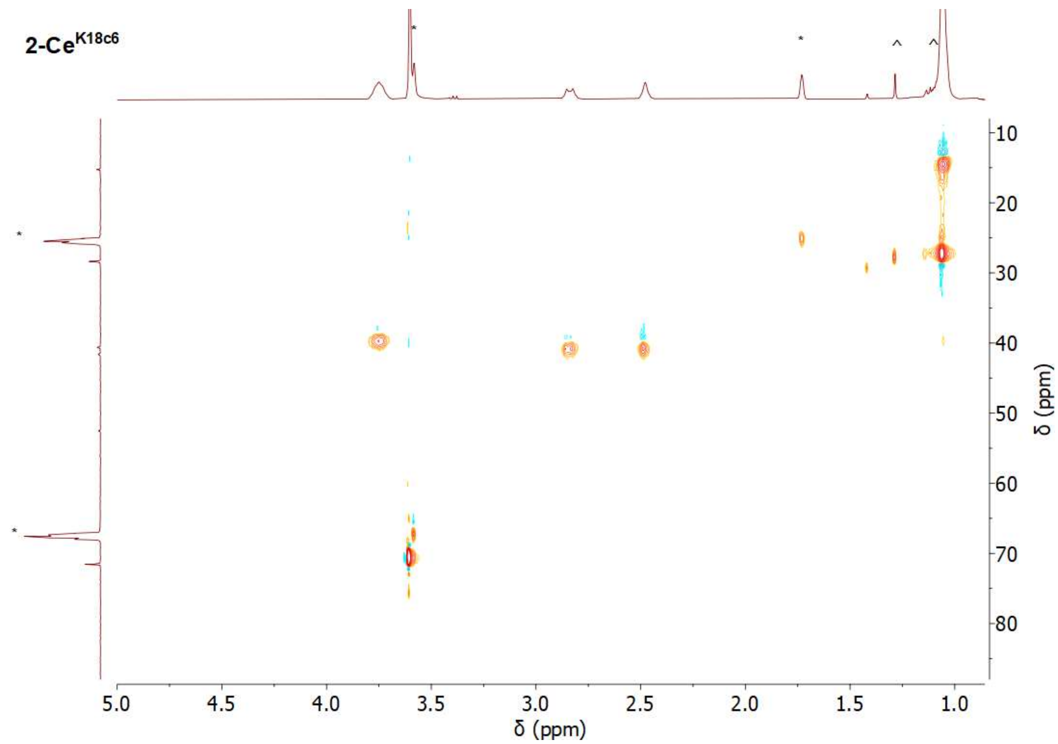


Figure S20. ^1H-^{13}C HSQC NMR of **2-Ce^{K18c6}** in THF-d_8. Note: the ^1H signal at 1.06 ppm is shown to be composed of two signals overlapping, assigned as the N-^{t}Bu protons and the N-CH_2-CH_3 protons.*=THF-d_8 ^ = *n*-pentane, H grease.

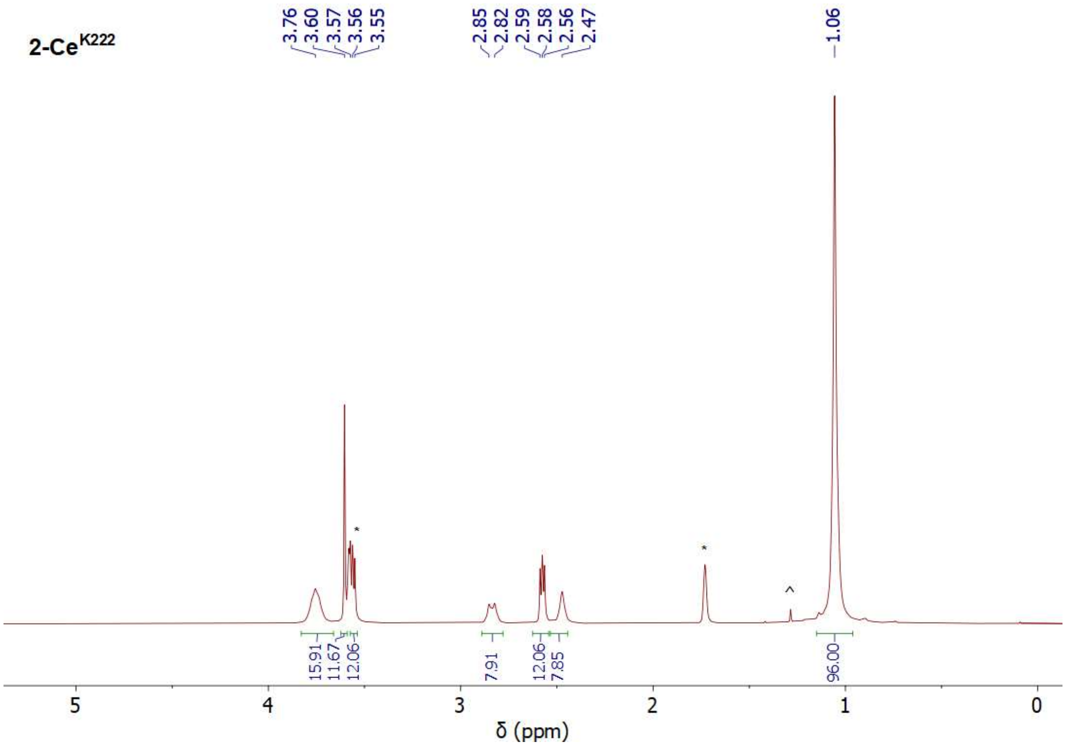


Figure S21. ^{1}H NMR of 2-Ce^{K222} in THF-d_8. * = THF-d_7, ^ = H grease.

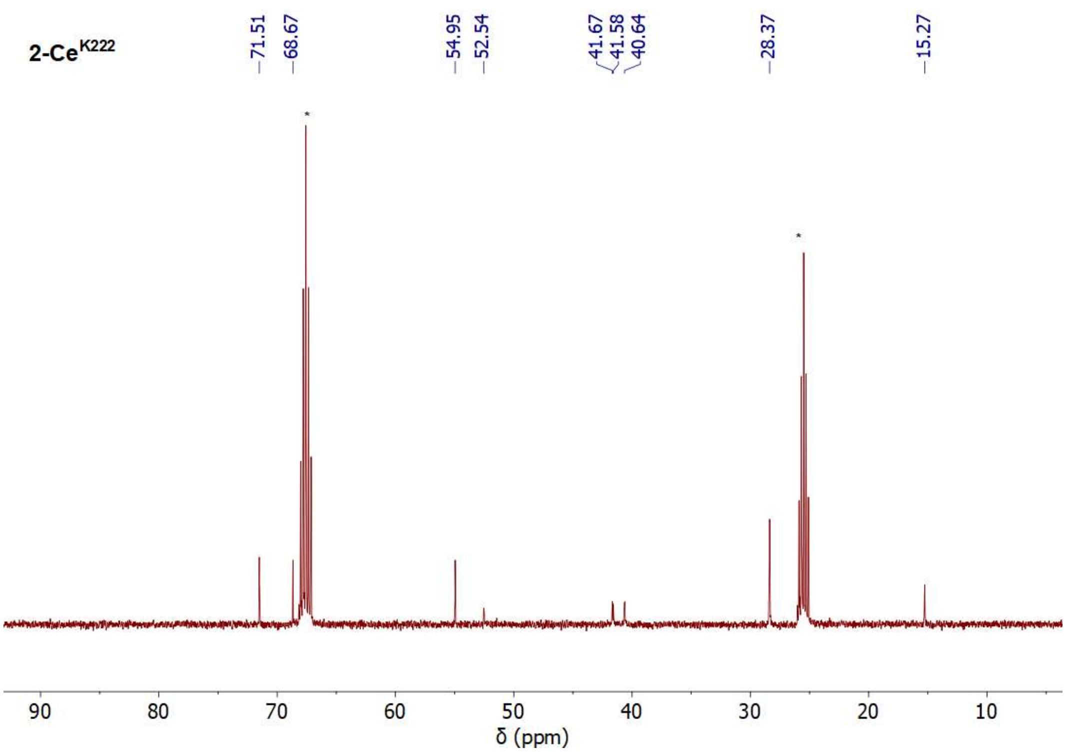


Figure S22. $^{13}C\{^{1}H\}$ NMR of 2-Ce^{K222} in THF-d_8. * = THF-d_8.

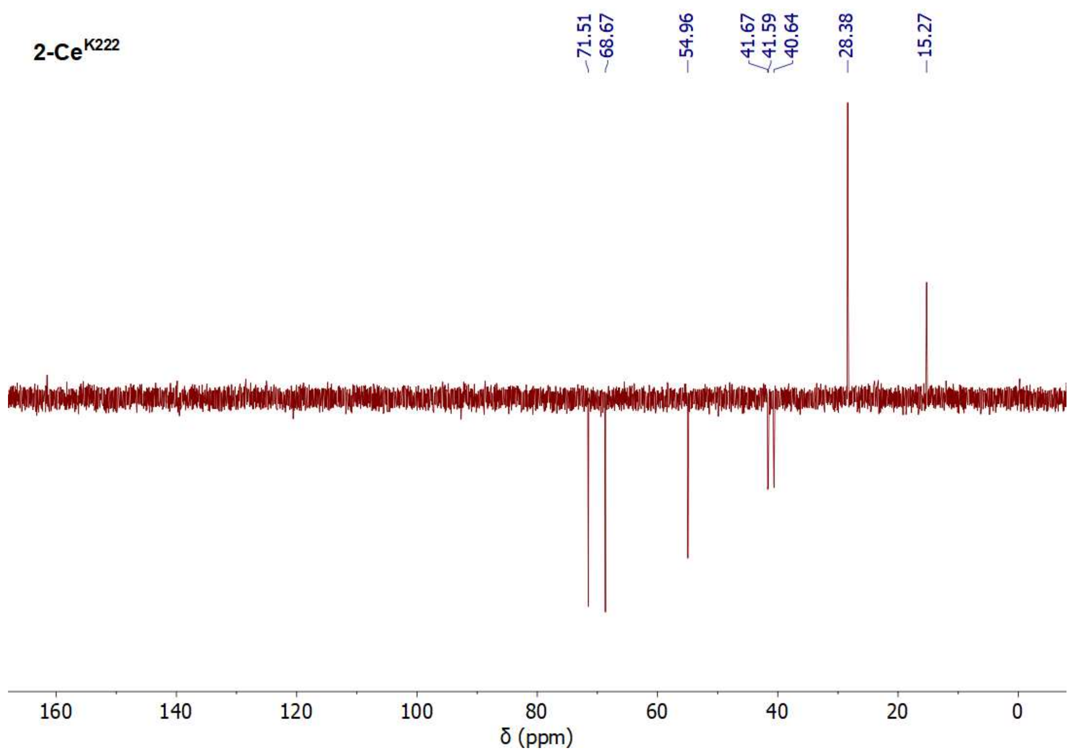


Figure S23. ^{13}C DEPT-135 NMR of **2-Ce^{K222}** in THF-d_8.

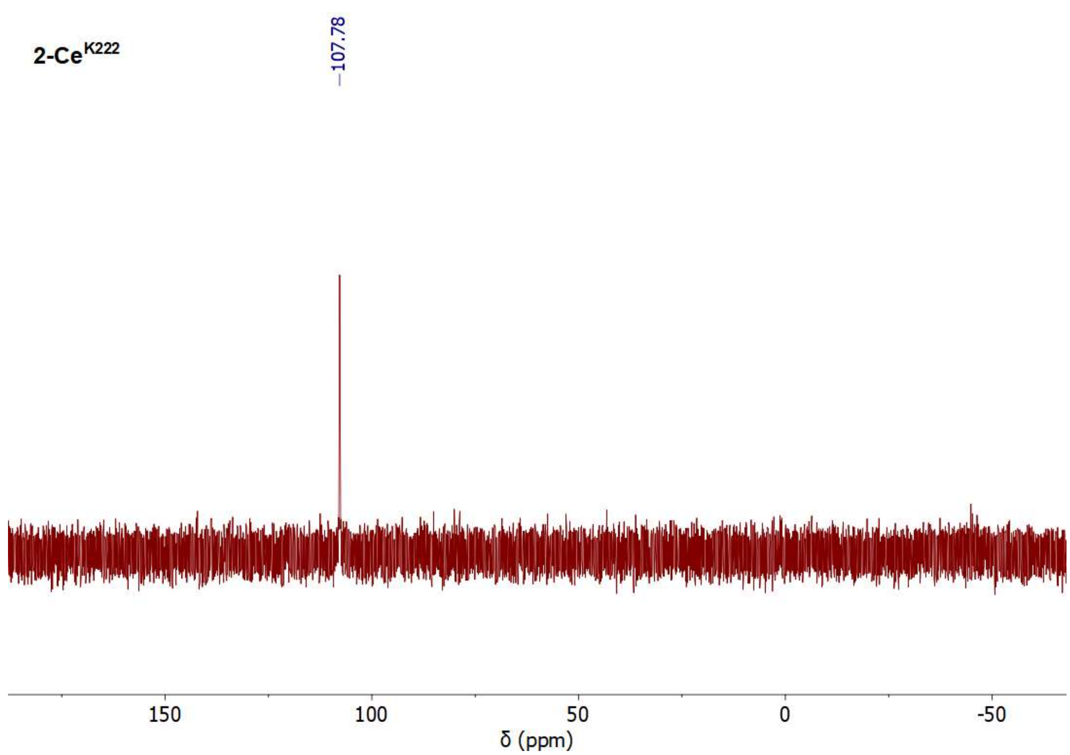


Figure S24. $^{31}P\{^{1}H\}$ NMR of **2-Ce^{K222}** in THF-d_8.

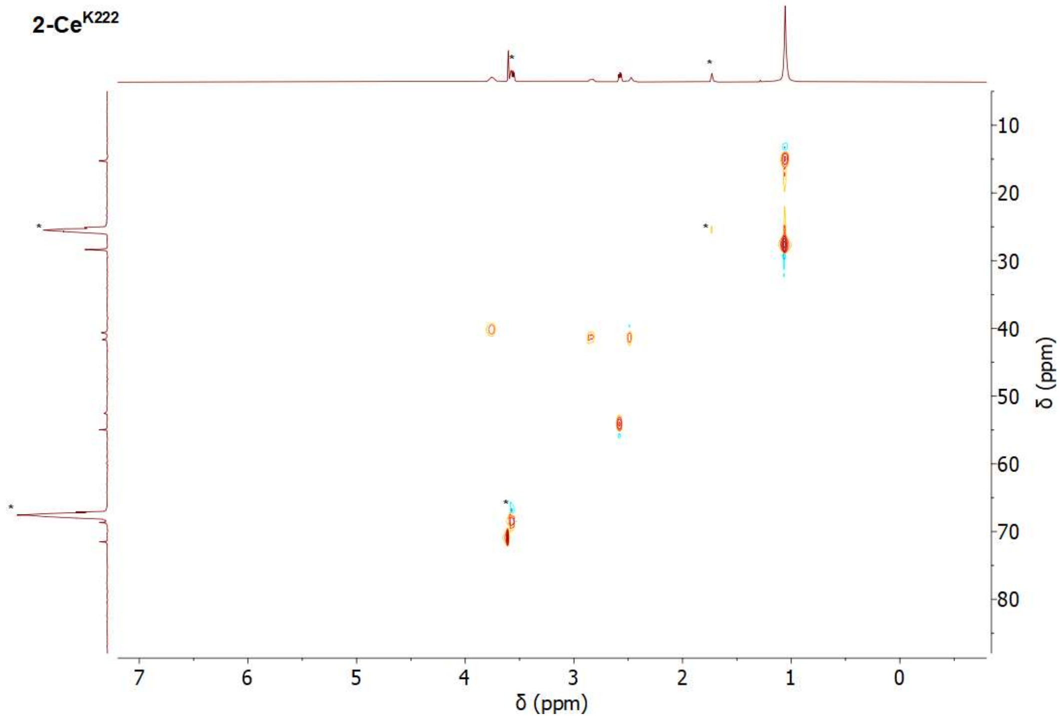


Figure S25. ^1H-^{13}C NMR of **2-Ce^{K222}** in THF-d_8. Notably, the ^1H signal at 1.06 ppm is shown to be composed of two signals overlapping, assigned as the N-^{t}Bu protons and the N-CH_2-CH_3 protons *=THF-d_8.

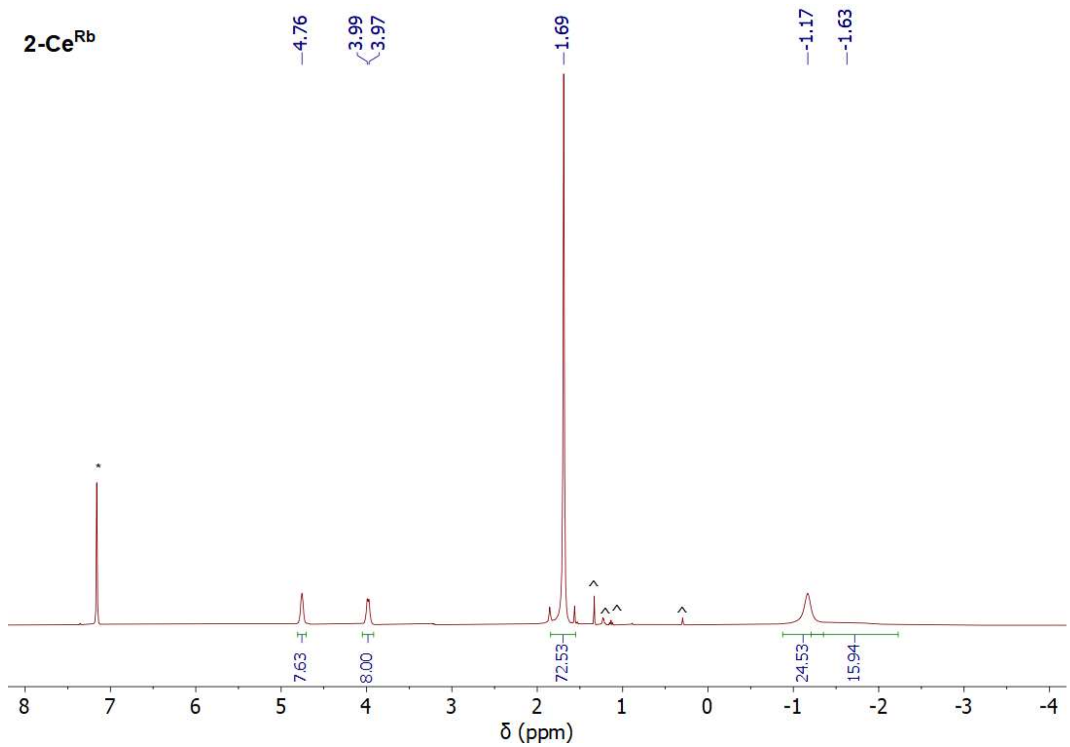


Figure S26. ^1H NMR of **2-Ce^{Rb}** in C_6D_6. * = C_6D_5H, ^ = *n*-pentane, Et_2O, silicone grease.

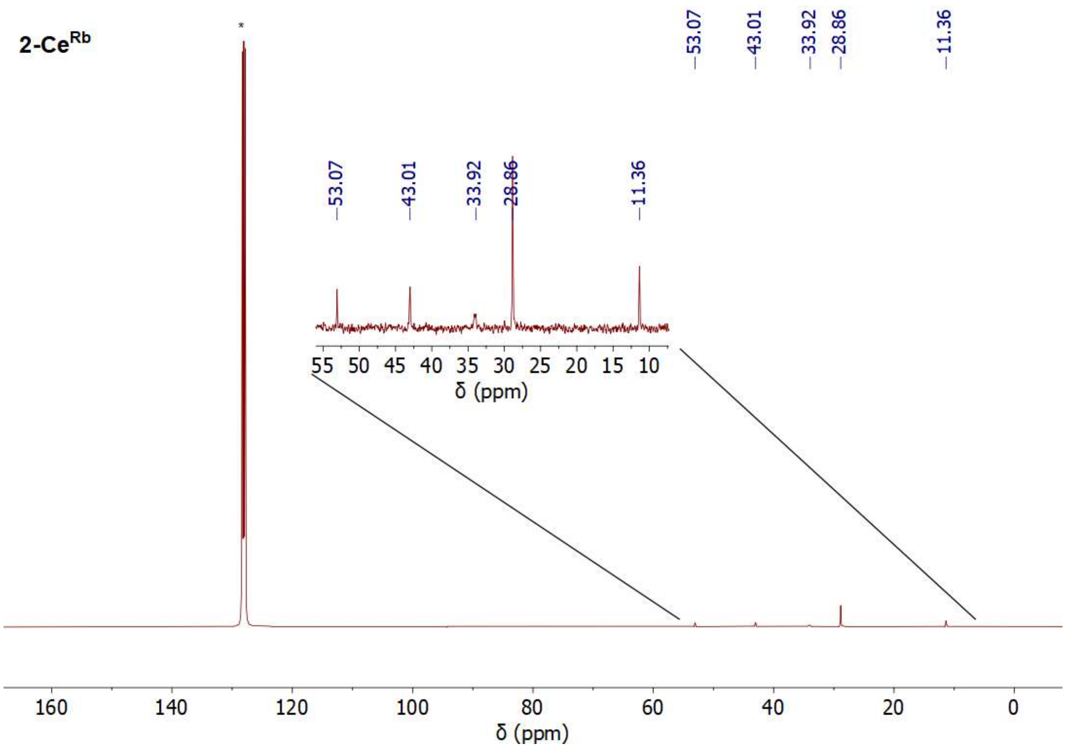


Figure S27. $^{13}C\{^1H\}$ NMR of **2-Ce^{Rb}** in C_6D_6. * = C_6D_6.

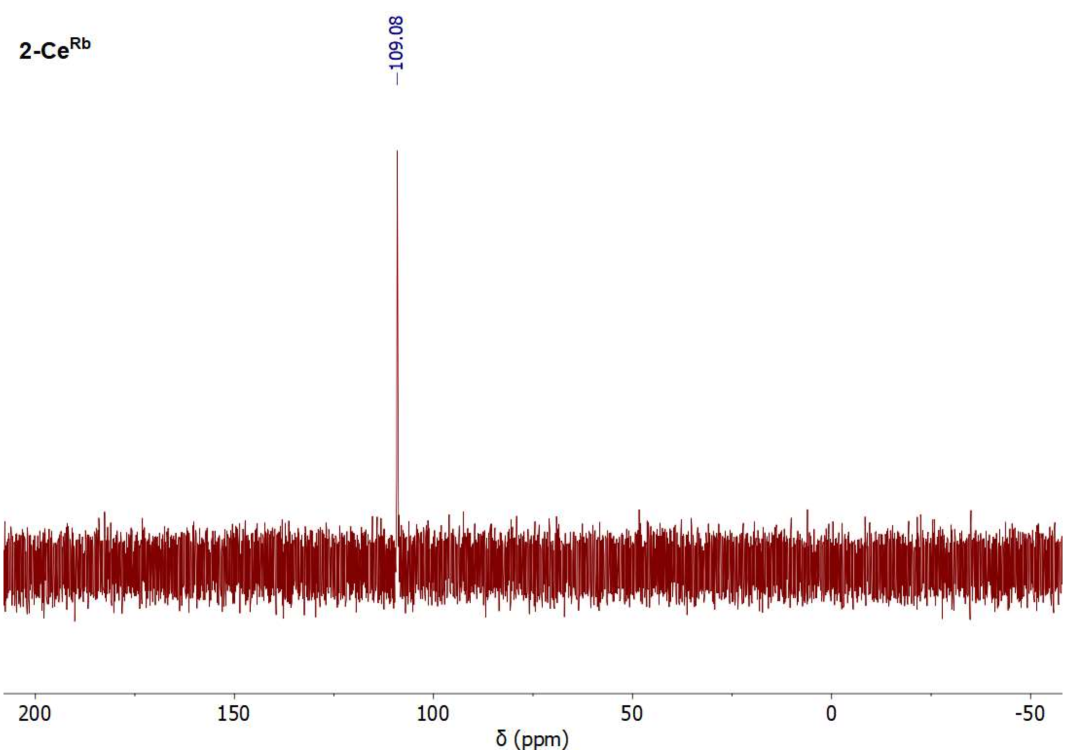


Figure S28. $^{31}P\{^1H\}$ NMR of **2-Ce^{Rb}** in C_6D_6.

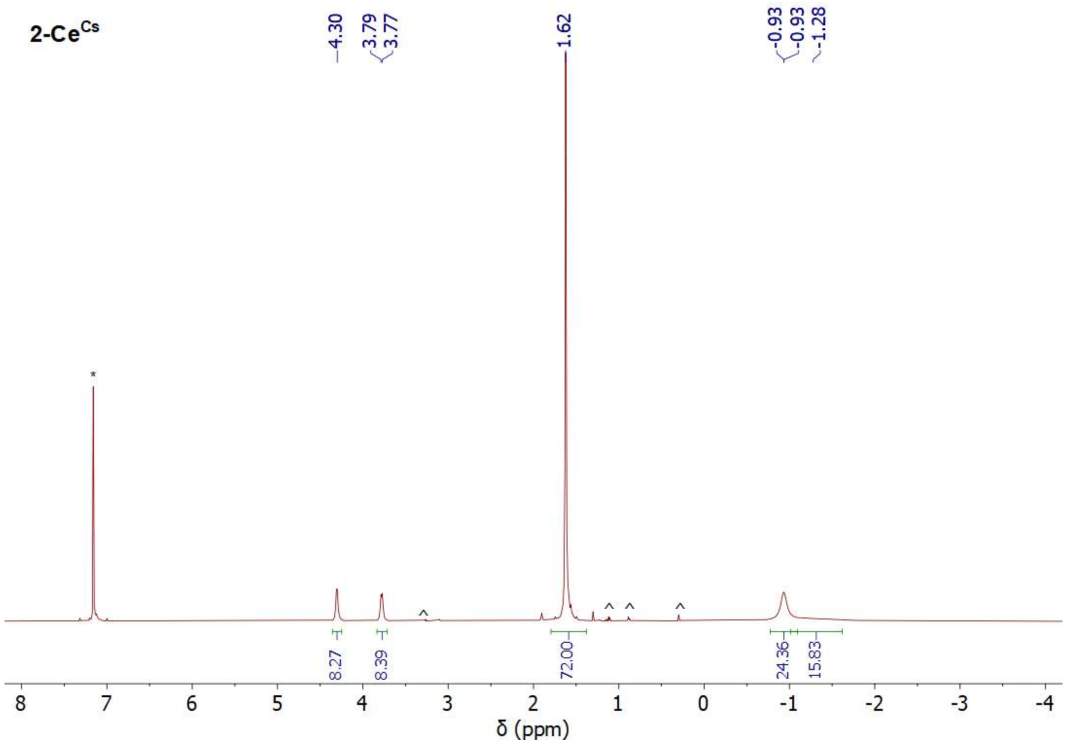


Figure S29. ^{1}H NMR of **2-Ce**^{Cs} in C_6D_6. * = C_6D_5H, ^ = *n*-pentane, silicone grease.

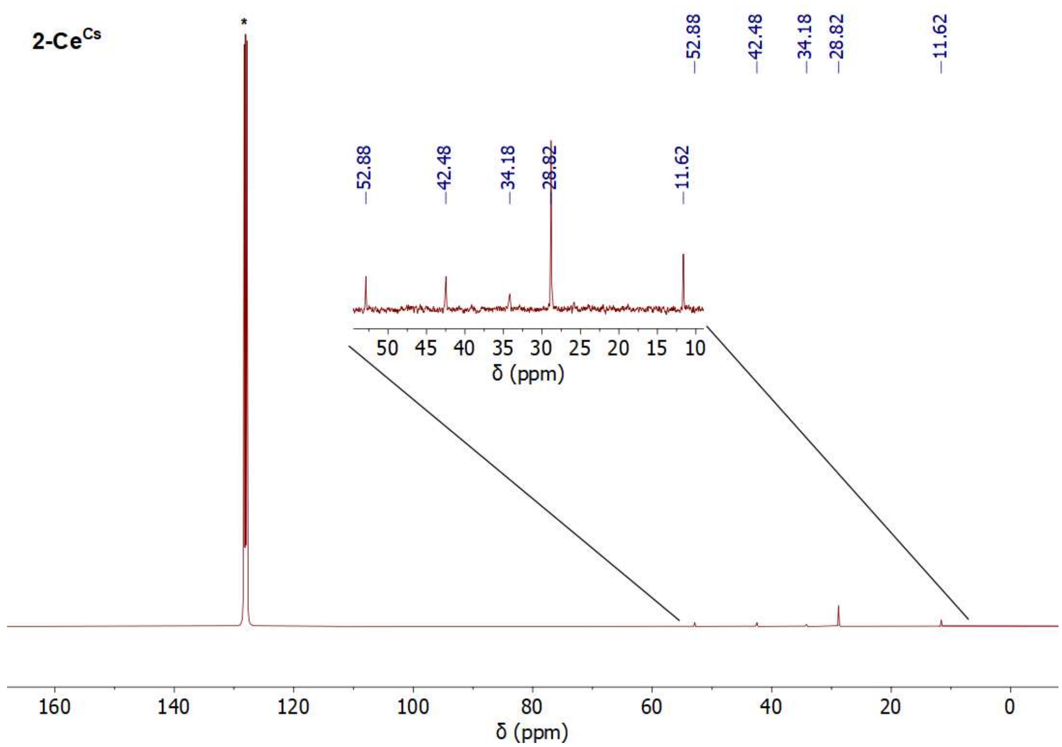


Figure S30. $^{13}C\{^{1}H\}$ NMR of **2-Ce**^{Cs} in C_6D_6. * = C_6D_6.

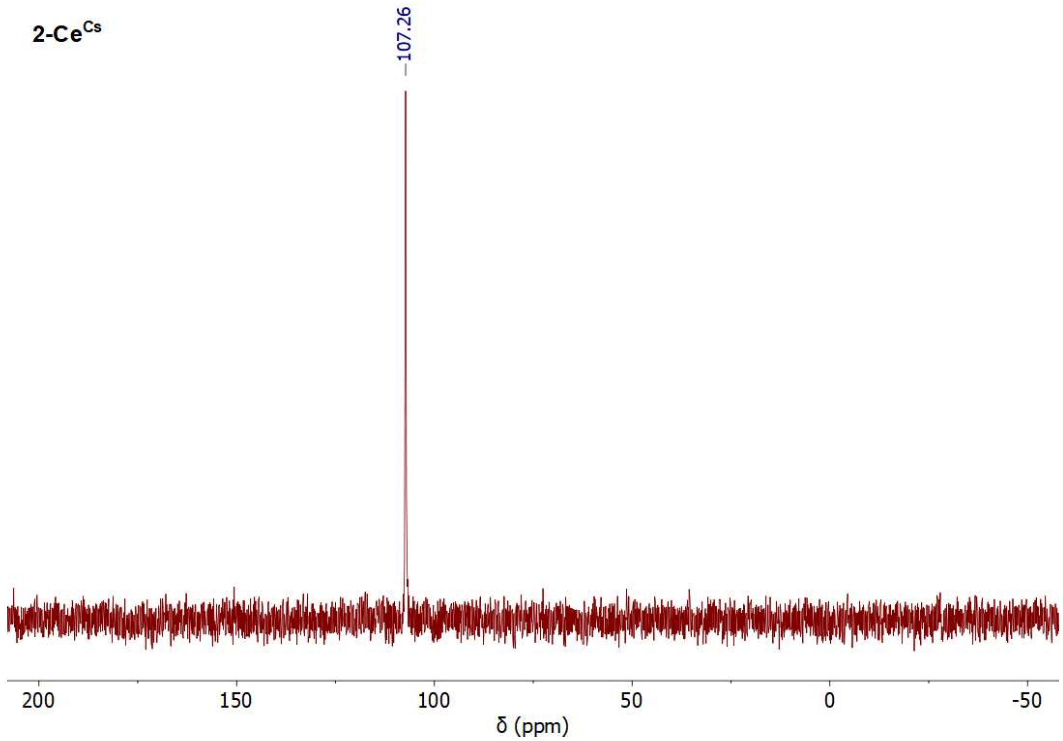


Figure S31. $^{31}P\{^{1}H\}$ NMR of **2-Ce^{Cs}** in C_6D_6.

Variable-Temperature NMR Spectra

General procedure: Samples were transferred to an NMR tube fitted with a J. Young tap, then inserted into the spectrometer at room temperature and subsequently cooled to -80°C. Spectra presented were sequentially measured with temperature increasing from low to high temperatures. Temperatures were corrected using a methanol calibration curve, and intermittently verified during the experiment using an external methanol calibration standard. The compounds reported herein are extremely sensitive to adventitious O_2/H_2O; upon cooling, generation of small amounts of HNP* and **1-Ce** is sometimes observed due to weakening of the Teflon/glass J. Young tap seal.

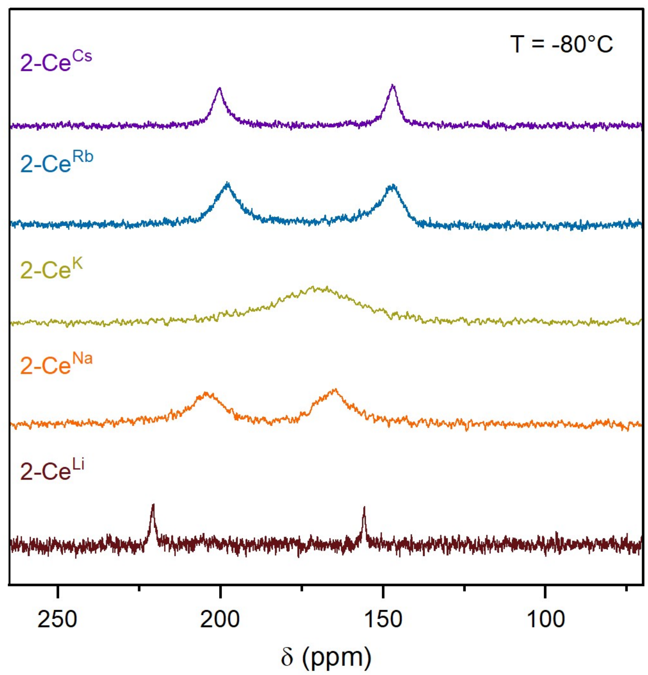


Figure S32. Low-temperature $^{31}P\{^{1}H\}$ NMR at -80°C in toluene-d_8

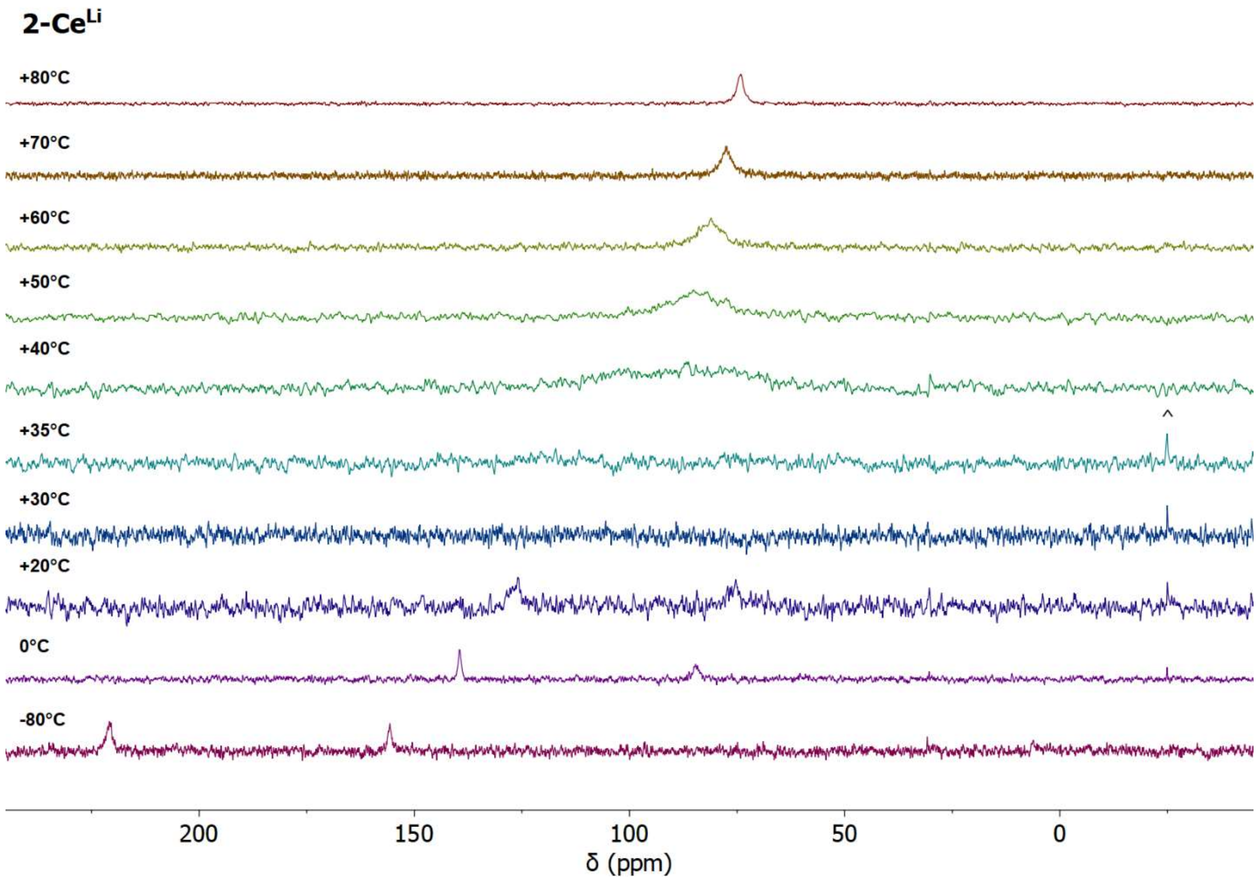


Figure S33. Variable-Temperature $^{31}P\{^{1}H\}$ NMR of **2-Ce^{Li}** in tol-d_8. ^ = **1-Ce.**

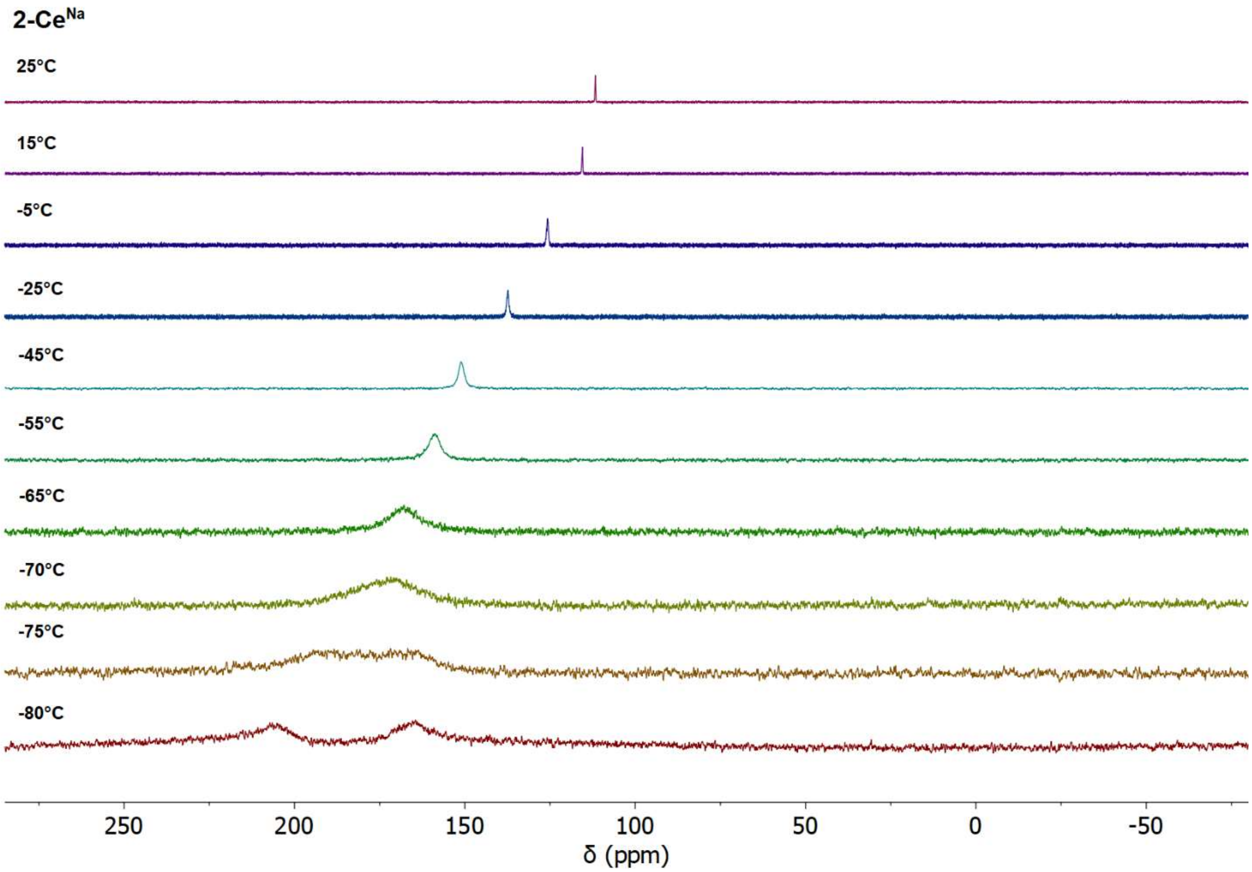


Figure S34. Variable-Temperature $^{31}P\{^{1}H\}$ NMR of **2-Ce^{Na}** in tol-d_8.

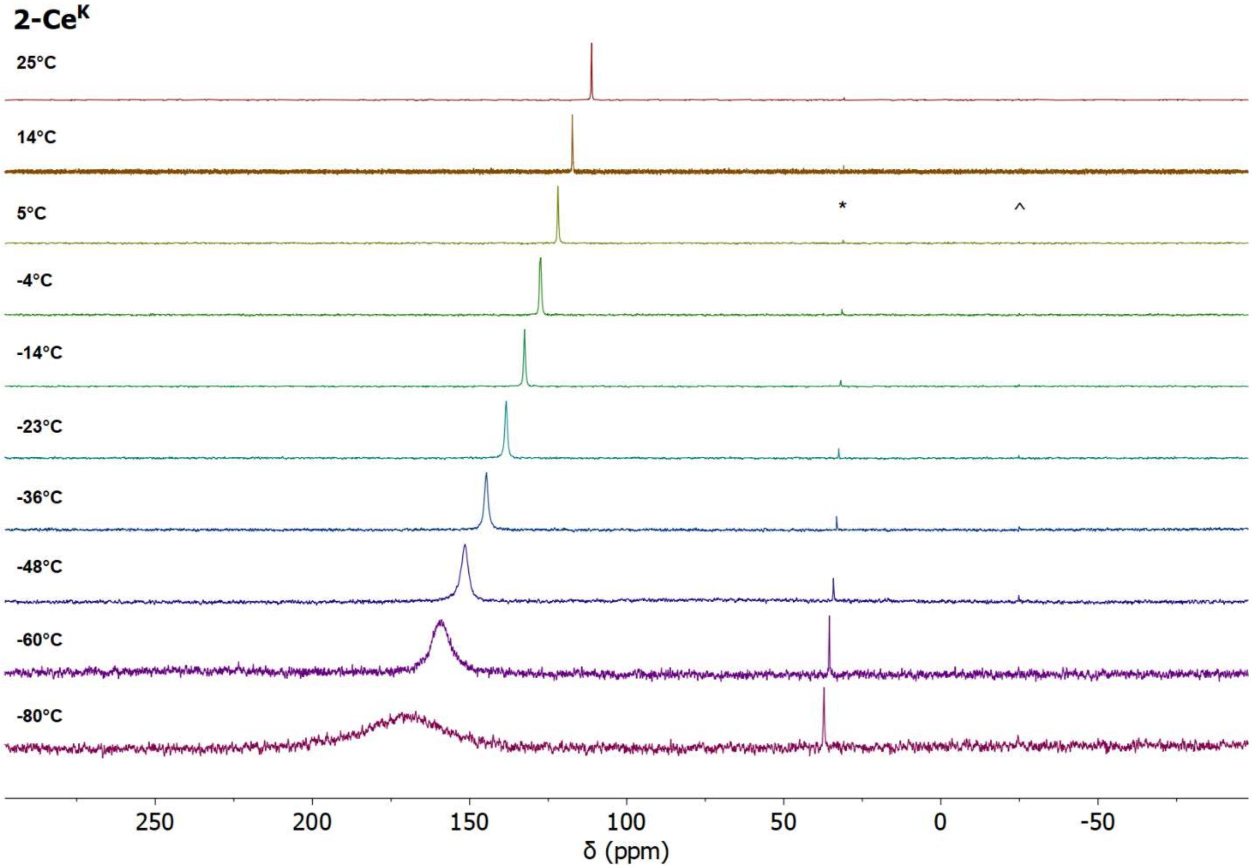


Figure S35. Variable-Temperature $^{31}P\{^{1}H\}$ NMR of **2-Ce^{K}** in tol-d_8. * = HNP*, ^ = **1-Ce.**

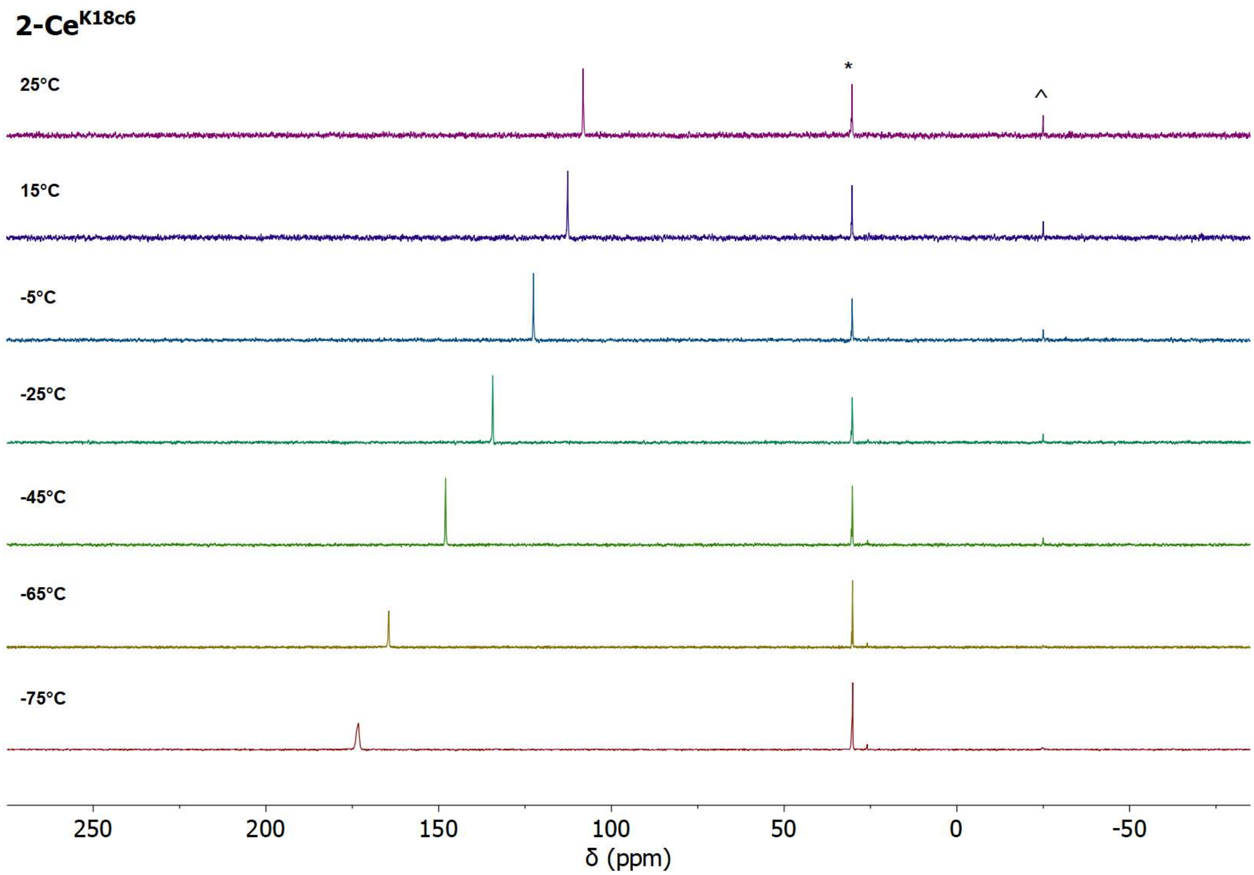


Figure S36. Variable-temperature $^{31}P\{^{1}H\}$ NMR of **2-Ce^{K18c6}** in THF-d_8. * = HNP*, ^ = **1-Ce**.

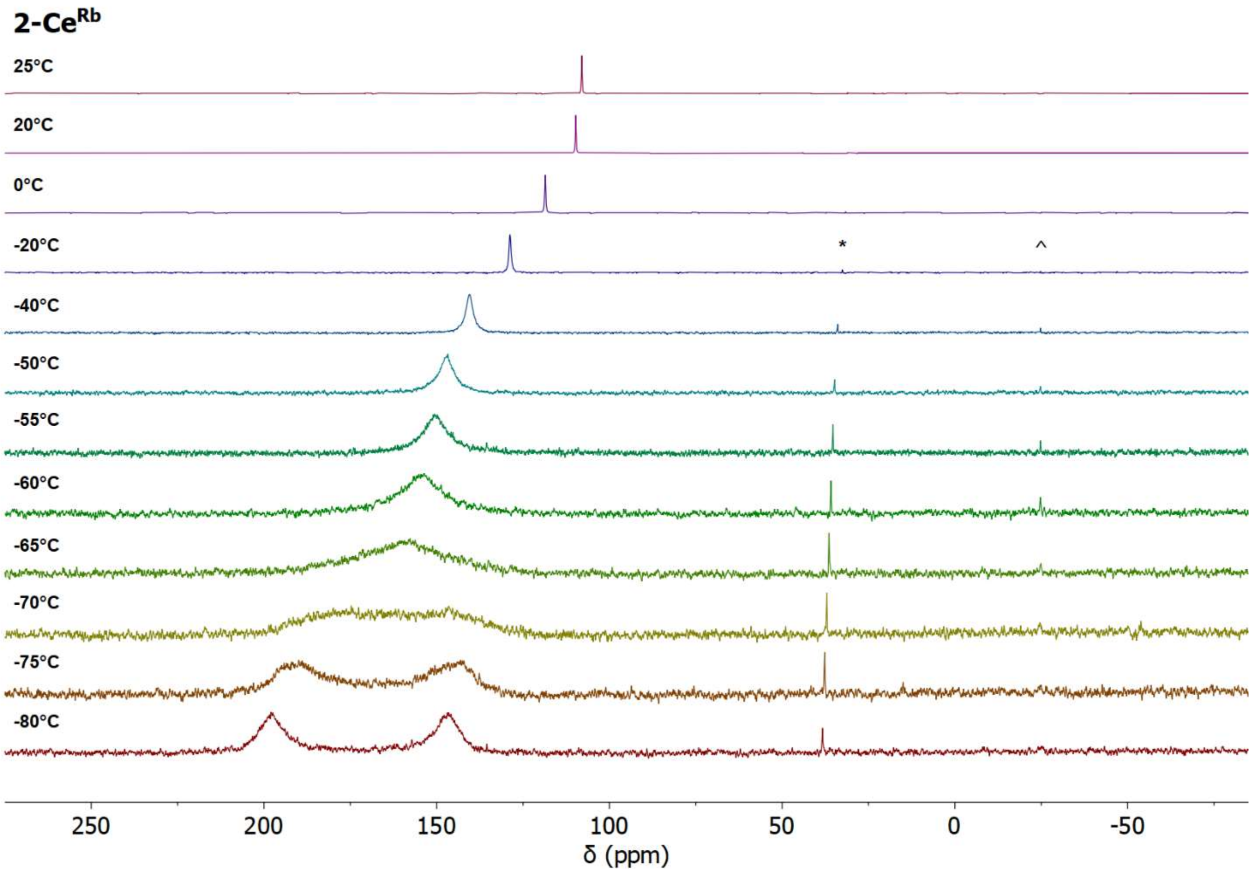


Figure S37. Variable-temperature $^{31}P\{^{1}H\}$ NMR of **2-Ce^{Rb}**. *= HNP*, ^ = **1-Ce.**

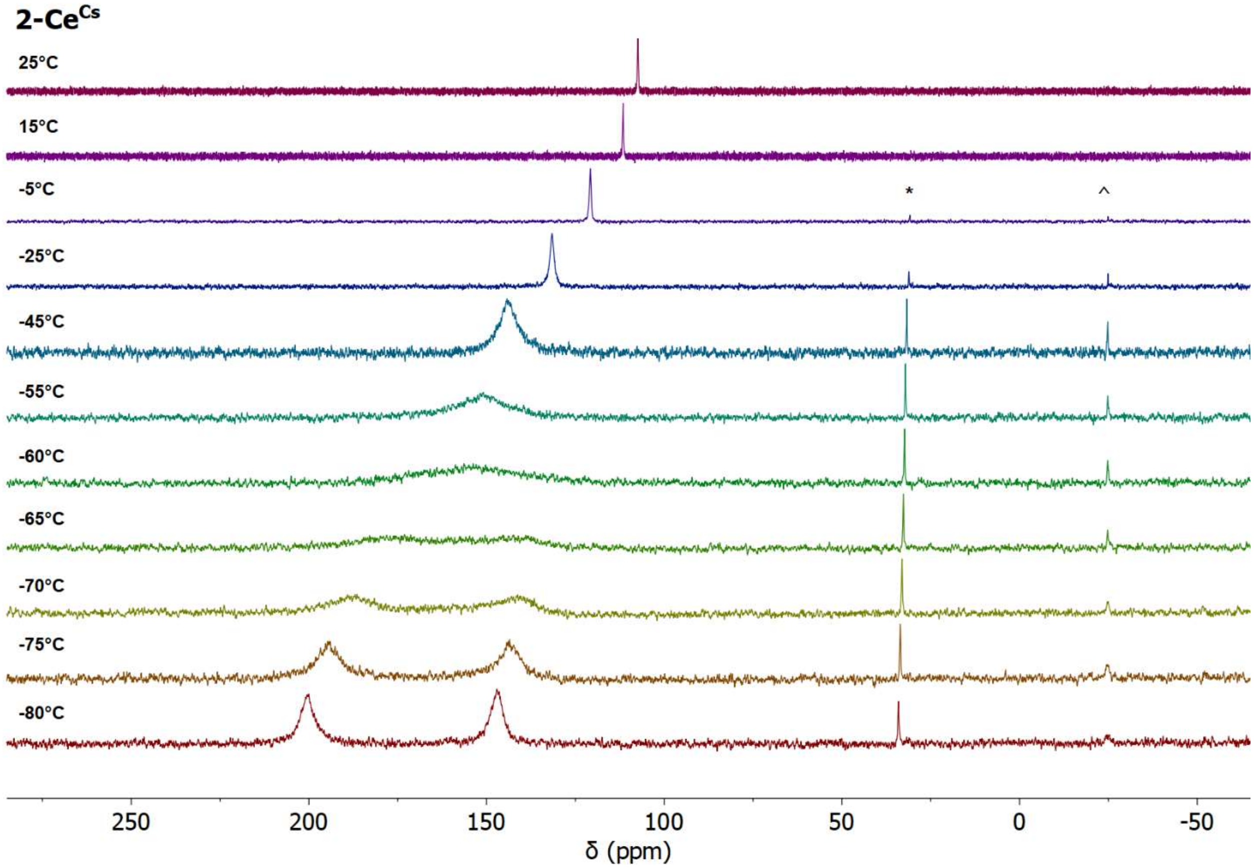


Figure S38. Variable-temperature $^{31}P\{^{1}H\}$ NMR of **2-Ce^{Cs}**. *= HNP*, ^ = **1-Ce.**

UV-Vis-NIR Spectra

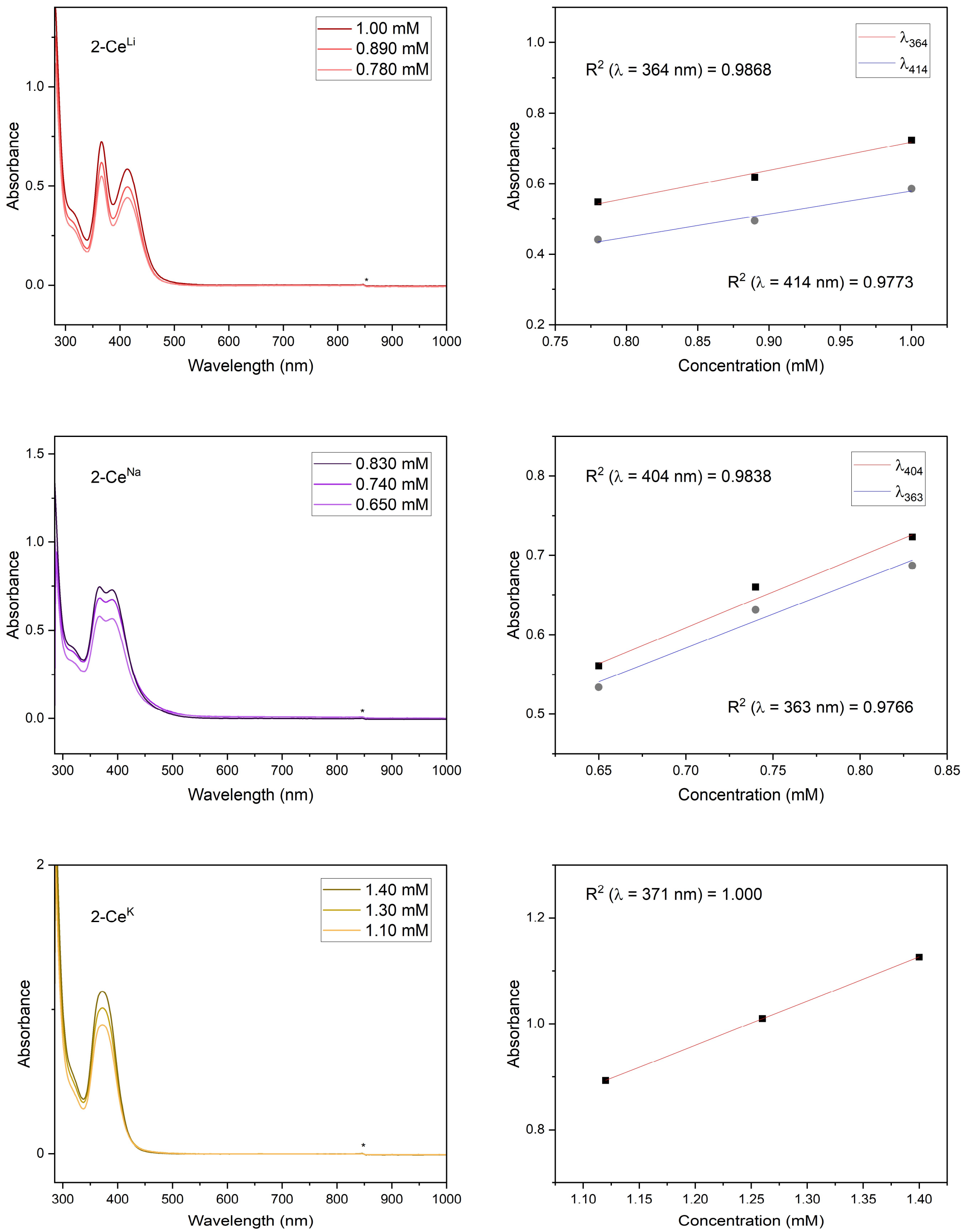


Figure S39. UV-Vis-NIR spectra at multiple concentrations (left) and linear regression analysis of absorbance at $λ_{max}$ (right) for **2-Ce^{Li}** (top), **2-Ce^{Na}** (middle), **2-Ce^{K}** (bottom) in toluene.

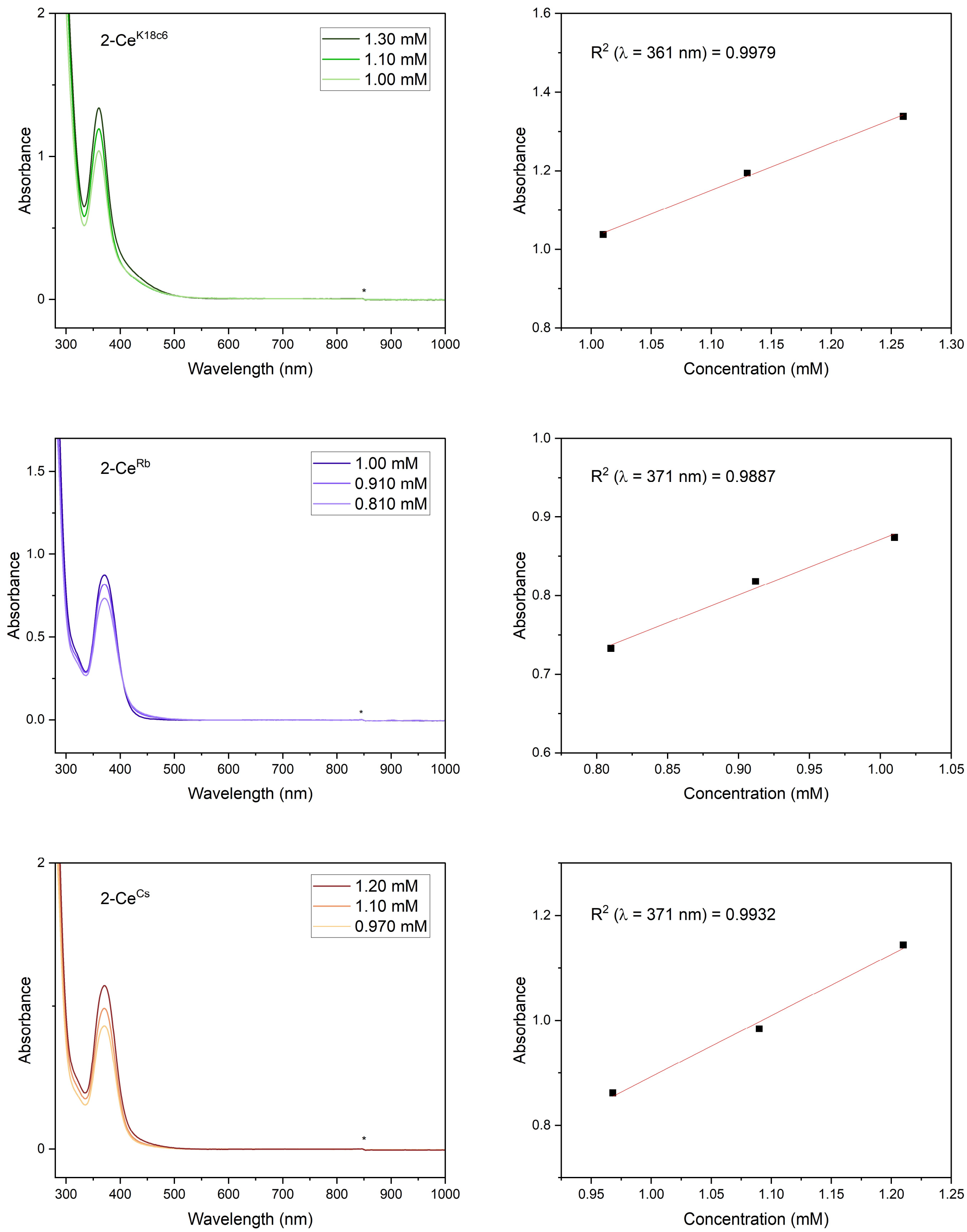


Figure S40. UV-Vis-NIR spectra at multiple concentrations (left) and linear regression analysis of absorbance at λ_{max} (right) for **2-Ce^{K18c6}** in THF (top), **2-Ce^{Rb}** (middle) and **2-Ce^{Cs}** (bottom) in toluene.

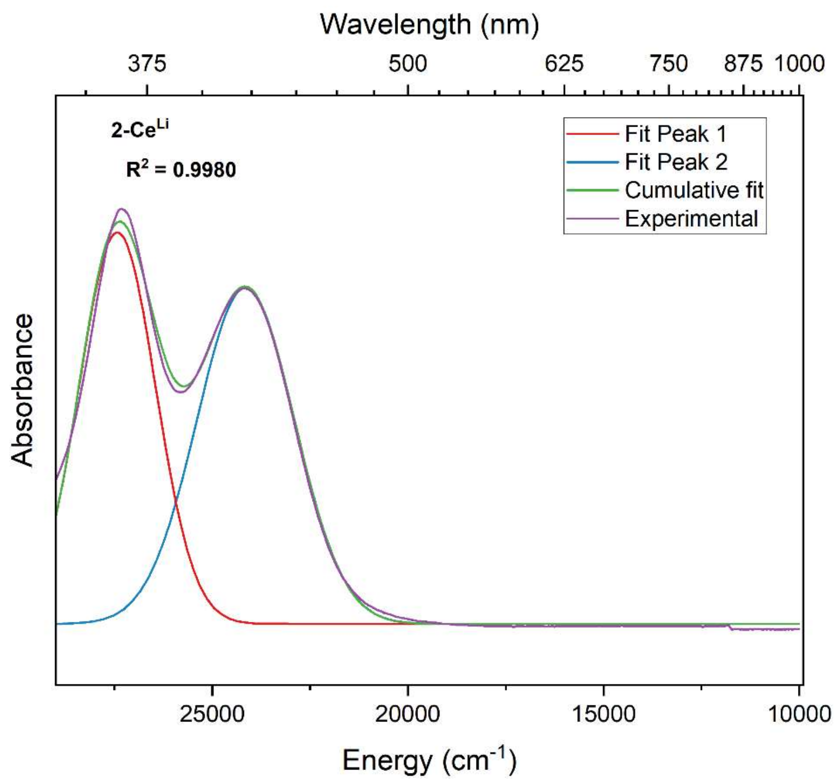


Figure S41. Gaussian fitting of UV-Vis-NIR spectrum of **2-Ce^{Li}** in toluene.

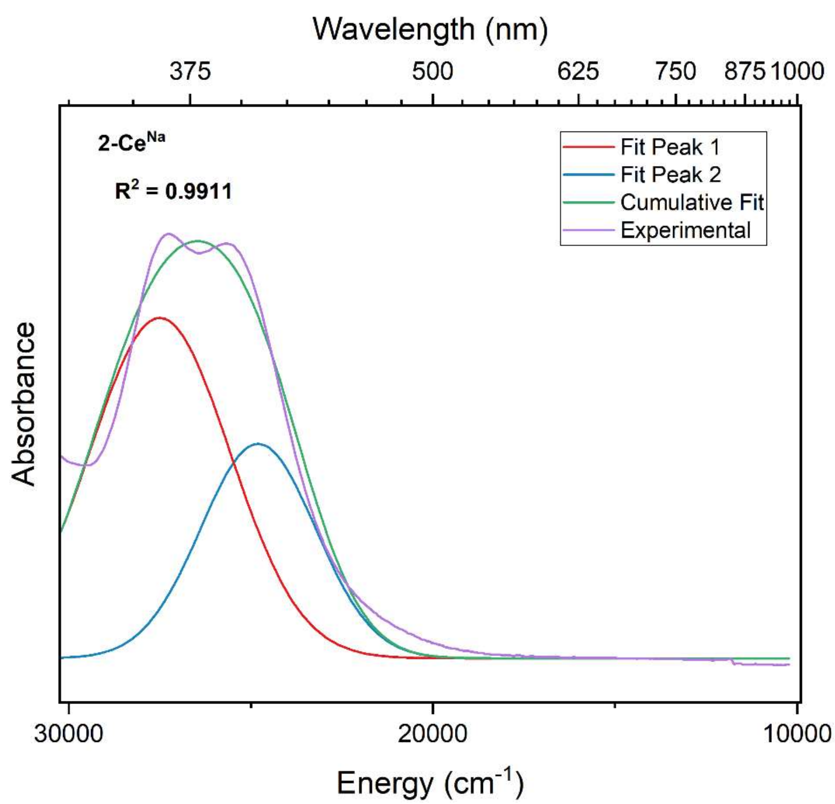


Figure S42. Gaussian fitting of UV-Vis-NIR spectrum of **2-Ce^{Na}** in toluene. Note: A satisfactory fit for this spectrum is complicated by large features on the edge of the UV window, in addition to trace amounts of highly absorbing **1-Ce.** Rather than over-parametrizing, a crude fit is presented showing two features present.

Table S1. Tabulated UV-Vis parameters.

	2-Ce^{Li}	**2-Ce^{Na}**	**2-Ce^{K}**	**2-Ce^{K18c6}**	**2-Ce^{Rb}**	**2-Ce^{Cs}**
λ (nm)	363	360	371	361	371	371
ε ($M^{1}cm^{-1}$)	800	900	800	1000	700	1000
FWHM (eV)	0.27	0.15	0.45	0.45	0.64	0.43
λ (nm)	414	393	-	-	-	-
ε ($M^{1}cm^{-1}$)	700	700	-	-	-	-
FWHM (eV)	0.39	0.68	-	-	-	-

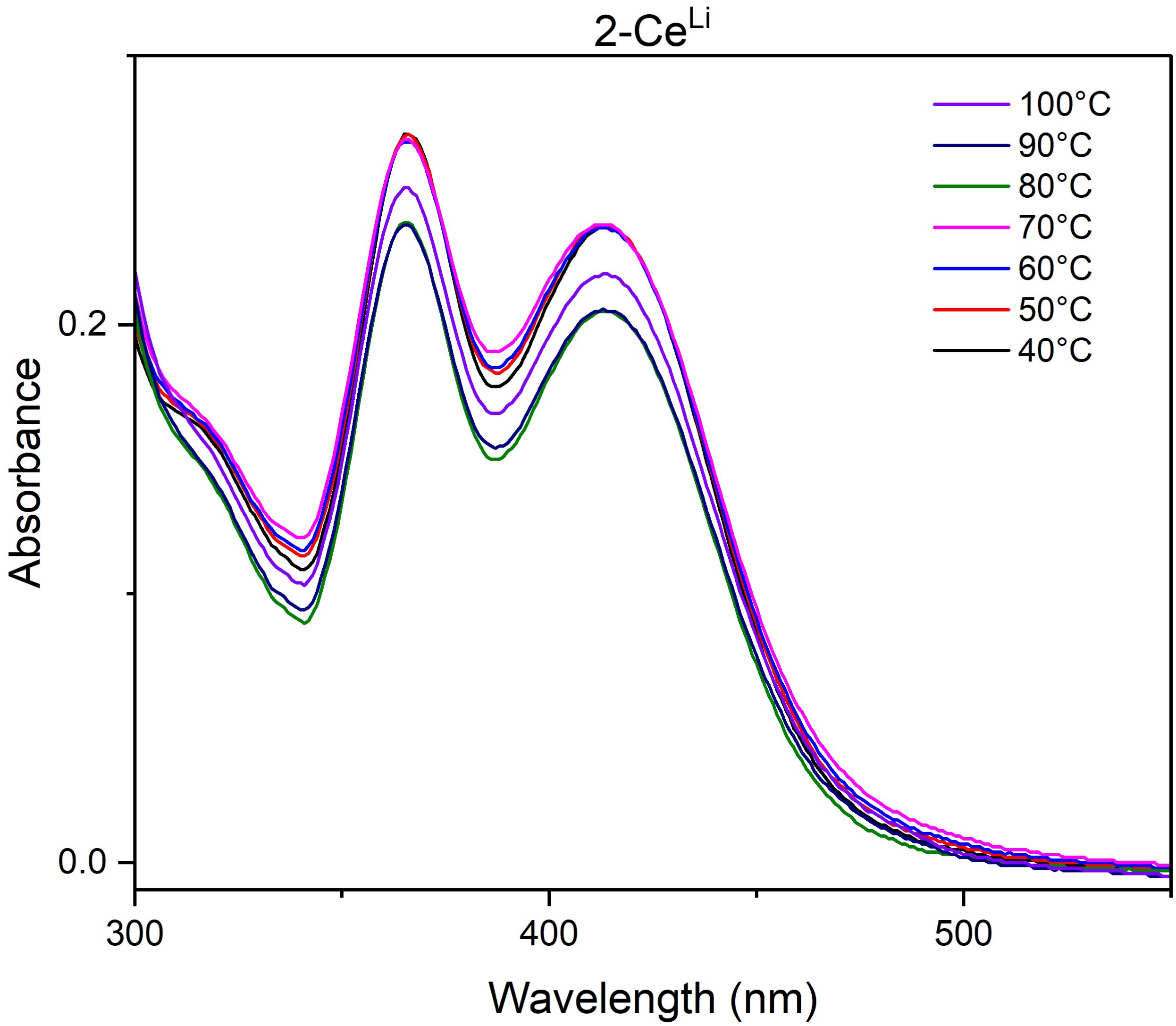


Figure S43. Variable-temperature UV-Vis spectra of **2-Ce^{Li}** in toluene.

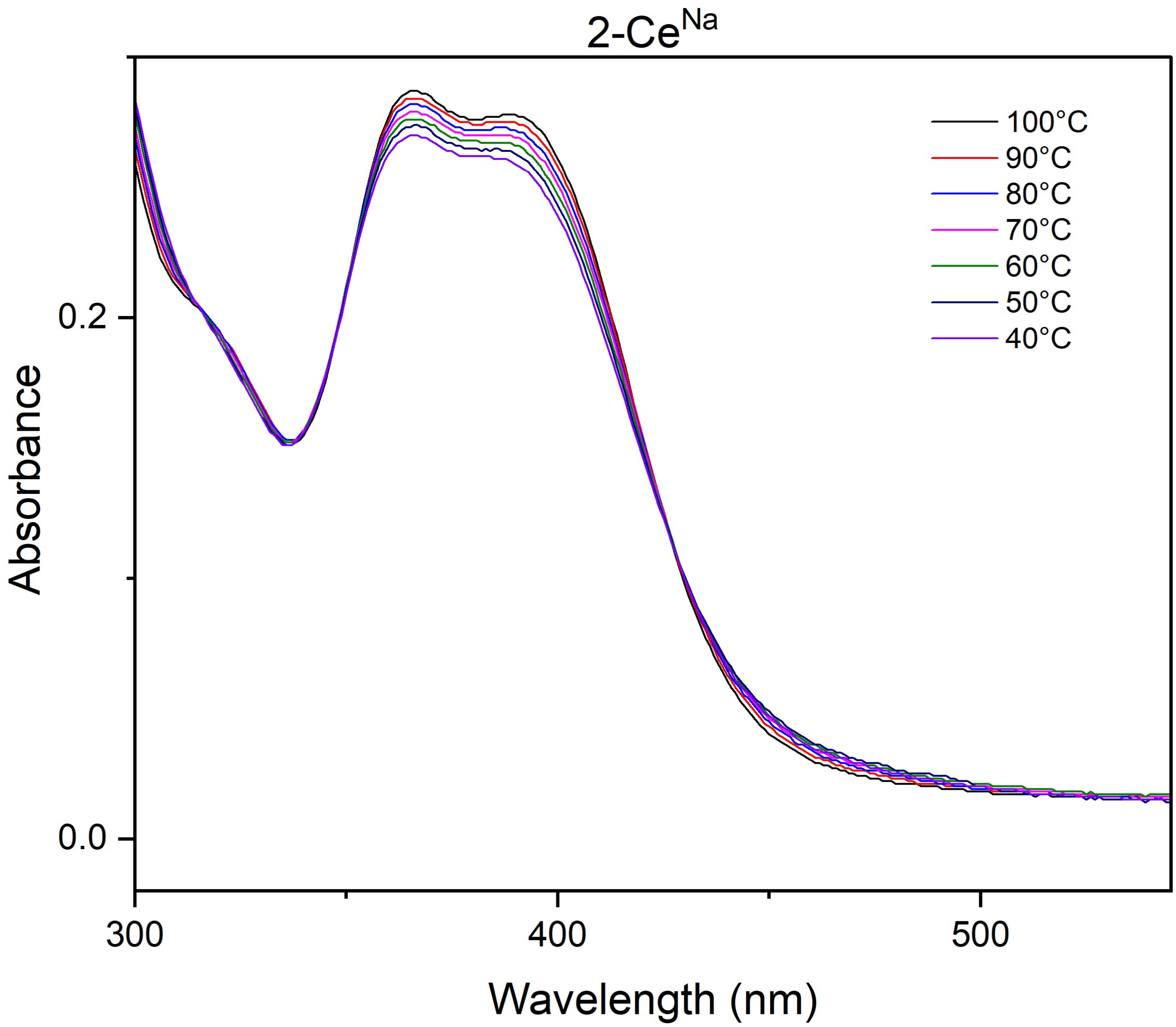


Figure S44. Variable-temperature UV-Vis spectra of **2-Ce^{Na}** in toluene.

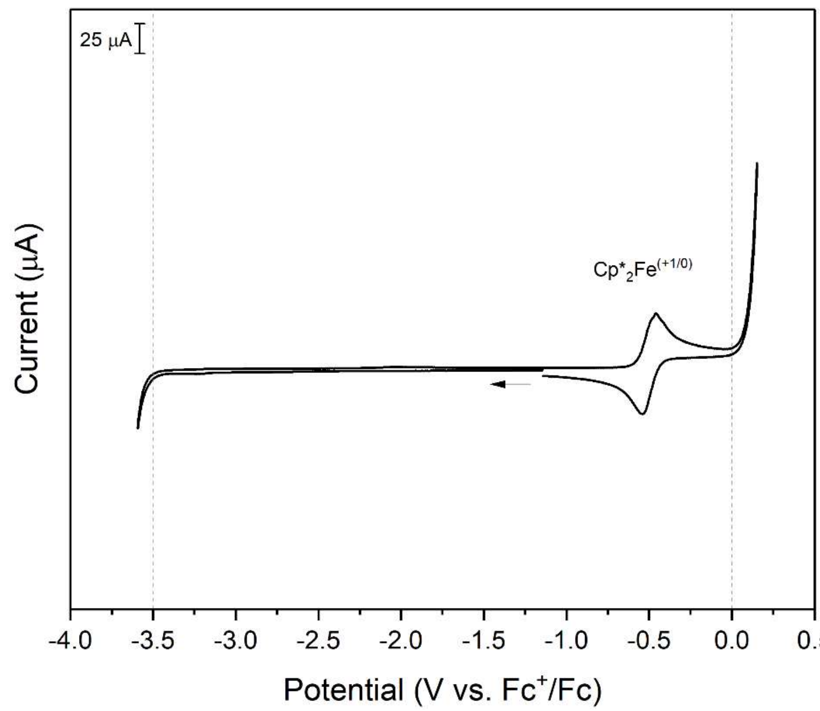


Figure S45. Cyclic voltammogram displaying electrochemical window of 50 mM [^{n}Bu$_4$N][BPh$_4$] in THF with internal reference decamethylferrocene, scan rate = 200 mV/s. Reference lines at -3.5 V and 0 V.

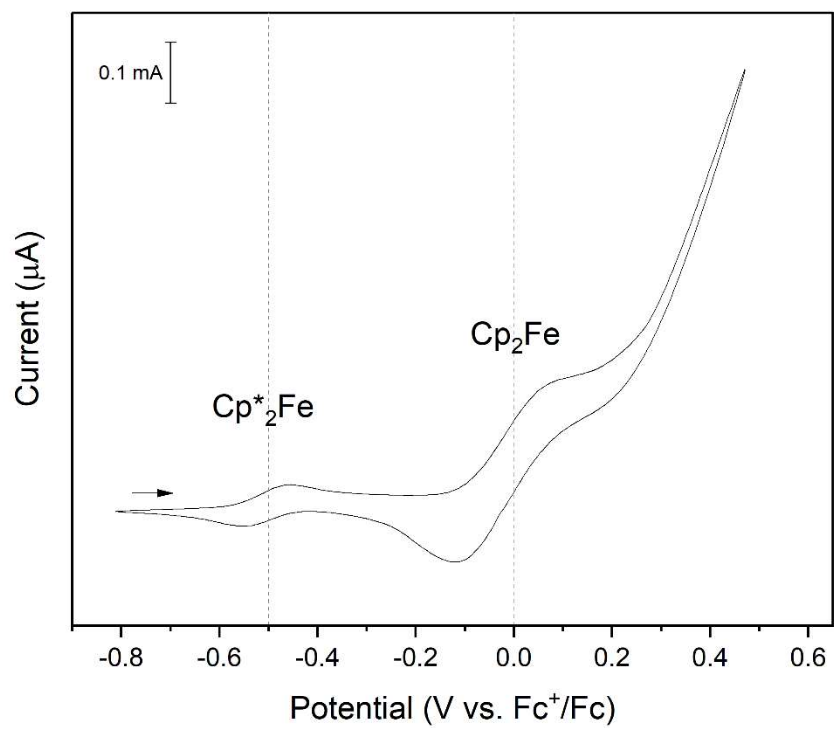
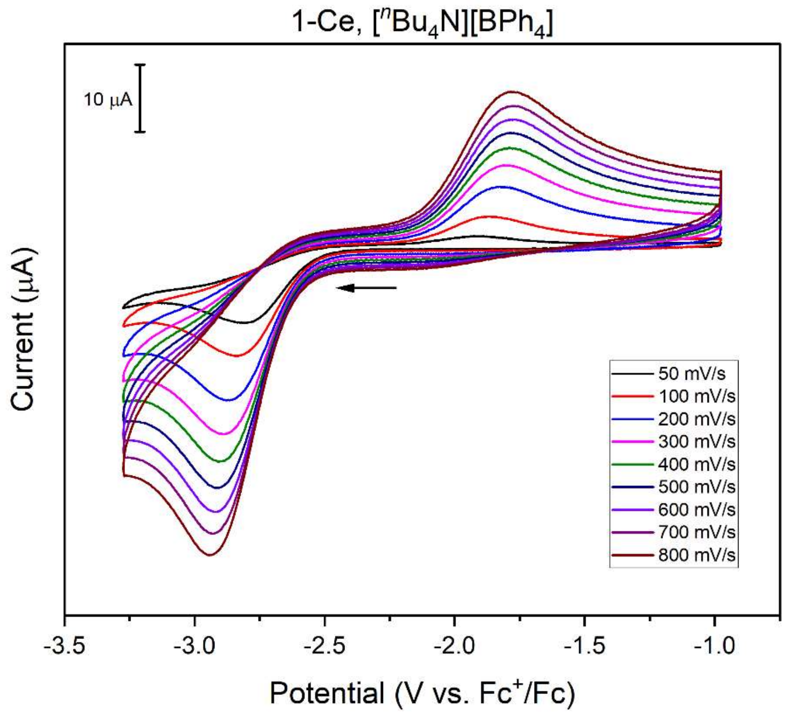


Figure S46. Cyclic voltammogram of decamethylferrocene vs. ferrocene in 50 mM [^{n}Bu$_4$N][BPh$_4$] in THF, scan rate = 200 mV/s.



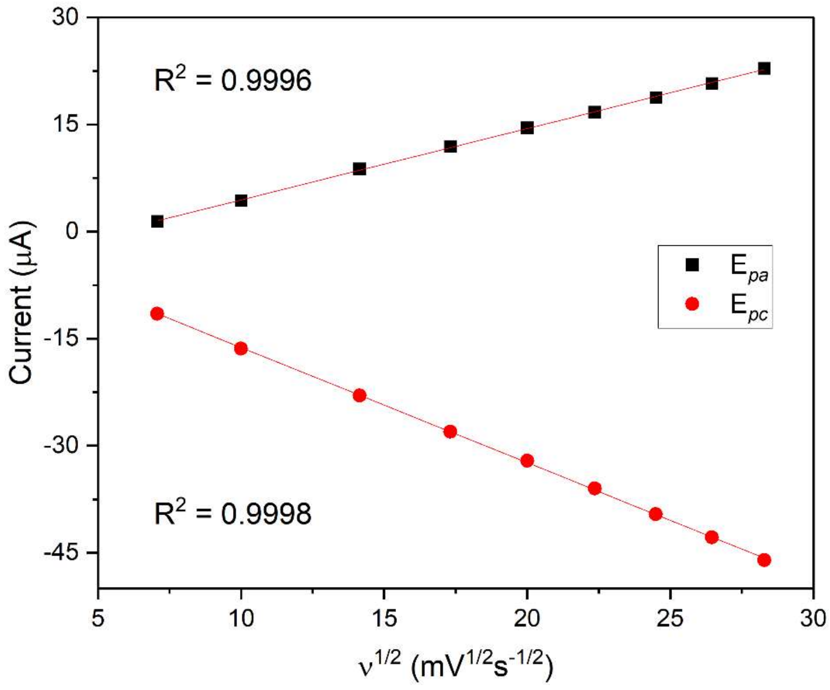


Figure S47. Scan-rate dependence of 3 mM **1-Ce** in 50 mM [^{n}Bu$_4$N][BPh$_4$] in THF (top) and Randles-Sevcik plot (bottom).

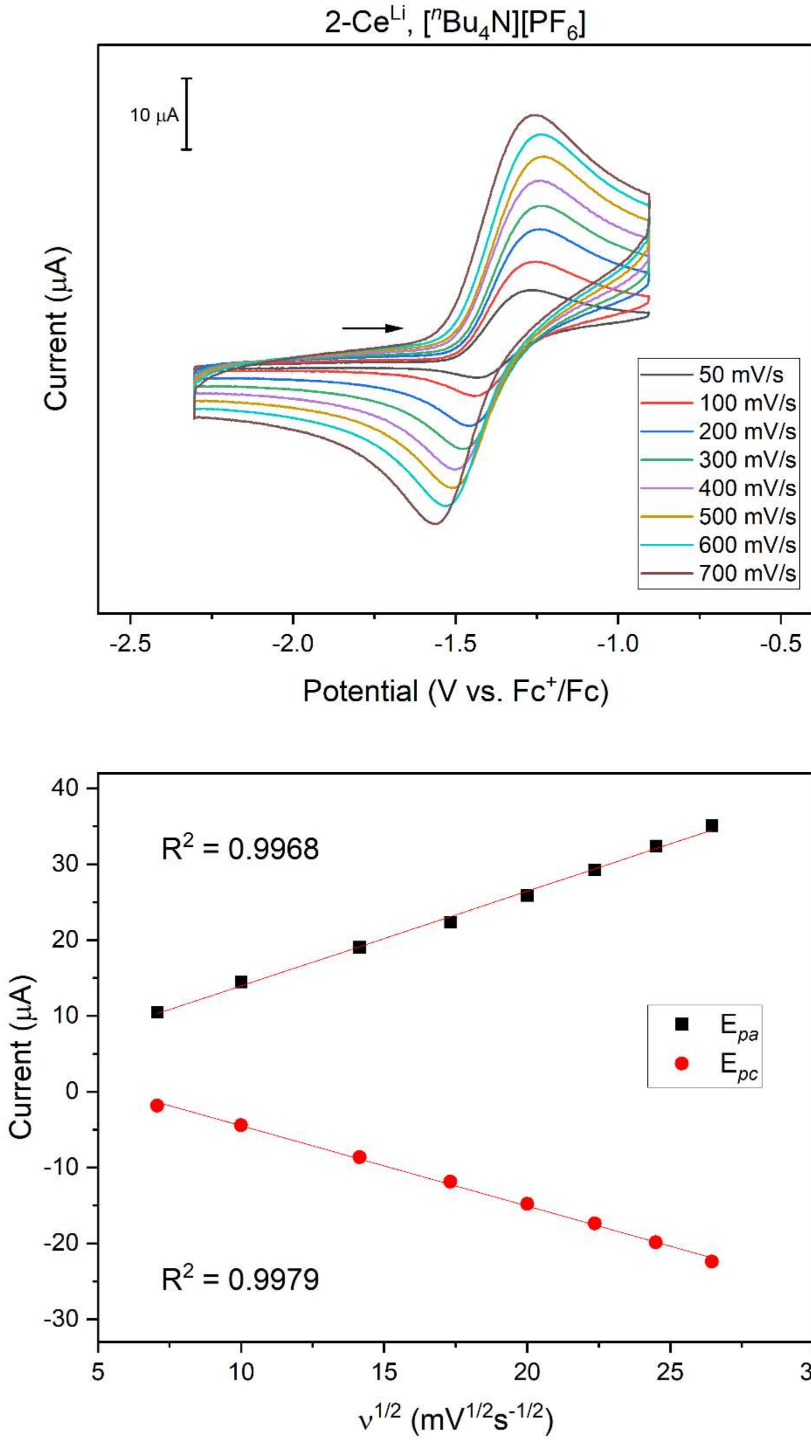


Figure S48. Scan-rate dependence of 3 mM **2-Ce^{Li}** in 50 mM [^{n}Bu$_4$N][PF$_6$] in THF (top) and Randles-Sevcik plot (bottom).

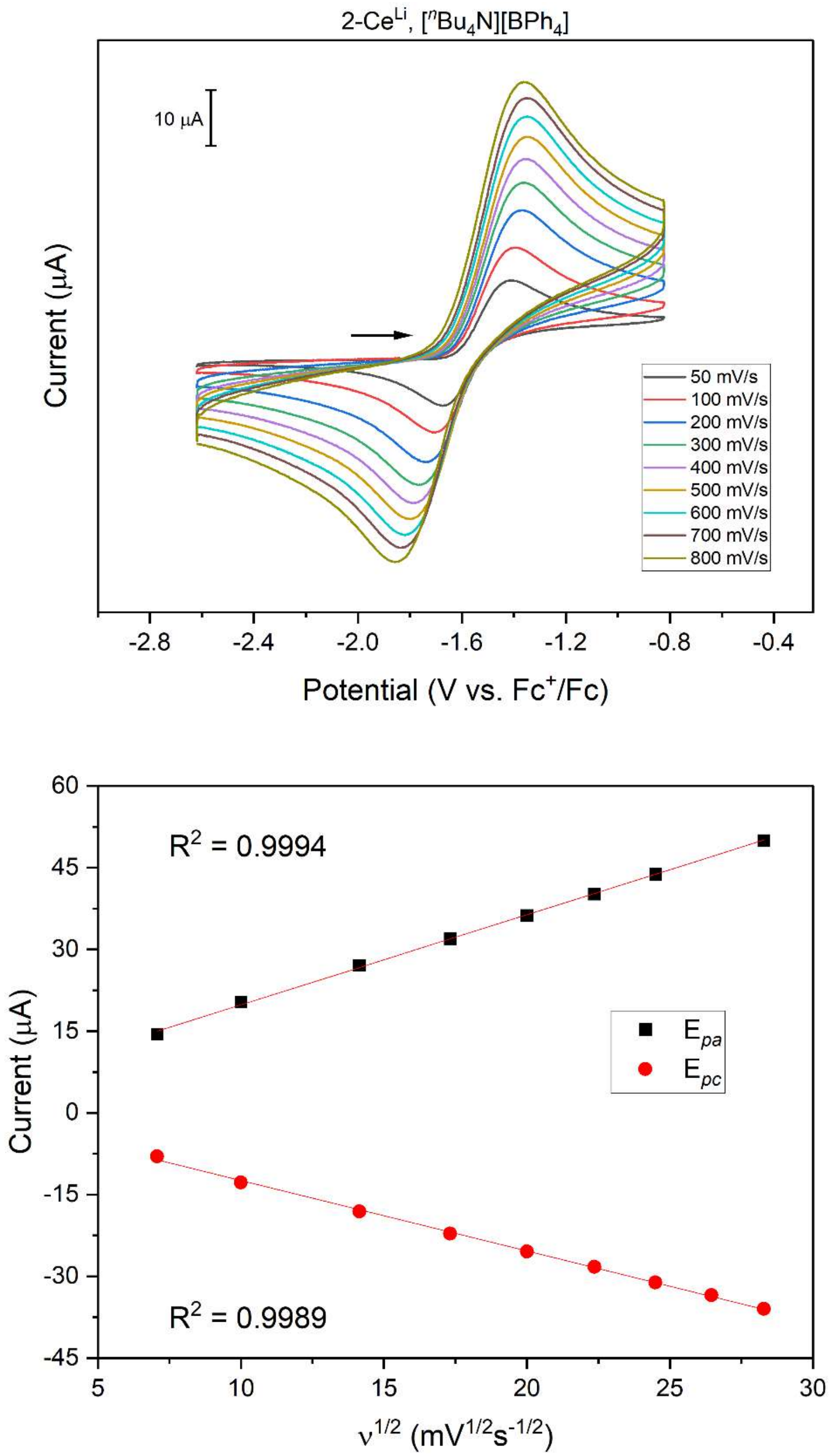
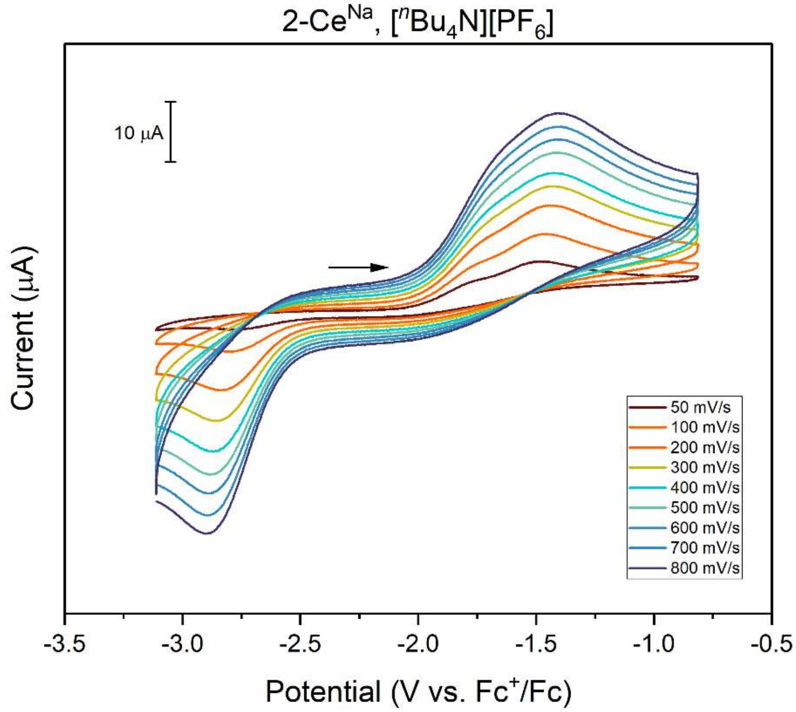


Figure S49. Scan-rate dependence of 3 mM **2-Ce^{Li}** in 50 mM [^{n}Bu$_4$N][BPh$_4$] in THF (top) and Randles-Sevcik plot (bottom).



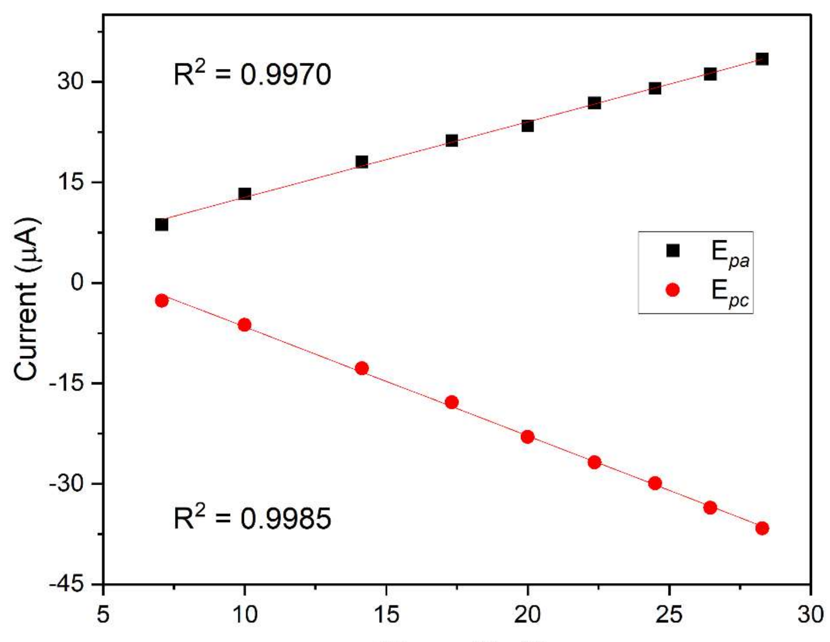
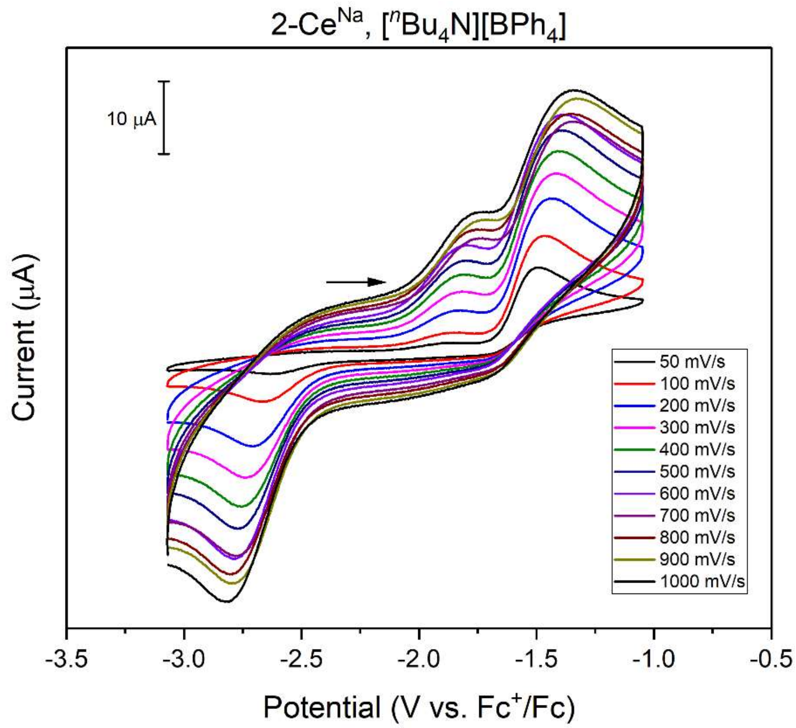


Figure S50. Scan-rate dependence of 3 mM **2-Ce^{Na}** in 100 mM [^{n}Bu$_4$N][PF$_6$] in THF (top) and Randles-Sevcik plot (bottom).



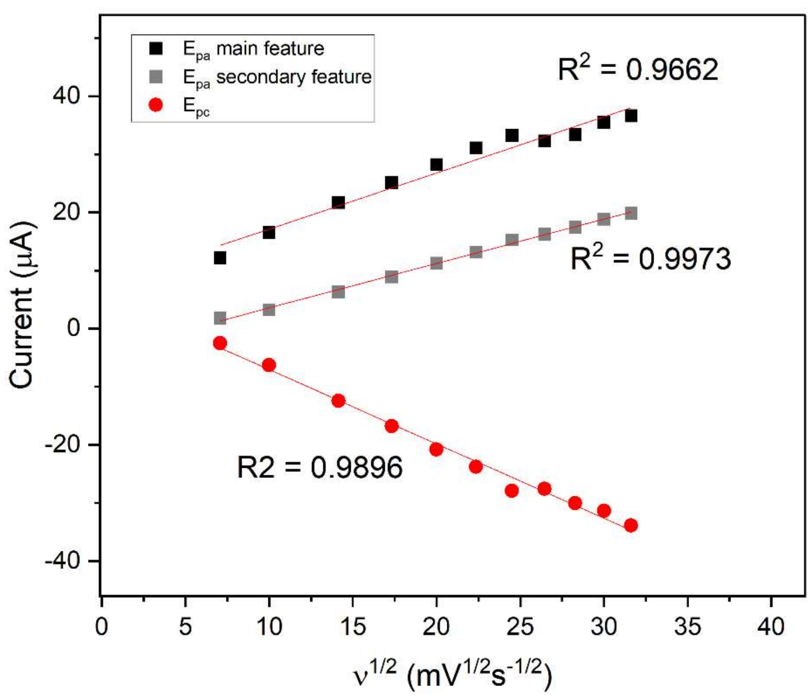
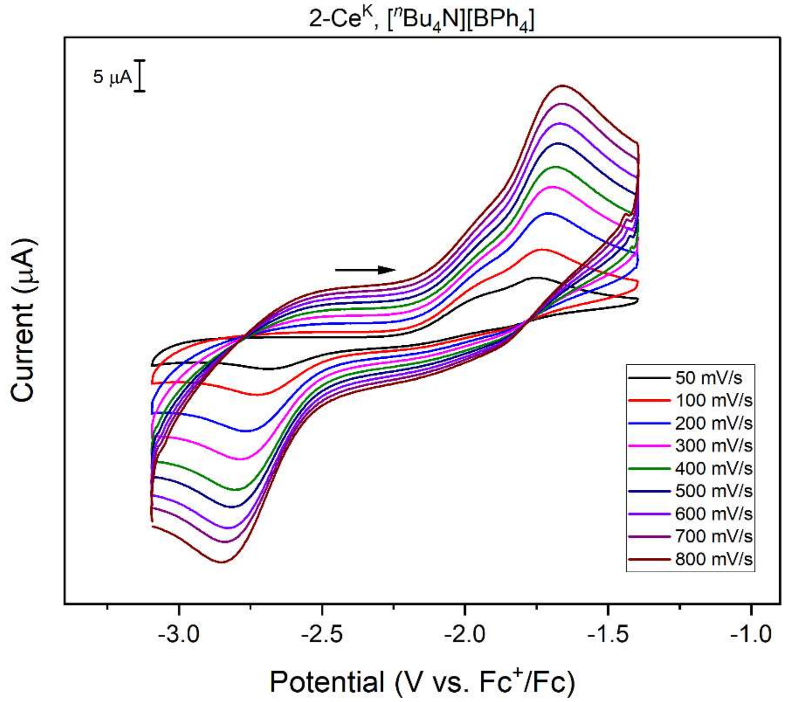


Figure S51. Scan-rate dependence of 3 mM **2-Ce^{Na}** in 50 mM [^{n}Bu$_4$N][BPh$_4$] in THF (top) and Randles-Sevcik plot (bottom).



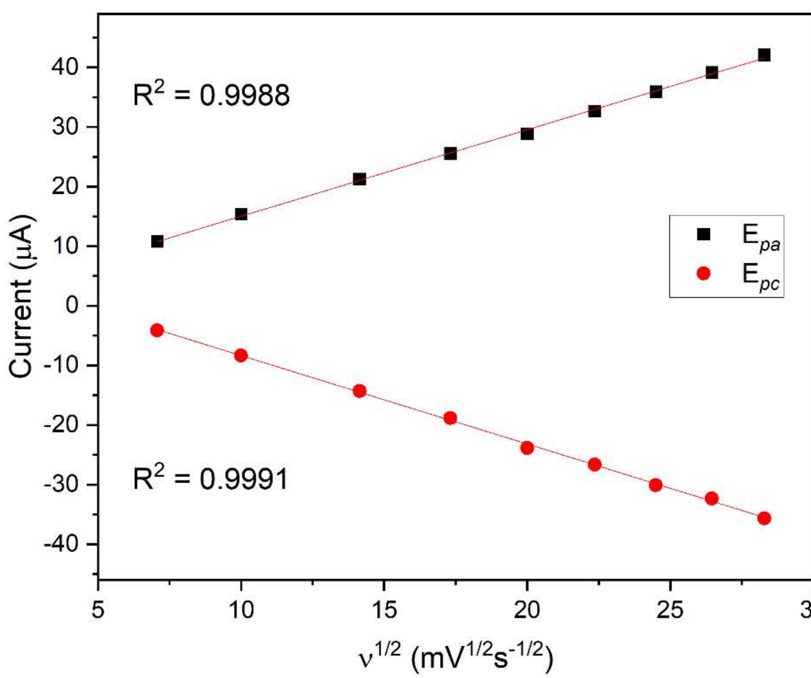


Figure S52. Scan-rate dependence of 3 mM **2-Ce^K** in 50 mM [^{n}Bu$_4$N][BPh$_4$] in THF (top) and Randles-Sevcik plot (bottom).

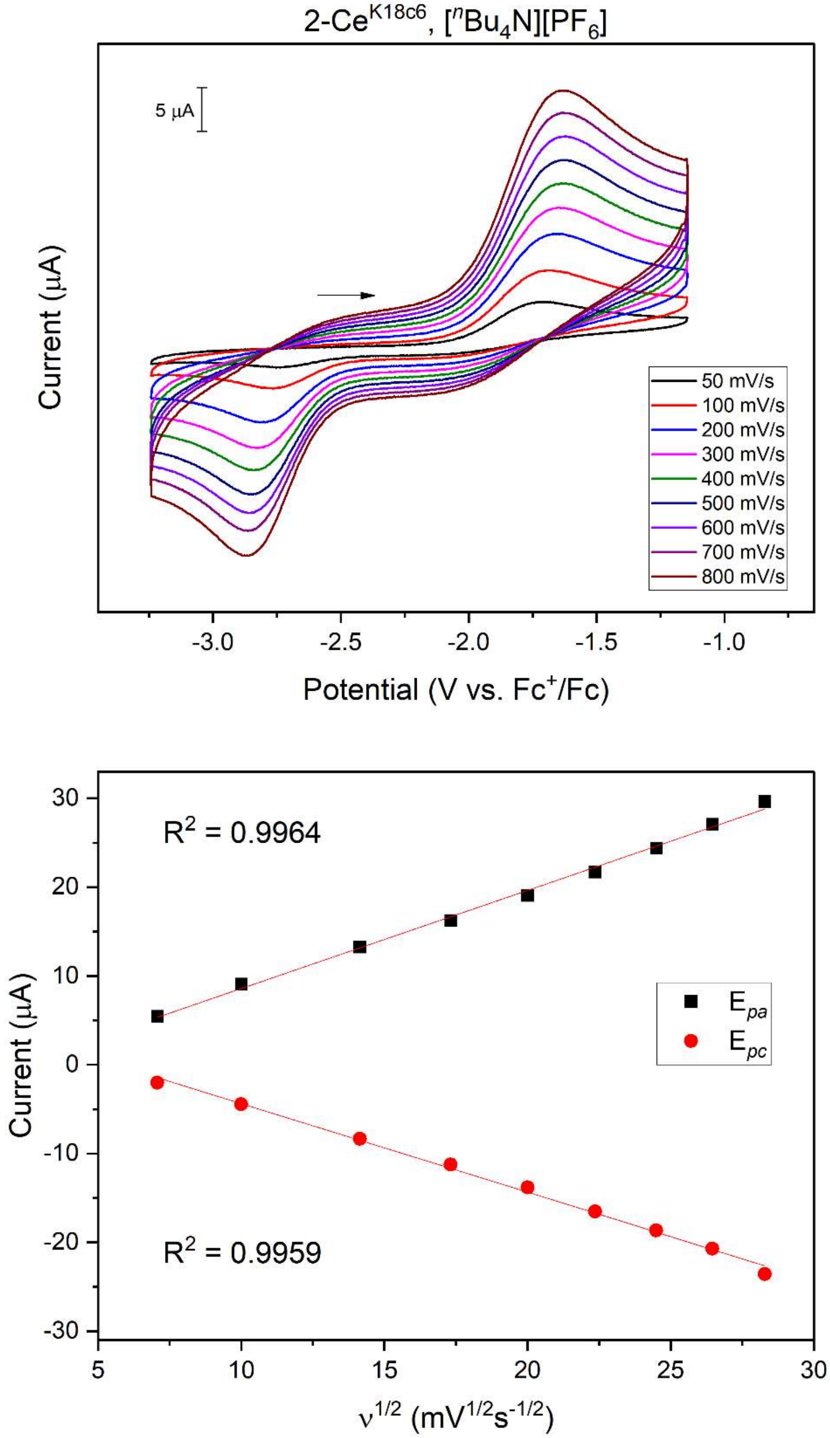
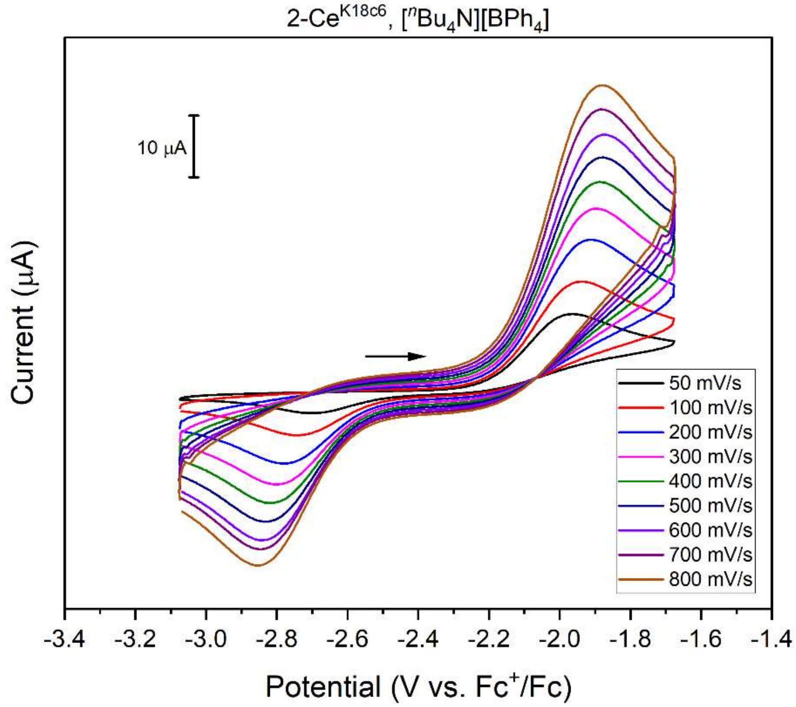


Figure S53. Scan-rate dependence of 3 mM **2-Ce^{K18c6}** in 100 mM [^{n}Bu$_4$N][PF$_6$] in THF (top) and Randles-Sevcik plot (bottom).



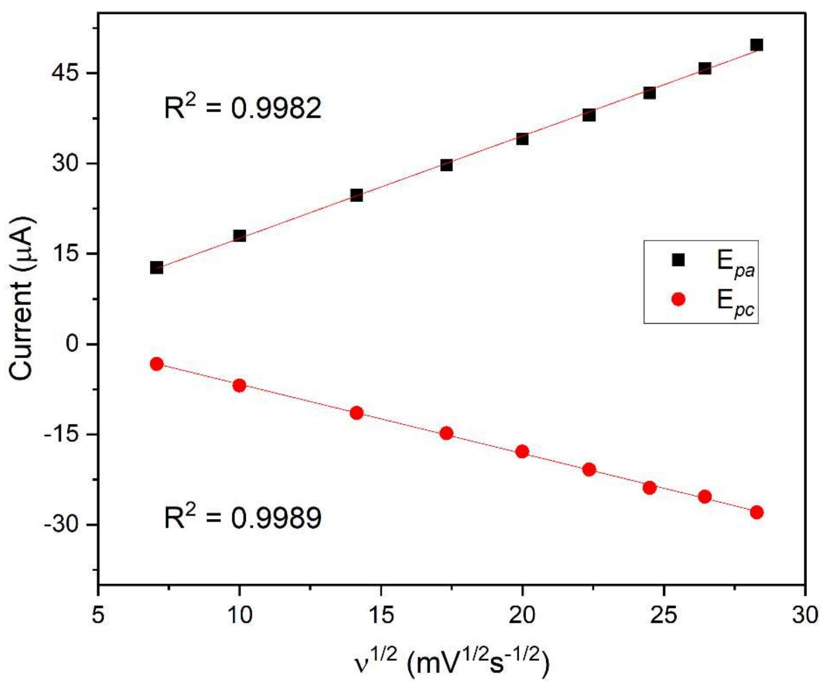
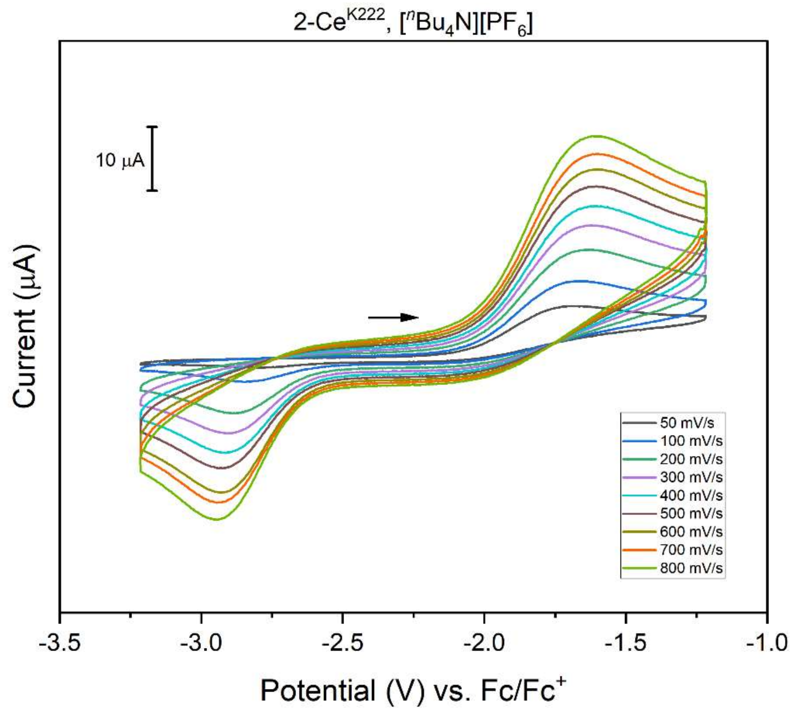


Figure S54. Scan-rate dependence of 3 mM **2-Ce^{K18c6}** in 50 mM [^{n}Bu$_4$N][BPh$_4$] in THF (top) and Randles-Sevcik plot (bottom).



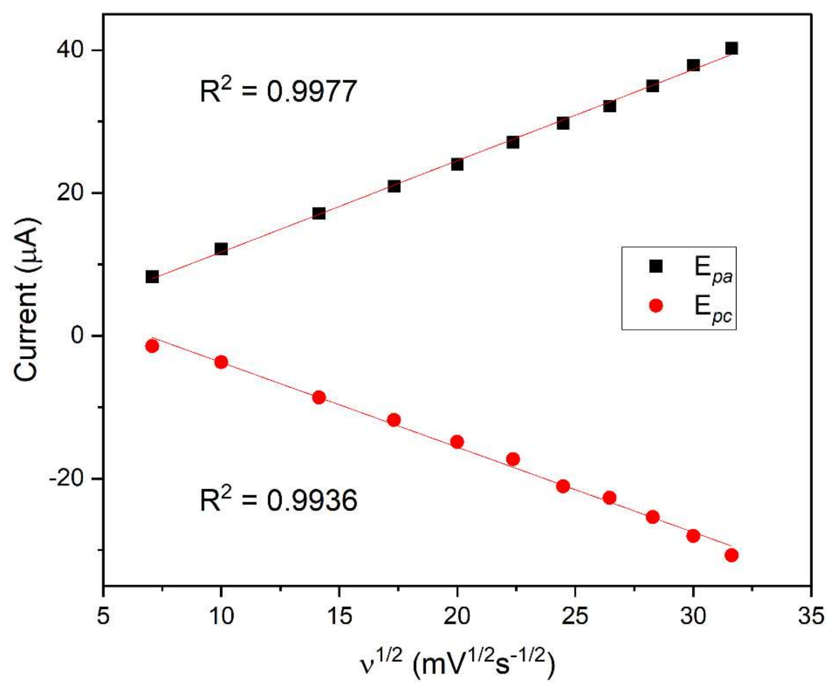


Figure S55. Scan-rate dependence of 3 mM **2-Ce^{K222}** in 100 mM [^{n}Bu$_4$N][PF$_6$] in THF (top) and Randles-Sevcik plot (bottom).

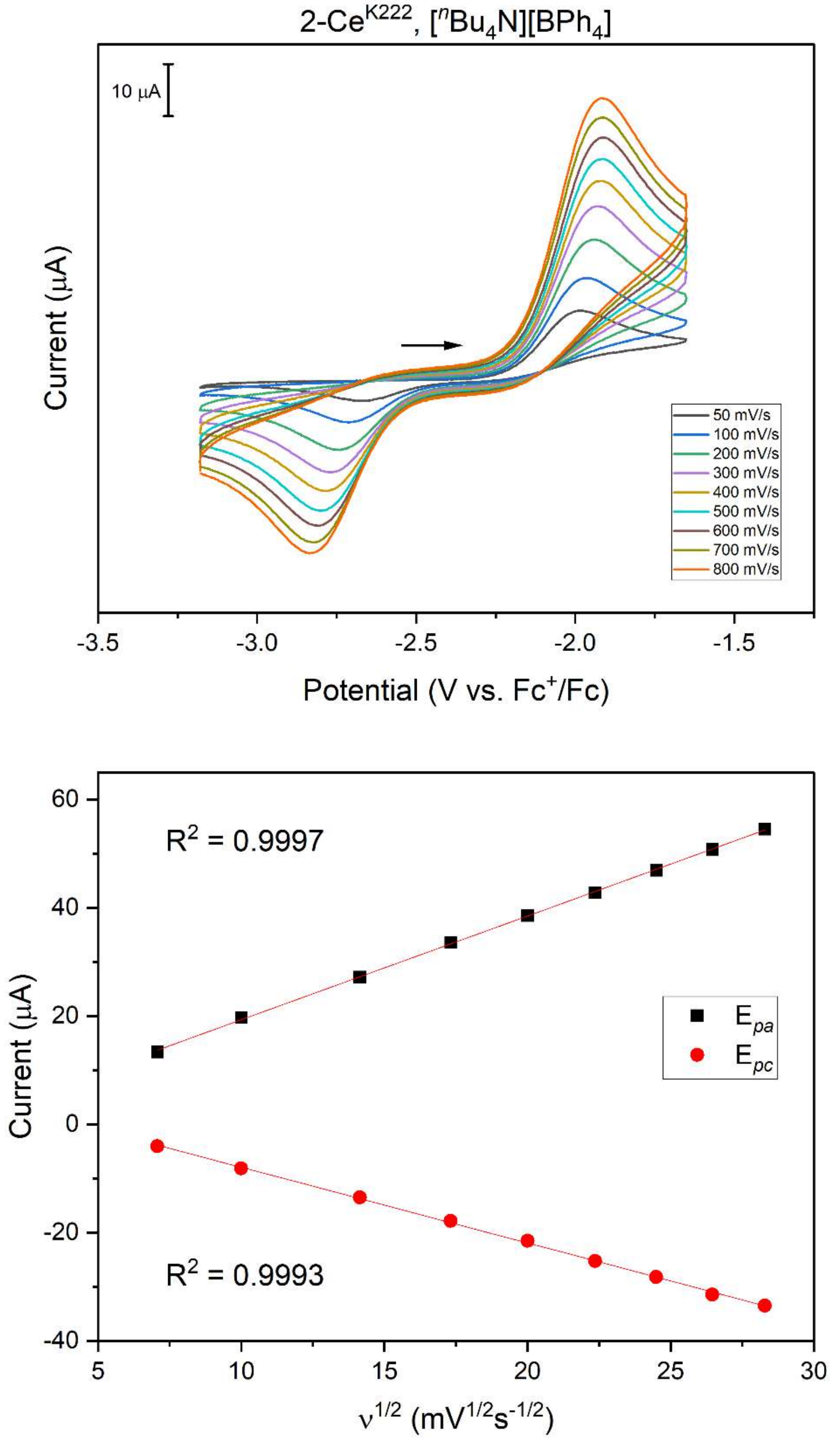
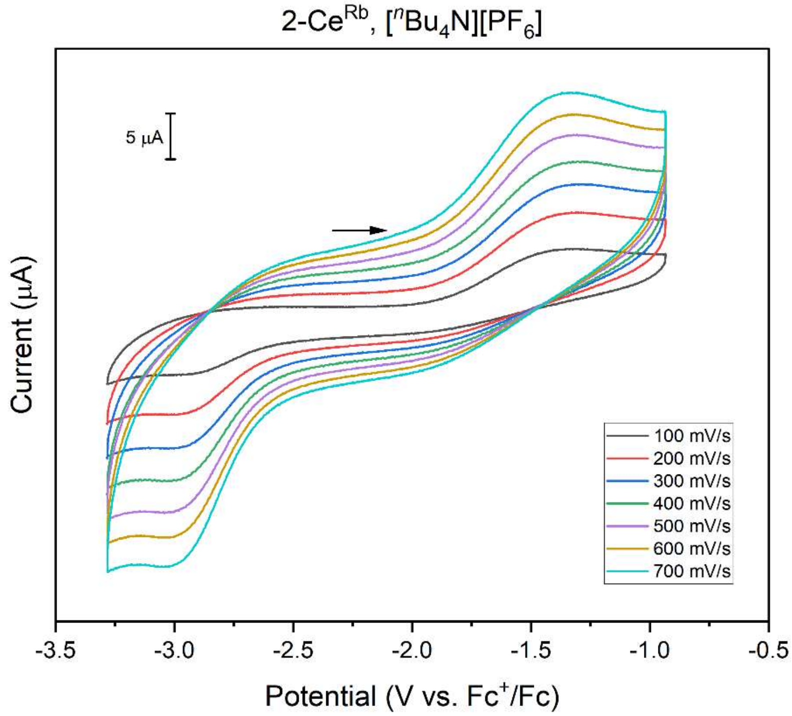


Figure S56. Scan-rate dependence of 3 mM **2-Ce^{K222}** in 50 mM [^{n}Bu$_4$N][BPh$_4$] in THF (top) and Randles-Sevcik plot (bottom).



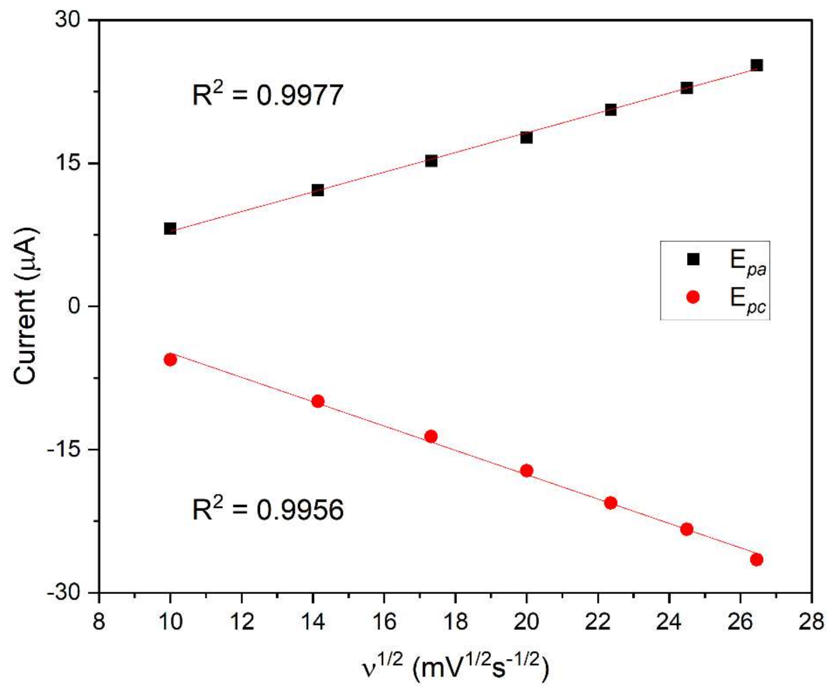
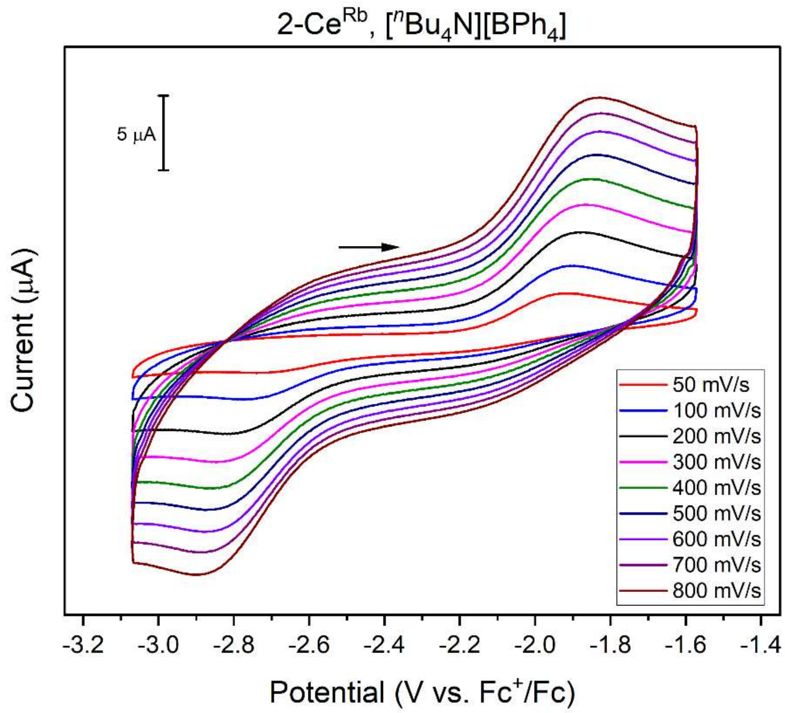


Figure S57. Scan-rate dependence of 3 mM **2-Ce^{Rb}** in 100 mM [^{n}Bu$_4$N][PF$_6$] in THF (top) and Randles-Sevcik plot (bottom).



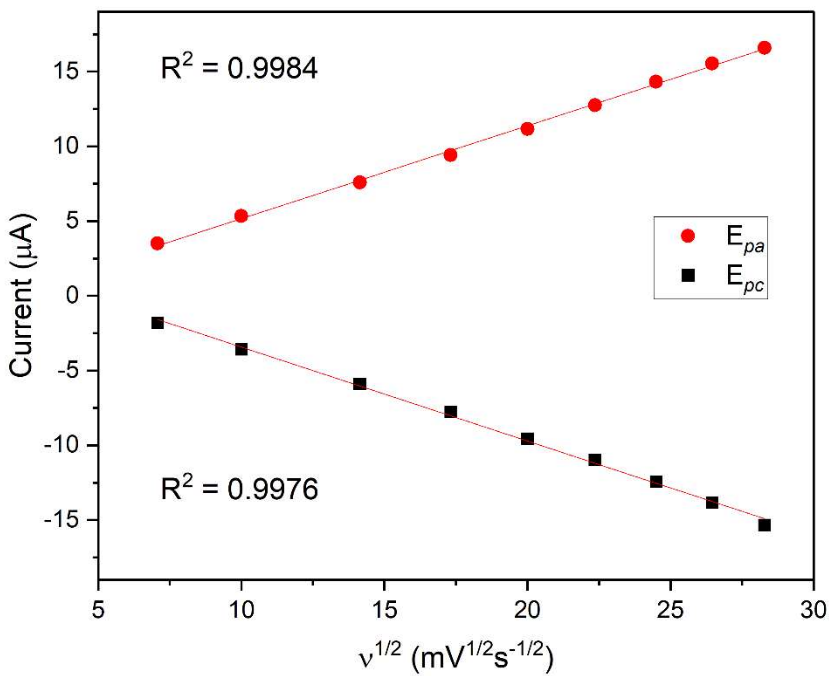
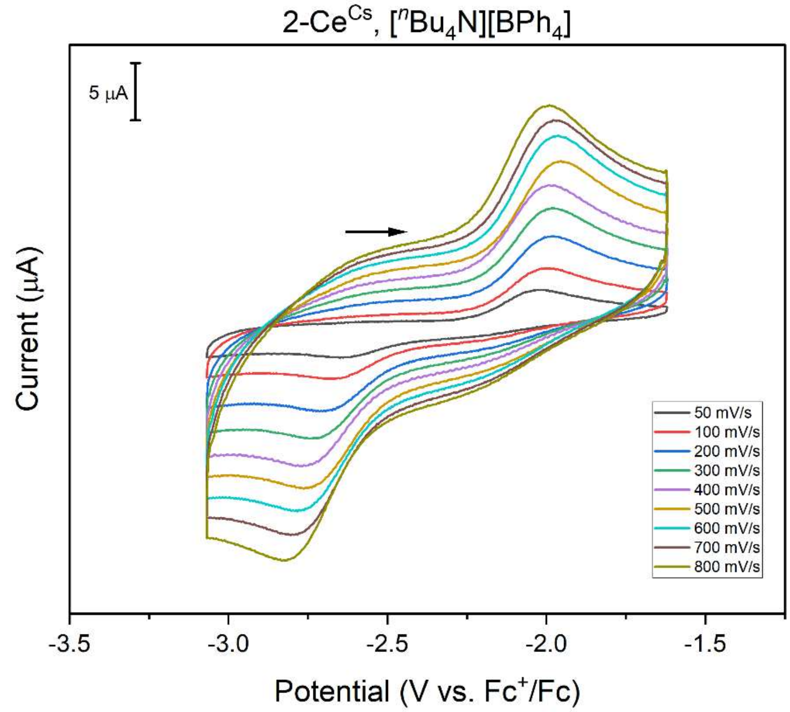


Figure S58. Scan-rate dependence of 1 mM **2-Ce^{Rb}** in 50 mM [$^{n}Bu_4N$][BPh_4] in THF (top) and Randles-Sevcik plot (bottom).



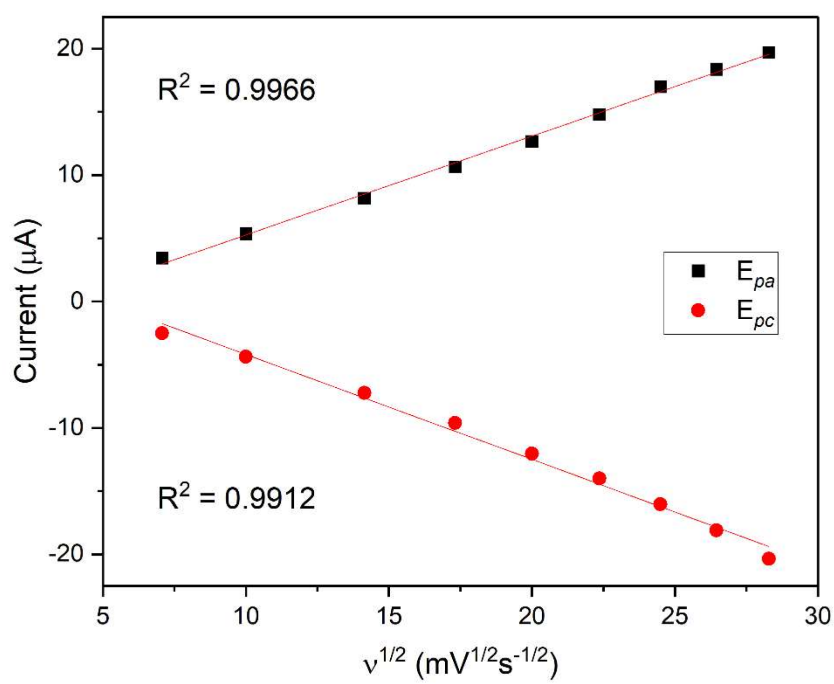


Figure S59. Scan-rate dependence of 1 mM **2-Ce^{Cs}** in 50 mM [^{n}Bu$_4$N][BPh$_4$] in THF (top) and Randles-Sevcik plot (bottom).

Differential Pulse Voltammetry

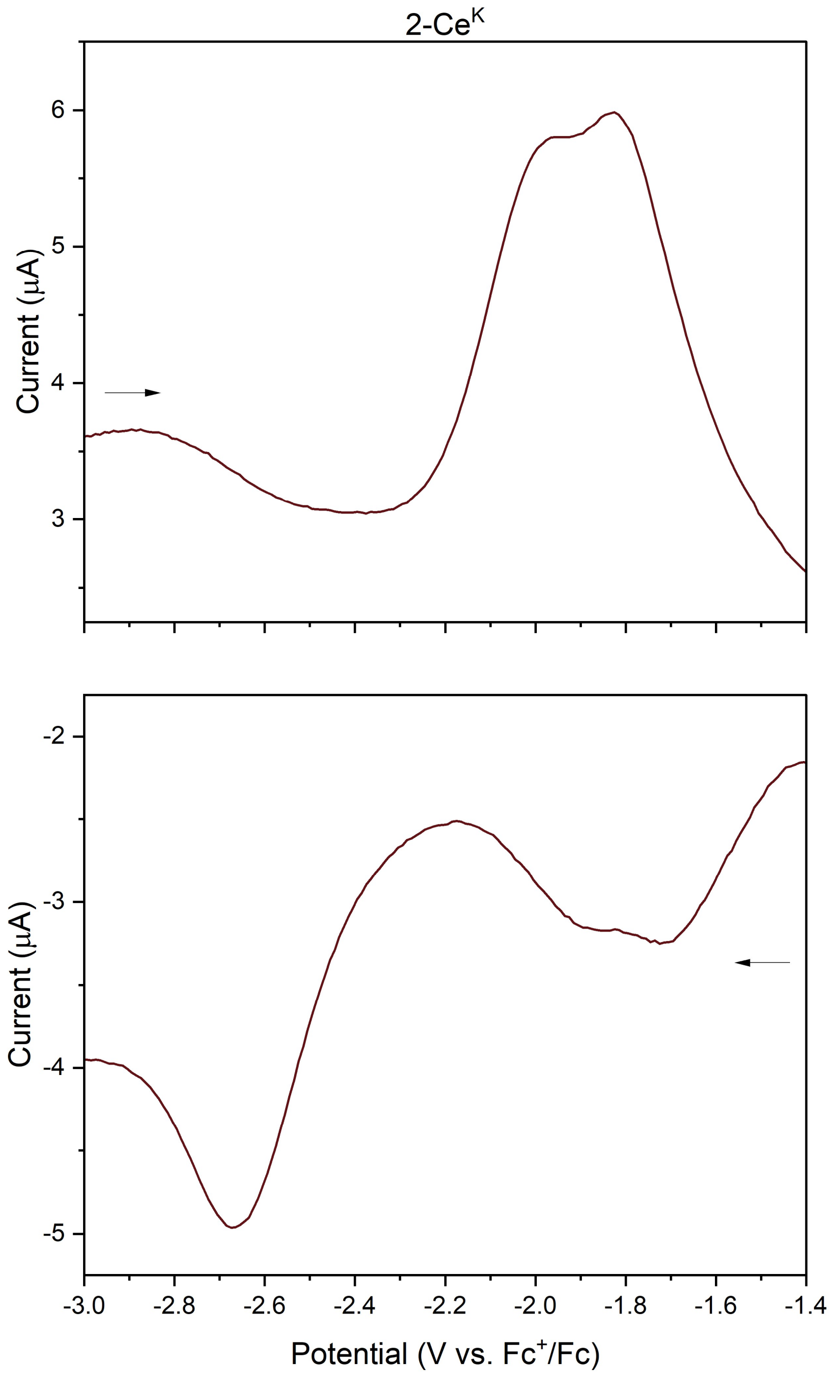


Figure S60. Differential pulse voltammogram of **2-Ce^{K}** in 50 mM [^{n}Bu$_4$N][BPh$_4$] in THF.

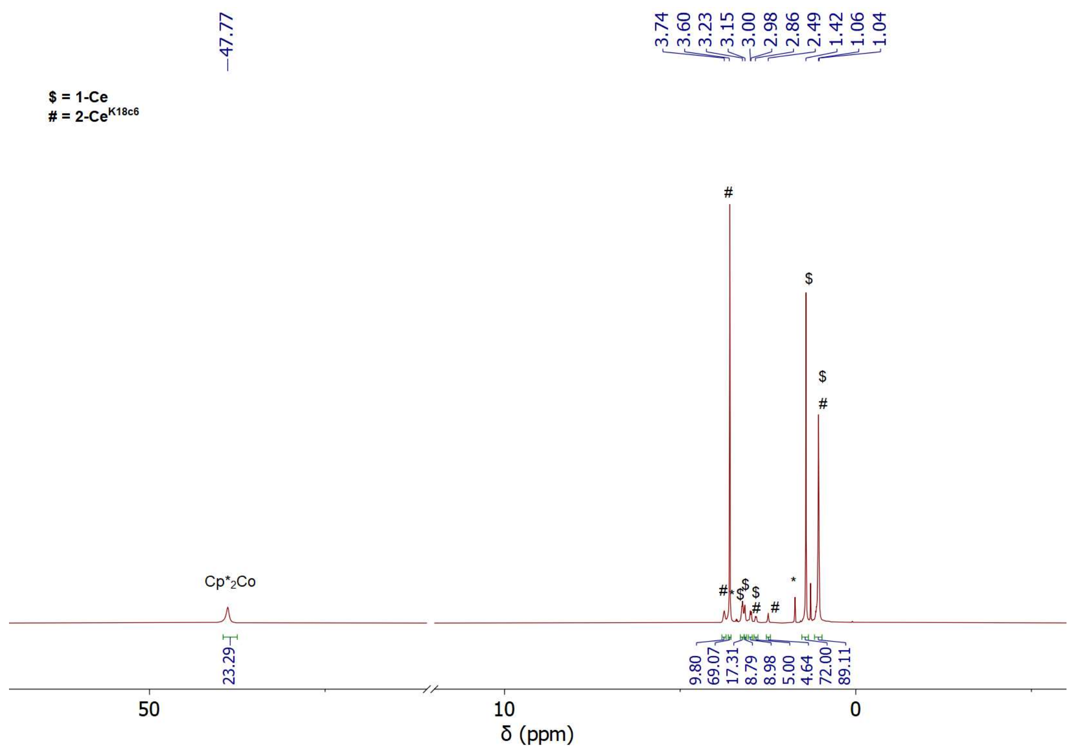


Figure S61. ^{1}H NMR spectrum of **2-Ce^{K18c6}** + [CoCp*$_2$][PF$_6$] in THF-d$_8$. * denotes THF-d$_7$.

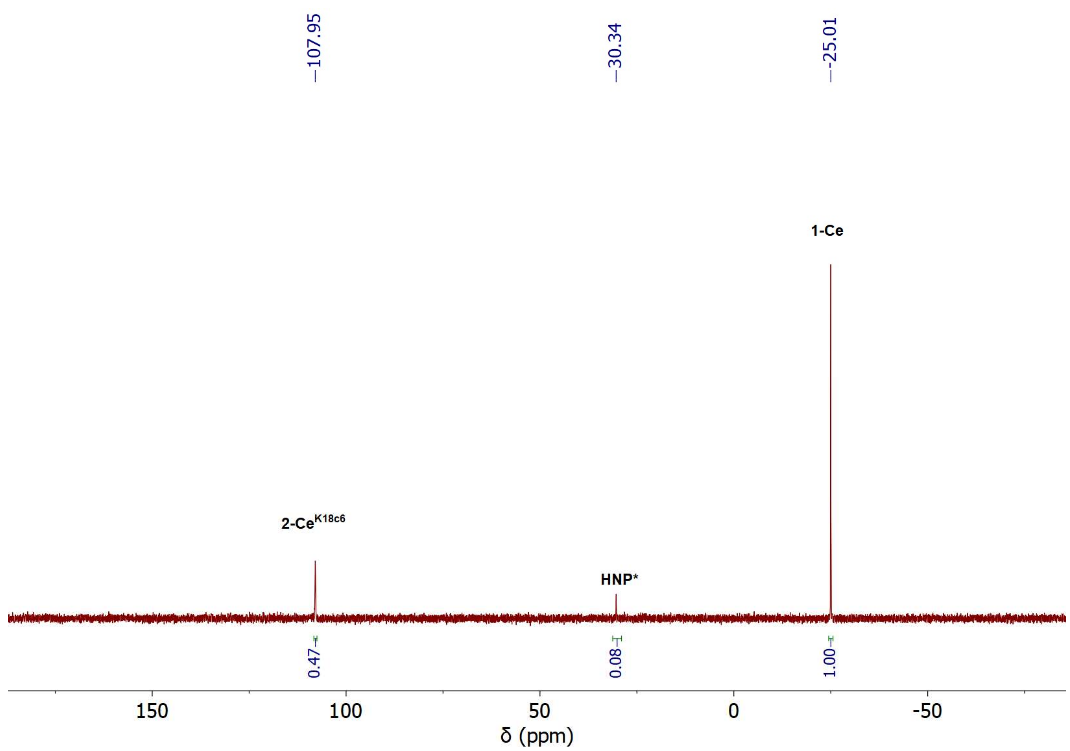


Figure S62. $^{31}P\{^{1}H\}$ NMR spectrum of **2-Ce^{K18c6}** + [CoCp*$_2$][PF$_6$] in THF-d$_8$.

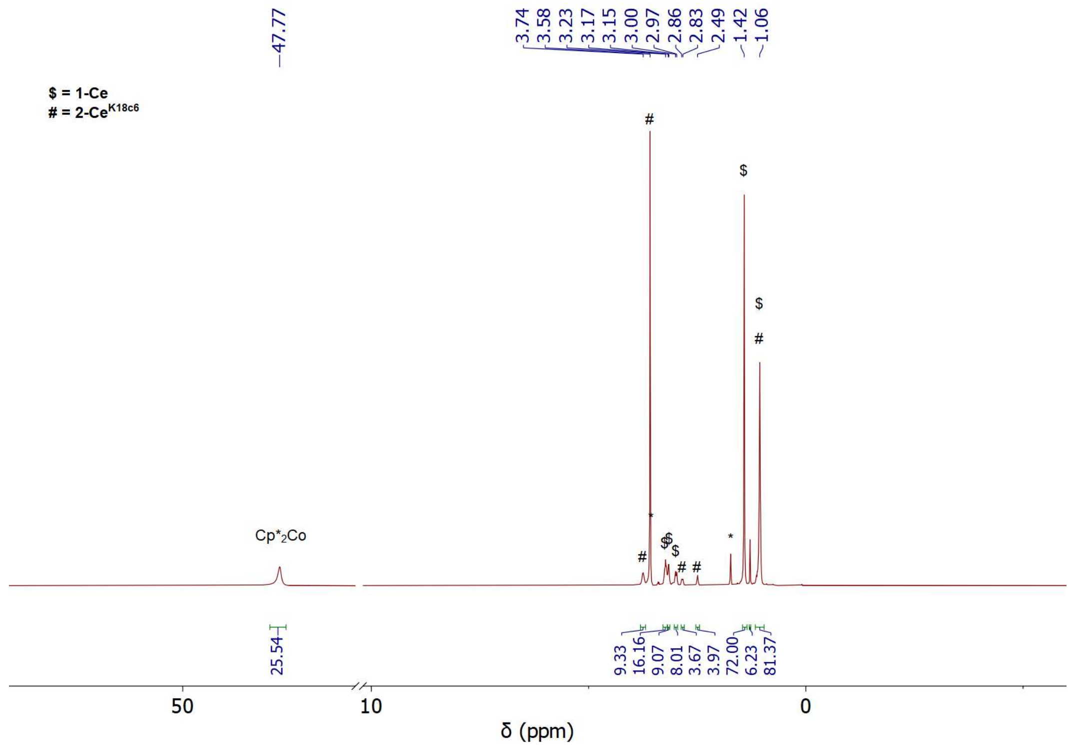


Figure S63. 1H NMR spectrum of **2-Ce**^{K18c6} + [CoCp*$_2$][PF$_6$] in THF-d$_8$ after heating at 60°C for 1h. * denotes THF-d$_7$.

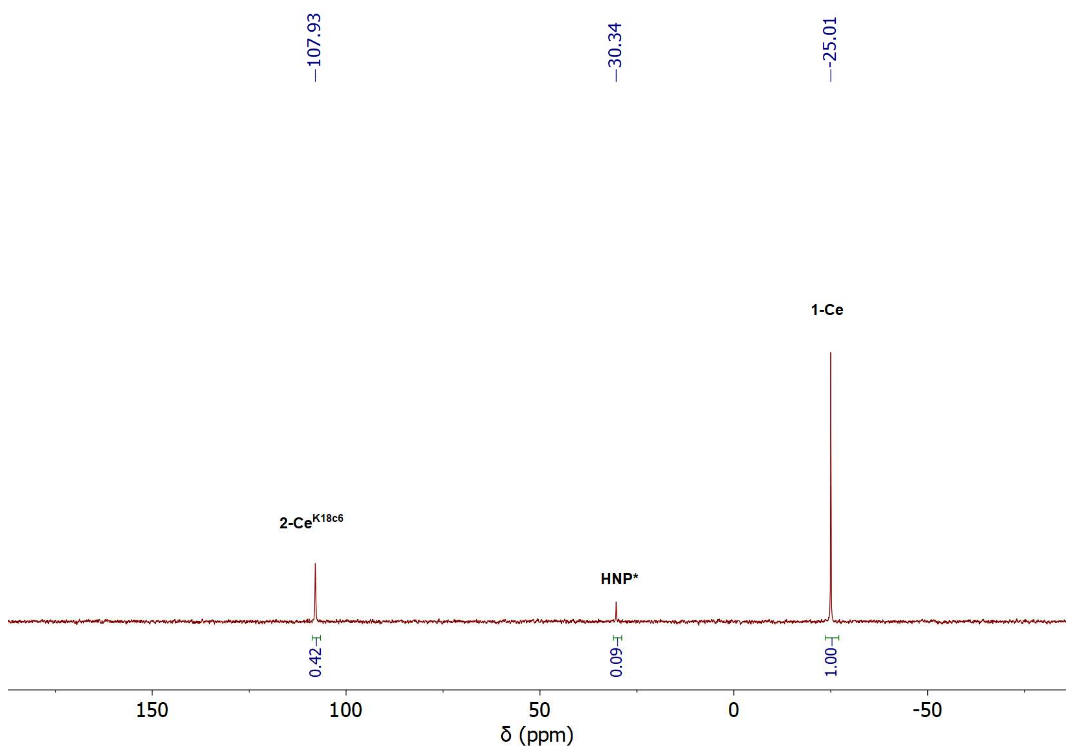


Figure S64. $^{31}P\{^{1}H\}$ NMR spectrum of **2-Ce**^{K18c6} + [CoCp*$_2$][PF$_6$] in THF-d$_8$ after heating at 60°C for 1h.

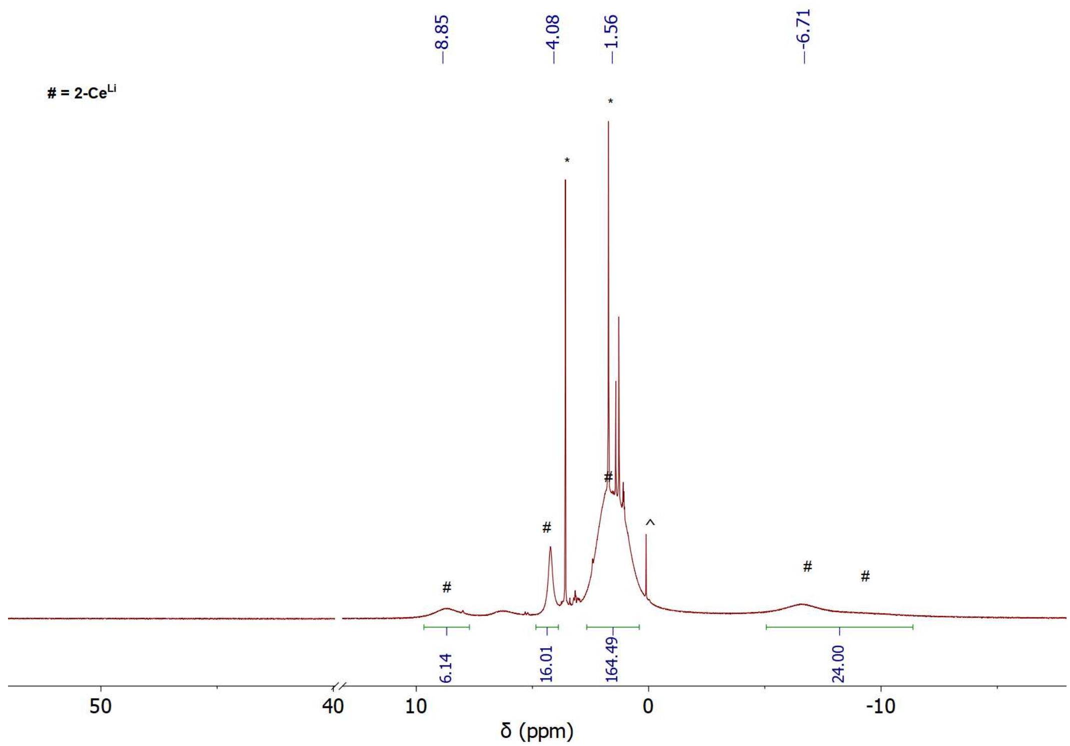


Figure S65. ^{1}H NMR spectrum of **2-Ce^{Li}** + $[CoCp^*_2][PF_6]$ in THF-d_8. * denotes THF-d_7, ^ denotes silicone grease. Note: There is no signal of $[CoCp^*_2]$ at 47.77 ppm.

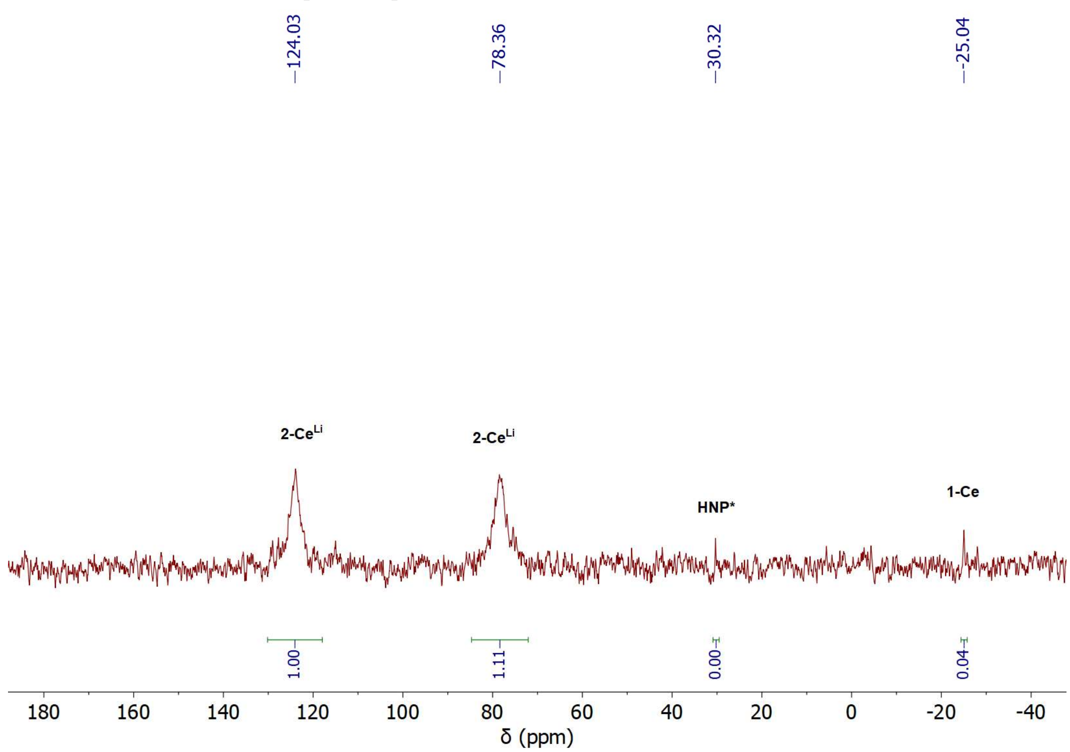


Figure S66. $^{31}P\{^{1}H\}$ NMR spectrum of **2-Ce^{Li}** + $[CoCp^*_2][PF_6]$ in THF-d_8.

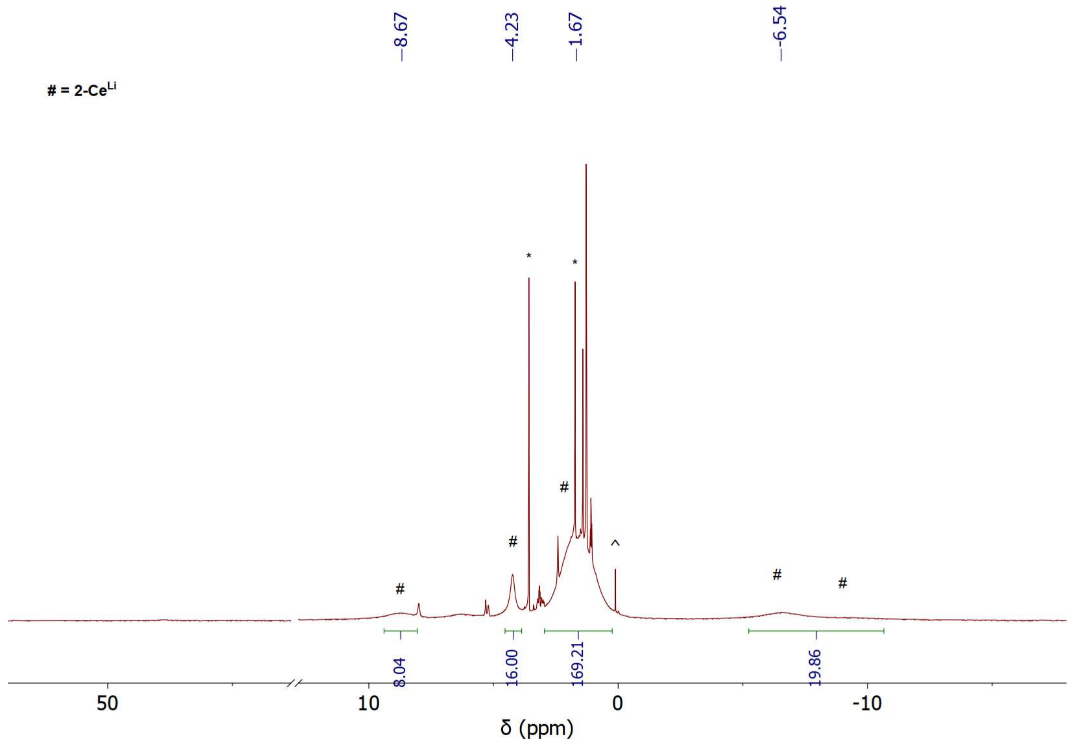


Figure S67. ^{1}H NMR spectrum of **2-Ce^{Li}** + [Co Cp*$_2$][PF$_6$] in THF-d$_8$ after heating at 60°C for 1h. * denotes THF-d$_7$, ^ denotes silicone grease. Note: There is no signal of [Co Cp*$_2$] at 47.77 ppm.

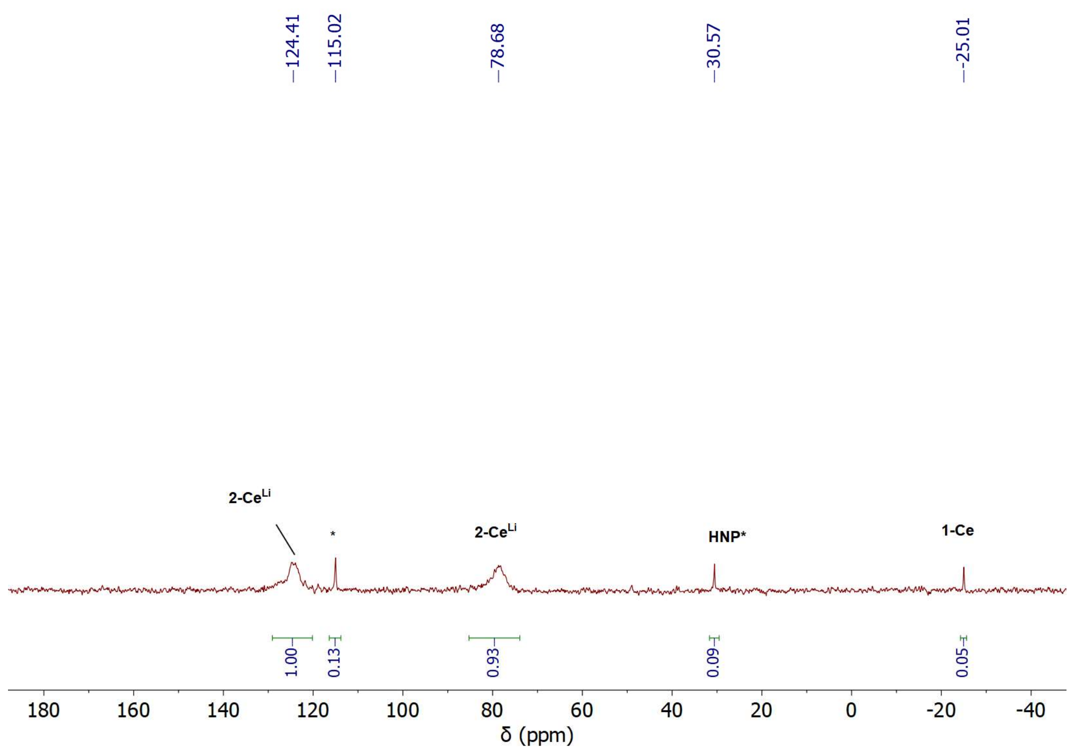


Figure S68. $^{31}P\{^{1}H\}$ NMR spectrum of **2-Ce^{Li}** + [Co Cp*$_2$][PF$_6$] in THF-d$_8$ after heating at 60°C for 1h.* denotes an unidentified side product.

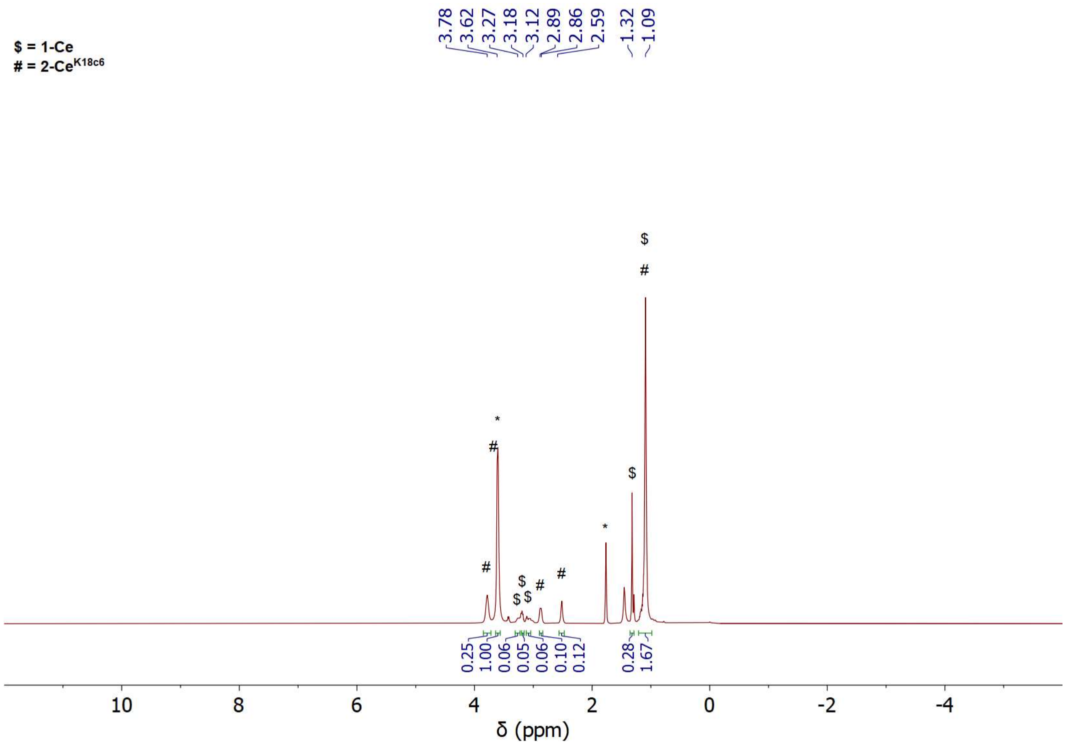


Figure S69. ^{1}H NMR spectrum of **2-Ce^{K18c6}** + benzophenone in THF-d_8. * denotes THF-d_7. Note: While there was not complete conversion to **1-Ce**, all benzophenone was consumed, suggesting side reactions are occurring, as supported by the presence of a significant amount of HNP*.

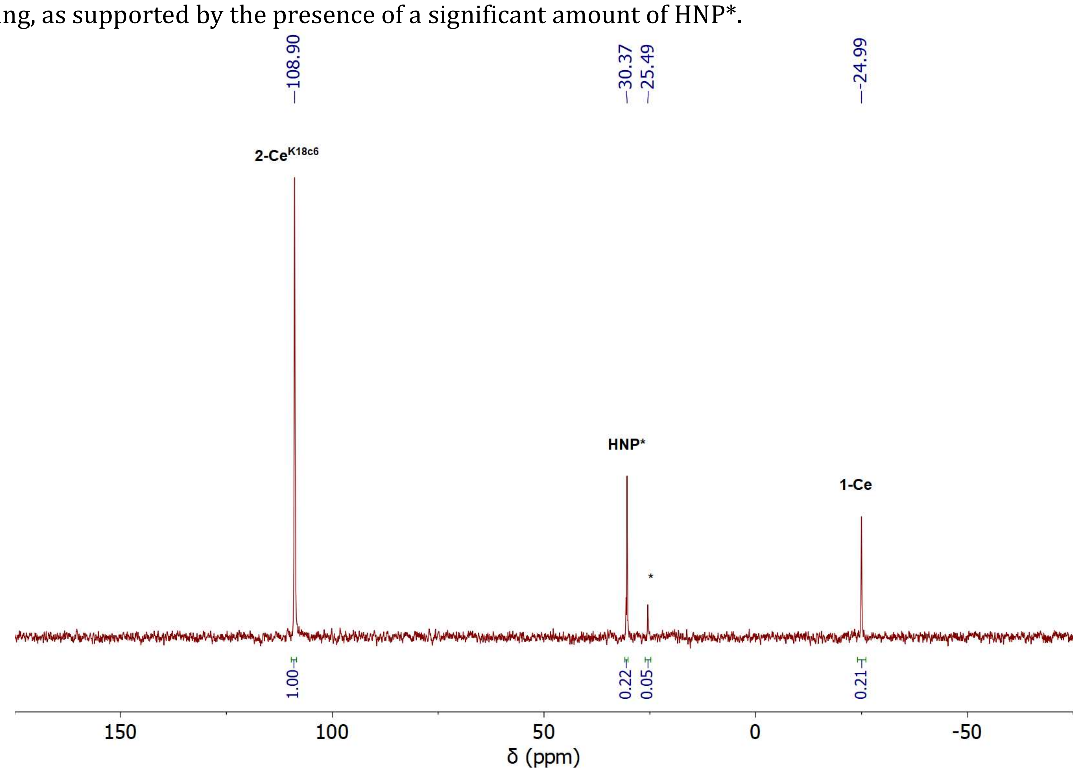


Figure S70. $^{31}P\{^{1}H\}$ NMR spectrum of **2-Ce^{K18c6}** + benzophenone in THF-d_8. * denotes an unidentified side product.

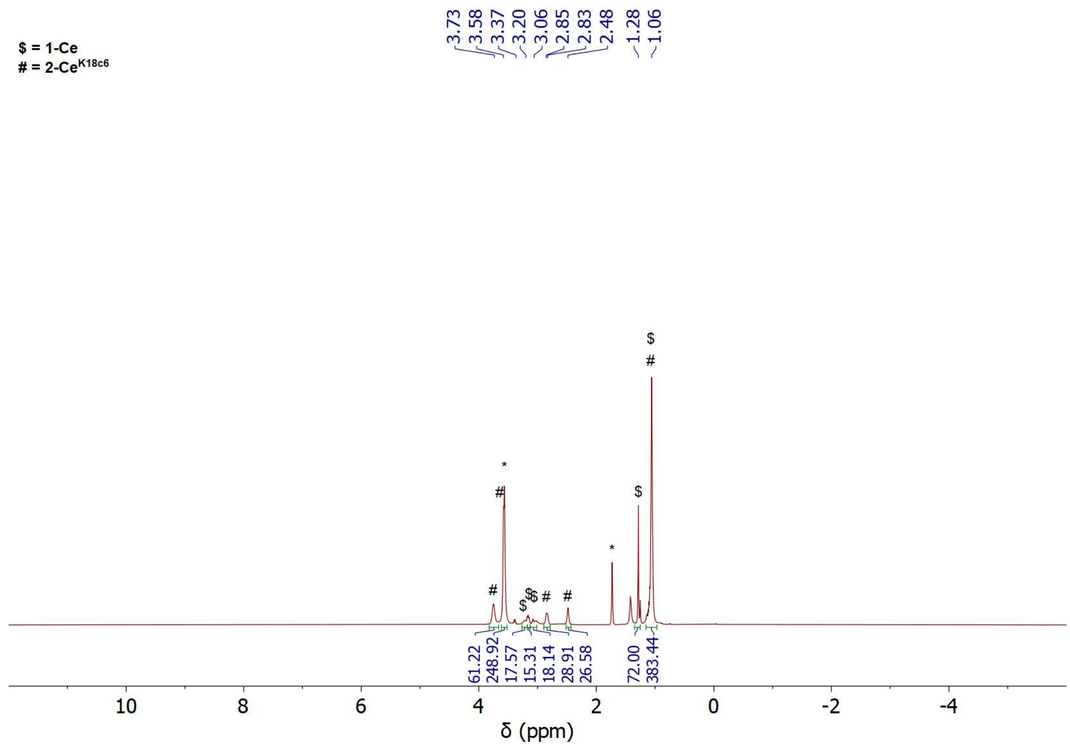


Figure S71. ^{1}H NMR spectrum of **2-Ce^{K18c6}** + benzophenone in THF-d_8 after heating at 60°C for 1h. * denotes THF-d_7. Note: While there was not complete conversion to **1-Ce**, all benzophenone was consumed, suggesting side reactions are occurring, as supported by the presence of a significant amount of HNP*.

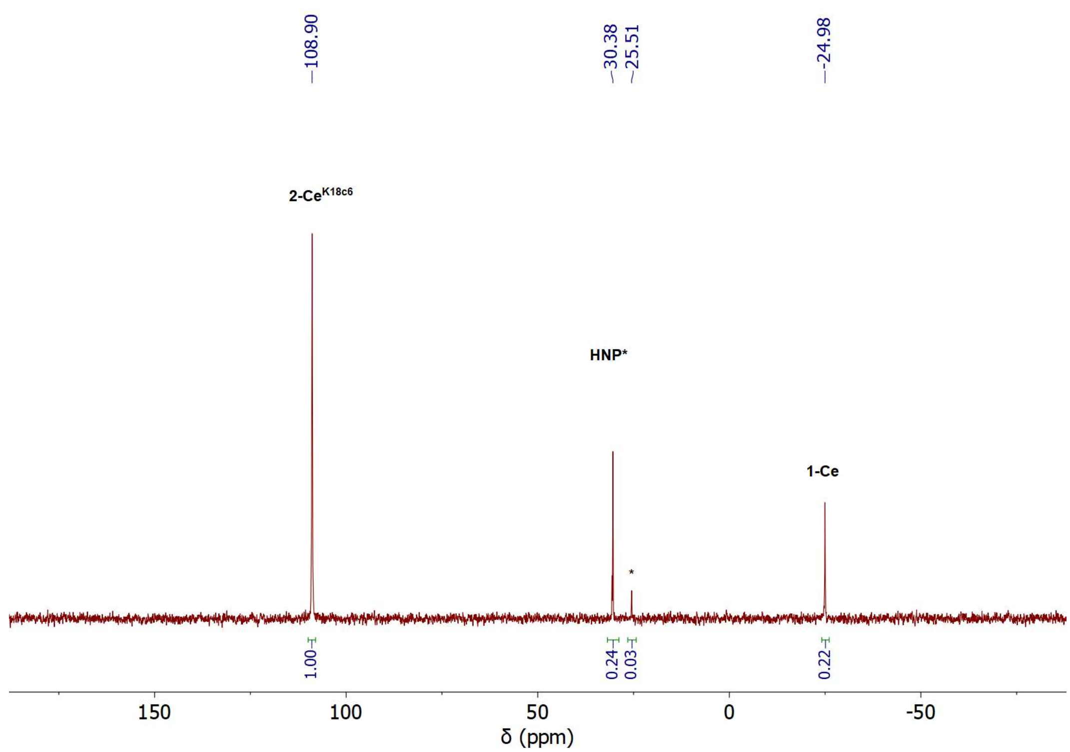


Figure S72. $^{31}P\{^{1}H\}$ NMR spectrum of **2-Ce^{K18c6}** + benzophenone in THF-d_8 after heating at 60°C for 1h. * denotes an unidentified side product.

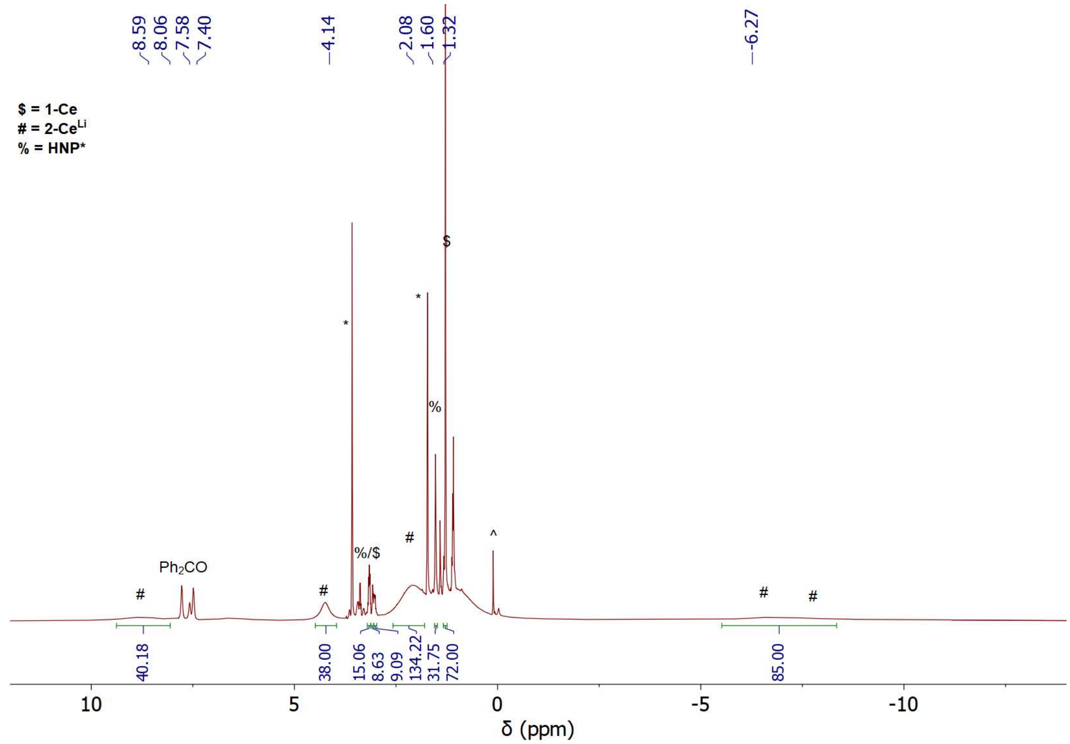


Figure S73. ^{1}H NMR spectrum of **2-Ce^{Li}** + benzophenone in THF-d_8.* denotes THF-d_7, ^ denotes silicone grease.

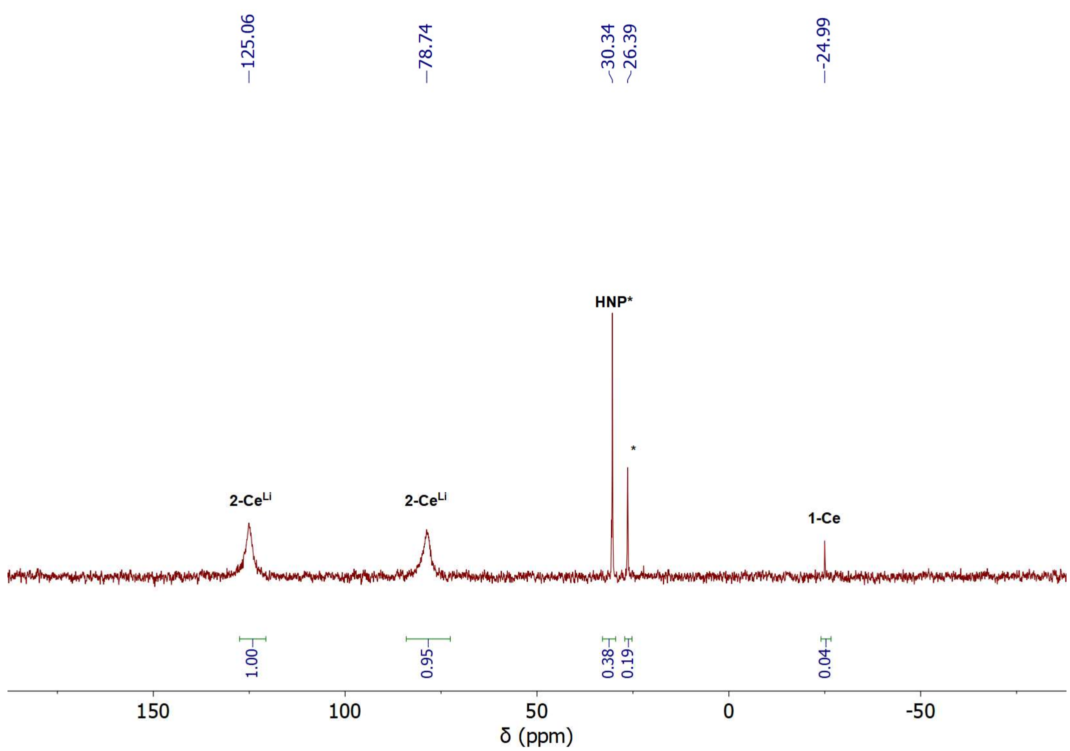


Figure S74. $^{31}P\{^{1}H\}$ NMR spectrum of **2-Ce^{Li}** + benzophenone in THF-d_8.* denotes an unidentified side product.

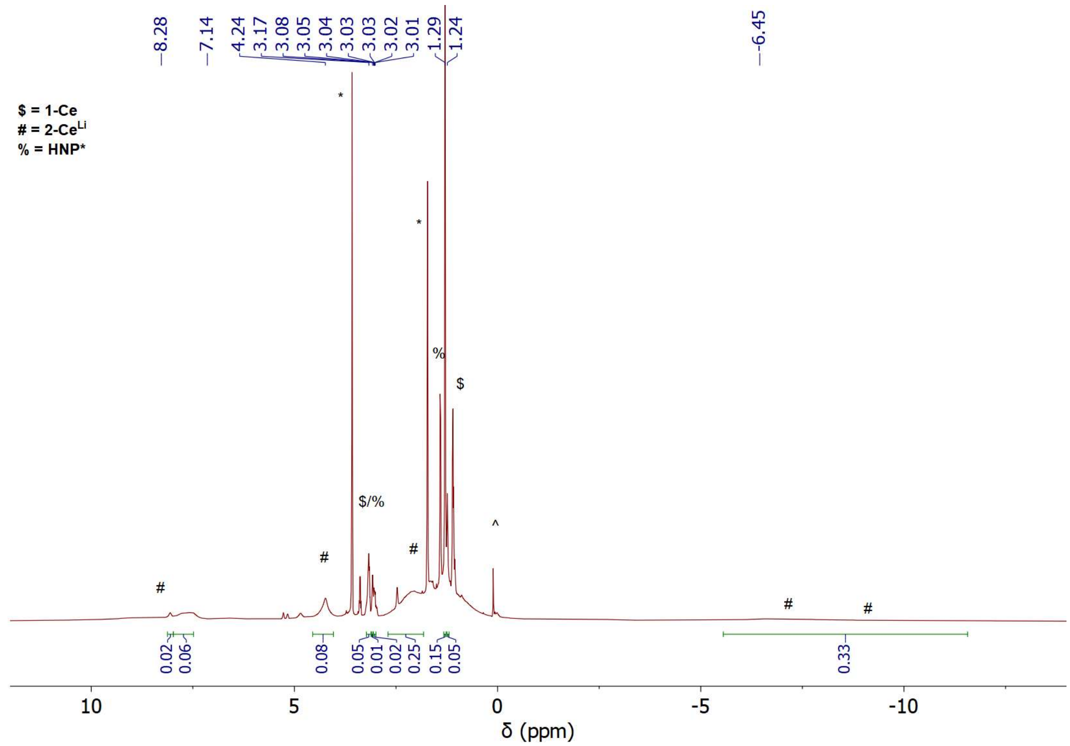


Figure S75. ^{1}H NMR spectrum of **2-Ce^{Li}** + benzophenone in THF-d_8 after heating at 60°C for 1h. * denotes THF-d_7, ^ denotes silicone grease.

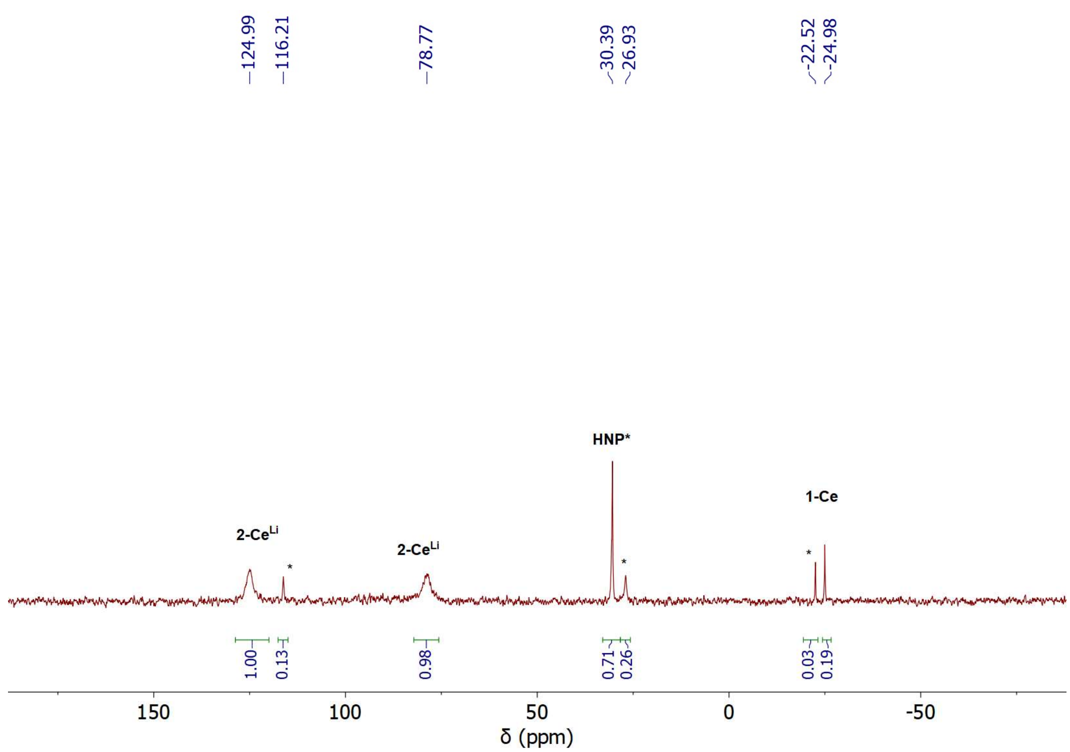


Figure S76. $^{31}P\{^{1}H\}$ NMR spectrum of **2-Ce^{Li}** + benzophenone in THF-d_8 after heating at 60°C for 1 h. * denotes unidentified side products.

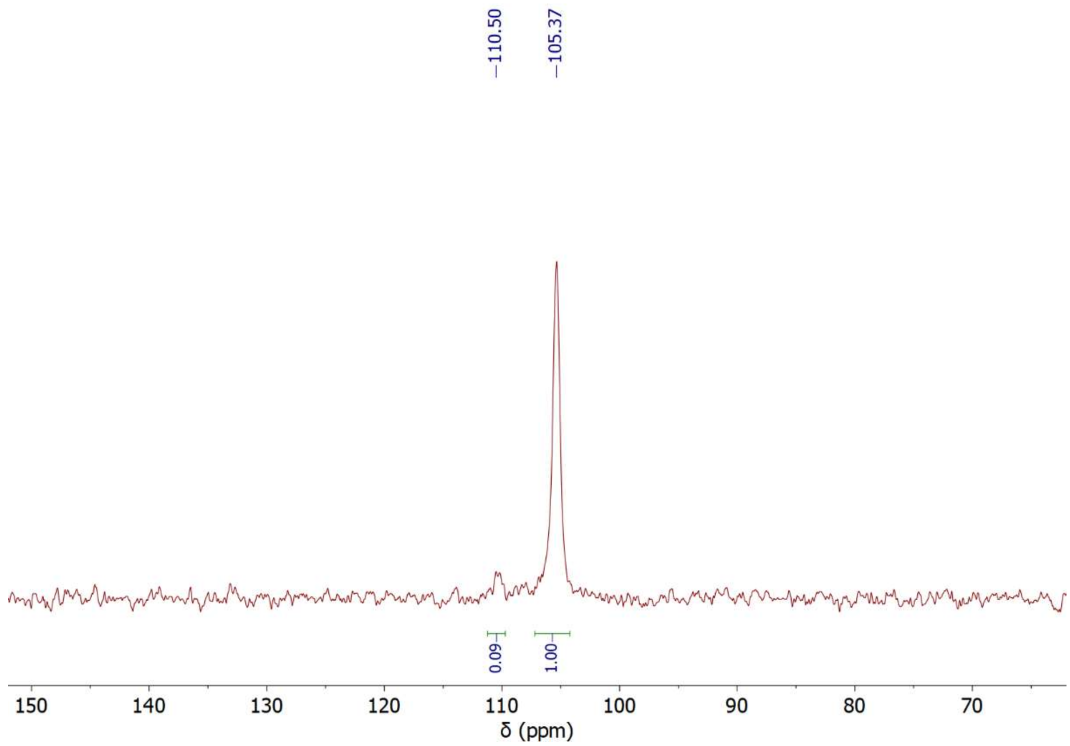


Figure S77. $^{31}P\{^{1}H\}$ NMR spectrum of **2-Ce^{Na}** at 3 mM concentration in 50 mM [$^{n}Bu_4N$][BPh_4] in THF-d_8. FWHM = 100 Hz for main feature at 105.37 ppm.

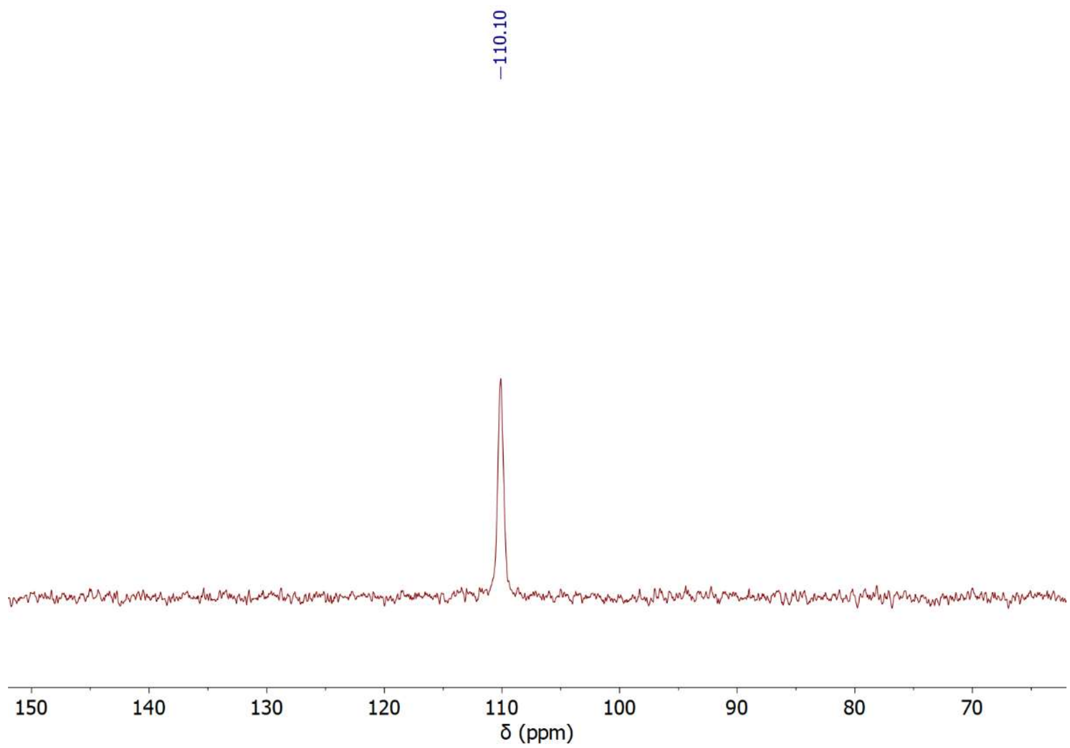


Figure S78. $^{31}P\{^{1}H\}$ NMR spectrum of **2-Ce^{K}** at 3 mM concentration in 50 mM [$^{n}Bu_4N$][BPh_4] in THF-d_8. FWHM = 80 Hz.

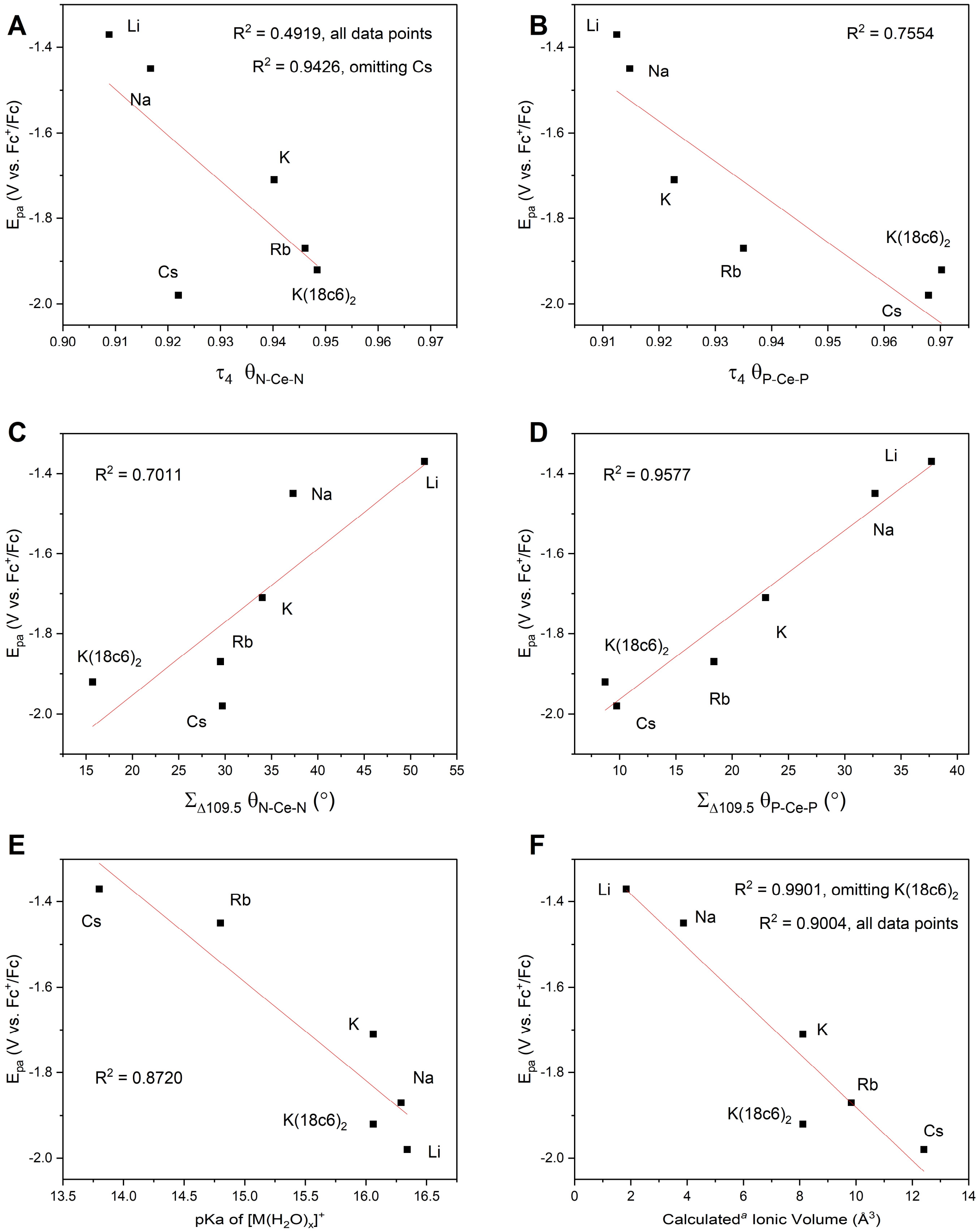


Figure S79. Oxidation potential (E_{pa}) plotted vs. **A**: τ_4 calculated using angles extracted from the Ce-N coordination sphere in the SC-XRD structures. **B**: τ_4 calculated using angles extracted from the Ce-P coordination sphere in the SC-XRD structures. **C**: $\Sigma_{\Delta 109.5}$ calculated using angles extracted from the Ce-N coordination sphere in the SC-XRD structures. **D**: $\Sigma_{\Delta 109.5}$ calculated using angles extracted from the Ce-P coordination sphere in the SC-XRD structures. **E**: pKa of $[M(H_2O)_x]^+$.[5] **F**: Ionic volume. Note: For **2-Ce^{Li}** and **2-Ce^{Cs}** two crystallographically unique molecules are in the asymmetric unit, parameters were calculated independently for each molecule and then averaged. [a]Calculated from Shannon ionic radius.[6]

Computational Details

The **2-Ce**$^{-}$, **1-Ce**, and **2-Ce**^{M} (M = Li, Na, K, Rb, Cs, [K(18c6)$_2$]) complexes were fully optimized in the gas phase without any constraints based on their XRD structures. Optimizations of the **2-Ce**^{Rb} and **2-Ce**^{Cs} complexes did not include the coordinated ether molecule present in their XRD structure. All structures were optimized by using the PBE0[7] hybrid DFT functional as implemented in the Gaussian16 software package (version A.03).[8] The ECP28MWB[9] small core quasi-relativistic pseudopotential and ECP28MWB_ANO[10] basis sets were used to describe Ce in all complexes. Rb and Cs were described with the ECP28MWB and ECP46MWB small core quasi-relativistic pseudopotentials[11] and ECP28MWB_ANO and ECP46MWB_ANO basis sets,[12] respectively. All remaining atoms were described with the all-electron Pople basis set 6-311G(d).[13] Harmonic frequency calculations were performed to confirm that the optimized structures were stationary points on the potential energy surface. The wavefunctions of the complexes were checked for stability to ensure that the calculations converged to their ground electronic states. In all calculations, spin contamination was found to be less than 0.2% with $\langle S^2 \rangle$ values being close to the corresponding values of the considered spin states, *i.e.,* doublet for **2-Ce**$^{-}$ and **2-Ce**^{M} (M = Li, Na, K, Rb, Cs, [K(18c6)$_2$]), and singlet for **1-Ce**.

The electron localization method employing Adaptive Natural Density Partitioning (AdNDP) analysis,[14] using the AdNDP 2.0 code,[15] was implemented to obtain a more chemically intuitive picture of the bonding interactions. Unpaired electrons, lone pairs of electrons, or traditional Lewis bonds can be recovered via AdNDP analysis as one-center one-electron (1c-1e), one-center two-electron (1c-2e), and two-center two-electron (2c-2e) interactions. AdNDP analysis also allows for the assignment of multicenter (nc-2e) bonds where n is equal to the number of atoms specified by the user. The occupation number (ON), which is the number of electrons occupying a particular identified localized state, serves as an indicator of bond strength. Previously, AdNDP was shown to be insensitive to the level of theory used.[16-18] Specifically, it was found that as long as the basis set is large enough to sufficiently describe electronic structure, AdNDP showed no qualitative dependency on the basis set. It was also shown that the AdNDP results obtained at either GGA or DFT hybrid functionals produce qualitatively the same bonding trends, in agreement with the results from CASSCF calculations.[16]

Time-dependent DFT calculations (TD-DFT)[19,20] of up to 200 excited states at the same level of theory for gas phase geometry optimizations were carried out to simulate the experimental UV-Vis spectrum of **2-Ce**^{K18c6} in THF and all other complexes in toluene. The computed spectra were plotted broadening the calculated excitation lines with Gaussian-type peaks using a half-width at half height of 0.15 eV for all figures containing TD-DFT spectra in the main text and the SI. Natural transition orbitals (NTOs),[21] which most of the time can yield single electron-hole representations of the electronic excitations, were employed to interpret the calculated excitation spectra and assess the character of the orbitals that play a role in each excitation.

To calculate the redox potentials of the complexes, single-point energy calculations in THF were performed using the self-consistent reaction field approach based on the integral equation formalism of the polarized continuum model (PCM).[22-24] Energies of solvation were used to calculate vertical detachment energy (VDE) and adiabatic detachment energy (ADE). VDE was computed as the energy difference between the original complex and its oxidized counterpart, which has the geometry of the original complex. ADE was computed as the energy difference between the original complex and its oxidized counterpart, the geometry of which was fully optimized. All redox potentials were referenced to a calculated absolute half-cell potential of a ferrocene couple Fc^{+}/Fc. The LANL08[25-27] basis set was used for Fe, and C/H atoms were described by the 6-311G(d) basis set.

MO energy level diagrams are based on the single-point energy calculations in THF. Chemissian 4.67[27] was used to plot the TD-DFT spectra and MO diagrams as well as visualize the NTOs. Chemcraft Version 1.8 (build 610b)[28] was used to visualize the molecular orbitals from the AdNDP analysis.

Table S2. Experimental *vs*. optimized bond lengths (Å) and angles (°). All Ce–N bonds are considered to be $N_{terminal}$ for **2-Ce^{K18c6}**, **2-Ce^{-}**, and **1-Ce.**

Bonds/ Metrics	**2-Ce$^{Li\ a}$**		**2-Ce^{Na}**		**2-Ce^{K}**		**2-Ce^{Rb}**		**2-Ce$^{Cs\ a}$**		**2-Ce^{K18c6}**		**2-Ce^{-}**		**1-Ce**	
	Exp.	Theor.	Exp.	Theor.	Exp.	Theor.	Exp.	Theor.	Exp.	Theor.	Exp.	Theor.	Exp.	Theor.	Exp.	Theor.
Ce–M^{+}	3.020 2.968	3.019 3.002	3.367	3.356	3.790	3.699	3.947	3.916	4.061 4.131	4.101 4.162	9.56	9.753	-	-	-	-
Avg. Ce–N_{capped}	2.395 2.343	2.406 2.412	2.372	2.405	2.376	2.404	2.380	2.409	2.393 2.361	2.409 2.396	-	-	-	-	-	-
Avg. Ce–$N_{terminal}$	2.302 2.304	2.292 2.286	2.297	2.294	2.313	2.303	2.329	2.306	2.311 2.332	2.311 2.316	2.339	2.350	2.339	2.345	2.237	2.192
Avg. N_{capped}–P	1.502 1.578	1.544 1.546	1.533	1.540	1.531	1.539	1.532	1.539	1.532 1.534	1.539 1.536	-	-	-	-	-	-
Avg. $N_{terminal}$–P	1.553 1.515	1.546 1.546	1.526	1.545	1.530	1.545	1.535	1.545	1.542 1.539	1.545 1.545	1.504	1.536	1.504	1.536	1.557	1.558
Avg. Ce–N_{capped}–P	173.5 164.7	169.5 169.9	172.3	173.6	168.2	169.5	161.9	166.4	163.5 165.3	165.4 166.1	-	-	-	-	-	-
Avg. Ce–$N_{terminal}$–P	166.3 172.3	170.7 171.1	173.2	172.4	168.1	174.3	174.8	177.0	170.7 171.6	173.0 174.9	169.0	167.7	169.0	168.5	163.0	169.0

[a]More than one crystallographically unique molecule is present in the asymmetric unit, metrics for each molecule are presented. The structure with its metrics given on top is denoted as (1) and the bottom is denoted as (2), here and elsewhere in the SI.

Table S3. Contribution of Ce atomic orbitals (%) in the bonds recovered by AdNDP. %Ce AOs in Ce–N–P π bonds represents the sum of the contribution for both the π and π_{orth} bonds.

	%Ce AOs in Ce–N σ bonds		%Ce AOs in Ce–N–P π bonds		Total		
	N_{capped}	$N_{terminal}$	N_{capped}	$N_{terminal}$	N_{capped}	$N_{terminal}$	Δ%Ce
2-Ce^{Li} [a]	7.08 7.02	8.17 8.25	0.66 0.70	3.57 3.73	7.75 7.72	11.74 11.98	3.99 4.26
2-Ce^{Na}	7.21	8.15	0.56	3.44	7.77	11.59	3.82
2-Ce^{K}	7.16	8.06	0.61	3.27	7.77	11.33	3.56
2-Ce^{Rb}	7.12	8.06	0.67	3.19	7.79	11.25	3.46
2-Ce^{Cs} [a]	7.10 7.18	7.99 7.98	0.70 0.72	3.08 3.01	7.79 7.89	11.07 10.99	3.28 3.10
2-Ce^{K18c6}	-	7.42	-	1.27	-	8.69	0.00
2-Ce^{-}	-	7.52	-	1.46	-	8.98	0.00

[a]More than one crystallographically unique molecule is present in the asymmetric unit, metrics for each molecule are presented.

Table S4. Difference between the Ce–N_{capped} and Ce–$N_{terminal}$ bond lengths (ΔCe–N, Å) for **2-Ce^{M}**, (M = Li, Na, K, Rb, Cs).

	2-Ce^{Li} [a]	**2-Ce^{Na}**	**2-Ce^{K}**	**2-Ce^{Rb}**	**2-Ce^{Cs}** [a]
Exp. ΔCe–N	0.093 0.038	0.075	0.063	0.051	0.029 0.082
Theor. ΔCe–N	0.114 0.126	0.112	0.101	0.103	0.080 0.097

[a]More than one crystallographically unique molecule is present in the asymmetric unit, metrics for each molecule are presented.

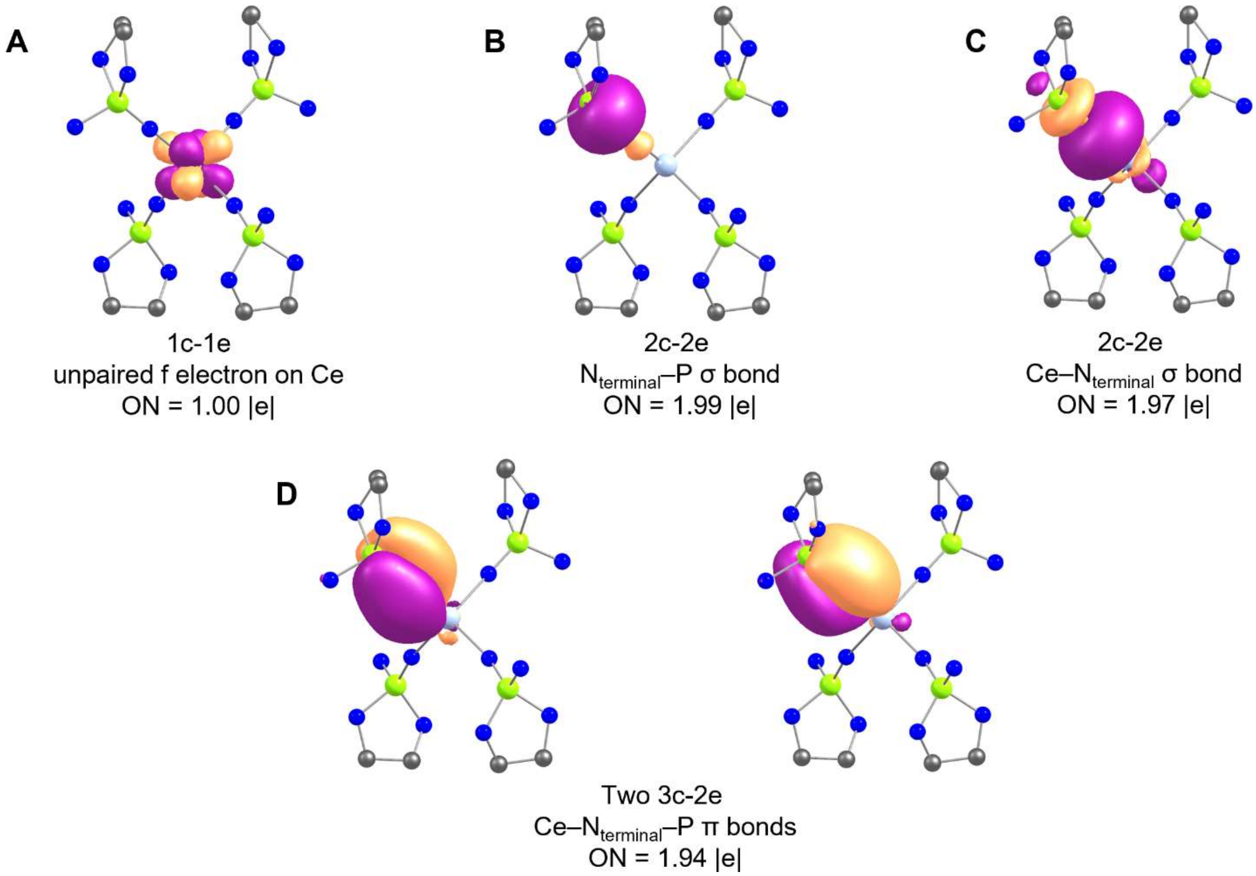


Figure S80. AdNDP analysis of the Ce–N–P interactions of **2-Ce**$^-$ displaying (**A**) an unpaired Ce 4*f* electron as one-center one-electron element, (**B**) two-center two-electron P–N σ bond, (**C**) two-center two-electron Ce–N σ bond, (**D**) three-center two-electron Ce–N–P π bonds. Side groups of the ligands (^{t}Bu, Et_2) are omitted for simplicity. An equivalent set of bonds (**B-D**) is identified for the other three ligands. ON stands for the occupation number.

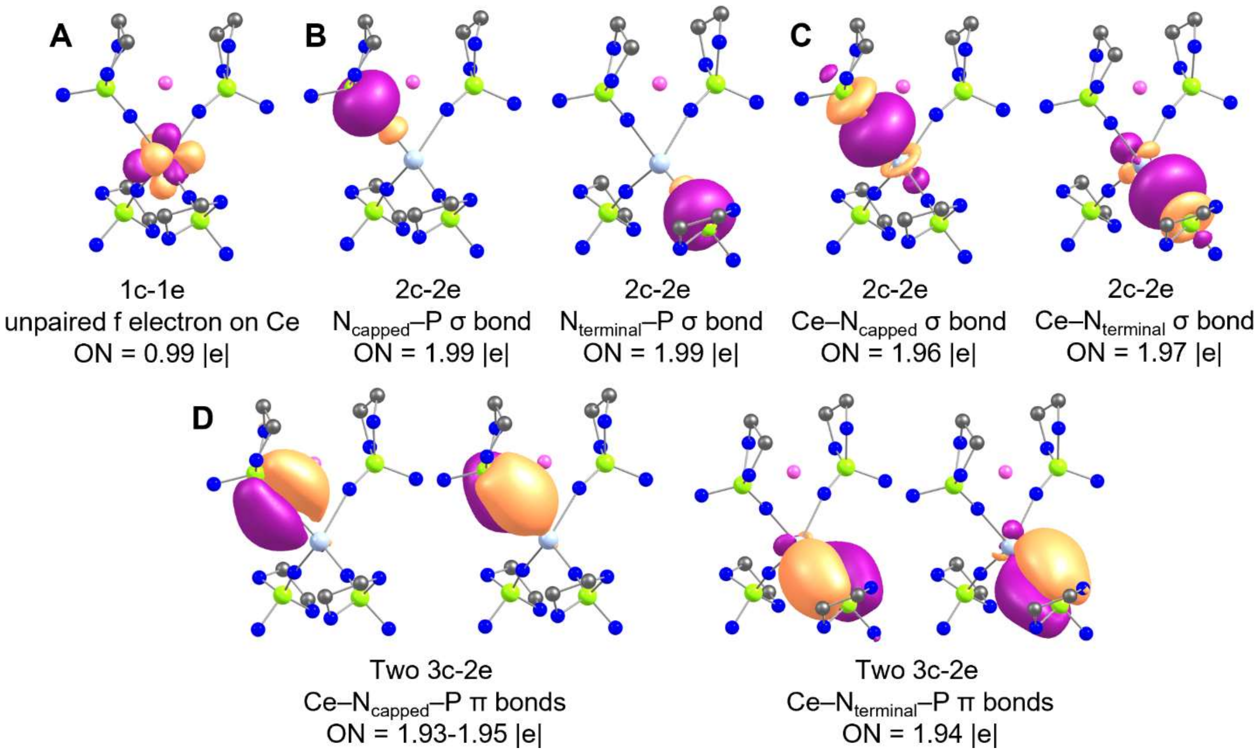


Figure S81. AdNDP analysis of the Ce–N–P interactions of **2-Ce^{Li}** (1) displaying (**A**) an unpaired Ce 4*f* electron as one-center one-electron element, (**B**) two-center two-electron P–N$_{capped/terminal}$ σ bonds, (**C**) two-center two-electron Ce–N$_{capped/terminal}$ σ bonds, (**D**) three-center two-electron Ce–N$_{capped/terminal}$–P π bonds. Side groups of the ligands (^{t}Bu, Et$_2$) are omitted for simplicity. Another equivalent set of bonds (**B-D**) is identified for each N$_{capped}$ and N$_{terminal}$ atom. Qualitatively similar bonds are found in all other **2-Ce^{M}** complexes. ON values for all other complexes are listed in the complimentary table below.

Table S5. ON values (|e|) of the bonds recovered by AdNDP analysis for each complex.

	1c-1e (unpaired 4f electron on Ce)	2c-2e N–P σ bond		2c-2e Ce–N σ bond		3c-2e Ce–N–P π bonds	
		N_{capped}	$N_{terminal}$	N_{capped}	$N_{terminal}$	N_{capped}	$N_{terminal}$
2-Ce^{Li} [a]	0.99 0.99	1.99 1.99	1.99 1.99	1.96 1.96	1.97 1.97	1.93-1.95 1.93-1.95	1.94 1.94
2-Ce^{Na}	0.99	1.99	1.99	1.96	1.97	1.94	1.94
2-Ce^{K}	0.99	1.99	1.99	1.96	1.97	1.93-1.94	1.94
2-Ce^{Rb}	0.99	1.99	1.99	1.97	1.97	1.93-1.94	1.94
2-Ce^{Cs} [a]	0.99 0.99	1.99 1.99	1.99 1.99	1.97 1.97	1.97 1.97	1.93-1.94 1.93-1.94	1.94 1.94
2-Ce^{K18c6}	0.99	-	1.99	-	1.97	-	1.93-1.94
2-Ce^{-}	1.00	-	1.99	-	1.97	-	1.94

[a]More than one crystallographically unique molecule is present in the asymmetric unit, metrics for each molecule are presented.

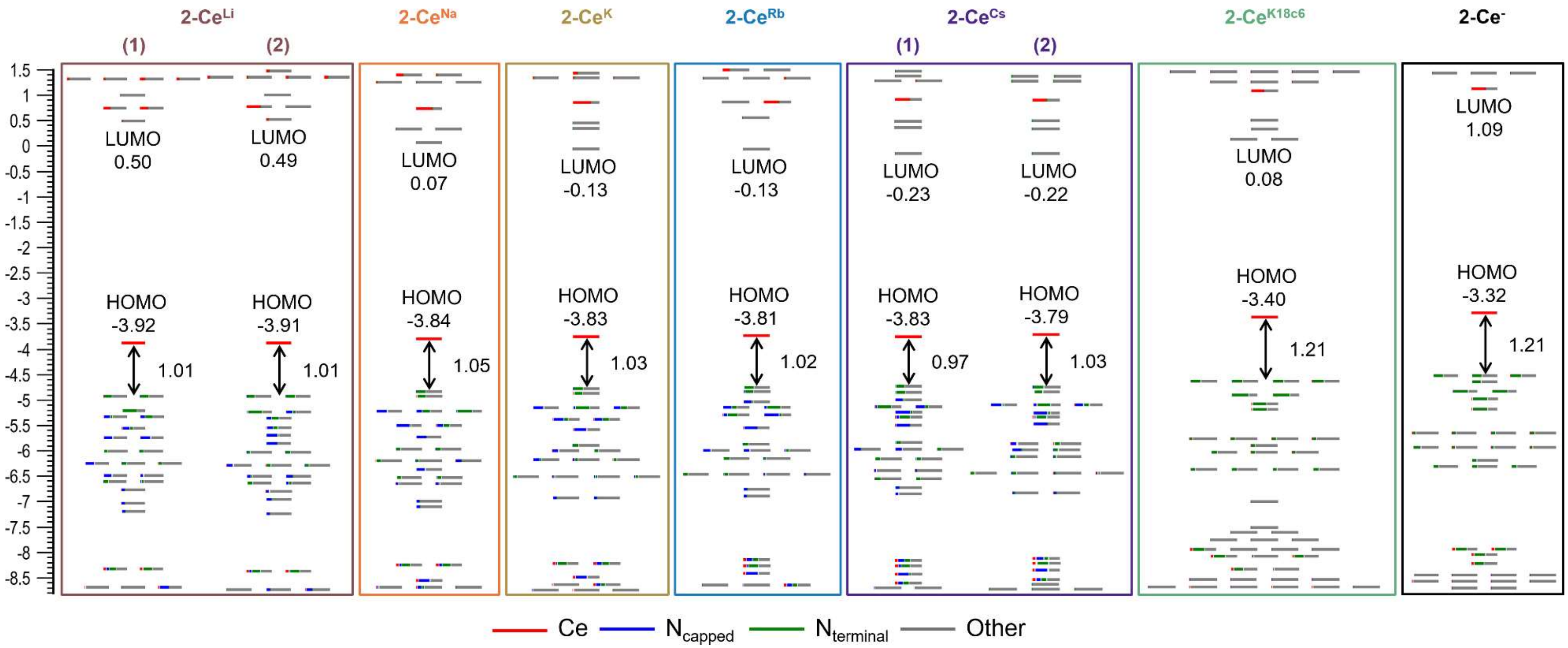


Figure S82. α MO energy diagrams for the studied Ce^{3+} imidophosphorane complexes. The gap between the Ce-dominant HOMO and the ligand-dominant HOMO-1 is indicated by the arrow. The y-axis scale shows energy values in eV, here and in all other MO diagrams in the SI. The red portion of the MO lines represents the percentage of Ce AOs in the MOs, the blue portion represents the N_{capped} AOs, the green portion represents the $N_{terminal}$ AOs, and the gray portion represents all other atoms AOs, here and in all other MO diagrams in the SI. Degeneracy of the MO energy levels is set to 0.085 eV for visualization purposes, here and in all other MO diagrams in the SI.

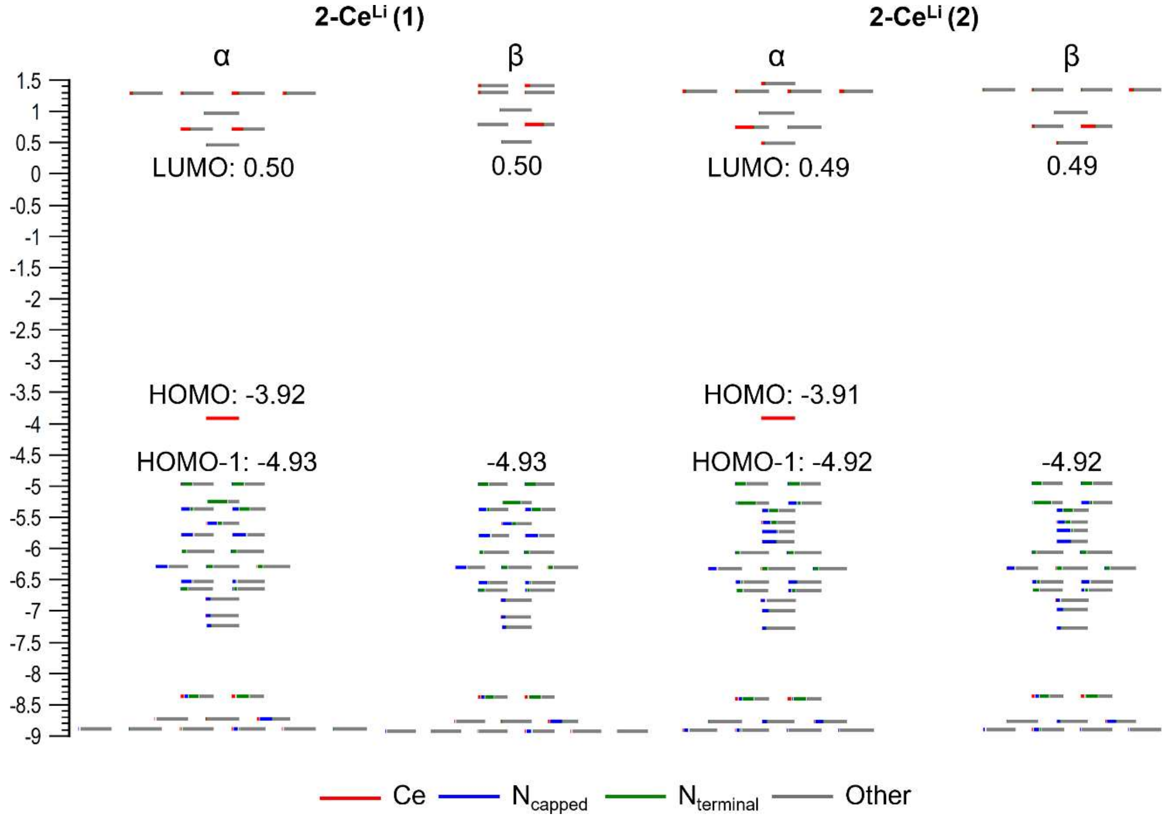


Figure S83. α and β MO energy levels for both crystallographically unique **2-Ce^Li** complexes.

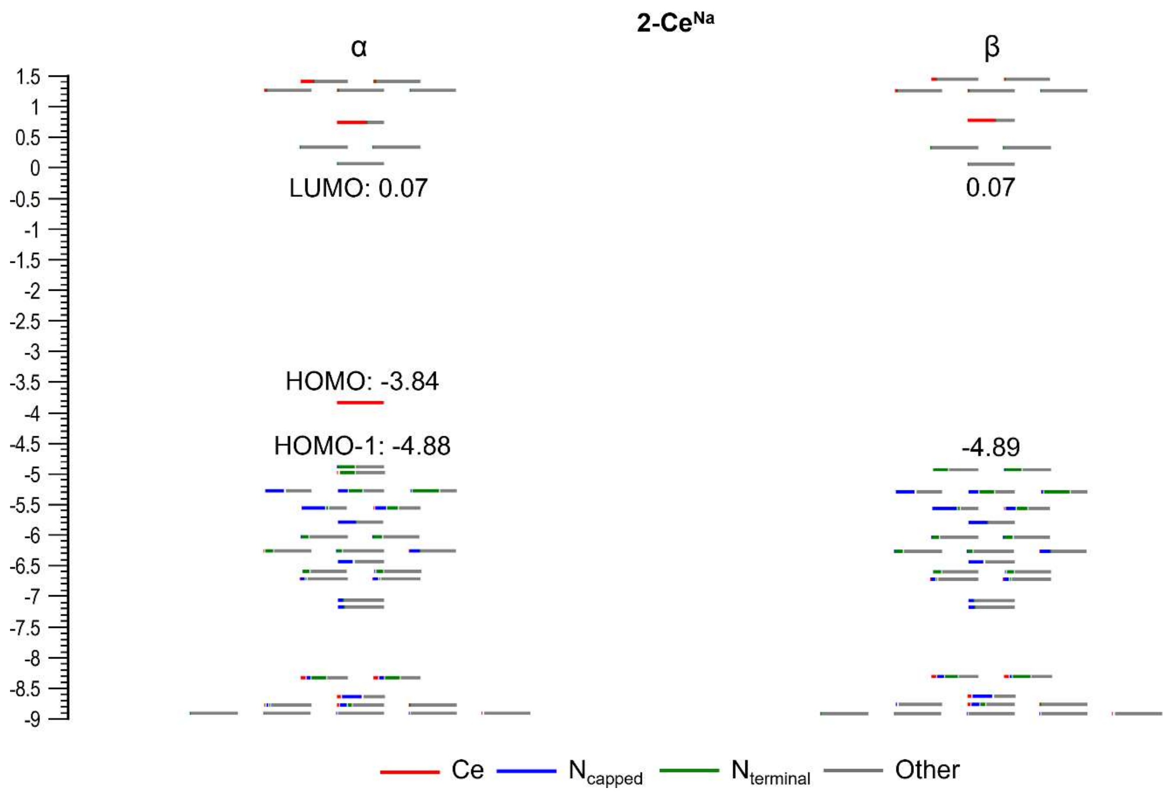


Figure S84. α and β MO energy levels for the **2-Ce^Na** complex.

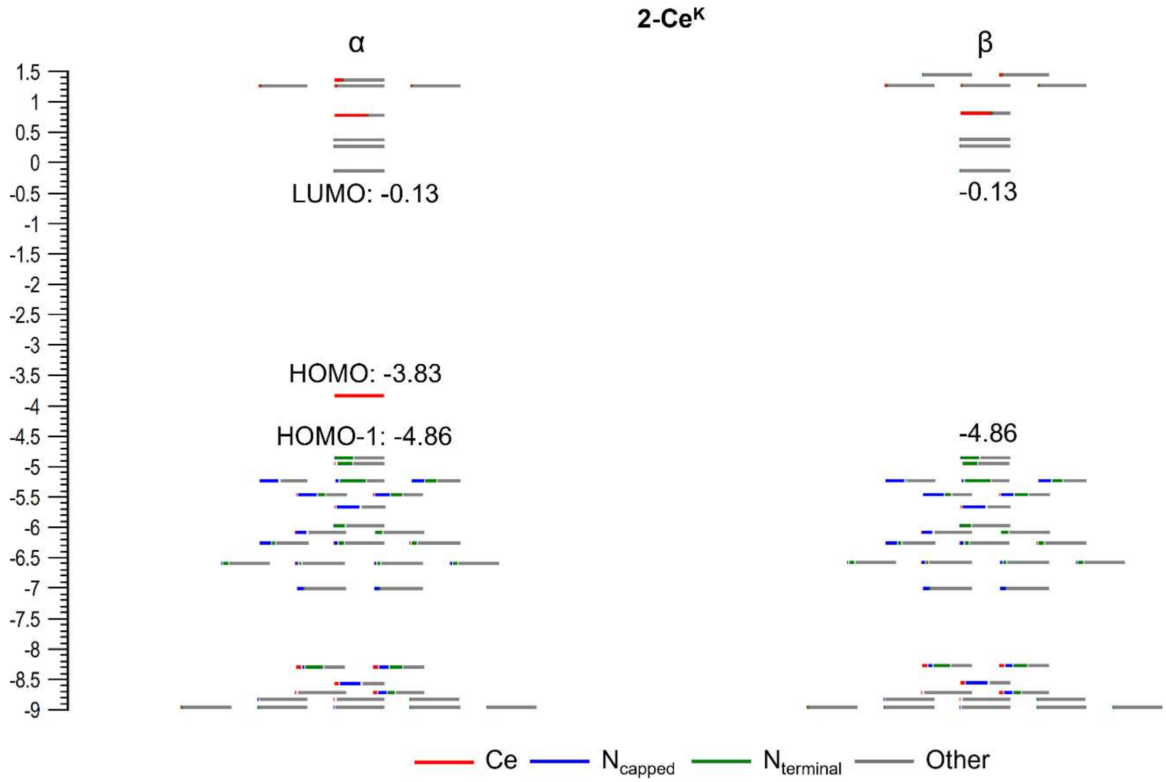


Figure S85. α and β MO energy levels for the **2-Ce**^{K} complex.

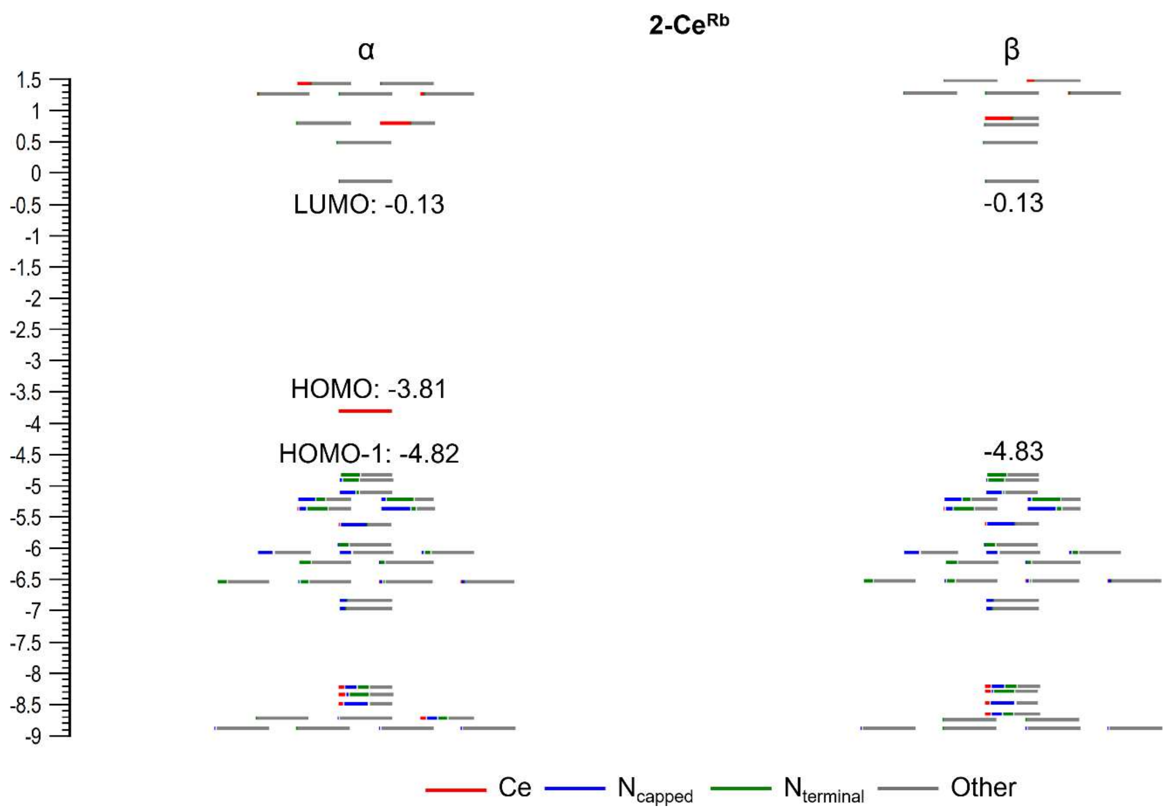


Figure S86. α and β MO energy levels for the **2-Ce**^{Rb} complex.

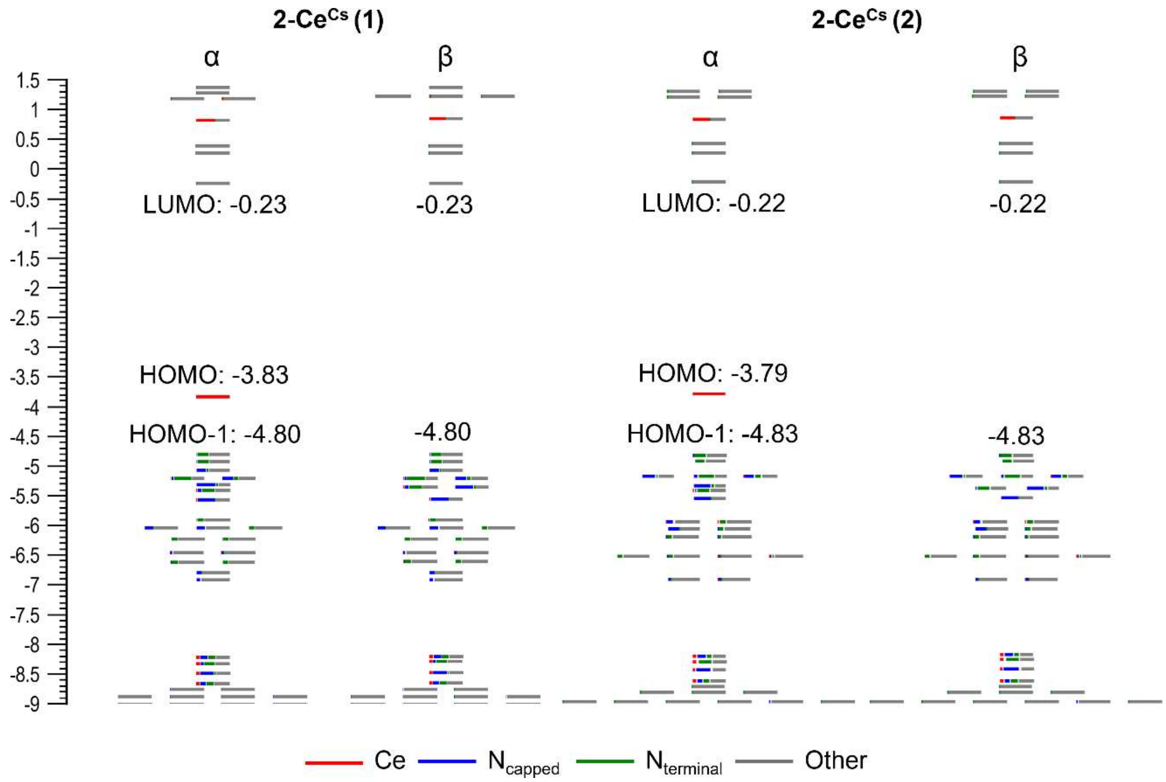


Figure S87. α and β MO energy levels for both crystallographically unique **2-Ce**^{Cs} complexes.

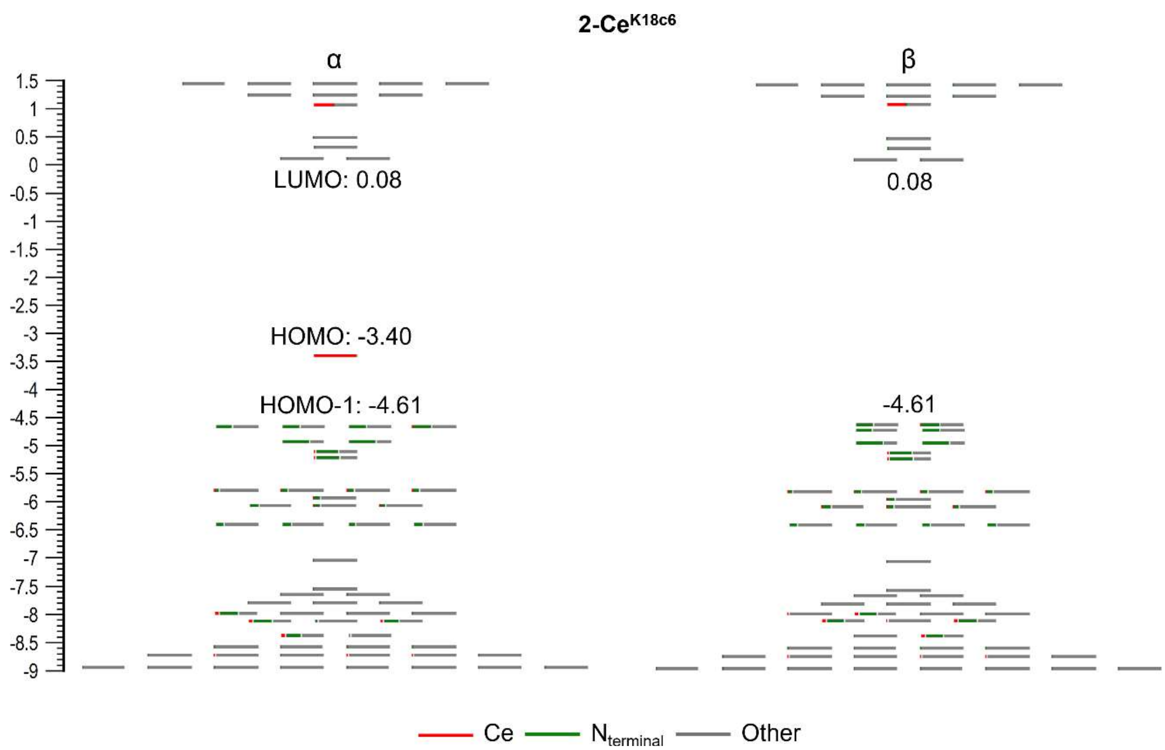


Figure S88. α and β MO energy levels for the **2-Ce**^{K18c6} complex.

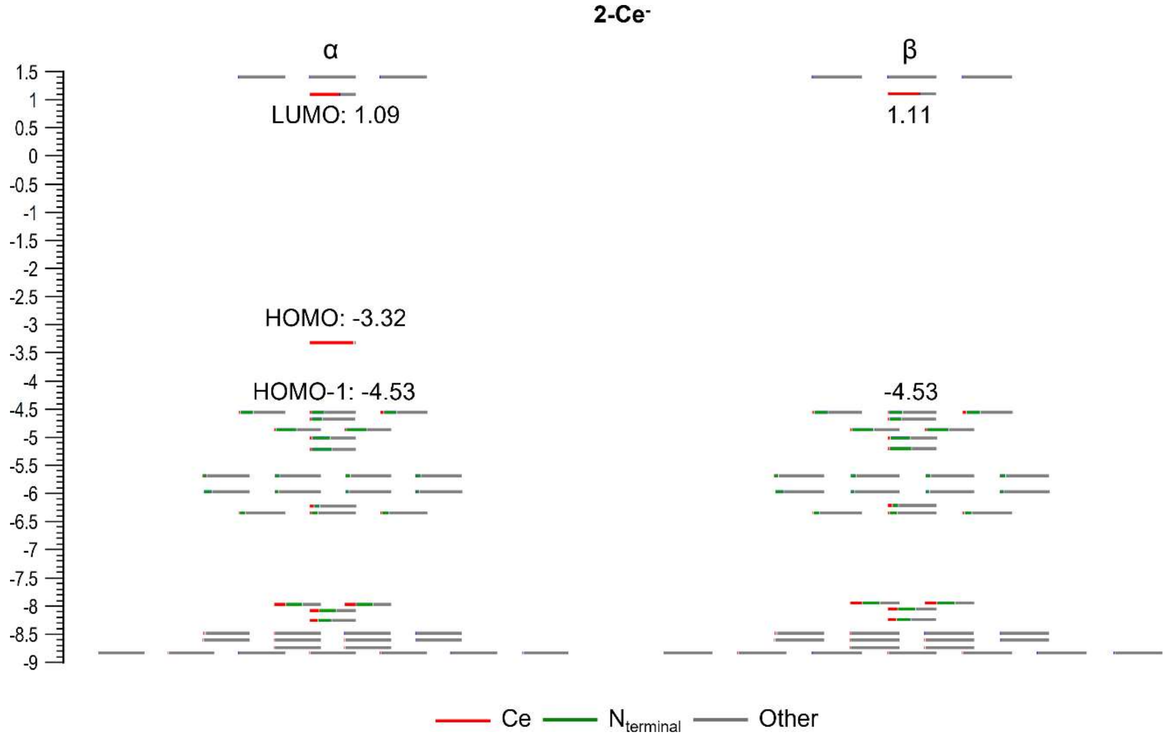


Figure S89. α and β MO energy levels for the **2-Ce**⁻ complex.

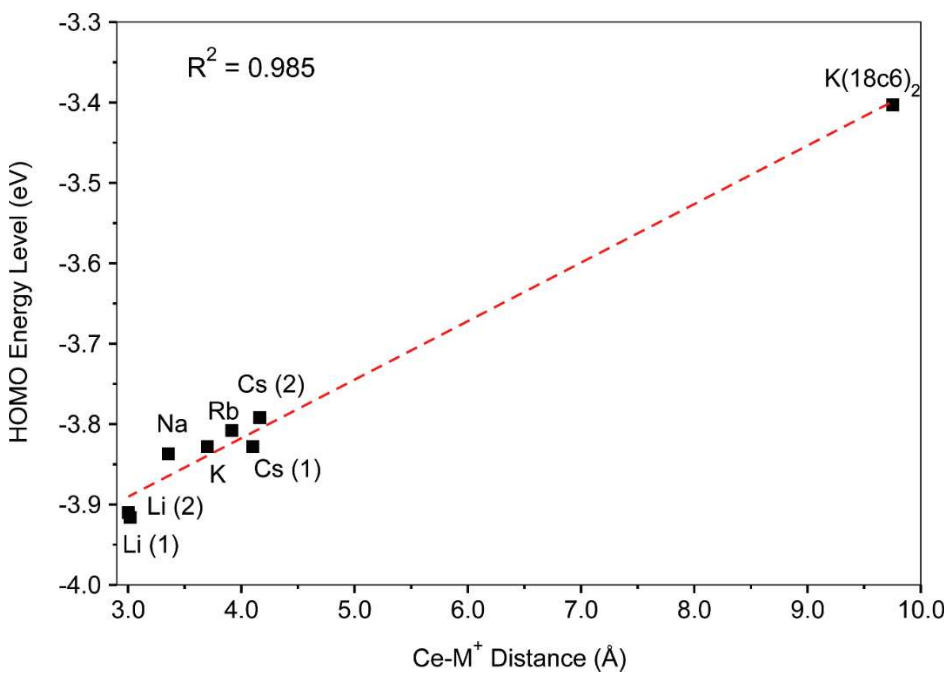


Figure S90. Correlation between the optimized Ce–M^+ distance and HOMO energy level.

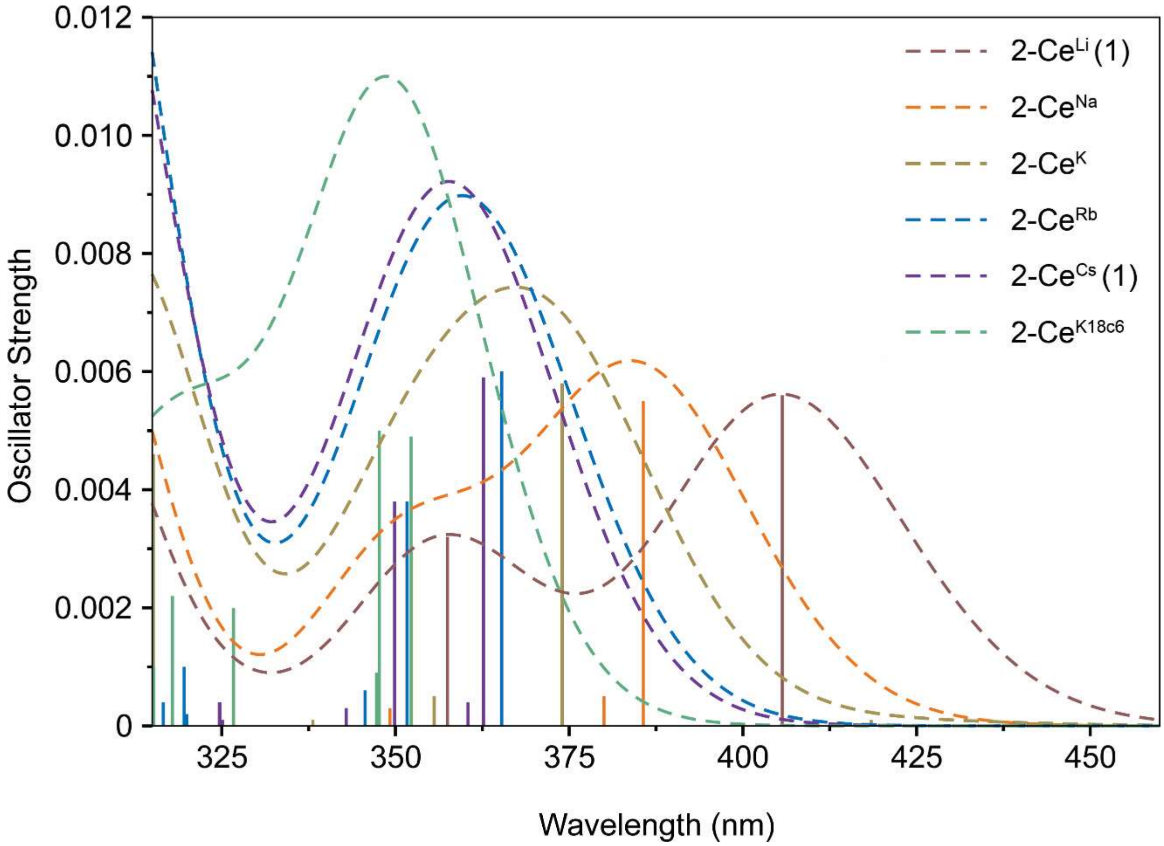


Figure S91. Calculated TD-DFT spectra overlayed with bars representing oscillator strength values. The half-width at half height is set to 0.15 eV, here and elsewhere in the SI. For clarity, the TD-DFT spectrum of only **2-Ce^{Li}** (1) and **2-Ce^{Cs}** (1) are shown for the complexes with crystallographically unique structures.

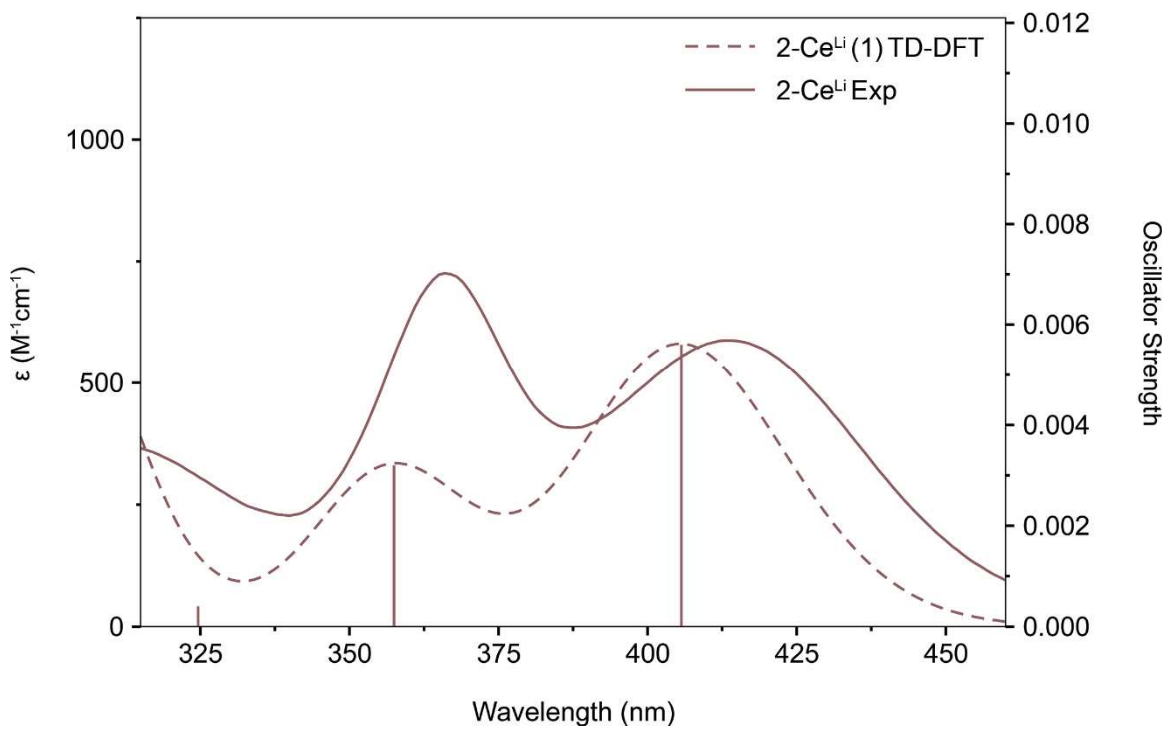


Figure S92. Overlap of TD-DFT and UV-Vis spectrum for **2-Ce^{Li}** (1).

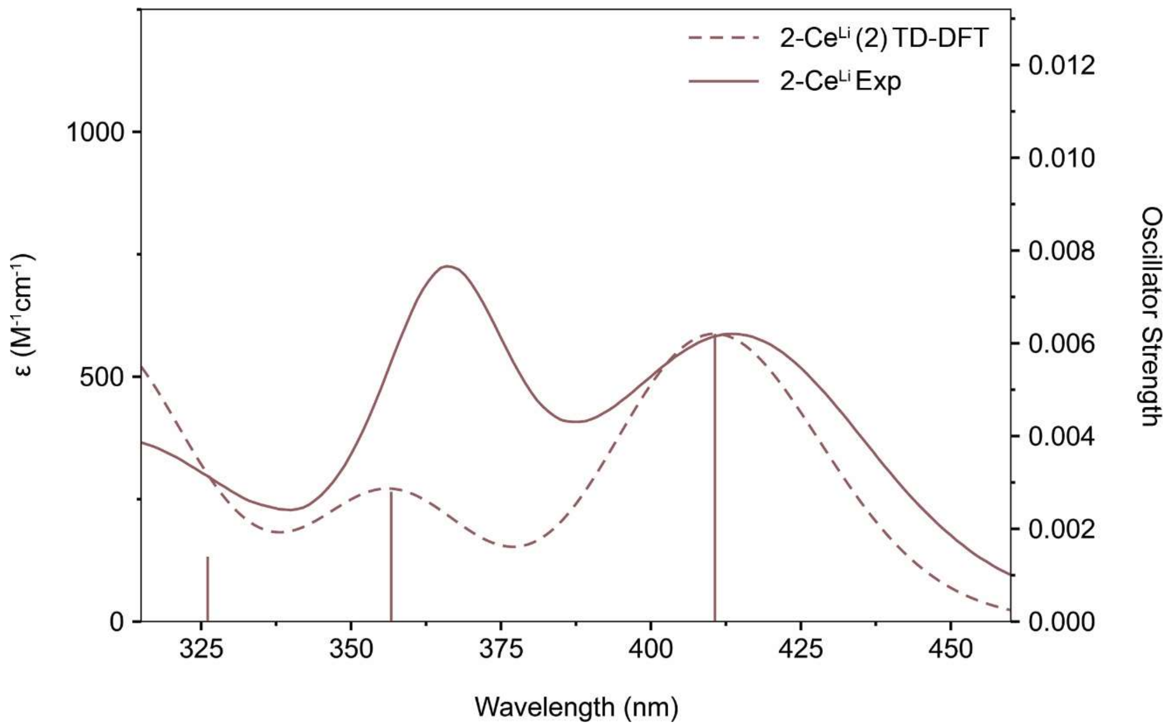


Figure S93. Overlap of TD-DFT and UV-Vis spectrum for **2-Ce^{Li}** (2).

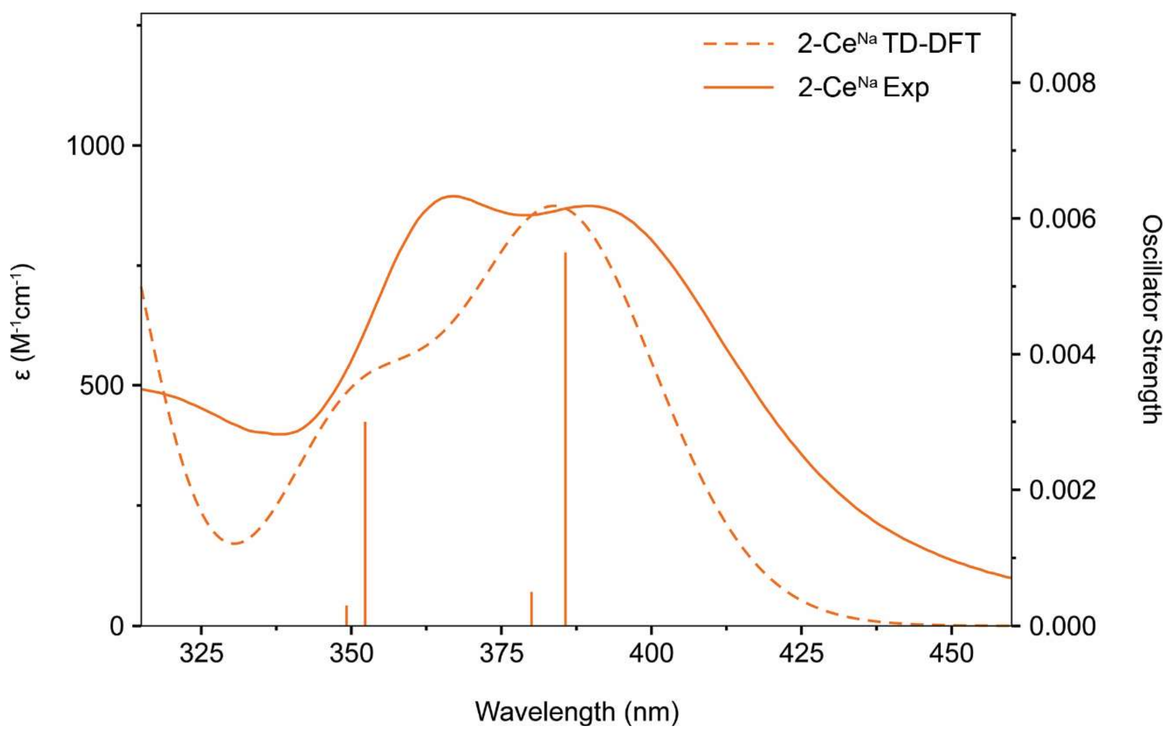


Figure S94. Overlap of TD-DFT and UV-Vis spectrum for **2-Ce^{Na}**.

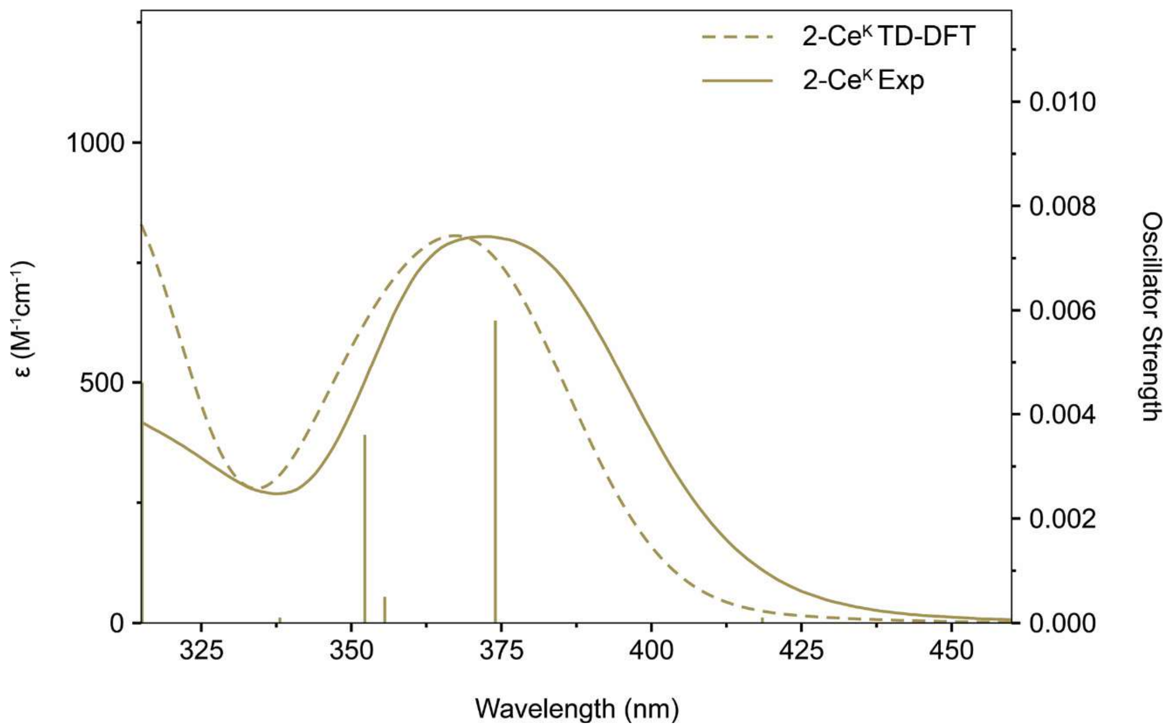


Figure S95. Overlap of TD-DFT and UV-Vis spectrum in for **2-Ce^{K}**.

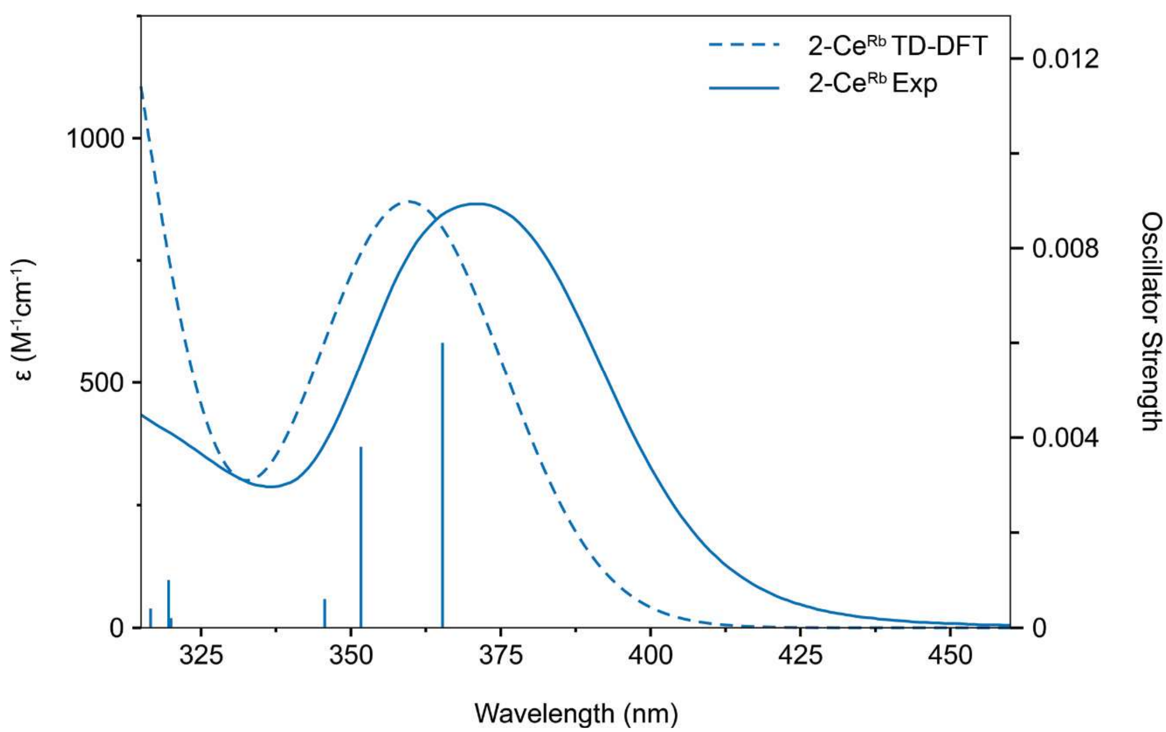


Figure S96. Overlap of TD-DFT and UV-Vis spectrum for **2-Ce^{Rb}**.

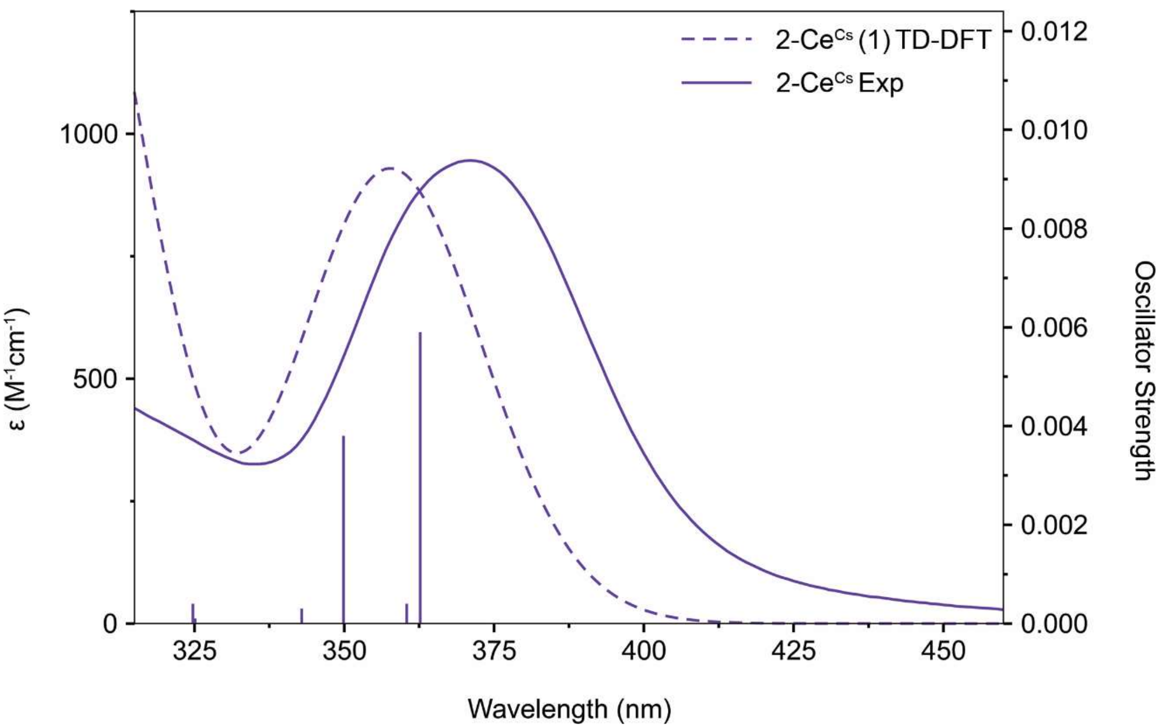


Figure S97. Overlap of TD-DFT and UV-Vis spectrum for **2-Ce^{Cs}** (1).

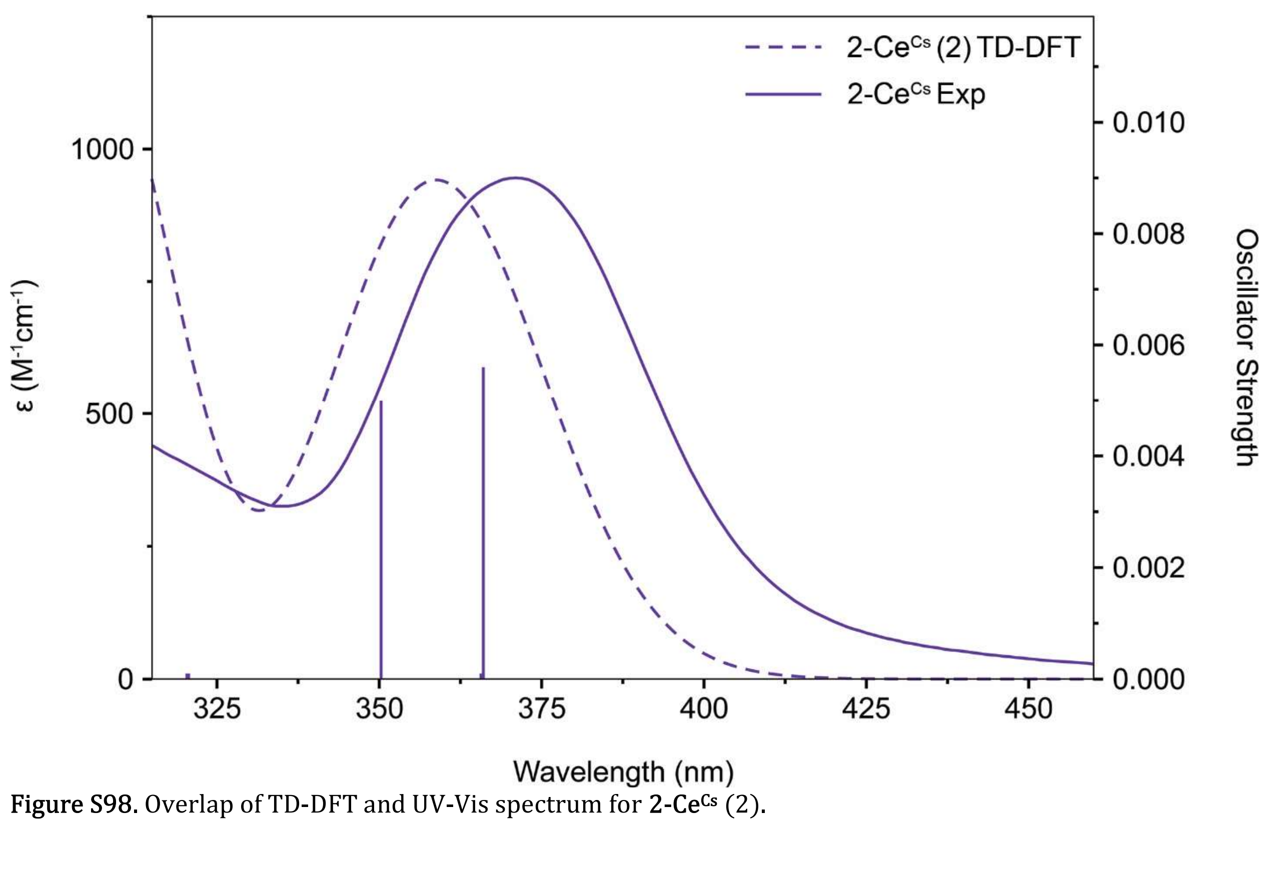


Figure S98. Overlap of TD-DFT and UV-Vis spectrum for **2-Ce^{Cs}** (2).

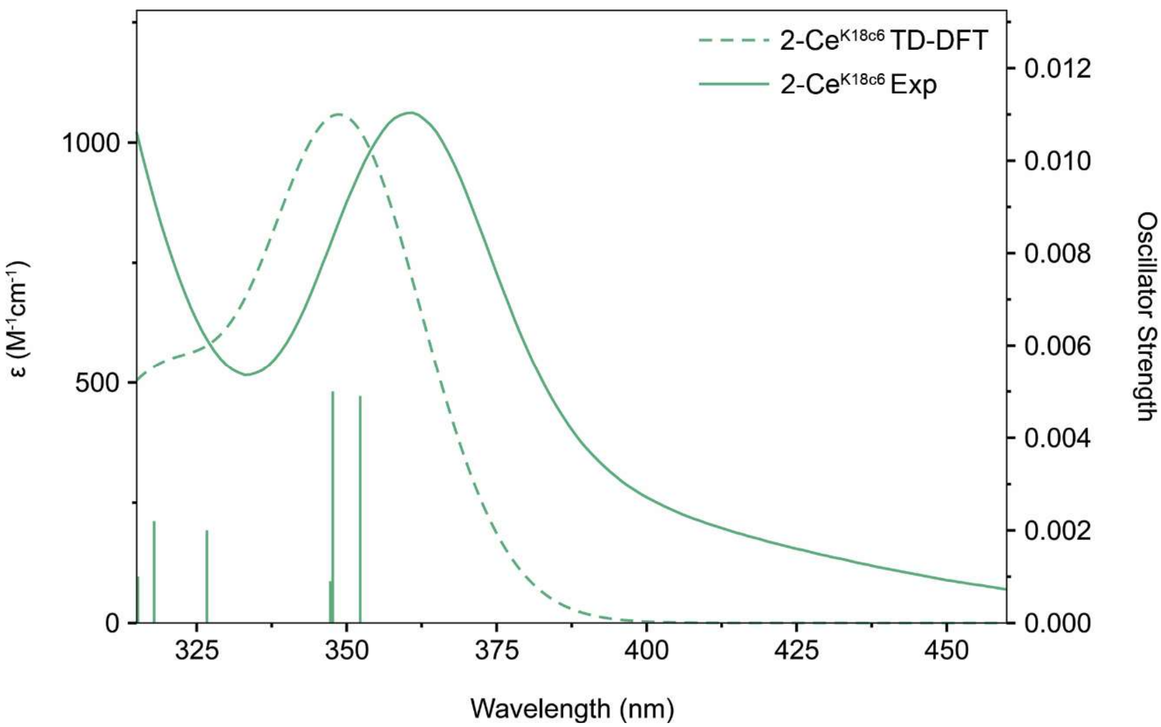


Figure S99. Overlap of TD-DFT and UV-Vis spectrum for **2-Ce**$^{\mathbf{K18c6}}$.

Table S6. Peak analysis of the 4*f*-5*d* transitions in the UV-Vis and calculated TD-DFT spectra.

Complex	Position of peaks/transitions Exp. [Theor.]	Gap between peaks/transitions Exp. [Theor.]
2-Ce$^{\mathbf{Li}}$ [a]	363/414 [357/406] [357/411]	51 [48] [54]
2-Ce$^{\mathbf{Na}}$	360/393 [352/385]	31 [33]
2-Ce$^{\mathbf{K}}$	371 [352/374]	[22]
2-Ce$^{\mathbf{Rb}}$	371 [352/365]	[13]
2-Ce$^{\mathbf{Cs}}$ [a]	371 [350/363] [350/366]	[13] [16]
2-Ce$^{\mathbf{K18c6}}$	361 [348/352]	[4]

[a]More than one crystallographically unique molecule is present in the asymmetric unit, metrics for each molecule are presented.

Table S7. Wavelength, probability (%NTO pair), oscillator strength (f), and the contribution of original principal Kohn-Sham orbitals for the major 4*f*-5*d* excited state transitions with the two largest amplitudes for each **2-Ce^M** complex.

	λ_{max} (nm)	%NTO pair	f	Major contributors
2-Ce^Li [a]	405.6 410.7	86% 86%	0.006 0.006	HOMO→LUMO+2 (38.4%) HOMO→LUMO+10 (17.6%) HOMO→LUMO+2 (34.8%) HOMO→LUMO+10 (17.6%)
	357.5 356.7	84% 86%	0.003 0.003	HOMO→LUMO+12 (34.8%) HOMO→LUMO+18 (14.4%) HOMO→LUMO+14 (25.0%) HOMO→LUMO+17 (18.5%)
2-Ce^Na	385.7	87%	0.005	HOMO→LUMO+3 (23.0%) HOMO→LUMO+12 (13.7%)
	352.3	86%	0.003	HOMO→LUMO+16 (25.0%) HOMO→LUMO+26 (13.7%)
2-Ce^K	374.0	87%	0.006	HOMO→LUMO+14 (22.1%) HOMO→LUMO+3 (15.2%)
	352.3	87%	0.004	HOMO→LUMO+13 (19.4%) HOMO→LUMO+27 (12.3%)
2-Ce^Rb	365.3	85%	0.006	HOMO→LUMO+16 (26.0%) HOMO→LUMO+3 (13.7%)
	351.7	85%	0.004	HOMO→LUMO+14 (20.3%) HOMO→LUMO+28 (11.6%)
2-Ce^Cs [a]	362.7 366.0	85% 87%	0.006 0.006	HOMO→LUMO+13 (19.4%) HOMO→LUMO+15 (9.6%) HOMO→LUMO+16 (23.0%) HOMO→LUMO+13 (19.4%)
	349.9 350.3	85% 86%	0.004 0.005	HOMO→LUMO+15 (14.4%) HOMO→LUMO+18 (13.0%) HOMO→LUMO+13 (24.0%) HOMO→LUMO+27 (13.7%)
2-Ce^K18c6	352.3	78%	0.005	HOMO→LUMO+30 (15.2%) HOMO→LUMO+36 (10.9%)
	347.7	81%	0.005	HOMO→LUMO+40 (13.0%) HOMO→LUMO+50 (11.6%)

[a]More than one crystallographically unique molecule is present in the asymmetric unit, metrics for each molecule are presented.

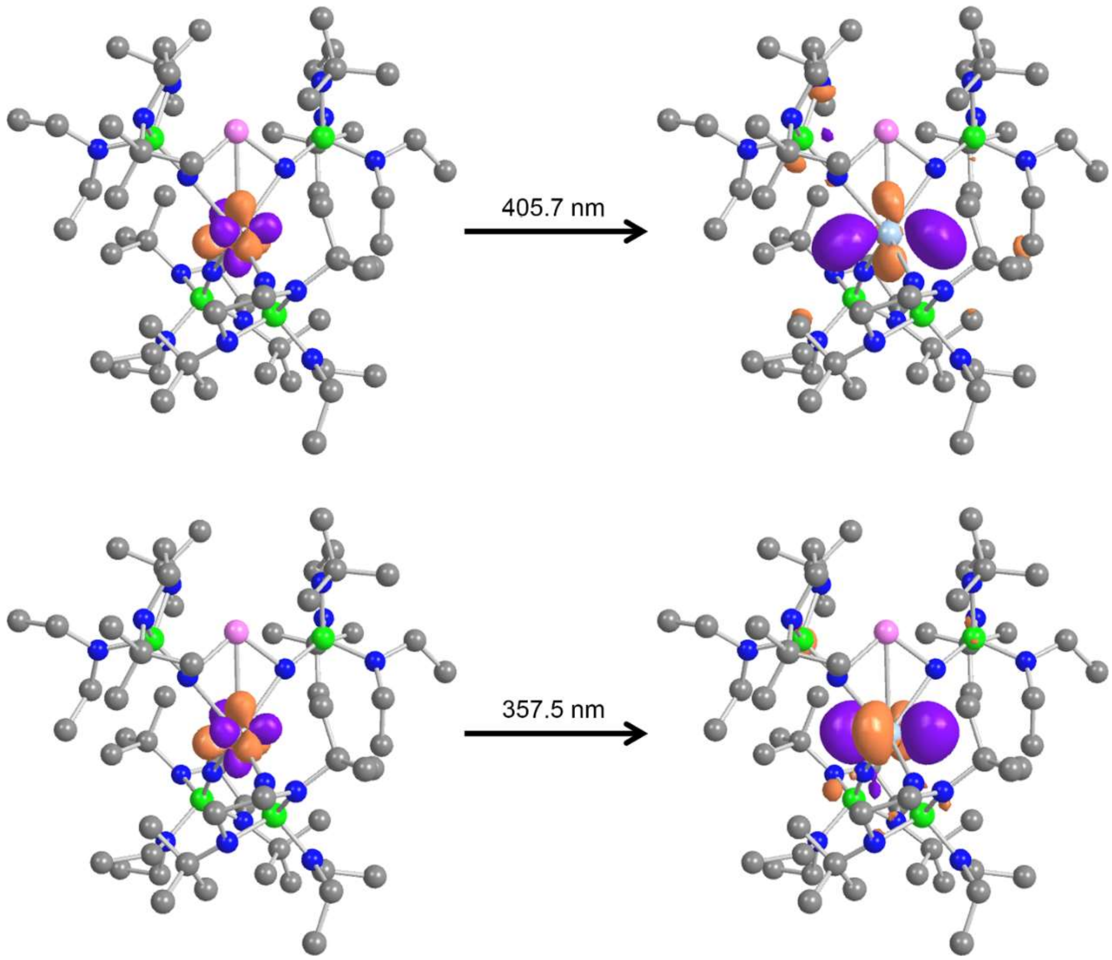


Figure S100. Dominant NTO pairs ("hole" (on the left) → "particle" (on the right)) corresponding to the $4f \rightarrow 5d$ transitions with the highest oscillator strength values within the ~340-450 nm range of **2-Ce^{Li}** (1). Cylinders connecting atoms do not necessarily represent bonds between atoms, here and in subsequent NTO figures. Atom colors are as follows here and in subsequent NTO figures: C, gray; N, dark blue; P, green; Ce, sky blue. The Li atom is colored pink.

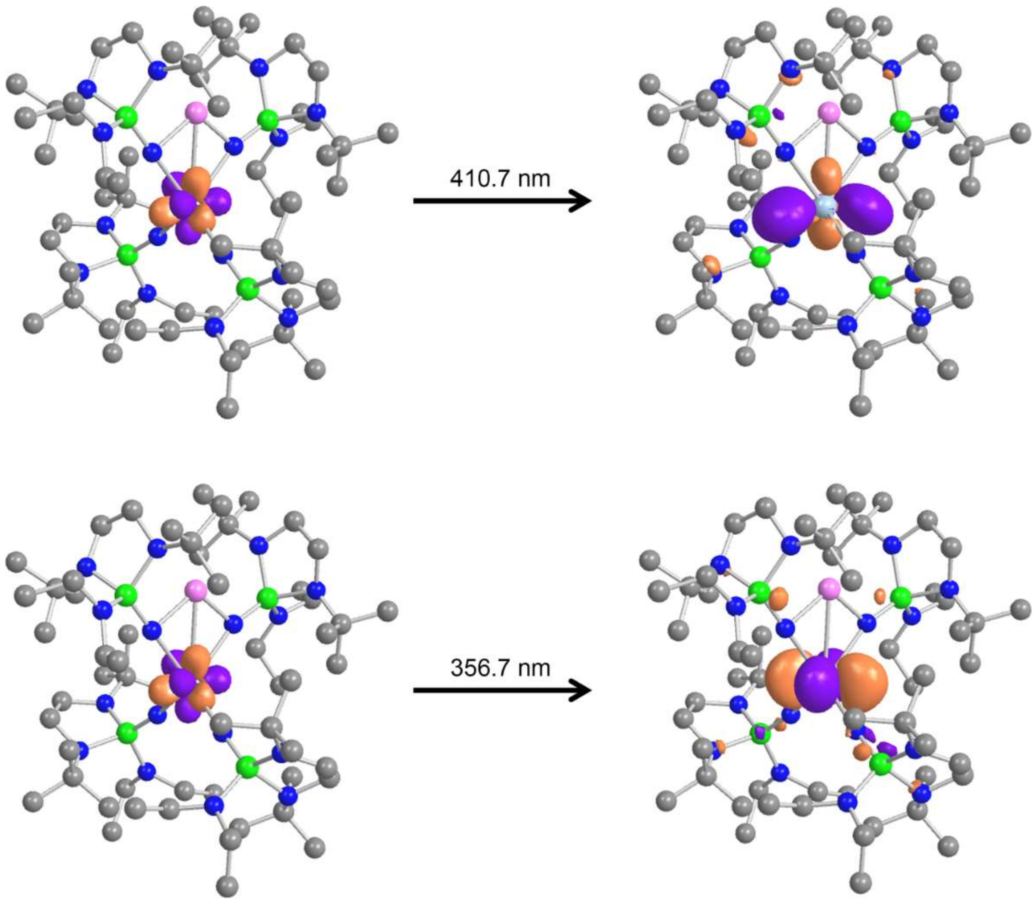


Figure S101. Dominant NTO pairs ("hole" (on the left) → "particle" (on the right)) corresponding to the 4f→ 5d transitions with the highest oscillator strength values within the ~340-450 nm range of **2-Ce**^{Li} (2).

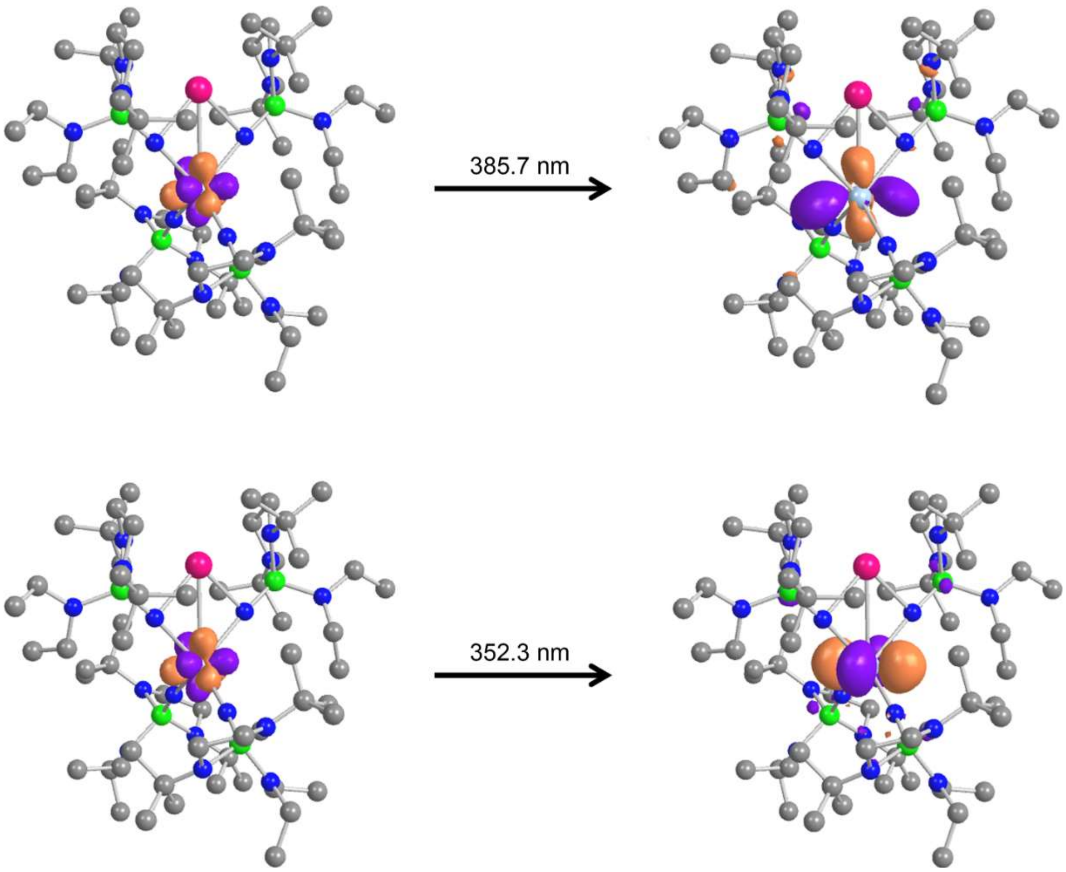


Figure S102. Dominant NTO pairs ("hole" (on the left) → "particle" (on the right)) corresponding to the $4f \rightarrow 5d$ transitions with the highest oscillator strength values within the ~340-450 nm range of **2-Ce^{Na}**. The Na atom is colored rose.

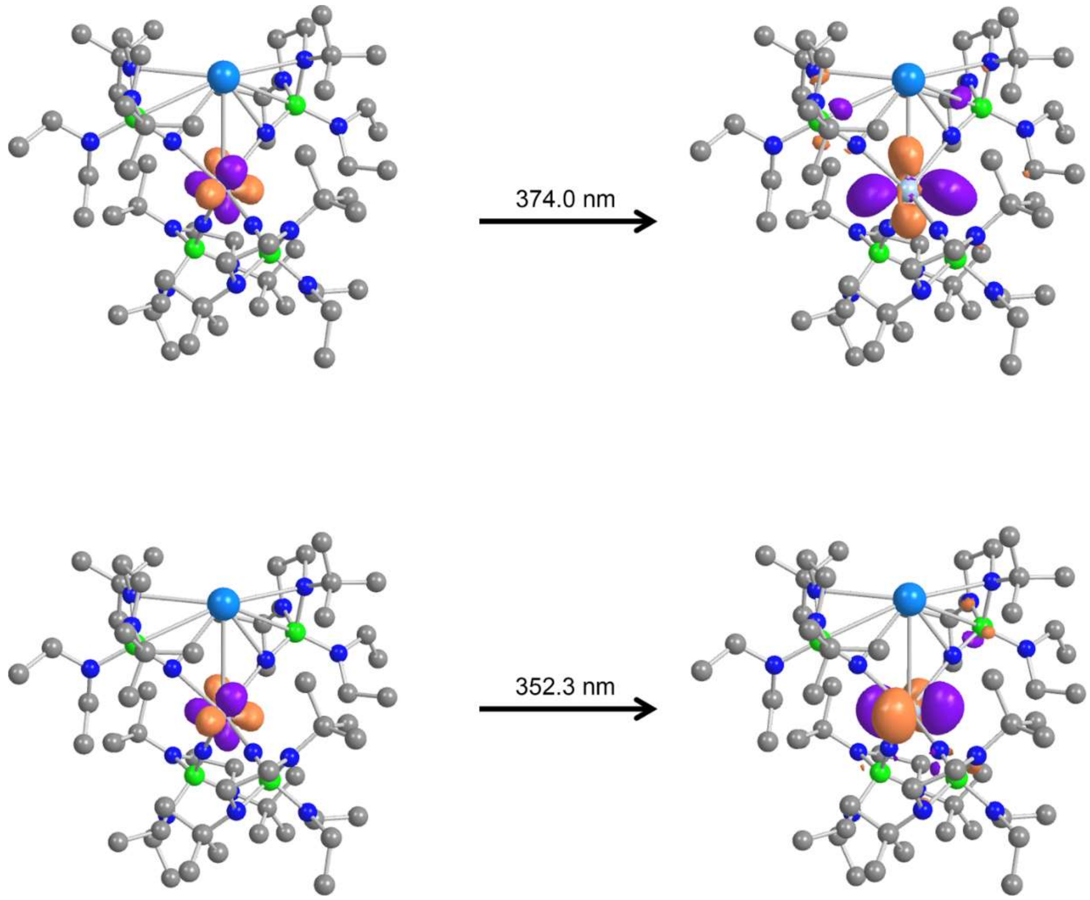


Figure S103. Dominant NTO pairs ("hole" (on the left) → "particle" (on the right)) corresponding to the $4f \rightarrow 5d$ transitions with the highest oscillator strength values within the ~340-450 nm range of **2-Ce^K^**. The K atom is colored blue.

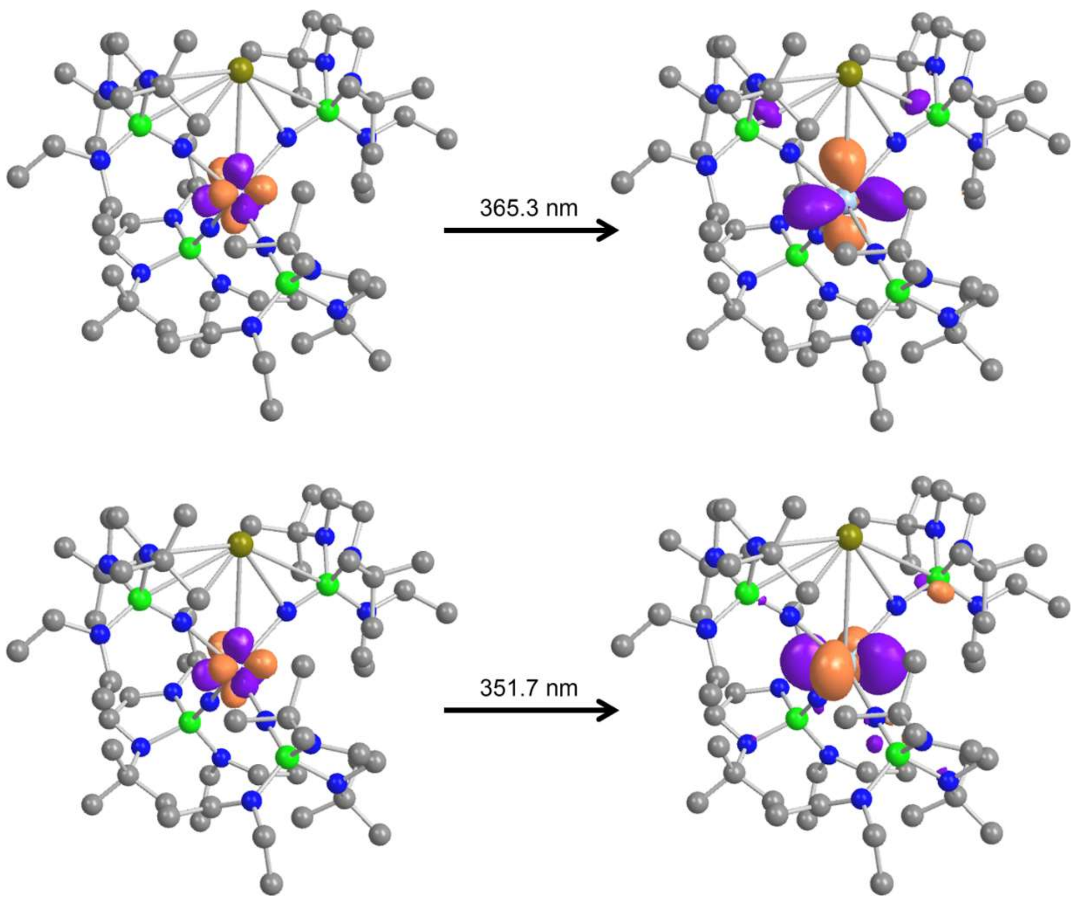


Figure S104. Dominant NTO pairs ("hole" (on the left) → "particle" (on the right)) corresponding to the $4f \rightarrow 5d$ transitions with the highest oscillator strength values within the ~340-450 nm range of **2-Ce^{Rb}**. The Rb atom is colored dark yellow.

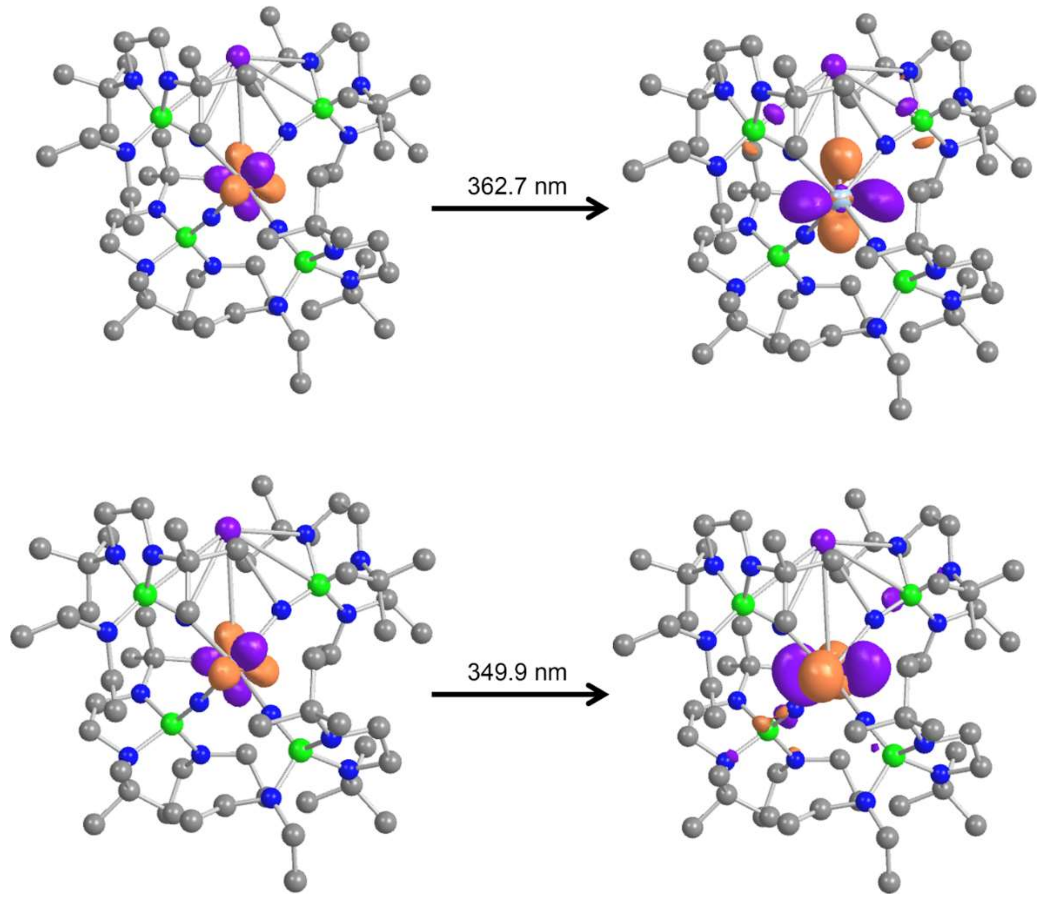


Figure S105. Dominant NTO pairs (“hole” (on the left) → “particle” (on the right)) corresponding to the $4f \rightarrow 5d$ transitions with the highest oscillator strength values within the ~340-450 nm range of **2-Ce^{Cs}** (1). The Cs atom is colored purple.

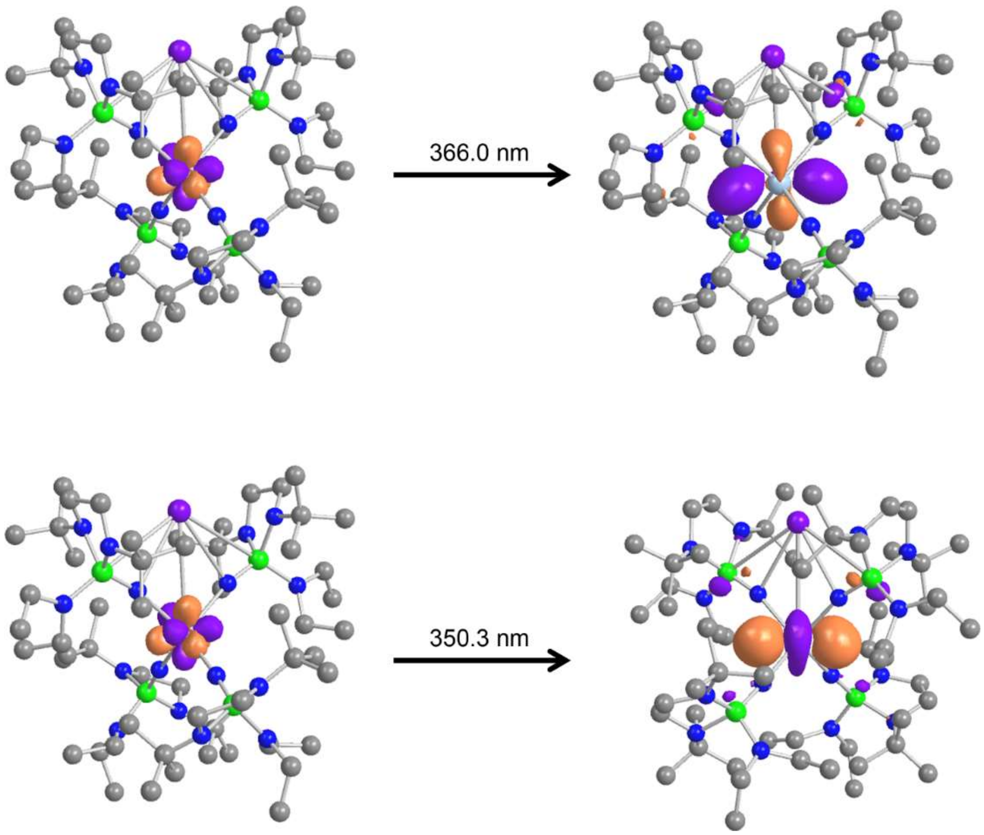


Figure S106. Dominant NTO pairs ("hole" (on the left) → "particle" (on the right)) corresponding to the $4f \rightarrow 5d$ transitions with the highest oscillator strength values within the ~340-450 nm range of **2-Ce^{Cs}** (2).

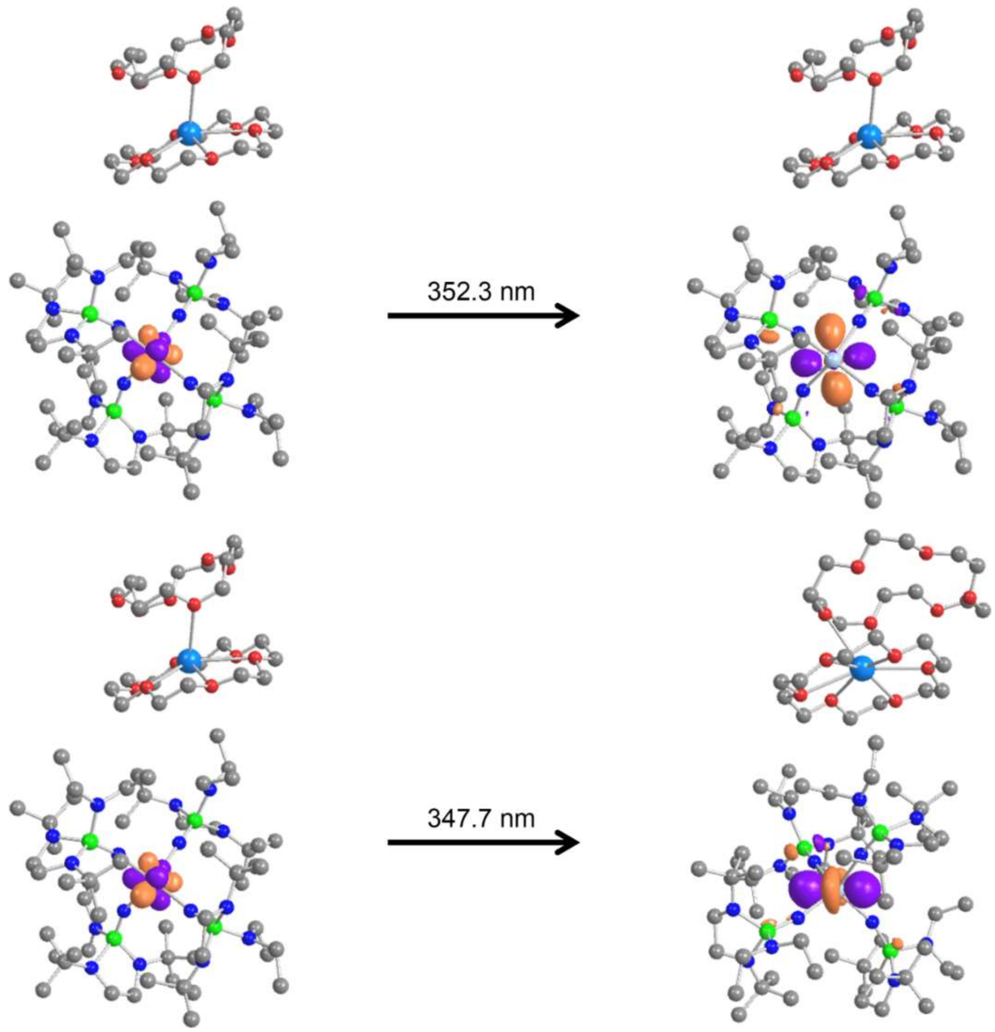


Figure S107. Dominant NTO pairs ("hole" (on the left) → "particle" (on the right)) corresponding to the $4f$→ $5d$ transitions with the highest oscillator strength values within the ∼340-450 nm range of **2-Ce**^{K18c6}. The K atom is colored blue, and the oxygen atoms are colored red.

Table S8. Experimental *vs.* calculated oxidation potentials representing the **2-Ce^{M}/1-Ce** (M^+ ejected) and the **2-Ce^{M}/1-Ce^{M+}** (M = Li, Na, K, Rb, Cs, [K(18c6)$_2$]) (M^+ retained) couples. Experimental values are reported based on the data obtained with BPh_4^- (PF_6^-) as the supporting electrolyte. VDEs and ADEs for each synthesized complex are reported for both M^+ ejected and M^+ retained when applicable. Calculated potentials are referenced to a Fc^+/Fc couple.

Complex	Exp. (V)	VDE (V) M^+ ejected	VDE (V) M^+ retained	ADE (V) M^+ ejected	ADE (V) M^+ retained
2-Ce^{Li} [a]	-1.37 (-1.23)	-0.35 -0.34	-0.69 -0.69	-1.56 -1.65	-1.34 -1.31
2-Ce^{Na}	-1.45 (-1.44)	-1.30	-0.76	-2.40	-1.38
2-Ce^{K}	-1.71 (-1.44)	-1.40	-0.77	-2.51	-1.43
2-Ce^{Rb}	-1.87 (-1.31*)	-1.79	-0.79	-2.94	-1.49
2-Ce^{Cs} [a]	-1.98 (-)	-1.83 -1.80	-0.78 -0.80	-2.91 -2.95	-1.46 -1.47
2-Ce^{K18c6}	-1.92 (-1.63)	-1.19		-1.98	
2-Ce^{-}	-1.83 (-1.63)	-1.29		-2.17	

[a]More than one crystallographically unique molecule is present in the asymmetric unit, metrics for each molecule are presented.
*Feature is not well defined

Table S9. Cartesian coordinates for the optimized geometries of **2-Ce^{-}** and **1-Ce.**

2-Ce^{-}				**1-Ce**			
58	0.000000000	0.000000000	-0.000053000	58	0.000000000	0.000000000	0.000000000
15	-2.917794000	1.002048000	2.323651000	15	-2.379942000	1.748064000	2.284442000
7	-4.452615000	0.963047000	1.584471000	7	-3.838556000	2.183742000	1.557068000
7	-2.997145000	2.407093000	3.312257000	7	-1.938250000	3.066750000	3.265546000
7	-1.756888000	0.780474000	1.343337000	7	-1.361320000	1.173688000	1.255385000
7	-3.119899000	0.000172000	3.736551000	7	-2.820965000	0.824512000	3.666962000
6	-4.601243000	0.532857000	0.210887000	6	-4.140942000	1.855625000	0.176674000
1	-5.108892000	-0.443972000	0.159302000	1	-4.903162000	1.063289000	0.129989000
1	-3.589953000	0.373697000	-0.169819000	1	-3.230085000	1.430027000	-0.248848000
6	-5.339390000	1.524795000	-0.678954000	6	-4.603787000	3.041644000	-0.657990000
1	-5.373926000	1.149813000	-1.706201000	1	-4.786683000	2.721454000	-1.687529000
1	-4.834350000	2.493498000	-0.690604000	1	-3.850284000	3.831700000	-0.680579000
1	-6.374071000	1.686747000	-0.357572000	1	-5.536991000	3.475898000	-0.286438000
6	-2.830168000	3.792415000	2.863693000	6	-1.505743000	4.408414000	2.843778000
6	-3.752472000	4.705829000	3.679475000	6	-2.256680000	5.473139000	3.650887000
1	-4.793763000	4.382835000	3.586729000	1	-3.338253000	5.359960000	3.535676000
1	-3.679844000	5.734937000	3.313828000	1	-1.981360000	6.470989000	3.297436000
1	-3.492041000	4.716544000	4.742023000	1	-2.019737000	5.429411000	4.717552000
6	-2.931280000	-1.462612000	3.687039000	6	-3.166086000	-0.610598000	3.622611000
6	-3.212365000	3.930551000	1.392390000	6	-1.799913000	4.636345000	1.364949000
1	-2.617237000	3.262114000	0.767156000	1	-1.352285000	3.857880000	0.744428000

1	-3.034117000	4.959211000	1.063790000	1	-1.382927000	5.599646000	1.057697000
1	-4.268261000	3.697827000	1.240233000	1	-2.873622000	4.655100000	1.174481000
6	-2.522888000	0.687479000	4.865714000	6	-2.043726000	1.278523000	4.806179000
1	-1.422029000	0.640508000	4.853451000	1	-1.015656000	0.885428000	4.794373000
1	-2.866345000	0.264687000	5.815424000	1	-2.510648000	0.973735000	5.746648000
6	-1.374244000	4.235396000	3.039624000	6	0.000000000	4.559900000	3.074214000
1	-1.053237000	4.156068000	4.083190000	1	0.267796000	4.401108000	4.122888000
1	-1.237142000	5.276953000	2.728615000	1	0.338228000	5.563616000	2.796653000
1	-0.725528000	3.598664000	2.436095000	1	0.540857000	3.829008000	2.471888000
6	-2.970068000	2.130798000	4.729241000	6	-2.021383000	2.788406000	4.683809000
1	-3.965153000	2.265084000	5.188198000	1	-2.934134000	3.217477000	5.127352000
1	-2.273577000	2.790831000	5.260748000	1	-1.164068000	3.203424000	5.225032000
6	-3.764429000	-2.093703000	4.809223000	6	-4.186802000	-0.896367000	4.729599000
1	-3.426546000	-1.781765000	5.801973000	1	-3.778272000	-0.718349000	5.728171000
1	-3.687972000	-3.185159000	4.769559000	1	-4.500810000	-1.943868000	4.692810000
1	-4.817186000	-1.816161000	4.706013000	1	-5.072125000	-0.266965000	4.608184000
6	-5.648029000	1.312641000	2.319372000	6	-4.864658000	2.860732000	2.330882000
1	-6.124424000	2.197859000	1.866120000	1	-5.020934000	3.875132000	1.932982000
1	-5.342675000	1.619236000	3.321042000	1	-4.485147000	2.990731000	3.345689000
6	-3.439165000	-2.019989000	2.358348000	6	-3.810072000	-0.967192000	2.285314000
1	-2.853162000	-1.642486000	1.518100000	1	-3.117133000	-0.823405000	1.453871000
1	-4.485692000	-1.758784000	2.190833000	1	-4.701477000	-0.367380000	2.096255000
1	-3.354878000	-3.110502000	2.367626000	1	-4.106078000	-2.019256000	2.299335000
6	-6.682233000	0.199484000	2.433769000	6	-6.202907000	2.138495000	2.393708000
1	-7.026484000	-0.146935000	1.454450000	1	-6.640602000	1.986728000	1.403030000
1	-7.561182000	0.553650000	2.983553000	1	-6.917012000	2.726607000	2.978239000
1	-6.270690000	-0.658574000	2.970412000	1	-6.102388000	1.161712000	2.872134000
6	-1.463020000	-1.864700000	3.859231000	6	-1.933982000	-1.495168000	3.826920000
1	-0.830673000	-1.376751000	3.113233000	1	-1.161332000	-1.278607000	3.084060000
1	-1.351518000	-2.947314000	3.748904000	1	-2.209759000	-2.549453000	3.739015000
1	-1.083399000	-1.600823000	4.851805000	1	-1.498095000	-1.359642000	4.821625000
15	1.001859000	2.918009000	-2.323612000	15	1.748064000	2.379942000	-2.284442000
7	0.962628000	4.452802000	-1.584382000	7	2.183742000	3.838556000	-1.557068000
7	2.406925000	2.997632000	-3.312179000	7	3.066750000	1.938250000	-3.265546000
7	0.780368000	1.757054000	-1.343326000	7	1.173688000	1.361320000	-1.255385000
7	0.000000000	3.120077000	-3.736531000	7	0.824512000	2.820965000	-3.666962000
6	0.532354000	4.601346000	-0.210815000	6	1.855625000	4.140942000	-0.176674000
1	-0.444434000	5.109078000	-0.159287000	1	1.063289000	4.903162000	-0.129989000
1	0.373078000	3.590045000	0.169814000	1	1.430027000	3.230085000	0.248848000
6	1.524260000	5.339369000	0.679162000	6	3.041644000	4.603787000	0.657990000
1	1.149131000	5.373967000	1.706353000	1	2.721454000	4.786683000	1.687529000
1	2.492894000	4.834200000	0.690955000	1	3.831700000	3.850284000	0.680579000
1	1.686397000	6.374025000	0.357790000	1	3.475898000	5.536991000	0.286438000

6	3.792294000	2.830933000	-2.863648000	6	4.408414000	1.505743000	-2.843778000
6	4.705455000	3.753168000	-3.679770000	6	5.473139000	2.256680000	-3.650887000
1	4.382350000	4.794439000	-3.587187000	1	5.359960000	3.338253000	-3.535676000
1	5.734636000	3.680735000	-3.314288000	1	6.470989000	1.981360000	-3.297436000
1	4.716004000	3.492511000	-4.742267000	1	5.429411000	2.019737000	-4.717552000
6	-1.462768000	2.931294000	-3.687137000	6	-0.610598000	3.166086000	-3.622611000
6	3.930537000	3.213531000	-1.392459000	6	4.636345000	1.799913000	-1.364949000
1	3.262289000	2.618428000	-0.767004000	1	3.857880000	1.352285000	-0.744428000
1	4.959273000	3.035580000	-1.063931000	1	5.599646000	1.382927000	-1.057697000
1	3.697611000	4.269417000	-1.240550000	1	4.655100000	2.873622000	-1.174481000
6	0.687407000	2.523211000	-4.865705000	6	1.278523000	2.043726000	-4.806179000
1	0.640561000	1.422346000	-4.853508000	1	0.885428000	1.015656000	-4.794373000
1	0.264592000	2.866678000	-5.815401000	1	0.973735000	2.510648000	-5.746648000
6	4.235507000	1.375049000	-3.039284000	6	4.559900000	0.000000000	-3.074214000
1	4.156122000	1.053772000	-4.082764000	1	4.401108000	-0.267796000	-4.122888000
1	5.277122000	1.238212000	-2.728362000	1	5.563616000	-0.338228000	-2.796653000
1	3.598957000	0.726376000	-2.435516000	1	3.829008000	-0.540857000	-2.471888000
6	2.130667000	2.970573000	-4.729168000	6	2.788406000	2.021383000	-4.683809000
1	2.264829000	3.965700000	-5.188066000	1	3.217477000	2.934134000	-5.127352000
1	2.790819000	2.274204000	-5.260687000	1	3.203424000	1.164068000	-5.225032000
6	-2.093807000	3.764420000	-4.809355000	6	-0.896367000	4.186802000	-4.729599000
1	-1.781552000	3.426733000	-5.802074000	1	-0.718349000	3.778272000	-5.728171000
1	-3.185253000	3.687681000	-4.769947000	1	-1.943868000	4.500810000	-4.692810000
1	-1.816550000	4.817233000	-4.705951000	1	-0.266965000	5.072125000	-4.608184000
6	1.312281000	5.648258000	-2.319187000	6	2.860732000	4.864658000	-2.330882000
1	2.197436000	6.124641000	-1.865798000	1	3.875132000	5.020934000	-1.932982000
1	1.619018000	5.342949000	-3.320829000	1	2.990731000	4.485147000	-3.345689000
6	-2.020414000	3.439023000	-2.358489000	6	-0.967192000	3.810072000	-2.285314000
1	-1.642977000	2.853007000	-1.518221000	1	-0.823405000	3.117133000	-1.453871000
1	-1.759363000	4.485568000	-2.190862000	1	-0.367380000	4.701477000	-2.096255000
1	-3.110916000	3.354602000	-2.367940000	1	-2.019256000	4.106078000	-2.299335000
6	0.199140000	6.682471000	-2.433676000	6	2.138495000	6.202907000	-2.393708000
1	-0.147390000	7.026685000	-1.454384000	1	1.986728000	6.640602000	-1.403030000
1	0.553381000	7.561441000	-2.983378000	1	2.726607000	6.917012000	-2.978239000
1	-0.658857000	6.270964000	-2.970443000	1	1.161712000	6.102388000	-2.872134000
6	-1.864652000	1.463005000	-3.859515000	6	-1.495168000	1.933982000	-3.826920000
1	-1.376892000	0.830686000	-3.113371000	1	-1.278607000	1.161332000	-3.084060000
1	-2.947291000	1.351391000	-3.749561000	1	-2.549453000	2.209759000	-3.739015000
1	-1.600398000	1.083445000	-4.852013000	1	-1.359642000	1.498095000	-4.821625000
15	2.917794000	-1.002048000	2.323651000	15	2.379942000	-1.748064000	2.284442000
7	4.452615000	-0.963047000	1.584471000	7	3.838556000	-2.183742000	1.557068000
7	2.997145000	-2.407093000	3.312257000	7	1.938250000	-3.066750000	3.265546000
7	1.756888000	-0.780474000	1.343337000	7	1.361320000	-1.173688000	1.255385000

7	3.119899000	-0.000172000	3.736551000	7	2.820965000	-0.824512000	3.666962000
6	4.601243000	-0.532857000	0.210887000	6	4.140942000	-1.855625000	0.176674000
1	5.108892000	0.443972000	0.159302000	1	4.903162000	-1.063289000	0.129989000
1	3.589953000	-0.373697000	-0.169819000	1	3.230085000	-1.430027000	-0.248848000
6	5.339390000	-1.524795000	-0.678954000	6	4.603787000	-3.041644000	-0.657990000
1	5.373926000	-1.149813000	-1.706201000	1	4.786683000	-2.721454000	-1.687529000
1	4.834350000	-2.493498000	-0.690604000	1	3.850284000	-3.831700000	-0.680579000
1	6.374071000	-1.686747000	-0.357572000	1	5.536991000	-3.475898000	-0.286438000
6	2.830168000	-3.792415000	2.863693000	6	1.505743000	-4.408414000	2.843778000
6	3.752472000	-4.705829000	3.679475000	6	2.256680000	-5.473139000	3.650887000
1	4.793763000	-4.382835000	3.586729000	1	3.338253000	-5.359960000	3.535676000
1	3.679844000	-5.734937000	3.313828000	1	1.981360000	-6.470989000	3.297436000
1	3.492041000	-4.716544000	4.742023000	1	2.019737000	-5.429411000	4.717552000
6	2.931280000	1.462612000	3.687039000	6	3.166086000	0.610598000	3.622611000
6	3.212365000	-3.930551000	1.392390000	6	1.799913000	-4.636345000	1.364949000
1	2.617237000	-3.262114000	0.767156000	1	1.352285000	-3.857880000	0.744428000
1	3.034117000	-4.959211000	1.063790000	1	1.382927000	-5.599646000	1.057697000
1	4.268261000	-3.697827000	1.240233000	1	2.873622000	-4.655100000	1.174481000
6	2.522888000	-0.687479000	4.865714000	6	2.043726000	-1.278523000	4.806179000
1	1.422029000	-0.640508000	4.853451000	1	1.015656000	-0.885428000	4.794373000
1	2.866345000	-0.264687000	5.815424000	1	2.510648000	-0.973735000	5.746648000
6	1.374244000	-4.235396000	3.039624000	6	0.000000000	-4.559900000	3.074214000
1	1.053237000	-4.156068000	4.083190000	1	-0.267796000	-4.401108000	4.122888000
1	1.237142000	-5.276953000	2.728615000	1	-0.338228000	-5.563616000	2.796653000
1	0.725528000	-3.598664000	2.436095000	1	-0.540857000	-3.829008000	2.471888000
6	2.970068000	-2.130798000	4.729241000	6	2.021383000	-2.788406000	4.683809000
1	3.965153000	-2.265084000	5.188198000	1	2.934134000	-3.217477000	5.127352000
1	2.273577000	-2.790831000	5.260748000	1	1.164068000	-3.203424000	5.225032000
6	3.764429000	2.093703000	4.809223000	6	4.186802000	0.896367000	4.729599000
1	3.426546000	1.781765000	5.801973000	1	3.778272000	0.718349000	5.728171000
1	3.687972000	3.185159000	4.769559000	1	4.500810000	1.943868000	4.692810000
1	4.817186000	1.816161000	4.706013000	1	5.072125000	0.266965000	4.608184000
6	5.648029000	-1.312641000	2.319372000	6	4.864658000	-2.860732000	2.330882000
1	6.124424000	-2.197859000	1.866120000	1	5.020934000	-3.875132000	1.932982000
1	5.342675000	-1.619236000	3.321042000	1	4.485147000	-2.990731000	3.345689000
6	3.439165000	2.019989000	2.358348000	6	3.810072000	0.967192000	2.285314000
1	2.853162000	1.642486000	1.518100000	1	3.117133000	0.823405000	1.453871000
1	4.485692000	1.758784000	2.190833000	1	4.701477000	0.367380000	2.096255000
1	3.354878000	3.110502000	2.367626000	1	4.106078000	2.019256000	2.299335000
6	6.682233000	-0.199484000	2.433769000	6	6.202907000	-2.138495000	2.393708000
1	7.026484000	0.146935000	1.454450000	1	6.640602000	-1.986728000	1.403030000
1	7.561182000	-0.553650000	2.983553000	1	6.917012000	-2.726607000	2.978239000
1	6.270690000	0.658574000	2.970412000	1	6.102388000	-1.161712000	2.872134000

6	1.463020000	1.864700000	3.859231000	6	1.933982000	1.495168000	3.826920000
1	0.830673000	1.376751000	3.113233000	1	1.161332000	1.278607000	3.084060000
1	1.351518000	2.947314000	3.748904000	1	2.209759000	2.549453000	3.739015000
1	1.083399000	1.600823000	4.851805000	1	1.498095000	1.359642000	4.821625000
15	-1.001859000	-2.918009000	-2.323612000	15	-1.748064000	-2.379942000	-2.284442000
7	-0.962628000	-4.452802000	-1.584382000	7	-2.183742000	-3.838556000	-1.557068000
7	-2.406925000	-2.997632000	-3.312179000	7	-3.066750000	-1.938250000	-3.265546000
7	-0.780368000	-1.757054000	-1.343326000	7	-1.173688000	-1.361320000	-1.255385000
7	0.000000000	-3.120077000	-3.736531000	7	-0.824512000	-2.820965000	-3.666962000
6	-0.532354000	-4.601346000	-0.210815000	6	-1.855625000	-4.140942000	-0.176674000
1	0.444434000	-5.109078000	-0.159287000	1	-1.063289000	-4.903162000	-0.129989000
1	-0.373078000	-3.590045000	0.169814000	1	-1.430027000	-3.230085000	0.248848000
6	-1.524260000	-5.339369000	0.679162000	6	-3.041644000	-4.603787000	0.657990000
1	-1.149131000	-5.373967000	1.706353000	1	-2.721454000	-4.786683000	1.687529000
1	-2.492894000	-4.834200000	0.690955000	1	-3.831700000	-3.850284000	0.680579000
1	-1.686397000	-6.374025000	0.357790000	1	-3.475898000	-5.536991000	0.286438000
6	-3.792294000	-2.830933000	-2.863648000	6	-4.408414000	-1.505743000	-2.843778000
6	-4.705455000	-3.753168000	-3.679770000	6	-5.473139000	-2.256680000	-3.650887000
1	-4.382350000	-4.794439000	-3.587187000	1	-5.359960000	-3.338253000	-3.535676000
1	-5.734636000	-3.680735000	-3.314288000	1	-6.470989000	-1.981360000	-3.297436000
1	-4.716004000	-3.492511000	-4.742267000	1	-5.429411000	-2.019737000	-4.717552000
6	1.462768000	-2.931294000	-3.687137000	6	0.610598000	-3.166086000	-3.622611000
6	-3.930537000	-3.213531000	-1.392459000	6	-4.636345000	-1.799913000	-1.364949000
1	-3.262289000	-2.618428000	-0.767004000	1	-3.857880000	-1.352285000	-0.744428000
1	-4.959273000	-3.035580000	-1.063931000	1	-5.599646000	-1.382927000	-1.057697000
1	-3.697611000	-4.269417000	-1.240550000	1	-4.655100000	-2.873622000	-1.174481000
6	-0.687407000	-2.523211000	-4.865705000	6	-1.278523000	-2.043726000	-4.806179000
1	-0.640561000	-1.422346000	-4.853508000	1	-0.885428000	-1.015656000	-4.794373000
1	-0.264592000	-2.866678000	-5.815401000	1	-0.973735000	-2.510648000	-5.746648000
6	-4.235507000	-1.375049000	-3.039284000	6	-4.559900000	0.000000000	-3.074214000
1	-4.156122000	-1.053772000	-4.082764000	1	-4.401108000	0.267796000	-4.122888000
1	-5.277122000	-1.238212000	-2.728362000	1	-5.563616000	0.338228000	-2.796653000
1	-3.598957000	-0.726376000	-2.435516000	1	-3.829008000	0.540857000	-2.471888000
6	-2.130667000	-2.970573000	-4.729168000	6	-2.788406000	-2.021383000	-4.683809000
1	-2.264829000	-3.965700000	-5.188066000	1	-3.217477000	-2.934134000	-5.127352000
1	-2.790819000	-2.274204000	-5.260687000	1	-3.203424000	-1.164068000	-5.225032000
6	2.093807000	-3.764420000	-4.809355000	6	0.896367000	-4.186802000	-4.729599000
1	1.781552000	-3.426733000	-5.802074000	1	0.718349000	-3.778272000	-5.728171000
1	3.185253000	-3.687681000	-4.769947000	1	1.943868000	-4.500810000	-4.692810000
1	1.816550000	-4.817233000	-4.705951000	1	0.266965000	-5.072125000	-4.608184000
6	-1.312281000	-5.648258000	-2.319187000	6	-2.860732000	-4.864658000	-2.330882000
1	-2.197436000	-6.124641000	-1.865798000	1	-3.875132000	-5.020934000	-1.932982000
1	-1.619018000	-5.342949000	-3.320829000	1	-2.990731000	-4.485147000	-3.345689000

6	2.020414000	-3.439023000	-2.358489000	6	0.967192000	-3.810072000	-2.285314000
1	1.642977000	-2.853007000	-1.518221000	1	0.823405000	-3.117133000	-1.453871000
1	1.759363000	-4.485568000	-2.190862000	1	0.367380000	-4.701477000	-2.096255000
1	3.110916000	-3.354602000	-2.367940000	1	2.019256000	-4.106078000	-2.299335000
6	-0.199140000	-6.682471000	-2.433676000	6	-2.138495000	-6.202907000	-2.393708000
1	0.147390000	-7.026685000	-1.454384000	1	-1.986728000	-6.640602000	-1.403030000
1	-0.553381000	-7.561441000	-2.983378000	1	-2.726607000	-6.917012000	-2.978239000
1	0.658857000	-6.270964000	-2.970443000	1	-1.161712000	-6.102388000	-2.872134000
6	1.864652000	-1.463005000	-3.859515000	6	1.495168000	-1.933982000	-3.826920000
1	1.376892000	-0.830686000	-3.113371000	1	1.278607000	-1.161332000	-3.084060000
1	2.947291000	-1.351391000	-3.749561000	1	2.549453000	-2.209759000	-3.739015000
1	1.600398000	-1.083445000	-4.852013000	1	1.359642000	-1.498095000	-4.821625000

Table S10. Cartesian coordinates for the optimized geometries of **2-Ce^{Li}** (1) and **2-Ce^{Li}** (2).

2-Ce^{Li} (1)				2-Ce^{Li} (2)			
58	0.320527000	-0.008360000	0.043575000	58	-0.308091000	0.030608000	-0.009127000
15	2.248049000	3.276419000	-0.353303000	15	-2.087460000	3.400175000	0.076355000
7	1.426509000	1.966847000	-0.315025000	7	-1.401290000	2.033558000	-0.155137000
7	3.553190000	3.220156000	-1.444357000	7	-3.399406000	3.672732000	-0.960495000
6	3.919831000	1.968055000	-2.075988000	7	-2.669369000	3.835265000	1.651589000
1	3.098575000	1.271108000	-1.899314000	7	-1.188233000	4.850749000	-0.011622000
1	4.806187000	1.541291000	-1.577954000	6	-3.420387000	2.893455000	2.504831000
6	4.200861000	2.080800000	-3.567600000	6	-0.303389000	5.258757000	-1.110416000
1	5.064746000	2.718578000	-3.777397000	6	-1.652825000	4.640485000	2.303436000
1	3.340682000	2.490834000	-4.103083000	1	-0.817945000	4.031115000	2.684204000
1	4.421096000	1.092591000	-3.984671000	1	-2.071098000	5.200542000	3.144544000
6	4.585187000	4.245295000	-1.410032000	6	-1.144343000	5.588477000	1.231583000
1	5.560014000	3.745495000	-1.506561000	1	-1.777237000	6.489428000	1.187079000
1	4.584044000	4.710198000	-0.418809000	1	-0.125946000	5.915615000	1.473738000
6	4.462798000	5.338493000	-2.463325000	6	-3.965411000	2.596974000	-1.748573000
1	5.297672000	6.043103000	-2.378396000	1	-4.936770000	2.281415000	-1.336023000
1	3.534361000	5.893553000	-2.319043000	1	-3.290672000	1.746048000	-1.636185000
1	4.467262000	4.934534000	-3.478686000	6	-4.138344000	2.928664000	-3.224345000
7	2.887500000	3.922961000	1.095942000	1	-3.190860000	3.232286000	-3.676595000
7	1.500383000	4.794814000	-0.725833000	1	-4.863570000	3.730696000	-3.393071000
6	3.690052000	3.198604000	2.088666000	1	-4.502411000	2.048588000	-3.763498000
6	0.502233000	4.925551000	-1.808380000	6	-4.057197000	4.964767000	-1.009838000
6	2.403569000	5.247785000	1.411252000	1	-4.015239000	5.356598000	-2.037645000
1	3.169116000	6.015690000	1.215483000	1	-3.470599000	5.657764000	-0.404529000
1	2.113977000	5.333587000	2.465536000	6	-5.502883000	4.979736000	-0.532549000
6	1.193491000	5.472125000	0.522393000	1	-5.929888000	5.979756000	-0.659365000
1	0.294514000	5.063551000	1.011254000	1	-5.568348000	4.718879000	0.525850000

1	1.031052000	6.540846000	0.359432000	1	-6.132238000	4.283531000	-1.095041000
6	4.435244000	2.039845000	1.428805000	6	-4.360562000	2.044975000	1.651086000
1	3.747039000	1.345948000	0.941404000	1	-5.058259000	2.666599000	1.088574000
1	4.994705000	1.485200000	2.187421000	1	-4.940978000	1.382416000	2.299213000
1	5.146499000	2.401652000	0.682365000	1	-3.806642000	1.423686000	0.944536000
6	2.783225000	2.650602000	3.194547000	6	-4.274962000	3.699257000	3.488698000
1	2.238803000	3.454344000	3.699998000	1	-3.668498000	4.275075000	4.193243000
1	3.357737000	2.110590000	3.954592000	1	-4.903769000	3.027059000	4.080413000
1	2.048862000	1.968691000	2.762367000	1	-4.924985000	4.394722000	2.951292000
6	4.731845000	4.142486000	2.698197000	6	-2.491591000	1.959680000	3.289539000
1	5.375396000	4.568432000	1.922972000	1	-1.835417000	1.417259000	2.604792000
1	5.366779000	3.592923000	3.399188000	1	-3.072985000	1.231029000	3.862529000
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6	-0.878932000	4.426262000	-1.373161000	6	-0.775119000	4.655518000	-2.431023000
1	-0.808501000	3.391783000	-1.029501000	1	-0.824209000	3.566988000	-2.370146000
1	-1.584173000	4.475759000	-2.208820000	1	-0.071433000	4.925110000	-3.224491000
1	-1.292380000	5.033954000	-0.563608000	1	-1.762376000	5.030910000	-2.706257000
6	0.950164000	4.129590000	-3.032567000	6	-0.336989000	6.783766000	-1.252970000
1	1.922601000	4.468382000	-3.390805000	1	-1.359903000	7.135984000	-1.414531000
1	0.218219000	4.261390000	-3.835427000	1	0.266878000	7.090825000	-2.111916000
1	1.019603000	3.064073000	-2.805151000	1	0.064892000	7.294085000	-0.373426000
6	0.401960000	6.398621000	-2.216976000	6	1.130550000	4.794183000	-0.836093000
1	-0.008315000	7.026311000	-1.421351000	1	1.509582000	5.202254000	0.105631000
1	-0.262607000	6.500890000	-3.080188000	1	1.810668000	5.114558000	-1.632805000
1	1.382953000	6.793783000	-2.493496000	1	1.158260000	3.704585000	-0.769894000
15	-2.639873000	0.367623000	2.597261000	3	2.665095000	-0.335562000	0.186023000
7	-1.670783000	0.135866000	1.416677000	7	1.632920000	-0.208334000	-1.450724000
7	-1.978319000	-0.107308000	4.087932000	15	2.487124000	-0.299468000	-2.740256000
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6	-1.785695000	0.652854000	6.472565000	6	4.106885000	-2.297624000	-3.153170000
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1	-1.017087000	-0.062619000	6.775425000	1	4.113821000	-2.788531000	-2.166182000
1	-2.401040000	0.857875000	7.354395000	6	4.991260000	-1.071342000	-3.129414000
7	-4.226858000	-0.337830000	2.341088000	1	5.901446000	-1.262178000	-2.549726000
7	-3.329175000	1.884078000	2.976797000	1	5.300292000	-0.818241000	-4.155548000
6	-4.496827000	-1.794720000	2.387103000	6	4.851902000	1.254255000	-2.234855000
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1	1.081652000	-7.121418000	1.416710000	1	-3.682289000	-0.466562000	-3.661443000
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1	1.072010000	1.347409000	-5.043558000	1	1.062285000	-3.572469000	4.233648000
1	0.080238000	0.270168000	-6.026144000	1	-0.532281000	-3.177535000	4.881542000
1	0.788476000	-0.312318000	-4.514936000	1	0.897333000	-2.963413000	5.887169000

Table S11. Cartesian coordinates for the optimized geometries of **2-Ce^{Na}** and **2-Ce^{K}**.

2-Ce^{Na}				2-Ce^{K}			
58	-0.284704000	-0.031760000	-0.030847000	58	-0.199123000	-0.016025000	-0.084211000
11	3.069606000	-0.123309000	0.021435000	19	3.340782000	0.962276000	0.359484000
15	2.366752000	-0.431273000	2.855980000	15	2.142409000	-0.598066000	2.998435000
7	1.381134000	-0.341328000	1.677524000	7	1.354649000	-0.216182000	1.732570000
7	3.947878000	0.272698000	2.510779000	7	3.531998000	0.448815000	3.325353000
7	3.094761000	-1.929338000	3.314557000	7	3.155048000	-1.990650000	3.067544000
7	1.790280000	0.203725000	4.316622000	7	1.195696000	-0.737866000	4.401134000
6	5.016494000	-0.566968000	3.029445000	6	4.675766000	-0.334088000	3.761583000
1	5.285530000	-0.313939000	4.065730000	1	4.679068000	-0.516599000	4.847363000
1	5.924529000	-0.470350000	2.426768000	1	5.617785000	0.162177000	3.508555000
6	4.496932000	-1.989072000	2.960043000	6	4.557729000	-1.644905000	3.020200000
1	4.659846000	-2.394194000	1.948254000	1	4.931833000	-1.522598000	1.988451000
1	5.054450000	-2.625857000	3.653661000	1	5.174903000	-2.414310000	3.494429000
6	4.214242000	1.734578000	2.500802000	6	3.422327000	1.806184000	3.910220000
6	3.057450000	2.486887000	1.847423000	6	2.268369000	2.570279000	3.269038000
1	2.921907000	2.230151000	0.791966000	1	2.451395000	2.786315000	2.212604000
1	3.261924000	3.559876000	1.888642000	1	2.146776000	3.533214000	3.772109000
1	2.107837000	2.304282000	2.350385000	1	1.323750000	2.031650000	3.327178000
6	5.479747000	1.994933000	1.674442000	6	4.714977000	2.579746000	3.618273000
1	6.385539000	1.636522000	2.170053000	1	5.566733000	2.210997000	4.195200000
1	5.603435000	3.069417000	1.514582000	1	4.582069000	3.633403000	3.878285000
1	5.421462000	1.517300000	0.689664000	1	4.980046000	2.530465000	2.556009000
6	4.424049000	2.318564000	3.902810000	6	3.209231000	1.791383000	5.429099000
1	3.502035000	2.275555000	4.481675000	1	2.235928000	1.372369000	5.680573000
1	4.727240000	3.367177000	3.828632000	1	3.251099000	2.810385000	5.825864000
1	5.207946000	1.795060000	4.456599000	1	3.979194000	1.211328000	5.944837000
6	2.340501000	-3.203467000	3.245774000	6	2.783501000	-3.331942000	2.567758000
6	2.301815000	-3.761837000	1.819257000	6	3.397447000	-3.591642000	1.188957000
1	1.810325000	-3.050116000	1.152556000	1	3.064733000	-2.833830000	0.474977000
1	1.734641000	-4.696594000	1.791785000	1	3.080633000	-4.566452000	0.809811000
1	3.301505000	-3.983057000	1.432477000	1	4.491278000	-3.593250000	1.214463000
6	0.902540000	-2.990798000	3.713741000	6	1.269529000	-3.483373000	2.452550000

1	0.861422000	-2.594083000	4.728668000	1	0.769326000	-3.258708000	3.395699000
1	0.377960000	-3.950064000	3.705707000	1	1.041111000	-4.518644000	2.186057000
1	0.368076000	-2.308760000	3.050931000	1	0.846464000	-2.835083000	1.684413000
6	3.006596000	-4.219946000	4.176699000	6	3.296522000	-4.382146000	3.560163000
1	3.997084000	-4.522766000	3.825653000	1	4.384528000	-4.357304000	3.669279000
1	2.396701000	-5.125735000	4.234556000	1	3.031107000	-5.387469000	3.219637000
1	3.110271000	-3.813338000	5.186751000	1	2.852858000	-4.228603000	4.547079000
6	0.411321000	0.662542000	4.416091000	6	-0.209266000	-0.356127000	4.376897000
1	-0.223764000	-0.114589000	4.867614000	1	-0.838912000	-1.248660000	4.490741000
1	0.049123000	0.795185000	3.395087000	1	-0.414965000	0.033843000	3.378417000
6	0.259729000	1.958049000	5.197088000	6	-0.595906000	0.672540000	5.429747000
1	-0.776376000	2.302057000	5.145919000	1	-1.665727000	0.887049000	5.362522000
1	0.893275000	2.746942000	4.782592000	1	-0.060785000	1.615283000	5.289180000
1	0.510394000	1.843673000	6.256013000	1	-0.399937000	0.323218000	6.448409000
6	2.537680000	0.088306000	5.560432000	6	1.703530000	-1.294802000	5.646395000
1	2.651341000	1.085361000	6.005914000	1	1.791798000	-0.512453000	6.413562000
1	3.547394000	-0.247469000	5.320713000	1	2.715804000	-1.655618000	5.455595000
6	1.948668000	-0.845319000	6.608590000	6	0.874519000	-2.435874000	6.222457000
1	0.912168000	-0.595011000	6.850148000	1	-0.131875000	-2.117572000	6.506171000
1	2.526164000	-0.769227000	7.535242000	1	1.358901000	-2.819393000	7.125614000
1	1.980077000	-1.885336000	6.281020000	1	0.775535000	-3.265009000	5.518387000
15	2.448131000	0.214616000	-2.855877000	15	2.470827000	0.985819000	-2.802184000
7	1.457512000	0.067991000	-1.685539000	7	1.518975000	0.628420000	-1.645748000
7	4.076172000	-0.366612000	-2.471907000	7	4.148505000	0.519931000	-2.561908000
7	3.085504000	1.741806000	-3.344163000	7	2.960373000	2.620297000	-3.110381000
7	1.904016000	-0.447096000	-4.314419000	7	1.951174000	0.471163000	-4.332180000
6	5.084122000	0.605818000	-2.856118000	6	5.066941000	1.591349000	-2.886718000
1	5.442759000	0.452319000	-3.884266000	1	5.391821000	1.566705000	-3.937776000
1	5.957466000	0.563561000	-2.193635000	1	5.973192000	1.547320000	-2.268984000
6	4.396548000	1.947599000	-2.759687000	6	4.299726000	2.868350000	-2.623413000
1	4.349763000	2.274993000	-1.705998000	1	4.330206000	3.116382000	-1.544255000
1	4.958081000	2.705580000	-3.311002000	1	4.763887000	3.705993000	-3.150098000
6	4.520173000	-1.782929000	-2.435563000	6	4.694044000	-0.856036000	-2.603666000
6	3.330676000	-2.737265000	-2.483011000	6	3.577939000	-1.888908000	-2.728439000
1	3.667454000	-3.752737000	-2.257393000	1	3.987781000	-2.891078000	-2.576106000
1	2.864341000	-2.751533000	-3.469131000	1	3.116643000	-1.863509000	-3.717352000
1	2.561178000	-2.466406000	-1.756700000	1	2.792493000	-1.722426000	-1.988641000
6	5.277418000	-2.022416000	-1.121822000	6	5.459769000	-1.125143000	-1.300463000
1	6.054953000	-1.271163000	-0.954895000	1	6.181662000	-0.331134000	-1.082459000
1	5.764878000	-3.002104000	-1.125982000	1	6.019164000	-2.063595000	-1.361360000
1	4.600933000	-2.019993000	-0.260241000	1	4.774651000	-1.226293000	-0.453626000
6	5.469660000	-2.124176000	-3.591011000	6	5.668587000	-1.046900000	-3.772844000
1	5.027798000	-1.882928000	-4.559239000	1	5.204541000	-0.787621000	-4.726421000

1	5.686918000	-3.195986000	-3.581038000	1	5.977108000	-2.094808000	-3.825567000
1	6.425826000	-1.599464000	-3.511705000	1	6.576419000	-0.447184000	-3.660901000
6	2.232530000	2.947852000	-3.486195000	6	2.004595000	3.749428000	-3.025895000
6	1.971016000	3.618642000	-2.136061000	6	1.701300000	4.129374000	-1.573554000
1	1.441795000	2.935411000	-1.467912000	1	1.223379000	3.292783000	-1.058898000
1	1.346846000	4.507089000	-2.267831000	1	1.017532000	4.982126000	-1.533930000
1	2.895824000	3.946005000	-1.650931000	1	2.605522000	4.421811000	-1.028132000
6	0.890120000	2.576878000	-4.106291000	6	0.696453000	3.373571000	-3.713172000
1	1.014887000	2.091043000	-5.074422000	1	0.862466000	3.085670000	-4.752353000
1	0.299033000	3.485868000	-4.248754000	1	0.018739000	4.231843000	-3.693617000
1	0.324735000	1.910045000	-3.454550000	1	0.204987000	2.547054000	-3.199077000
6	2.933820000	3.930534000	-4.428781000	6	2.597726000	4.954353000	-3.761683000
1	3.845987000	4.352118000	-3.997748000	1	3.455497000	5.388281000	-3.240237000
1	2.269186000	4.770595000	-4.648760000	1	1.844112000	5.742103000	-3.844667000
1	3.191530000	3.442231000	-5.372813000	1	2.911054000	4.674804000	-4.771745000
6	0.766918000	-1.361871000	-4.303594000	6	0.899980000	-0.533009000	-4.432516000
1	0.628483000	-1.724588000	-3.283283000	1	0.772260000	-0.990008000	-3.449282000
1	1.025739000	-2.236252000	-4.918711000	1	1.243562000	-1.330188000	-5.108778000
6	-0.545545000	-0.759227000	-4.781739000	6	-0.447730000	-0.001893000	-4.895770000
1	-1.324808000	-1.527593000	-4.798893000	1	-1.166894000	-0.822670000	-4.971954000
1	-0.470922000	-0.332600000	-5.784135000	1	-0.394534000	0.490453000	-5.868742000
1	-0.875809000	0.030231000	-4.104661000	1	-0.843201000	0.718491000	-4.178600000
6	2.765340000	-0.497179000	-5.482381000	6	2.816118000	0.619711000	-5.488269000
1	3.208512000	-1.502899000	-5.577897000	1	3.349132000	-0.326229000	-5.684943000
1	3.587631000	0.202780000	-5.317076000	1	3.571952000	1.368472000	-5.242100000
6	2.088426000	-0.154850000	-6.801636000	6	2.116235000	1.044318000	-6.771173000
1	1.308140000	-0.874257000	-7.061124000	1	1.417717000	0.284788000	-7.129835000
1	2.827354000	-0.172338000	-7.608931000	1	2.858364000	1.200718000	-7.560486000
1	1.638559000	0.840318000	-6.776666000	1	1.564150000	1.977301000	-6.634556000
15	-2.578546000	-3.093188000	-0.215505000	15	-2.050925000	-3.320357000	-0.766395000
7	-1.694131000	-1.826854000	-0.270568000	7	-1.285238000	-1.989953000	-0.581337000
7	-3.252785000	-3.629953000	1.291161000	7	-2.839599000	-4.092167000	0.575815000
7	-1.904932000	-4.640555000	-0.487567000	7	-1.209896000	-4.764644000	-1.125989000
7	-3.893711000	-3.037497000	-1.284226000	7	-3.243715000	-3.246526000	-1.972755000
6	-2.408690000	-4.682556000	1.825752000	6	-2.003332000	-5.169244000	1.070172000
1	-2.941850000	-5.274344000	2.575126000	1	-2.591781000	-5.894657000	1.639104000
1	-1.493476000	-4.287838000	2.294064000	1	-1.194918000	-4.806564000	1.722738000
6	-2.038416000	-5.544639000	0.632280000	6	-1.412717000	-5.824317000	-0.165394000
1	-1.104315000	-6.082685000	0.833530000	1	-0.471538000	-6.326305000	0.089643000
1	-2.820004000	-6.300586000	0.450897000	1	-2.099120000	-6.595897000	-0.551686000
6	-3.837837000	-2.687046000	2.265217000	6	-3.590608000	-3.322008000	1.585850000
6	-4.635731000	-1.609647000	1.533213000	6	-4.406212000	-2.227789000	0.900916000
1	-5.101789000	-0.942609000	2.263978000	1	-4.995540000	-1.689896000	1.648487000

1	-5.425286000	-2.047045000	0.920296000	1	-5.093362000	-2.647776000	0.164733000
1	-3.993091000	-1.006188000	0.889205000	1	-3.760454000	-1.504800000	0.398767000
6	-2.766309000	-2.007946000	3.126419000	6	-2.662090000	-2.675585000	2.620200000
1	-2.042585000	-1.494893000	2.489356000	1	-1.927555000	-2.041620000	2.119532000
1	-2.224861000	-2.727281000	3.747431000	1	-2.122245000	-3.425233000	3.206683000
1	-3.221150000	-1.274077000	3.799112000	1	-3.234821000	-2.062335000	3.323076000
6	-4.805037000	-3.455197000	3.171631000	6	-4.568830000	-4.261008000	2.299081000
1	-5.325774000	-2.761775000	3.838877000	1	-5.213816000	-3.688085000	2.971985000
1	-4.293438000	-4.185902000	3.804146000	1	-4.058728000	-5.013193000	2.907072000
1	-5.552321000	-3.984414000	2.574178000	1	-5.203215000	-4.779331000	1.574746000
6	-1.074112000	-5.040942000	-1.629314000	6	-0.228508000	-4.961381000	-2.199691000
6	0.408769000	-4.913117000	-1.266306000	6	1.187677000	-4.805265000	-1.637347000
1	0.635093000	-3.875378000	-1.013443000	1	1.311350000	-3.800576000	-1.228731000
1	1.050368000	-5.221657000	-2.098829000	1	1.945461000	-4.967879000	-2.411484000
1	0.664696000	-5.536092000	-0.403996000	1	1.376702000	-5.524810000	-0.834463000
6	-1.363588000	-4.160065000	-2.842377000	6	-0.434562000	-3.940862000	-3.316311000
1	-2.388656000	-4.295250000	-3.191953000	1	-1.400710000	-4.081340000	-3.804463000
1	-0.683342000	-4.428945000	-3.656375000	1	0.352989000	-4.059794000	-4.066706000
1	-1.219045000	-3.104282000	-2.604666000	1	-0.392989000	-2.921554000	-2.928277000
6	-1.390497000	-6.490322000	-2.012262000	6	-0.394340000	-6.360283000	-2.802824000
1	-1.134742000	-7.196334000	-1.217311000	1	-0.182479000	-7.153614000	-2.080613000
1	-0.817346000	-6.776156000	-2.899272000	1	0.296660000	-6.489388000	-3.641170000
1	-2.453182000	-6.606984000	-2.243353000	1	-1.411755000	-6.503109000	-3.178038000
6	-4.285323000	-1.798426000	-1.923341000	6	-3.703935000	-1.978045000	-2.498828000
1	-3.496230000	-1.077218000	-1.702929000	1	-2.976966000	-1.228870000	-2.178564000
1	-5.207449000	-1.400445000	-1.470999000	1	-4.666552000	-1.688427000	-2.048089000
6	-4.477909000	-1.907221000	-3.429573000	6	-3.843514000	-1.954397000	-4.014466000
1	-5.299344000	-2.577273000	-3.701662000	1	-4.645264000	-2.607390000	-4.372721000
1	-3.570588000	-2.269318000	-3.919547000	1	-2.915930000	-2.264547000	-4.502532000
1	-4.715406000	-0.923700000	-3.846761000	1	-4.079319000	-0.940604000	-4.351715000
6	-4.736930000	-4.199166000	-1.491834000	6	-3.957468000	-4.440153000	-2.385124000
1	-4.268936000	-5.043729000	-0.983645000	1	-3.441841000	-5.300682000	-1.956133000
1	-4.742083000	-4.460265000	-2.561254000	1	-3.870091000	-4.554955000	-3.476053000
6	-6.173441000	-4.056946000	-1.007658000	6	-5.428288000	-4.491897000	-1.994132000
1	-6.207402000	-3.918646000	0.075090000	1	-5.539820000	-4.515411000	-0.908271000
1	-6.743582000	-4.959533000	-1.250249000	1	-5.895873000	-5.394201000	-2.401595000
1	-6.686799000	-3.211869000	-1.476087000	1	-5.988361000	-3.633202000	-2.376775000
15	-2.257554000	3.244509000	0.193704000	15	-2.654111000	2.884827000	0.457513000
7	-1.426402000	1.942658000	0.199559000	7	-1.682688000	1.691102000	0.327644000
7	-3.083485000	3.756917000	-1.246242000	7	-3.454722000	3.533093000	-0.941526000
7	-1.493438000	4.771765000	0.317273000	7	-2.075508000	4.444051000	0.865337000
7	-3.446005000	3.272491000	1.407067000	7	-3.905219000	2.610284000	1.572758000
6	-2.291487000	4.778370000	-1.904272000	6	-2.737025000	4.712960000	-1.385374000

1	-2.897570000	5.357377000	-2.606316000	1	-3.359406000	5.332787000	-2.036616000
1	-1.435955000	4.358832000	-2.458792000	1	-1.813449000	4.464641000	-1.933401000
6	-1.790247000	5.662987000	-0.781007000	6	-2.391440000	5.459898000	-0.112491000
1	-0.901875000	6.220038000	-1.100316000	1	-1.544122000	6.134169000	-0.284476000
1	-2.563407000	6.402278000	-0.512453000	1	-3.246536000	6.080680000	0.203448000
6	-3.799406000	2.803921000	-2.116443000	6	-4.020807000	2.663097000	-1.990498000
6	-4.572557000	1.802925000	-1.261313000	6	-4.705105000	1.455965000	-1.352808000
1	-3.900153000	1.192367000	-0.655691000	1	-3.990444000	0.833566000	-0.810906000
1	-5.141683000	1.132020000	-1.910261000	1	-5.160507000	0.841566000	-2.134371000
1	-5.274143000	2.308626000	-0.596226000	1	-5.490938000	1.763362000	-0.661307000
6	-2.842650000	2.037582000	-3.035886000	6	-2.944317000	2.163896000	-2.958590000
1	-2.324227000	2.704086000	-3.731134000	1	-2.481858000	2.984535000	-3.514558000
1	-3.385333000	1.299309000	-3.634016000	1	-3.371338000	1.472866000	-3.691645000
1	-2.092094000	1.519287000	-2.435092000	1	-2.162655000	1.644678000	-2.399593000
6	-4.813424000	3.576557000	-2.966084000	6	-5.081490000	3.450167000	-2.766482000
1	-5.466294000	4.180852000	-2.330069000	1	-5.831109000	3.860930000	-2.084500000
1	-5.436063000	2.877718000	-3.532502000	1	-5.588432000	2.792872000	-3.479214000
1	-4.333841000	4.238731000	-3.692102000	1	-4.652921000	4.275832000	-3.341159000
6	-0.606200000	5.252030000	1.384166000	6	-1.292544000	4.827085000	2.045995000
6	0.834721000	5.324157000	0.866985000	6	0.166759000	5.064884000	1.642355000
1	1.169593000	4.331837000	0.561637000	1	0.591013000	4.145818000	1.234474000
1	1.509351000	5.700768000	1.643505000	1	0.767397000	5.380502000	2.501986000
1	0.924437000	5.992595000	0.005733000	1	0.252139000	5.845056000	0.880376000
6	-0.642942000	4.314895000	2.587108000	6	-1.337482000	3.732146000	3.108674000
1	-1.629416000	4.307841000	3.053034000	1	-2.348530000	3.602146000	3.497174000
1	0.084755000	4.654202000	3.329731000	1	-0.682951000	4.008497000	3.940630000
1	-0.398736000	3.290583000	2.296798000	1	-1.004040000	2.774236000	2.703200000
6	-1.047143000	6.645600000	1.847680000	6	-1.864350000	6.110757000	2.659291000
1	-0.973840000	7.388987000	1.048739000	1	-1.794407000	6.962461000	1.976708000
1	-0.410222000	6.986877000	2.669348000	1	-1.310142000	6.372967000	3.565594000
1	-2.080139000	6.629925000	2.205354000	1	-2.914748000	5.977732000	2.932244000
6	-3.826039000	2.063334000	2.108280000	6	-4.188536000	1.278516000	2.065295000
1	-3.107895000	1.297008000	1.810693000	1	-3.354681000	0.649673000	1.747640000
1	-4.814147000	1.711404000	1.773085000	1	-5.089972000	0.866231000	1.585216000
6	-3.834585000	2.197953000	3.624483000	6	-4.351739000	1.197690000	3.576478000
1	-4.574875000	2.921971000	3.978858000	1	-5.221727000	1.755552000	3.936526000
1	-2.855150000	2.507485000	3.998394000	1	-3.468115000	1.585632000	4.089576000
1	-4.081161000	1.235232000	4.082925000	1	-4.489618000	0.155784000	3.881864000
6	-4.219528000	4.471278000	1.669024000	6	-4.822244000	3.671603000	1.942119000
1	-3.790586000	5.279654000	1.075107000	1	-4.445983000	4.600688000	1.511589000
1	-4.087557000	4.770052000	2.720651000	1	-4.794574000	3.814896000	3.033506000
6	-5.708187000	4.371550000	1.364579000	6	-6.266939000	3.472356000	1.503989000
1	-5.877504000	4.196928000	0.299986000	1	-6.344923000	3.456572000	0.414953000

1	-6.209751000	5.305845000	1.636610000	1	-6.888406000	4.294002000	1.874452000
1	-6.193864000	3.566798000	1.924279000	1	-6.693353000	2.541831000	1.890379000

Table S12. Cartesian coordinates for the optimized geometries of **2-Ce^{Rb}** and **2-Ce^{K18c6}**.

2-Ce^{Rb}				2-Ce^{K18c6}			
58	-0.220951000	0.030364000	0.015016000	58	-3.402939000	0.092382000	-0.070130000
15	2.184160000	0.619259000	3.047957000	15	-5.767906000	2.995839000	-0.751544000
15	1.748797000	-2.333603000	-2.426072000	7	-4.631359000	2.053226000	-0.317552000
15	-0.915307000	3.504715000	-1.517684000	7	-6.682023000	2.685737000	-2.164645000
15	-3.520249000	-1.711218000	0.922824000	7	-7.233235000	3.131403000	0.181475000
7	1.335773000	0.162443000	1.846698000	7	-5.269901000	4.611963000	-0.959354000
7	1.157716000	-1.337075000	-1.414725000	6	-8.233466000	2.270517000	-0.423872000
7	-0.622507000	2.105764000	-0.928459000	1	-9.240404000	2.538887000	-0.090564000
7	-2.206971000	-0.963959000	0.601824000	1	-8.070741000	1.206567000	-0.191490000
7	3.695349000	1.392708000	2.668402000	6	-8.093117000	2.492180000	-1.919650000
7	3.030548000	-0.525439000	4.054328000	1	-8.485164000	1.626103000	-2.465461000
7	1.358815000	1.564442000	4.184598000	1	-8.682588000	3.372033000	-2.229310000
7	1.975638000	-4.006244000	-2.031529000	6	-7.209286000	3.190502000	1.655489000
7	3.485772000	-2.157735000	-2.725575000	6	-6.070784000	4.097469000	2.116666000
7	0.929655000	-2.408947000	-3.913275000	1	-5.104413000	3.691179000	1.813944000
7	0.359606000	4.487512000	-2.102451000	1	-6.082687000	4.167977000	3.209001000
7	-1.467564000	4.810484000	-0.512146000	1	-6.168282000	5.104471000	1.708216000
7	-2.019287000	3.476410000	-2.807868000	6	-7.015539000	1.812391000	2.296805000
7	-3.496846000	-3.178412000	1.799446000	1	-7.831684000	1.128500000	2.050903000
7	-4.451550000	-2.457953000	-0.338766000	1	-6.984191000	1.901748000	3.388224000
7	-4.646120000	-0.761126000	1.766759000	1	-6.076616000	1.368617000	1.958673000
6	4.805255000	0.906368000	3.456189000	6	-8.528451000	3.799023000	2.142904000
1	4.965295000	1.491560000	4.375231000	1	-8.710583000	4.761393000	1.656034000
1	5.745803000	0.941251000	2.891632000	1	-8.490454000	3.960765000	3.224743000
6	4.452972000	-0.522435000	3.817125000	1	-9.385240000	3.148674000	1.945542000
1	4.764306000	-1.209913000	3.003336000	6	-6.142771000	2.381015000	-3.495240000
1	5.007578000	-0.835205000	4.706118000	6	-4.725981000	2.933473000	-3.647389000
6	2.421958000	-1.797610000	4.490118000	1	-4.718484000	4.021635000	-3.556776000
6	0.979233000	-1.553553000	4.917247000	1	-4.341012000	2.665628000	-4.636065000
1	0.933127000	-0.830840000	5.734628000	1	-4.051876000	2.522541000	-2.892312000
1	0.535446000	-2.491989000	5.261143000	6	-7.023022000	3.044038000	-4.561092000
1	0.378122000	-1.184248000	4.084759000	1	-8.044901000	2.653987000	-4.553599000
6	3.189609000	-2.340082000	5.698684000	1	-6.610393000	2.859460000	-5.557758000
1	3.278684000	-1.574424000	6.474694000	1	-7.069819000	4.126036000	-4.405892000
1	4.193271000	-2.689729000	5.440274000	6	-6.114885000	0.867075000	-3.723277000
1	2.653210000	-3.193335000	6.122565000	1	-5.499424000	0.379358000	-2.963679000
6	2.434047000	-2.837527000	3.365101000	1	-5.709857000	0.623862000	-4.710913000

1	1.839904000	-2.471570000	2.525715000	1	-7.118080000	0.434308000	-3.665792000
1	2.001049000	-3.785472000	3.697390000	6	-3.991143000	5.066143000	-0.458244000
1	3.454884000	-3.056176000	3.028205000	1	-3.438853000	4.168503000	-0.171417000
6	3.865924000	2.697662000	1.996154000	1	-4.115619000	5.665845000	0.459357000
6	4.672025000	2.484236000	0.708376000	6	-3.183599000	5.874835000	-1.464762000
1	5.610586000	1.953576000	0.903030000	1	-3.683788000	6.805328000	-1.752173000
1	4.929503000	3.437685000	0.237608000	1	-2.996348000	5.298332000	-2.375001000
1	4.086449000	1.917531000	-0.020802000	1	-2.217433000	6.149902000	-1.030952000
6	4.628785000	3.680450000	2.893141000	6	-6.162044000	5.598692000	-1.532042000
1	4.132768000	3.798930000	3.859225000	1	-7.046547000	5.072736000	-1.894094000
1	4.670286000	4.663026000	2.415101000	1	-5.694724000	6.043335000	-2.425037000
1	5.660036000	3.365840000	3.077463000	6	-6.595892000	6.716366000	-0.592075000
6	2.522434000	3.326035000	1.633175000	1	-7.189378000	6.319685000	0.234272000
1	1.908512000	2.671388000	1.012604000	1	-7.211562000	7.444775000	-1.130652000
1	2.699551000	4.250328000	1.076352000	1	-5.742920000	7.257555000	-0.170592000
1	1.946828000	3.572748000	2.527202000	15	-5.283526000	-3.187171000	-0.879703000
6	-0.020911000	1.960694000	3.965663000	7	-4.614433000	-1.810805000	-0.721542000
1	-0.322749000	1.516894000	3.016244000	7	-4.625415000	-4.611951000	-0.123732000
1	-0.082145000	3.049714000	3.832941000	7	-6.816266000	-3.515123000	-0.172490000
6	-0.990470000	1.536865000	5.060020000	7	-5.484572000	-3.673947000	-2.505153000
1	-1.991601000	1.905902000	4.821375000	6	-6.780045000	-4.558397000	0.830559000
1	-0.722067000	1.943438000	6.040074000	1	-7.260847000	-5.479883000	0.464144000
1	-1.048218000	0.450563000	5.150475000	1	-7.301293000	-4.259676000	1.747545000
6	1.971433000	1.971115000	5.436027000	6	-5.313736000	-4.814076000	1.136033000
1	3.024782000	1.689716000	5.406369000	1	-4.969641000	-4.117831000	1.917110000
1	1.542887000	1.399110000	6.274080000	1	-5.171721000	-5.833556000	1.508217000
6	1.847734000	3.458229000	5.741338000	6	-7.956278000	-2.586289000	-0.174615000
1	2.246408000	4.071655000	4.929386000	6	-7.980797000	-1.780578000	-1.472028000
1	2.402346000	3.700923000	6.652905000	1	-7.071376000	-1.185992000	-1.579286000
1	0.810194000	3.761911000	5.902700000	1	-8.837965000	-1.099518000	-1.460294000
6	3.369814000	-4.368096000	-1.921001000	1	-8.069842000	-2.435621000	-2.340547000
1	3.533529000	-5.416263000	-2.188729000	6	-7.866225000	-1.617255000	1.006814000
1	3.767335000	-4.233738000	-0.897102000	1	-7.839068000	-2.147639000	1.963279000
6	4.107433000	-3.460991000	-2.878677000	1	-8.731240000	-0.945429000	1.029582000
1	5.171990000	-3.428435000	-2.626214000	1	-6.957952000	-1.018042000	0.923566000
1	4.026599000	-3.856330000	-3.902681000	6	-9.264232000	-3.379636000	-0.080789000
6	4.072324000	-1.071872000	-3.543798000	1	-9.360818000	-4.084835000	-0.910447000
6	3.376380000	0.250487000	-3.243978000	1	-10.115939000	-2.693812000	-0.120603000
1	2.301367000	0.205267000	-3.409954000	1	-9.343610000	-3.942147000	0.853705000
1	3.791326000	1.032492000	-3.885342000	6	-3.192942000	-4.942686000	-0.171856000
1	3.523209000	0.566879000	-2.208594000	6	-2.624656000	-4.581954000	-1.542458000
6	3.983242000	-1.341544000	-5.051188000	1	-3.159785000	-5.100471000	-2.341421000
1	4.469549000	-2.280664000	-5.328762000	1	-1.572890000	-4.879982000	-1.588984000

1	4.481989000	-0.542716000	-5.608480000	1	-2.682651000	-3.506947000	-1.723632000
1	2.944743000	-1.382209000	-5.377244000	6	-3.029386000	-6.455648000	0.017625000
6	5.553929000	-0.913308000	-3.175581000	1	-3.353402000	-6.788364000	1.007710000
1	5.686612000	-0.804483000	-2.093364000	1	-1.976573000	-6.737192000	-0.088542000
1	5.960514000	-0.015574000	-3.648952000	1	-3.608759000	-7.000920000	-0.732677000
1	6.165196000	-1.756181000	-3.507426000	6	-2.393083000	-4.207952000	0.908748000
6	1.030917000	-4.743300000	-1.164204000	1	-2.547191000	-3.129038000	0.832999000
6	-0.406277000	-4.392430000	-1.533341000	1	-1.323197000	-4.416921000	0.804112000
1	-0.612825000	-3.330565000	-1.390916000	1	-2.691657000	-4.524148000	1.912373000
1	-1.087851000	-4.954329000	-0.889269000	6	-4.860971000	-2.916830000	-3.569207000
1	-0.619614000	-4.656867000	-2.570541000	1	-3.967220000	-3.449434000	-3.939839000
6	1.258898000	-4.407325000	0.311263000	1	-4.509252000	-1.983342000	-3.125967000
1	2.281014000	-4.638390000	0.630028000	6	-5.780035000	-2.629589000	-4.748164000
1	0.586945000	-4.982929000	0.952600000	1	-6.679366000	-2.099769000	-4.425297000
1	1.061913000	-3.346583000	0.479225000	1	-6.089037000	-3.545909000	-5.261018000
6	1.221726000	-6.247110000	-1.382738000	1	-5.265881000	-2.003744000	-5.484617000
1	1.163063000	-6.495356000	-2.446592000	6	-5.897040000	-5.027561000	-2.834412000
1	0.432938000	-6.796870000	-0.862151000	1	-5.643951000	-5.679939000	-1.992615000
1	2.176457000	-6.612696000	-0.994233000	1	-5.285666000	-5.371697000	-3.682800000
6	-0.083681000	-1.417536000	-4.242937000	6	-7.373638000	-5.203233000	-3.166596000
1	-0.150690000	-0.736669000	-3.392319000	1	-7.983637000	-4.940427000	-2.300991000
1	-1.063467000	-1.906026000	-4.319193000	1	-7.585102000	-6.246932000	-3.427292000
6	0.193499000	-0.637066000	-5.520742000	1	-7.687772000	-4.576233000	-4.004480000
1	0.322708000	-1.291414000	-6.388648000	15	-2.475436000	0.086335000	3.684653000
1	1.089742000	-0.017894000	-5.432675000	7	-2.720242000	-0.056612000	2.175360000
1	-0.645926000	0.027404000	-5.740945000	7	-2.336218000	1.642536000	4.456711000
6	1.168802000	-3.455002000	-4.896799000	7	-3.649278000	-0.381773000	4.845650000
1	1.777913000	-4.221197000	-4.414203000	7	-1.065523000	-0.731301000	4.204332000
1	1.757211000	-3.072957000	-5.744542000	6	-4.153338000	0.717053000	5.640859000
6	-0.091453000	-4.111342000	-5.446353000	1	-3.793062000	0.655461000	6.681107000
1	0.187040000	-4.936041000	-6.109292000	1	-5.249276000	0.726744000	5.673591000
1	-0.704226000	-3.420118000	-6.030386000	6	-3.646467000	1.986784000	4.981635000
1	-0.717284000	-4.517454000	-4.648698000	1	-4.345078000	2.298119000	4.189906000
6	0.481047000	5.759929000	-1.427890000	1	-3.580515000	2.800036000	5.710729000
1	0.089894000	6.585552000	-2.045163000	6	-4.403121000	-1.641195000	4.838997000
1	1.525459000	5.996093000	-1.190928000	6	-3.544614000	-2.766143000	4.268761000
6	-0.328897000	5.633754000	-0.152207000	1	-3.230770000	-2.536736000	3.248815000
1	0.289083000	5.178519000	0.638486000	1	-4.125088000	-3.693782000	4.250142000
1	-0.649050000	6.619056000	0.197615000	1	-2.655297000	-2.930326000	4.881661000
6	-2.507484000	4.629580000	0.517854000	6	-5.670270000	-1.507982000	3.990451000
6	-3.593885000	3.688861000	0.003083000	1	-6.312349000	-0.696922000	4.347356000
1	-4.052674000	4.071967000	-0.909379000	1	-6.260078000	-2.431056000	4.015815000
1	-4.376140000	3.587973000	0.760357000	1	-5.401181000	-1.295541000	2.954213000

1	-3.194755000	2.693550000	-0.201607000	6	-4.772098000	-2.014912000	6.278544000
6	-3.157677000	5.985684000	0.810336000	1	-3.875895000	-2.080056000	6.903202000
1	-2.464661000	6.689678000	1.279244000	1	-5.270451000	-2.988885000	6.294394000
1	-3.998620000	5.857277000	1.498508000	1	-5.454387000	-1.292728000	6.735192000
1	-3.533789000	6.439195000	-0.110707000	6	-1.563590000	2.748664000	3.861735000
6	-1.924242000	4.051427000	1.809264000	6	-0.310085000	2.207717000	3.178617000
1	-1.419973000	3.107770000	1.594412000	1	0.308576000	1.638217000	3.875192000
1	-2.711952000	3.871278000	2.547375000	1	0.278830000	3.047221000	2.796765000
1	-1.199267000	4.731725000	2.266248000	1	-0.569615000	1.561736000	2.337900000
6	1.389756000	4.107456000	-3.073993000	6	-1.117603000	3.687846000	4.988460000
6	0.916205000	2.941992000	-3.939085000	1	-1.965061000	4.156789000	5.495835000
1	0.639986000	2.081134000	-3.326241000	1	-0.497186000	4.495507000	4.586039000
1	1.720836000	2.643902000	-4.617713000	1	-0.535652000	3.141253000	5.736159000
1	0.050065000	3.225918000	-4.539072000	6	-2.378122000	3.538134000	2.832269000
6	2.667425000	3.697079000	-2.334695000	1	-2.778518000	2.873892000	2.062429000
1	3.036609000	4.507012000	-1.698069000	1	-1.753321000	4.294325000	2.346117000
1	3.469429000	3.436326000	-3.033292000	1	-3.215906000	4.064436000	3.297425000
1	2.457063000	2.835093000	-1.698881000	6	-0.150673000	-1.280481000	3.233492000
6	1.688542000	5.291129000	-4.000883000	1	0.798728000	-0.714903000	3.228950000
1	0.780344000	5.621344000	-4.512942000	1	-0.614584000	-1.116465000	2.257328000
1	2.417854000	4.996424000	-4.761430000	6	0.153093000	-2.762621000	3.418101000
1	2.106269000	6.146329000	-3.462392000	1	0.662686000	-2.974853000	4.365025000
6	-2.842606000	2.313108000	-3.063115000	1	0.799280000	-3.118750000	2.607605000
1	-3.875928000	2.478216000	-2.719426000	1	-0.762812000	-3.355892000	3.389937000
1	-2.438828000	1.508101000	-2.445973000	6	-0.749847000	-0.879571000	5.606888000
6	-2.869042000	1.883637000	-4.522810000	1	-0.743238000	-1.946925000	5.883290000
1	-3.357262000	2.619554000	-5.169164000	1	-1.566113000	-0.431426000	6.175399000
1	-3.423445000	0.945838000	-4.626245000	6	0.567576000	-0.251125000	6.045920000
1	-1.856920000	1.722703000	-4.901977000	1	0.743031000	-0.442248000	7.109894000
6	-2.275727000	4.665447000	-3.598138000	1	1.422678000	-0.660356000	5.496065000
1	-2.077073000	4.446550000	-4.658661000	1	0.552993000	0.830859000	5.895809000
1	-1.542410000	5.419805000	-3.309266000	15	-0.228734000	0.420400000	-2.318244000
6	-3.674642000	5.252508000	-3.467029000	7	-1.440802000	0.230724000	-1.399758000
1	-4.454065000	4.527430000	-3.720094000	7	-0.344946000	0.355634000	-4.029825000
1	-3.789691000	6.104446000	-4.145017000	7	0.598493000	1.958636000	-2.436526000
1	-3.855338000	5.605870000	-2.449872000	7	1.040514000	-0.679334000	-1.981736000
6	-4.657118000	-1.802778000	-1.644861000	6	0.069094000	2.649459000	-3.600063000
6	-4.925649000	-0.313099000	-1.440779000	1	0.719653000	3.475794000	-3.901949000
1	-5.798271000	-0.149871000	-0.806421000	1	-0.939128000	3.057617000	-3.425743000
1	-5.115183000	0.158958000	-2.408977000	6	0.009398000	1.593487000	-4.687293000
1	-4.068626000	0.186709000	-0.985242000	1	-0.729283000	1.878628000	-5.444823000
6	-5.889484000	-2.416036000	-2.317282000	1	0.986090000	1.513777000	-5.194949000
1	-5.734275000	-3.460362000	-2.601946000	6	0.821006000	2.784849000	-1.235477000

1	-6.129181000	-1.866187000	-3.232313000	6	1.327527000	1.904836000	-0.095392000
1	-6.755218000	-2.367932000	-1.650902000	1	1.540149000	2.530949000	0.776146000
6	-3.442161000	-1.963135000	-2.565383000	1	0.575647000	1.168368000	0.195119000
1	-2.551168000	-1.558191000	-2.081377000	1	2.243219000	1.382242000	-0.378280000
1	-3.602147000	-1.432033000	-3.509204000	6	-0.448026000	3.509776000	-0.779925000
1	-3.251295000	-3.012366000	-2.810323000	1	-0.264845000	4.068508000	0.143656000
6	-4.174577000	-3.881534000	-0.359501000	1	-0.792787000	4.225170000	-1.530188000
1	-4.976487000	-4.431466000	-0.860250000	1	-1.250298000	2.791117000	-0.602376000
1	-3.231830000	-4.118264000	-0.875411000	6	1.910639000	3.816274000	-1.550708000
6	-4.082639000	-4.296945000	1.098123000	1	2.187617000	4.360954000	-0.641995000
1	-3.470330000	-5.202115000	1.193311000	1	2.800768000	3.317551000	-1.947663000
1	-5.085416000	-4.539848000	1.487187000	1	1.582406000	4.559496000	-2.282193000
6	-2.856486000	-3.412986000	3.099148000	6	-1.082756000	-0.655381000	-4.797017000
6	-1.487040000	-4.065902000	2.888096000	6	-1.085840000	-1.986190000	-4.050817000
1	-1.577023000	-5.004806000	2.332233000	1	-1.657469000	-2.724748000	-4.619724000
1	-1.002526000	-4.293960000	3.843807000	1	-0.068103000	-2.362746000	-3.922332000
1	-0.843111000	-3.392348000	2.319681000	1	-1.546723000	-1.883028000	-3.066650000
6	-2.666742000	-2.101699000	3.858308000	6	-0.386314000	-0.871279000	-6.144936000
1	-2.086719000	-1.385483000	3.272036000	1	-0.890088000	-1.666091000	-6.703146000
1	-2.132316000	-2.299112000	4.792208000	1	-0.401010000	0.026126000	-6.770037000
1	-3.627624000	-1.646035000	4.102523000	1	0.657075000	-1.166607000	-5.996439000
6	-3.739702000	-4.329011000	3.953282000	6	-2.528301000	-0.203496000	-5.023569000
1	-4.735390000	-3.896010000	4.085066000	1	-3.085709000	-0.941697000	-5.608962000
1	-3.293984000	-4.459626000	4.943845000	1	-3.028794000	-0.068007000	-4.063202000
1	-3.855544000	-5.323827000	3.514095000	1	-2.571716000	0.746673000	-5.565336000
6	-4.672209000	1.214984000	3.282729000	6	0.984731000	-1.507190000	-0.800829000
1	-5.689859000	1.072904000	3.659492000	1	0.006869000	-1.323015000	-0.348585000
1	-4.472991000	2.290932000	3.297692000	1	1.739116000	-1.182564000	-0.061573000
1	-3.983846000	0.733872000	3.982018000	6	1.158060000	-2.996992000	-1.063569000
6	-4.490846000	0.674099000	1.871316000	1	1.066570000	-3.555928000	-0.126237000
1	-5.187848000	1.194415000	1.195464000	1	0.391252000	-3.364924000	-1.748361000
1	-3.485413000	0.901913000	1.511978000	1	2.138288000	-3.235365000	-1.492362000
6	-5.869320000	-1.343109000	2.284676000	6	2.192556000	-0.793106000	-2.842805000
1	-5.926512000	-1.167138000	3.369929000	1	2.221498000	-1.789850000	-3.315967000
1	-5.799861000	-2.425204000	2.164512000	1	2.066675000	-0.080872000	-3.659616000
6	-7.154481000	-0.851357000	1.632591000	6	3.530156000	-0.537641000	-2.156193000
1	-7.184069000	-1.126609000	0.576297000	1	4.358436000	-0.666522000	-2.861765000
1	-7.267146000	0.234523000	1.705738000	1	3.574009000	0.481616000	-1.763925000
1	-8.022652000	-1.303002000	2.123516000	1	3.690408000	-1.229331000	-1.321393000
37	3.523549000	-1.081000000	0.294939000	19	6.319645000	-0.647496000	0.135156000
				8	10.519186000	-2.000637000	-0.264024000
				8	8.236998000	-2.155475000	1.591852000
				8	8.135997000	0.505773000	2.394219000

8	11.641101000	0.534143000	-1.229219000
6	11.522879000	2.882915000	-1.573512000
1	12.070767000	2.993717000	-0.628199000
1	11.856864000	3.683866000	-2.251763000
8	10.133575000	2.951692000	-1.379719000
6	8.967888000	-3.247661000	1.076982000
1	8.451112000	-3.535049000	0.159415000
1	8.928167000	-4.097286000	1.775883000
6	8.511403000	-1.843507000	2.938617000
1	9.592748000	-1.765692000	3.106443000
1	8.138462000	-2.637896000	3.604091000
6	9.900304000	4.152323000	0.772707000
1	10.973972000	4.125610000	1.016237000
1	9.513126000	5.107039000	1.143567000
6	10.418848000	-2.953390000	0.764791000
1	10.961910000	-2.603223000	1.656175000
1	10.893436000	-3.900527000	0.458622000
6	9.680594000	4.119129000	-0.730742000
1	8.607749000	4.163011000	-0.928985000
1	10.143315000	5.014013000	-1.178708000
6	11.861473000	-1.760344000	-0.612157000
1	12.335659000	-2.694572000	-0.952919000
1	12.425394000	-1.400555000	0.261438000
6	11.962823000	-0.742278000	-1.716078000
1	12.996341000	-0.754755000	-2.097747000
1	11.300071000	-1.021668000	-2.549396000
6	11.864276000	1.547405000	-2.178477000
1	11.251209000	1.380419000	-3.076973000
1	12.920636000	1.553732000	-2.490296000
6	7.811786000	-0.541894000	3.280737000
1	6.729668000	-0.673465000	3.207692000
1	8.048703000	-0.268756000	4.319961000
6	9.866725000	1.888745000	1.446216000
1	10.954018000	2.034412000	1.537611000
1	9.685775000	1.372650000	0.499992000
8	9.224029000	3.146803000	1.484394000
6	9.431549000	1.029622000	2.600420000
1	10.163180000	0.215094000	2.686030000
1	9.456550000	1.609275000	3.534440000
8	4.514673000	-0.669589000	2.366207000
8	4.748894000	-2.986244000	0.759665000
8	6.586489000	-3.163492000	-1.379664000
8	7.289354000	-0.688734000	-2.548041000

				8	6.880785000	1.748079000	-1.195365000
				8	5.050517000	1.707874000	0.958866000
				6	3.667640000	-1.790684000	2.508513000
				1	2.784472000	-1.676029000	1.868520000
				1	3.318500000	-1.879186000	3.547316000
				6	4.403635000	-3.042831000	2.126489000
				1	5.309856000	-3.169374000	2.738488000
				1	3.744079000	-3.901241000	2.317839000
				6	5.230750000	-4.214194000	0.273075000
				1	4.473967000	-5.000887000	0.407145000
				1	6.133629000	-4.517364000	0.824165000
				6	5.535576000	-4.087197000	-1.193720000
				1	5.820361000	-5.074944000	-1.586115000
				1	4.639489000	-3.752719000	-1.733626000
				6	6.943581000	-3.019780000	-2.736868000
				1	6.052618000	-2.798846000	-3.340212000
				1	7.388490000	-3.952656000	-3.114795000
				6	7.934807000	-1.896795000	-2.875177000
				1	8.801744000	-2.061602000	-2.220339000
				1	8.289315000	-1.869298000	-3.917154000
				6	8.085085000	0.455122000	-2.776191000
				1	8.449934000	0.459593000	-3.814734000
				1	8.952771000	0.468203000	-2.103310000
				6	7.242436000	1.680090000	-2.554820000
				1	7.825329000	2.567290000	-2.838334000
				1	6.344351000	1.633267000	-3.186703000
				6	5.990239000	2.806927000	-0.916925000
				1	5.042052000	2.658034000	-1.450408000
				1	6.417516000	3.763873000	-1.252358000
				6	5.747809000	2.869763000	0.564972000
				1	6.704226000	2.945199000	1.099134000
				1	5.145438000	3.762837000	0.787237000
				6	4.720115000	1.709890000	2.329106000
				1	4.179188000	2.630963000	2.590104000
				1	5.635407000	1.669355000	2.936343000
				6	3.821004000	0.540985000	2.616971000
				1	3.494851000	0.580052000	3.666097000
				1	2.927958000	0.596441000	1.982942000

Table S13. Cartesian coordinates for the optimized geometries of 2-Ce^{Cs} (1) and 2-Ce^{Cs} (2).

2-Ce^{Cs} (1)				2-Ce^{Cs} (2)			
58	-0.268438000	0.025801000	0.020715000	58	0.271143000	0.003455000	0.000699000

15	-3.431585000	-1.607574000	1.468011000	15	2.441663000	3.128353000	-0.617248000
15	-1.197139000	3.008828000	-2.240391000	15	2.521709000	-3.070617000	0.619442000
15	1.648994000	-2.710103000	-2.028114000	15	-2.032331000	-0.899053000	-3.020895000
15	2.139620000	1.437603000	2.767775000	15	-2.057539000	0.850695000	3.019216000
7	-0.881223000	1.755128000	-1.394184000	7	1.568316000	1.865133000	-0.452482000
7	1.114336000	-1.547193000	-1.174994000	7	1.619035000	-1.827666000	0.453588000
7	1.340897000	0.698337000	1.678239000	7	-1.316772000	-0.472746000	-1.730032000
7	-2.135285000	-0.906965000	1.001984000	7	-1.328726000	0.442657000	1.729887000
55	3.696258000	-0.938267000	0.430182000	55	-3.890178000	-0.041224000	-0.003474000
7	0.739024000	-3.045206000	-3.425856000	7	3.669513000	2.948245000	-1.779669000
6	-0.290741000	-2.118313000	-3.870977000	6	4.055468000	1.639777000	-2.263369000
1	-0.316941000	-1.299764000	-3.148873000	1	3.274902000	0.948924000	-1.938658000
1	-1.271288000	-2.607385000	-3.814760000	1	4.988357000	1.301679000	-1.785327000
6	-0.084083000	-1.568956000	-5.276296000	6	4.220430000	1.564145000	-3.774606000
1	0.813501000	-0.949413000	-5.343930000	1	4.419080000	0.531646000	-4.077927000
1	-0.935499000	-0.943945000	-5.559628000	1	5.054961000	2.171800000	-4.137903000
1	-0.000825000	-2.362485000	-6.025752000	1	3.314577000	1.898270000	-4.286819000
6	0.922694000	-4.252838000	-4.217616000	6	4.490834000	4.075552000	-2.177031000
1	1.543205000	-4.932974000	-3.631269000	1	4.036500000	4.978920000	-1.767808000
1	1.477991000	-4.039473000	-5.143350000	1	4.446274000	4.189403000	-3.271059000
6	-0.367688000	-4.971350000	-4.592523000	6	5.949044000	4.012472000	-1.742377000
1	-0.991313000	-4.386068000	-5.272923000	1	6.451530000	3.111304000	-2.106623000
1	-0.970745000	-5.211009000	-3.714105000	1	6.029787000	4.031826000	-0.653725000
1	-0.126136000	-5.909218000	-5.101699000	1	6.497524000	4.873852000	-2.137371000
7	-2.243000000	2.702765000	-3.551755000	7	3.743395000	-2.861952000	1.783301000
6	-2.594352000	1.339219000	-3.893999000	6	4.097132000	-1.544842000	2.268328000
1	-2.370035000	0.724642000	-3.020017000	1	3.301889000	-0.872361000	1.940795000
1	-1.948097000	0.974623000	-4.711795000	1	5.023536000	-1.185273000	1.793386000
6	-4.046253000	1.157907000	-4.310602000	6	4.254916000	-1.465211000	3.780121000
1	-4.283481000	1.707723000	-5.226272000	1	3.354762000	-1.819018000	4.289167000
1	-4.729469000	1.493287000	-3.526526000	1	4.429647000	-0.428480000	4.083759000
1	-4.247401000	0.100232000	-4.510108000	1	5.101321000	-2.054185000	4.146695000
6	-2.405481000	3.689297000	-4.608459000	6	4.590142000	-3.969767000	2.182151000
1	-2.359321000	3.164739000	-5.574602000	1	4.158530000	-4.883364000	1.771014000
1	-1.543397000	4.363043000	-4.592321000	1	4.545403000	-4.085490000	3.275977000
6	-3.676412000	4.525590000	-4.539347000	6	6.047585000	-3.871664000	1.751463000
1	-3.724015000	5.214306000	-5.390438000	1	6.615251000	-4.720219000	2.147091000
1	-3.682566000	5.118446000	-3.623374000	1	6.527608000	-2.959247000	2.117965000
1	-4.578682000	3.909829000	-4.555303000	1	6.131782000	-3.887945000	0.663012000
7	-4.593991000	-0.538618000	2.093083000	7	-1.046490000	-0.929087000	-4.407058000
6	-4.435523000	0.896626000	1.989108000	6	0.267900000	-0.304251000	-4.387238000
1	-5.090326000	1.304504000	1.203063000	1	1.042558000	-1.072864000	-4.502470000
1	-3.411574000	1.072924000	1.653508000	1	0.407431000	0.116141000	-3.389491000

6	-4.701570000	1.643858000	3.289339000	6	0.468230000	0.774980000	-5.442540000
1	-4.530186000	2.714969000	3.146096000	1	0.321088000	0.396795000	-6.459069000
1	-4.042618000	1.301086000	4.090266000	1	1.488561000	1.162951000	-5.386849000
1	-5.734525000	1.530363000	3.632434000	1	-0.212443000	1.617410000	-5.298374000
6	-5.840475000	-1.035554000	2.644761000	6	-1.445925000	-1.567707000	-5.651395000
1	-5.914948000	-0.748750000	3.705611000	1	-1.721610000	-0.818857000	-6.409989000
1	-5.791236000	-2.125181000	2.643083000	1	-2.345556000	-2.149515000	-5.445256000
6	-7.100435000	-0.576140000	1.922970000	6	-0.397312000	-2.497379000	-6.249389000
1	-7.199981000	0.513290000	1.912671000	1	-0.090610000	-3.266549000	-5.536900000
1	-7.986671000	-0.978940000	2.423832000	1	0.501385000	-1.965480000	-6.571351000
1	-7.114867000	-0.922658000	0.887378000	1	-0.810885000	-2.997644000	-7.130271000
7	2.972541000	0.574430000	4.030197000	7	-1.076258000	0.902390000	4.408079000
7	3.642376000	2.159920000	2.276599000	6	-1.494223000	1.529592000	5.652140000
6	4.403056000	0.569519000	3.849872000	1	-1.753357000	0.773338000	6.409225000
1	4.926577000	0.494757000	4.807162000	1	-2.407334000	2.089437000	5.444428000
6	4.739403000	1.885499000	3.175361000	6	-0.470257000	2.484026000	6.253850000
1	4.869762000	2.668699000	3.938591000	1	0.440612000	1.974051000	6.577087000
1	5.693476000	1.809311000	2.636903000	1	-0.898075000	2.972523000	7.134532000
6	2.373517000	-0.576386000	4.732403000	1	-0.181104000	3.261693000	5.543251000
6	3.110368000	-0.802783000	6.055551000	6	0.253231000	0.310462000	4.390507000
1	4.128941000	-1.175650000	5.914230000	1	1.008388000	1.097833000	4.508387000
1	2.576641000	-1.548296000	6.651152000	1	0.405308000	-0.105002000	3.392582000
1	3.158094000	0.124198000	6.634191000	6	0.477857000	-0.765018000	5.444758000
6	2.444551000	-1.851559000	3.884338000	1	-0.181784000	-1.623592000	5.298030000
1	2.023329000	-2.706813000	4.420327000	1	0.319418000	-0.391967000	6.461481000
1	3.481272000	-2.111286000	3.637333000	1	1.507500000	-1.127849000	5.390651000
6	0.913658000	-0.274858000	5.051217000	7	-2.938146000	2.341835000	3.122128000
1	0.828943000	0.623862000	5.665560000	7	-3.529203000	-0.052566000	3.381252000
1	0.478938000	-1.111299000	5.604419000	6	-4.358617000	2.151417000	3.299322000
1	0.329032000	-0.136197000	4.140134000	1	-4.911471000	2.141192000	2.340343000
6	3.798667000	3.295819000	1.345487000	1	-4.799275000	2.949005000	3.905980000
6	4.540007000	4.458829000	2.016621000	6	-4.515399000	0.817035000	3.995315000
1	4.038259000	4.769455000	2.936021000	1	-4.363031000	0.941517000	5.078021000
1	4.565324000	5.319150000	1.342078000	1	-5.531027000	0.433400000	3.854832000
1	5.576151000	4.209470000	2.262960000	6	-2.512992000	3.561412000	2.404931000
6	4.616084000	2.830200000	0.133613000	6	-3.194813000	4.778119000	3.037581000
1	5.558149000	2.363161000	0.442123000	1	-4.272809000	4.801729000	2.853523000
1	4.868839000	3.668586000	-0.522601000	1	-2.776181000	5.695024000	2.614095000
6	2.446230000	3.811709000	0.858092000	1	-3.028240000	4.797211000	4.118606000
1	1.842722000	3.022699000	0.406332000	6	-2.881680000	3.491034000	0.918673000
1	2.607533000	4.590852000	0.108171000	1	-2.315886000	2.687777000	0.441262000
1	1.870883000	4.243995000	1.678009000	1	-2.637002000	4.426293000	0.409275000
7	-3.428455000	-2.860726000	2.663671000	1	-3.956157000	3.323882000	0.777200000

7	-4.273899000	-2.630974000	0.381895000	6	-1.004446000	3.747392000	2.528530000
6	-3.463567000	-4.152714000	2.007765000	1	-0.710542000	3.854143000	3.574543000
1	-3.818111000	-4.930953000	2.689560000	1	-0.709241000	4.654399000	1.994079000
1	-2.473704000	-4.459616000	1.635807000	1	-0.457179000	2.910418000	2.092012000
6	-4.424333000	-3.991840000	0.841904000	6	-3.533349000	-1.457830000	3.845154000
1	-4.180423000	-4.716958000	0.055713000	6	-3.347226000	-1.578183000	5.362908000
1	-5.457161000	-4.198069000	1.166234000	1	-2.401487000	-1.133341000	5.672509000
6	-2.671510000	-2.770754000	3.924245000	1	-3.341127000	-2.630469000	5.662679000
6	-3.336211000	-3.674810000	4.968565000	1	-4.154748000	-1.089989000	5.915834000
1	-2.853306000	-3.542180000	5.941554000	6	-4.875396000	-2.101952000	3.472106000
1	-3.259483000	-4.735652000	4.714766000	1	-5.721181000	-1.655934000	4.001480000
1	-4.394877000	-3.422635000	5.073369000	1	-4.862956000	-3.165311000	3.726406000
6	-2.707962000	-1.341036000	4.458009000	6	-2.432833000	-2.250926000	3.149293000
1	-3.734555000	-1.018695000	4.640289000	1	-2.542512000	-2.233907000	2.063517000
1	-2.243805000	-0.644275000	3.756768000	1	-2.474694000	-3.292839000	3.477715000
1	-2.159868000	-1.293019000	5.403623000	1	-1.438329000	-1.865956000	3.370103000
6	-1.212673000	-3.195652000	3.734694000	7	3.245290000	3.849462000	0.746657000
1	-0.657459000	-3.101012000	4.672924000	7	1.737768000	4.637287000	-1.015827000
1	-0.736171000	-2.568855000	2.978072000	6	2.492906000	5.004388000	1.196329000
1	-1.137735000	-4.240259000	3.418296000	1	3.122227000	5.680534000	1.781857000
6	-4.630171000	-2.305845000	-1.003329000	1	1.627149000	4.728178000	1.817446000
6	-3.554154000	-2.824041000	-1.963170000	6	2.021532000	5.691696000	-0.070838000
1	-2.599010000	-2.345293000	-1.739427000	1	1.133142000	6.300532000	0.136789000
1	-3.817743000	-2.611309000	-3.005063000	1	2.803947000	6.374070000	-0.443349000
1	-3.419608000	-3.906491000	-1.870971000	6	3.891885000	3.033540000	1.791255000
6	-5.977329000	-2.948424000	-1.350260000	6	4.904048000	3.902246000	2.545258000
1	-5.935929000	-4.040906000	-1.320141000	1	5.598504000	4.378639000	1.847518000
1	-6.279306000	-2.661252000	-2.361747000	1	5.483423000	3.284328000	3.237683000
1	-6.756855000	-2.620519000	-0.657033000	1	4.424178000	4.685009000	3.139120000
6	-4.762636000	-0.795352000	-1.185854000	6	4.654806000	1.879895000	1.145041000
1	-5.545790000	-0.383255000	-0.547551000	1	3.980557000	1.205048000	0.614374000
1	-5.020521000	-0.577206000	-2.224715000	1	5.167806000	1.302494000	1.918824000
1	-3.828112000	-0.281881000	-0.949792000	1	5.404126000	2.245457000	0.441156000
7	0.084046000	3.940048000	-2.905241000	6	2.873937000	2.461794000	2.783707000
7	-1.878914000	4.437430000	-1.535471000	1	2.351262000	3.252028000	3.331291000
6	0.120882000	5.306239000	-2.437953000	1	3.370894000	1.825872000	3.523199000
1	-0.233005000	6.009120000	-3.209725000	1	2.129259000	1.866297000	2.252011000
1	1.135358000	5.613466000	-2.153629000	6	0.864321000	4.935239000	-2.156632000
6	-0.793171000	5.352442000	-1.227808000	6	-0.588585000	5.013463000	-1.677884000
1	-1.167657000	6.366791000	-1.067668000	1	-0.890102000	4.047659000	-1.269756000
1	-0.231928000	5.052997000	-0.328016000	1	-1.265216000	5.278063000	-2.497664000
6	1.178172000	3.443486000	-3.743016000	1	-0.710063000	5.769502000	-0.895530000
6	1.544275000	4.491633000	-4.799874000	6	1.268331000	6.270950000	-2.791262000

1	0.678010000	4.746220000	-5.417093000	1	1.137030000	7.113334000	-2.106266000
1	2.323913000	4.099109000	-5.459550000	1	0.650505000	6.467910000	-3.672548000
1	1.927444000	5.413948000	-4.354703000	1	2.314166000	6.250242000	-3.110167000
6	0.756848000	2.168616000	-4.470541000	6	0.973100000	3.851788000	-3.226614000
1	0.442953000	1.396078000	-3.764791000	1	1.973319000	3.827430000	-3.661926000
1	1.600115000	1.783058000	-5.050518000	1	0.254629000	4.058983000	-4.025346000
1	-0.066261000	2.361332000	-5.161741000	1	0.759309000	2.864658000	-2.811163000
6	2.403783000	3.145531000	-2.874709000	7	-2.876813000	-2.411142000	-3.124408000
1	2.727936000	4.038285000	-2.332280000	7	-3.524259000	-0.031687000	-3.387446000
1	3.249844000	2.799045000	-3.477811000	6	-4.301129000	-2.254510000	-3.304174000
1	2.150953000	2.376190000	-2.142217000	1	-4.855599000	-2.255431000	-2.346088000
6	-2.993095000	4.386528000	-0.565351000	1	-4.721863000	-3.063300000	-3.910135000
6	-2.498825000	4.067703000	0.847670000	6	-4.487940000	-0.925395000	-4.002704000
1	-1.958796000	3.119276000	0.846093000	1	-4.329793000	-1.047878000	-5.084803000
1	-3.342033000	3.991656000	1.540283000	1	-5.512749000	-0.565812000	-3.865384000
1	-1.831090000	4.844895000	1.230398000	6	-2.424615000	-3.619036000	-2.404019000
6	-3.704752000	5.743637000	-0.556220000	6	-2.797304000	-3.554088000	-0.918490000
1	-3.066706000	6.548848000	-0.181833000	1	-2.252209000	-2.735954000	-0.442323000
1	-4.581168000	5.699631000	0.097296000	1	-2.530911000	-4.481861000	-0.406292000
1	-4.042120000	6.013592000	-1.560140000	1	-3.875700000	-3.412456000	-0.779163000
6	-4.009197000	3.325961000	-0.983313000	6	-0.911986000	-3.770480000	-2.525251000
1	-4.395410000	3.521042000	-1.983967000	1	-0.614505000	-3.873811000	-3.570601000
1	-4.847194000	3.334519000	-0.280373000	1	-0.596386000	-4.668638000	-1.987504000
1	-3.569729000	2.326425000	-0.971404000	1	-0.384630000	-2.919686000	-2.090988000
7	1.258583000	2.594730000	3.637228000	6	-3.077097000	-4.852582000	-3.034986000
6	1.814570000	3.274553000	4.792832000	1	-4.154505000	-4.900866000	-2.852344000
1	2.870139000	3.010220000	4.867137000	1	-2.637843000	-5.758617000	-2.608990000
1	1.354898000	2.891678000	5.717784000	1	-2.908601000	-4.870042000	-4.115736000
6	1.667925000	4.790516000	4.765506000	6	-3.560920000	1.372513000	-3.853138000
1	2.100851000	5.223538000	3.860266000	6	-3.374902000	1.495363000	-5.370741000
1	2.178308000	5.230510000	5.627716000	1	-2.418323000	1.072753000	-5.678195000
1	0.622340000	5.105608000	4.812890000	1	-3.393247000	2.547135000	-5.671801000
6	-0.107836000	2.919406000	3.274299000	1	-4.169626000	0.987481000	-5.924480000
1	-0.360803000	2.284944000	2.424425000	6	-4.918643000	1.985036000	-3.483580000
1	-0.165348000	3.956449000	2.912699000	1	-5.752570000	1.518315000	-4.013908000
6	-1.127595000	2.720732000	4.385908000	1	-4.930966000	3.048047000	-3.739298000
1	-2.118565000	3.012953000	4.029619000	1	-5.109908000	1.903895000	-2.408430000
1	-0.908752000	3.328602000	5.269438000	6	-2.480870000	2.192358000	-3.156325000
1	-1.180380000	1.676654000	4.700430000	1	-2.591860000	2.174750000	-2.070689000
7	3.360474000	-2.611507000	-2.467871000	1	-2.546467000	3.232448000	-3.486621000
7	1.903320000	-4.286301000	-1.351468000	1	-1.477108000	1.830580000	-3.374390000
6	3.981217000	-3.921489000	-2.400770000	7	3.342971000	-3.772428000	-0.743767000
1	5.057673000	-3.844728000	-2.216040000	7	1.851944000	-4.595332000	1.016666000

1	3.849816000	-4.506481000	-3.324228000	6	2.617464000	-4.943954000	-1.194798000
6	3.302515000	-4.627305000	-1.249298000	1	3.262473000	-5.605087000	-1.780378000
1	3.457740000	-5.707835000	-1.322943000	1	1.745963000	-4.687169000	-1.816253000
1	3.753997000	-4.304398000	-0.291838000	6	2.161164000	-5.642591000	0.071622000
6	3.894183000	-1.705545000	-3.509148000	1	1.287423000	-6.271927000	-0.136957000
6	5.400429000	-1.512890000	-3.283618000	1	2.958995000	-6.306555000	0.444660000
1	5.616216000	-1.226467000	-2.248583000	6	3.972647000	-2.941823000	-1.787188000
1	5.773261000	-0.714968000	-3.931510000	6	5.006135000	-3.787042000	-2.538950000
1	5.980570000	-2.410151000	-3.513078000	1	5.710024000	-4.247044000	-1.839674000
6	3.230887000	-0.337284000	-3.405864000	1	5.572426000	-3.156048000	-3.230398000
1	2.145568000	-0.392801000	-3.471964000	1	4.545728000	-4.580863000	-3.133543000
1	3.593600000	0.304433000	-4.213427000	6	4.707392000	-1.770720000	-1.139707000
6	3.695693000	-2.241489000	-4.932708000	1	4.016771000	-1.111656000	-0.610275000
1	4.141397000	-3.231491000	-5.062439000	1	5.208134000	-1.181549000	-1.912659000
1	4.172391000	-1.574858000	-5.658045000	1	5.463812000	-2.118745000	-0.434524000
1	2.637002000	-2.305793000	-5.179381000	6	2.943705000	-2.393989000	-2.781762000
6	1.005379000	-4.846905000	-0.318953000	1	2.439765000	-3.196230000	-3.329429000
6	1.208764000	-6.363344000	-0.250152000	1	3.427420000	-1.747752000	-3.521068000
1	1.110858000	-6.813967000	-1.242280000	1	2.185109000	-1.814742000	-2.251856000
1	0.449218000	-6.806173000	0.399731000	6	0.984659000	-4.914150000	2.156573000
1	2.183354000	-6.640863000	0.161366000	6	-0.465518000	-5.026722000	1.676359000
6	1.284694000	-4.231829000	1.055575000	1	-0.789528000	-4.068372000	1.267885000
1	2.320020000	-4.400407000	1.372645000	1	-1.136497000	-5.307197000	2.495495000
1	0.641118000	-4.673441000	1.820566000	1	-0.568389000	-5.785416000	0.893915000
1	1.088003000	-3.158327000	1.024852000	6	1.419539000	-6.240104000	2.791263000
6	-0.446555000	-4.583550000	-0.700804000	1	1.308886000	-7.085162000	2.105920000
1	-0.668689000	-3.516315000	-0.731063000	1	0.805702000	-6.451888000	3.671894000
1	-1.107371000	-5.039889000	0.040477000	1	2.464277000	-6.194711000	3.111181000
1	-0.675719000	-5.018135000	-1.674851000	6	1.066611000	-3.828796000	3.227003000
1	4.041564000	2.117233000	-0.463313000	1	2.065424000	-3.781076000	3.663590000
1	1.869816000	-1.712934000	2.966334000	1	0.352226000	-4.053066000	4.024779000
1	3.464380000	0.161637000	-2.462635000	1	0.830196000	-2.846786000	2.811695000
1	4.764069000	-0.280142000	3.235996000	1	-5.066448000	-2.023816000	2.396704000

Table S14: Single-crystal X-ray Crystallography Data

	2-Ce^{Li}	**2-Ce^{Na}**	**2-Ce^{K18c6}**	**2-Ce^{Rb}**	**2-Ce^{Cs}**
Formula	$C_{56}H_{128}CeLiN_{16}P_4$	$C_{56}H_{128}CeN_{16}NaP_4$	$C_{80}H_{176}CeKN_{16}O_{12}P_4$	$C_{56}H_{128}CeN_{16}P_4Rb$	$C_{56}H_{128}CeCsN_{16}P_4$
Formula Weight/gmol^{-1}	1296.70	1312.75	1857.50	1375.23	1422.64
Collection Temperature/K	100(2)	100(2)	100(2)	100(2)	100(2)
Space Group [System]	P2$_1$/c [monoclinic]	P2$_1$/n [monoclinic]	P2$_1$/c [monoclinic]	P-1 [triclinic]	P1 [triclinic]
Resolution/Å	0.83	0.70	0.85	0.82	0.61
a/Å	28.658(6)	14.1551(7)	20.5497(14)	13.8280(10)	13.915(3)
b/Å	22.627(5)	23.2285(12)	18.8590(12)	13.9994(10)	13.928(2)
c/Å	25.312(5)	22.8762(12)	28.366(2)	23.9161(17)	24.247(5)
α/°	90	90	90	95.768(3)	105.027(7)
β/°	115.73(3)	99.179(2)	107.014(2)	105.731(3)	96.887(7)
γ/°	90	90	90	108.564(3)	109.734(6)
Volume/Å^3	14786(7)	7425.4(7)	10512.1(12)	4135.0(5)	4159.3(14)
Z [Z']	4 [1]	2 [0.5]	4 [1]	1 [0.5]	1 [1]
ρ/gcm^{-3}	1.198	1.207	1.220	1.253	1.253
μ/mm^{-1}	0.748	0.751	0.594	1.262	1.102
F(000)	5744.0	2904.0	4172.0	1672.0	1663.0
Crystal Size/mm^3	0.348 x 0.29 x 0.224	0.426 x 0.374 x 0.228	0.3 x 0.3 x 0.2	0.477 x 0.311 x 0.256	0.308 x 0.28 x 0.18
Radiation Type	MoKα(λ=0.71073)	MoKα(λ=0.71073)	MoKα(λ=0.71073)	MoKα(λ=0.71073)	MoKα(λ=0.71073)
Physical Description	Yellow prism	Yellow prism	Colorless prism	Colorless prism	Colorless plate
Collection 2θ range/°	3.688 to 50.734	3.402 to 61.016	3.61 to 49.426	3.886 to 51.362	4.000 to 71.262
Index Ranges	$-34\leq h\leq 34$; $-27\leq k\leq 26$; $-30\leq l\leq 30$	$-17\leq h\leq 20$; $-33\leq k\leq 33$; $-32\leq l\leq 32$	$-24\leq h\leq 24$; $-22\leq k\leq 22$; $-33\leq l\leq 33$	$-16\leq h\leq 16$; $-17\leq k\leq 17$; $-29\leq l\leq 29$	$-22\leq h\leq 22$; $-22\leq k\leq 22$; $-39\leq l\leq 39$
Reflections Collected	249753	225204	265941	85806	112618
Independent Reflections	27060 [R_{int}=0.0772, R_{sigma}=0.0415]	22555 [R_{int}=0.07184, R_{sigma}=0.0361]	17753 [R_{int}=0.1297, R_{sigma}=0.0431]	15631 [R_{int}=0.0619, R_{sigma}=0.0431]	64250 [R_{int}=0.0558, R_{sigma}=0.0741]
Data/Restraints/Parameters	27060/7411/2160	22555/2567/1020	17753/1443/1337	15631/180/871	64250/445/1658
Goodness of Fit	1.146	1.036	1.158	1.094	1.101
Final R Indices (I ≥2σ)	R_1=0.0858, wR_2=0.1805	R_1=0.0446, wR_2=0.1069	R_1=0.1296, wR_2=0.2645	R_1=0.0856, wR_2=0.2284	R_1=0.0538, wR_2=0.1183
Final R Indices (all data)	R_1=0.0931, wR_2=0.1847	R_1=0.0536, wR_2=0.1145	R_1 = 0.1389, wR_2=0.2699	R_1=0.0987, wR_2=0.2432	R_1=0.0588, wR_2=0.1363
Largest Diff. Peak/Hole/eA^3	2.0/-1.6	2.0/-1.6	2.2/-2.2	5.4/-2.9	3.6/-3.6
Completeness to 2θ/%	99.9	100	99.1	99.6	100
CCDC Number	2248373	2248374	2248368	2248375	2248365

Crystallography Details:

Crystals suitable for X-ray diffraction were coated in paratone or Cargille-NVH oil in a glovebox and transferred to the diffractometer in a 20 mL capped vial. Crystals were mounted on a nylon loop on a Bruker D8 VENTURE diffractometer dual wavelength Mo/Cu four-circle diffractometer with a microfocus sealed X-ray tube using a mirror optics as monochromator and a Bruker PHOTON II detector. The diffractometer is equipped with an Oxford Cryostream 800 cryostat and crystals were cooled and kept at T = 100(2) K during data collection. All data were integrated with SAINT and a multi-scan absorption correction using SADABS was applied.[29] The structures were solved with the ShelXT structure solution program using the Intrinsic Phasing solution method and refined by full-matrix least-squares methods against F^2 using SHELXL-2014[30] and by using Olex2 1.5-alpha[31] as the graphical interface. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were refined isotropically on calculated positions using a riding model with their Uiso values constrained to 1.5 times the Ueq of their pivot atoms for terminal sp3 carbon atoms and 1.2 times for all other carbon atoms. Disordered moieties were refined using bond lengths restraints and displacement parameter restraints. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.

2-Ce^{Li}

The Li-Ce-structure of **2-Ce^{Li}** was found to be complicated by superlattice reflections. Initially, a smaller monoclinic cell was identified, but it did not capture all the reflections. Subsequently, a much larger triclinic cell was used, which captured all the data. However, it was later discovered that the data had monoclinic symmetry. A low symmetry cerium structure with 18 residues obtained with the triclinic cell was correct.

From this preliminary structure and the 2/m Laue symmetry, we identified a smaller cell in P21/c that contains two independent molecules with some of the ligands disordered, and it indexed most of the reflections. This cell was larger than the small monoclinic cell, and some weak superlattice reflections were present. The large triclinic cell transforms into an even larger cell with the correct Laue symmetry (2/m), but would result in a cumbersome and unyielding model, and hence we decided that the smaller cell (with correct Laue symmetry and with superlattice data) was the best cell for studying the chemical structure.

It is possible that there was a phase transition close to the data collection temperature. The Ce atom Ce2 is lifted off its mean position by either dynamic or static disorder and could be modeled by splitting it into two parts. However, instead of doing this, it was modeled as one component with an elongated ellipsoid representing the disorder. This was done so that the metal-ligand geometries could be analyzed (splitting the Ce atom would create two additional sets of metal-ligand bonds). The complexity of the model, correlated parameters would be extreme, and reliable bond distances and angles could not be obtained. Instead, the equilibrium position gave more reliable and simplified geometries.

For this structural model of **2-Ce^{Li}** in P21/c, there are two molecules with four ligands each. There are eight components to the ligand disorder (i.e., two groups of atoms), and at least one of the Li atoms and one of the Ce atoms could be split, resulting in as many as 16 components to the disorder. We identified the components that can be thought of as representing the two unique CeL4-Li group of atoms (two CeL4 tetrahedra). The distortions and geometries of the ligands were straightforward to analyze once this was done. Finally, all the atoms (except H) were refined anisotropically.

2-Ce^{K18c6}

Despite having good signal-to-noise (I/sigma), R_{int} and R_1 are higher because the reflections were, on the whole, very broad indicating a high-degree of crystal mosaicity. The diffraction data for this structure is highly broadened with poor peak profiles, indicating extensive crystal decomposition. Overall data for the **2-Ce^{K18c6}** structure suffers from broadened (and weakened) data. As a result, the merging R-values were large. A very large number of reflections were collected in order to improve the overall data quality (and this gave better I/sigma for the low angle data). It was observed that the reflections are not affected by the decay equally. It is observed the higher angle data is weakened the most to the point that the higher angle data are impacted at a much higher level, with the data above 1.1 Å being the most troublesome. However, a satisfactory model is obtained by including the larger number of reflections with no salient alerts.

2-Ce^{Rb}

The oblate N4 atom is not due to weak data. Instead, it must arise from the intensities of some of the twinned reflections being incorrect. The intensities consist of overlaps, partial overlaps and isolated reflections (from one component only). The intensities are increased by a factor from the other twin domain. The twin law corrects the intensities by presuming that the intensities have been treated equally during the integration. The data integration process is affected by the twinning. The errors in the integration of the twin cannot be completely approximated by the twin law and the corrected data, even though the twin law is valid, presumes that there were no errors in integrating the twinned reflections. The ADP is a measure of the spread of electron density around an atom in a crystal structure. This distortion is be caused by a combination of factors, including weak data. In this case, the crystals were twinned. Twinning is the main factor causing extra electron density at the N4 atom, which is then reflected in the ADP values. The weak data could also be contributing to the distortion of the thermal ellipsoids of the atomic positions although other atoms are fine. The twinning operation involves a 180-degree rotation around an axis that is parallel to the b-axis 0 1 0. This is the axis that bisects the Ce-N bond with the prolate N. It is a reflection through a plane perpendicular to the axis h0l plane. This is known as the 100 reflection twin, also called the spinel twin or normal twin. In this type of twinning, the twin domains are related by a reflection through a common twin plane, resulting in a mirror image relationship between the two domains. The 100 reflection twin is commonly observed in crystals with low symmetry and this one with its triclinic unit cell is one such example.

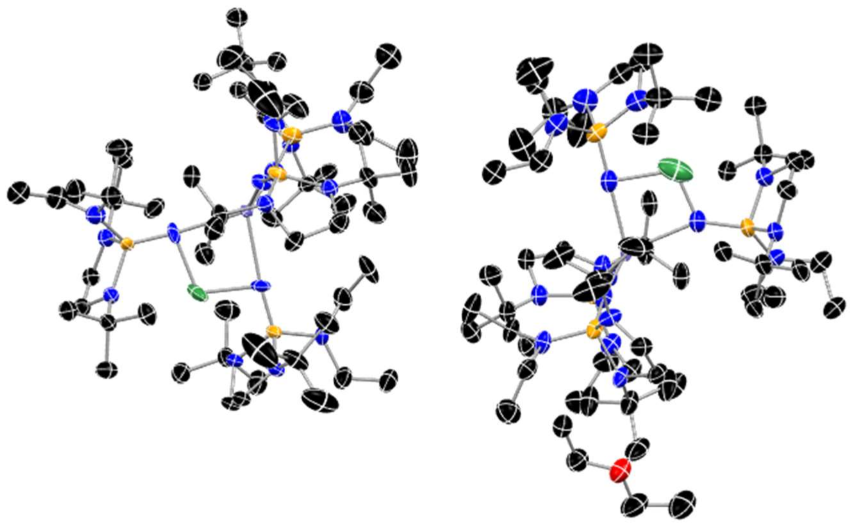

Figure S108. Asymmetric unit of **2-Ce^{Li}**. C atoms are shown in black, N in blue, O in red, P in orange, Li in green, and Ce in light blue. H atoms are omitted for clarity. Thermal ellipsoids drawn at 50% probability level.

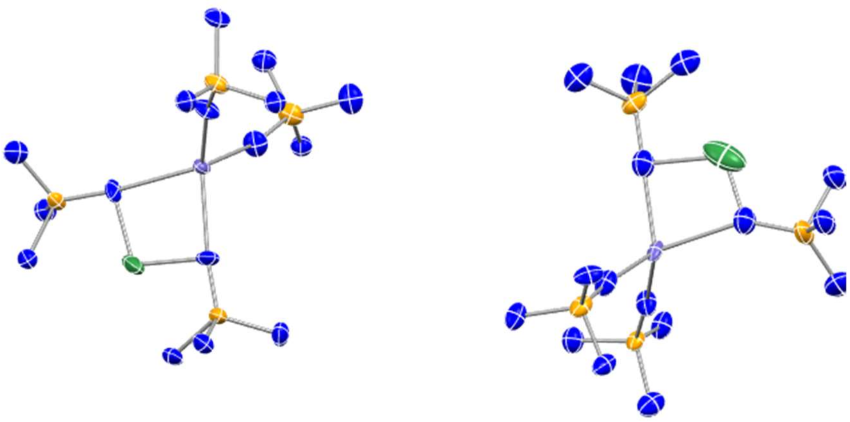

Figure S109. Truncated asymmetric unit of **2-Ce^{Li}**. N atoms are shown in blue, P in orange, Li in green, and Ce in light blue. H atoms are omitted for clarity. Thermal ellipsoids drawn at 50% probability level.

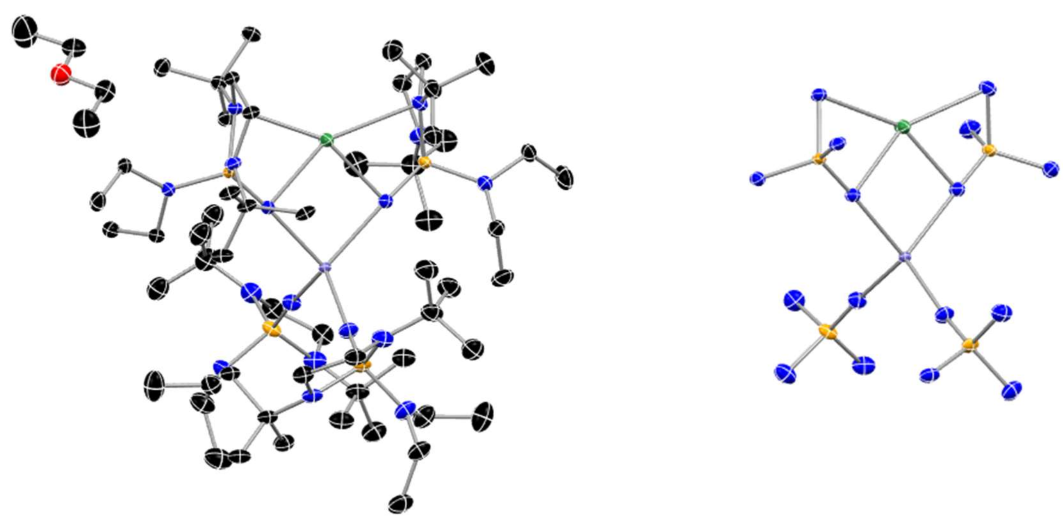

Figure S110. Asymmetric unit of **2-Ce^{Na}** (left) and truncated asymmetric unit of **2-Ce^{Na}** (right). C atoms are shown in black, N in blue, O in red, P in orange, Na in green, and Ce in light blue. H atoms are omitted for clarity. Thermal ellipsoids drawn at 50% probability level.

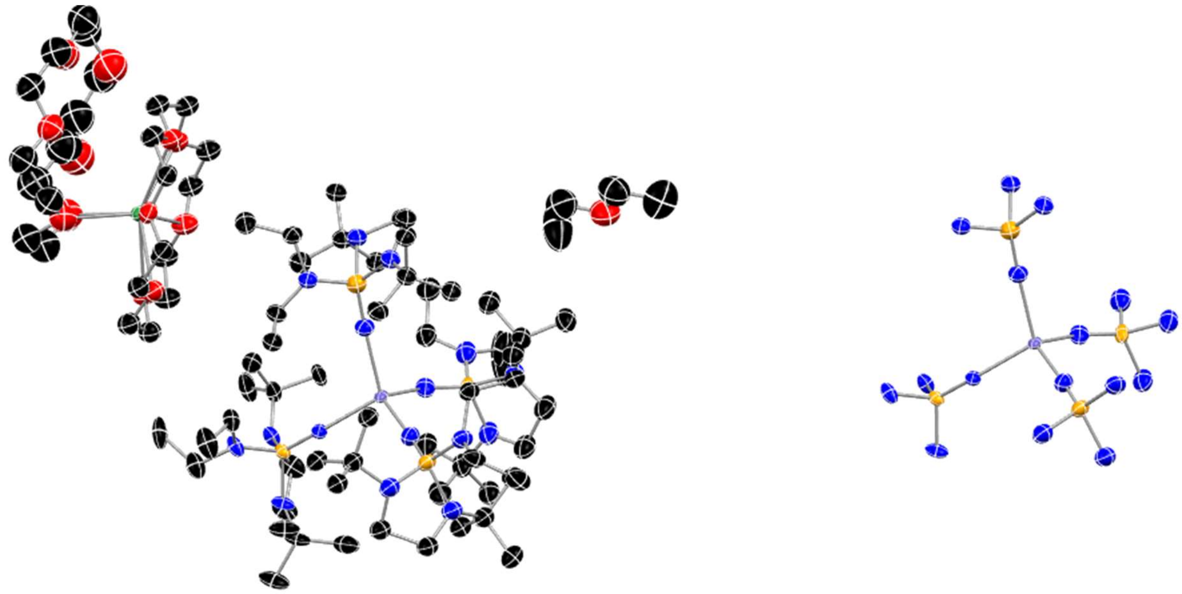

Figure S111. Asymmetric unit of **2-Ce**^{K18c6} (left) and truncated asymmetric unit of **2-Ce**^{K18c6} (right). C atoms are shown in black, N in blue, O in red, P in orange, K in green, and Ce in light blue. Hydrogen atoms are omitted for clarity. Thermal ellipsoids drawn at 50% probability level.

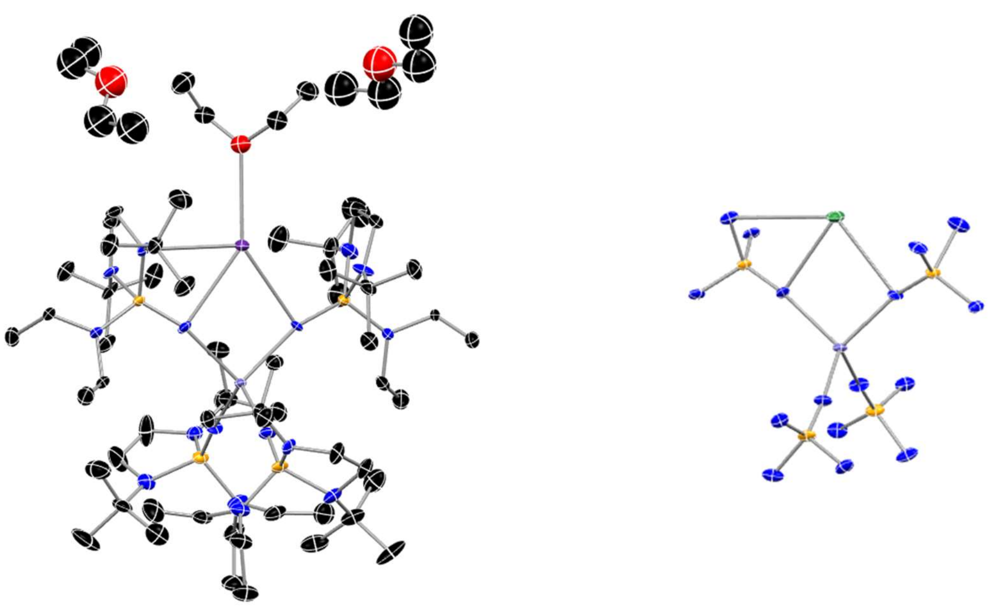

Figure S112. Asymmetric unit of **2-Ce**^{Rb} (left) and truncated asymmetric unit of **2-Ce**^{Rb} (right). C atoms are shown in black, N in blue, O in red, P in orange, Rb in green, and Ce in light blue. H atoms are omitted for clarity. Thermal ellipsoids drawn at 50% probability level.

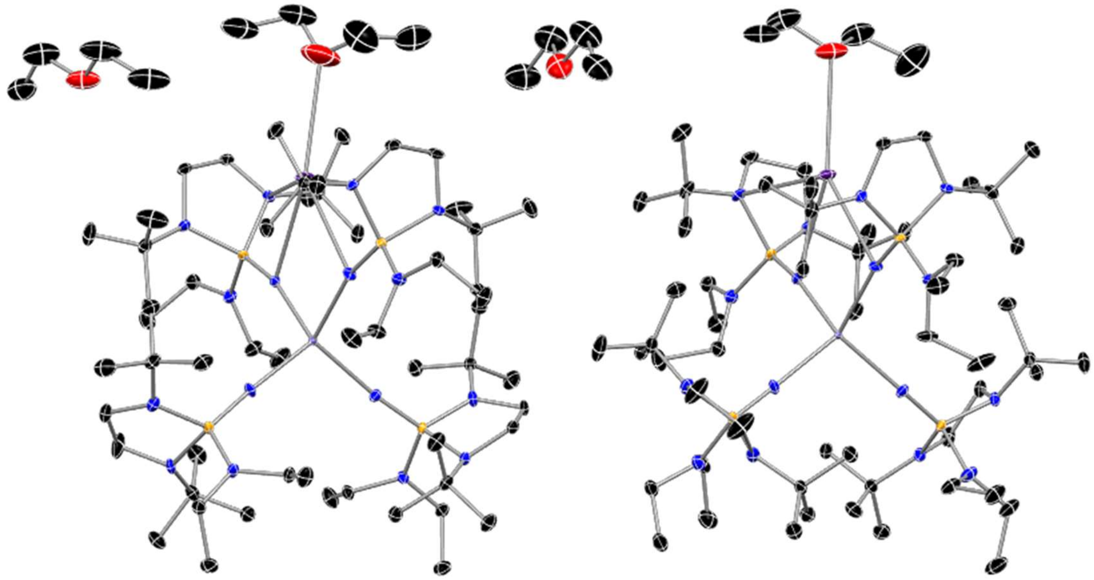

Figure S113. Asymmetric unit of **2-Ce^{Cs}**. C atoms are shown in black, N in blue, O in red, P in orange, Cs in purple, and Ce in light blue. H atoms are omitted for clarity. Thermal ellipsoids drawn at 50% probability level.

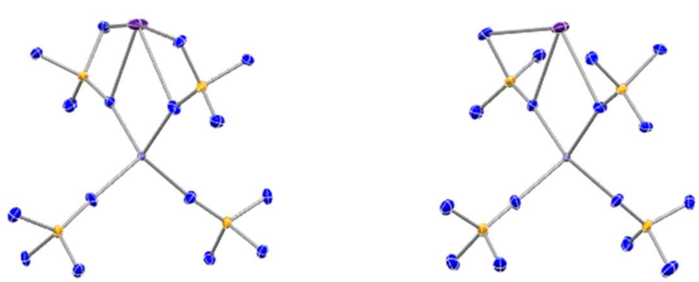

Figure S114. Truncated asymmetric unit of **2-Ce^{Cs}**. N atoms are shown in blue, P in orange, Cs in purple, and Ce in light blue. H atoms are omitted for clarity. Thermal ellipsoids drawn at 50% probability level.

Table S15. Bond distances for **2-Ce^{Li}**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ce1	N2	2.300(4)	N3_1	C3_1	1.473(10)
Ce1	N3	2.392(4)	N4_1	C11_1	1.466(10)
Ce1	Li1	3.021(11)	N4_1	C13_1	1.454(10)
Ce1	N1	2.305(5)	C1_1	C2_1	1.524(2)
Ce1	N1B	2.305(5)	C3_1	C4_1	1.546(12)
Ce1	N17_3	2.400(4)	C3_1	C5_1	1.510(11)
Ce1	N17_4	2.400(4)	C3_1	C6_1	1.549(12)
Ce2	N9	2.315(6)	C7_1	C8_1	1.530(13)
Ce2	Li2	2.968(17)	C7_1	C9_1	1.518(12)
Ce2	N1_1	2.272(5)	C7_1	C10_1	1.533(13)
Ce2	N1_2	2.515(9)	C11_1	C12_1	1.528(2)
Ce2	N17_6	2.293(6)	C13_1	C14_1	1.527(2)
Ce2	N17_7	2.293(6)	N1_2	P1_2	1.544(8)
Ce2	N17_8	2.412(6)	P1_2	N2_2	1.672(9)
Ce2	N17_9	2.325(8)	P1_2	N3_2	1.700(9)
P2	N2	1.517(4)	P1_2	N4_2	1.706(8)
P2	N20	1.656(4)	N2_2	C1_2	1.439(12)
P2	N22	1.702(3)	N2_2	C7_2	1.486(11)
P2	N21'	1.636(14)	N3_2	C2_2	1.484(12)
N20	C201	1.499(10)	N3_2	C3_2	1.468(11)
N20	C203	1.465(9)	N4_2	C11_2	1.439(11)
C201	C202	1.527(2)	N4_2	C13_2	1.461(11)
C203	C204	1.528(2)	C1_2	C2_2	1.520(12)
N21	C21	1.523(17)	C3_2	C4_2	1.526(13)
N21	C23	1.510(17)	C3_2	C5_2	1.529(13)
N22	C22	1.486(17)	C3_2	C6_2	1.547(12)
N22	C24	1.475(15)	C7_2	C8_2	1.536(14)
C21	C211	1.57(2)	C7_2	C9_2	1.540(14)
C21	C212	1.54(2)	C7_2	C10_2	1.518(14)
C21	C213	1.52(2)	C11_2	C12_2	1.506(12)
C22	C221	1.56(3)	C13_2	C14_2	1.526(12)
C22	C222	1.53(2)	N17_3	P17_3	1.565(7)
C22	C223	1.55(2)	P17_3	N47_3	1.722(8)
C23	C24	1.5242(16)	P17_3	N57_3	1.702(8)
N21'	C21'	1.42(2)	P17_3	N67_3	1.647(8)
N21'	C23'	1.44(2)	N47_3	C17_3	1.474(11)
N22'	C22'	1.49(2)	N47_3	C77_3	1.500(10)
N22'	C24'	1.41(2)	N57_3	C27_3	1.469(11)
C21'	C21A	1.56(2)	N57_3	C37_3	1.484(10)
C21'	C21B	1.52(2)	N67_3	C117_3	1.474(3)
C21'	C21C	1.53(2)	N67_3	C137_3	1.487(10)
C22'	C22A	1.57(2)	C17_3	C27_3	1.525(2)
C22'	C22B	1.54(2)	C37_3	C47_3	1.529(4)
C22'	C22C	1.55(3)	C37_3	C57_3	1.529(4)
C23'	C24'	1.525(2)	C37_3	C67_3	1.530(4)
P3	N3	1.507(4)	C77_3	C87_3	1.544(11)
P3	N30	1.677(4)	C77_3	C97_3	1.524(12)
P3	N31	1.725(6)	C77_3	C107_3	1.520(12)
P3	N32	1.732(5)	C117_3	C127_3	1.518(8)
N3	Li1	2.000(15)	C137_3	C147_3	1.521(12)
N30	C301	1.474(3)	N17_4	P17_4	1.495(6)
N30	C303	1.472(3)	P17_4	N47_4	1.684(5)
C301	C302	1.534(11)	P17_4	N57_4	1.712(6)
N31	C31	1.493(10)	P17_4	N67_4	1.644(5)

N31	C33	1.462(9)	N47_4	C17_4	1.448(8)
N31	Li1	2.529(14)	N47_4	C77_4	1.498(9)
N32	C32	1.449(10)	N57_4	C27_4	1.448(9)
N32	C34	1.429(8)	N57_4	C37_4	1.465(9)
C31	C311	1.537(11)	N67_4	C117_4	1.477(3)
C31	C312	1.518(10)	N67_4	C137_4	1.475(3)
C31	C313	1.512(11)	C17_4	C27_4	1.5245(15)
C32	C321	1.529(4)	C37_4	C47_4	1.542(11)
C32	C322	1.530(4)	C37_4	C57_4	1.537(10)
C32	C323	1.529(4)	C37_4	C67_4	1.526(10)
C33	C34	1.524(2)	C77_4	C87_4	1.527(10)
P5	N9	1.531(7)	C77_4	C97_4	1.535(10)
P5	N50	1.677(6)	C77_4	C107_4	1.528(11)
P5	N51	1.716(6)	C117_4	C127_4	1.526(3)
P5	N52	1.687(6)	C137_4	C147_4	1.527(3)
N50	C501	1.473(3)	N17_6	P17_6	1.580(7)
N50	C503	1.473(3)	P17_6	N47_6	1.698(9)
N51	C51	1.499(7)	P17_6	N57_6	1.735(9)
N51	C53	1.465(9)	P17_6	N67_6	1.682(9)
N52	C52	1.480(7)	N47_6	C17_6	1.437(12)
N52	C54	1.434(9)	N47_6	C77_6	1.495(11)
C51	C511	1.526(3)	N57_6	C27_6	1.487(12)
C51	C512	1.526(3)	N57_6	C37_6	1.483(11)
C51	C513	1.526(3)	N67_6	C117_6	1.466(11)
C52	C521	1.526(3)	N67_6	C137_6	1.431(11)
C52	C522	1.526(3)	C17_6	C27_6	1.535(12)
C52	C523	1.526(3)	C37_6	C47_6	1.530(6)
C53	C54	1.524(2)	C37_6	C57_6	1.530(6)
C501	C502	1.520(11)	C37_6	C67_6	1.530(6)
C503	C504	1.509(12)	C77_6	C87_6	1.531(13)
Li1	N17_3	2.009(15)	C77_6	C97_6	1.539(12)
Li1	N47_3	2.666(17)	C77_6	C107_6	1.508(13)
Li1	N17_4	2.009(15)	C117_6	C127_6	1.515(13)
Li1	P17_4	2.673(15)	C137_6	C147_6	1.525(13)
Li2	N1_1	2.09(2)	N17_7	P17_7	1.498(6)
Li2	N3_1	2.56(2)	P17_7	N47_7	1.697(7)
Li2	N1_2	1.56(2)	P17_7	N57_7	1.714(6)
Li2	P1_2	2.63(3)	P17_7	N67_7	1.661(6)
Li2	N17_8	1.76(2)	N47_7	C17_7	1.447(10)
Li2	N17_9	2.16(2)	N47_7	C77_7	1.486(10)
N1	P1	1.588(8)	N57_7	C27_7	1.462(9)
P1	N4	1.689(5)	N57_7	C37_7	1.475(9)
P1	N5	1.711(6)	N67_7	C117_7	1.462(9)
P1	N6	1.640(5)	N67_7	C137_7	1.453(9)
N4	C1	1.451(8)	C17_7	C27_7	1.524(2)
N4	C7	1.494(8)	C37_7	C47_7	1.522(11)
N5	C2	1.443(9)	C37_7	C57_7	1.529(11)
N5	C3	1.464(9)	C37_7	C67_7	1.537(11)
N6	C11	1.472(3)	C77_7	C87_7	1.533(12)
N6	C13	1.472(3)	C77_7	C97_7	1.528(11)
C1	C2	1.5237(16)	C77_7	C107_7	1.529(12)
C3	C4	1.542(10)	C117_7	C127_7	1.527(2)
C3	C5	1.537(10)	C137_7	C147_7	1.528(2)
C3	C6	1.527(10)	N17_8	P17_8	1.577(5)
C7	C8	1.528(10)	P17_8	N47_8	1.702(3)
C7	C9	1.535(10)	P17_8	N57_8	1.702(3)
C7	C10	1.530(11)	P17_8	N67_8	1.660(7)
C11	C12	1.527(2)	N47_8	C17_8	1.450(10)

C13	C14	1.528(2)	N47_8	C77_8	1.514(10)
N1B	P1B	1.467(9)	N57_8	C27_8	1.467(9)
P1B	N4B	1.739(9)	N57_8	C37_8	1.462(10)
P1B	N5B	1.687(8)	N67_8	C117_8	1.474(3)
P1B	N6B	1.680(9)	N67_8	C137_8	1.473(3)
N4B	C1B	1.493(11)	C17_8	C27_8	1.524(2)
N4B	C7B	1.510(10)	C37_8	C47_8	1.542(11)
N5B	C2B	1.461(10)	C37_8	C57_8	1.530(11)
N5B	C3B	1.468(10)	C37_8	C67_8	1.535(12)
N6B	C11B	1.459(11)	C77_8	C87_8	1.527(12)
N6B	C13B	1.455(10)	C77_8	C97_8	1.511(11)
C1B	C2B	1.525(11)	C77_8	C107_8	1.534(12)
C3B	C4B	1.530(12)	C117_8	C127_8	1.528(2)
C3B	C5B	1.516(12)	C137_8	C147_8	1.529(2)
C3B	C6B	1.549(12)	N17_9	P17_9	1.567(9)
C7B	C8B	1.530(12)	P17_9	N47_9	1.673(9)
C7B	C9B	1.510(12)	P17_9	N57_9	1.684(9)
C7B	C10B	1.536(12)	P17_9	N67_9	1.792(8)
C11B	C12B	1.536(13)	N47_9	C17_9	1.460(12)
C13B	C14B	1.521(13)	N47_9	C77_9	1.492(11)
C303	C304	1.527(3)	N57_9	C27_9	1.485(12)
C303	C30D	1.527(2)	N57_9	C37_9	1.485(11)
O1	C91	1.396(9)	N67_9	C117_9	1.473(3)
O1	C93	1.421(10)	N67_9	C137_9	1.474(3)
C91	C92	1.505(10)	C17_9	C27_9	1.527(12)
C93	C94'	1.507(13)	C37_9	C47_9	1.530(4)
C93	C94	1.493(16)	C37_9	C57_9	1.531(12)
N1_1	P1_1	1.577(5)	C37_9	C67_9	1.530(4)
P1_1	N2_1	1.702(3)	C77_9	C87_9	1.523(14)
P1_1	N3_1	1.702(3)	C77_9	C97_9	1.534(13)
P1_1	N4_1	1.677(8)	C77_9	C107_9	1.536(13)
N2_1	C1_1	1.455(10)	C117_9	C127_9	1.518(8)
N2_1	C7_1	1.489(10)	C137_9	C147_9	1.518(8)
N3_1	C2_1	1.479(10)			

Table S16. Bond angles for **2-Ce^{Li}**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N2	Ce1	N3	114.24(19)	C11_1	N4_1	P1_1	123.7(7)
N2	Ce1	Li1	124.4(3)	C13_1	N4_1	P1_1	118.8(7)
N2	Ce1	N1	113.8(2)	C13_1	N4_1	C11_1	117.3(8)
N2	Ce1	N1B	113.8(2)	N2_1	C1_1	C2_1	105.3(7)
N2	Ce1	N17_3	114.98(18)	N3_1	C2_1	C1_1	104.6(6)
N2	Ce1	N17_4	114.98(18)	N3_1	C3_1	C4_1	110.6(9)
N3	Ce1	Li1	41.4(3)	N3_1	C3_1	C5_1	112.1(8)
N3	Ce1	N17_3	82.93(19)	N3_1	C3_1	C6_1	110.4(8)
N3	Ce1	N17_4	82.93(19)	C4_1	C3_1	C6_1	106.3(9)
N1	Ce1	N3	113.5(2)	C5_1	C3_1	C4_1	107.6(9)
N1	Ce1	Li1	121.8(3)	C5_1	C3_1	C6_1	109.6(9)
N1	Ce1	N17_4	113.9(2)	N2_1	C7_1	C8_1	110.2(9)
N1B	Ce1	N3	113.5(2)	N2_1	C7_1	C9_1	111.1(10)
N1B	Ce1	Li1	121.8(3)	N2_1	C7_1	C10_1	109.9(8)
N1B	Ce1	N17_3	113.9(2)	C8_1	C7_1	C10_1	109.7(10)
N17_3	Ce1	Li1	41.6(3)	C9_1	C7_1	C8_1	109.1(9)
N17_4	Ce1	Li1	41.6(3)	C9_1	C7_1	C10_1	106.9(10)
N9	Ce2	Li2	127.7(4)	N4_1	C11_1	C12_1	113.3(9)
N9	Ce2	N1_2	121.0(2)	N4_1	C13_1	C14_1	113.6(9)
N9	Ce2	N17_8	119.8(2)	Li2	N1_2	Ce2	90.3(7)
N9	Ce2	N17_9	115.8(2)	P1_2	N1_2	Ce2	154.2(6)

N1_1	Ce2	N9	114.7(2)	P1_2	N1_2	Li2	115.5(10)
N1_1	Ce2	Li2	44.6(5)	N1_2	P1_2	N2_2	121.3(6)
N1_1	Ce2	N17_7	112.6(2)	N1_2	P1_2	N3_2	118.4(6)
N1_1	Ce2	N17_8	81.0(2)	N1_2	P1_2	N4_2	109.5(5)
N1_2	Ce2	Li2	31.7(5)	N2_2	P1_2	N3_2	93.0(5)
N17_6	Ce2	N9	112.2(2)	N2_2	P1_2	N4_2	106.5(6)
N17_6	Ce2	Li2	120.1(4)	N3_2	P1_2	N4_2	106.3(6)
N17_6	Ce2	N1_2	116.0(2)	C1_2	N2_2	P1_2	113.7(7)
N17_6	Ce2	N17_9	109.1(2)	C1_2	N2_2	C7_2	117.9(8)
N17_7	Ce2	N9	112.2(2)	C7_2	N2_2	P1_2	127.7(8)
N17_7	Ce2	Li2	120.1(4)	C2_2	N3_2	P1_2	109.4(7)
N17_7	Ce2	N17_8	113.0(2)	C3_2	N3_2	P1_2	125.4(8)
N17_8	Ce2	Li2	36.4(5)	C3_2	N3_2	C2_2	115.9(9)
N17_9	Ce2	Li2	46.1(5)	C11_2	N4_2	P1_2	119.9(8)
N17_9	Ce2	N1_2	77.9(3)	C11_2	N4_2	C13_2	119.4(9)
N2	P2	N20	113.5(2)	C13_2	N4_2	P1_2	118.3(8)
N2	P2	N22	124.6(3)	N2_2	C1_2	C2_2	107.5(9)
N2	P2	N21'	126.6(6)	N3_2	C2_2	C1_2	104.3(9)
N20	P2	N22	107.2(2)	N3_2	C3_2	C4_2	112.9(10)
N21'	P2	N20	103.4(5)	N3_2	C3_2	C5_2	109.9(10)
P2	N2	Ce1	165.7(4)	N3_2	C3_2	C6_2	109.7(10)
C201	N20	P2	118.3(4)	C4_2	C3_2	C5_2	108.6(10)
C203	N20	P2	121.8(5)	C4_2	C3_2	C6_2	108.2(10)
C203	N20	C201	114.7(6)	C5_2	C3_2	C6_2	107.3(10)
N20	C201	C202	114.3(8)	N2_2	C7_2	C8_2	111.7(11)
N20	C203	C204	113.6(8)	N2_2	C7_2	C9_2	107.5(10)
C21	N21	P2	129.0(8)	N2_2	C7_2	C10_2	111.8(10)
C23	N21	P2	117.7(6)	C8_2	C7_2	C9_2	108.4(10)
C23	N21	C21	112.1(9)	C10_2	C7_2	C8_2	108.0(11)
C22	N22	P2	118.4(8)	C10_2	C7_2	C9_2	109.4(11)
C24	N22	P2	110.2(6)	N4_2	C11_2	C12_2	114.8(12)
C24	N22	C22	112.6(9)	N4_2	C13_2	C14_2	113.8(11)
N21	C21	C211	106.1(14)	Li1	N17_3	Ce1	86.0(4)
N21	C21	C212	109.7(13)	P17_3	N17_3	Ce1	163.2(4)
C212	C21	C211	109.1(16)	P17_3	N17_3	Li1	105.9(5)
C213	C21	N21	111.9(12)	N17_3	P17_3	N47_3	106.1(5)
C213	C21	C211	109.6(15)	N17_3	P17_3	N57_3	128.7(5)
C213	C21	C212	110.4(16)	N17_3	P17_3	N67_3	111.0(5)
N22	C22	C221	112.8(14)	N57_3	P17_3	N47_3	92.7(4)
N22	C22	C222	108.9(12)	N67_3	P17_3	N47_3	110.7(5)
N22	C22	C223	108.4(12)	N67_3	P17_3	N57_3	105.6(6)
C222	C22	C221	108.7(15)	P17_3	N47_3	Li1	78.3(5)
C222	C22	C223	111.2(13)	C17_3	N47_3	Li1	131.0(8)
C223	C22	C221	106.8(16)	C17_3	N47_3	P17_3	110.5(6)
N21	C23	C24	100.9(10)	C17_3	N47_3	C77_3	113.4(7)
N22	C24	C23	105.4(11)	C77_3	N47_3	Li1	96.1(7)
C21'	N21'	P2	124.4(12)	C77_3	N47_3	P17_3	124.9(7)
C21'	N21'	C23'	123.4(14)	C27_3	N57_3	P17_3	111.5(6)
C23'	N21'	P2	111.3(10)	C27_3	N57_3	C37_3	115.2(7)
C22'	N22'	P2	124.0(10)	C37_3	N57_3	P17_3	123.8(6)
C24'	N22'	P2	108.2(10)	C117_3	N67_3	P17_3	126.5(7)
C24'	N22'	C22'	115.8(13)	C117_3	N67_3	C137_3	108.5(8)
N21'	C21'	C21A	113.3(16)	C137_3	N67_3	P17_3	120.1(7)
N21'	C21'	C21B	110.2(15)	N47_3	C17_3	C27_3	105.1(7)
N21'	C21'	C21C	109.8(15)	N57_3	C27_3	C17_3	104.1(7)
C21B	C21'	C21A	106.5(17)	N57_3	C37_3	C47_3	111.0(8)
C21B	C21'	C21C	110.7(16)	N57_3	C37_3	C57_3	109.9(7)
C21C	C21'	C21A	106.3(16)	N57_3	C37_3	C67_3	108.6(8)

N22'	C22'	C22A	109.0(13)	C47_3	C37_3	C67_3	110.9(9)
N22'	C22'	C22B	109.6(14)	C57_3	C37_3	C47_3	108.4(8)
N22'	C22'	C22C	110.3(16)	C57_3	C37_3	C67_3	108.1(8)
C22B	C22'	C22A	106.4(16)	N47_3	C77_3	C87_3	110.1(9)
C22B	C22'	C22C	110.1(17)	N47_3	C77_3	C97_3	111.7(9)
C22C	C22'	C22A	111.3(15)	N47_3	C77_3	C107_3	111.0(9)
N21'	C23'	C24'	110.3(12)	C97_3	C77_3	C87_3	107.9(9)
N22'	C24'	C23'	106.4(13)	C107_3	C77_3	C87_3	107.5(9)
N3	P3	N30	112.9(2)	C107_3	C77_3	C97_3	108.6(9)
N3	P3	N31	111.6(3)	C77_3	C107_3	Li1	91.8(8)
N3	P3	N32	121.8(3)	N67_3	C117_3	C127_3	108.0(8)
N30	P3	N31	111.8(3)	N67_3	C137_3	C147_3	113.4(10)
N30	P3	N32	104.9(2)	Li1	N17_4	Ce1	86.0(4)
N31	P3	N32	92.0(3)	P17_4	N17_4	Ce1	173.8(3)
P3	N3	Ce1	173.2(3)	P17_4	N17_4	Li1	98.3(5)
P3	N3	Li1	98.5(5)	N17_4	P17_4	N47_4	120.7(4)
Li1	N3	Ce1	86.4(4)	N17_4	P17_4	N57_4	113.0(4)
C301	N30	P3	121.6(4)	N17_4	P17_4	N67_4	115.4(3)
C303	N30	P3	121.2(4)	N47_4	P17_4	N57_4	92.6(3)
C303	N30	C301	117.0(5)	N67_4	P17_4	N47_4	108.5(3)
N30	C301	C302	114.9(6)	N67_4	P17_4	N57_4	103.1(3)
P3	N31	Li1	75.3(4)	P17_4	N47_4	Li1	70.4(4)
C31	N31	P3	124.2(5)	C17_4	N47_4	Li1	126.2(6)
C31	N31	Li1	99.0(5)	C17_4	N47_4	P17_4	113.2(4)
C33	N31	P3	111.2(5)	C17_4	N47_4	C77_4	115.6(5)
C33	N31	C31	114.6(5)	C77_4	N47_4	Li1	96.6(6)
C33	N31	Li1	128.1(6)	C77_4	N47_4	P17_4	126.4(4)
C32	N32	P3	124.1(4)	C27_4	N57_4	P17_4	112.9(4)
C34	N32	P3	111.4(4)	C27_4	N57_4	C37_4	119.9(6)
C34	N32	C32	119.7(4)	C37_4	N57_4	P17_4	124.8(6)
N31	C31	C311	110.3(6)	C117_4	N67_4	P17_4	116.3(5)
N31	C31	C312	109.0(7)	C137_4	N67_4	P17_4	120.6(5)
N31	C31	C313	113.3(7)	C137_4	N67_4	C117_4	120.4(6)
C312	C31	C311	106.0(7)	N47_4	C17_4	C27_4	106.9(5)
C313	C31	C311	109.0(8)	N57_4	C27_4	C17_4	106.4(6)
C313	C31	C312	108.9(7)	N57_4	C37_4	C47_4	109.3(7)
N32	C32	C321	113.0(6)	N57_4	C37_4	C57_4	111.5(7)
N32	C32	C322	107.9(6)	N57_4	C37_4	C67_4	110.9(7)
N32	C32	C323	108.7(7)	C57_4	C37_4	C47_4	107.2(8)
C321	C32	C322	108.2(7)	C67_4	C37_4	C47_4	110.2(8)
C323	C32	C321	109.0(7)	C67_4	C37_4	C57_4	107.7(8)
C323	C32	C322	110.1(10)	N47_4	C77_4	C87_4	111.3(7)
N31	C33	C34	104.5(5)	N47_4	C77_4	C97_4	110.0(6)
N32	C34	C33	107.1(5)	N47_4	C77_4	C107_4	109.1(7)
N9	P5	N50	113.4(3)	C87_4	C77_4	C97_4	108.9(8)
N9	P5	N51	120.9(3)	C87_4	C77_4	C107_4	109.0(7)
N9	P5	N52	119.8(3)	C107_4	C77_4	C97_4	108.6(7)
N50	P5	N51	103.9(3)	N67_4	C117_4	C127_4	114.1(7)
N50	P5	N52	104.6(3)	N67_4	C137_4	C147_4	114.5(6)
N52	P5	N51	90.9(3)	P17_6	N17_6	Ce2	160.2(4)
P5	N9	Ce2	172.2(4)	N17_6	P17_6	N47_6	125.6(6)
C501	N50	P5	121.9(5)	N17_6	P17_6	N57_6	120.8(5)
C501	N50	C503	116.7(6)	N17_6	P17_6	N67_6	108.5(5)
C503	N50	P5	121.3(4)	N47_6	P17_6	N57_6	90.8(5)
C51	N51	P5	121.7(4)	N67_6	P17_6	N47_6	104.2(6)
C53	N51	P5	109.2(4)	N67_6	P17_6	N57_6	103.9(6)
C53	N51	C51	114.3(5)	C17_6	N47_6	P17_6	114.4(6)
C52	N52	P5	125.9(4)	C17_6	N47_6	C77_6	118.2(8)

C54	N52	P5	114.6(4)	C77_6	N47_6	P17_6	125.7(8)
C54	N52	C52	118.9(5)	C27_6	N57_6	P17_6	108.6(7)
N51	C51	C511	108.2(4)	C37_6	N57_6	P17_6	122.7(7)
N51	C51	C512	108.0(5)	C37_6	N57_6	C27_6	114.7(8)
N51	C51	C513	111.6(4)	C117_6	N67_6	P17_6	119.5(9)
C511	C51	C512	108.7(4)	C137_6	N67_6	P17_6	120.7(9)
C511	C51	C513	109.5(5)	C137_6	N67_6	C117_6	119.1(10)
C512	C51	C513	110.9(6)	N47_6	C17_6	C27_6	107.2(8)
N52	C52	C521	111.5(4)	N57_6	C27_6	C17_6	103.1(8)
N52	C52	C522	109.4(4)	N57_6	C37_6	C47_6	111.1(8)
N52	C52	C523	109.4(4)	N57_6	C37_6	C57_6	109.6(8)
C522	C52	C521	108.4(5)	N57_6	C37_6	C67_6	110.1(8)
C523	C52	C521	108.2(6)	C57_6	C37_6	C47_6	107.8(9)
C523	C52	C522	109.9(6)	C67_6	C37_6	C47_6	109.1(9)
N51	C53	C54	104.3(6)	C67_6	C37_6	C57_6	109.1(9)
N52	C54	C53	106.7(6)	N47_6	C77_6	C87_6	109.2(10)
N50	C501	C502	114.1(6)	N47_6	C77_6	C97_6	108.7(10)
N50	C503	C504	114.8(7)	N47_6	C77_6	C107_6	110.7(9)
N3	Li1	N31	71.4(5)	C87_6	C77_6	C97_6	109.0(10)
N3	Li1	N17_3	104.6(5)	C107_6	C77_6	C87_6	110.7(10)
N3	Li1	N47_3	171.3(7)	C107_6	C77_6	C97_6	108.4(10)
N3	Li1	N17_4	104.6(5)	N67_6	C117_6	C127_6	112.7(11)
N3	Li1	P17_4	138.0(6)	N67_6	C137_6	C147_6	115.3(12)
N31	Li1	N47_3	117.3(5)	P17_7	N17_7	Ce2	172.5(4)
N31	Li1	P17_4	149.3(6)	N17_7	P17_7	N47_7	116.5(5)
N17_3	Li1	N31	164.6(7)	N17_7	P17_7	N57_7	117.3(4)
N17_3	Li1	N47_3	66.7(5)	N17_7	P17_7	N67_7	117.6(4)
N17_4	Li1	N31	164.6(7)	N47_7	P17_7	N57_7	90.6(3)
N17_4	Li1	P17_4	33.6(3)	N67_7	P17_7	N47_7	104.5(4)
N1_1	Li2	N3_1	72.1(7)	N67_7	P17_7	N57_7	106.4(4)
N1_2	Li2	P1_2	32.1(6)	C17_7	N47_7	P17_7	115.2(5)
N1_2	Li2	N17_9	109.0(10)	C17_7	N47_7	C77_7	116.9(7)
N17_8	Li2	N1_1	104.1(8)	C77_7	N47_7	P17_7	126.6(6)
N17_8	Li2	N3_1	170.1(10)	C27_7	N57_7	P17_7	111.9(5)
N17_9	Li2	P1_2	141.0(9)	C27_7	N57_7	C37_7	116.6(5)
P1	N1	Ce1	166.8(4)	C37_7	N57_7	P17_7	123.7(5)
N1	P1	N4	117.4(5)	C117_7	N67_7	P17_7	120.2(6)
N1	P1	N5	117.5(5)	C137_7	N67_7	P17_7	120.4(6)
N1	P1	N6	114.9(4)	C137_7	N67_7	C117_7	119.4(7)
N4	P1	N5	92.2(3)	N47_7	C17_7	C27_7	107.3(6)
N6	P1	N4	108.5(3)	N57_7	C27_7	C17_7	105.5(6)
N6	P1	N5	103.5(4)	N57_7	C37_7	C47_7	110.9(8)
C1	N4	P1	112.1(4)	N57_7	C37_7	C57_7	110.8(7)
C1	N4	C7	115.9(5)	N57_7	C37_7	C67_7	106.9(8)
C7	N4	P1	126.5(4)	C47_7	C37_7	C57_7	108.7(8)
C2	N5	P1	113.7(4)	C47_7	C37_7	C67_7	111.2(9)
C2	N5	C3	120.4(6)	C57_7	C37_7	C67_7	108.2(8)
C3	N5	P1	125.1(5)	N47_7	C77_7	C87_7	110.4(8)
C11	N6	P1	117.2(5)	N47_7	C77_7	C97_7	109.1(8)
C13	N6	P1	121.3(5)	N47_7	C77_7	C107_7	111.0(8)
C13	N6	C11	121.0(6)	C97_7	C77_7	C87_7	109.8(9)
N4	C1	C2	106.6(5)	C97_7	C77_7	C107_7	108.2(9)
N5	C2	C1	107.3(5)	C107_7	C77_7	C87_7	108.3(8)
N5	C3	C4	109.4(7)	N67_7	C117_7	C127_7	111.4(8)
N5	C3	C5	111.6(7)	N67_7	C137_7	C147_7	112.1(8)
N5	C3	C6	110.8(7)	Li2	N17_8	Ce2	89.2(7)
C5	C3	C4	107.2(8)	P17_8	N17_8	Ce2	150.0(4)
C6	C3	C4	110.1(8)	P17_8	N17_8	Li2	120.8(8)

C6	C3	C5	107.6(8)	N17_8	P17_8	N47_8	120.2(5)
N4	C7	C8	111.4(6)	N17_8	P17_8	N57_8	101.1(4)
N4	C7	C9	110.1(6)	N17_8	P17_8	N67_8	124.4(4)
N4	C7	C10	109.2(7)	N57_8	P17_8	N47_8	93.2(3)
C8	C7	C9	108.8(8)	N67_8	P17_8	N47_8	105.2(4)
C8	C7	C10	108.8(7)	N67_8	P17_8	N57_8	107.0(3)
C10	C7	C9	108.4(7)	C17_8	N47_8	P17_8	111.0(5)
N6	C11	C12	114.3(7)	C17_8	N47_8	C77_8	115.7(6)
N6	C13	C14	114.6(7)	C77_8	N47_8	P17_8	121.6(6)
P1B	N1B	Ce1	170.6(5)	C27_8	N57_8	P17_8	112.2(4)
N1B	P1B	N4B	122.7(6)	C37_8	N57_8	P17_8	126.0(5)
N1B	P1B	N5B	122.0(6)	C37_8	N57_8	C27_8	118.5(6)
N1B	P1B	N6B	109.5(6)	C117_8	N67_8	P17_8	121.5(6)
N5B	P1B	N4B	90.9(4)	C137_8	N67_8	P17_8	123.3(6)
N6B	P1B	N4B	102.9(6)	C137_8	N67_8	C117_8	113.3(7)
N6B	P1B	N5B	106.0(6)	N47_8	C17_8	C27_8	106.1(7)
C1B	N4B	P1B	106.0(6)	N57_8	C27_8	C17_8	106.0(7)
C1B	N4B	C7B	114.2(8)	N57_8	C37_8	C47_8	110.9(9)
C7B	N4B	P1B	117.9(7)	N57_8	C37_8	C57_8	111.9(8)
C2B	N5B	P1B	113.9(6)	N57_8	C37_8	C67_8	111.4(8)
C2B	N5B	C3B	117.3(7)	C57_8	C37_8	C47_8	107.1(8)
C3B	N5B	P1B	128.8(7)	C57_8	C37_8	C67_8	107.1(9)
C11B	N6B	P1B	122.4(8)	C67_8	C37_8	C47_8	108.2(8)
C13B	N6B	P1B	120.5(8)	N47_8	C77_8	C87_8	111.0(8)
C13B	N6B	C11B	117.1(9)	N47_8	C77_8	C107_8	108.8(8)
N4B	C1B	C2B	102.3(7)	C87_8	C77_8	C107_8	107.2(8)
N5B	C2B	C1B	104.9(7)	C97_8	C77_8	N47_8	109.6(8)
N5B	C3B	C4B	110.4(9)	C97_8	C77_8	C87_8	110.4(9)
N5B	C3B	C5B	112.4(9)	C97_8	C77_8	C107_8	109.8(9)
N5B	C3B	C6B	109.2(9)	N67_8	C117_8	C127_8	109.1(7)
C4B	C3B	C6B	107.8(10)	N67_8	C137_8	C147_8	110.5(7)
C5B	C3B	C4B	109.2(10)	Li2	N17_9	Ce2	82.9(6)
C5B	C3B	C6B	107.7(10)	P17_9	N17_9	Ce2	177.3(5)
N4B	C7B	C8B	110.6(8)	P17_9	N17_9	Li2	95.7(8)
N4B	C7B	C9B	108.8(9)	N17_9	P17_9	N47_9	123.4(6)
N4B	C7B	C10B	109.5(9)	N17_9	P17_9	N57_9	126.2(6)
C8B	C7B	C10B	108.0(9)	N17_9	P17_9	N67_9	104.2(4)
C9B	C7B	C8B	111.0(9)	N47_9	P17_9	N57_9	94.1(5)
C9B	C7B	C10B	109.0(9)	N47_9	P17_9	N67_9	103.3(6)
N6B	C11B	C12B	111.4(11)	N57_9	P17_9	N67_9	102.2(6)
N6B	C13B	C14B	114.4(11)	C17_9	N47_9	P17_9	112.9(7)
N30	C303	C304	114.7(9)	C17_9	N47_9	C77_9	117.4(8)
N30	C303	C30D	118.4(8)	C77_9	N47_9	P17_9	129.5(8)
C91	O1	C93	111.0(7)	C27_9	N57_9	P17_9	111.8(7)
O1	C91	C92	109.2(7)	C27_9	N57_9	C37_9	114.6(8)
O1	C93	C94'	110.8(11)	C37_9	N57_9	P17_9	125.8(7)
O1	C93	C94	109.6(13)	C117_9	N67_9	P17_9	111.5(7)
Li2	N1_1	Ce2	85.6(6)	C117_9	N67_9	C137_9	116.1(9)
P1_1	N1_1	Ce2	179.5(4)	C137_9	N67_9	P17_9	109.1(7)
P1_1	N1_1	Li2	94.7(7)	N47_9	C17_9	C27_9	106.9(8)
N1_1	P1_1	N2_1	121.0(4)	N57_9	C27_9	C17_9	105.1(8)
N1_1	P1_1	N3_1	114.8(4)	N57_9	C37_9	C47_9	111.1(9)
N1_1	P1_1	N4_1	114.5(4)	N57_9	C37_9	C57_9	108.7(9)
N2_1	P1_1	N3_1	92.2(4)	N57_9	C37_9	C67_9	111.2(9)
N4_1	P1_1	N2_1	104.0(4)	C47_9	C37_9	C57_9	108.9(9)
N4_1	P1_1	N3_1	107.5(4)	C47_9	C37_9	C67_9	108.6(9)
C1_1	N2_1	P1_1	111.1(5)	C67_9	C37_9	C57_9	108.3(9)
C1_1	N2_1	C7_1	116.5(6)	N47_9	C77_9	C87_9	113.5(11)

C7_1	N2_1	P1_1	125.6(6)	N47_9	C77_9	C97_9	110.0(10)
P1_1	N3_1	Li2	76.4(5)	N47_9	C77_9	C107_9	109.7(10)
C2_1	N3_1	Li2	120.8(8)	C87_9	C77_9	C97_9	107.3(10)
C2_1	N3_1	P1_1	112.8(5)	C87_9	C77_9	C107_9	108.5(10)
C3_1	N3_1	Li2	96.0(7)	C97_9	C77_9	C107_9	107.7(10)
C3_1	N3_1	P1_1	128.8(6)	N67_9	C117_9	C127_9	112.5(9)
C3_1	N3_1	C2_1	114.1(6)	N67_9	C137_9	C147_9	111.9(10)

Table S17. Bond lengths for **2-Ce^{Na}**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ce1	N1A	2.3594(12)	C41A	C42A	1.520(3)
Ce1	N2A	2.3850(13)	C39A	C40A	1.514(3)
Ce1	N4A	2.3069(13)	P1B	N1B	1.5298(15)
Ce1	N3A	2.2864(13)	P1B	N5B	1.7167(14)
Ce1	N1B	2.3594(12)	P1B	N6B	1.7163(14)
Ce1	N4B	2.3069(13)	P1B	N7B	1.6733(16)
Ce1	N3B	2.2864(13)	N1B	Na1B	2.368(6)
Na1A	N1A	2.404(6)	N5B	C1B	1.457(2)
Na1A	N5A	2.692(6)	N5B	C7B	1.4769(18)
Na1A	N2A	2.362(6)	N5B	Na1B	2.743(6)
Na1A	N8A	2.672(6)	N6B	C2B	1.450(2)
P1A	N1A	1.5347(15)	N6B	C3B	1.4902(18)
P1A	N5A	1.7131(14)	N7B	C13B	1.462(2)
P1A	N6A	1.7155(14)	N7B	C11B	1.470(2)
P1A	N7A	1.6752(16)	C1B	C2B	1.510(3)
N5A	C1A	1.459(2)	C7B	C10B	1.529(2)
N5A	C7A	1.4798(18)	C7B	C8B	1.547(2)
N6A	C2A	1.452(2)	C7B	C9B	1.532(2)
N6A	C3A	1.4881(18)	C3B	C4B	1.543(3)
N7A	C13A	1.462(2)	C3B	C5B	1.524(2)
N7A	C11A	1.471(2)	C3B	C6B	1.506(2)
C1A	C2A	1.510(3)	C13B	C14B	1.520(3)
C7A	C8A	1.525(2)	C11B	C12B	1.514(3)
C7A	C9A	1.548(2)	P2B	N2B	1.5315(15)
C7A	C10A	1.532(2)	P2B	N8B	1.7149(14)
C3A	C4A	1.543(3)	P2B	N9B	1.7151(14)
C3A	C5A	1.524(2)	P2B	N10B	1.6741(16)
C3A	C6A	1.507(2)	N2B	Na1B	2.402(6)
C13A	C14A	1.521(3)	N8B	C15B	1.463(2)
C11A	C12A	1.514(3)	N8B	C21B	1.4775(18)
P2A	N2A	1.5306(16)	N9B	C16B	1.453(2)
P2A	N8A	1.7190(15)	N9B	C17B	1.4825(18)
P2A	N9A	1.7107(15)	N10B	C27B	1.458(2)
P2A	N10A	1.6780(17)	N10B	C25B	1.469(2)
N8A	C15A	1.465(2)	C15B	C16B	1.506(3)
N8A	C21A	1.4777(19)	C21B	C22B	1.523(2)
N9A	C16A	1.447(2)	C21B	C23B	1.549(2)
N9A	C17A	1.4766(19)	C21B	C24B	1.535(2)
N10A	C27A	1.460(2)	C17B	C18B	1.547(3)
N10A	C25A	1.470(2)	C17B	C19B	1.521(3)
C15A	C16A	1.509(3)	C17B	C20B	1.511(2)
C21A	C22A	1.525(3)	C27B	C28B	1.518(3)
C21A	C23A	1.550(2)	C25B	C26B	1.513(3)
C21A	C24A	1.534(2)	P4B	N4B	1.5258(15)
C17A	C18A	1.547(3)	P4B	N15B	1.7196(14)
C17A	C19A	1.524(3)	P4B	N14B	1.7087(14)
C17A	C20A	1.511(3)	P4B	N16B	1.6813(16)

C27A	C28A	1.518(3)	N15B	C44B	1.462(2)
C25A	C26A	1.514(3)	N15B	C45B	1.4817(18)
P4A	N4A	1.5261(16)	N14B	C43B	1.437(2)
P4A	N15A	1.7158(15)	N14B	C49B	1.4724(18)
P4A	N14A	1.7101(15)	N16B	C55B	1.457(2)
P4A	N16A	1.6836(17)	N16B	C53B	1.470(2)
N15A	C44A	1.460(2)	C44B	C43B	1.510(3)
N15A	C45A	1.4801(19)	C45B	C46B	1.528(2)
N14A	C43A	1.441(2)	C45B	C47B	1.545(2)
N14A	C49A	1.4753(19)	C45B	C48B	1.529(2)
N16A	C55A	1.458(2)	C49B	C52B	1.550(3)
N16A	C53A	1.469(2)	C49B	C50B	1.526(3)
C44A	C43A	1.509(3)	C49B	C51B	1.511(3)
C45A	C46A	1.528(2)	C55B	C56B	1.523(3)
C45A	C47A	1.545(2)	C53B	C54B	1.512(3)
C45A	C48A	1.530(2)	P3B	N3B	1.5254(15)
C49A	C52A	1.549(3)	P3B	N12B	1.7123(14)
C49A	C50A	1.525(3)	P3B	N11B	1.7091(14)
C49A	C51A	1.511(3)	P3B	N13B	1.6864(16)
C55A	C56A	1.521(3)	N12B	C30B	1.461(2)
C53A	C54A	1.513(3)	N12B	C31B	1.4778(18)
P3A	N3A	1.5276(16)	N11B	C29B	1.437(2)
P3A	N12A	1.7183(15)	N11B	C35B	1.4703(18)
P3A	N11A	1.7058(14)	N13B	C41B	1.460(2)
P3A	N13A	1.6819(17)	N13B	C39B	1.470(2)
N12A	C30A	1.463(2)	C30B	C29B	1.510(3)
N12A	C31A	1.4793(19)	C31B	C32B	1.529(2)
N11A	C29A	1.436(2)	C31B	C33B	1.545(2)
N11A	C35A	1.4688(19)	C31B	C34B	1.531(2)
N13A	C41A	1.458(2)	C35B	C36B	1.549(3)
N13A	C39A	1.468(2)	C35B	C37B	1.528(3)
C30A	C29A	1.508(3)	C35B	C38B	1.512(3)
C31A	C32A	1.529(2)	C41B	C42B	1.520(3)
C31A	C33A	1.544(2)	C39B	C40B	1.512(3)
C31A	C34A	1.530(2)	O1S_1	C2S_1	1.419(2)
C35A	C38A	1.550(3)	O1S_1	C3S_1	1.4191(19)
C35A	C36A	1.525(2)	C1S_1	C2S_1	1.519(2)
C35A	C37A	1.515(2)	C3S_1	C4S_1	1.518(2)

Table S18. Bond angles for **2-Ce^{Na}**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1A	Ce1	N2A	89.99(6)	N11A	C35A	C37A	110.5(2)
N4A	Ce1	N1B	113.59(7)	C36A	C35A	C38A	107.0(2)
N3A	Ce1	N4A	110.47(7)	C37A	C35A	C38A	108.4(2)
N3A	Ce1	N1B	110.23(6)	C37A	C35A	C36A	109.5(2)
N4B	Ce1	N1A	113.59(7)	N13A	C41A	C42A	113.4(3)
N4B	Ce1	N2A	117.21(7)	N13A	C39A	C40A	114.5(3)
N3B	Ce1	N1A	110.23(6)	N1B	P1B	N5B	115.82(12)
N3B	Ce1	N2A	113.82(7)	N1B	P1B	N6B	119.00(12)
N3B	Ce1	N4B	110.47(7)	N1B	P1B	N7B	113.53(11)
N1A	Na1A	N5A	65.25(13)	N6B	P1B	N5B	92.04(9)
N1A	Na1A	N8A	153.2(3)	N7B	P1B	N5B	108.15(11)
N2A	Na1A	N1A	89.5(2)	N7B	P1B	N6B	105.92(11)
N2A	Na1A	N5A	154.5(3)	Ce1	N1B	Na1B	90.98(14)
N2A	Na1A	N8A	65.40(13)	P1B	N1B	Ce1	173.94(12)
N8A	Na1A	N5A	140.1(3)	P1B	N1B	Na1B	95.00(17)
N1A	P1A	N5A	116.12(14)	P1B	N5B	Na1B	78.41(16)
N1A	P1A	N6A	119.72(14)	C1B	N5B	P1B	111.79(13)

N1A	P1A	N7A	112.57(13)	C1B	N5B	C7B	117.84(15)
N5A	P1A	N6A	92.13(10)	C1B	N5B	Na1B	114.0(3)
N7A	P1A	N5A	108.33(13)	C7B	N5B	P1B	124.79(14)
N7A	P1A	N6A	105.79(13)	C7B	N5B	Na1B	101.2(2)
Ce1	N1A	Na1A	89.98(14)	C2B	N6B	P1B	111.62(13)
P1A	N1A	Ce1	173.85(14)	C2B	N6B	C3B	117.40(17)
P1A	N1A	Na1A	94.76(17)	C3B	N6B	P1B	121.39(14)
P1A	N5A	Na1A	81.05(17)	C13B	N7B	P1B	120.90(15)
C1A	N5A	Na1A	120.4(3)	C13B	N7B	C11B	116.11(17)
C1A	N5A	P1A	111.89(14)	C11B	N7B	P1B	122.28(16)
C1A	N5A	C7A	116.81(17)	N5B	C1B	C2B	105.91(16)
C7A	N5A	Na1A	95.7(2)	N6B	C2B	C1B	105.78(17)
C7A	N5A	P1A	124.45(16)	N5B	C7B	C10B	111.15(17)
C2A	N6A	P1A	111.64(15)	N5B	C7B	C8B	109.92(17)
C2A	N6A	C3A	117.62(18)	N5B	C7B	C9B	111.08(17)
C3A	N6A	P1A	122.12(15)	C10B	C7B	C8B	107.56(17)
C13A	N7A	P1A	120.48(17)	C10B	C7B	C9B	108.65(18)
C13A	N7A	C11A	115.7(2)	C9B	C7B	C8B	108.38(18)
C11A	N7A	P1A	122.50(18)	N6B	C3B	C4B	109.15(17)
N5A	C1A	C2A	105.90(18)	N6B	C3B	C5B	110.09(17)
N6A	C2A	C1A	105.82(18)	N6B	C3B	C6B	110.29(17)
N5A	C7A	C8A	110.84(19)	C5B	C3B	C4B	107.95(15)
N5A	C7A	C9A	109.62(19)	C6B	C3B	C4B	109.23(16)
N5A	C7A	C10A	111.31(19)	C6B	C3B	C5B	110.09(16)
C8A	C7A	C9A	107.8(2)	N7B	C13B	C14B	113.9(2)
C8A	C7A	C10A	108.9(2)	N7B	C11B	C12B	116.0(2)
C10A	C7A	C9A	108.2(2)	N2B	P2B	N8B	115.92(13)
C7A	C8A	Na1A	80.6(2)	N2B	P2B	N9B	118.98(13)
N6A	C3A	C4A	109.08(19)	N2B	P2B	N10B	113.44(12)
N6A	C3A	C5A	110.66(19)	N8B	P2B	N9B	91.99(9)
N6A	C3A	C6A	110.02(19)	N10B	P2B	N8B	108.58(13)
C5A	C3A	C4A	107.5(2)	N10B	P2B	N9B	105.57(13)
C6A	C3A	C4A	109.3(2)	Ce1	N2B	Na1B	89.53(15)
C6A	C3A	C5A	110.2(2)	P2B	N2B	Ce1	170.17(14)
N7A	C13A	C14A	113.4(2)	P2B	N2B	Na1B	94.37(18)
N7A	C11A	C12A	114.7(2)	C15B	N8B	P2B	111.89(14)
N2A	P2A	N8A	114.29(16)	C15B	N8B	C21B	116.83(17)
N2A	P2A	N9A	121.66(16)	C21B	N8B	P2B	125.61(16)
N2A	P2A	N10A	112.37(14)	C16B	N9B	P2B	111.36(15)
N9A	P2A	N8A	91.52(11)	C16B	N9B	C17B	117.32(18)
N10A	P2A	N8A	110.18(15)	C17B	N9B	P2B	122.85(15)
N10A	P2A	N9A	104.76(15)	C27B	N10B	P2B	121.30(17)
Na1A	N2A	Ce1	90.37(15)	C27B	N10B	C25B	116.33(19)
P2A	N2A	Ce1	170.71(15)	C25B	N10B	P2B	122.22(17)
P2A	N2A	Na1A	95.02(18)	N8B	C15B	C16B	105.94(18)
P2A	N8A	Na1A	80.34(17)	N9B	C16B	C15B	105.47(18)
C15A	N8A	Na1A	117.5(3)	N8B	C21B	C22B	111.66(18)
C15A	N8A	P2A	111.85(16)	N8B	C21B	C23B	109.83(18)
C15A	N8A	C21A	115.36(19)	N8B	C21B	C24B	110.65(18)
C21A	N8A	Na1A	96.5(2)	C22B	C21B	C23B	107.64(19)
C21A	N8A	P2A	127.72(18)	C22B	C21B	C24B	108.9(2)
C16A	N9A	P2A	112.00(17)	C24B	C21B	C23B	108.05(19)
C16A	N9A	C17A	118.4(2)	N9B	C17B	C18B	109.15(19)
C17A	N9A	P2A	124.64(17)	N9B	C17B	C19B	110.93(19)
C27A	N10A	P2A	120.1(2)	N9B	C17B	C20B	110.33(19)
C27A	N10A	C25A	116.0(2)	C19B	C17B	C18B	107.99(17)
C25A	N10A	P2A	122.4(2)	C20B	C17B	C18B	108.54(17)
N8A	C15A	C16A	105.1(2)	C20B	C17B	C19B	109.84(17)

N9A	C16A	C15A	105.3(2)	N10B	C27B	C28B	114.3(2)
N8A	C21A	C22A	111.6(2)	N10B	C25B	C26B	116.2(2)
N8A	C21A	C23A	109.6(2)	N4B	P4B	N15B	116.99(13)
N8A	C21A	C24A	111.3(2)	N4B	P4B	N14B	119.24(14)
C22A	C21A	C23A	108.0(2)	N4B	P4B	N16B	113.43(13)
C22A	C21A	C24A	108.7(2)	N14B	P4B	N15B	91.89(9)
C24A	C21A	C23A	107.6(2)	N16B	P4B	N15B	106.81(13)
N9A	C17A	C18A	109.1(2)	N16B	P4B	N14B	105.93(13)
N9A	C17A	C19A	111.7(2)	P4B	N4B	Ce1	169.90(14)
N9A	C17A	C20A	110.0(2)	C44B	N15B	P4B	111.00(14)
C19A	C17A	C18A	107.2(2)	C44B	N15B	C45B	117.24(18)
C20A	C17A	C18A	108.8(2)	C45B	N15B	P4B	123.44(16)
C20A	C17A	C19A	109.9(2)	C43B	N14B	P4B	113.15(14)
N10A	C27A	C28A	115.2(3)	C43B	N14B	C49B	119.97(17)
N10A	C25A	C26A	115.7(3)	C49B	N14B	P4B	124.34(16)
N4A	P4A	N15A	118.58(16)	C55B	N16B	P4B	121.14(17)
N4A	P4A	N14A	120.03(17)	C55B	N16B	C53B	116.43(19)
N4A	P4A	N16A	111.92(15)	C53B	N16B	P4B	121.57(18)
N14A	P4A	N15A	91.72(11)	N15B	C44B	C43B	105.76(18)
N16A	P4A	N15A	106.10(15)	N14B	C43B	C44B	106.50(18)
N16A	P4A	N14A	106.05(15)	N15B	C45B	C46B	110.71(19)
P4A	N4A	Ce1	173.05(16)	N15B	C45B	C47B	109.74(17)
C44A	N15A	P4A	111.54(16)	N15B	C45B	C48B	110.83(18)
C44A	N15A	C45A	117.4(2)	C46B	C45B	C47B	107.68(19)
C45A	N15A	P4A	122.77(18)	C46B	C45B	C48B	108.99(19)
C43A	N14A	P4A	113.19(16)	C48B	C45B	C47B	108.81(19)
C43A	N14A	C49A	119.40(19)	N14B	C49B	C52B	109.51(19)
C49A	N14A	P4A	125.37(18)	N14B	C49B	C50B	110.89(19)
C55A	N16A	P4A	120.5(2)	N14B	C49B	C51B	111.04(19)
C55A	N16A	C53A	116.3(2)	C50B	C49B	C52B	107.51(16)
C53A	N16A	P4A	122.0(2)	C51B	C49B	C52B	108.27(16)
N15A	C44A	C43A	105.8(2)	C51B	C49B	C50B	109.52(17)
N14A	C43A	C44A	106.5(2)	N16B	C55B	C56B	113.8(2)
N15A	C45A	C46A	110.1(2)	N16B	C53B	C54B	116.3(2)
N15A	C45A	C47A	109.9(2)	N3B	P3B	N12B	117.68(13)
N15A	C45A	C48A	110.9(2)	N3B	P3B	N11B	119.36(14)
C46A	C45A	C47A	108.1(2)	N3B	P3B	N13B	112.81(13)
C46A	C45A	C48A	109.1(2)	N11B	P3B	N12B	91.95(9)
C48A	C45A	C47A	108.7(2)	N13B	P3B	N12B	107.15(13)
N14A	C49A	C52A	109.2(2)	N13B	P3B	N11B	105.42(13)
N14A	C49A	C50A	111.1(2)	P3B	N3B	Ce1	176.45(14)
N14A	C49A	C51A	110.6(2)	C30B	N12B	P3B	111.50(14)
C50A	C49A	C52A	107.2(2)	C30B	N12B	C31B	117.69(18)
C51A	C49A	C52A	108.4(2)	C31B	N12B	P3B	124.54(15)
C51A	C49A	C50A	110.3(2)	C29B	N11B	P3B	113.04(14)
N16A	C55A	C56A	113.7(3)	C29B	N11B	C35B	120.12(17)
N16A	C53A	C54A	115.7(3)	C35B	N11B	P3B	124.51(15)
N3A	P3A	N12A	116.95(15)	C41B	N13B	P3B	120.33(17)
N3A	P3A	N11A	120.58(16)	C41B	N13B	C39B	116.17(19)
N3A	P3A	N13A	112.29(14)	C39B	N13B	P3B	121.24(19)
N11A	P3A	N12A	91.64(11)	N12B	C30B	C29B	105.87(18)
N13A	P3A	N12A	107.27(15)	N11B	C29B	C30B	106.48(18)
N13A	P3A	N11A	105.73(15)	N12B	C31B	C32B	110.79(19)
P3A	N3A	Ce1	172.84(15)	N12B	C31B	C33B	109.97(18)
C30A	N12A	P3A	110.25(16)	N12B	C31B	C34B	110.85(19)
C30A	N12A	C31A	117.1(2)	C32B	C31B	C33B	107.64(19)
C31A	N12A	P3A	123.25(17)	C32B	C31B	C34B	108.77(19)
C29A	N11A	P3A	113.77(15)	C34B	C31B	C33B	108.7(2)

C29A	N11A	C35A	120.55(18)	N11B	C35B	C36B	109.62(19)
C35A	N11A	P3A	125.67(17)	N11B	C35B	C37B	110.93(19)
C41A	N13A	P3A	120.57(19)	N11B	C35B	C38B	111.08(19)
C41A	N13A	C39A	116.2(2)	C37B	C35B	C36B	107.47(16)
C39A	N13A	P3A	122.4(2)	C38B	C35B	C36B	108.30(16)
N12A	C30A	C29A	105.9(2)	C38B	C35B	C37B	109.34(17)
N11A	C29A	C30A	107.64(19)	N13B	C41B	C42B	113.7(2)
N12A	C31A	C32A	110.2(2)	N13B	C39B	C40B	116.1(2)
N12A	C31A	C33A	110.0(2)	N1B	Na1B	N2B	89.4(2)
N12A	C31A	C34A	111.3(2)	N1B	Na1B	N8B	154.7(3)
C32A	C31A	C33A	107.8(2)	N2B	Na1B	N8B	65.38(13)
C32A	C31A	C34A	108.8(2)	C2S_1	O1S_1	C3S_1	113.5(3)
C34A	C31A	C33A	108.7(2)	O1S_1	C2S_1	C1S_1	108.7(2)
N11A	C35A	C38A	109.5(2)	O1S_1	C3S_1	C4S_1	108.7(3)
N11A	C35A	C36A	111.9(2)				

Table S19. Bond lengths for **2-Ce**^{K18c6}.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ce1	N1_4	2.326(7)	P1_5	N1_5	1.547(7)
Ce1	N1_5	2.319(7)	P1_5	N6_5	1.694(9)
Ce1	N3_7	2.334(8)	P1_5	N5_5	1.711(9)
Ce1	N2_8	2.376(7)	P1_5	N7_5	1.684(11)
Ce1	N1_9	2.376(7)	N6_5	C2_5	1.413(14)
Ce1	N4_10	2.326(7)	N6_5	C3_5	1.463(9)
K1A	O1S	2.728(12)	N5_5	C1_5	1.409(14)
K1A	O2	2.708(15)	N5_5	C7_5	1.463(9)
K1A	O1C_2	2.816(13)	N7_5	C11_5	1.443(13)
K1A	O2C_2	2.908(12)	N7_5	C13_5	1.440(14)
K1A	O5C_2	2.856(12)	C1_5	C2_5	1.502(12)
K1A	O6C_2	2.862(13)	C7_5	C10_5	1.525(16)
K1B	O1S	2.824(12)	C7_5	C9_5	1.497(15)
K1B	O1C_3	2.876(12)	C7_5	C8_5	1.535(14)
K1B	O2C_3	2.891(12)	C3_5	C6_5	1.528(7)
K1B	O3C_3	2.863(11)	C3_5	C5_5	1.529(7)
K1B	O4C_3	2.850(12)	C3_5	C4_5	1.528(7)
K1B	O5C_3	2.826(12)	C11_5	C12_5	1.5265(19)
K1B	O6C_3	2.873(13)	C13_5	C14_5	1.5262(18)
O2S	C2S	1.424(4)	P3_7	N3_7	1.527(8)
O2S	C3S	1.425(4)	P3_7	N12_7	1.704(8)
O1S	C1S	1.424(4)	P3_7	N11_7	1.694(8)
O1S	C12S	1.424(4)	P3_7	N13_7	1.673(9)
O2	C11S	1.425(3)	N12_7	C30_7	1.458(12)
O2	C10S	1.424(3)	N12_7	C31_7	1.476(13)
O3S	C4S	1.423(4)	N11_7	C29_7	1.452(11)
O3S	C5S	1.426(4)	N11_7	C35_7	1.483(15)
C6S	O4S	1.419(4)	N13_7	C39_7	1.465(13)
C6S	C5S	1.5050(2)	N13_7	C41_7	1.472(14)
O4S	C7S	1.427(4)	C29_7	C30_7	1.520(13)
C1S	C2S	1.5050(2)	C35_7	C36_7	1.521(13)
C12S	C11S	1.5050(2)	C35_7	C38_7	1.534(14)
C8S	C7S	1.5050(2)	C35_7	C37_7	1.545(12)
C8S	O5S	1.425(4)	C31_7	C34_7	1.543(13)
C3S	C4S	1.5050(2)	C31_7	C33_7	1.537(13)
C9S	O5S	1.423(4)	C31_7	C32_7	1.533(12)
C9S	C10S	1.5050(2)	C39_7	C40_7	1.524(14)
O1T	C1T	1.425(2)	C41_7	C42_7	1.531(15)
O1T	C3T	1.425(2)	P2_8	N2_8	1.438(12)

C1T	C2T	1.505(2)	P2_8	N9_8	1.76(2)
C4T	C3T	1.505(2)	P2_8	N8_8	1.72(2)
O1C_2	C1C_2	1.4248(15)	P2_8	N10_8	1.70(2)
O1C_2	C12C_2	1.4250(16)	N9_8	C16_8	1.47(3)
O2C_2	C2C_2	1.4250(15)	N9_8	C17_8	1.47(3)
O2C_2	C3C_2	1.4246(15)	N8_8	C15_8	1.47(3)
O3C_2	C4C_2	1.4246(15)	N8_8	C21_8	1.53(3)
O3C_2	C5C_2	1.4248(16)	N10_8	C25_8	1.51(3)
O4C_2	C6C_2	1.4242(15)	N10_8	C27_8	1.45(3)
O4C_2	C7C_2	1.4246(15)	C15_8	C16_8	1.57(3)
O5C_2	C8C_2	1.425(3)	C21_8	C24_8	1.55(4)
O5C_2	C9C_2	1.424(3)	C21_8	C23_8	1.47(3)
O6C_2	C10C_2	1.424(3)	C21_8	C22_8	1.56(3)
O6C_2	C11C_2	1.423(3)	C17_8	C20_8	1.528(6)
C1C_2	C2C_2	1.498(12)	C17_8	C19_8	1.528(6)
C3C_2	C4C_2	1.509(12)	C17_8	C18_8	1.528(6)
C5C_2	C6C_2	1.499(11)	C25_8	C26_8	1.48(3)
C7C_2	C8C_2	1.518(12)	C27_8	C28_8	1.525(2)
C9C_2	C10C_2	1.530(15)	P1_9	N1_9	1.552(7)
C11C_2	C12C_2	1.510(12)	P1_9	N5_9	1.695(9)
O1C_3	C1C_3	1.4251(15)	P1_9	N6_9	1.706(9)
O1C_3	C12C_3	1.4252(16)	P1_9	N7_9	1.687(11)
O2C_3	C2C_3	1.4248(15)	N5_9	C2_9	1.420(14)
O2C_3	C3C_3	1.4252(15)	N5_9	C7_9	1.466(10)
O3C_3	C4C_3	1.4247(15)	N6_9	C1_9	1.402(14)
O3C_3	C5C_3	1.4248(16)	N6_9	C3_9	1.456(10)
O4C_3	C6C_3	1.4248(15)	N7_9	C11_9	1.446(14)
O4C_3	C7C_3	1.4246(15)	N7_9	C13_9	1.443(14)
O5C_3	C8C_3	1.425(3)	C1_9	C2_9	1.504(13)
O5C_3	C9C_3	1.424(3)	C3_9	C4_9	1.526(16)
O6C_3	C10C_3	1.425(3)	C3_9	C5_9	1.498(16)
O6C_3	C11C_3	1.424(3)	C3_9	C6_9	1.536(14)
C1C_3	C2C_3	1.499(12)	C7_9	C8_9	1.528(6)
C3C_3	C4C_3	1.508(12)	C7_9	C9_9	1.528(6)
C5C_3	C6C_3	1.498(11)	C7_9	C10_9	1.528(6)
C7C_3	C8C_3	1.519(12)	C11_9	C12_9	1.525(4)
C9C_3	C10C_3	1.529(15)	C13_9	C14_9	1.5248(18)
C11C_3	C12C_3	1.510(12)	P4_10	N4_10	1.504(18)
P1_4	N1_4	1.549(7)	P4_10	N14_10	1.69(2)
P1_4	N5_4	1.693(9)	P4_10	N15_10	1.79(2)
P1_4	N6_4	1.711(9)	P4_10	N16_10	1.68(2)
P1_4	N7_4	1.685(11)	N14_10	C43_10	1.44(3)
N5_4	C2_4	1.413(14)	N14_10	C49_10	1.49(3)
N5_4	C7_4	1.460(10)	N15_10	C44_10	1.52(3)
N6_4	C1_4	1.408(14)	N15_10	C45_10	1.46(3)
N6_4	C3_4	1.461(10)	N16_10	C53_10	1.46(3)
N7_4	C11_4	1.441(14)	N16_10	C55_10	1.48(3)
N7_4	C13_4	1.438(14)	C44_10	C43_10	1.506(12)
C1_4	C2_4	1.506(12)	C45_10	C46_10	1.50(4)
C3_4	C4_4	1.526(16)	C45_10	C48_10	1.60(3)
C3_4	C5_4	1.497(16)	C45_10	C47_10	1.57(3)
C3_4	C6_4	1.535(14)	C49_10	C52_10	1.51(3)
C7_4	C8_4	1.530(7)	C49_10	C51_10	1.57(3)
C7_4	C9_4	1.530(7)	C49_10	C50_10	1.51(3)
C7_4	C10_4	1.528(7)	C53_10	C54_10	1.525(2)
C11_4	C12_4	1.5250(19)	C55_10	C56_10	1.524(2)
C13_4	C14_4	1.5236(18)			

Table S20. Bond angles for **2-Ce**K18c6.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1_4	Ce1	N3_7	110.2(3)	N5_4	C7_4	C8_4	111.1(9)
N1_4	Ce1	N1_9	109.9(3)	N5_4	C7_4	C9_4	111.0(9)
N1_5	Ce1	N1_4	105.5(3)	N5_4	C7_4	C10_4	110.5(9)
N1_5	Ce1	N3_7	107.3(3)	C8_4	C7_4	C9_4	106.8(9)
N1_5	Ce1	N2_8	116.0(3)	C10_4	C7_4	C8_4	107.3(9)
N1_5	Ce1	N1_9	116.0(3)	C10_4	C7_4	C9_4	110.0(9)
N1_5	Ce1	N4_10	105.5(3)	N7_4	C11_4	C12_4	116.2(10)
N3_7	Ce1	N2_8	107.8(3)	N7_4	C13_4	C14_4	124.2(10)
N3_7	Ce1	N1_9	107.8(3)	N1_5	P1_5	N6_5	120.7(5)
N4_10	Ce1	N3_7	110.2(3)	N1_5	P1_5	N5_5	119.4(4)
N4_10	Ce1	N2_8	109.9(3)	N1_5	P1_5	N7_5	113.3(5)
O1S	K1A	O1C_2	101.6(4)	N6_5	P1_5	N5_5	91.2(4)
O1S	K1A	O2C_2	79.5(4)	N7_5	P1_5	N6_5	103.6(5)
O1S	K1A	O5C_2	128.7(4)	N7_5	P1_5	N5_5	105.3(5)
O1S	K1A	O6C_2	146.9(4)	P1_5	N1_5	Ce1	157.3(5)
O2	K1A	O1S	61.7(3)	C2_5	N6_5	P1_5	113.8(7)
O2	K1A	O1C_2	77.7(4)	C2_5	N6_5	C3_5	119.0(8)
O2	K1A	O2C_2	113.2(4)	C3_5	N6_5	P1_5	125.2(7)
O2	K1A	O5C_2	95.1(4)	C1_5	N5_5	P1_5	112.3(7)
O2	K1A	O6C_2	86.6(4)	C1_5	N5_5	C7_5	119.0(9)
O1C_2	K1A	O2C_2	58.7(3)	C7_5	N5_5	P1_5	121.9(7)
O1C_2	K1A	O5C_2	118.2(4)	C11_5	N7_5	P1_5	121.5(7)
O1C_2	K1A	O6C_2	59.4(3)	C13_5	N7_5	P1_5	119.5(8)
O5C_2	K1A	O2C_2	148.3(4)	C13_5	N7_5	C11_5	117.8(9)
O5C_2	K1A	O6C_2	58.9(3)	N5_5	C1_5	C2_5	107.4(9)
O6C_2	K1A	O2C_2	107.0(4)	N6_5	C2_5	C1_5	109.1(9)
O1S	K1B	O1C_3	90.4(4)	N5_5	C7_5	C10_5	112.0(9)
O1S	K1B	O2C_3	80.8(4)	N5_5	C7_5	C9_5	110.2(9)
O1S	K1B	O3C_3	76.9(4)	N5_5	C7_5	C8_5	110.4(8)
O1S	K1B	O4C_3	106.1(4)	C10_5	C7_5	C8_5	106.7(9)
O1S	K1B	O5C_3	127.2(4)	C9_5	C7_5	C10_5	106.6(9)
O1S	K1B	O6C_3	130.1(4)	C9_5	C7_5	C8_5	110.9(10)
O1C_3	K1B	O2C_3	58.3(3)	N6_5	C3_5	C6_5	111.0(8)
O3C_3	K1B	O1C_3	116.7(3)	N6_5	C3_5	C5_5	110.8(8)
O3C_3	K1B	O2C_3	58.5(3)	N6_5	C3_5	C4_5	110.3(8)
O3C_3	K1B	O6C_3	149.8(4)	C6_5	C3_5	C5_5	107.1(8)
O4C_3	K1B	O1C_3	160.1(4)	C4_5	C3_5	C6_5	107.5(8)
O4C_3	K1B	O2C_3	112.6(3)	C4_5	C3_5	C5_5	110.0(8)
O4C_3	K1B	O3C_3	58.6(3)	N7_5	C11_5	C12_5	115.5(9)
O4C_3	K1B	O6C_3	114.5(4)	N7_5	C13_5	C14_5	122.7(10)
O5C_3	K1B	O1C_3	117.3(4)	N3_7	P3_7	N12_7	121.7(4)
O5C_3	K1B	O2C_3	151.8(4)	N3_7	P3_7	N11_7	121.8(5)
O5C_3	K1B	O3C_3	119.4(4)	N3_7	P3_7	N13_7	112.7(4)
O5C_3	K1B	O4C_3	61.2(2)	N11_7	P3_7	N12_7	90.7(4)
O5C_3	K1B	O6C_3	59.0(3)	N13_7	P3_7	N12_7	103.6(4)
O6C_3	K1B	O1C_3	58.5(3)	N13_7	P3_7	N11_7	102.6(5)
O6C_3	K1B	O2C_3	107.4(4)	P3_7	N3_7	Ce1	167.1(5)
C2S	O2S	C3S	110.0(7)	C30_7	N12_7	P3_7	109.1(7)
C1S	O1S	K1A	130.8(6)	C30_7	N12_7	C31_7	113.2(8)
C1S	O1S	K1B	127.5(6)	C31_7	N12_7	P3_7	122.5(6)
C12S	O1S	K1A	120.3(6)	C29_7	N11_7	P3_7	113.1(7)
C12S	O1S	K1B	124.0(6)	C29_7	N11_7	C35_7	118.7(9)
C12S	O1S	C1S	108.6(7)	C35_7	N11_7	P3_7	123.5(7)
C11S	O2	K1A	97.6(8)	C39_7	N13_7	P3_7	121.0(7)
C11S	O2	K1B	94.6(8)	C39_7	N13_7	C41_7	115.8(9)
C10S	O2	K1A	130.3(9)	C41_7	N13_7	P3_7	123.1(7)

C10S	O2	K1B	132.7(9)	N11_7	C29_7	C30_7	107.3(8)
C10S	O2	C11S	101.3(9)	N12_7	C30_7	C29_7	103.9(9)
C4S	O3S	C5S	120.3(8)	N11_7	C35_7	C36_7	109.0(9)
O4S	C6S	C5S	121.3(12)	N11_7	C35_7	C38_7	112.0(10)
C6S	O4S	C7S	111.4(12)	N11_7	C35_7	C37_7	107.6(10)
O1S	C1S	C2S	115.2(9)	C36_7	C35_7	C38_7	109.6(12)
O1S	C12S	C11S	101.1(8)	C36_7	C35_7	C37_7	107.2(10)
O5S	C8S	C7S	139.6(15)	C38_7	C35_7	C37_7	111.3(11)
O2S	C2S	C1S	107.3(8)	N12_7	C31_7	C34_7	108.6(8)
O4S	C7S	C8S	105.4(9)	N12_7	C31_7	C33_7	108.6(9)
O2S	C3S	C4S	113.5(10)	N12_7	C31_7	C32_7	113.9(9)
O3S	C4S	C3S	117.4(8)	C33_7	C31_7	C34_7	107.9(10)
O3S	C5S	C6S	108.4(7)	C32_7	C31_7	C34_7	108.2(10)
O2	C11S	K1A	56.4(7)	C32_7	C31_7	C33_7	109.4(9)
O2	C11S	K1B	61.0(7)	N13_7	C39_7	C40_7	113.4(10)
O2	C11S	C12S	124.7(9)	N13_7	C41_7	C42_7	114.1(10)
C12S	C11S	K1A	94.4(6)	N2_8	P2_8	N9_8	117.6(9)
C12S	C11S	K1B	92.5(6)	N2_8	P2_8	N8_8	122.6(10)
O5S	C9S	C10S	104.7(10)	N2_8	P2_8	N10_8	117.0(9)
C9S	O5S	C8S	107.0(8)	N8_8	P2_8	N9_8	90.8(10)
O2	C10S	C9S	97.5(10)	N10_8	P2_8	N9_8	103.8(10)
C1T	O1T	C3T	109.7(13)	N10_8	P2_8	N8_8	100.4(10)
O1T	C1T	C2T	103.6(15)	P2_8	N2_8	Ce1	176.8(7)
O1T	C3T	C4T	108.5(15)	C16_8	N9_8	P2_8	106.4(16)
C1C_2	O1C_2	K1A	119.9(8)	C16_8	N9_8	C17_8	117.3(18)
C12C_2	O1C_2	K1A	118.3(8)	C17_8	N9_8	P2_8	117.3(15)
C12C_2	O1C_2	C1C_2	110.7(5)	C15_8	N8_8	P2_8	111.3(16)
C2C_2	O2C_2	K1A	105.7(9)	C15_8	N8_8	C21_8	121.0(19)
C2C_2	O2C_2	C3C_2	110.9(5)	C21_8	N8_8	P2_8	122.8(17)
C3C_2	O2C_2	K1A	112.7(8)	C25_8	N10_8	P2_8	119.3(15)
C4C_2	O3C_2	K1A	118.5(8)	C27_8	N10_8	P2_8	122.2(17)
C4C_2	O3C_2	C5C_2	111.1(5)	C27_8	N10_8	C25_8	114.2(19)
C5C_2	O3C_2	K1A	117.2(7)	N8_8	C15_8	C16_8	107(2)
C6C_2	O4C_2	K1A	111.8(9)	N9_8	C16_8	C15_8	100(2)
C6C_2	O4C_2	C7C_2	111.6(5)	N8_8	C21_8	C24_8	109(2)
C7C_2	O4C_2	K1A	100.1(7)	N8_8	C21_8	C22_8	107(2)
C8C_2	O5C_2	K1A	115.6(8)	C24_8	C21_8	C22_8	108(2)
C9C_2	O5C_2	K1A	117.5(9)	C23_8	C21_8	N8_8	110(2)
C9C_2	O5C_2	C8C_2	112.0(8)	C23_8	C21_8	C24_8	113(2)
C10C_2	O6C_2	K1A	115.0(10)	C23_8	C21_8	C22_8	109(2)
C11C_2	O6C_2	K1A	109.4(10)	N9_8	C17_8	C20_8	109.1(17)
C11C_2	O6C_2	C10C_2	111.2(5)	N9_8	C17_8	C19_8	105.6(17)
O1C_2	C1C_2	C2C_2	107.4(11)	N9_8	C17_8	C18_8	112.6(17)
O2C_2	C2C_2	K1A	51.7(7)	C19_8	C17_8	C20_8	107.9(18)
O2C_2	C2C_2	C1C_2	108.4(11)	C18_8	C17_8	C20_8	111.8(18)
C1C_2	C2C_2	K1A	84.6(8)	C18_8	C17_8	C19_8	109.4(19)
O2C_2	C3C_2	C4C_2	110.3(11)	C26_8	C25_8	N10_8	113.2(19)
O3C_2	C4C_2	C3C_2	105.1(10)	N10_8	C27_8	C28_8	112(2)
O3C_2	C5C_2	C6C_2	109.8(10)	N1_9	P1_9	N5_9	121.6(5)
O4C_2	C6C_2	C5C_2	104.9(10)	N1_9	P1_9	N6_9	118.6(5)
O4C_2	C7C_2	K1A	56.2(6)	N1_9	P1_9	N7_9	112.8(5)
O4C_2	C7C_2	C8C_2	105.9(11)	N5_9	P1_9	N6_9	91.4(5)
C8C_2	C7C_2	K1A	85.8(8)	N7_9	P1_9	N5_9	103.6(6)
O5C_2	C8C_2	C7C_2	109.3(10)	N7_9	P1_9	N6_9	105.8(5)
O5C_2	C9C_2	C10C_2	106.1(13)	P1_9	N1_9	Ce1	163.1(5)
O6C_2	C10C_2	C9C_2	110.2(12)	C2_9	N5_9	P1_9	112.6(8)
O6C_2	C11C_2	C12C_2	107.5(12)	C2_9	N5_9	C7_9	117.2(9)
O1C_2	C12C_2	C11C_2	110.5(12)	C7_9	N5_9	P1_9	124.8(8)

C1C_3	O1C_3	K1B	118.4(8)	C1_9	N6_9	P1_9	114.7(7)
C12C_3	O1C_3	K1B	118.0(8)	C1_9	N6_9	C3_9	121.0(9)
C12C_3	O1C_3	C1C_3	110.6(5)	C3_9	N6_9	P1_9	124.0(8)
C2C_3	O2C_3	K1B	108.3(9)	C11_9	N7_9	P1_9	120.2(8)
C2C_3	O2C_3	C3C_3	110.4(5)	C13_9	N7_9	P1_9	118.4(8)
C3C_3	O2C_3	K1B	111.4(8)	C13_9	N7_9	C11_9	116.9(10)
C4C_3	O3C_3	K1B	119.0(8)	N6_9	C1_9	C2_9	107.5(10)
C4C_3	O3C_3	C5C_3	111.0(5)	N5_9	C2_9	C1_9	108.2(10)
C5C_3	O3C_3	K1B	116.2(7)	N6_9	C3_9	C4_9	112.7(10)
C6C_3	O4C_3	K1B	111.6(9)	N6_9	C3_9	C5_9	110.4(9)
C7C_3	O4C_3	K1B	101.5(7)	N6_9	C3_9	C6_9	110.4(9)
C7C_3	O4C_3	C6C_3	111.2(5)	C4_9	C3_9	C6_9	106.4(10)
C8C_3	O5C_3	K1B	113.6(8)	C5_9	C3_9	C4_9	106.1(10)
C9C_3	O5C_3	K1B	118.0(9)	C5_9	C3_9	C6_9	110.7(10)
C9C_3	O5C_3	C8C_3	112.1(8)	N5_9	C7_9	C8_9	111.2(8)
C10C_3	O6C_3	K1B	114.8(10)	N5_9	C7_9	C9_9	111.0(8)
C11C_3	O6C_3	K1B	111.3(10)	N5_9	C7_9	C10_9	109.9(8)
C11C_3	O6C_3	C10C_3	110.8(5)	C8_9	C7_9	C9_9	107.2(9)
O1C_3	C1C_3	C2C_3	106.9(11)	C8_9	C7_9	C10_9	107.5(9)
O2C_3	C2C_3	C1C_3	108.1(11)	C10_9	C7_9	C9_9	109.9(9)
O2C_3	C3C_3	C4C_3	110.5(11)	N7_9	C11_9	C12_9	115.8(10)
O3C_3	C4C_3	C3C_3	105.1(10)	N7_9	C13_9	C14_9	122.9(11)
O3C_3	C5C_3	C6C_3	109.9(10)	N4_10	P4_10	N14_10	122.8(12)
O4C_3	C6C_3	C5C_3	105.1(10)	N4_10	P4_10	N15_10	120.7(11)
O4C_3	C7C_3	K1B	54.5(6)	N4_10	P4_10	N16_10	112.2(11)
O4C_3	C7C_3	C8C_3	105.7(11)	N14_10	P4_10	N15_10	90.4(11)
C8C_3	C7C_3	K1B	85.4(8)	N16_10	P4_10	N14_10	105.3(12)
O5C_3	C8C_3	C7C_3	108.9(10)	N16_10	P4_10	N15_10	101.7(12)
O5C_3	C9C_3	C10C_3	106.2(13)	P4_10	N4_10	Ce1	174.7(8)
O6C_3	C10C_3	C9C_3	110.4(12)	C43_10	N14_10	P4_10	114.5(16)
O6C_3	C11C_3	C12C_3	107.5(11)	C43_10	N14_10	C49_10	118.2(19)
O1C_3	C12C_3	C11C_3	110.3(12)	C49_10	N14_10	P4_10	127.3(17)
N1_4	P1_4	N5_4	121.0(6)	C44_10	N15_10	P4_10	104.6(15)
N1_4	P1_4	N6_4	119.3(6)	C45_10	N15_10	P4_10	121.7(16)
N1_4	P1_4	N7_4	113.2(5)	C45_10	N15_10	C44_10	114.2(19)
N5_4	P1_4	N6_4	91.0(5)	C53_10	N16_10	P4_10	118.7(17)
N7_4	P1_4	N5_4	103.7(6)	C53_10	N16_10	C55_10	118(2)
N7_4	P1_4	N6_4	105.5(6)	C55_10	N16_10	P4_10	114.2(16)
P1_4	N1_4	Ce1	178.5(5)	C43_10	C44_10	N15_10	102.0(19)
C2_4	N5_4	P1_4	114.0(7)	N14_10	C43_10	C44_10	105.6(19)
C2_4	N5_4	C7_4	119.8(9)	N15_10	C45_10	C46_10	109(2)
C7_4	N5_4	P1_4	126.2(8)	N15_10	C45_10	C48_10	113(2)
C1_4	N6_4	P1_4	112.4(8)	N15_10	C45_10	C47_10	109(2)
C1_4	N6_4	C3_4	119.7(10)	C46_10	C45_10	C48_10	110(2)
C3_4	N6_4	P1_4	122.2(8)	C46_10	C45_10	C47_10	109(2)
C11_4	N7_4	P1_4	121.6(9)	C47_10	C45_10	C48_10	107(2)
C13_4	N7_4	P1_4	119.2(8)	N14_10	C49_10	C52_10	111(2)
C13_4	N7_4	C11_4	118.7(10)	N14_10	C49_10	C51_10	105(2)
N6_4	C1_4	C2_4	106.9(10)	N14_10	C49_10	C50_10	105(2)
N5_4	C2_4	C1_4	108.7(10)	C52_10	C49_10	C51_10	110(2)
N6_4	C3_4	C4_4	112.2(10)	C50_10	C49_10	C52_10	113(2)
N6_4	C3_4	C5_4	110.1(9)	C50_10	C49_10	C51_10	113(2)
N6_4	C3_4	C6_4	110.5(9)	N16_10	C53_10	C54_10	109.2(19)
C4_4	C3_4	C6_4	106.6(10)	N16_10	C55_10	C56_10	124.0(19)
C5_4	C3_4	C4_4	106.5(10)	C55_10	C56_10	K1A	163.8(16)
C5_4	C3_4	C6_4	110.9(10)				

Table S21. Bond lengths for **2-Ce^{Rb}**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ce1	N1	2.380(7)	C6	Rb1	3.564(14)
Ce1	N2	2.381(7)	C7	C8	1.519(14)
Ce1	N3	2.335(7)	C7	C9	1.549(13)
Ce1	N4	2.322(7)	C7	C10	1.535(14)
Ce1	Rb1	3.9474(9)	C8	Rb1	3.571(10)
P1	N1	1.535(7)	C11	C12	1.520(15)
P1	N5	1.697(8)	C13	C14	1.531(12)
P1	N6	1.730(8)	C15	C16	1.508(13)
P1	N7	1.660(8)	C17	C18	1.507(13)
P1	Rb1	3.469(2)	C17	C19	1.543(14)
P2	N2	1.529(7)	C17	C20	1.523(15)
P2	N8	1.717(7)	C21	C22	1.510(14)
P2	N9	1.713(7)	C21	C23	1.535(15)
P2	N10	1.689(8)	C21	C24	1.557(12)
P2	Rb1	3.411(2)	C27	C28	1.514(13)
P3	N3	1.533(7)	C25	C26	1.522(13)
P3	N11	1.695(8)	C29	C30	1.514(14)
P3	N12	1.724(8)	C31	C32	1.518(17)
P3	N13	1.685(8)	C31	C33	1.549(15)
P4	N4	1.538(7)	C31	C34	1.529(16)
P4	N14	1.718(8)	C35	C36	1.539(12)
P4	N15	1.704(8)	C35	C37	1.524(13)
P4	N16	1.675(8)	C35	C38	1.545(13)
N1	Rb1	2.939(7)	C41	C42	1.522(17)
N2	Rb1	2.896(7)	C39	C40	1.525(15)
N5	C1	1.461(12)	C43	C44	1.514(16)
N5	C7	1.469(13)	C43	C45	1.526(15)
N5	Rb1	3.545(9)	C43	C46	1.534(16)
N6	C2	1.424(13)	C47	C48	1.431(11)
N6	C3	1.473(12)	C49	C50	1.532(14)
N7	C11	1.439(12)	C49	C51	1.522(14)
N7	C13	1.465(11)	C49	C52	1.527(14)
N8	C15	1.447(11)	C53	C54	1.534(17)
N8	C21	1.476(12)	C55	C56	1.485(15)
N9	C16	1.477(11)	Rb1	O1SB	2.884(10)
N9	C17	1.490(11)	Rb1	O1SC	2.903(10)
N9	Rb1	3.219(8)	O1S	C1S	1.422(2)
N10	C27	1.471(11)	O1S	C3S	1.422(2)
N10	C25	1.461(11)	C1S	C2S	1.5202(15)
N11	C29	1.461(11)	C3S	C4S	1.5200(16)
N11	C35	1.458(12)	O1	C1A	1.4210(17)
N12	C30	1.456(13)	O1	C1C	1.4207(17)
N12	C31	1.485(13)	C1A	C1B	1.5203(15)
N13	C41	1.461(12)	C1C	C1D	1.5203(15)
N13	C39	1.461(12)	O1SE	C1SE	1.421(2)
N14	C48	1.434(12)	O1SE	C3SE	1.421(2)
N14	C49	1.486(13)	C1SE	C2SE	1.520(2)
N15	C43	1.482(13)	C3SE	C4SE	1.520(2)
N15	C47	1.438(13)	O1SB	C1SB	1.422(2)
N16	C54	1.463(12)	O1SB	C3SB	1.422(2)
N16	C55	1.456(12)	C1SB	C2SB	1.520(2)
C1	C2	1.490(15)	C3SB	C4SB	1.520(2)
C2	Rb1	3.627(12)	O1SC	C1SC	1.422(2)
C3	C4	1.561(17)	O1SC	C3SC	1.422(2)
C3	C5	1.478(17)	C1SC	C2SC	1.5202(16)
C3	C6	1.518(15)	C3SC	C4SC	1.5202(15)

Table S22. Bond angles for **2-Ce**^{Rb}.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	Ce1	N2	94.6(2)	N5	C1	C2	106.7(8)
N1	Ce1	Rb1	47.86(18)	N6	C2	C1	108.8(8)
N2	Ce1	Rb1	46.80(18)	N6	C2	Rb1	81.4(6)
N3	Ce1	N1	112.8(3)	C1	C2	Rb1	88.4(6)
N3	Ce1	N2	113.7(3)	N6	C3	C4	109.5(9)
N3	Ce1	Rb1	123.45(19)	N6	C3	C5	112.2(10)
N4	Ce1	N1	112.9(3)	N6	C3	C6	109.8(9)
N4	Ce1	N2	113.0(3)	C5	C3	C4	105.5(10)
N4	Ce1	N3	109.2(3)	C5	C3	C6	112.6(11)
N4	Ce1	Rb1	127.31(19)	C6	C3	C4	107.0(10)
N1	P1	N5	118.0(4)	C3	C6	Rb1	107.5(7)
N1	P1	N6	120.7(4)	N5	C7	C8	109.8(8)
N1	P1	N7	113.9(4)	N5	C7	C9	109.6(8)
N1	P1	Rb1	57.3(3)	N5	C7	C10	112.6(7)
N5	P1	N6	91.0(4)	C8	C7	C9	108.9(8)
N5	P1	Rb1	78.5(3)	C8	C7	C10	108.4(8)
N6	P1	Rb1	83.3(3)	C10	C7	C9	107.5(9)
N7	P1	N5	107.0(4)	C7	C8	Rb1	101.2(6)
N7	P1	N6	103.1(4)	N7	C11	C12	114.4(9)
N7	P1	Rb1	171.2(3)	N7	C13	C14	114.1(8)
N2	P2	N8	120.6(4)	N8	C15	C16	105.8(7)
N2	P2	N9	116.3(4)	N9	C16	C15	105.7(7)
N2	P2	N10	114.3(4)	N9	C17	C18	110.7(8)
N2	P2	Rb1	57.6(3)	N9	C17	C19	111.3(8)
N8	P2	Rb1	92.0(3)	N9	C17	C20	108.4(8)
N9	P2	N8	91.3(4)	C18	C17	C19	108.6(9)
N9	P2	Rb1	68.9(3)	C18	C17	C20	110.0(9)
N10	P2	N8	103.9(4)	C20	C17	C19	107.8(9)
N10	P2	N9	107.4(4)	N8	C21	C22	111.2(8)
N10	P2	Rb1	163.8(3)	N8	C21	C23	111.5(9)
N3	P3	N11	121.1(4)	N8	C21	C24	108.6(7)
N3	P3	N12	121.2(4)	C22	C21	C23	109.7(8)
N3	P3	N13	113.1(4)	C22	C21	C24	107.3(8)
N11	P3	N12	90.4(4)	C23	C21	C24	108.4(8)
N13	P3	N11	103.9(4)	N10	C27	C28	113.3(8)
N13	P3	N12	103.6(4)	N10	C25	C26	114.4(8)
N4	P4	N14	121.3(4)	N11	C29	C30	106.1(7)
N4	P4	N15	120.8(4)	N12	C30	C29	104.7(8)
N4	P4	N16	112.4(4)	N12	C31	C32	109.3(9)
N15	P4	N14	91.0(4)	N12	C31	C33	107.7(9)
N16	P4	N14	103.5(4)	N12	C31	C34	112.6(9)
N16	P4	N15	104.5(4)	C32	C31	C33	108.8(10)
Ce1	N1	Rb1	95.2(2)	C32	C31	C34	108.8(9)
P1	N1	Ce1	160.4(5)	C34	C31	C33	109.6(11)
P1	N1	Rb1	96.6(3)	N11	C35	C36	110.3(7)
Ce1	N2	Rb1	96.4(2)	N11	C35	C37	111.0(8)
P2	N2	Ce1	163.4(5)	N11	C35	C38	109.7(8)
P2	N2	Rb1	95.9(3)	C36	C35	C38	107.7(8)
P3	N3	Ce1	174.0(5)	C37	C35	C36	108.6(8)
P4	N4	Ce1	175.5(5)	C37	C35	C38	109.5(8)
P1	N5	Rb1	73.5(3)	N13	C41	C42	114.5(9)
C1	N5	P1	114.6(6)	N13	C39	C40	114.6(9)
C1	N5	C7	118.7(7)	N15	C43	C44	110.5(9)
C1	N5	Rb1	92.0(5)	N15	C43	C45	109.4(10)
C7	N5	P1	126.7(6)	N15	C43	C46	110.6(8)
C7	N5	Rb1	103.6(5)	C44	C43	C45	107.3(10)

C2	N6	P1	112.7(7)	C44	C43	C46	110.0(10)
C2	N6	C3	118.6(8)	C45	C43	C46	109.1(11)
C3	N6	P1	124.3(7)	C48	C47	N15	110.6(9)
C11	N7	P1	122.7(6)	C47	C48	N14	110.6(9)
C11	N7	C13	115.7(7)	N14	C49	C50	110.6(8)
C13	N7	P1	121.5(6)	N14	C49	C51	111.0(8)
C15	N8	P2	113.5(6)	N14	C49	C52	108.9(8)
C15	N8	C21	115.6(7)	C51	C49	C50	108.8(9)
C21	N8	P2	122.5(6)	C51	C49	C52	108.0(9)
P2	N9	Rb1	81.3(3)	C52	C49	C50	109.5(9)
C16	N9	P2	112.1(6)	N16	C54	C53	114.2(9)
C16	N9	C17	116.2(7)	N16	C55	C56	114.6(9)
C16	N9	Rb1	106.1(5)	N2	Rb1	N1	73.68(18)
C17	N9	P2	125.5(6)	N2	Rb1	O1SC	148.6(3)
C17	N9	Rb1	107.2(5)	O1SB	Rb1	N1	142.8(4)
C27	N10	P2	121.9(6)	O1SB	Rb1	N2	143.0(3)
C25	N10	P2	121.4(6)	O1SC	Rb1	N1	136.9(3)
C25	N10	C27	116.1(7)	C1S	O1S	C3S	114.7(7)
C29	N11	P3	113.8(6)	O1S	C1S	C2S	112.6(9)
C35	N11	P3	125.2(6)	O1S	C3S	C4S	114.3(9)
C35	N11	C29	117.6(7)	C1C	O1	C1A	114.8(7)
C30	N12	P3	108.3(6)	O1	C1A	C1B	112.6(9)
C30	N12	C31	115.5(8)	O1	C1C	C1D	114.4(9)
C31	N12	P3	121.3(7)	C3SE	O1SE	C1SE	114.7(7)
C41	N13	P3	121.2(6)	O1SE	C1SE	C2SE	112.6(9)
C41	N13	C39	116.6(8)	O1SE	C3SE	C4SE	114.3(9)
C39	N13	P3	122.2(7)	C1SB	O1SB	Rb1	119.3(9)
C48	N14	P4	111.3(7)	C3SB	O1SB	Rb1	125.7(9)
C48	N14	C49	118.4(8)	C3SB	O1SB	C1SB	114.7(7)
C49	N14	P4	123.6(6)	O1SB	C1SB	C2SB	112.6(9)
C43	N15	P4	123.7(6)	O1SB	C3SB	C4SB	114.3(9)
C47	N15	P4	111.5(7)	C1SC	O1SC	Rb1	117.0(9)
C47	N15	C43	118.4(9)	C1SC	O1SC	C3SC	114.7(7)
C54	N16	P4	121.8(6)	C3SC	O1SC	Rb1	127.7(9)
C55	N16	P4	121.1(6)	O1SC	C1SC	C2SC	112.6(9)
C55	N16	C54	117.1(8)	O1SC	C3SC	C4SC	114.3(9)

Table S23. Bond lengths for **2-Ce^{Cs}**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ce1	N2	2.326(6)	N1_2	C1_2	1.450(9)
Ce1	N3	2.388(5)	N1_2	C3_2	1.481(9)
Ce1	N4	2.398(5)	N2_2	C2_2	1.467(9)
Ce1	N9	2.295(6)	N2_2	C7_2	1.477(9)
Cs1	N3	3.068(6)	C1_2	C2_2	1.518(11)
Cs1	N4	3.052(6)	C3_2	C4_2	1.529(11)
Cs1	O1_19	3.155(8)	C3_2	C5_2	1.557(11)
Cs1	N1_1	3.327(6)	C3_2	C6_2	1.523(11)
P1	N9	1.541(6)	C7_2	C8_2	1.535(11)
P1	N1_26	1.689(6)	C7_2	C9_2	1.539(10)
P1	N1_3	1.726(6)	C7_2	C10_2	1.522(12)
P1	N2_3	1.700(6)	N1_3	C1_3	1.455(9)
P2	N2	1.544(6)	N1_3	C3_3	1.474(9)
P2	N1_24	1.688(7)	N2_3	C2_3	1.461(12)
P2	N1_4	1.709(7)	N2_3	C7_3	1.474(9)
P2	N2_4	1.717(6)	C1_3	C2_3	1.523(12)
P3	N3	1.534(6)	C3_3	C4_3	1.525(10)
P3	N1_23	1.685(6)	C3_3	C5_3	1.548(11)

P3	N1_1	1.731(6)	C3_3	C6_3	1.525(11)
P3	N2_1	1.727(6)	C7_3	C8_3	1.540(11)
P4	N4	1.532(6)	C7_3	C9_3	1.535(12)
P4	N1_2	1.734(6)	C7_3	C10_3	1.530(15)
P4	N2_2	1.701(5)	N1_4	C1_4	1.426(11)
P4	N1_14	1.682(6)	N1_4	C3_4	1.473(10)
Ce2	N5	2.315(6)	N2_4	C2_4	1.445(12)
Ce2	N6	2.348(5)	N2_4	C7_4	1.465(9)
Ce2	N7	2.364(5)	C1_4	C2_4	1.448(13)
Ce2	N8	2.358(5)	C3_4	C4_4	1.521(11)
Cs2	N7	3.067(6)	C3_4	C5_4	1.552(11)
Cs2	N8	3.080(7)	C3_4	C6_4	1.532(13)
Cs2	O2	3.136(9)	C7_4	C8_4	1.530(11)
Cs2	N2_5	3.323(6)	C7_4	C9_4	1.541(11)
P5	N5	1.541(6)	C7_4	C10_4	1.532(12)
P5	N1_20	1.689(5)	N1_5	C1_5	1.452(9)
P5	N1_6	1.720(5)	N1_5	C3_5	1.479(9)
P5	N2_6	1.698(6)	N2_5	C2_5	1.464(10)
P6	N6	1.536(6)	N2_5	C7_5	1.490(9)
P6	N1_21	1.687(6)	C1_5	C2_5	1.524(11)
P6	N1_15	1.709(6)	C3_5	C4_5	1.527(12)
P6	N2_15	1.702(6)	C3_5	C5_5	1.520(14)
P7	N7	1.538(5)	C3_5	C6_5	1.535(11)
P7	N1_22	1.687(6)	C7_5	C8_5	1.547(11)
P7	N1_7	1.695(5)	C7_5	C9_5	1.526(12)
P7	N2_7	1.749(6)	C7_5	C10_5	1.533(12)
P8	N8	1.530(6)	N1_6	C1_6	1.461(9)
P8	N1_25	1.699(6)	N1_6	C3_6	1.480(9)
P8	N1_5	1.719(6)	N2_6	C2_6	1.448(8)
P8	N2_5	1.733(6)	N2_6	C7_6	1.483(9)
O2	C5	1.422(3)	C1_6	C2_6	1.525(11)
O2	C7	1.420(3)	C3_6	C4_6	1.545(10)
C5	C6	1.520(3)	C3_6	C5_6	1.534(11)
C7	C8	1.519(3)	C3_6	C6_6	1.533(10)
O1_18	C2_18	1.395(13)	C7_6	C8_6	1.528(11)
O1_18	C3_18	1.457(14)	C7_6	C9_6	1.531(9)
C1_18	C2_18	1.524(3)	C7_6	C10_6	1.542(9)
C3_18	C4_18	1.524(3)	N1_7	C1_7	1.464(9)
O1_19	C2_19	1.449(7)	N1_7	C3_7	1.492(9)
O1_19	C3_19	1.450(7)	N2_7	C2_7	1.456(8)
C1_19	C2_19	1.526(3)	N2_7	C7_7	1.487(9)
C3_19	C4_19	1.525(3)	C1_7	C2_7	1.515(10)
O1_27	C2_27	1.401(17)	C3_7	C4_7	1.550(13)
O1_27	C3_27	1.434(15)	C3_7	C5_7	1.530(11)
C1_27	C2_27	1.525(17)	C3_7	C6_7	1.540(11)
C3_27	C4_27	1.534(18)	C7_7	C8_7	1.531(10)
N1_20	C11_20	1.450(8)	C7_7	C9_7	1.547(12)
N1_20	C13_20	1.460(7)	C7_7	C10_7	1.520(10)
C11_20	C12_20	1.524(9)	N1_15	C1_15	1.437(10)
C13_20	C14_20	1.523(10)	N1_15	C3_15	1.472(9)
N1_21	C11_21	1.443(7)	N2_15	C2_15	1.449(10)
N1_21	C13_21	1.467(8)	N2_15	C7_15	1.455(11)
C11_21	C12_21	1.534(10)	C1_15	C2_15	1.452(13)
C13_21	C14_21	1.527(10)	C3_15	C4_15	1.528(11)
N1_22	C11_22	1.457(9)	C3_15	C5_15	1.531(10)
N1_22	C13_22	1.463(8)	C3_15	C6_15	1.569(11)
C11_22	C12_22	1.537(10)	C7_15	C8_15	1.535(13)
C13_22	C14_22	1.518(10)	C7_15	C9_15	1.538(12)

N1_23	C11_23	1.469(9)	C7_15	C10_15	1.535(12)
N1_23	C13_23	1.462(8)	N1_14	C11_14	1.458(8)
C11_23	C12_23	1.522(9)	N1_14	C13_14	1.454(10)
C13_23	C14_23	1.511(10)	C11_14	C12_14	1.495(13)
N1_24	C11_24	1.453(10)	C13_14	C14_14	1.525(14)
N1_24	C13_24	1.469(9)	N1_1	C1_1	1.466(10)
C11_24	C12_24	1.524(11)	N1_1	C3_1	1.488(9)
C13_24	C14_24	1.526(10)	N2_1	C2_1	1.460(10)
N1_25	C11_25	1.466(8)	N2_1	C7_1	1.484(9)
N1_25	C13_25	1.460(9)	C1_1	C2_1	1.492(11)
C11_25	C12_25	1.523(10)	C3_1	C4_1	1.536(13)
C13_25	C14_25	1.533(10)	C3_1	C5_1	1.548(12)
N1_26	C11_26	1.462(5)	C3_1	C6_1	1.521(11)
N1_26	C13_26	1.462(5)	C7_1	C8_1	1.542(11)
C11_26	C12_26	1.505(10)	C7_1	C9_1	1.535(11)
C13_26	C14_26	1.491(12)	C7_1	C10_1	1.518(13)

Table S24. Bond angles for **2-Ce^{Cs}**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N2	Ce1	N3	109.2(2)	N2_2	C7_2	C9_2	107.5(7)
N2	Ce1	N4	116.1(2)	N2_2	C7_2	C10_2	111.9(6)
N3	Ce1	N4	97.08(19)	C8_2	C7_2	C9_2	109.0(6)
N9	Ce1	N2	106.8(2)	C10_2	C7_2	C8_2	108.4(8)
N9	Ce1	N3	116.6(2)	C10_2	C7_2	C9_2	109.2(7)
N9	Ce1	N4	111.2(2)	C7_2	C9_2	Cs1	101.3(4)
N3	Cs1	O1_19	144.2(2)	C1_3	N1_3	P1	108.9(4)
N3	Cs1	N1_1	51.11(14)	C1_3	N1_3	C3_3	115.5(7)
N4	Cs1	N3	71.75(13)	C3_3	N1_3	P1	122.2(5)
N4	Cs1	O1_19	142.4(2)	C2_3	N2_3	P1	113.8(5)
N4	Cs1	N1_1	121.81(14)	C2_3	N2_3	C7_3	118.8(6)
O1_19	Cs1	N1_1	95.8(2)	C7_3	N2_3	P1	126.2(6)
N9	P1	N1_26	113.6(3)	N1_3	C1_3	C2_3	104.7(7)
N9	P1	N1_3	122.3(3)	N2_3	C2_3	C1_3	106.2(6)
N9	P1	N2_3	119.1(3)	N1_3	C3_3	C4_3	108.5(6)
N1_26	P1	N1_3	102.2(3)	N1_3	C3_3	C5_3	109.4(7)
N1_26	P1	N2_3	105.4(3)	N1_3	C3_3	C6_3	111.7(5)
N2_3	P1	N1_3	90.6(3)	C4_3	C3_3	C5_3	108.3(6)
N2	P2	N1_24	114.2(4)	C6_3	C3_3	C4_3	110.2(8)
N2	P2	N1_4	120.5(4)	C6_3	C3_3	C5_3	108.6(6)
N2	P2	N2_4	120.6(3)	N2_3	C7_3	C8_3	110.1(7)
N1_24	P2	N1_4	104.5(3)	N2_3	C7_3	C9_3	109.4(7)
N1_24	P2	N2_4	102.6(3)	N2_3	C7_3	C10_3	110.6(7)
N1_4	P2	N2_4	90.8(3)	C9_3	C7_3	C8_3	110.4(7)
N3	P3	N1_23	113.9(3)	C10_3	C7_3	C8_3	108.3(7)
N3	P3	N1_1	115.9(3)	C10_3	C7_3	C9_3	108.0(8)
N3	P3	N2_1	121.5(3)	C1_4	N1_4	P2	112.9(5)
N1_23	P3	N1_1	109.8(3)	C1_4	N1_4	C3_4	119.4(7)
N1_23	P3	N2_1	102.3(3)	C3_4	N1_4	P2	125.0(5)
N2_1	P3	N1_1	90.7(3)	C2_4	N2_4	P2	110.0(6)
N4	P4	N1_2	121.9(3)	C2_4	N2_4	C7_4	116.9(7)
N4	P4	N2_2	117.6(3)	C7_4	N2_4	P2	123.3(5)
N4	P4	N1_14	112.8(3)	N1_4	C1_4	C2_4	109.8(8)
N2_2	P4	N1_2	90.8(3)	N2_4	C2_4	C1_4	109.7(8)
N1_14	P4	N1_2	103.5(3)	N1_4	C3_4	C4_4	109.1(7)
N1_14	P4	N2_2	107.3(3)	N1_4	C3_4	C5_4	110.1(6)
P2	N2	Ce1	173.1(4)	N1_4	C3_4	C6_4	110.9(6)
Ce1	N3	Cs1	95.38(18)	C4_4	C3_4	C5_4	108.9(7)
P3	N3	Ce1	165.9(4)	C4_4	C3_4	C6_4	109.7(8)

P3	N3	Cs1	98.2(3)	C6_4	C3_4	C5_4	108.0(7)
Ce1	N4	Cs1	95.59(18)	N2_4	C7_4	C8_4	111.5(7)
P4	N4	Ce1	161.1(4)	N2_4	C7_4	C9_4	108.7(7)
P4	N4	Cs1	101.9(3)	N2_4	C7_4	C10_4	109.7(6)
P1	N9	Ce1	168.4(4)	C8_4	C7_4	C9_4	110.5(6)
N5	Ce2	N6	110.8(2)	C8_4	C7_4	C10_4	108.4(7)
N5	Ce2	N7	112.6(2)	C10_4	C7_4	C9_4	108.1(7)
N5	Ce2	N8	113.7(2)	C1_5	N1_5	P8	114.0(5)
N6	Ce2	N7	113.62(19)	C1_5	N1_5	C3_5	116.4(6)
N6	Ce2	N8	110.6(2)	C3_5	N1_5	P8	122.8(5)
N8	Ce2	N7	94.79(19)	P8	N2_5	Cs2	84.4(2)
N7	Cs2	N8	68.86(13)	C2_5	N2_5	Cs2	113.3(5)
N7	Cs2	O2	146.8(3)	C2_5	N2_5	P8	110.7(4)
N7	Cs2	N2_5	118.12(15)	C2_5	N2_5	C7_5	116.1(6)
N8	Cs2	O2	141.0(3)	C7_5	N2_5	Cs2	103.2(4)
N8	Cs2	N2_5	50.96(14)	C7_5	N2_5	P8	123.9(5)
O2	Cs2	N2_5	94.8(3)	N1_5	C1_5	C2_5	105.5(6)
N5	P5	N1_20	112.6(3)	N2_5	C2_5	C1_5	105.6(6)
N5	P5	N1_6	120.4(3)	N1_5	C3_5	C4_5	107.2(7)
N5	P5	N2_6	120.7(3)	N1_5	C3_5	C5_5	111.3(7)
N1_20	P5	N1_6	104.0(3)	N1_5	C3_5	C6_5	111.1(6)
N1_20	P5	N2_6	104.3(3)	C4_5	C3_5	C6_5	108.6(8)
N2_6	P5	N1_6	91.7(3)	C5_5	C3_5	C4_5	109.8(10)
N6	P6	N1_21	113.5(3)	C5_5	C3_5	C6_5	108.8(8)
N6	P6	N1_15	120.8(3)	N2_5	C7_5	C8_5	112.2(5)
N6	P6	N2_15	121.0(4)	N2_5	C7_5	C9_5	108.3(8)
N1_21	P6	N1_15	104.1(3)	N2_5	C7_5	C10_5	111.2(6)
N1_21	P6	N2_15	103.0(3)	C9_5	C7_5	C8_5	108.7(7)
N2_15	P6	N1_15	90.8(3)	C9_5	C7_5	C10_5	108.0(7)
N7	P7	N1_22	113.6(3)	C10_5	C7_5	C8_5	108.3(8)
N7	P7	N1_7	120.9(3)	C7_5	C9_5	Cs2	79.9(5)
N7	P7	N2_7	116.1(3)	C1_6	N1_6	P5	108.7(5)
N1_22	P7	N1_7	103.6(3)	C1_6	N1_6	C3_6	116.1(5)
N1_22	P7	N2_7	108.8(3)	C3_6	N1_6	P5	121.9(4)
N1_7	P7	N2_7	91.1(3)	C2_6	N2_6	P5	114.3(5)
N8	P8	N1_25	113.4(3)	C2_6	N2_6	C7_6	117.5(6)
N8	P8	N1_5	121.9(3)	C7_6	N2_6	P5	128.1(4)
N8	P8	N2_5	115.6(3)	N1_6	C1_6	C2_6	105.8(5)
N1_25	P8	N1_5	103.6(3)	N2_6	C2_6	C1_6	105.3(5)
N1_25	P8	N2_5	108.5(3)	N1_6	C3_6	C4_6	108.6(5)
N1_5	P8	N2_5	91.2(3)	N1_6	C3_6	C5_6	109.7(5)
P5	N5	Ce2	172.4(4)	N1_6	C3_6	C6_6	112.6(6)
P6	N6	Ce2	170.7(4)	C5_6	C3_6	C4_6	107.0(7)
Ce2	N7	Cs2	98.18(17)	C6_6	C3_6	C4_6	109.3(6)
P7	N7	Ce2	165.6(3)	C6_6	C3_6	C5_6	109.4(6)
P7	N7	Cs2	95.7(3)	N2_6	C7_6	C8_6	109.5(6)
Ce2	N8	Cs2	97.99(19)	N2_6	C7_6	C9_6	110.9(6)
P8	N8	Ce2	165.1(4)	N2_6	C7_6	C10_6	110.2(6)
P8	N8	Cs2	96.7(3)	C8_6	C7_6	C9_6	109.7(7)
C5	O2	Cs2	111.8(6)	C8_6	C7_6	C10_6	108.3(6)
C7	O2	Cs2	134.9(6)	C9_6	C7_6	C10_6	108.2(6)
C7	O2	C5	113.3(4)	C1_7	N1_7	P7	113.4(5)
O2	C5	Cs2	48.4(4)	C1_7	N1_7	C3_7	116.7(5)
O2	C5	C6	108.3(4)	C3_7	N1_7	P7	124.3(4)
C6	C5	Cs2	102.8(9)	P7	N2_7	Cs2	82.80(19)
O2	C7	C8	108.8(4)	C2_7	N2_7	Cs2	109.7(4)
C2_18	O1_18	C3_18	112.7(10)	C2_7	N2_7	P7	111.1(4)
O1_18	C2_18	C1_18	109.7(12)	C2_7	N2_7	C7_7	116.0(5)

O1_18	C3_18	C4_18	108.4(14)	C7_7	N2_7	Cs2	105.3(4)
C2_19	O1_19	Cs1	119.9(9)	C7_7	N2_7	P7	125.2(5)
C2_19	O1_19	C3_19	110.0(8)	N1_7	C1_7	C2_7	106.1(5)
C3_19	O1_19	Cs1	112.7(8)	N2_7	C2_7	C1_7	104.6(5)
O1_19	C2_19	C1_19	107.8(13)	N1_7	C3_7	C4_7	111.0(7)
O1_19	C3_19	C4_19	107.4(13)	N1_7	C3_7	C5_7	111.5(6)
C2_27	O1_27	C3_27	112.2(12)	N1_7	C3_7	C6_7	108.1(6)
O1_27	C2_27	C1_27	108.9(14)	C5_7	C3_7	C4_7	108.6(7)
O1_27	C3_27	C4_27	108.9(13)	C5_7	C3_7	C6_7	107.5(8)
C11_20	N1_20	P5	121.7(4)	C6_7	C3_7	C4_7	110.1(9)
C11_20	N1_20	C13_20	117.3(5)	N2_7	C7_7	C8_7	112.1(6)
C13_20	N1_20	P5	120.6(4)	N2_7	C7_7	C9_7	108.2(6)
N1_20	C11_20	C12_20	113.0(6)	N2_7	C7_7	C10_7	110.2(6)
N1_20	C13_20	C14_20	114.8(6)	C8_7	C7_7	C9_7	107.8(7)
C11_21	N1_21	P6	120.7(5)	C10_7	C7_7	C8_7	109.2(7)
C11_21	N1_21	C13_21	117.2(5)	C10_7	C7_7	C9_7	109.2(7)
C13_21	N1_21	P6	122.0(4)	C1_15	N1_15	P6	111.4(6)
N1_21	C11_21	C12_21	113.5(6)	C1_15	N1_15	C3_15	116.2(6)
N1_21	C13_21	C14_21	114.8(6)	C3_15	N1_15	P6	122.7(4)
C11_22	N1_22	P7	121.8(4)	C2_15	N2_15	P6	112.9(6)
C11_22	N1_22	C13_22	116.1(5)	C2_15	N2_15	C7_15	117.7(6)
C13_22	N1_22	P7	122.1(5)	C7_15	N2_15	P6	124.8(5)
N1_22	C11_22	C12_22	112.4(7)	N1_15	C1_15	C2_15	109.8(7)
N1_22	C13_22	C14_22	114.6(6)	N2_15	C2_15	C1_15	109.3(6)
C11_23	N1_23	P3	121.4(4)	N1_15	C3_15	C4_15	108.6(6)
C13_23	N1_23	P3	122.0(5)	N1_15	C3_15	C5_15	109.5(5)
C13_23	N1_23	C11_23	116.5(6)	N1_15	C3_15	C6_15	111.5(7)
N1_23	C11_23	C12_23	113.9(6)	C4_15	C3_15	C5_15	107.9(7)
N1_23	C13_23	C14_23	116.1(6)	C4_15	C3_15	C6_15	111.0(6)
C11_24	N1_24	P2	120.1(5)	C5_15	C3_15	C6_15	108.2(6)
C11_24	N1_24	C13_24	116.0(6)	N2_15	C7_15	C8_15	110.9(7)
C13_24	N1_24	P2	120.7(6)	N2_15	C7_15	C9_15	109.8(8)
N1_24	C11_24	C12_24	113.9(8)	N2_15	C7_15	C10_15	110.7(6)
N1_24	C13_24	C14_24	116.1(6)	C8_15	C7_15	C9_15	110.0(7)
C11_25	N1_25	P8	121.4(5)	C10_15	C7_15	C8_15	107.8(8)
C13_25	N1_25	P8	122.3(4)	C10_15	C7_15	C9_15	107.5(8)
C13_25	N1_25	C11_25	116.3(6)	C11_14	N1_14	P4	121.6(5)
N1_25	C11_25	C12_25	113.3(7)	C13_14	N1_14	P4	122.0(4)
N1_25	C13_25	C14_25	114.7(7)	C13_14	N1_14	C11_14	116.3(6)
C11_26	N1_26	P1	121.3(4)	N1_14	C11_14	C12_14	116.3(7)
C13_26	N1_26	P1	119.9(5)	N1_14	C13_14	C14_14	113.9(8)
C13_26	N1_26	C11_26	118.8(6)	P3	N1_1	Cs1	85.2(2)
N1_26	C11_26	C12_26	113.9(6)	C1_1	N1_1	Cs1	108.9(5)
N1_26	C13_26	C14_26	116.9(7)	C1_1	N1_1	P3	111.5(5)
C1_2	N1_2	P4	111.7(4)	C1_1	N1_1	C3_1	116.8(5)
C1_2	N1_2	C3_2	116.8(6)	C3_1	N1_1	Cs1	104.2(4)
C3_2	N1_2	P4	122.9(4)	C3_1	N1_1	P3	123.6(5)
P4	N2_2	Cs1	73.4(2)	C2_1	N2_1	P3	112.0(5)
C2_2	N2_2	Cs1	95.7(4)	C2_1	N2_1	C7_1	117.0(6)
C2_2	N2_2	P4	114.2(4)	C7_1	N2_1	P3	122.3(5)
C2_2	N2_2	C7_2	118.5(5)	N1_1	C1_1	C2_1	105.5(6)
C7_2	N2_2	Cs1	106.8(4)	N2_1	C2_1	C1_1	104.8(7)
C7_2	N2_2	P4	126.9(5)	N1_1	C3_1	C4_1	108.1(7)
N1_2	C1_2	Cs1	85.1(4)	N1_1	C3_1	C5_1	110.0(5)
N1_2	C1_2	C2_2	105.4(6)	N1_1	C3_1	C6_1	113.0(6)
C2_2	C1_2	Cs1	93.0(4)	C4_1	C3_1	C5_1	108.0(7)
N2_2	C2_2	C1_2	105.7(5)	C6_1	C3_1	C4_1	108.2(7)
N1_2	C3_2	C4_2	110.0(6)	C6_1	C3_1	C5_1	109.3(7)

N1_2	C3_2	C5_2	111.3(6)	C3_1	C5_1	Cs1	82.3(5)
N1_2	C3_2	C6_2	109.2(6)	N2_1	C7_1	C8_1	108.0(6)
C4_2	C3_2	C5_2	108.7(7)	N2_1	C7_1	C9_1	110.6(7)
C6_2	C3_2	C4_2	108.2(6)	N2_1	C7_1	C10_1	110.4(6)
C6_2	C3_2	C5_2	109.4(6)	C9_1	C7_1	C8_1	110.0(7)
C3_2	C5_2	Cs1	111.4(5)	C10_1	C7_1	C8_1	109.0(8)
N2_2	C7_2	C8_2	110.7(7)	C10_1	C7_1	C9_1	108.9(7)

References

1. Rice, N. T.; Popov, I. A.; Russo, D. R.; Bacsa, J.; Batista, E. R.; Yang, P.; Telser, J.; La Pierre, H. S, *J. Am. Chem. Soc.* **2019**, 141 (*33*), 13222-13233.

2. Gompa, T. P.; Rice, N. T.; Russo, D. R.; Aguirre Quintana, L. M.; Yik, B. J.; Bacsa, J.; La Pierre, H. S., *Dalton Trans.* **2019**, 48 (*23*), 8030- 8033.

3. Evans, W. J.; Kozimor, S. A.; Ziller, J. W.; Kaltsoyannis, N., *J. Am. Chem. Soc.* **2004**, 126 (*44*), 14533-14547.

4. Johnson, S. A.; Kiernicki, J. J.; Fanwick, P. E.; Bart, S. C., *Organometallics* **2015**, 34 (*12*), 2889-2895.

5. Perrin, D. D., *Ionisation Constants of Inorganic Acids and Bases in Aqueous Solution*. Pergamon, **1982**.

6. Shannon, R., *Acta Crystallogr. A* **1976**, 32 (*5*), 751-767.

7. Perdew, J. P.; Emzerhof, M.; Burke, K., *J. Chem. Phys*. **1996**, *105*, 9982.

8. Gaussian 16, Revision A.03, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2016**.

9. Cao, X.; Dolg, M., *J. Chem. Phys*. **2001**, *115*, 7348.

10. Dolg, M.; Stoll, H.; Preuss, H., *J. Chem. Phys*. **1989**, *90*, 1730.

11. Unpublished: A. Bergner, Arbeitsbericht **1990**.

12. Leininger, T.; Nicklass, A.; K"uchle, W.; Stoll, H.; Dolg, M.; Bergner, A., *Chem. Phys. Lett.* **1996**, *255*, 274-280.

13. Krishnan, R.; Binkley, J. S.; Seeger, R.; Pople, J. A., *J. Chem. Phys.* **1980,** *72*, 650-654.

14. Zubarev, D. Y.; Boldyrev, A. I., *Phys. Chem. Chem. Phys*. **2008**, *10*, 5207-5217.

15. Tkachenko, N. V.; Boldyrev, A. I., *Phys. Chem. Chem. Phys*. **2019**, *21*, 9590-9596.

16. Kelley, M. P.; Popov, I. A.; Jung, J.; Batista, E. R.; Yang, P., *Nat. Commun*. **2020**, *11*, 1558.

17. Kulichenko, M.; Fedik, N.; Boldyrev, A.; Muñoz-Castro, A., *Chem. Eur. J.* **2020**, *26*, 2263-2268.

18. Sergeeva, A. P.; Boldyrev, A. I., *Comments Inorg. Chem.* **2010**, *31*, 2-12.

19. Runge, E.; Gross, E. K. U., *Phys. Rev. Lett.* **1984**, *52*, 997-1000.

20. Casida, M. E., *Recent Advances in Density Functional Methods, Part I*, World Scientific Singapore, **1995**; pp. 155-192.

21. Martin, R. L., *J. Chem. Phys*. **2003**, *118*, 4775-4777.

22. Cancès, E., *J. Chem. Phys.* **1997**, *107*, 3032.

23. Mennucci, B; Cancès, E.; Tomasi, J., *J. Phys. Chem. B* **1997**, *101*, 10506-10517.

24. Cancès, E.; Mennucci, B., *J. Mat. Chem.* **1998**, *23*, 309-326.

25. Hay, P. J.; Wadt, W. R., *J. Chem. Phys*. **1985**, *82*, 299-310.

26. Roy, L. E.; Hay, P. J.; Martin, R. L., *J. Chem. Theory Comput*. **2008**, *4*, 1029-1031.

27. Skripnikov, L. *Chemissian v4.67*.

28. G. A. Zhurko, *Chemcraft - Graphical Software for Visualization of Quantum Chemistry Computations*, 2005.

29. a) Krause, L., Herbst-Irmer, R., Sheldrick, G., Stalke, D., *J. Appl .Crystallogr.* **2015**, 48, 3-10. b) Bruker, V8.40B ed., Bruker AXS Inc., Madison, Wisconsin, USA.

30. Sheldrick, G. *Acta Crystallogr.. A* **2015**, 71, 3-8.

31. Dolomanov, O., Bourhis, L., Gildea, R., Howard, J., Puschmann, H., *J. Appl. Crystallogr*. **2009**, 42, 339-341.