Supporting Information

Controlled Monodefluorination and Alkylation of C(sp^3)-F Bonds by Lanthanide Photocatalysts: Importance of Metal – Ligand Cooperativity

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S1 General Details

All moisture and air sensitive materials were manipulated using standard high-vacuum Schlenk-line techniques and MBraun gloveboxes and stored under an atmosphere of dried and deoxygenated dinitrogen. All glassware items, cannulae and Fisherbrand 1.2 μm retention glass microfibre filters were dried in a 160 °C oven overnight before use.

Hexanes, tetrahydrofuran (THF), diethyl ether (Et_2O) and toluene for use with moisture and air sensitive compounds were dried using an MBRAUN SPS 800 Manual solvent purification system and stored over activated 3 Å molecular sieves. Benzene-d_6, pyridine-d_5 were purchased from Cambridge Isotope Laboratories and were refluxed over potassium metal for 24 hours, freeze-pump-thaw degassed and purified by trap-to-trap distillation prior to use. THF-D_8 was purchased from Cambridge Isotope Laboratories and dried over sodium/benzophenone before being freeze-pump-thaw degassed and purified by trap-to-trap distillation prior to use. All solvents were purchased from Sigma-Aldrich or Fisher Scientific and stored over 3 Å molecular sieves for 4 hours before being used.

$PhICl_2$ was prepared according to the literature procedure[1] and stored at –30 °C. Dihydrocarbyl magnesium reagents[2], [**H_2L**]Br, **HL**, **HLMes** and **HL^{t}Bu**[3], KC_5Me_4H,[4] lanthanide triiodides (Ln = La, Ce, Nd, Sm),[5,6] lanthanide tris(tetramethylcyclopentadienyl) complexes (Ln = La, Ce, Nd, Sm),[5,7,8] and *ortho*-substituted benzotrifluoride 1-CF_3-2-(C_3H_5)C_6H_4 (**9**),[9] were all prepared using published methods. All other chemicals were purchased from commercial suppliers and degassed and/or dried under vacuum or over 3 Å molecular sieves for 12 hours before use.

The station for photochemical reactions was equipped with a fan to maintain constant temperature, and unless otherwise stated, a single 40 W Kessil A160WE Tuna Blue lamp. The reactions were conducted in J-Young valved NMR tubes fixed at a distance of 7.5 cm from the light source.

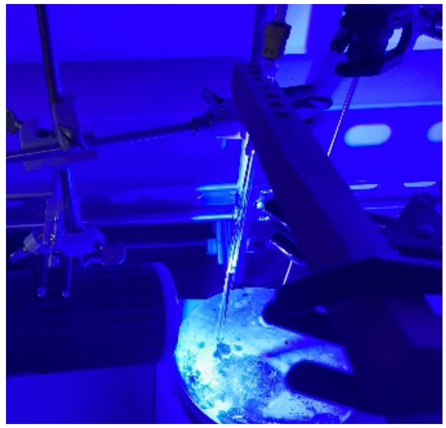


Figure S1. Reaction set-up for photochemical reactions.

NMR spectra were recorded on Bruker Avance 400, 500 and 600 MHz spectrometers and are referenced to residual protio solvent (3.58 and 1.72 ppm for THF-D_8, 7.16 ppm for C_6D_6) for ^{1}H NMR spectroscopy. THF was used as solvents for No Deuterium (NoD) NMR experiments,[10] and was referenced to added tetramethylsilane (0.00 ppm for both ^{1}H and ^{13}C{^{1}H} NMR spectroscopic experiments). Quantitative ^{1}H NMR data were acquired with a minimum of eight scans, with the delay time set to 5x the longest T_1 value present. Chemical shifts are quoted in ppm and coupling constants in Hz. Tetrakis(trimethylsilyl)silane (TMS*) was used as internal standards for quantitative ^{1}H NMR spectroscopy. NMR spectra were taken at 25°C unless otherwise noted. Structural assignments were performed using HSQC and HMBC NMR spectroscopic experiments when necessary. Elemental analyses were carried out by the microanalytic services in the College of Chemistry at the University of California, Berkeley. Difficulty in acquiring elemental analyses of organolanthanides is well reported.[11] Multiple attempts to collect data have been made but poor carbon combustion has been a problem. GC-MS measurements were acquired using an Agilent 7890B GC-MS system; LC-MS data LCMS was collected with the ACQUITY™ UPLC™ H-Class PLUS System; HRMS data was collected using a PerkinElmer HRMS.

Figure S2. 10 mm pathlength quartz cell fused with a J-Young valve used for collecting photophysical data of all air sensitive compounds.

Quartz cells with a 10 mm pathlength equipped with a J-Young valve were used to contain samples prepared under a dinitrogen atmosphere for electronic absorption spectra (UV-Vis) and fluorescence measurements. UV-Vis measurements were collected on an Agilent Varian Cary 50 UV-Vis spectrophotometer. Emission and excitation spectra were collected on Fluorolog®-3 spectrofluorometer.

Single crystal X-ray diffraction data of **1-Ce** were collected using an Excalibur Eos diffractometer, fitted with a CCD area detector and using MoKα radiation (λ = 0.71073 Å) at 170 K. X-ray diffraction data for **3-Ce** were collected at beamline 12.2.1 of the Advanced Light Source (ALS) at Lawrence Berkeley National Lab, using a Bruker D8 diffractometer coupled to a Bruker PhotonII CPAD detector with Si(111)-monochromated synchrotron radiation (17 keV radiation). Single crystal X-ray diffraction data of all other compounds were collected using a Rigaku Xtalab Synergy-S diffractometer fitted with a HyPix-6000HE photon counting detector using MoKα (λ = 0.71073 Å) or CuKα (λ = 0.1.5418Å) radiation. All structures were solved using SHELXT in Olex2 and refined using SHELXL in Olex2.[13,14] Absorption corrections were completed using CrysAlis PRO (Rigaku Oxford Diffraction) software. Analytical numeric absorption corrections used a multifaceted crystal model based on expressions derived by Clark and Reid.[15] Numerical absorption correction was based on a Gaussian integration over a multifaceted crystal model.

Cyclic voltammetry (CV) was performed inside a glovebox under nitrogen atmosphere, using an EC Epsilon (BASi) potentiostat. The working electrodes were glassy carbon with an area of 0.071 cm^2 that were polished with Al_2O_3 (1 um, 0.3 um, 0.05 um) and rinsed with ultrapure water and acetone before the measurements. The counter electrode was a platinum wire. The reference electrode (Ag/Ag^+) consisted of a silver wire in a reservoir of the electrolyte solution to which a small amount of $AgBF_4$ was added, connected to the sample solution by a frit. Potentials were calibrated to the Fc/Fc^+ redox couple in each electrolyte solution. Experiments were performed in $TBAPF_6$ in THF (0.1 M) or in $TBABPh_4$ in THF (0.085 M, close to saturation) at room temperature. Analyte concentrations were kept at around 5 mM for the measurements.

S2 Experimental Procedures and Characterization

Synthesis of **KL**

To a cold (-78 °C), magnetically stirred, cream slurry of 2.13 g of $[H_2L1]Br$ in THF (50 mL) was added a cold suspension of 2.16 g of KN'' in THF (100 mL) dropwise over ten minutes. The mixture was allowed to warm to room temperature, with stirring, overnight. After this period, the orange solution was isolated from the pale grey powder (KBr) by filtration. Concentration of the solution to 5 ml and the subsequent addition of 10 ml of pentane provided a cream powder. This powder was isolated by filtration and washed with pentane (3 x 20 ml) to afford [KL1]. Yield: 1.56 g (82%)

^{1}H NMR (500 MHz, pyridine-d_5, 300 K): δ 7.49 (d, J_{H-H} = 2.9, 1H, $CH(5)_{Ph}$), 7.34 (d, J_{H-H} = 2.9, 1H, $CH(3)_{Ph}$), 7.33 (d, J_{H-H} = 1.6, 1H, $CH_{Im(Ph)}$), 7.10 (d, J_{H-H} = 1.6, 1H, $CH_{Im(iPr)}$), 4.51 (sept, J_{H-H} = 6.7, 1H, CH_{iPr}), 1.69 (s, 9H, CH_{3tBu}), 1.38 (s, 9H, CH_{3tBu}), 1.30 (d, J_{H-H} = 6.7, 6H, CH_{3iPr}). ^{13}C{^{1}H} NMR (125.8 MHz, pyridine-d_5, 300 K): δ 206.3 (s, C-K), 163.4 (s, C-O), 138.6 (s, C_{Ph}), 131.4 (s, C_{Ph}), 127.6 (s, C_{Ph}), 122.7 (s, $CH_{Im(Ph)}$), 122.1 (s, CH_{Ph}), 122.0 (s, CH_{Ph}), 114.6 (s, $CH_{Im(iPr)}$), 51.8 (s, CH_{iPr}), 35.7 (s, C_{tBu}), 33.7 (s, C_{tBu}), 32.2 (s, CH_{3tBu}), 30.0 (s, CH_{3tBu}), 24.0 (s, CH_{3iPr}).

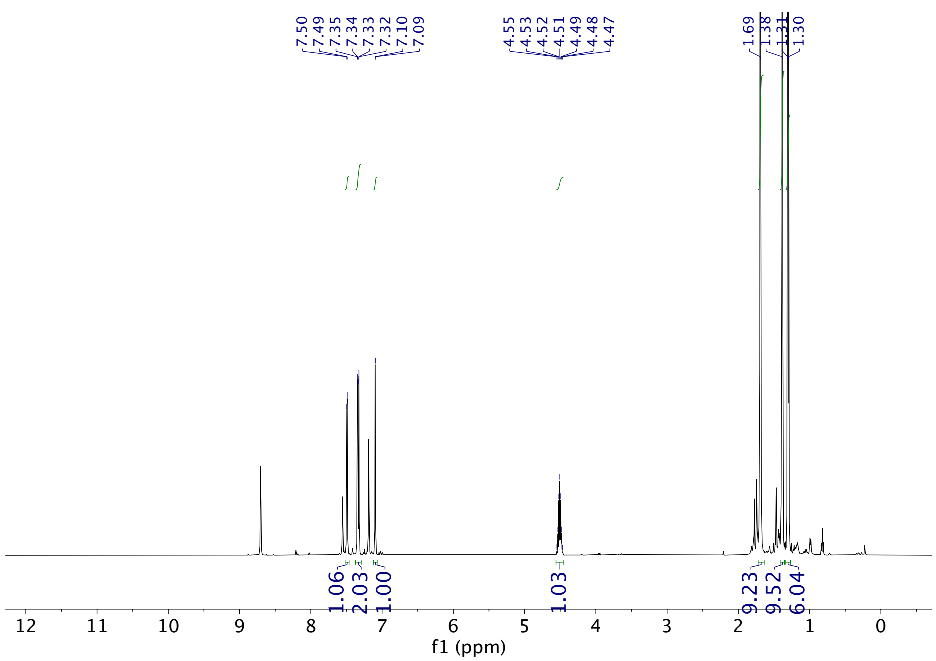


Figure S3. ^{1}H NMR in pyridine-D_5 of **KL.**

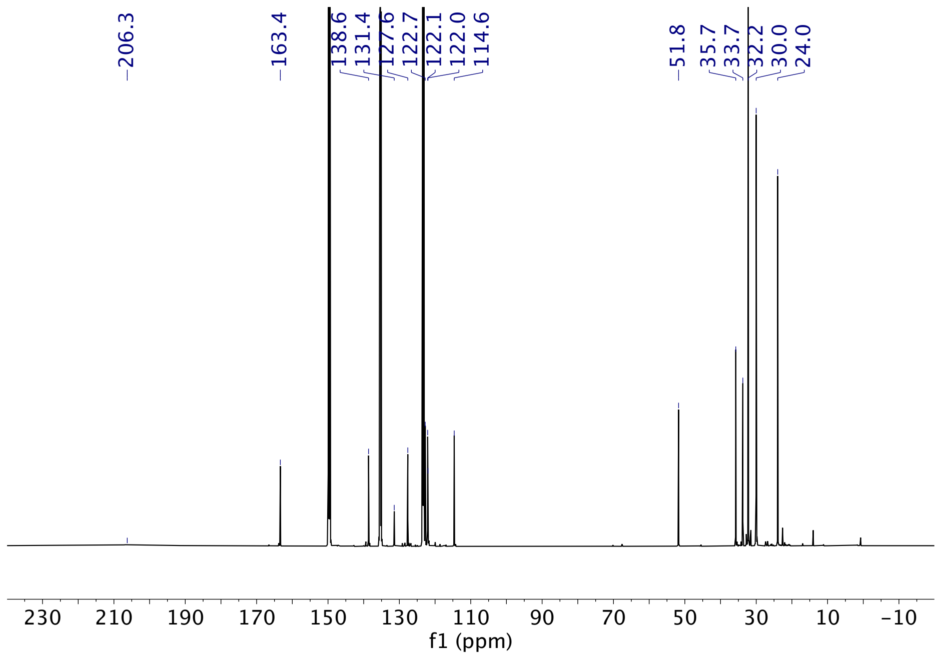


Figure S4. $^{13}C\{^1H\}$ NMR in pyridine-D_5 of **KL.**

Synthesis of **CeL(Cp^{Me4})$_2$ (1-Ce)**

In a glovebox, to a magnetically stirred green solution of **Ce(Cp^{Me4})$_3$ (2-Ce)** (1.212 g, 2.40 mmol, 1 equiv.) in toluene (50 mL), **HL** (0.756 g, 2.40 mmol, 1 equiv.) was added and the solution stirred overnight. After this time, volatiles were removed by vacuum evaporation and the orange solid washed with cold (–30°C) hexane (2 x 5 ml) to afford **CeL(Cp^{Me4})$_2$**. Yield: 1.37 g (82%). Diffraction quality crystals were grown from a concentrated hexane solution at –30°C.

^{1}H NMR (500 MHz, C_6D_6, 298 K): δ 16.66 (s, 2H, CH_{Cp}), 12.59 (s, 1H, CH_{Im}), 11.03 (s, 1H, CH_{Ph}), 8.39 (s, 1H, CH_{Ph}), 7.29 (s, 6H, CH_{3Cp}), 4.53 (s, 1H, CH_{Im}), 2.05 (s, 9H, CH_{3tBu}), 1.57 (s, 6H, CH_{3Cp}), 0.59 (s, 6H, CH_{3Cp}), -3.84 (s, 6H, CH_{3Cp}), -4.27 (s, 9H, CH_{3tBu}), -8.23 (d, J_{H-H} = 6.7, 6H, CH_{3iPr}), -41.41 (s, 1H, CH_{iPr}). Anal. Calcd for $C_{38}H_{55}CeN_2O$: C, 65.58, H, 7.97, N, 4.03. Found: C, 64.11; H, 7.82; N, 4.03.

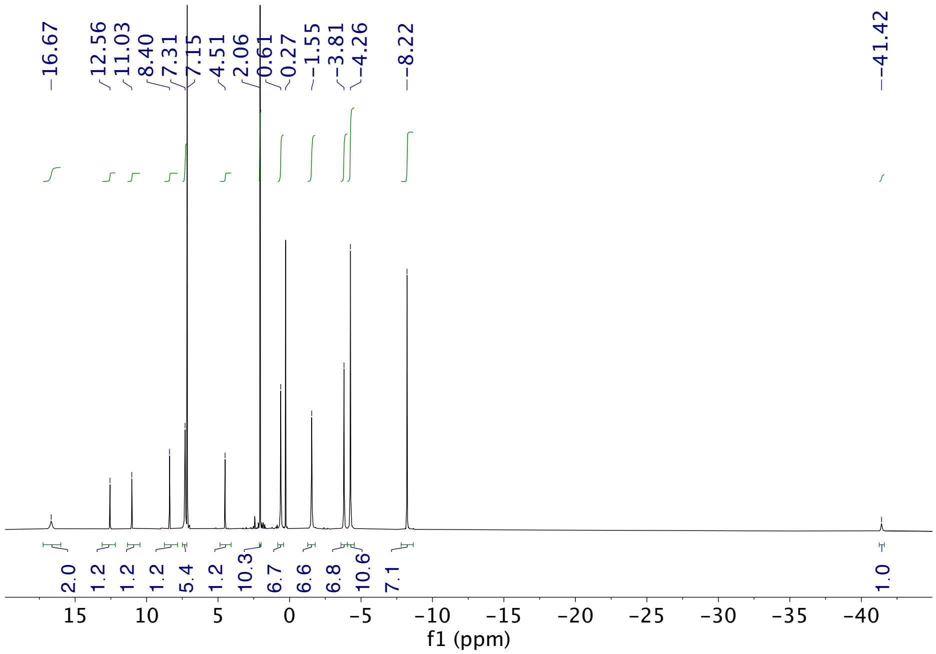


Figure S5. ^{1}H NMR in C_6D_6 of **1-Ce**.

<u>Synthesis of **CeLMes(Cp^{Me4})$_2$ (1-CeMes)**</u>

In a glovebox, to a magnetically stirred green solution of **Ce(Cp^{Me4})$_3$ (2-Ce)** (38.4 mg, 0.0760 mmol, 1 equiv.) in toluene (50 mL), **HLMes** (30.0 mg, 0.0760 mmol, 1 equiv.) was added and the solution stirred overnight. After this time, volatiles were removed by vacuum evaporation and the orange solid washed with cold (–30°C) hexane (2 x 2 ml) to afford **CeLMes(Cp^{Me4})$_2$**. Yield: 45.2 mg (77%).

^{1}H NMR (400 MHz, C_6D_6, 298 K): δ 17.69 (br s, 2H, CH_{Cp}), 13.33 (s, 1H, CH_{Im}), 11.49 (s, 1H, CH_{Ph}), 8.46 (s, 1H, CH_{Ph}), 8.34(s, 6H, CH_{3Cp}), 5.50 (s, 1H, CH_{Im}), 3.62 (s, 6H, CH_{3Mes}) 2.07 (s, 9H, CH_{3tBu}), 0.36 (s, 2H, CH_{Mes}), -1.54 (s, 3H, CH_{3Mes}), -3.14 (s, 6H, CH_{3Cp}), -3.36 (s, 6H, CH_{3Cp}), -4.31 (s, 9H, CH_{3tBu}), -7.53 (br s, 6H, CH_{3Cp}). Anal. Calcd for $C_{44}H_{61}CeN_2O$: C, 68.27, H, 7.94, N, 3.62. Found: C, 63.83; H, 7.85; N, 3.92.

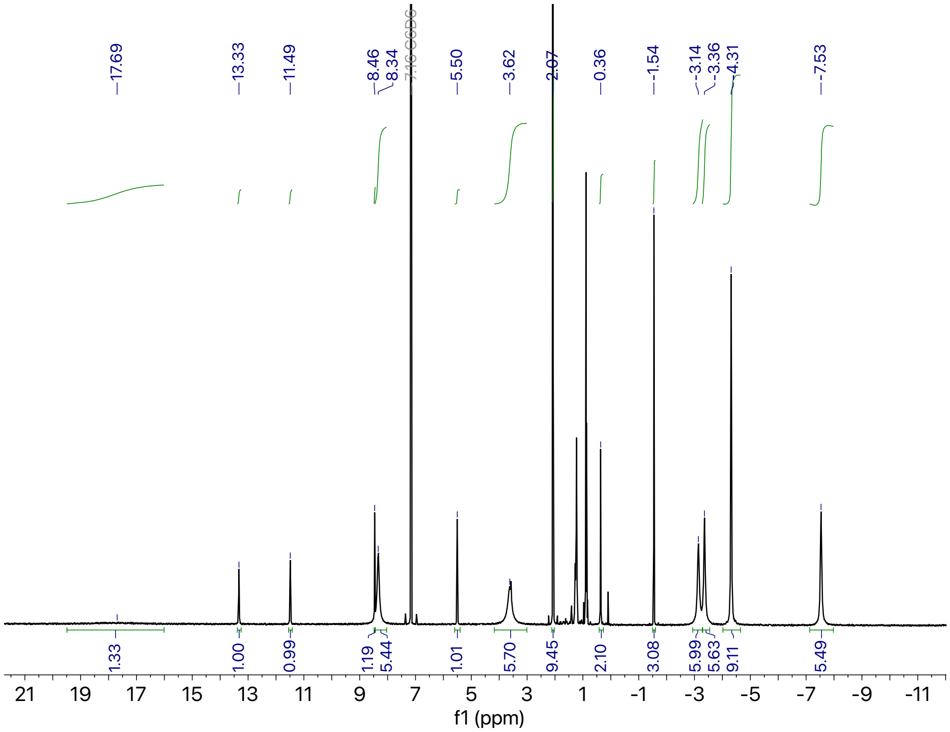


Figure S6. ^{1}H NMR in C_6D_6 of **1-CeMes**.

Synthesis of **CeL^{t}Bu(Cp^{Me4})$_2$ (1-Ce^{t}Bu)**

In a glovebox, to a magnetically stirred green solution of **Ce(Cp^{Me4})$_3$ (2-Ce)** (125 mg, 0.254 mmol, 1 equiv.) in toluene (50 mL), **HL^{t}Bu** (83.9 mg, 0.254 mmol, 1 equiv.) was added and the solution stirred overnight. After this time, volatiles were removed by vacuum evaporation and the orange solid washed with cold (–30°C) hexane (2 x 2 ml) to afford **CeL^{t}Bu(Cp^{Me4})$_2$**. Yield: 83.9 mg (78%).

^{1}H NMR (400 MHz, C_6D_6) δ 17.58 (br s, 2H, CH_{Cp}), 13.06 (s, 1H, CH_{Im}), 11.31 (s, 1H, CH_{Ph}), 8.49 (s, 1H, CH_{Ph}), 7.97 (s, 6H, CH_{3Cp}), 4.51 (s, 1H, CH_{Im}), 2.15 (s, 9H, $CH_{3tBu(Ph)}$), 0.46 (s, 9H, CH_{3tBu}), -1.65 (s, 6H, CH_{3Cp}), -4.28 (s, 6H, CH_{3Cp}), -4.51 (s, 9H, $CH_{3tBu(Ph)}$), -8.67 (s, 6H, CH_{3Cp}).

Anal. Calcd for $C_{39}H_{58}CeN_2O$: C, 65.88, H, 8.22, N, 3.94. Found: C, 65.75; H,8.43; N, 4.14.

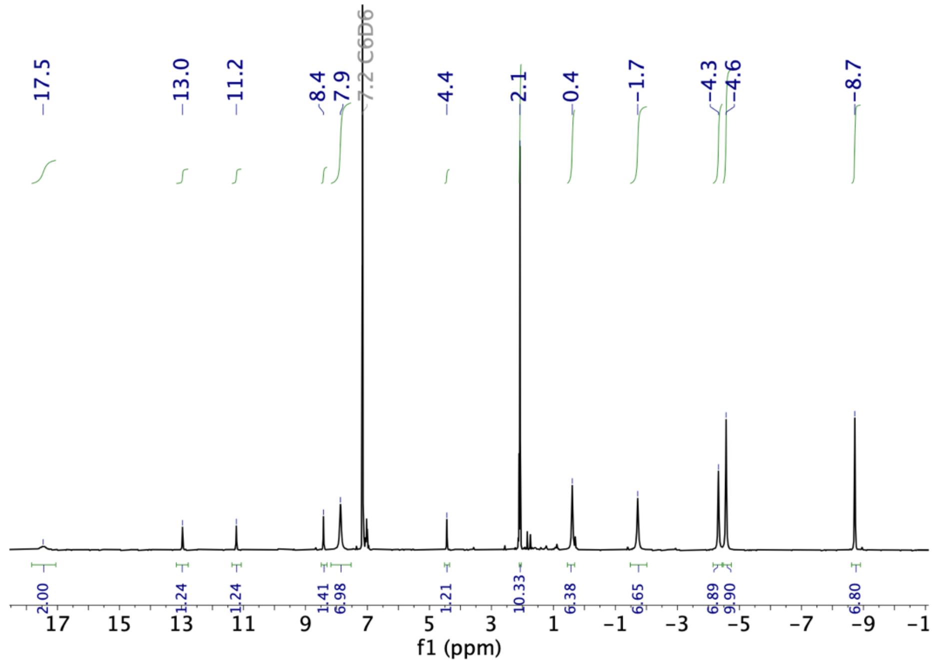


Figure S7. ^{1}H NMR in C_6D_6 of **1-Ce^{t}Bu**.

<u>Synthesis of **[(Cp^{Me4})$_2$CeCl]$_2$ (3-Ce)**</u>

Method A: In a glovebox a vial was charged with **(Cp^{Me4})$_3$Ce** (47.0 mg, 0.0933 mmol, 1.00 equiv.) in THF (5 mL), resulting in a green solution. With stirring, a colorless solution of $PhICl_2$ (13.5 mg, 0.0484 mmol, 0.52 equiv.) in THF (1 mL) was added dropwise. Upon addition, the color of the solution quickly changed from green to orange-yellow. After stirring for 2 hours at room temperature, the volatiles were removed under vacuum, resulting in a pink-orange powder which was subsequently washed with hexanes (2 x 0.5 mL). The powder was redissolved in a minimum of THF (1 mL), and the bright orange-yellow solution was filtered through glass fiber into a 1 mL vial, layered with hexanes (3 mL) and stored at –30 °C for 3 days to yield large orange blocks of **[(Cp^{Me4})$_2$CeCl]$_2$** that were dried *in vacuo*. Yield: 54%. Crystals grown via this method were suitable for X-ray diffraction studies.

Method B: A Teflon-stoppered ampoule was charged with $CeCl_3$ (11.5 mg, 0.0467 mmol, 1.00 equiv.) **(Cp^{Me4})$_3$Ce** (47.0 mg, 0.0933 mmol, 2.00 equiv.) and THF (5 mL), resulting in a green slurry. The ampoule was sealed and heated to 70°C for 24 hours, resulting in a color change from green to yellow. The volatiles were removed under vacuum, resulting in a pink-orange powder, which was subsequently washed with hexanes (2 x 0.5 mL). The powder was redissolved in a minimum of THF (1 mL), and the bright orange-yellow solution was filtered through glass fiber into a 1 mL vial, layered with hexanes (3 mL) and stored at –30 °C for 3 days to yield large orange blocks of **$[(Cp^{Me4})_2CeCl]_2$** that were dried under vacuum. Yield: 54%

Note: $[(Cp^{Me4})_2CeCl]_2$ is dichroic, appearing as a pink solid when isolated as a powder and orange-yellow in THF solution.

^{1}H NMR (500 MHz, THF-D_8) δ 8.79 (br. s, 6H, **CH_{3Cp}**), 6.83 (br. s, 1H, **H**$_{Cp}$), –0.93 (br. s, 6H, **CH_{3Cp}**).

Anal. Calcd for: $C_{36}H_{52}Ce_2Cl_2$: C, 51.72; H, 6.27. Found: C, 51.28; H, 6.09.

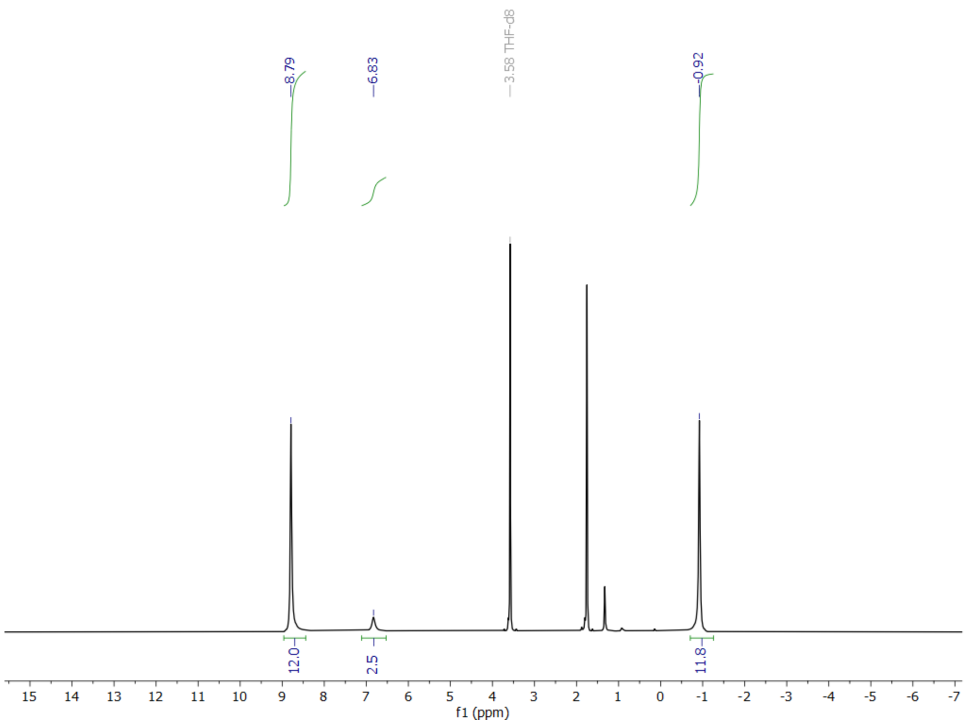


Figure S8. ^{1}H NMR in THF-D_8 of **3-Ce**.

<u>Synthesis of **$CeCp^{Me4}{}_2(OAr)$ (4-Ce)** (OAr = 1-O-2,6-$^tBu_2$-4-Me-C_6H_2)</u>

In a glovebox, a vial was charged with **3-Ce** (31.5 mg, 0.0377 mmol, 1 equiv.), sodium 2,6-di-*tert*-butyl-4-methylphenolate (18.3 mg, 0.0754 mmol, 2 equiv.) and hexanes (5 mL). The reaction was stirred at room temperature for 48 hours and following a gradual color change from yellow to deep red, volatiles were removed under vacuum. The red residue was extracted into hexane before being dried to give a red powder identified as $(Cp^{Me4})_2Ce(OAr)$ by ^1H NMR spectroscopy. Yield: 88% Diffraction quality crystals were grown from a concentrated hexane solution at –30°C.

^1H NMR (400 MHz, C_6D_6): δ 28.01 (br. s, 2H, H_{Cp}), 6.57 (s, 2H, $H_{m\text{-}Ph}$), 3.18 (br. s, 12H, CH_{3Cp}), 2.18 (s, 3H, $3H_{p\text{-}Ph}$), -4.18 (br. s, 12H, CH_{3Cp}), -6.26 (br. s, 18H, CH_{3tBu}).

Anal. Calcd for: $C_{33}H_{49}CeO$: C, 65.86; H, 8.21. Found: C, 66.00; H, 8.03.

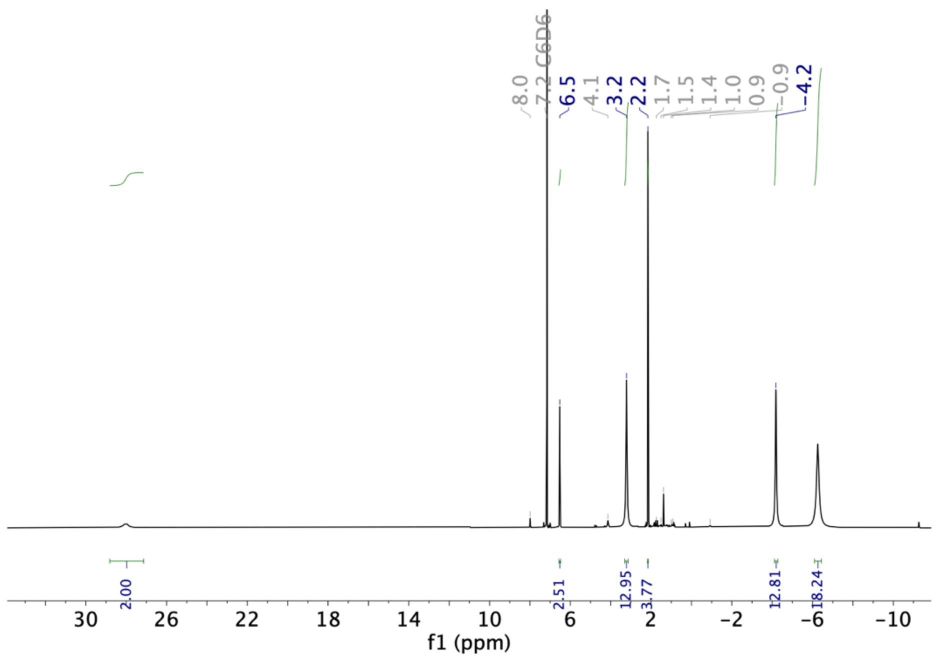


Figure S9. ^1H NMR in C_6D_6 of **4-Ce**.

Synthesis of **$(Cp^{Me4})_2Ce(OTf)(THF)$ (5-Ce)**

In a glovebox, a teflon-stoppered ampoule was charged with **2-Ce** (1.0442 g, 2.073 mmol, 2.01 equiv.), $Ce(OTf)_3$ (0.6065 g, 1.033 mmol, 1.00 equiv.) and THF (30 mL), resulting in a dark green slurry. The ampoule was sealed and placed in a 70 ºC oil bath with stirring for 20 hours, during which time the color changed from dark green to a bright yellow. The reaction mixture was then cooled to room temperature before being filtered through glass fiber. The yellow filtrate was dried under vacuum to yield a pale-yellow powder which was washed with hexanes (2 x 4 mL) before drying under vacuum again, yielding **5-Ce.** 89%

yield. X-ray quality crystals of **5-Ce** were grown by layering a concentrated THF solution with hexanes and storing at –30 °C for 3 days.

Note: 5-Ce is thermochromic, appearing pale yellow when cold (–30 °C) and bright yellow at room temperature in either solution or solid state.

^{1}H NMR (500 MHz, THF-D_8) δ 11.68 (br. s, 12H), 10.78 (br. s, 2H), –4.50 (br. s, 12H).^{19}F NMR (471 MHz, THF-D_8) δ –96.2 (s). Anal. Calcd for: $C_{23}H_{34}CeF_3O_4S$: C, 43.76; H, 5.68. Found: C, 42.63; H, 5.33.

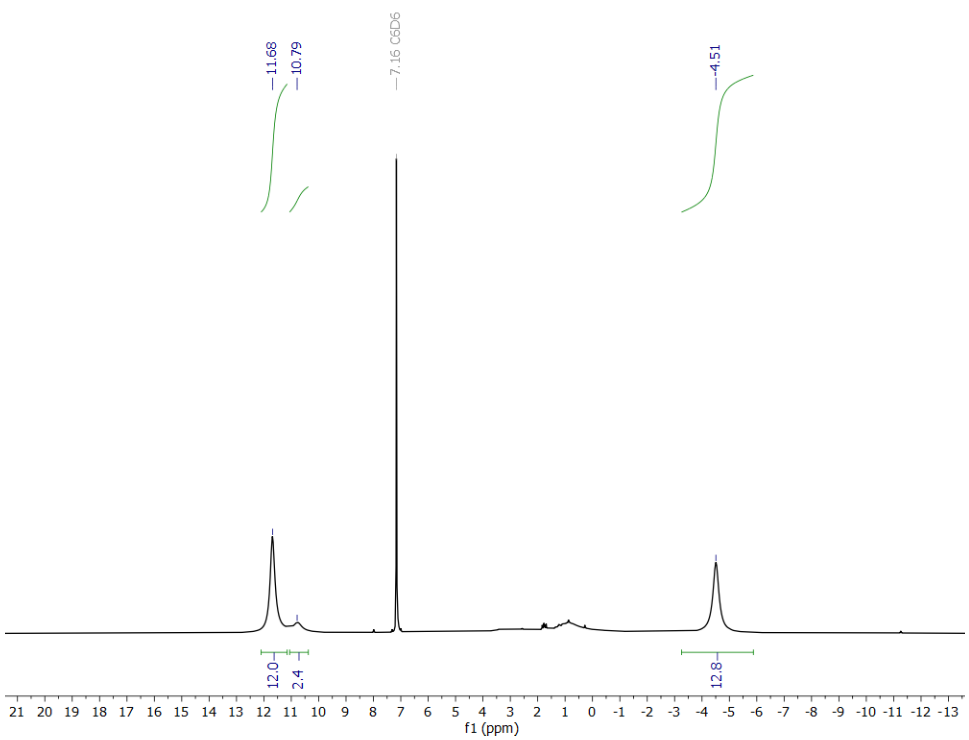


Figure S10. ^{1}H NMR in C_6D_6 of **5-Ce**.

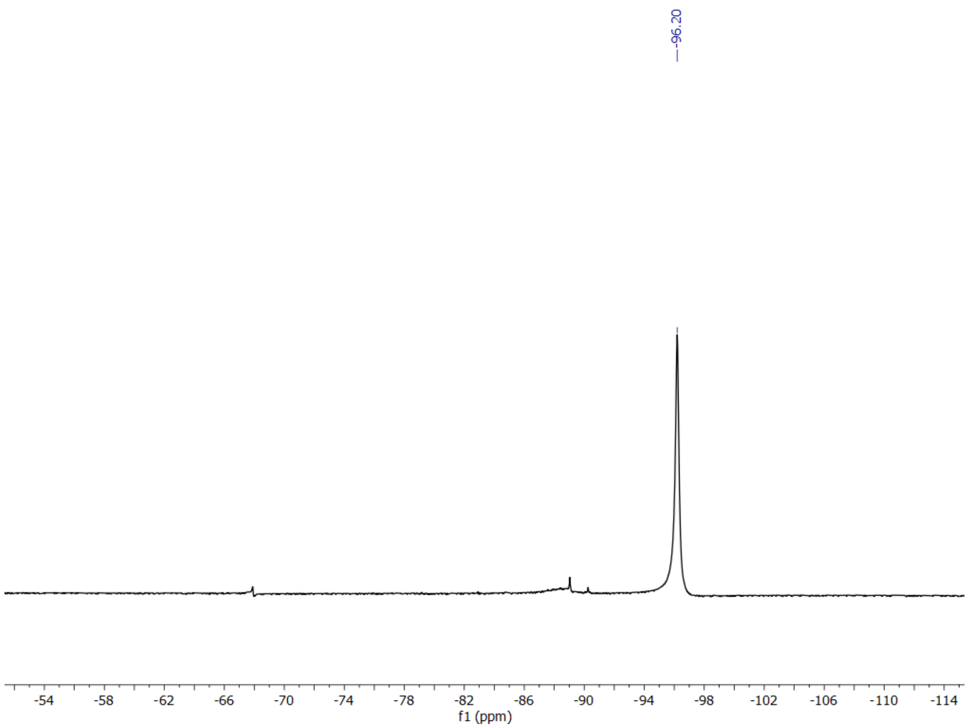


Figure S11. ^{19}F NMR in THF-D$_8$ of **5-Ce**.

<u>Synthesis of **$(Cp^{Me4})_2Ce(CH_2Ph)(THF)$ (6-Ce)**</u>

In a glovebox, a 20 mL vial was charged with **(5-Ce)** (262.4 mg, 0.4354 mmol, 1.00 equiv.) dissolved in THF (8 mL), yielding a bright yellow solution. With stirring, a THF solution (2 mL) of $MgBn_2(THF)_2$ (80.6 mg, 0.2298 mmol, 0.53 equiv.) was added dropwise, resulting in a darkening of the color to a golden yellow. The solution was stirred at room temperature for 1 hour before being dried under vacuum to yield a bright yellow residue, which was extracted with hexanes (20 mL). The yellow solution was filtered and concentrated, then stored at –30 ºC overnight to yield a bright yellow microcrystalline solid. After decanting the supernatant, the solid was dried under vacuum to yield **$(Cp^{Me4})_2Ce(CH_2Ph)(THF)$**. 88% yield. X-ray quality crystals were grown by cooling a hexanes solution to –30 °C for 3 days.

Note: In our hands, **$(Cp^{Me4})_2Ce(CH_2Ph)(THF)$** decomposes to a dark brown material upon prolonged exposure to vacuum (i.e. >3 hours), presumably due to irreversible loss of coordinated THF. Moreover, the complex is dichroic in solution, appearing yellow when concentrated but green when dilute in hexane solution.

^{1}H NMR (500 MHz, C_6D_6) δ 15.62 (br. s, 2H), 5.14 (br. s, 12H), 3.04 (br. s, 12H), 0.14 (br. s, 2H), –1.20 (br. s, 4H), –2.65 (t, J = 6.8 Hz, 1H, $\mathbf{H}_{p\text{-}Ar}$), –4.33 (br. s, 4H), –4.67 (br. s, 2H), –11.27 (br. s, 2H).

Anal. Calcd for: $C_{29}H_{42}CeO$: C, 63.7; H, 7.74. Found: C, 58.02; H, 6.79. [Multiple attempts]

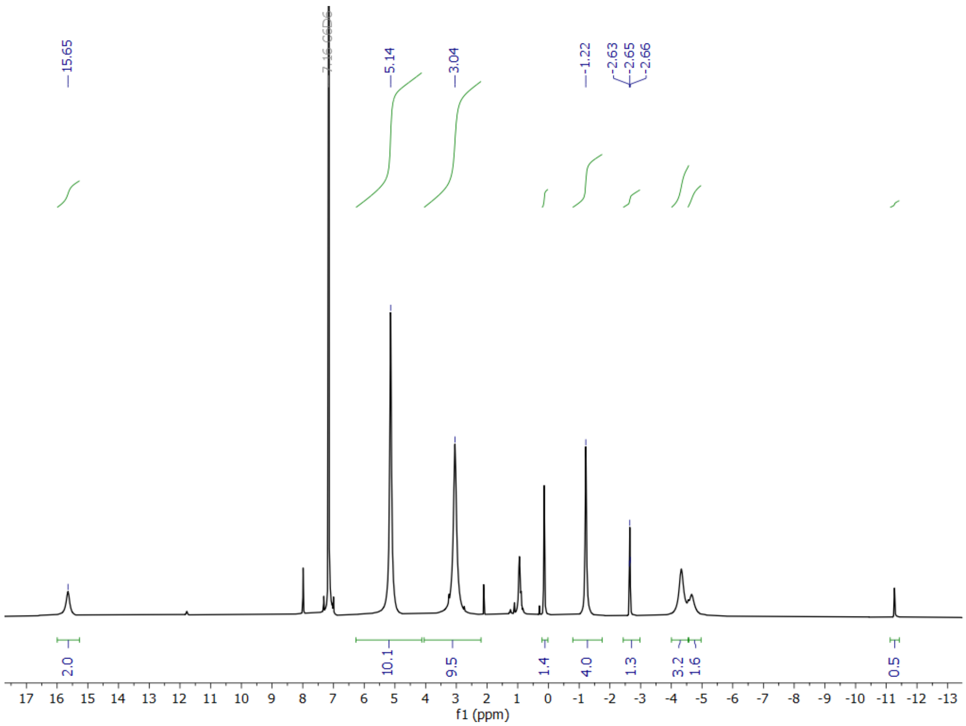


Figure S12. ^{1}H NMR in C_6D_6 of **6-Ce**.

<u>Synthesis of **LaL(Cp^{Me4})$_2$ (1-La)**</u>

In a glovebox, to a magnetically stirred solution of **La(Cp^{Me4})$_3$ (2-La)** (1.212 g, 2.40 mmol, 1 equiv.) in toluene (50 mL), **HL** (0.756 g, 2.40 mmol, 1 equiv). was added and the solution stirred overnight. After this time, volatiles were removed by vacuum evaporation and the cream solid washed with cold (–30°C) hexane (2 x 5 ml) to afford **LaL(Cp^{Me4})$_2$**. Yield: 74%. Diffraction quality crystals were grown from a concentrated toluene solution at –30°C.

^{1}H NMR (500 MHz, C_6D_6, 298 K) : δ 7.50 (1H, d, $J_{H\text{-}H}$ = 2.4, CH_{Im}), 7.10 (1H, d, $J_{H\text{-}H}$ = 2.5, CH_{Im}), 6.73 (1H, d, $J_{H\text{-}H}$ = 1.7, CH_{Ph}), 6.26 (1H, d, $J_{H\text{-}H}$ = 1.8, CH_{Ph}), 5.77 (2H, s, CH_{Cp}), 4.41 (1H, sept, $J_{H\text{-}H}$ = 6.8, H_{iPr}), 2.23

(6H, s, CH_{3Cp}), 2.21 (6H, s, CH_{3Cp}), 2.11 (6H, s, CH_{3Cp}), 1.97 (6H, s, CH_{3Cp}), 1.87 (9H, s, CH_{3tBu}), 1.69 (9H, s, CH_{3tBu}), 1.39 (9H, s, CH_{3tBu}), 1.17 (6H, d, $J_{H\text{-}H}$ = 6.8, CH_{iPr}). $^{13}C\{^{1}H\}$ NMR (125 MHz, C_6D_6, 298 K): δ 154.1 (s, C-O), 138.9 (s, C_{Ph}), 136.5 (s, C_{Ph}), 128.4 (s, NCN), 123.4 (s, C_{PhH}), 122.5 (s, C_{im}), 121.8 (s, Cp), 120.7 (s, Cp), 119.8 (s, Cp), 118.8 (s, Cp), 118.5 (s, C_{im}), 114.7 (s, C_{PhH}), 111.9 (s, CpH), 52.9 (s, iPrCH), 36.2 (s, C_{CH3}), 34.3 (s, C_{CH3}), 32.1 (s, C_{tBu}), 30.6 (s, C_{tBu}), 24.0 (s, iPr_{CH3}), 13.0 (s, CpMe), 12.9 (s, CpMe), 11.4 (s, CpMe), 10.07 (s, CpMe).

Anal. Calcd for: $C_{38}H_{55}LaN_2O$: C, 65.79, H, 7.85, N, 4.04. Found: C, 66.07 H; 8.03; N, 3.67.

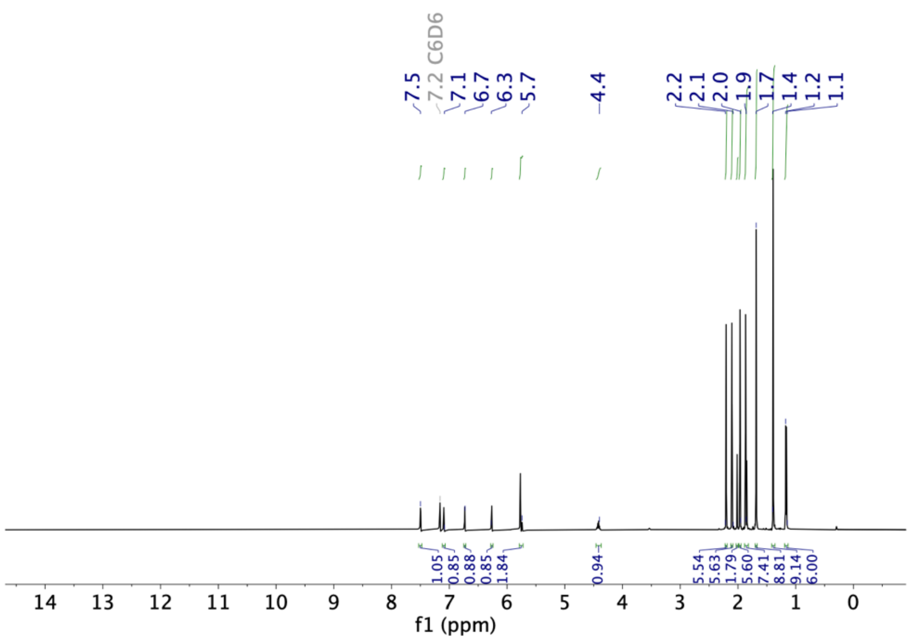


Figure S13. ^{1}H NMR in C_6D_6 of **1-La**.

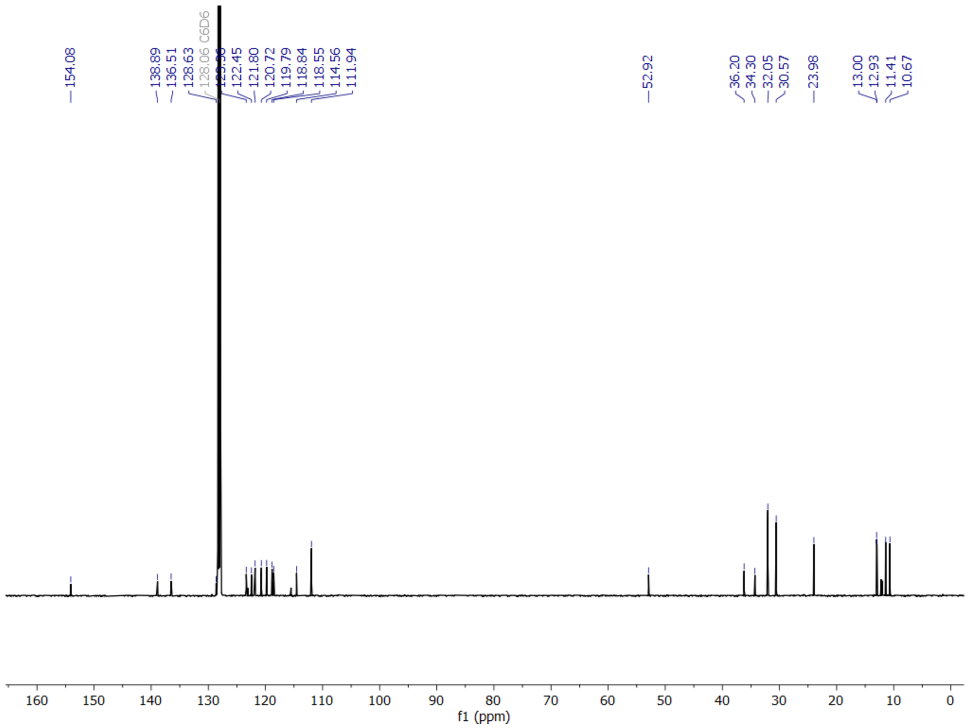


Figure S14. $^{13}C\{^1H\}$ NMR in C_6D_6 of **1-La**.

<u>Synthesis of **[(Cp^{Me4})$_2$LaCl]$_2$ (3-La)**</u>

Method A: In a glovebox, to a magnetically stirred solution of La(Cp^{Me4})$_3$ (**2-La**) (40.0 mg, 0.0575 mmol, 1 equiv.) in toluene (2 mL), benzyl chloride (6.66 µL, 0.0579 mmol, 1 equiv.). was added and the solution stirred overnight. After this time, volatiles were removed by vacuum evaporation and the white solid washed with cold (-20°C) hexane (2 x 5 ml) to afford [(Cp^{Me4})$_2$La(µ–Cl)]$_2$ Yield: 79%. Diffraction quality crystals were grown from a concentrated toluene solution at –30°C.

Method B: In a glovebox a vial was charged with **2-La** (40.0 mg, 0.0575 mmol, 1.00 equiv.) in THF (5 mL). With stirring, a colorless solution of $PhICl_2$ (7.92 mg, 0.0288 mmol, 0.52 equiv.) in THF (1 mL) was added dropwise. After stirring for 2 hours at room temperature, the volatiles were removed under vacuum, resulting in a cream powder which was subsequently washed with hexanes (2 x 0.5 mL). The powder was redissolved in a minimum of THF (1 mL), and the colorless solution was filtered through glass fiber into a 4 mL vial, layered with hexanes (3 mL) and stored at –30 °C for 3 days to yield large colorless blocks of **[(Cp^{Me4})$_2$LaCl]$_2$** that were dried *in vacuo*. Yield: 63%.

^{1}H NMR (400 MHz, THF-H_8, 298 K): δ 5.51 (2H, s, CH_{3Cp}), 1.99 (6H, s, CH_{3Cp}), 1.90 (6H, s, C_5Me_4H).

$^{13}C\{^{1}H\}$ NMR (125 MHz, THF-H_8, 298 K): δ 122.0 (s, C_{Cp}), 122.0 (s, C_{Cp}), 112.9 (s, C_{HCp}), 12.5 (s, C_{H3Cp})

Anal. Calcd for $C_{36}Cl_2H_{52}La_2$: C, 51.88; H, 6.29; Found: C, 49.03; H, 5.69. [Multiple attempts]

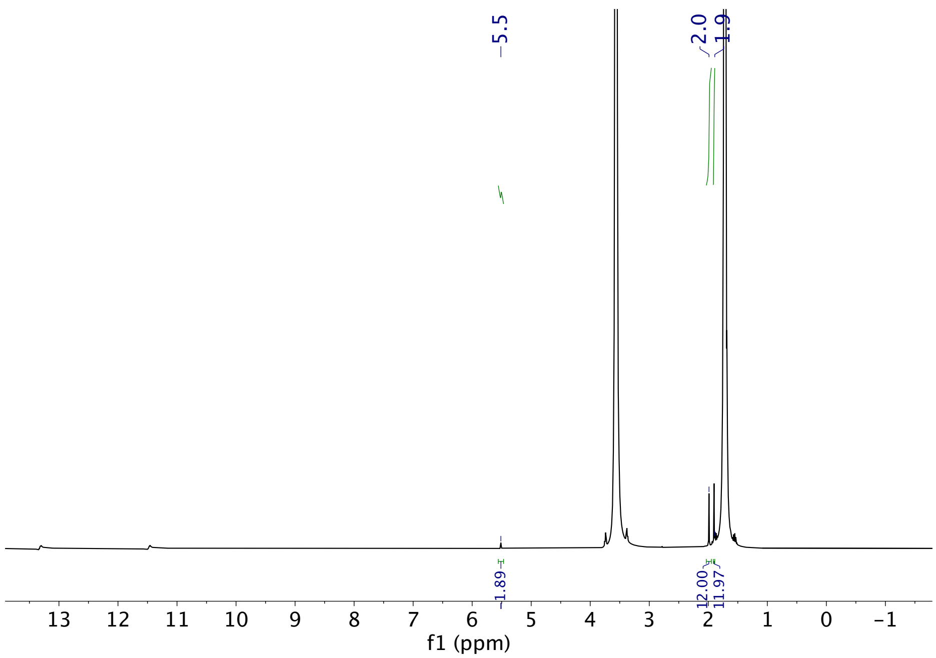


Figure S15. ^{1}H NoD NMR in THF-H_8 of **3-La**. Solvent artifacts are observed between 11.5 and 13.5 ppm.

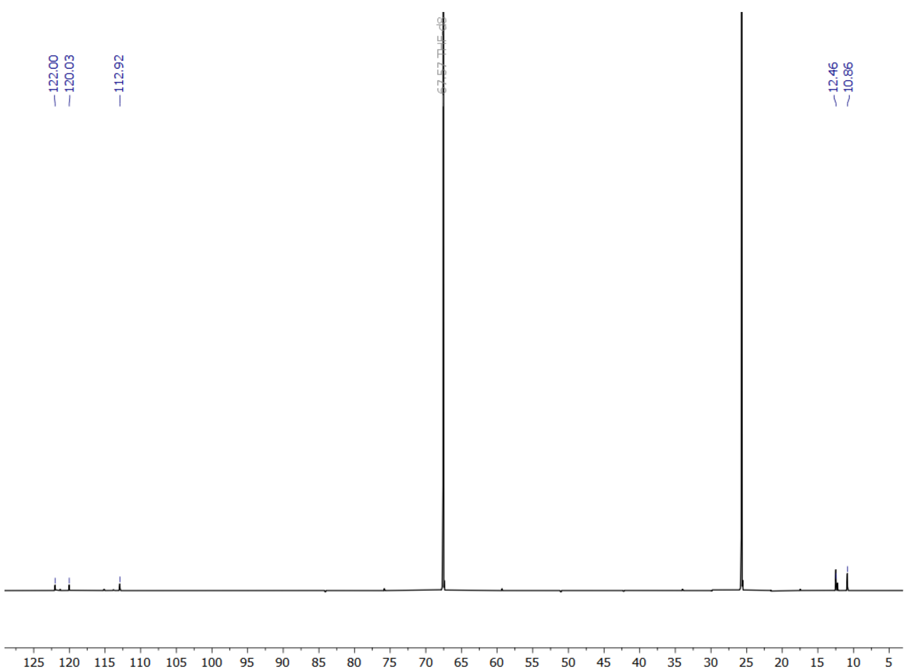


Figure S16. $^{13}C\{^{1}H\}$ NoD NMR in THF-D_8 of **3-La**.

Synthesis of **$NdL(Cp^{Me4})_2$ (1-Nd)**

In a glovebox, to a magnetically stirred solution of **$Nd(Cp^{Me4})_3$** (54.9 mg, 0.108 mmol, 1 equiv.) in toluene (50 mL), **HL** (34.1 mg, 0.108 mmol, 1 equiv). was added and the blue solution stirred overnight. After this time a color change to green was observed, volatiles were removed by vacuum evaporation and the resulting blue solid washed with cold (–30°C) hexane (2 x 2 ml) to afford **$NdL(Cp^{Me4})_2$**. Yield: 64%. Diffraction quality crystals were grown from a concentrated toluene solution at –30 °C.

Anal. Calcd for: $C_{38}H_{55}N_2ONd$: C, 65.19; H, 7.92; N, 4.00. Found: C, 65.47; H, 7.73; N, 3.82.

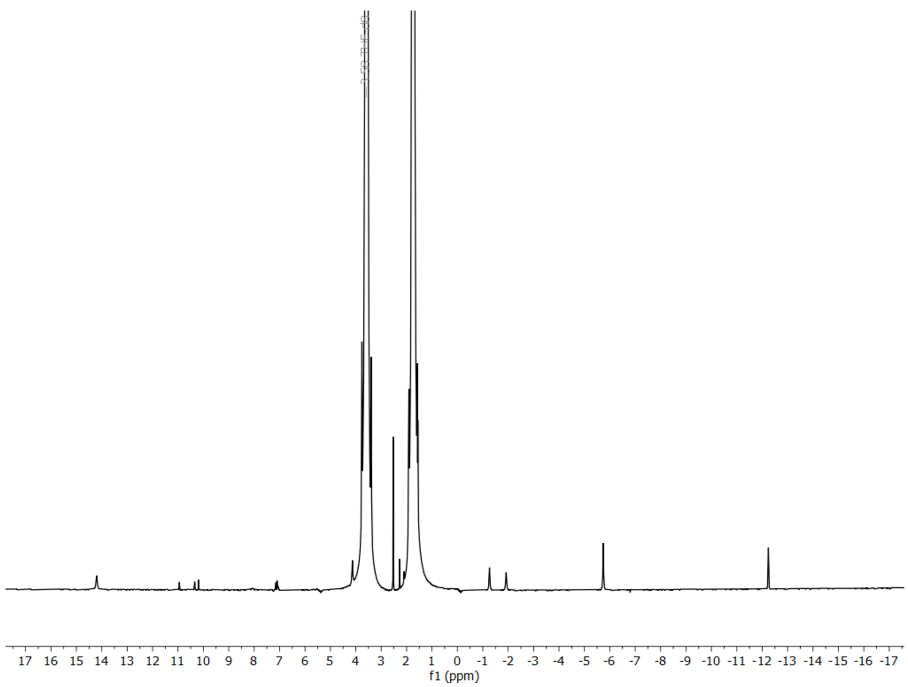


Figure S17. [1]H NoD NMR in THF of **1-Nd**.

Synthesis of **$SmL(Cp^{Me4})_2$ (1-Sm)**

In a glovebox, to a magnetically stirred solution of **$Sm(Cp^{Me4})_3$** (24.0 mg, 0.0460 mmol, 1 equiv.) in toluene (2 mL), **HL** (14.7 mg, 0.046 mmol, 1 equiv). was added and the red solution stirred overnight. After this time, volatiles were removed by vacuum evaporation and the yellow solid washed with cold (**–**30°C) hexane (2 x 2 ml) to afford **$SmL(Cp^{Me4})_2$**. Yield: 59%. Diffraction quality crystals were grown from a concentrated toluene solution at –30°C.

Anal. Calcd for: $C_{38}H_{55}N_2OSm$: C, 64.54; H, 7.98; N, 4.00. Found: C, 64.75; H, 8.43; N, 4.40.

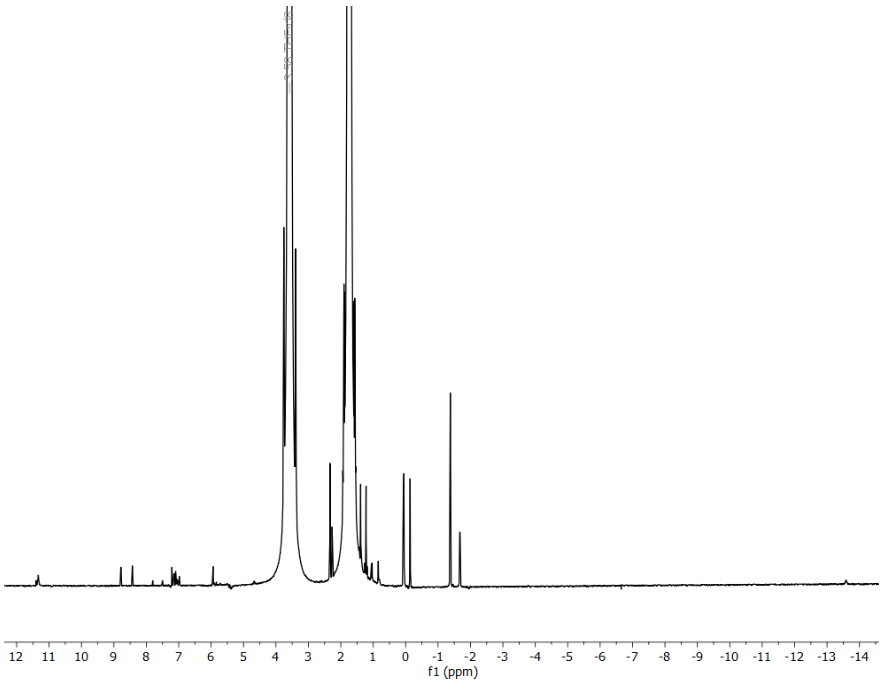


Figure S18. ^{1}H NoD NMR in THF of **1-Sm**.

Synthesis of **[MgBnL]$_2$ (7-Mg)**

To a cold (–78 °C) solution of **HL** (31.4 mg, 0.01 mmol, 1 equiv.) in THF (2 mL) was added a cold solution of $MgBn_2(THF)_2$ (35.0 mg, 0.01 mmol, 1 equiv.) dropwise over ten minutes. The mixture was allowed to warm to room temperature, with stirring, overnight. After this period, volatiles were removed by vacuum evaporation, and the cream powder washed with cold hexanes. Yield: 59%. Diffraction quality crystals were grown from a concentrated toluene solution at –30°C.

^{1}H NMR (500 MHz, C_6D_6, 298 K) : δ 7.59 (1H, d, $J_{H\text{-}H}$ = 2.6, CH_{im}), 6.94 (d, $J_{H\text{-}H}$ = 2.4, 1H, CH_{im}), 6.86 (2H, t, $J_{H\text{-}H}$ = 7.5, CH_{Bn}), 6.69 (2H, d, $J_{H\text{-}H}$ = 7.6, CH_{Bn}), 6.56 (1H, d, $J_{H\text{-}H}$ = 1.7, CH_{Ph}), 6.53 (1H, $J_{H\text{-}H}$ =7.2, CH_{Bn}), 5.82 (1H, d, $J_{H\text{-}H}$ = 1.7, CH_{Ph}), 3.13 (1H, h, $J_{H\text{-}H}$ = 6.6, CH_{iPr}), 2.00 (2H, dd, $J_{H\text{-}H}$ = 8.9, CH_{2Bn}), 1.83 (9H, s, CH_{3tBu}), 1.35 (9H, s, CH_{3tBu}), 0.71 (3H, d, $J_{H\text{-}H}$ = 6.6, CH_{3iPr}), 0.62 (3H, d, $J_{H\text{-}H}$ = 6.6, CH_{3iPr}). $^{13}C\{^1H\}$ NMR (125 MHz, C_6D_6, 298 K): δ 156.3 (s, C-O), 142.7 (s, C_{Ph}), 140.8 (s, C_{Ph}), 130.7 (s, NCN), 124.1 (s, C_{Bn}), 123.8 (s, C_{Bn}) 123.7 (s, C_{im}), 119.7 (s, C_{Ph}), 118.9 (s, C_{im}), 117.7 (s, C_{PhH}), 116.5 (s, C_{PhH}), 116.3 (s, C_{Bn}), 51.9 (s, C_{HiPr}), 36.2 (s, C_{CH3}), 34.5 (s, C_{CH3}), 31.8 (s, C_{tBu}), 32.6 (s, C_{tBu}), 25.1 (s, C_{H2Bn}), 23.8 (s, C_{iPr}), 23.3 (s, C_{iPr})

Anal. Calcd for: $C_{54}H_{74}Mg_2N_4O_2$: C, 75.43; H, 8.68; N, 6.52. Found: C, 71.67; H, 8.26; N,6.35.

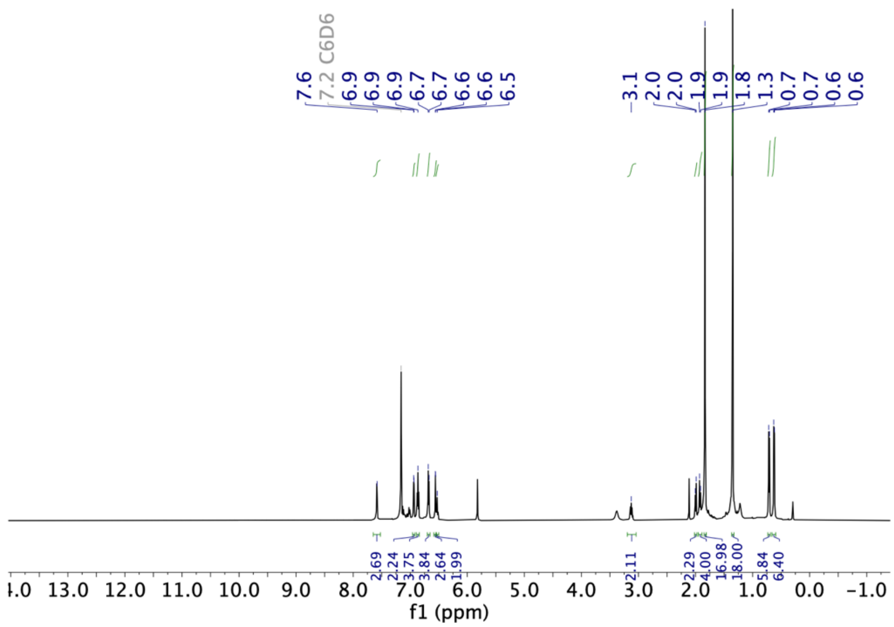


Figure S19. ^{1}H NMR in C_6D_6 of **7-Mg**.

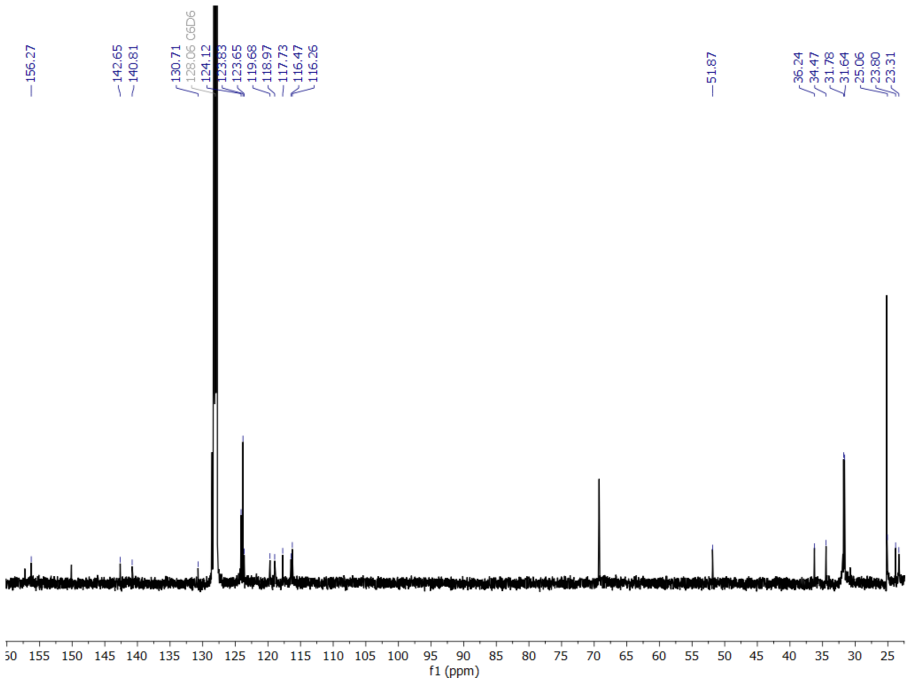


Figure S20. $^{13}C\{^1H\}$ NMR in C_6D_6 of **7-Mg**.

<u>Synthesis of **[MgL]$_2$ (8-Mg)**</u>

To a solution of **HL** (62.8 mg, 0.01 mmol, 2 equiv.) in THF (2 mL) was added a solution of $MgBn_2(THF)_2$ (35.0 mg, 0.01 mmol, 1 equiv.). The mixture was stirred overnight. After this period, volatiles were removed by vacuum evaporation, and the cream powder washed with cold hexanes. Yield: 74% Diffraction quality crystals were grown from a concentrated toluene solution at –30°C.

^1H NMR (500 MHz, C_6D_6, 298 K) : δ 7.57 (2H, d, $J_{H\text{-}H}$ = 2.5, CH_{im}), 7.2 (2H, d, $J_{H\text{-}H}$ = 2.5, CH_{im}), 7.00 (2H, d, $J_{H\text{-}H}$ = 1.8, CH_{Ph}), 6.22 (2H, d, $J_{H\text{-}H}$ = 2.0, CH_{Ph}), 4.18 (2H, br s, CH_{iPr}), 1.78 (18H, s, CH_{3tBu}), 1.43 (18H, s, CH_{3tBu}), 1.01 (6H, d, $J_{H\text{-}H}$ = 6.7, CH_{3iPr}), 0.90 (6H, d, $J_{H\text{-}H}$ = 6.8, CH_{3iPr}). $^{13}C\{^1H\}$ NMR (125 MHz, C_6D_6, 298 K): δ 156.8 (s, C_O), 141.7 (C_{Ph}), 134.4 (s, NCN), 129.3 (s, C_{Ph}), 128.6 (s, C_{Ph}), 125.7 (s, C_{Ph}), 122.3 (s, C_{Ph}), 120.6 (s, CH_{im}), 116.5 (s, CH_{im}), 115.5 (s, C_{Ph}), 52.5 (s,CH_{iPr}), 36.4 (s, C_{tBu}), 34.3 (s, C_{tBu}), 32.2 (s, $C_{(CH3)3}$), 30.2 (s, $C_{(CH3)3}$), 23.9 (s, C_{iPr}), 23.4 (C_{iPr}).

Anal. Calcd for: $C_{40}H_{58}N_4O_2Mg$: C,73.77; H, 8.98; N, 8.60. Found: C, 71.45; H, 9.22; N, 7.27. [Multiple attempts]

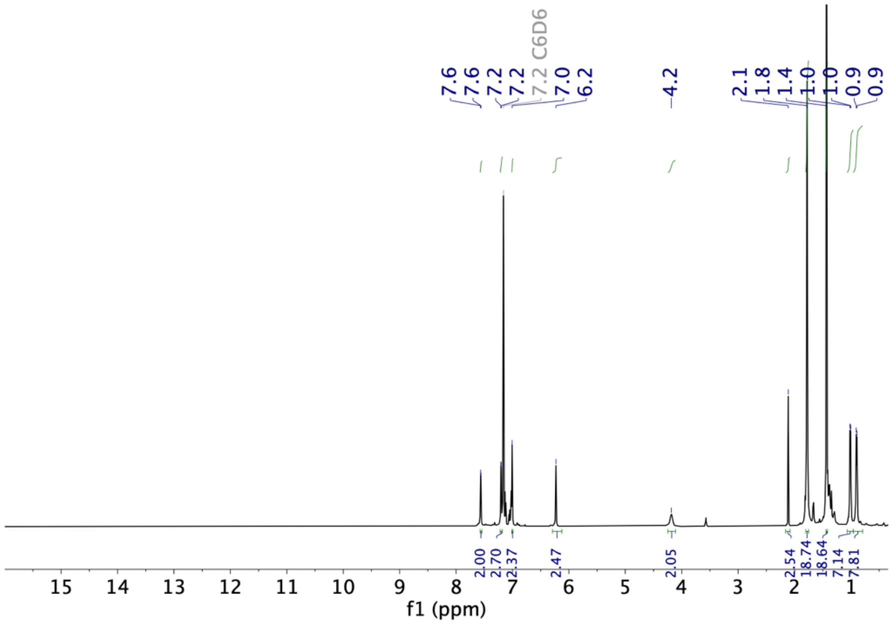


Figure S21. ^{1}H NMR in C_6D_6 of **8-Mg.**

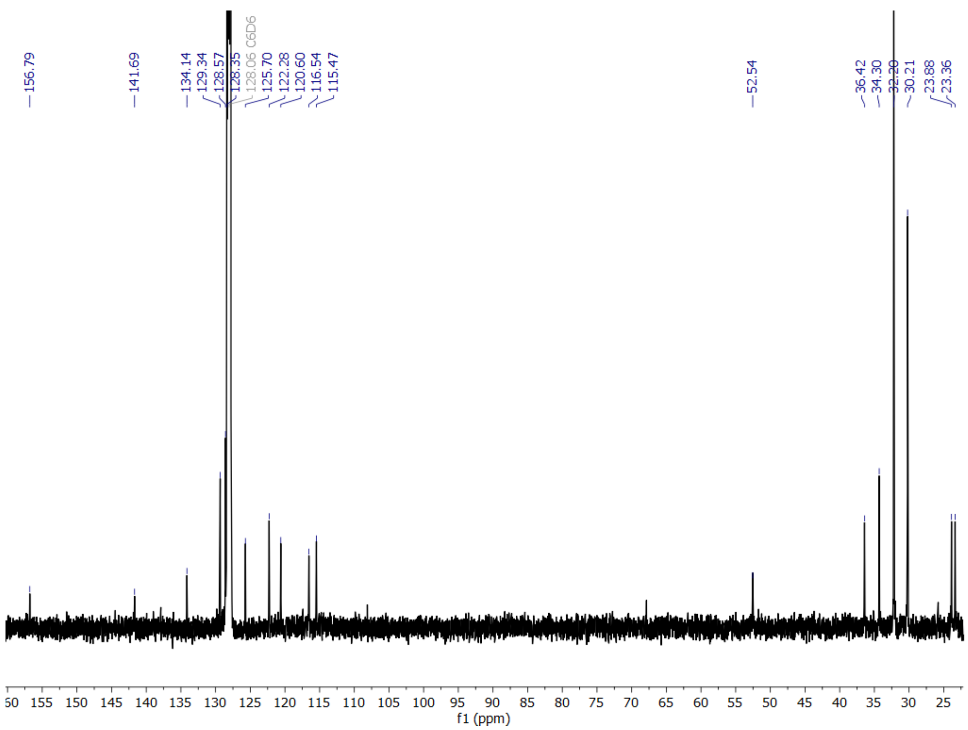


Figure S22. ^{13}C{^{1}H} NMR in C_6D_6 of **8-Mg.**

S3 Absorption and Fluorescence Data

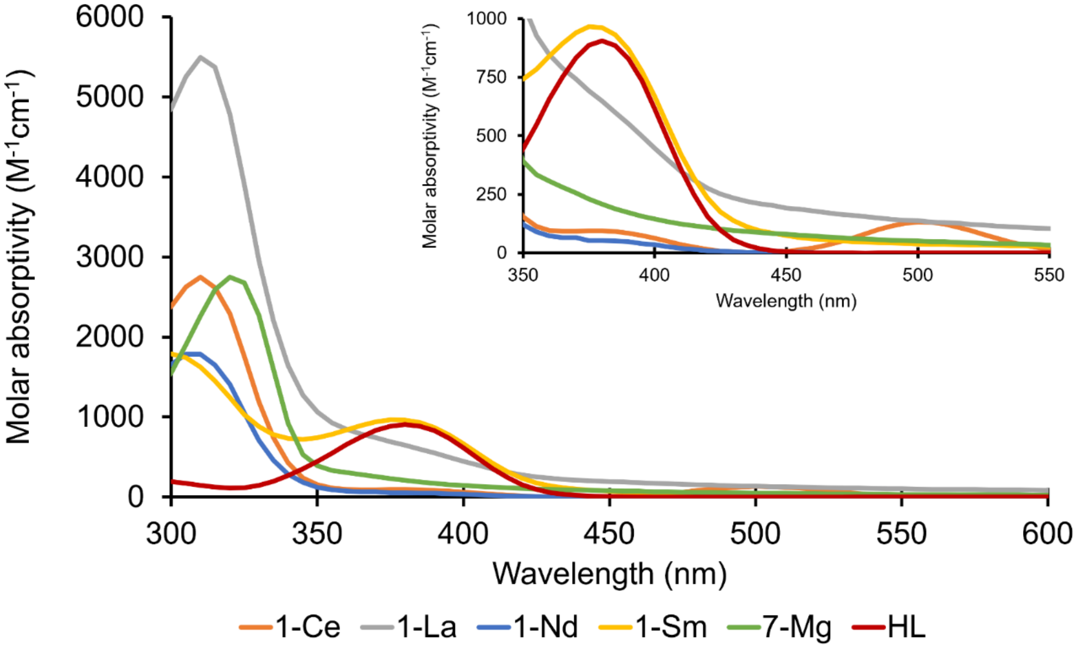


Figure S23: Overlaid UV-Vis spectra of **1-Ce** (orange), **1-La** (grey), **1-Nd** (blue), **1-Sm** (yellow), **7-Mg** (green) and proligand **HL** (red) in THF Cerium metal-centered absorption at 505 nm expanded for clarity.

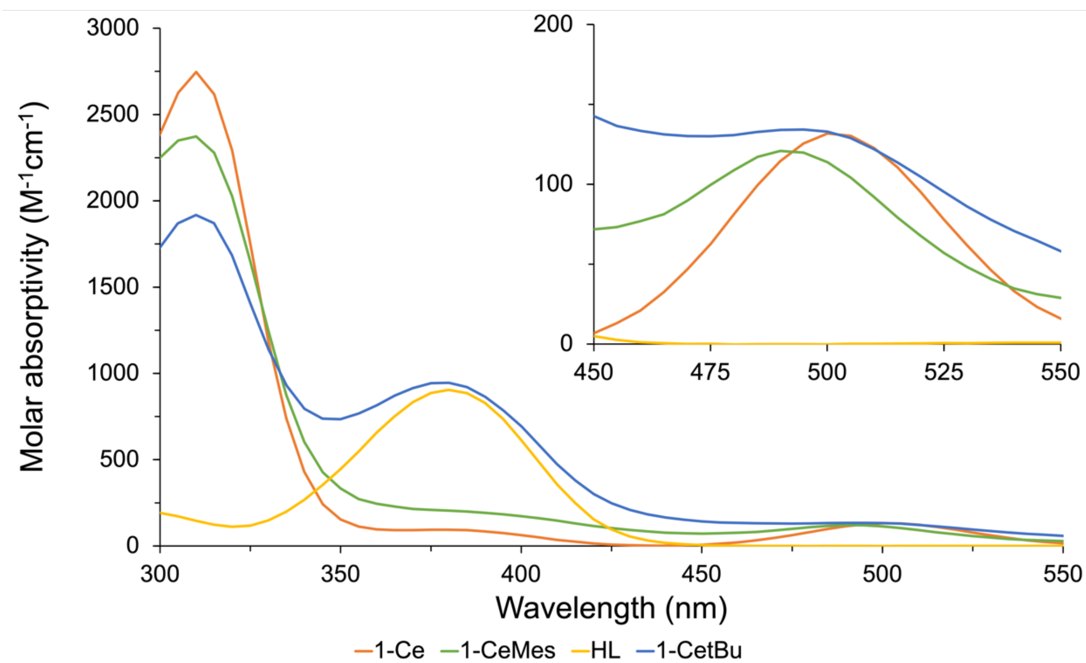


Figure S24: Overlaid UV-Vis spectra of **1-Ce** (orange), **1-CeMes** (green), **1-Ce^{t}Bu** (blue), and **HL** (yellow), in THF Cerium metal-centered absorptions expanded for clarity

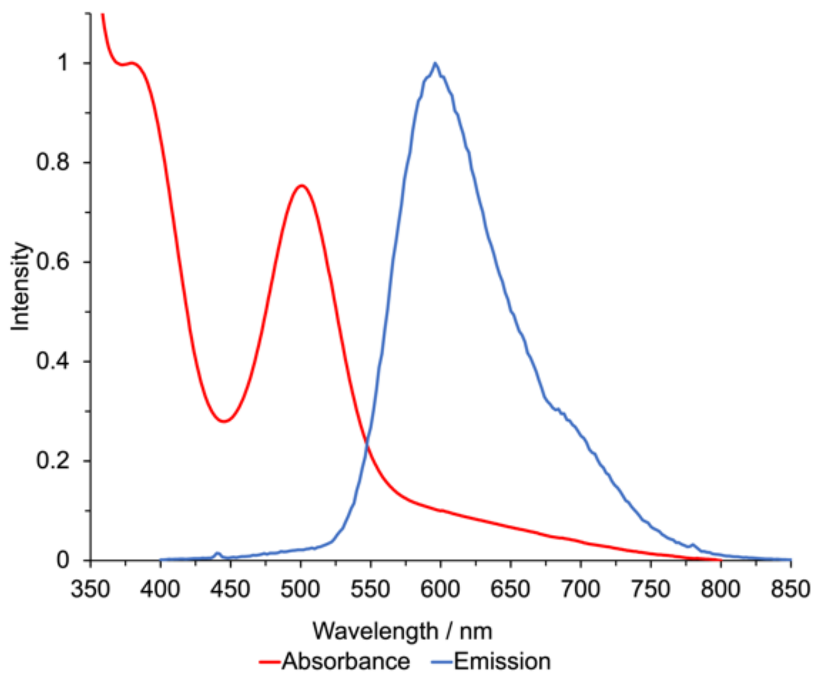


Figure S25. Absorption (red) and emission (blue) spectra of **1-Ce** recorded in THF. The emission spectrum was collected with an excitation wavelength of 390 nm and calibrated to the detector efficiency.

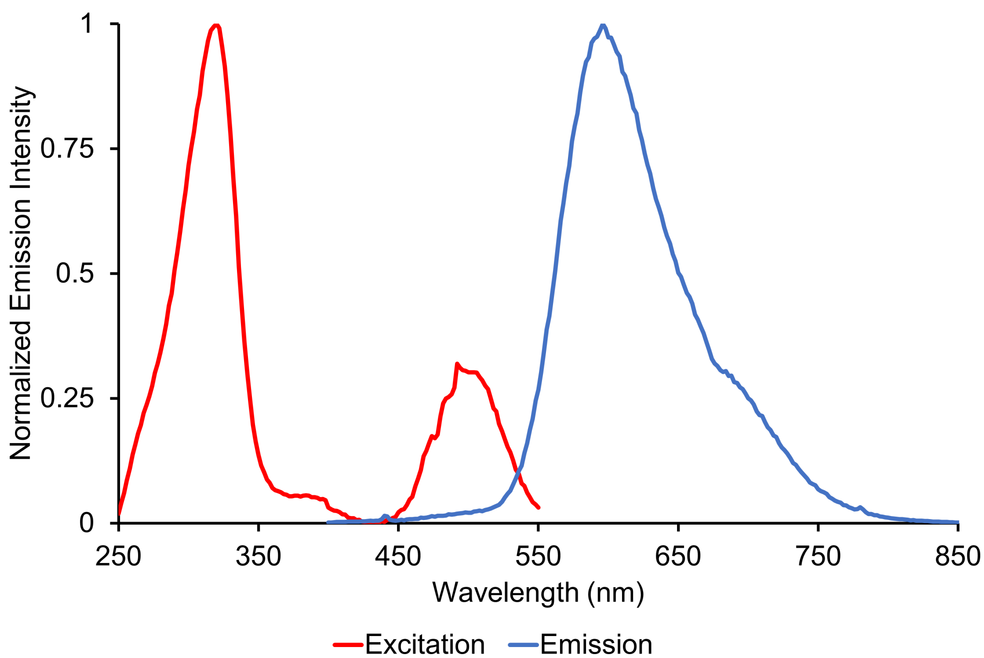


Figure S26. Emission and excitation spectra of **1-Ce** recorded in THF. The emission spectrum was collected with an excitation wavelength of 390 nm; the excitation was monitored at an emission wavelength of 600 nm. All data were calibrated to the detector efficiency and normalized.

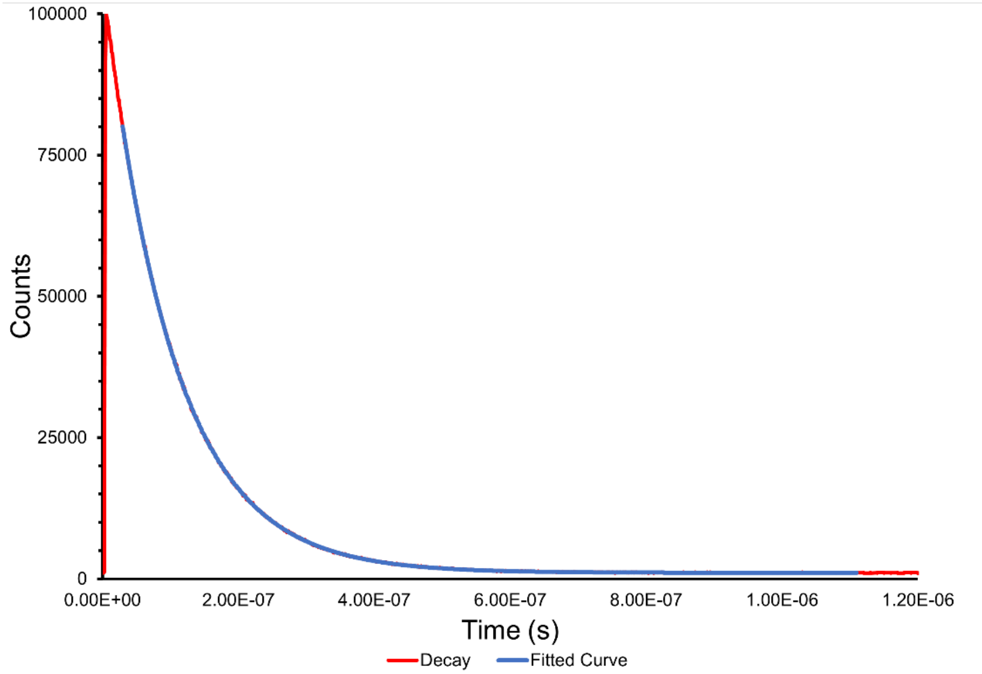


Figure S27. Lifetime decay of **1-Ce** recorded in toluene. τ1[ns]= 101.941 ±0.039.

S4 Electrochemistry

S4.1 Cyclic Voltammograms

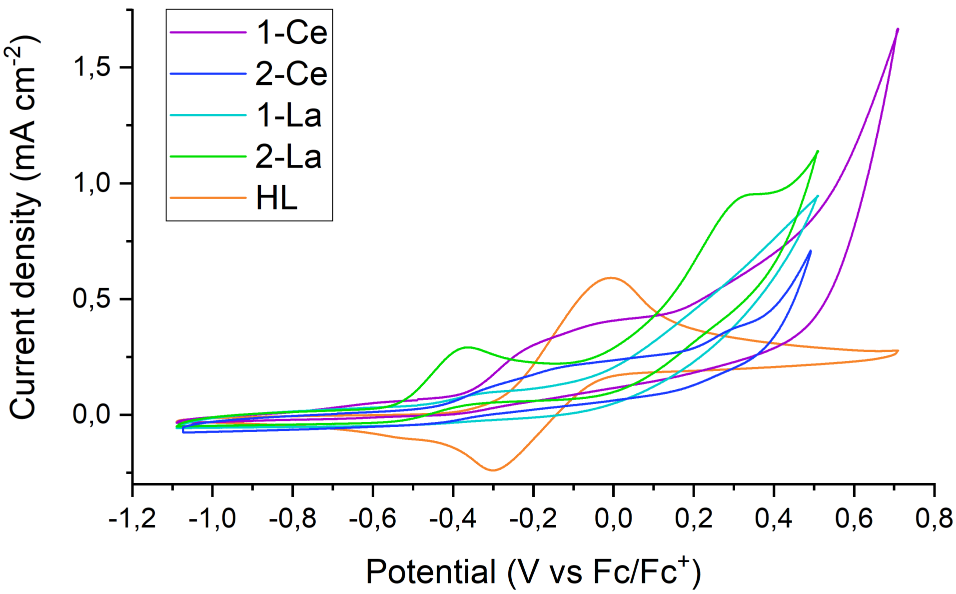


Figure S28. Cyclic voltammograms of **1-Ce** (purple), **2-Ce** (dark blue), **1-La** (light blue), **2-La** (green) and HL (orange) in THF with 0.1 M [^{n}Bu$_4$N][PF$_6$] supporting electrolyte. [analyte] = ca. 5 mM; v = 0.1 V/sec.

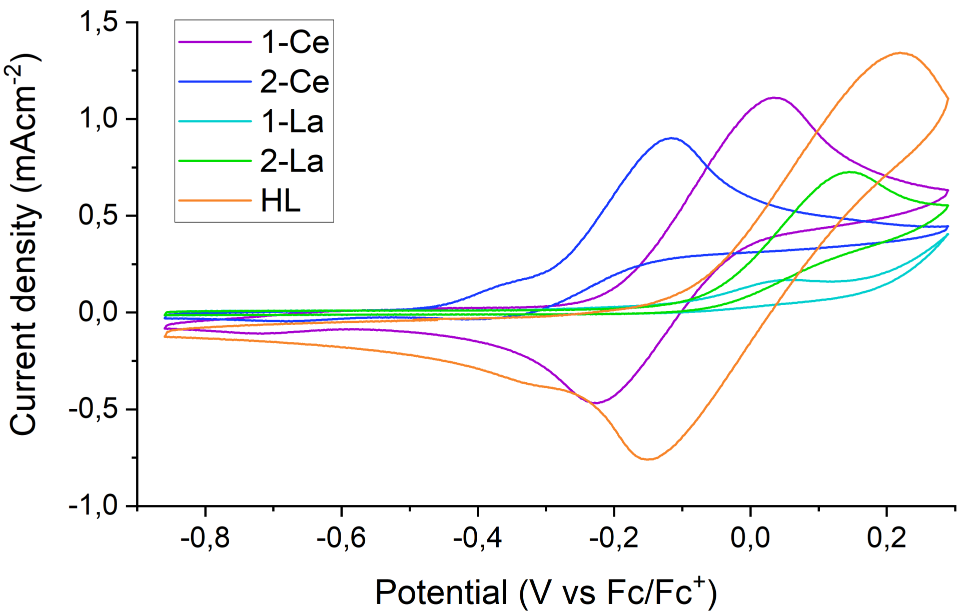


Figure S29. Cyclic voltammograms of **1-Ce** (purple), **2-Ce** (dark blue), **1-La** (light blue), **2-La** (green) and **HL** (orange) in THF with 0.085 M [^{n}Bu$_4$N][BPh$_4$] supporting electrolyte. [analyte] = ca. 5 mM; v = 0.5 V/sec.

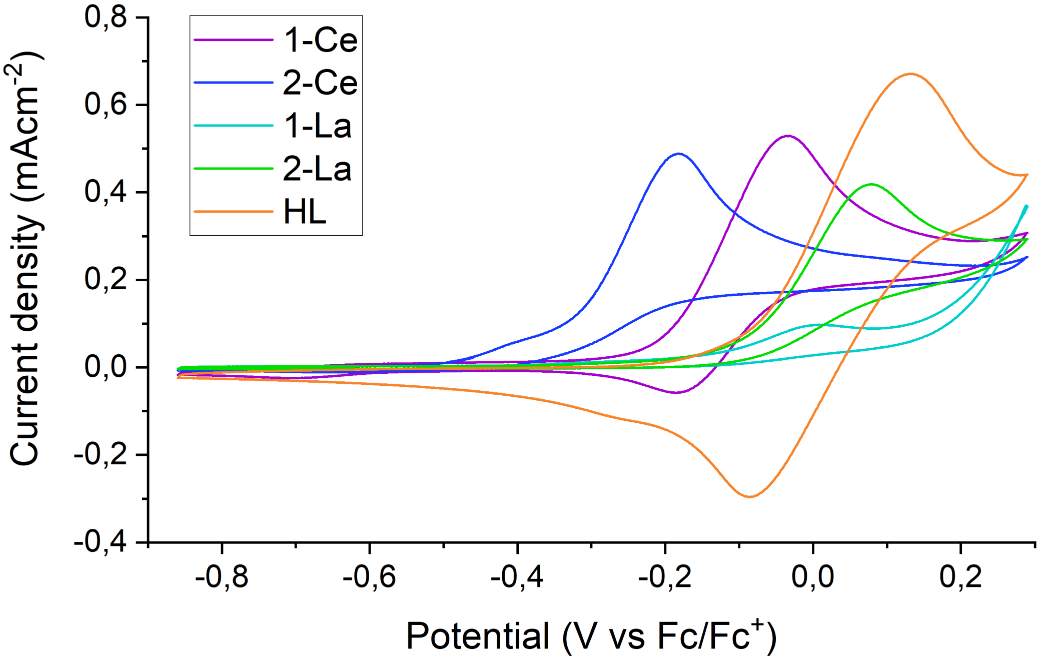


Figure S30. Cyclic voltammograms of **1-Ce** (purple), **2-Ce** (dark blue), **1-La** (light blue), **2-La** (green) and **HL** (orange) in THF with 0.085 M [$^{n}Bu_4N$ BPh_4] supporting electrolyte. [analyte] = ca. 5 mM; v = 0.1 V/sec.

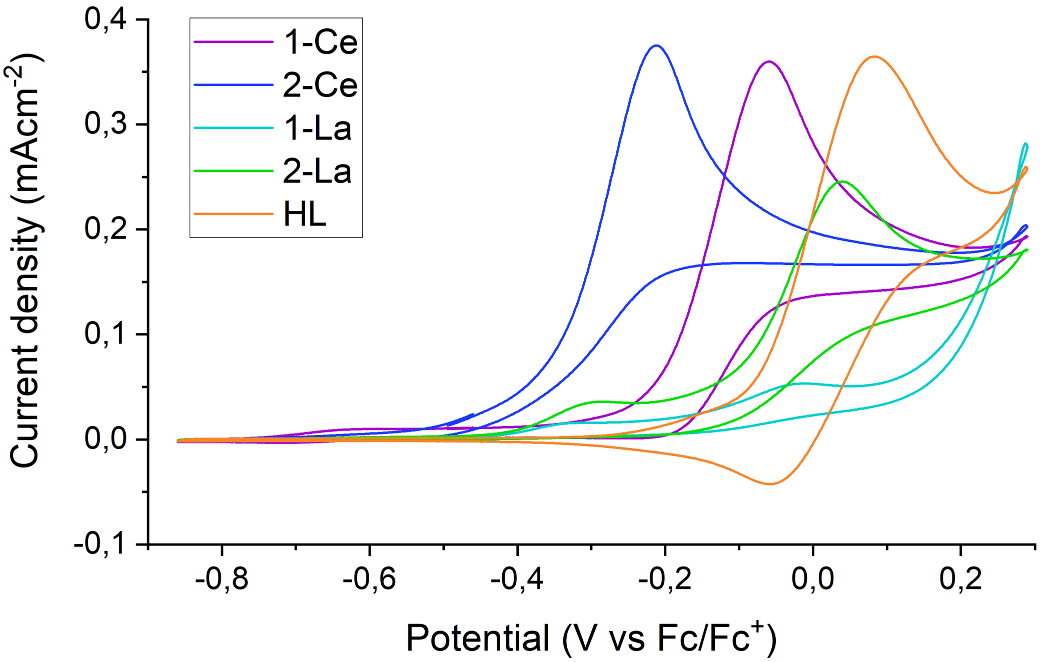


Figure S31. Cyclic voltammograms of **1-Ce** (purple), **2-Ce** (dark blue), **1-La** (light blue), **2-La** (green) and HL (orange) in THF with 0.085 M [$^{n}Bu_4N$][BPh_4] supporting electrolyte. [analyte] = ca. 5 mM; v = 0.02 V/sec.

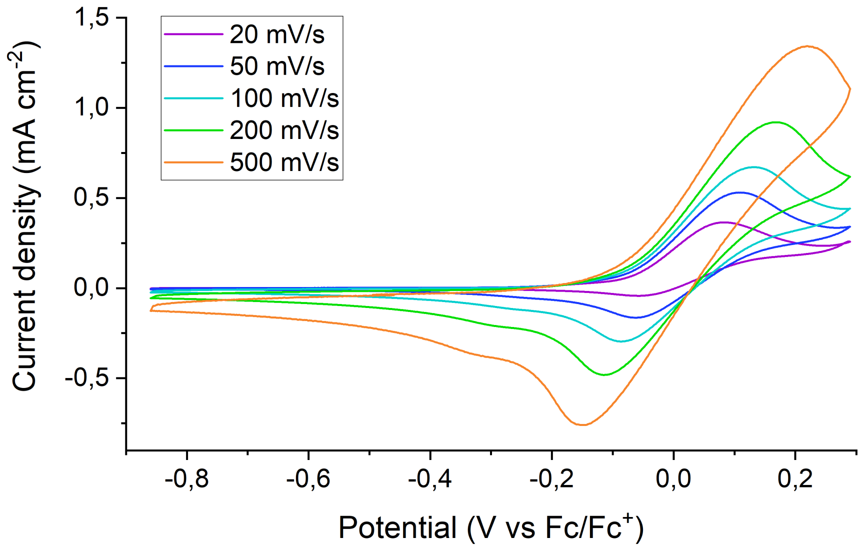


Figure S32. Cyclic voltammograms **HL** in THF with 0.085 M [$^{n}Bu_4N$][BPh_4] supporting electrolyte at different scan speeds between 0.02 and 0.5 V/sec. [analyte] = ca. 5 mM. The $E_{1/2}$ of the partially reversible HL/$HL^{+\cdot}$ redox couple was determined to be −0.00 V vs. Fc/Fc^+. Irreversibility of the redox feature is observed at slow scan speeds, which is attributed to a chemical reaction of the oxidized species.

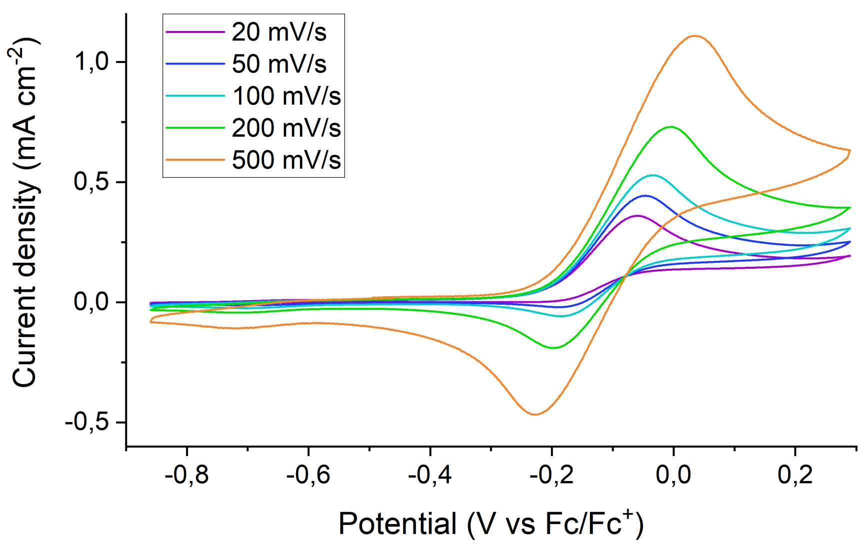


Figure S33. Cyclic voltammograms **1-Ce** in THF with 0.085 M [$^{n}Bu_4N$][BPh_4] supporting electrolyte at different scan speeds between 0.02 and 0.5 V/sec. [analyte] = ca. 5 mM. The $E_{1/2}$ of the partially reversible Ce^{III}/Ce^{IV} redox couple was determined to be −0.15 V vs. Fc/Fc^+. Irreversibility of the redox feature is observed at slow scan speeds, which is attributed to a chemical reaction of the oxidized species similar to the case of HL/$HL^{+\cdot}$.

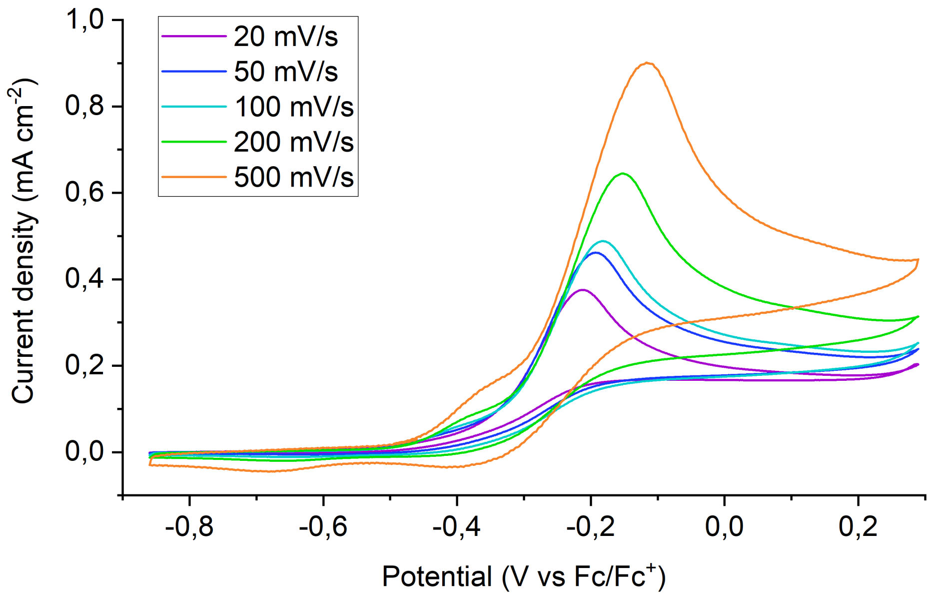


Figure S34. Cyclic voltammograms **2-Ce** in THF with 0.085 M [^{n}Bu$_4$N][BPh$_4$] supporting electrolyte at different scan speeds between 0.02 and 0.5 V/sec. [analyte] = ca. 5 mM. A fully irreversible oxidation is observed with an onset around -0.3 V vs. Fc/Fc$^+$.

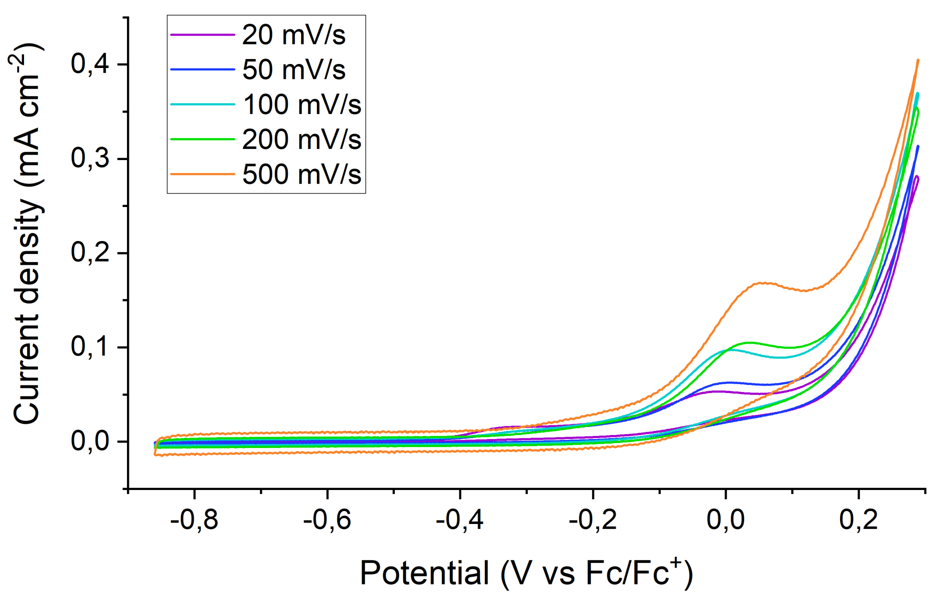


Figure S35. Cyclic voltammograms **1-La** in THF with 0.085 M [^{n}Bu$_4$N BPh$_4$] supporting electrolyte at different scan speeds between 0.02 and 0.5 V/sec. [analyte] = ca. 5 mM. A minor component shows an irreversible oxidation with an onset around -0.15 V vs. Fc/Fc$^+$, followed by a larger increase in oxidative current which is attributed to the main component (**1-La**) with an onset around 0.15 V Fc/Fc$^+$.

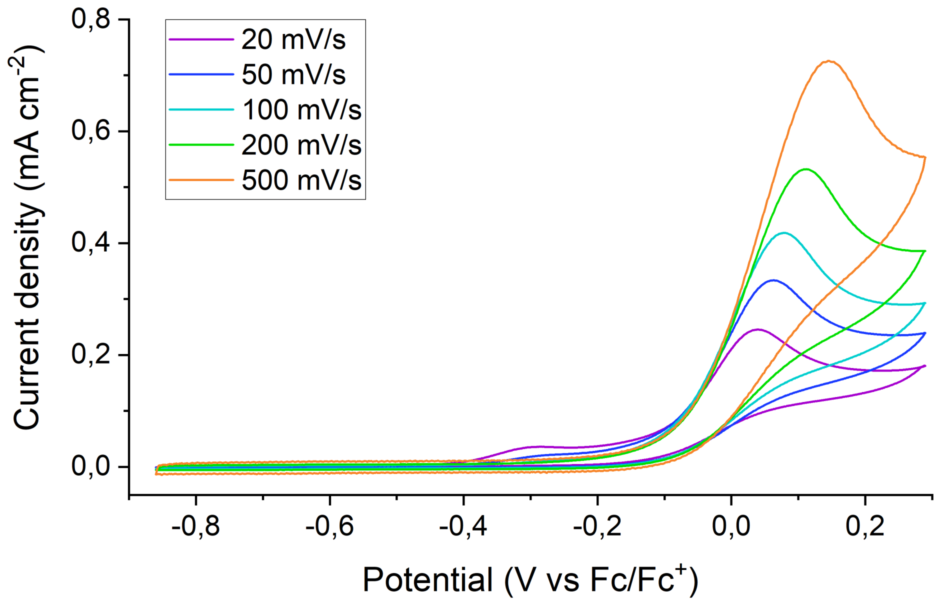


Figure S36. Cyclic voltammograms **2-La** in THF with 0.085 M [^{n}Bu$_4$N BPh$_4$] supporting electrolyte at different scan speeds between 0.02 and 0.5 V/sec. [analyte] = ca. 5 mM. A fully irreversible oxidation is observed with an onset around -0.05 V vs. Fc/Fc$^+$.

S4.2 Rehm Weller Calculation for **1-Ce**

The excited-state reduction potential (E*1/2red) of 1-Ce was calculated using the Rehm-Weller formalism (Equation 1)

$$E^*_{1/2red} = E_{1/2red} - E_{0,0} + \omega \quad (1)$$

$E_{1/2red}$ is the ground state reduction potential between the Ce^{III}/Ce^{IV} redox couple. $E_{0,0}$ is the energy difference between 0th vibrational states of ground state and excited states which can be approximated by emission energy. ω is the work function which describes electrostatic interactions due to the separation of charges upon the redox event. ω is relatively small and is generally omitted.

$E_{1/2red}$ was determined for **1-Ce** in THF solution by a cyclic voltammetry experiment at scan speeds between 0.02 and 0.5 V/sec. (Figure S33) The $E_{1/2red}$ of the Ce^{III}/Ce^{IV} redox couple was determined to be −0.15 V vs. Fc/Fc$^+$. $E_{0,0}$ was determined by the emission maximum (Figure S26) at 605 nm resulting in a value of 2.05 V. Therefore:

$E_{1/2}^* = E_{1/2} - E_{0,0}$
$E_{1/2} = -0.15$ V (Fc/Fc$^+$)
$E_{0,0} = 2.05$ V
$E_{1/2}^* = -0.15$ V -2.05 V)
$E_{1/2}^* = -2.2$ V

S5 Stoichiometric C-F activation of $PhCF_3$

S5.1 Preliminary reactions

S5.1.1 General procedure and results

In a glovebox, a Young NMR tube was charged with metal complex (0.0100 mmol, 1 equiv.) and THF (0.5 mL). $PhCF_3$ (1.23 μL, 0.0100 mmol, 1 equiv.) was then added using a micropipette. The sample was then irradiated with light and monitored periodically by ^1H and ^{19}F NMR spectroscopy. Final time point measurements were collected after 48 hours. Little conversion was seen in these reactions, hypothesized to be due to binding competition with THF solvent.

Table S1. Calculated conversion of $PhCF_3$ to $PhCF_2H$ with yields determined by ^{19}F NMR spectroscopy.

Complex	Conversion to $PhCF_2H$, %
1-Ce	2.7
2-Ce	0.2
3-Ce	0
4-Ce	2.7
5-Ce	0
6-Ce	3.6 (7.4% $PhCF_2CH_2Ph$)
1-La	0.8
7-Mg	10 (4.0% $PhCF_2CH_2Ph$)
8-Mg	0

S5.1.2 ^{19}F NMR spectra

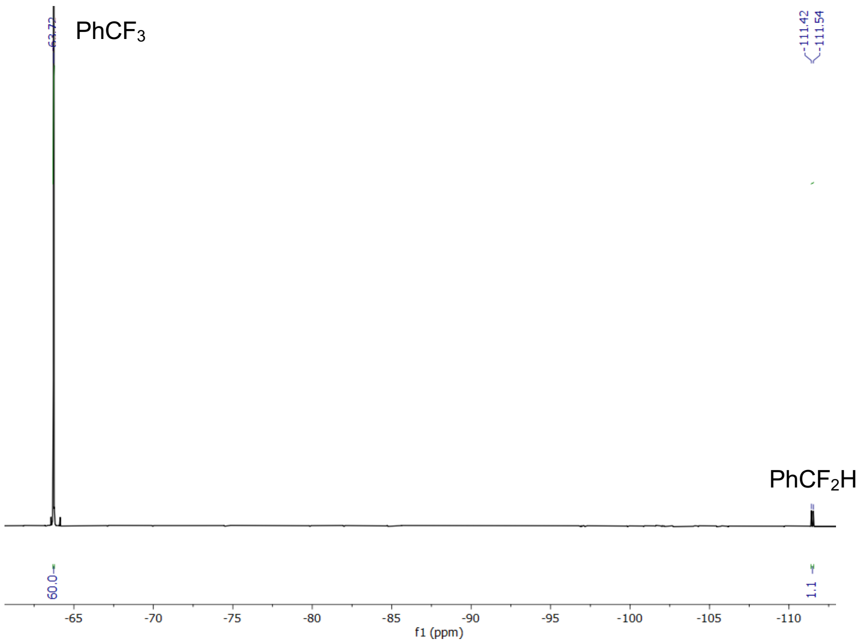


Figure S37. ^{19}F NMR in THF- H_8 **1-Ce** with 1 equiv. $PhCF_3$ following 48 hours of irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

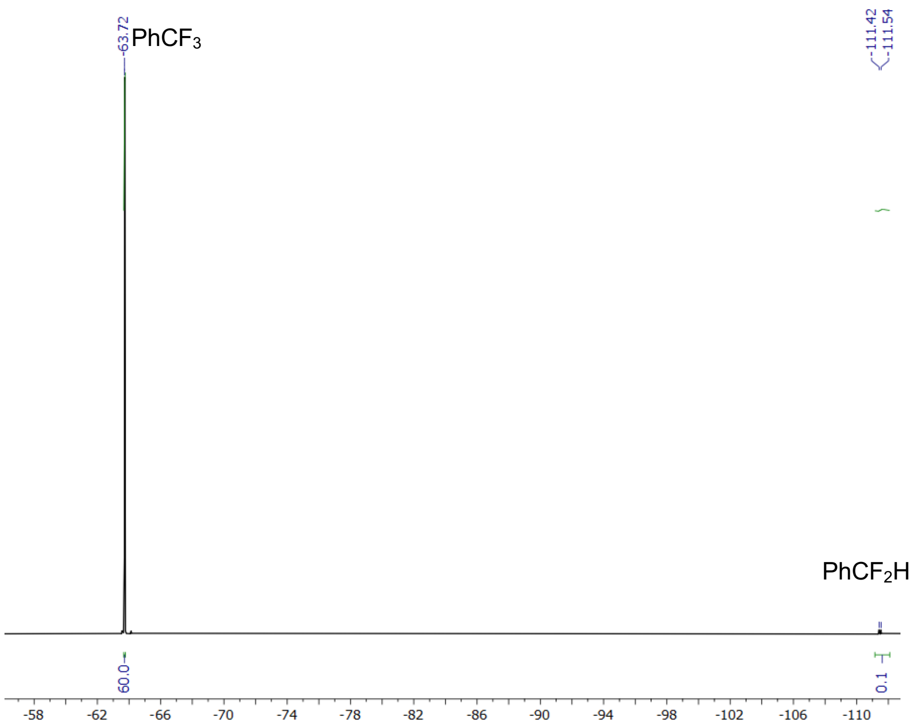


Figure S38. ^{19}F NMR in THF- H_8 **2-Ce** with 1 equiv. $PhCF_3$ following 48 hours of irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

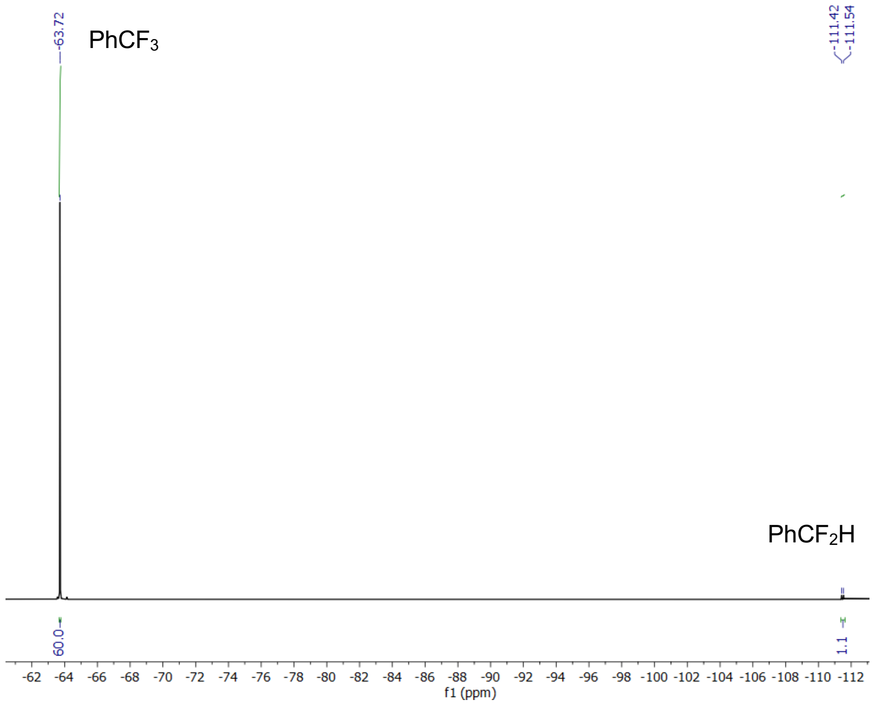


Figure S39. [19]F NMR in THF-H_8 **4-Ce** with 5 equiv. $PhCF_3$ following 48 hours of irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

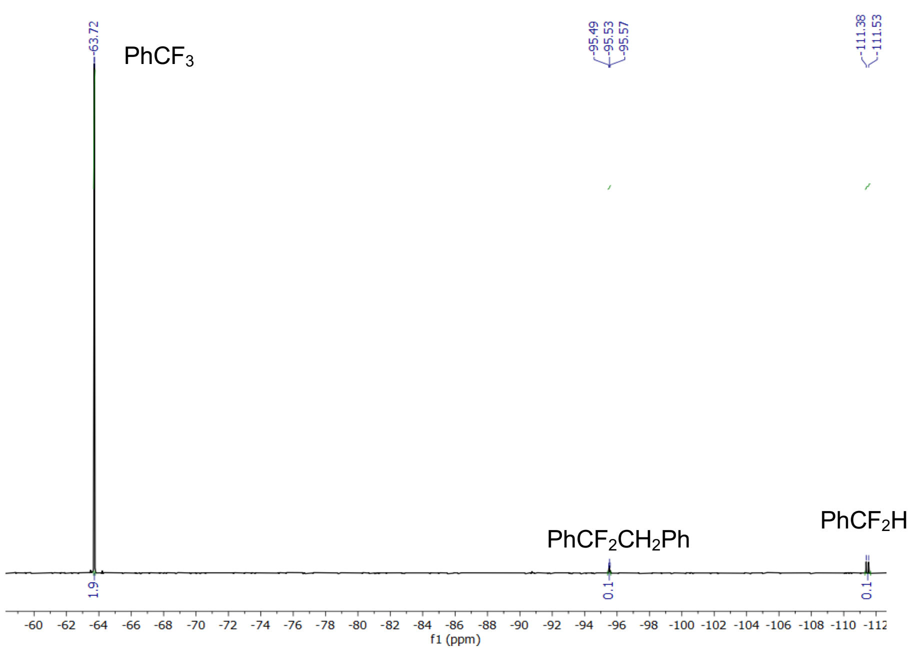


Figure S40.[19]F NMR in THF-H_8 **6-Ce** with 1 equiv. $PhCF_3$ following 48 hours of irradiation under a 40 W Kessil A160WE Tuna Blue lamp. Generation of $PhCF_2CH_2Ph$ is observed via benzyl radicals released from **6-Ce** under irradiation.

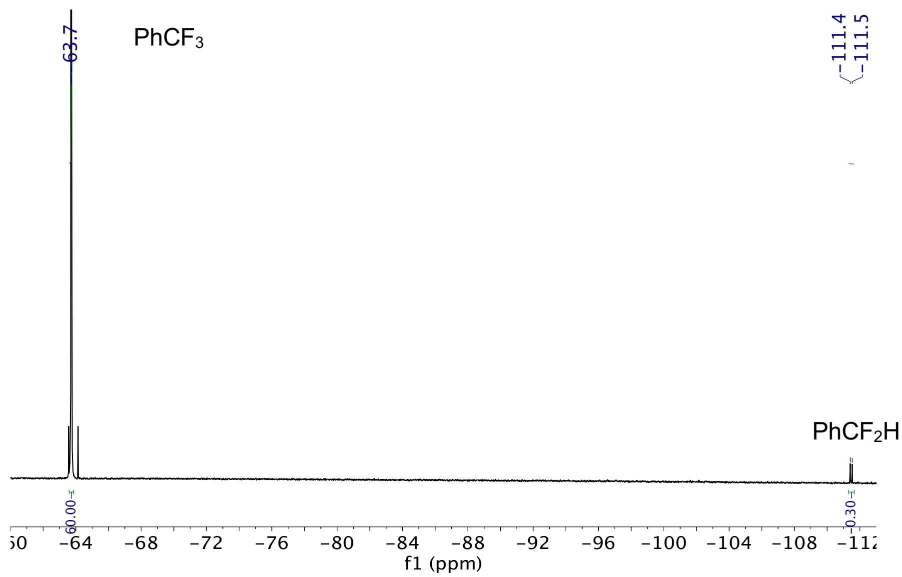


Figure S41.[19]F NMR in THF-H$_8$ **1-La** with 1 equiv. PhCF$_3$ following 48 hours of irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

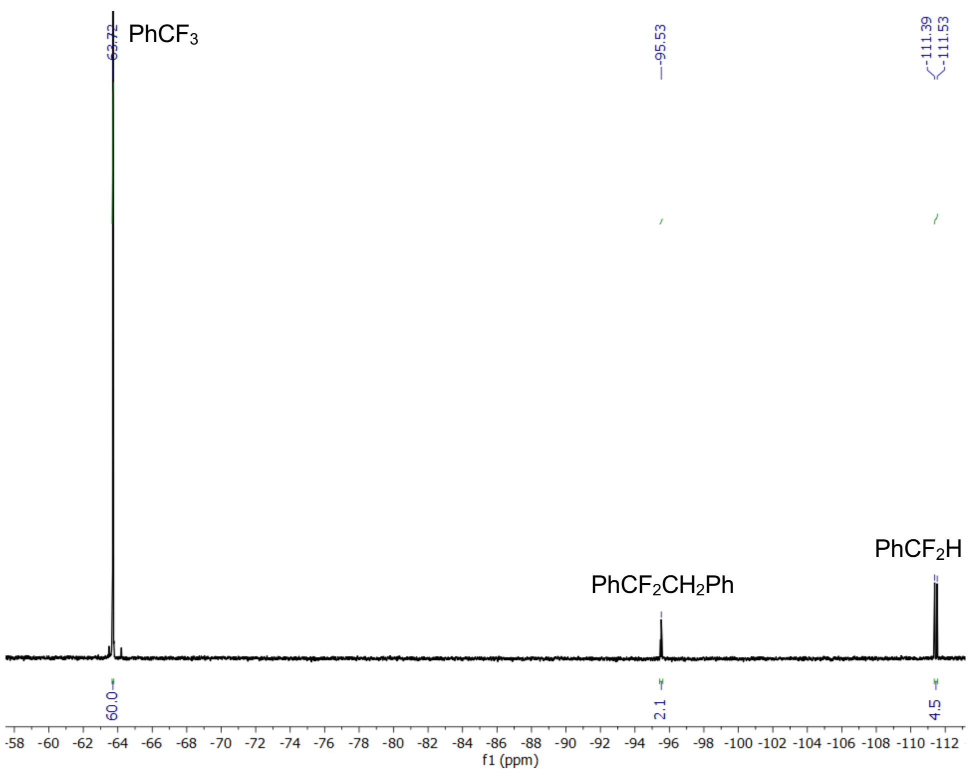


Figure S42. [19]F NMR in THF- H$_8$ **7-Mg** with 1 equiv. PhCF$_3$ following 48 hours of irradiation under a 40 W Kessil A160WE Tuna Blue lamp. Generation of PhCF$_2$CH$_2$Ph is observed via benzyl radicals released from **7-Mg** under irradiation.

S5.2 Optimized reactions

S5.2.1 General procedure and results

In a glovebox, a Young NMR tube was charged with metal complex (0.0100 mmol, 1 equiv.) and THF (0.5 mL). $PhCF_3$ (6.23 μL, 0.0500 mmol, 5 equiv.) was then added using a micropipette. The sample was then irradiated with light and monitored periodically by ^{1}H and ^{19}F NMR spectroscopy. Final time point measurements were collected after 120 hours.

Table S2. Calculated conversion of $PhCF_3$ to $PhCF_2H$ with yields determined by ^{19}F NMR spectroscopy.

Complex	Conversion to $PhCF_2H$, %
1-Ce	75
2-Ce	5
1-La	10
7-Mg	19 (6% $PhCF_2CH_2Ph$ arising from Bn transfer from the catalyst)

S5.2.2 ^{19}F NMR spectra

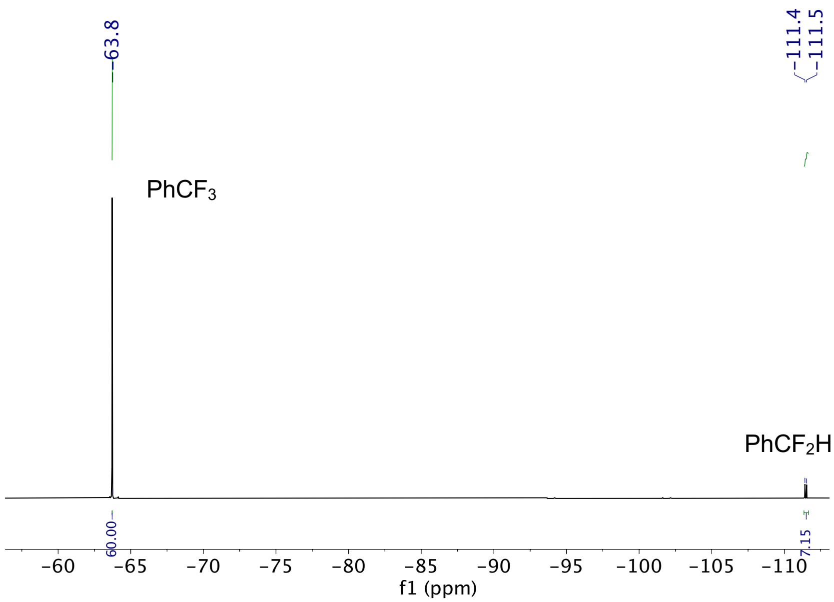


Figure S43. ^{19}F NMR in THF-H_8 **1-Ce** with 5 equiv. $PhCF_3$ following 120 hours of irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

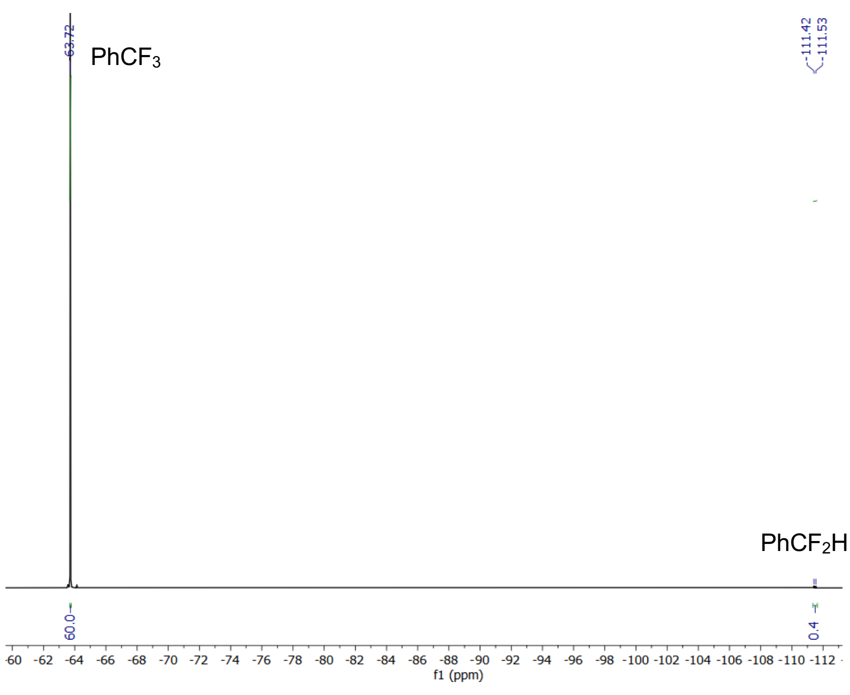


Figure S44. ^{19}F NMR in THF-H_8 **2-Ce** with 5 equiv. $PhCF_3$ following 120 hours of irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

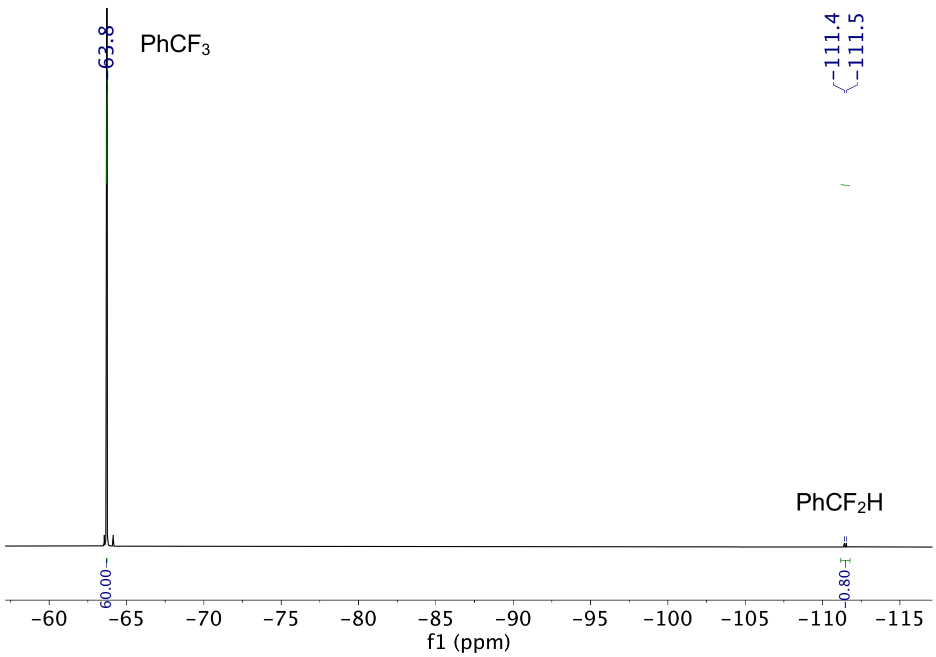


Figure S45. [19]F NMR in THF-H8 **1-La** with 5 equiv. $PhCF_3$ following 120 hours of irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

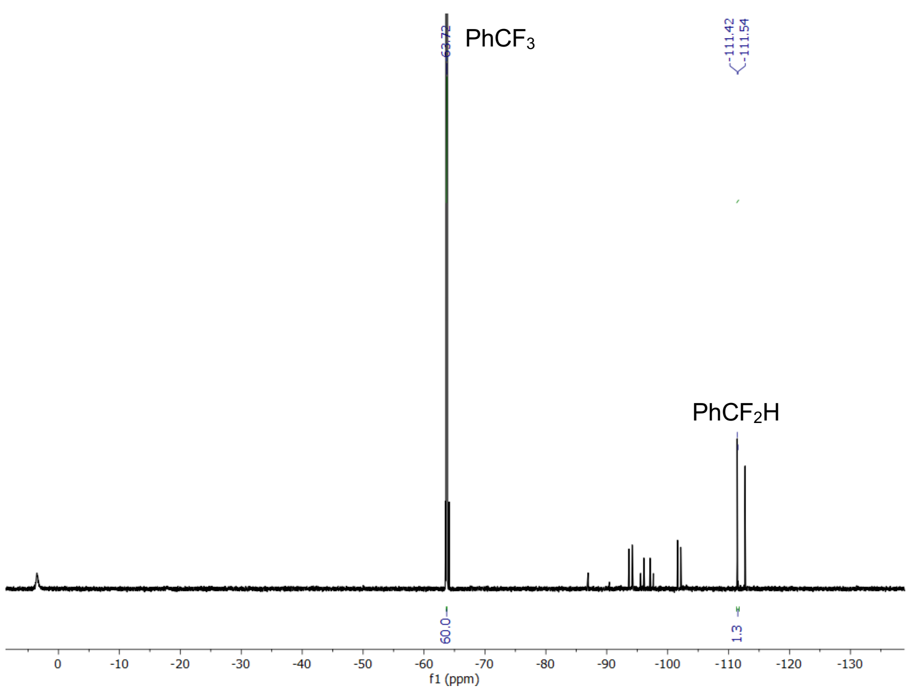


Figure S46. [19]F NMR in THF-H8 **2-La** with 5 equiv. $PhCF_3$ following 120 hours of irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

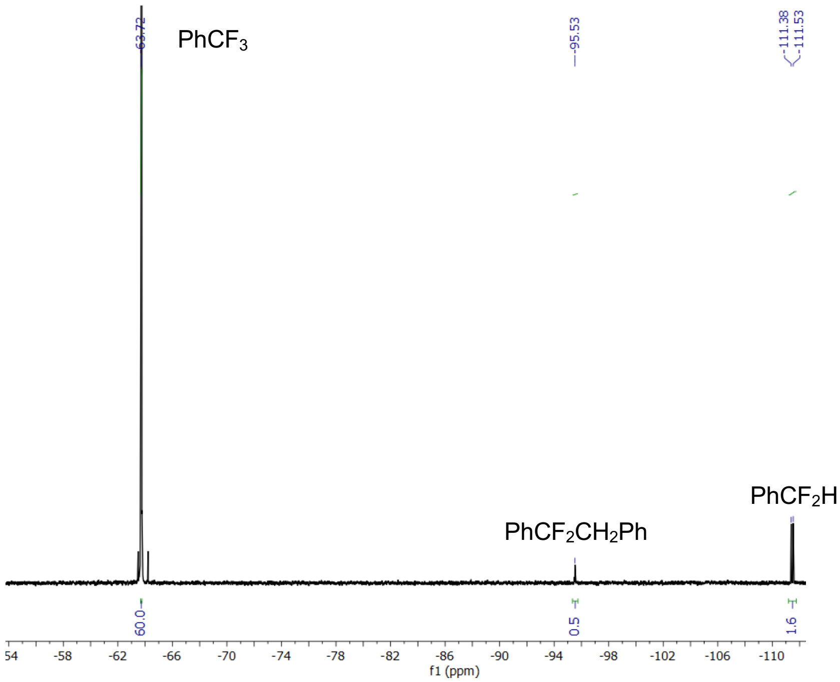


Figure S47. [19]F NMR in THF-H_8 **7-Mg** with 5 equiv. $PhCF_3$ following 120 hours of irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

S5.3 Substrate scope

S5.3.1 General procedure and ^{19}F NMR Spectra

In a glovebox, a Young NMR tube was charged with metal complex (0.0100 mmol, 1 equiv.) and THF (0.5 mL). Fluorinated substrate (0.0500 mmol, 5 equiv.) was then added using a micropipette. The sample was then irradiated with a 40 W Kessil A160WE Tuna Blue lamp and monitored by ^{1}H and ^{19}F NMR spectroscopy after 20 hours. Approximately 25% conversion of hexafluorobenzene to C_6F_5H, trace reaction for trifluoromethoxybenzene; 1,3-bis(trifluoromethyl)benzene;1 ,4-bis(trifluoromethyl)benzene, perfluoro(methylcyclohexane).

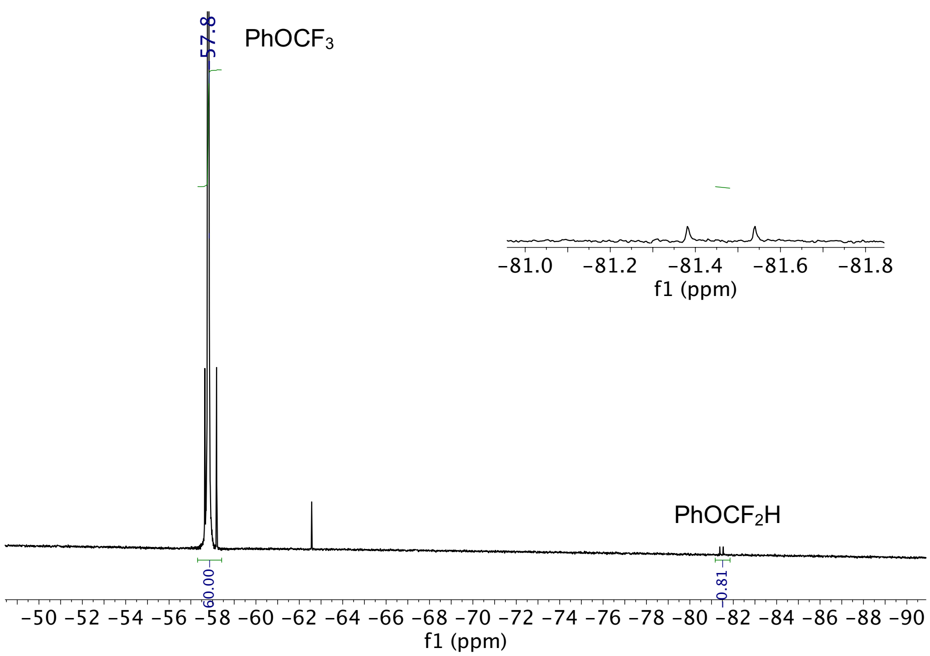


Figure S48. ^{19}F NMR in THF-H_8 **1-Ce** with 5 equiv. trifluoromethoxybenzene following 20 hours of irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

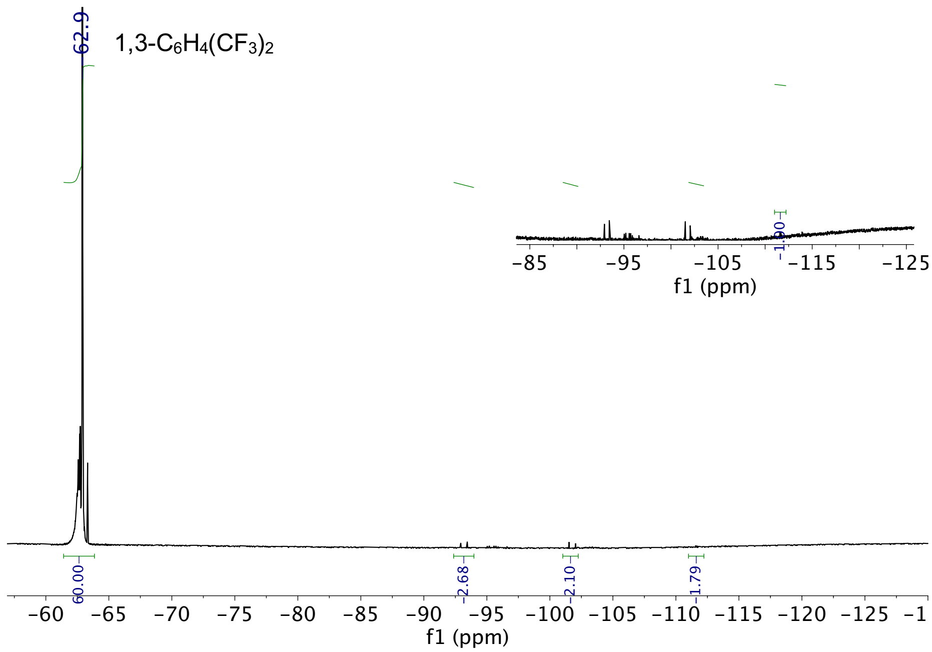


Figure S49. ^{19}F NMR in THF-H_8 **1-Ce** with 5 equiv. 1,3-bis(trifluoromethyl)benzene following 20 hours of irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

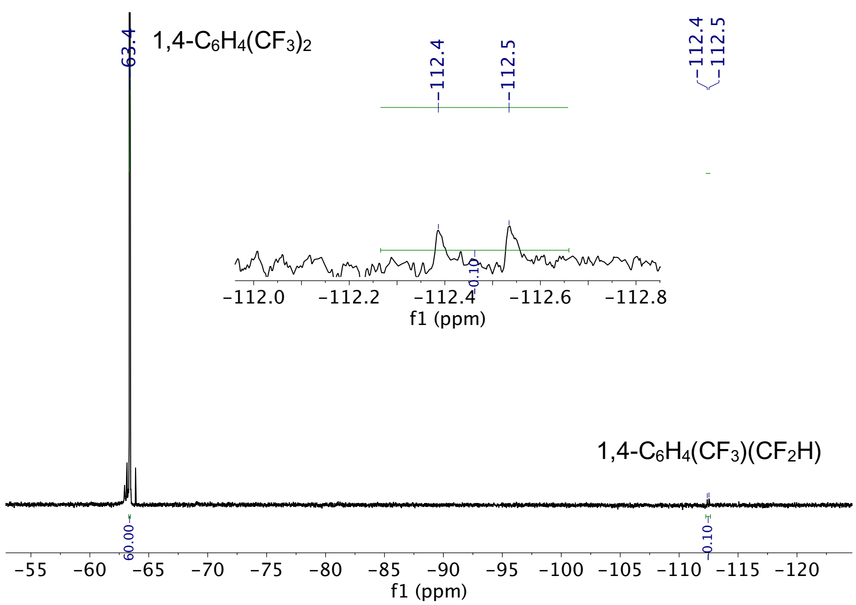


Figure S50. ^{19}F NMR in THF-H_8 **1-Ce** with 5 equiv. 1,4-bis(trifluoromethyl)benzene following 20 hours of irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

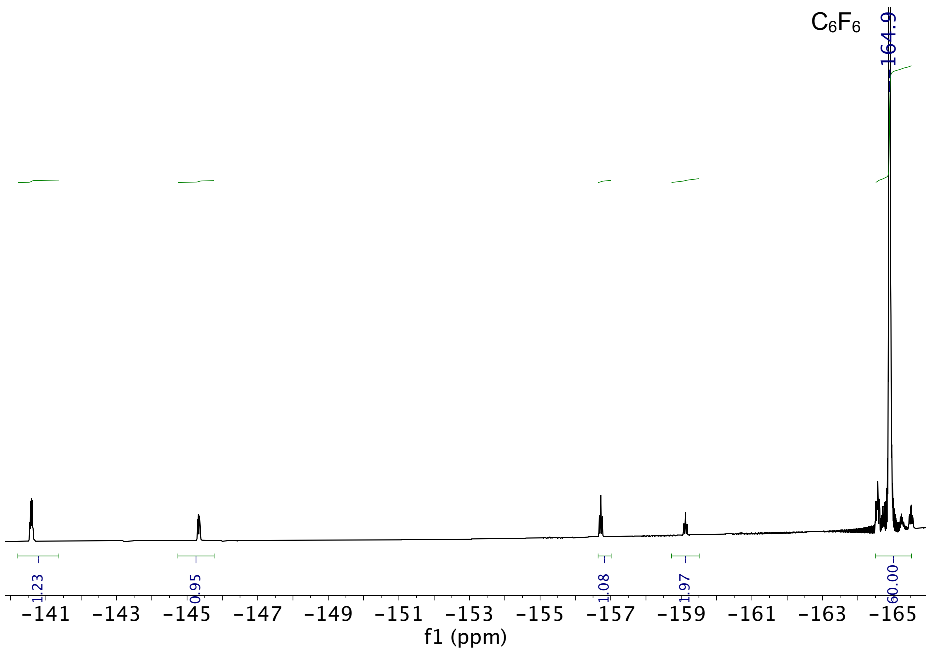


Figure S51. [19]F NMR in THF-H_8 **1-Ce** with 5 equiv. hexafluorobenzene following 20 hours of irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

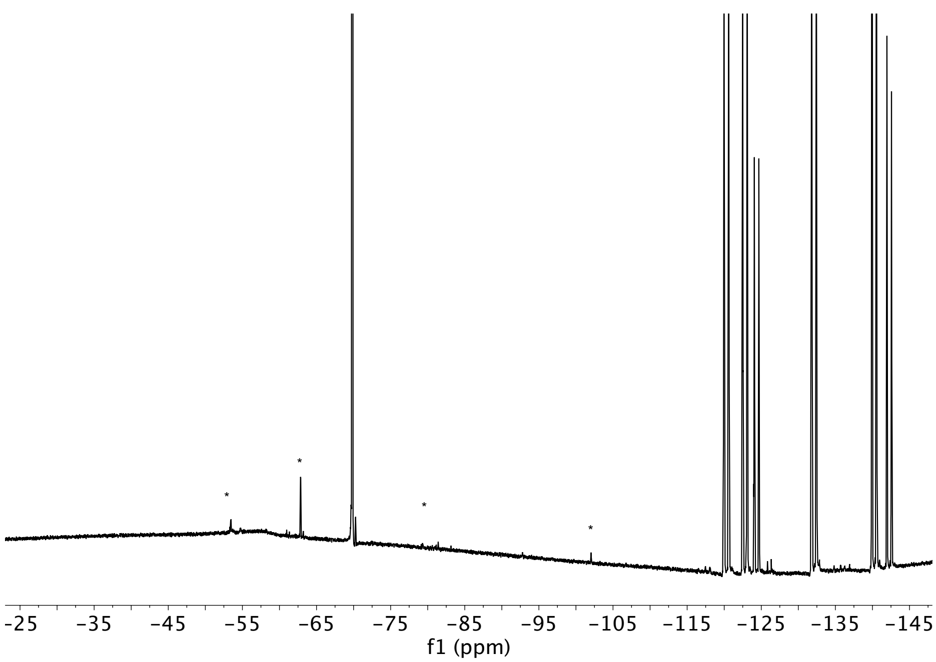


Figure S52. [19]F NMR in THF-H_8 **1-Ce** with 5 equiv. perfluoro(methylcyclohexane) following 16 hours of irradiation under a 40 W Kessil A160WE Tuna Blue lamp, new peaks marked *.

S6 Catalytic alkyl coupling

S6.1 20 mol% catalytic reactions with $MgBn_2(THF)_2$

S6.1.1 General procedure and results

In a glovebox, a vial was charged with $MgBn_2(THF)_2$, $PhCF_3$ (6.13 μL , 0.0500 mmol, 1 equiv.) and THF (0.5 mL). The solution was then used to dissolve the catalyst (0.0100 mmol, 0.2 equiv.), and the reaction mixture transferred to a Young NMR tube. The sample was irradiated with a 40 W Kessil A160WE Tuna Blue lamp and monitored periodically by ^{1}H and ^{19}F NMR spectroscopy, with a final time point being measured after 48 hours.

Table S3. Defluoroalkylative coupling of $PhCF_3$ with dibenzyl magnesium mediated by metal catalysts, with yields determined by ^{19}F NMR spectroscopy.

Catalyst [20 mol%]	**Conversion to $PhCF_2CH_2Ph$ and $PhCF_2H$ after 48 hours(%)**	**$PhCF_2CH_2Ph$: $PhCF_2H$**	**Conversion to $PhCF_2CH_2Ph$ and $PhCF_2H$ (%) after (x) hours**
1-Ce	51	2:1	91% (80 hours)
2-Ce	6	7:5	n/a
3-Ce	18	7:5	46% (80 hours)
4-Ce	41	3:1	65% (80 hours)
5-Ce	18	5:2	n/a
6-Ce	33	3:1	n/a
1-La	67	9:5	72% (60 hours)
2-La	19	1:1	n/a
1-Nd	32	3:2	87% (140 hours)
1-Sm	12	2:3	n/a
7-Mg	24	6:5	56% (80 hours)
8-Mg	13	1:1	n/a

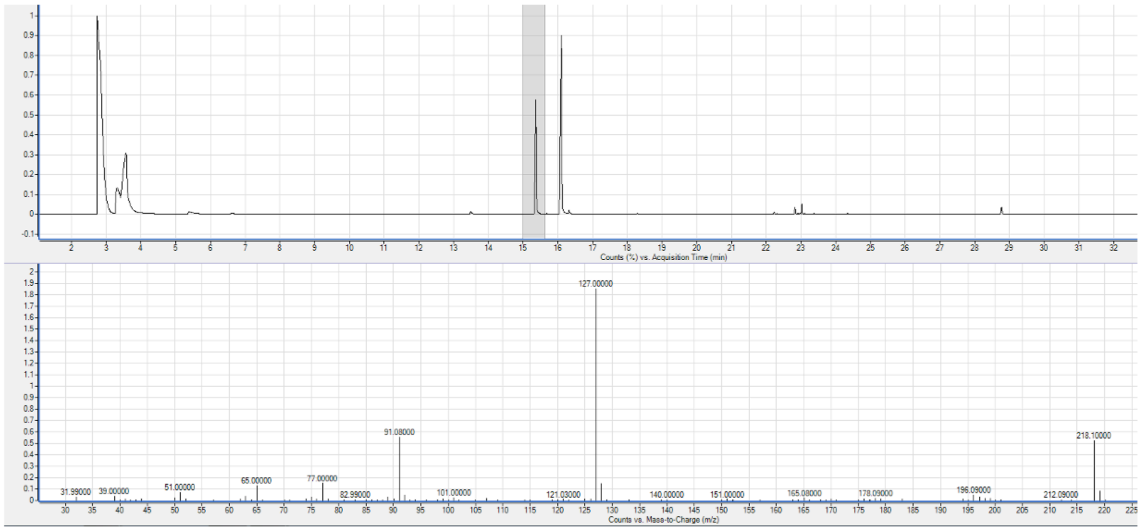


Figure S53. GCMS trace of the products of reaction of **1-Ce** in THF-H_8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 16 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp. m/z ($PhCF_2^-$) = 127, m/z ($PhCF_2CH_2Ph$) = 218

S6.1.2 ^{19}F NMR spectra

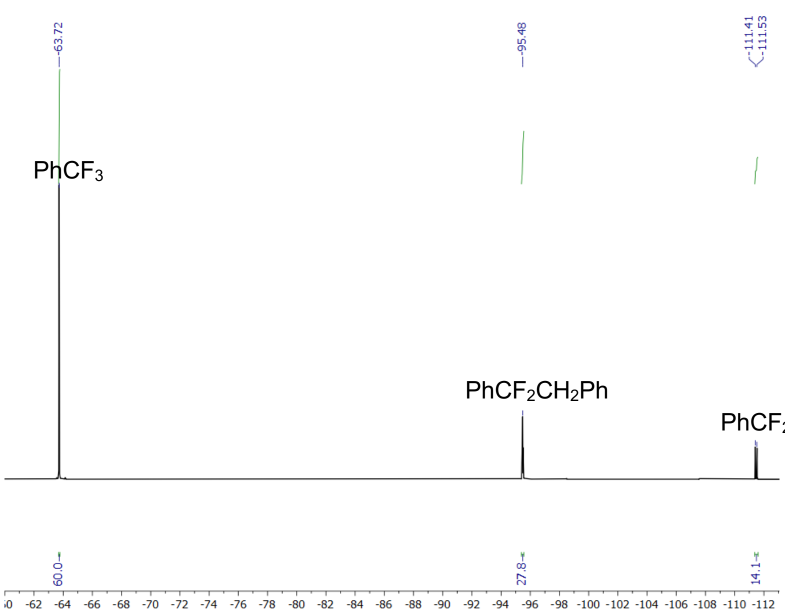


Figure S54. ^{19}F NMR of 20 mol% **1-Ce** in THF-H_8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 48 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

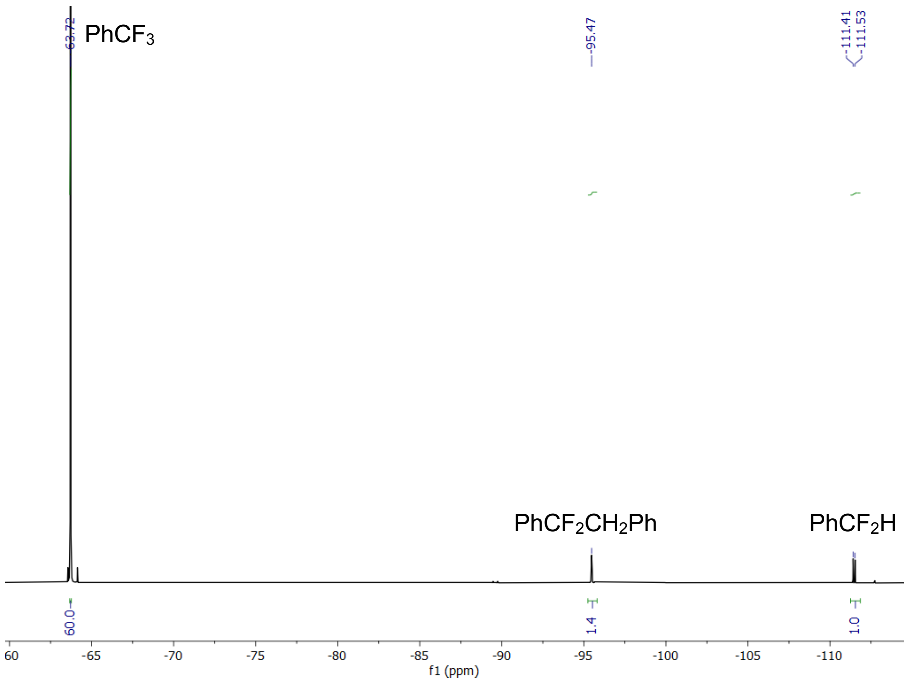


Figure S55. [19]F NMR of 20 mol% **2-Ce** in THF-H_8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 48 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

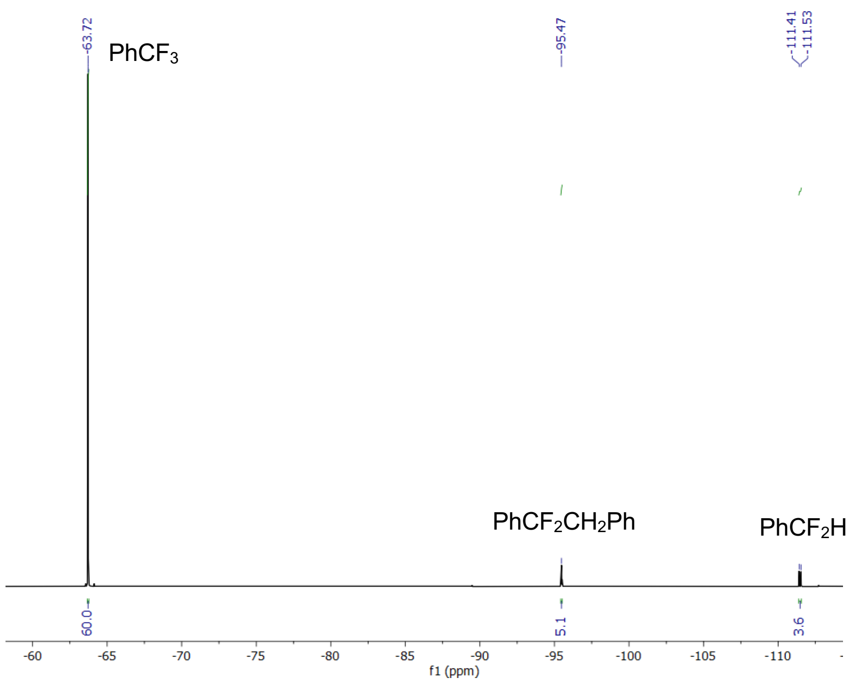


Figure S56. [19]F NMR of 20 mol% **3-Ce** in THF-H_8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 48 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

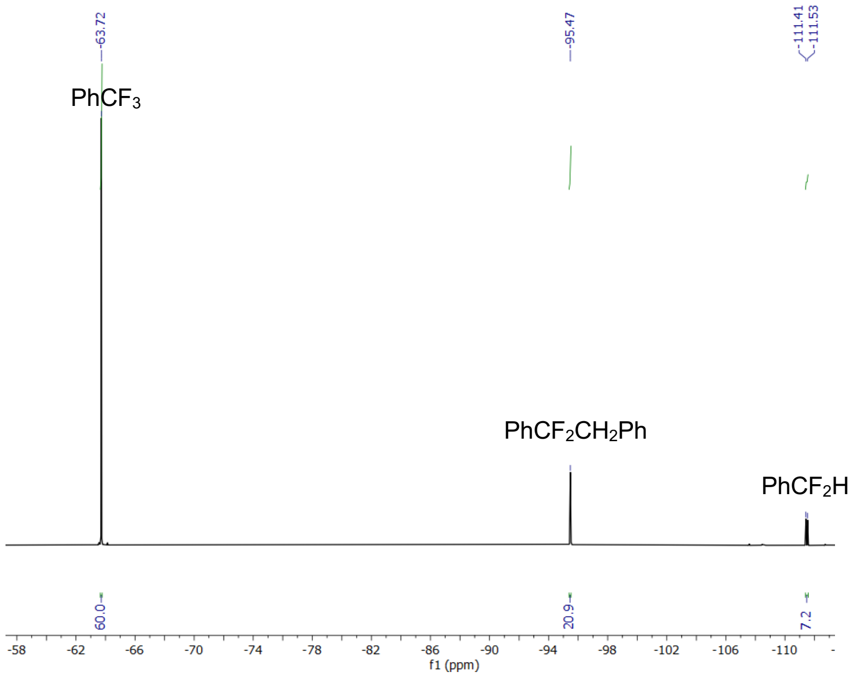


Figure S57. [19]F NMR of 20 mol% **4-Ce** in THF-H8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 48 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

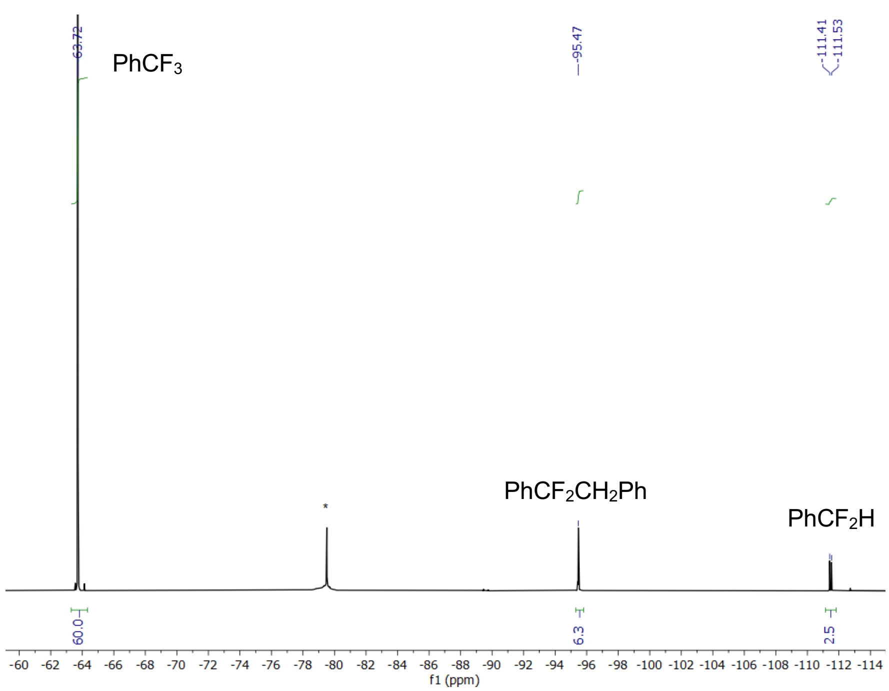


Figure S58. [19]F NMR of 20 mol% **5-Ce** in THF-H8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 48 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp. Residual triflate is marked with *.

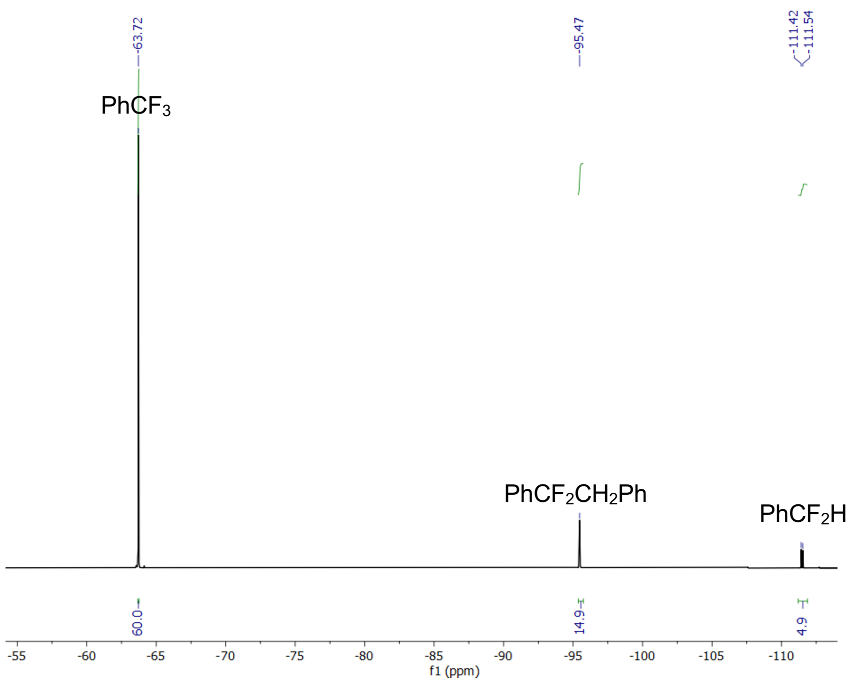


Figure S59. [19]F NMR of 20 mol% **6-Ce** in THF-H_8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 48 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

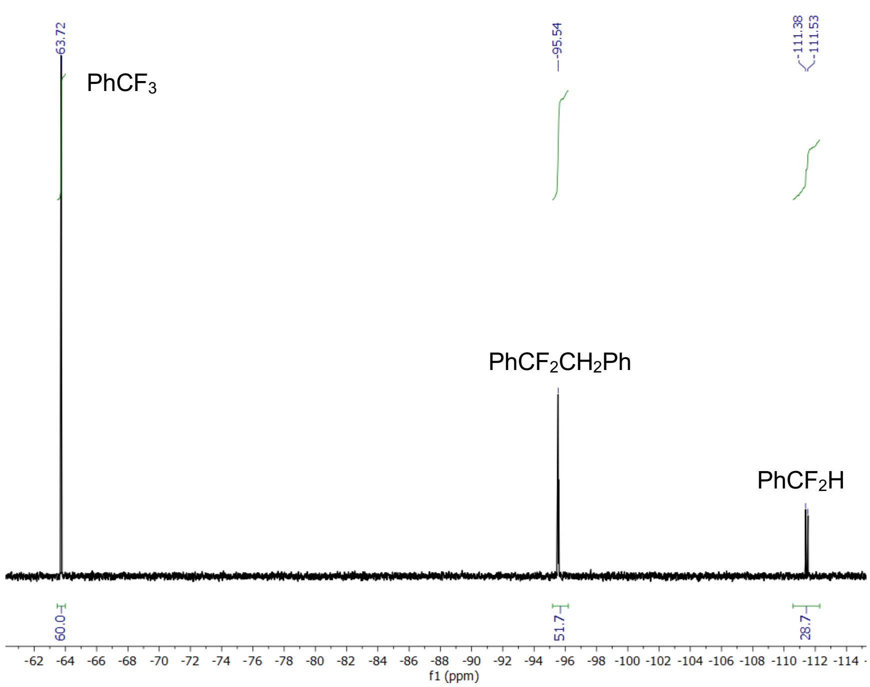


Figure S60. [19]F NMR of 20 mol% **1-La** in THF-H_8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 48 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

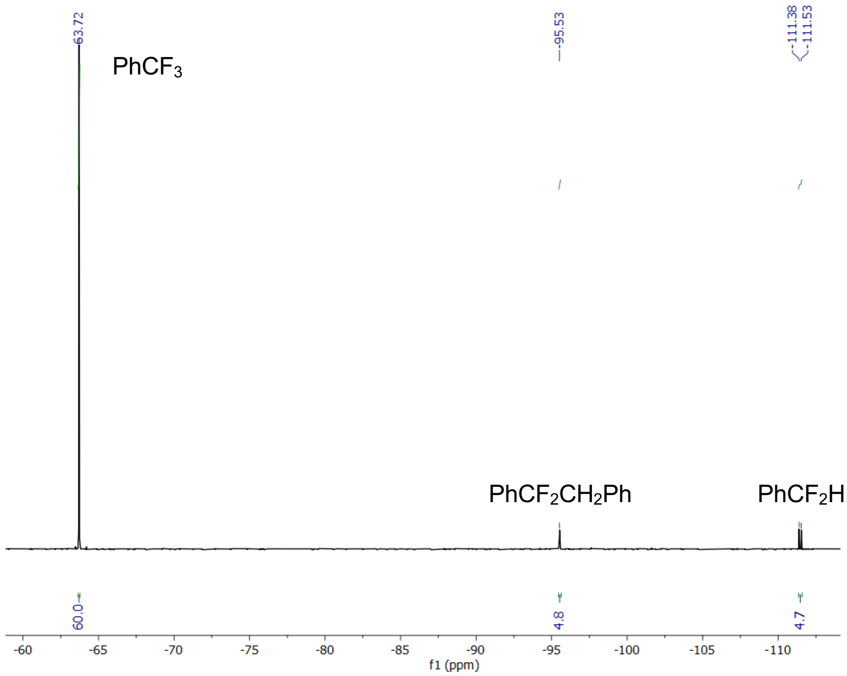


Figure S61. ^{19}F NMR of 20 mol% **2-La** in THF-H_8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 48 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

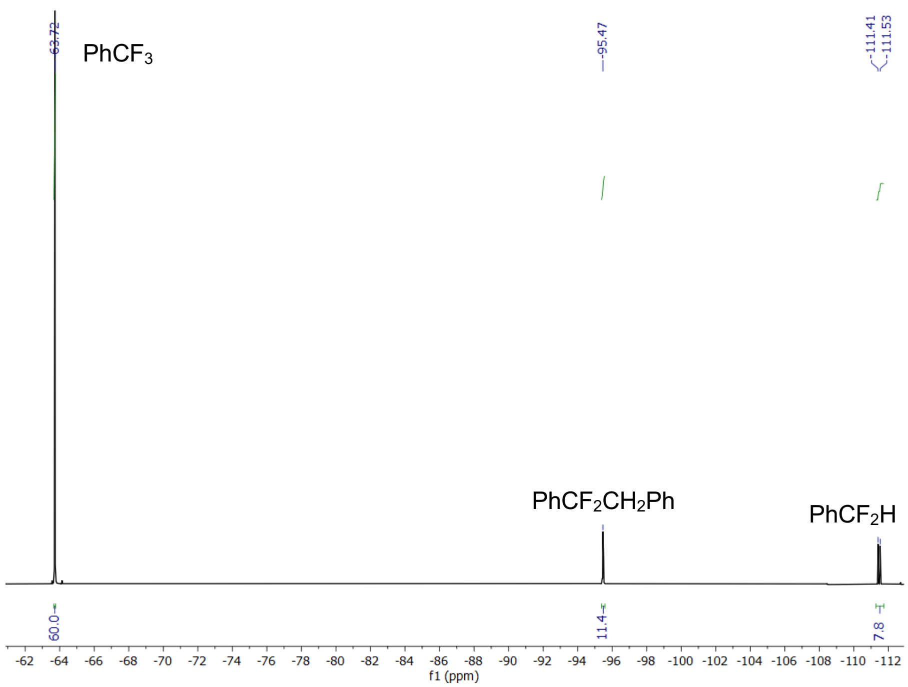


Figure S62. ^{19}F NMR of 20 mol% **1-Nd** in THF-H_8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 48 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

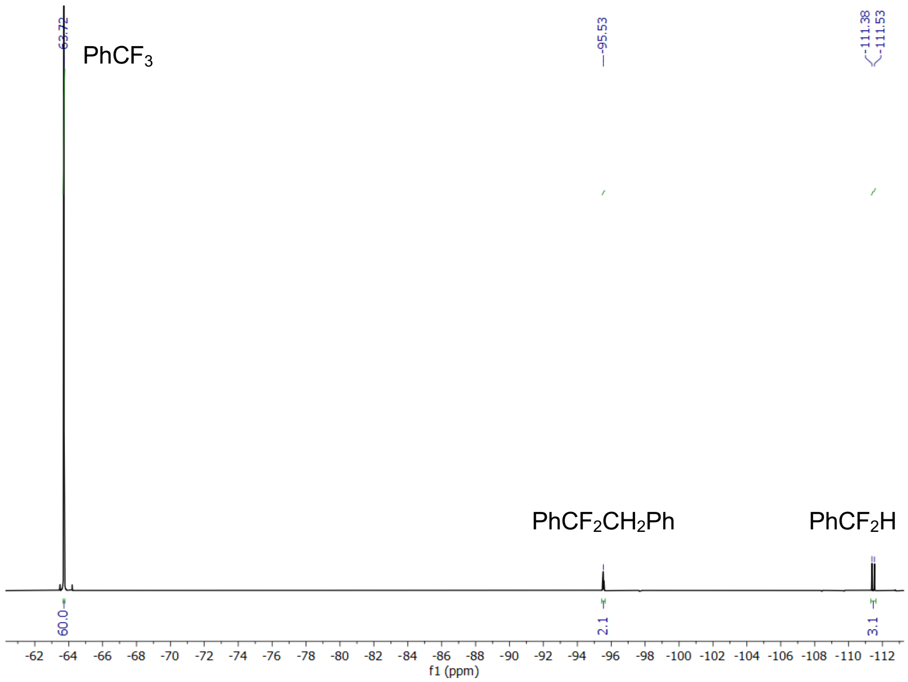


Figure S63. ^{19}F NMR of 20 mol% **1-Sm** in THF-H_8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 48 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

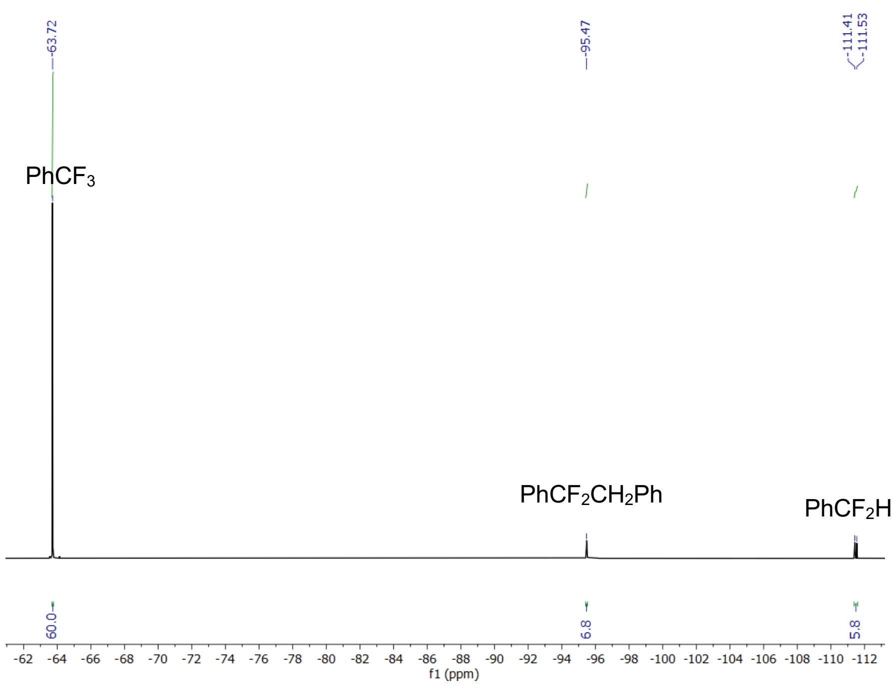


Figure S64. ^{19}F NMR of 20 mol% **7-Mg** in THF-H_8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 48 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

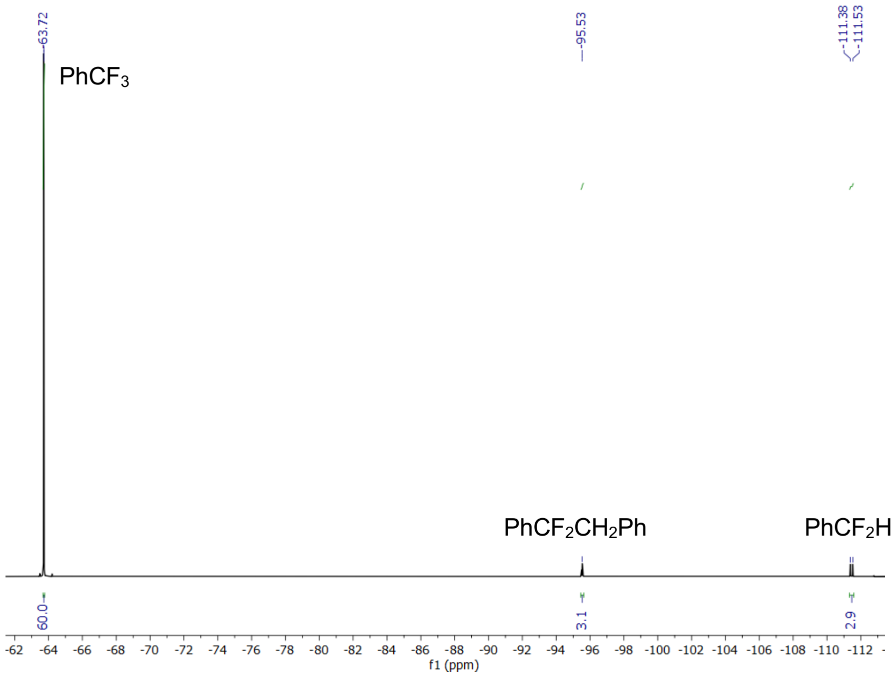


Figure S65. ^{19}F NMR of 20 mol% **8-Mg** in THF-H_8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 48 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

<u>S6.2 20 mol% reactions of **1-Ce** with other metal dialkyl reagents</u>

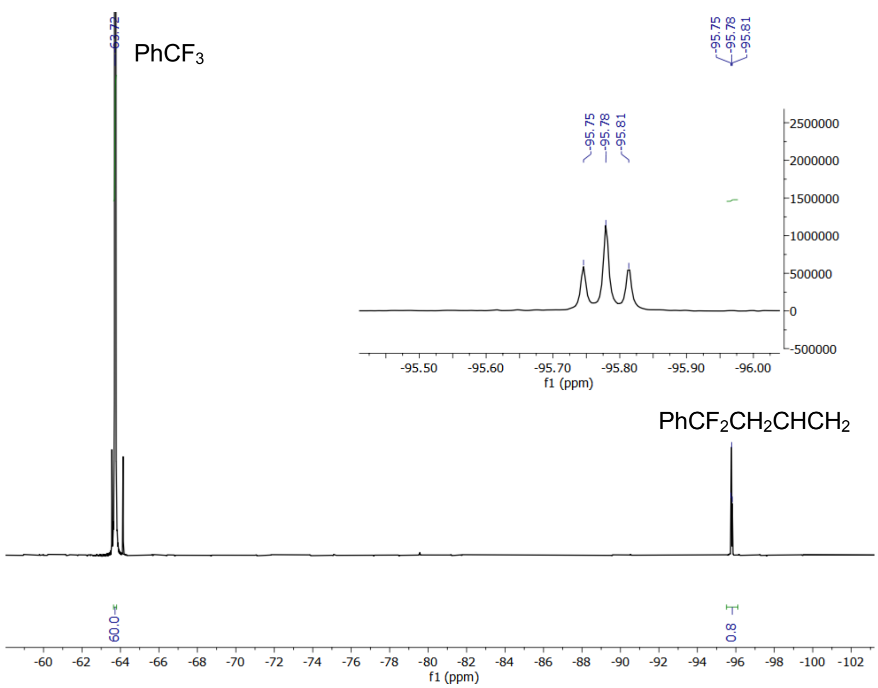


Figure S66. ^{19}F NMR of 20 mol% **1-Ce** in THF-H_8 with 1 equiv. $Mg(allyl)_2(THF)_2$ and 5 equiv. $PhCF_3$ after 18 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp at room temperature.

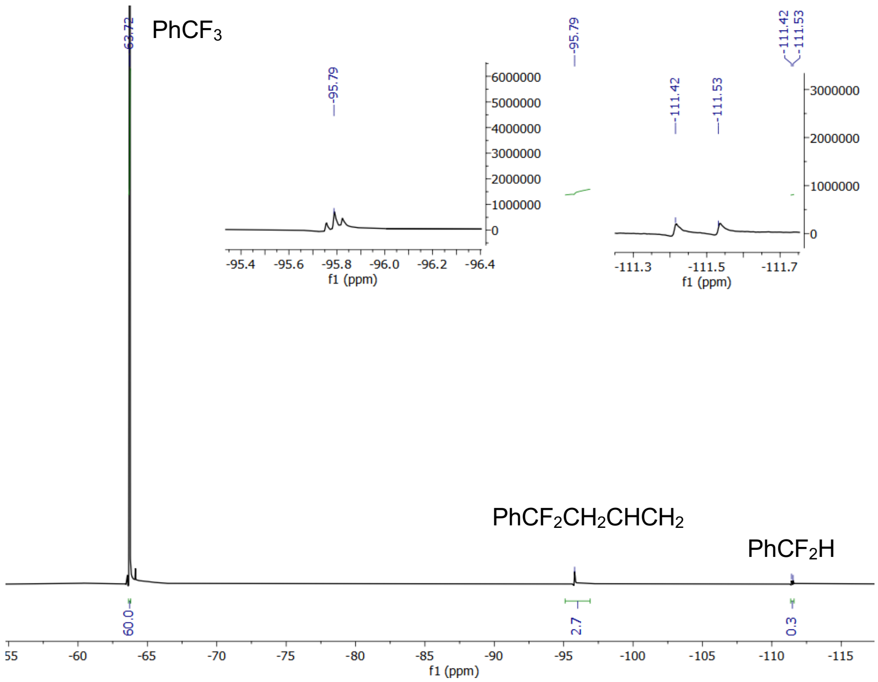


Figure S67. [19]F NMR of 20 mol% **1-Ce** in THF-H8 with 1 equiv. $Bu_3Sn(allyl)$ and 5 equiv. $PhCF_3$ after 48 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp at 70°C.

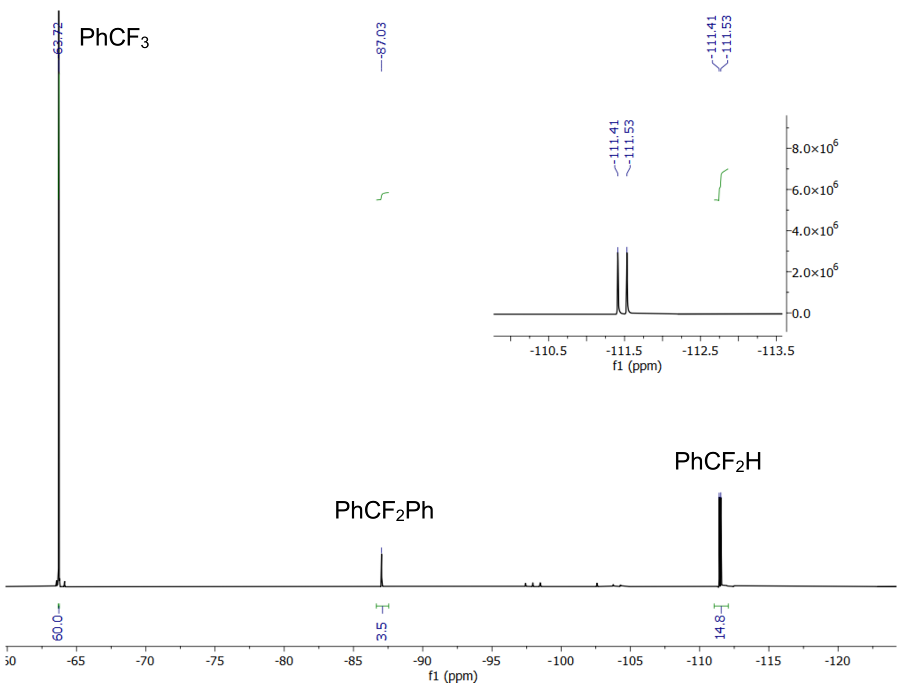


Figure S68. [19]F NMR of 20 mol% **1-Ce** in THF-H8 with 1 equiv. $Mg(phenyl)_2(THF)_2$ and 5 equiv. $PhCF_3$ after 48 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp at 70°C.

S6.3. 1 mol% catalytic reactions with **1-Ce**, **1-La, 1-Nd, 1-Sm** and **7-Mg**

S6.3.1 General procedure and results

In a glovebox, a vial was charged with $MgBn_2(THF)_2$ in THF (0.5 mL) and $PhCF_3$ (6.13 μL, 0.0500 mmol, 1 equiv.). The solution was then used to dissolve the catalyst, and the reaction mixture transferred to a Young NMR tube with a capillary containing 1,2-difluorobenzene as internal standard. The sample was irradiated with a 40 W Kessil A160WE Tuna Blue lamp and monitored periodically by ^1H and ^{19}F NMR spectroscopy every 21 hours.

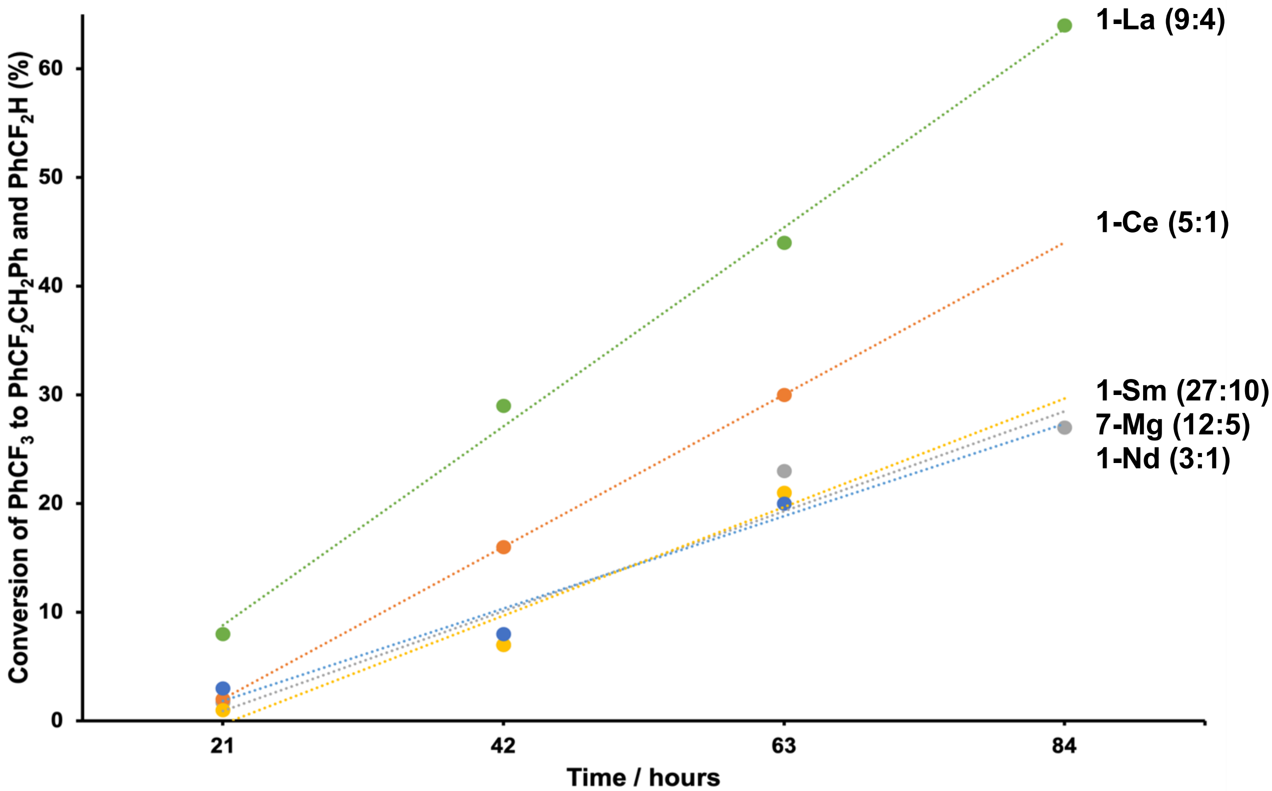


Figure S69. Graph of the conversion of $PhCF_3$ to $PhCF_2CH_2Ph$ and $PhCF_2H$ mediated by 1 mol% loading of **1-La, 1-Ce, 1-Nd, 1-Sm** and **7-Mg**, with 1 equiv. $PhCF_3$ and 1 equiv. $MgBn_2(THF)_2$ after irradiation under a 40 W Kessil A160WE Tuna Blue lamp at room temperature. $PhCF_2CH_2Ph$:$PhCF_2H$ product ration after 63 hours irradiation written in parentheses after complex label.

S6.3.2 ^{19}F NMR spectra

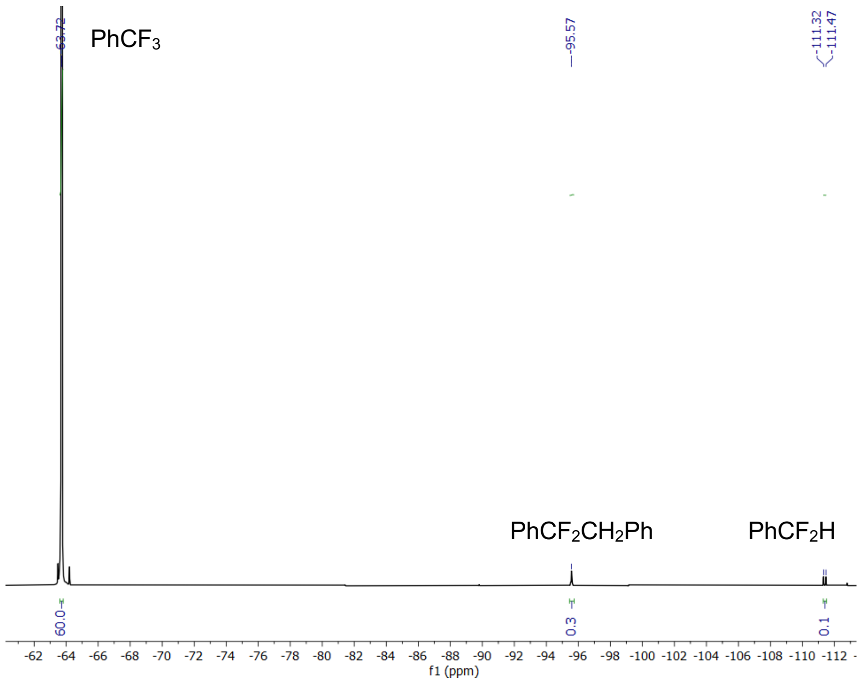


Figure S70. ^{19}F NMR of 1 mol% **1-Ce** in THF-H_8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 21 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

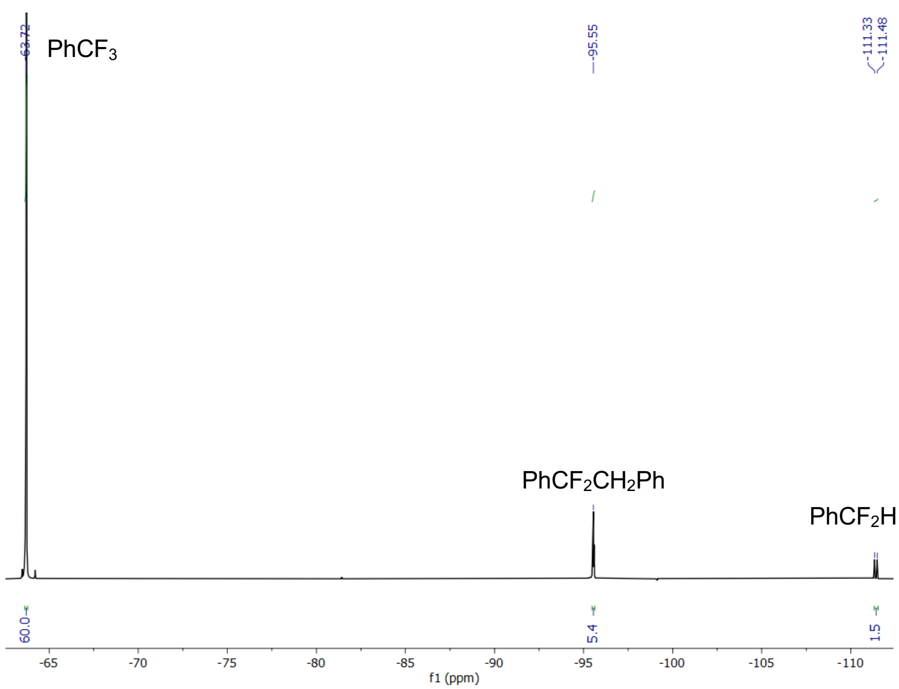


Figure S71. ^{19}F NMR of 1 mol% **1-Ce** in THF-H_8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 42 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

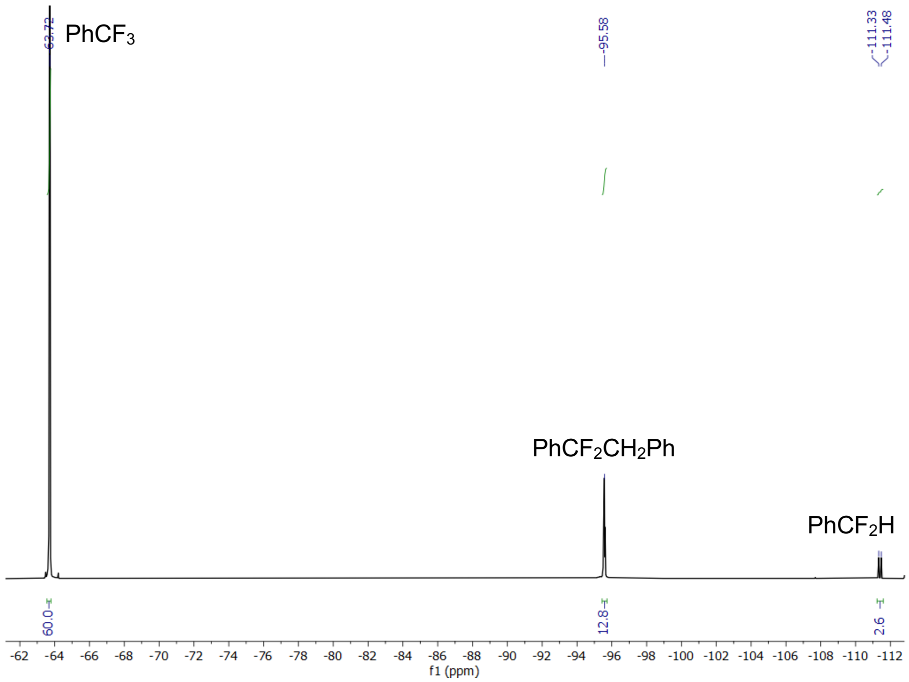


Figure S72. [19]F NMR of 1 mol% **1-Ce** in THF-H_8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 63 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

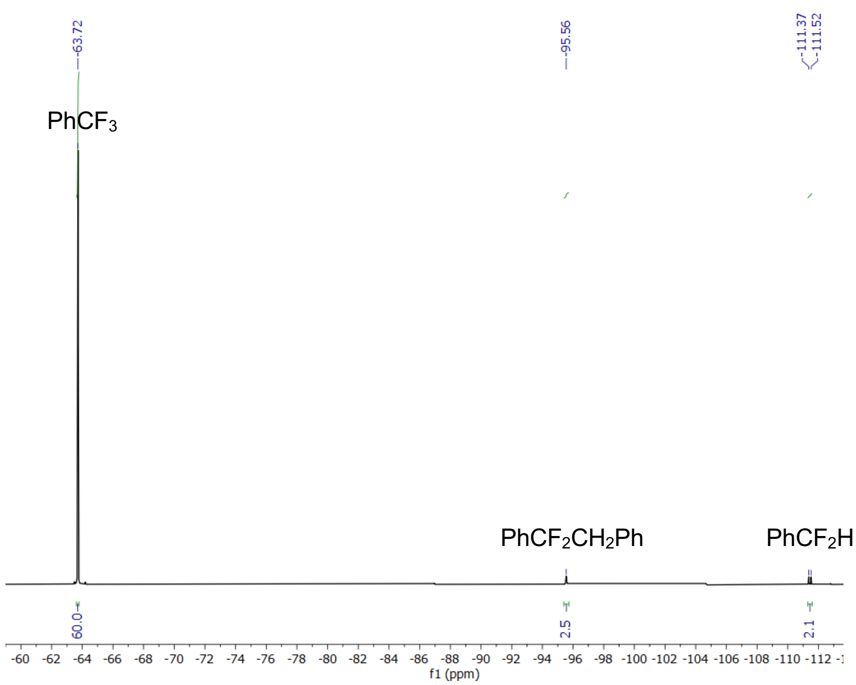


Figure S73. [19]F NMR of 1 mol% **1-La** in THF-H_8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 21 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

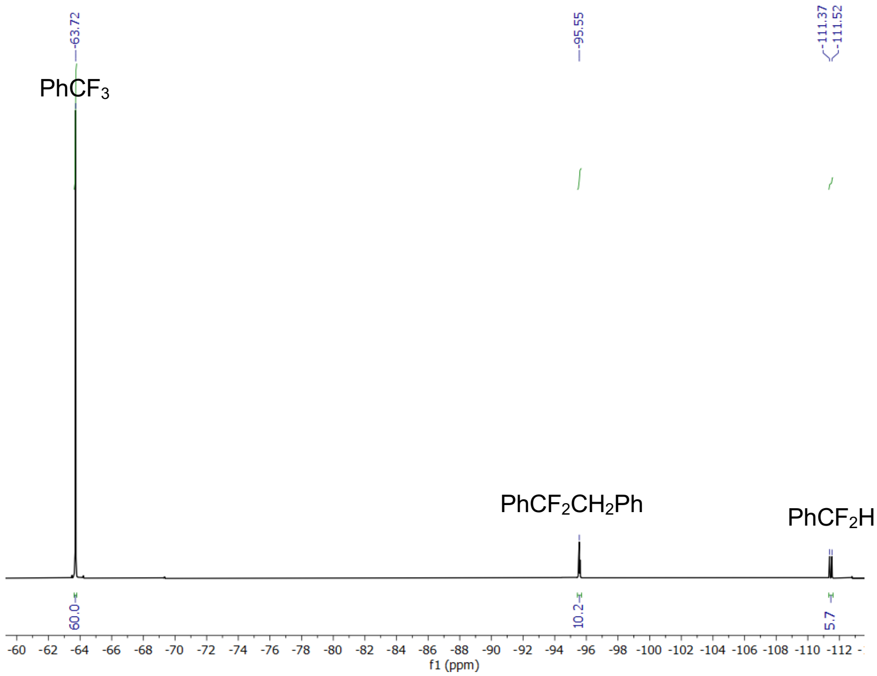


Figure S74. [19]F NMR of 1 mol% **1-La** in THF-H_8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 42 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

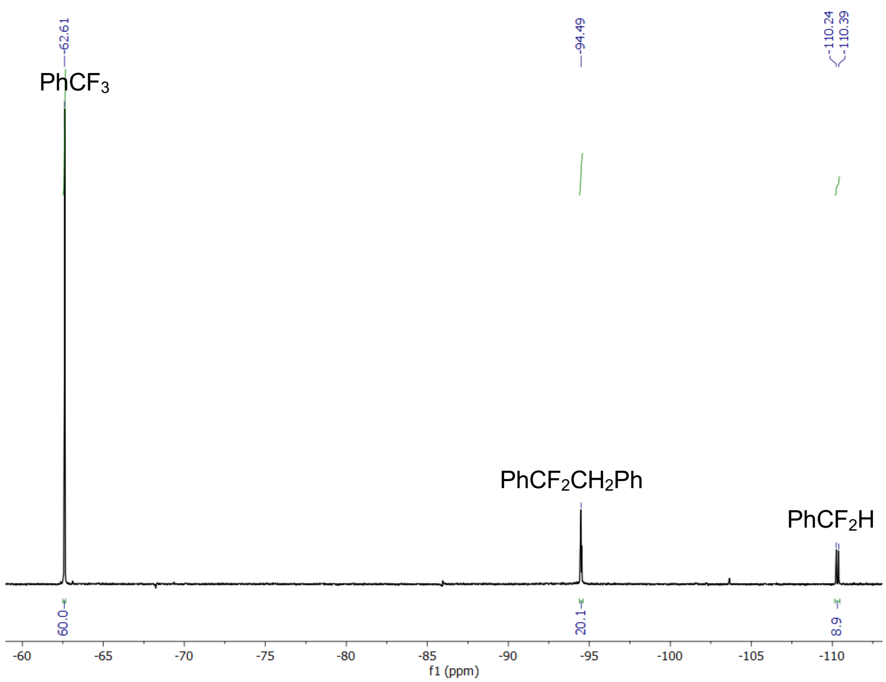


Figure S75. [19]F NMR of 1 mol% **1-La** in THF-H_8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 63 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

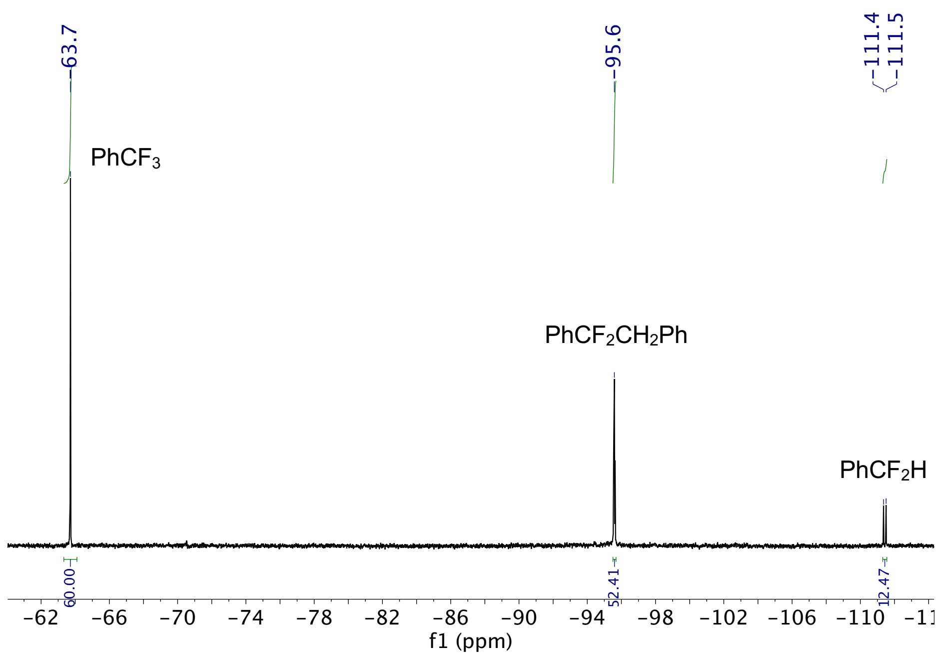


Figure S76. [19]F NMR of 1 mol% **1-La** in THF-H_8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 84 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

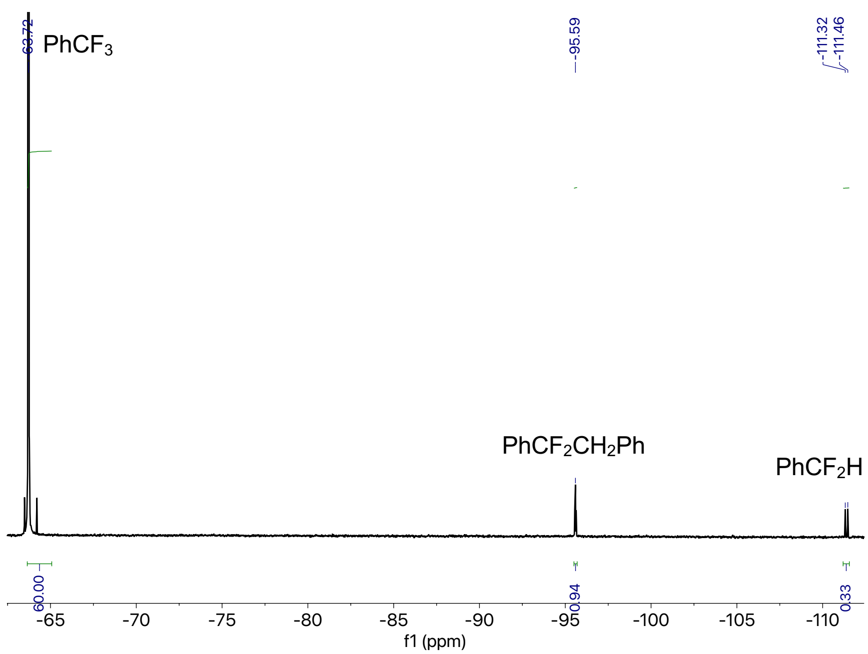


Figure S77. [19]F NMR of 1 mol% **1-Nd** in THF-H_8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 21 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

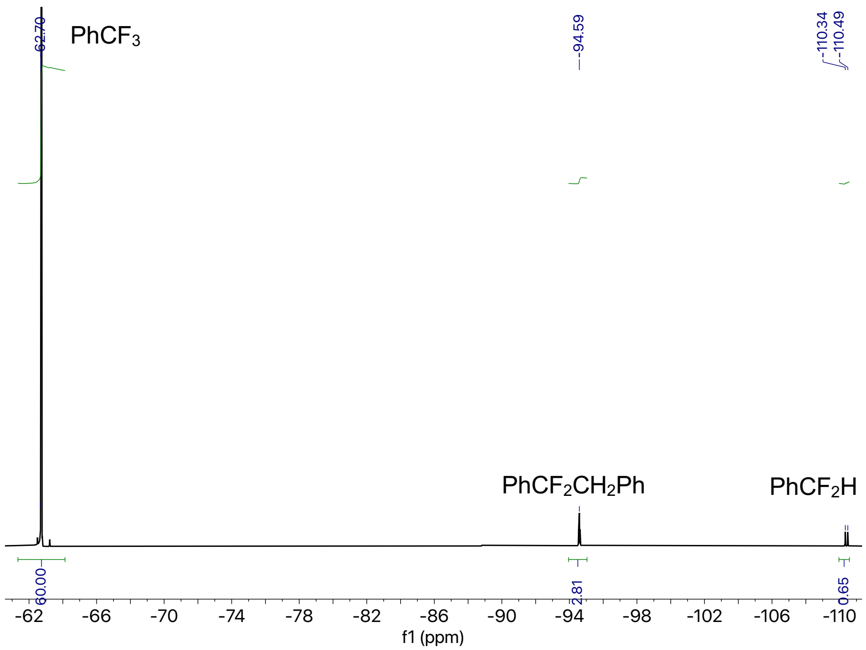


Figure S78. [19]F NMR of 1 mol% **1-Nd** in THF-H_8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 42 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

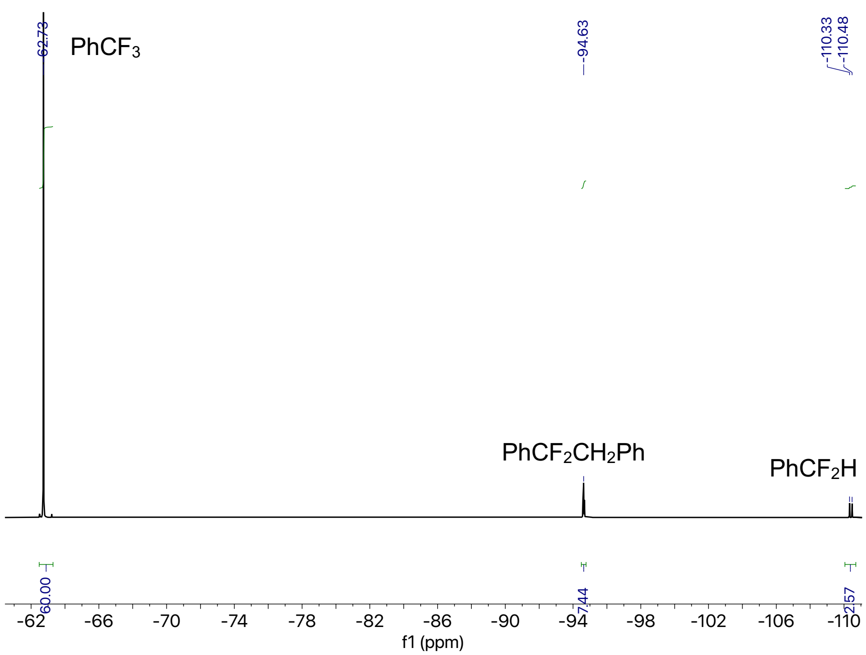


Figure S79. [19]F NMR of 1 mol% **1-Nd** in THF-H_8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 63 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

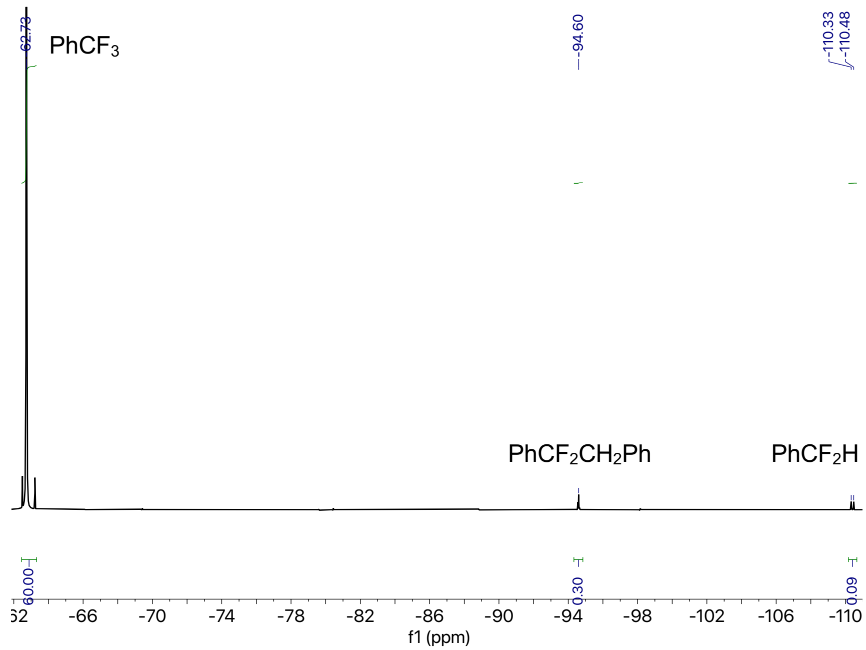


Figure S80. [19]F NMR of 1 mol% **1-Sm** in THF-H_8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 21 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

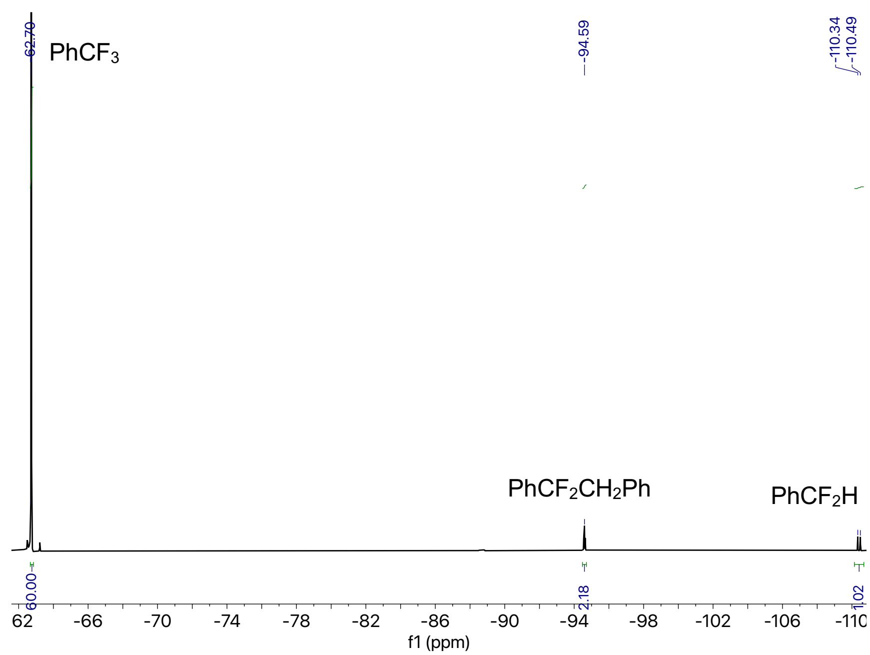


Figure S81. [19]F NMR of 1 mol% **1-Sm** in THF-H_8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 42 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

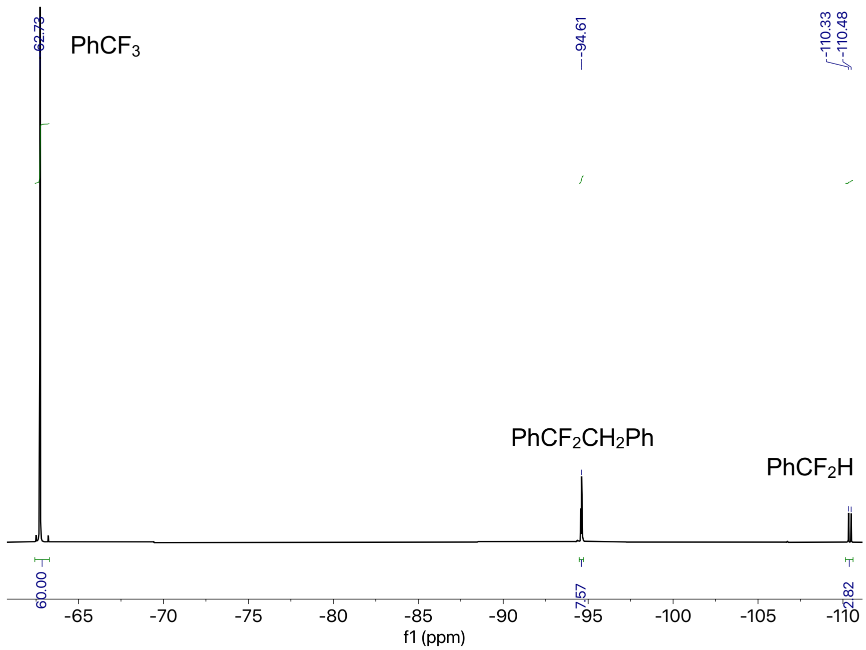


Figure S82. [19]F NMR of 1 mol% **1-Sm** in THF-H_8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 63 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

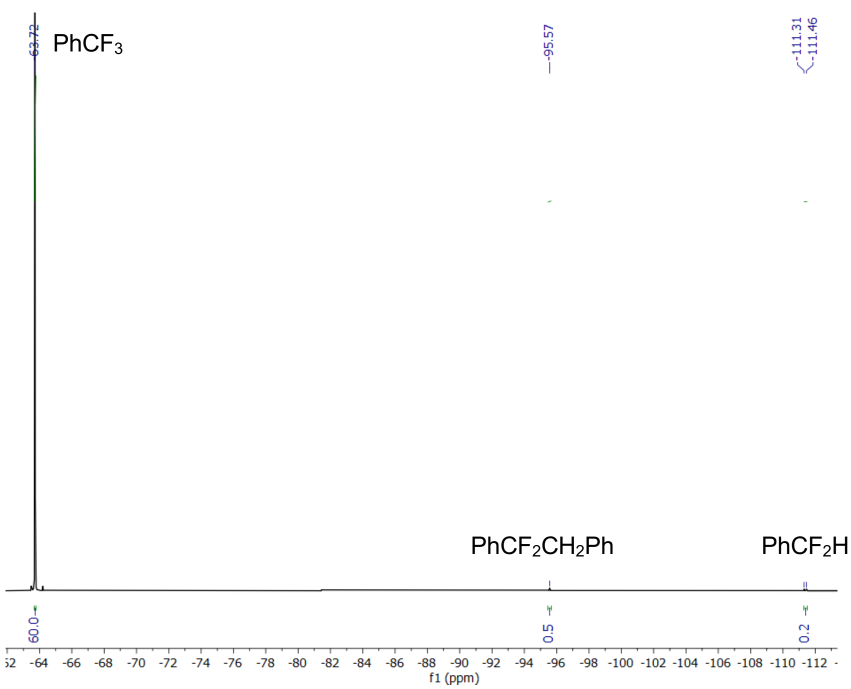


Figure S83. [19]F NMR of 1 mol% **7-Mg** in THF-H_8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 21 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

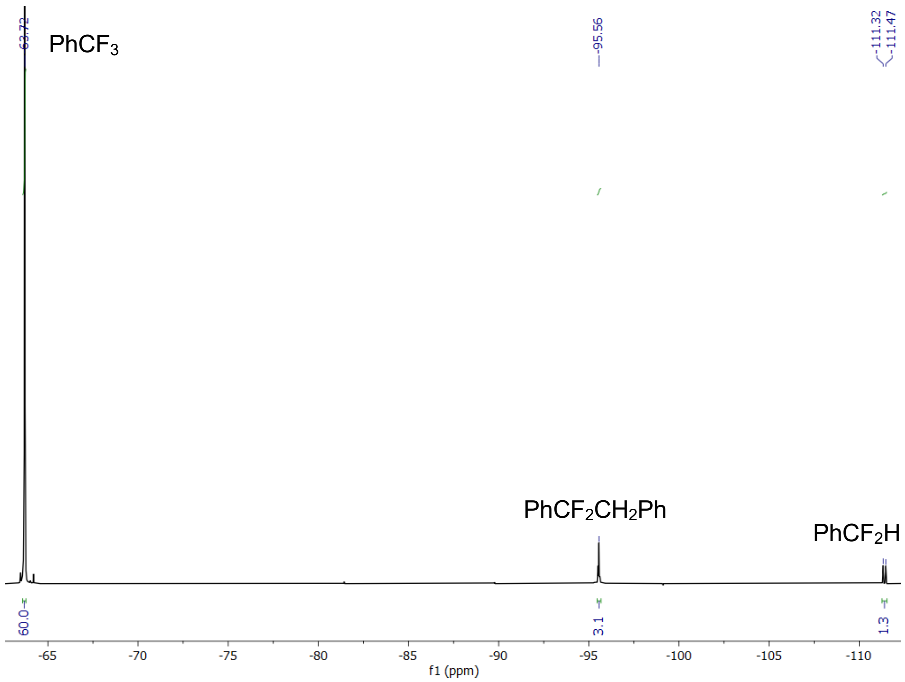


Figure S84. [19]F NMR of 1 mol% **7-Mg** in THF-H_8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 42 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

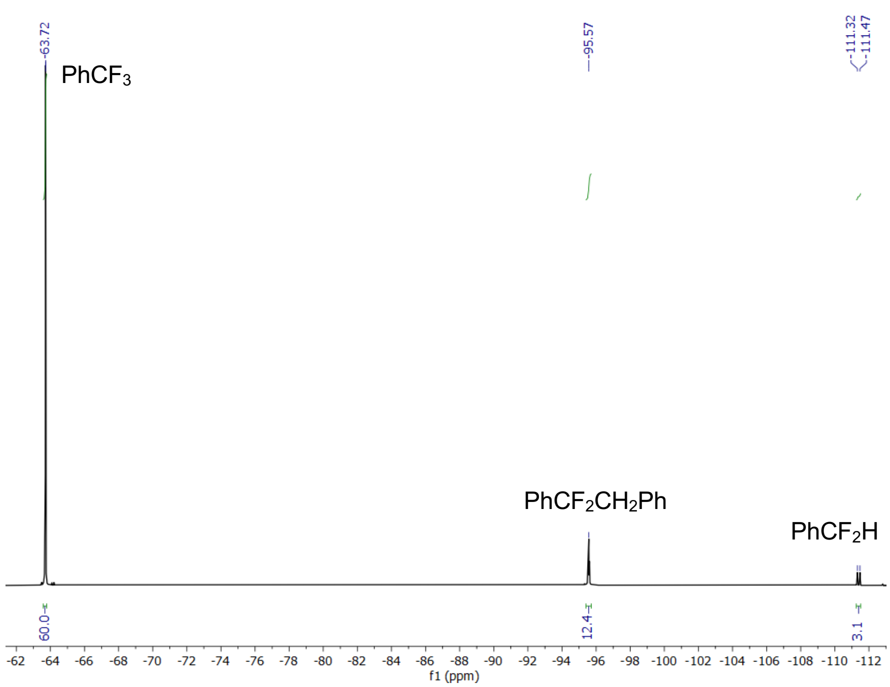


Figure S85. [19]F NMR of 1 mol% **7-Mg** in THF-H_8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 84 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

S6.4 1 mol% catalytic reactions with **1-Ce**, **1-La** and **7-Mg** in THF-D_8

S6.4.1 General procedure and results

In a glovebox, a vial was charged with $MgBn_2(THF)_2$ in THF-D_8 (0.5 mL) and $PhCF_3$ (6.13 µL , 0.0500 mmol, 1 equiv.). The solution was then used to dissolve the catalyst, and the reaction mixture transferred to a Young NMR tube with a capillary containing 1,2-difluorobenzene. The sample was irradiated with a 40 W Kessil A160WE Tuna Blue lamp and monitored by ^{1}H and ^{19}F NMR spectroscopy after 42 hours.

Table S4. Defluoroalkylative coupling of $PhCF_3$ with dibenzyl magnesium mediated by 1 mol% catalyst loading of **1-Ce**, **1-La** and **7-Mg** in THF-D_8 followed by 42 hours irradiation, with yields determined by ^{19}F NMR spectroscopy.

Catalyst [1 mol%]	**Conversion of $PhCF_3$ to $PhCF_2CH_2Ph$ and $PhCF_2H$ (%)**	**$PhCF_2CH_2Ph$: $PhCF_2H$ ratio**
1-Ce	13	11:1
1-La	16	11:1
7-Mg	10	8:1

S6.4.2 ^{19}F NMR spectra

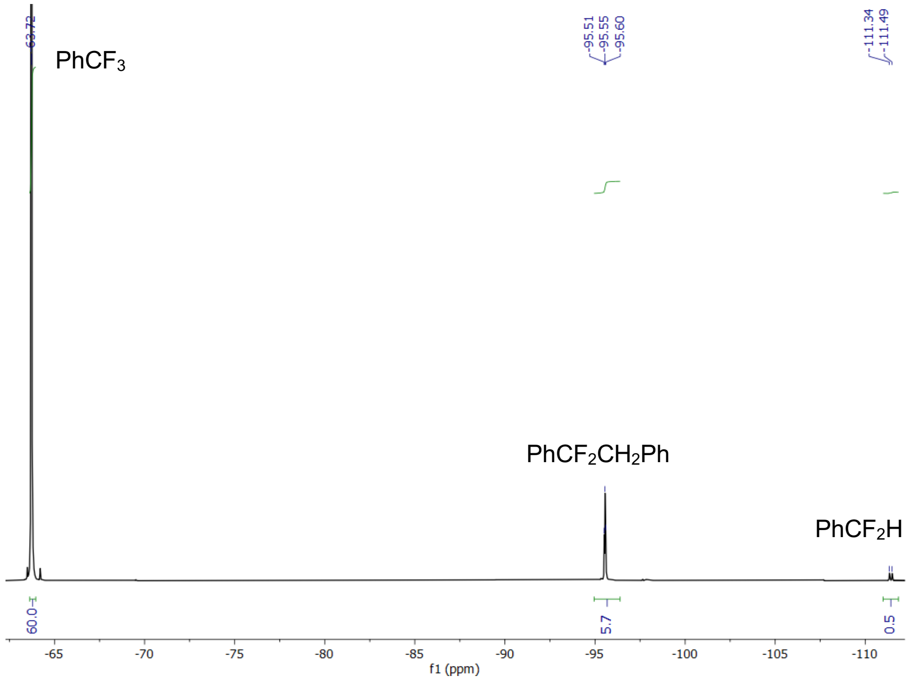


Figure S86. ^{19}F NMR of 1 mol% **1-Ce** in THF-D_8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 42 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

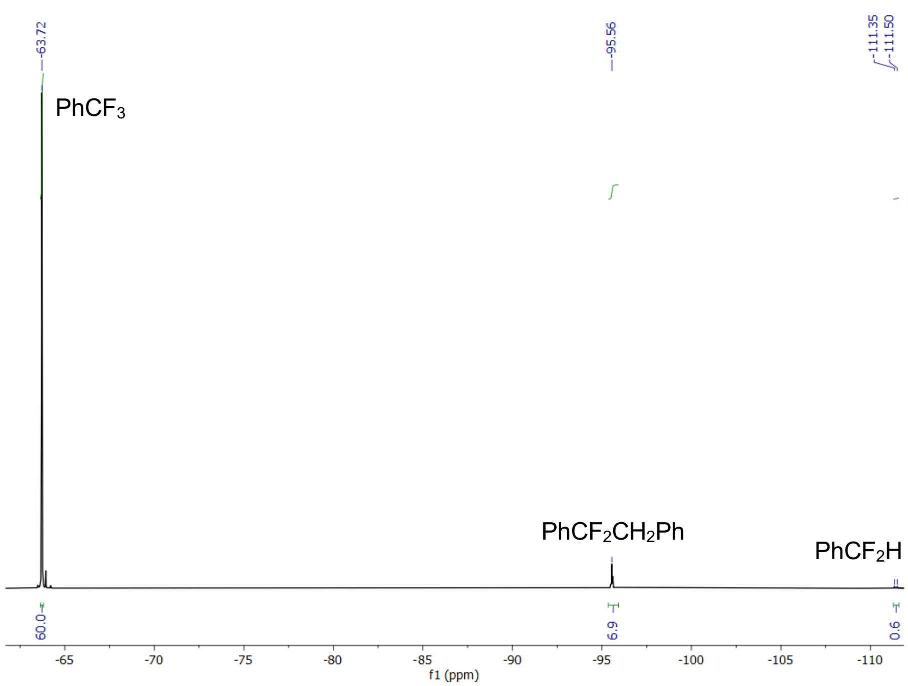


Figure S87. ^{19}F NMR of 1 mol% **1-La** in THF-D_8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 42 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

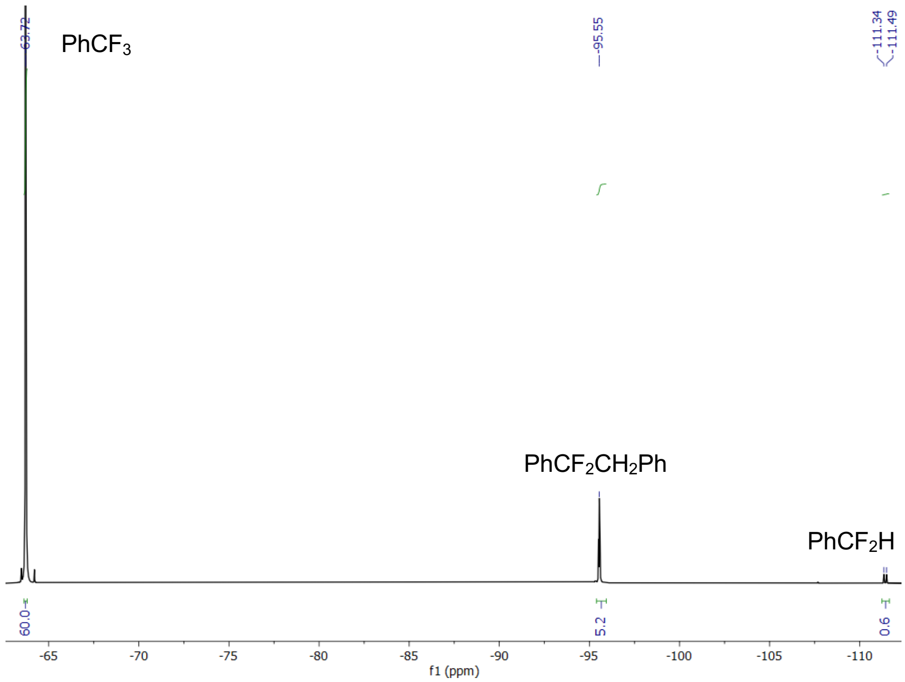


Figure S88. ^{19}F NMR of 1 mol% **7-Mg** in THF-D_8 with $MgBn_2(THF)_2$ and $PhCF_3$ after 42 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

S7 Stoichiometric alkene coupling

S7.1. Preliminary reactions

S7.1.1 General procedure and results

In a glovebox, a Young NMR tube was charged with catalyst (0.0100 mmol, 1 equiv.) and THF (0.5 mL). Alkene (0.0100 mmol, 1 equiv.) was then added using a micropipette. The sample was then irradiated with 40 W Kessil A160WE Tuna Blue lamp and monitored periodically by ^{1}H and ^{19}F NMR spectroscopy, with a final time point being taken after 100 hours irradiation.

Table S5. Defluoroalkylative coupling of $PhCF_3$ with alkenes mediated by **1-Ln**, with yields determined by ^{19}F NMR spectroscopy.

Entry	Complex	Alkene R Identity	Yield of alkylated product (%)	Yield of $PhCF_2H$ byproduct (%)
1	**1-Ce**	^{t}Bu	13	8
2	**1-Ce**	$SiMe_3$	27	6
3	**1-La**	$SiMe_3$	1	Not detected
4	**1-Ce**	$Si(OMe)_3$	19	7

S7.1.2 ^{19}F NMR Spectra

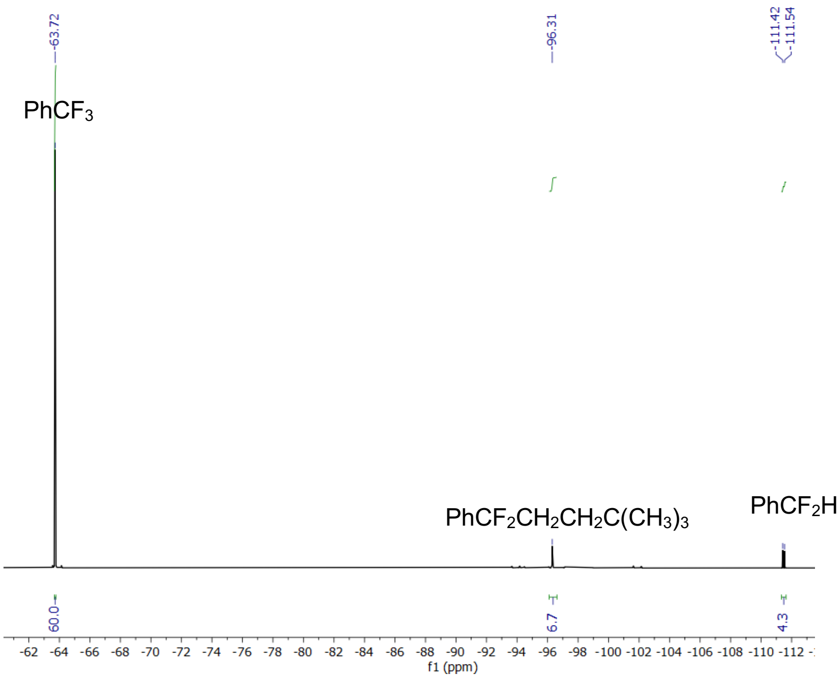


Figure S89. ^{19}F NMR in THF-H_8 **1-Ce** with 1 equiv. 3,3-dimethylbut-1-ene and 1 equiv. $PhCF_3$ following 300 hours of irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

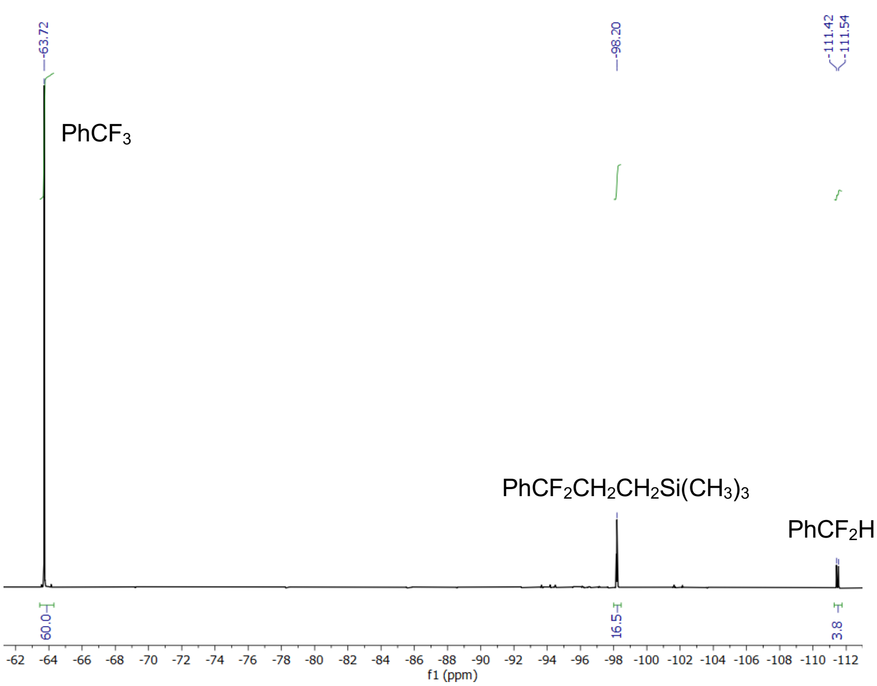


Figure S90. ^{19}F NMR in THF-H_8 **1-Ce** with 1 equiv. trimethyl(vinyl)silane and 1 equiv. $PhCF_3$ following 300 hours of irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

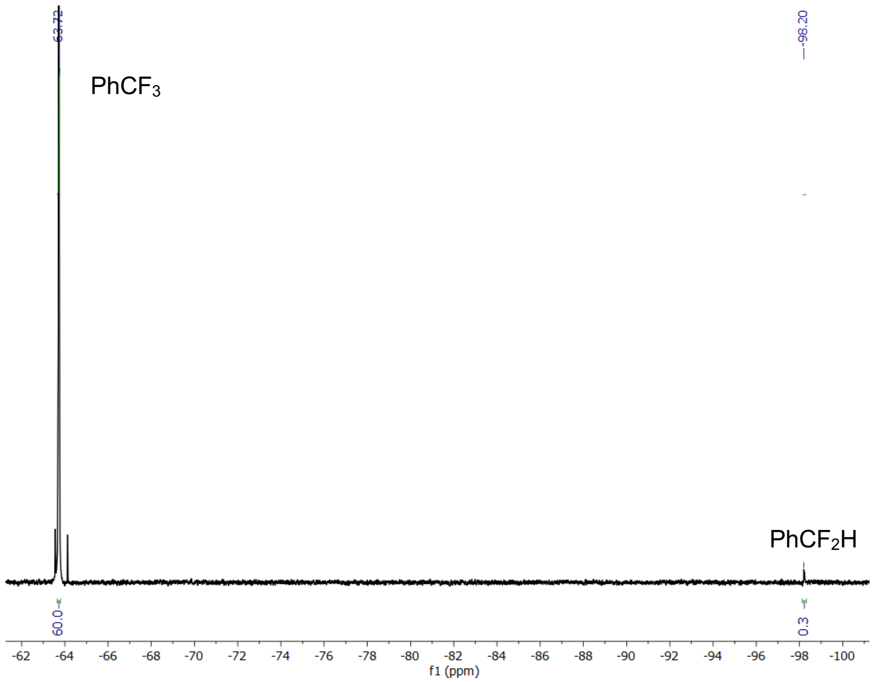


Figure S91. [19]F NMR in THF-H_8 **1-La** with 1 equiv. trimethyl(vinyl)silane and 1 equiv. $PhCF_3$ following 300 hours of irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

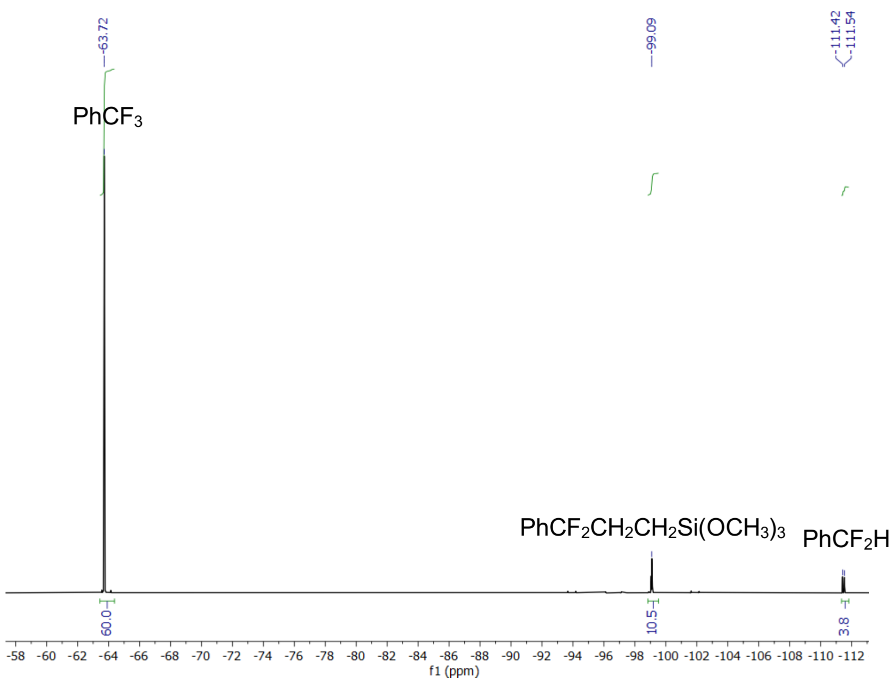


Figure S92. [19]F NMR in THF-H_8 **1-Ce** with 1 equiv. trimethoxy(vinyl)silane and 1 equiv. $PhCF_3$ following 300 hours of irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

S7.2. Optimized reactions

S7.2.1 General procedure

In a glovebox, a Young NMR tube was charged with catalyst (0.0500 mmol, 5 equiv.) and THF (0.5 mL). Alkene (0.0500 mmol, 5 equiv.) was then added using a micropipette. The sample was then irradiated with light and monitored periodically by ^{1}H and ^{19}F NMR spectroscopy, with a final time point being taken after 100 hours irradiation.

S7.2.2 ^{19}F NMR Spectra

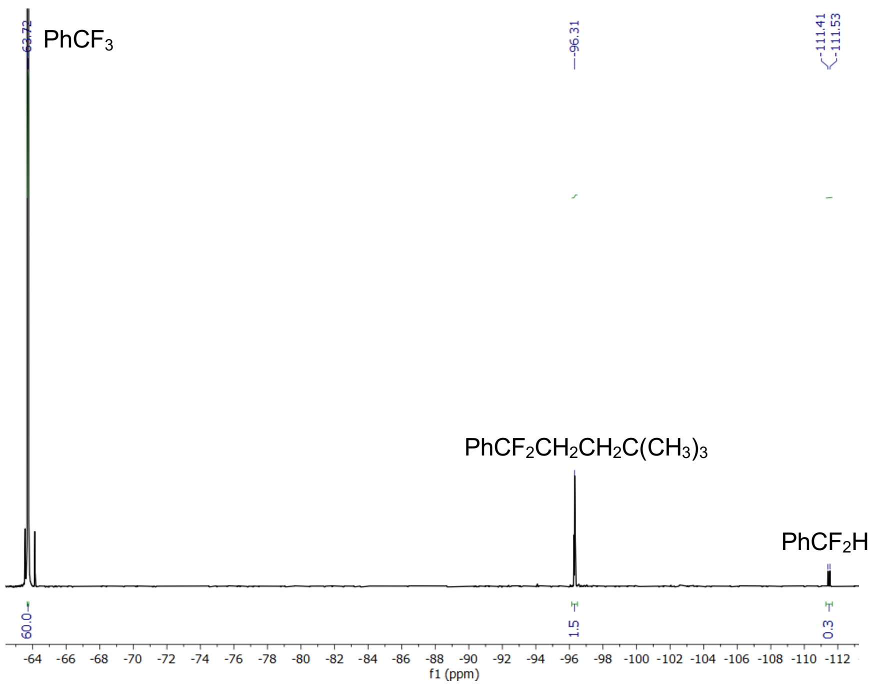


Figure S93. ^{19}F NMR in THF-H_8 **1-Ce** with 5 equiv. 3,3-dimethylbut-1-ene and 5 equiv. $PhCF_3$ following 70 hours of irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

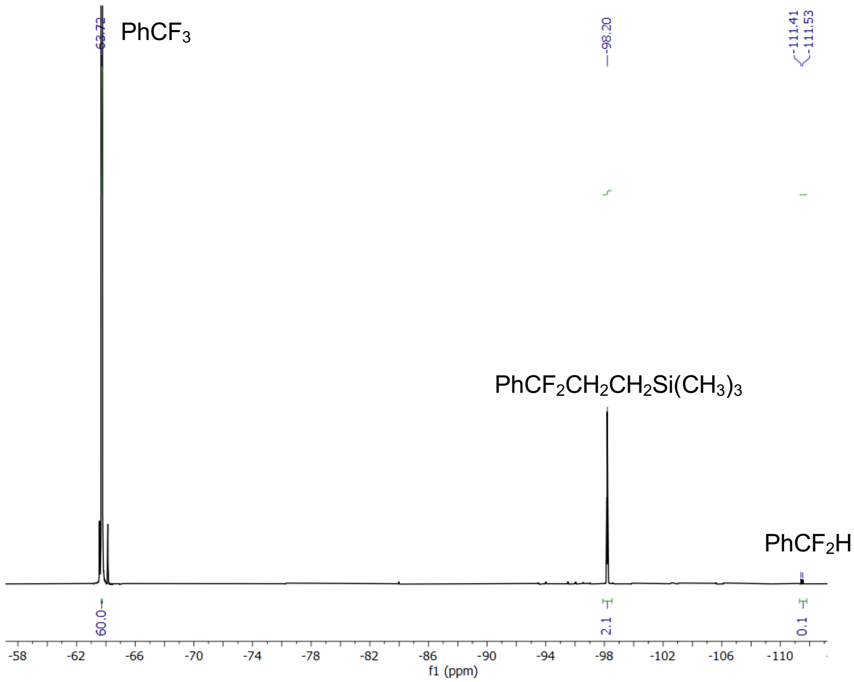


Figure S94. [19]F NMR in THF-H8 **1-Ce** with 5 equiv. trimethyl(vinyl)silane and 5 equiv. $PhCF_3$ following 100 hours of irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

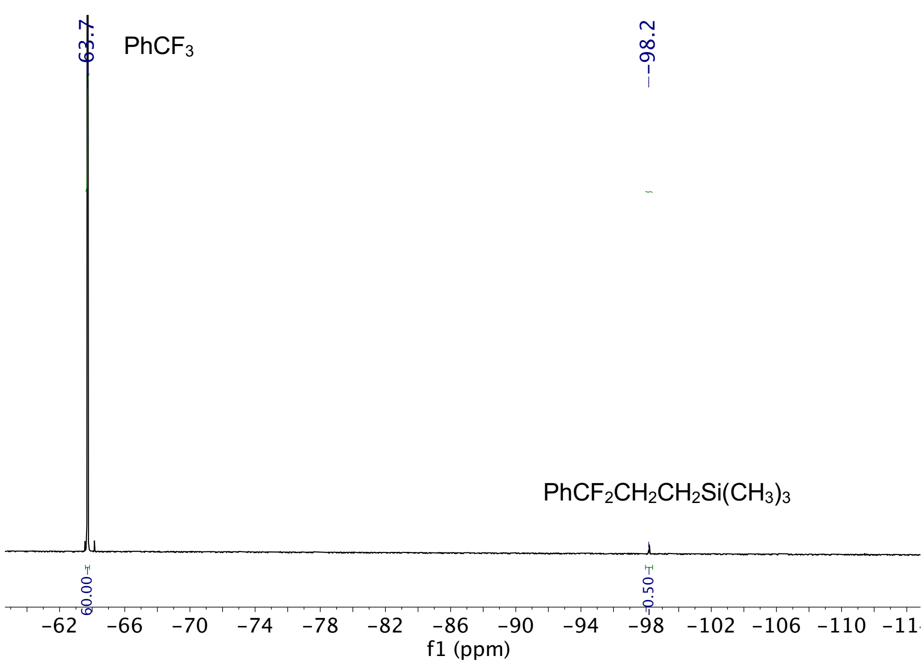


Figure S95. [19]F NMR in THF-H8 **1-La** with 5 equiv. trimethyl(vinyl)silane and 5 equiv. $PhCF_3$ following 100 hours of irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

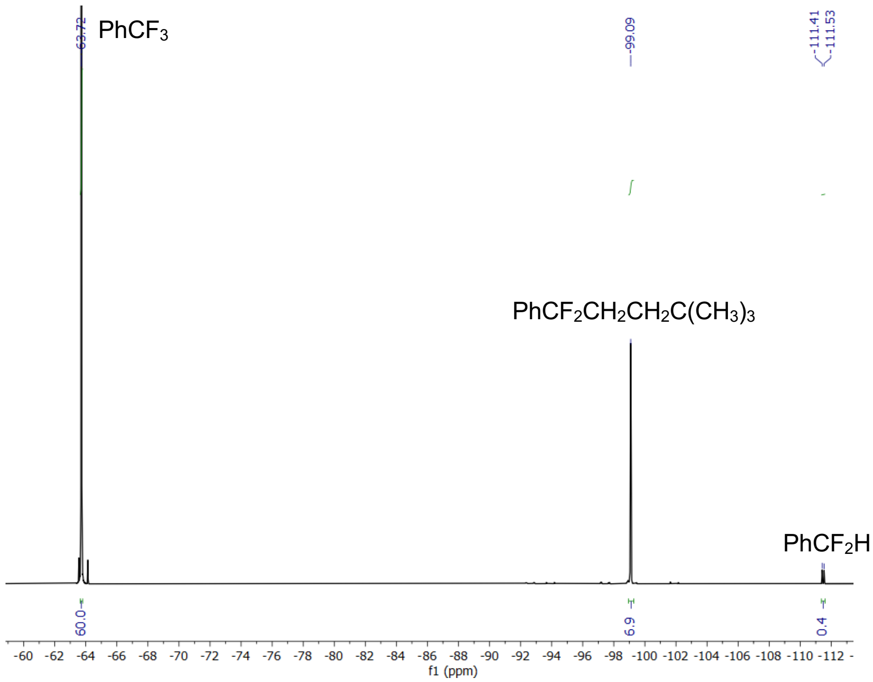


Figure S96. ^{19}F NMR in THF-H$_8$ **1-Ce** with 5 equiv. trimethoxy(vinyl)silane and 5 equiv. PhCF$_3$ following 100 hours of irradiation under a 40 W Kessil A160WE Tuna Blue lamp.

S8 Miscellaneous and Control reactions

S8.NMR spectroscopic investigation of possible interactions between $PhCF_3$ and **1-Ce** and **1-La**

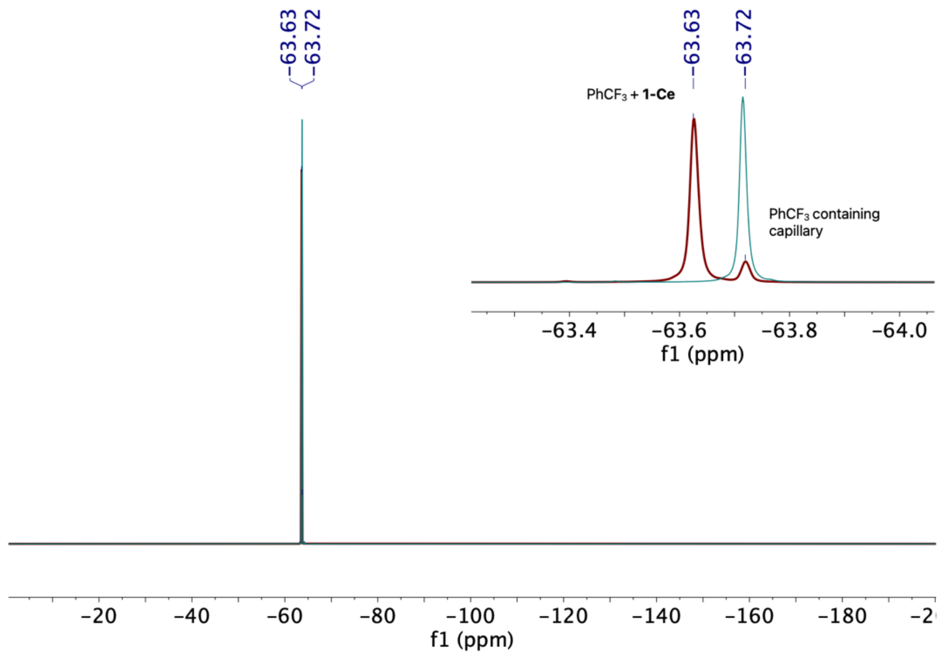


Figure S97.[19]F NMR spectrum of a 325 μM solution of $PhCF_3$ in THF-H_8 in a Young-tapped NMR tube with a capillary containing the same 325 μM solution of $PhCF_3$ in THF-H_8 before (green trace) and after (red trace) the addition of 0.01 mmol **1-Ce.** A shift is seen between $PhCF_3$ inside and outside the capillary which could be attributed to an interaction between $PhCF_3$ and **1-Ce**.

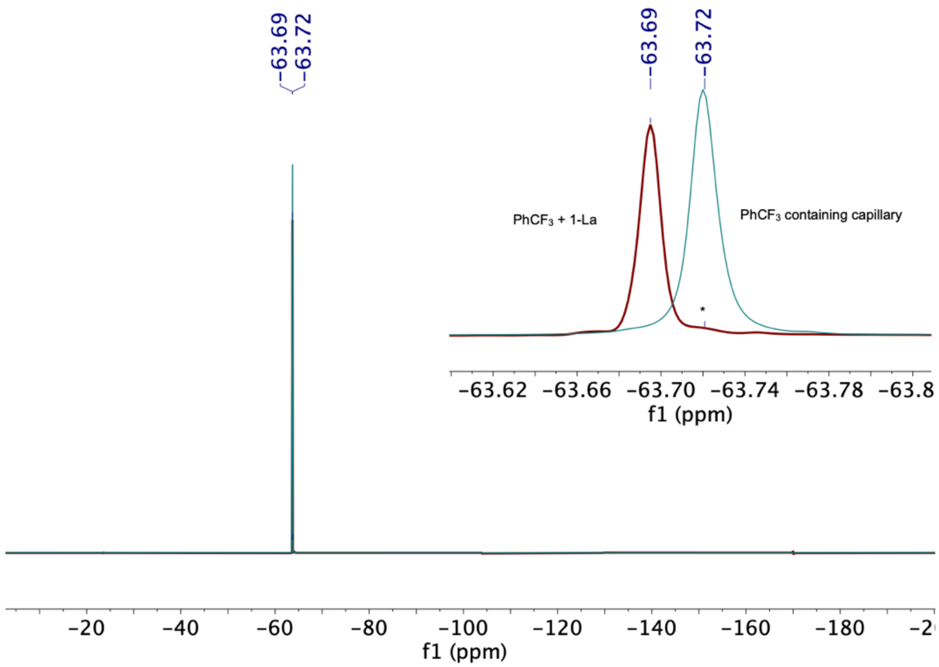


Figure S98. ^{19}F NMR spectrum of a 325 μM solution of $PhCF_3$ in THF-H_8 in a Young-tapped NMR tube with a capillary containing the same 325 μM solution of $PhCF_3$ in THF-H_8 before (green trace) and after (red trace) the addition of 0.01 mmol **1-La**. A shoulder marked (*) seen following addition of **1-La**, which could be attributed to an interaction between $PhCF_3$ and **1-La.**

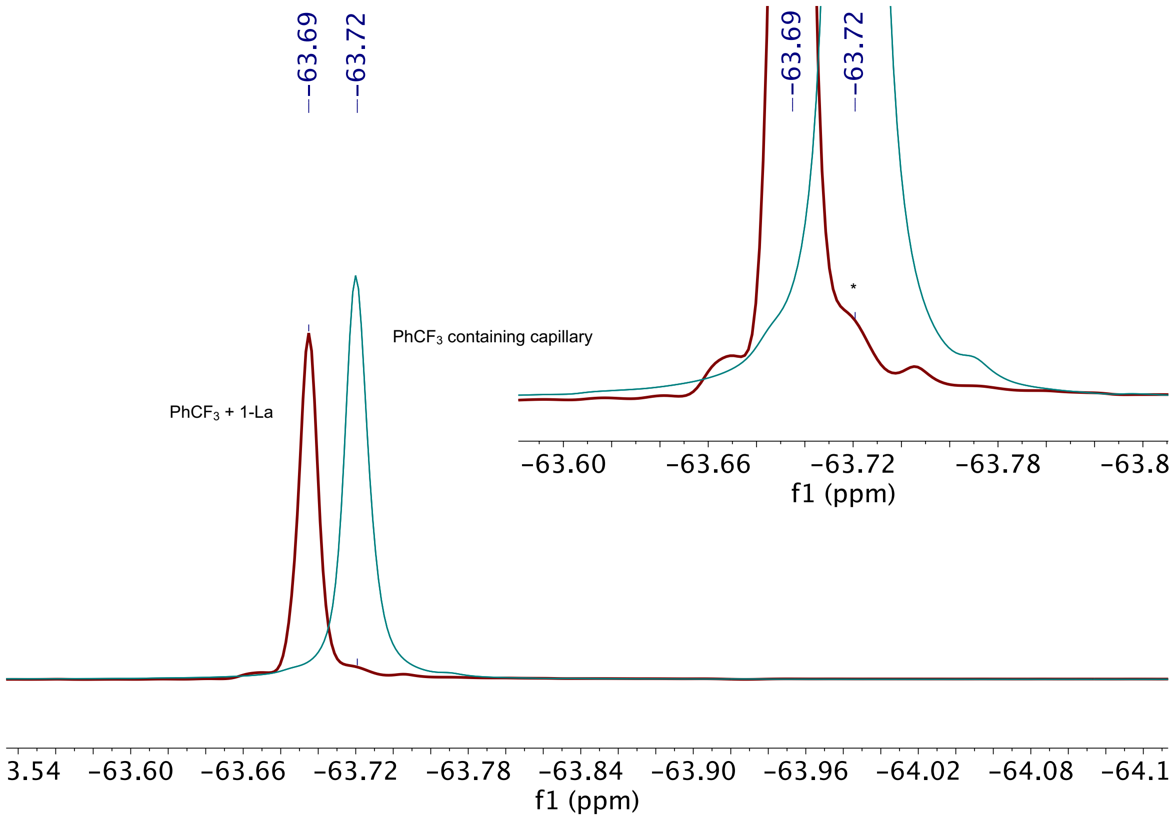


Figure S99. Additional ^{19}F NMR spectrum of 325 μM solution of $PhCF_3$ in THF-H_8 in a Young-tapped NMR tube with a capillary containing the same 325 μM solution of $PhCF_3$ in THF-H_8 before (green trace) and after (red trace) the addition of 0.01 mmol **1-La**. The shoulder marked (*) seen following addition of **1-La**, which could be attributed to an interaction between $PhCF_3$ and **1-La** is highlighted**.**

S8.2 Radical trapping experiments

S8.2.1 Independent synthesis of 1,1-difluoro-2,3-dihydro-1H-indene (**10**)

Following a literature method, diethylaminosulfur trifluoride (2.70 mL, 0.0205 mol, 3 equiv.), was added dropwise to an ice-cold solution of 2-methyl-2,3-dihydro-1*H*-inden-1-one (0.940 mL, 0.0680, 1 equiv.) in dichloromethane (20 mL). The reaction mixture was warmed to room temperature and then heated to reflux for 36 hours. The solution was cooled and added dropwise to a saturated aqueous sodium hydrogencarbonate, extracted with dichloromethane (3 x 10 mL), washed with brine, and dried over magnesium sulfate. Volatiles were removed under vacuum to give a low yield of crude product, identified as containing **10** by ^{19}F NMR, LCMS, and HRMS.

^{19}F NMR (470 MHz, $CDCl_3$) δ -96.07 (dd, *J* = 15.2, 4.4 Hz), -96.60 (dd, *J* = 15.3, 4.4 Hz), -98.78 (d, *J* = 14.3 Hz), -99.31 (d, *J* = 14.2 Hz). m/z=168. HRMS Calcd [2M+MeCN+H]$^+$ 378.1942; found [2M+MeCN+H]$^+$ 378.1948. Residual = 1.586 ppm.

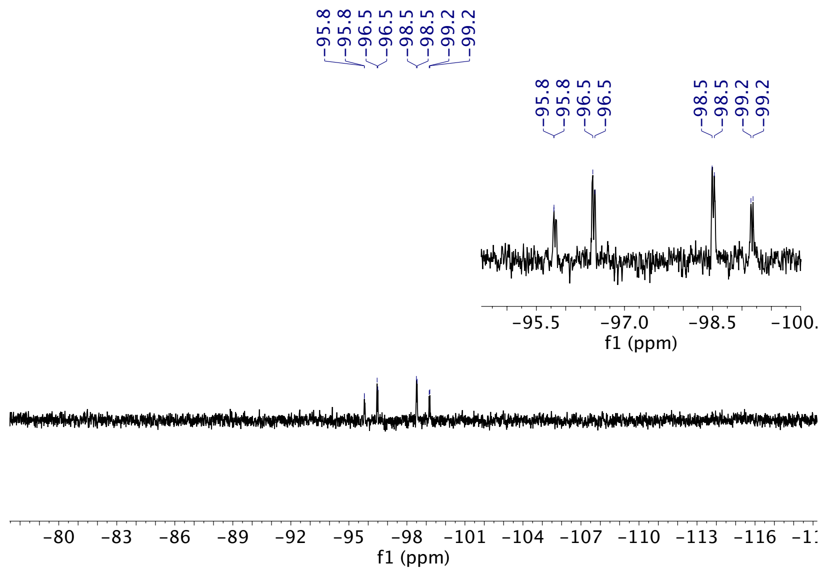


Figure S100.^{19}F NMR in $CDCl_3$ of 1,1-difluoro-2,3-dihydro-1H-indene **10** made from the independent synthesis.

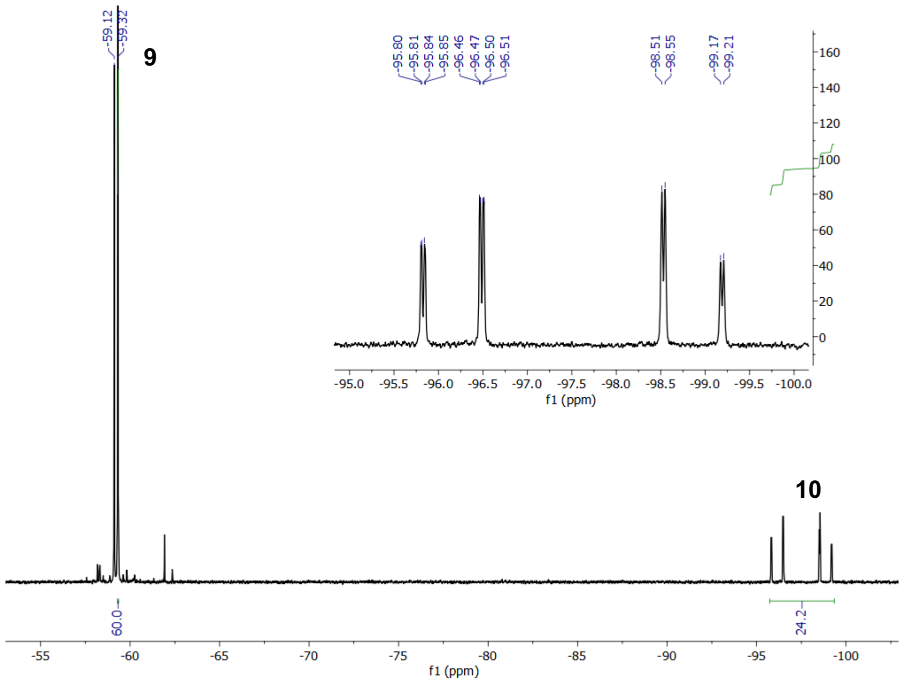


Figure S101.[19]F NMR in THF-H_8 of **1-Ce** with 5 equiv. **9**, following 6 days irradiation with a 40 W Kessil A160WE Tuna Blue lamp at 70 °C.

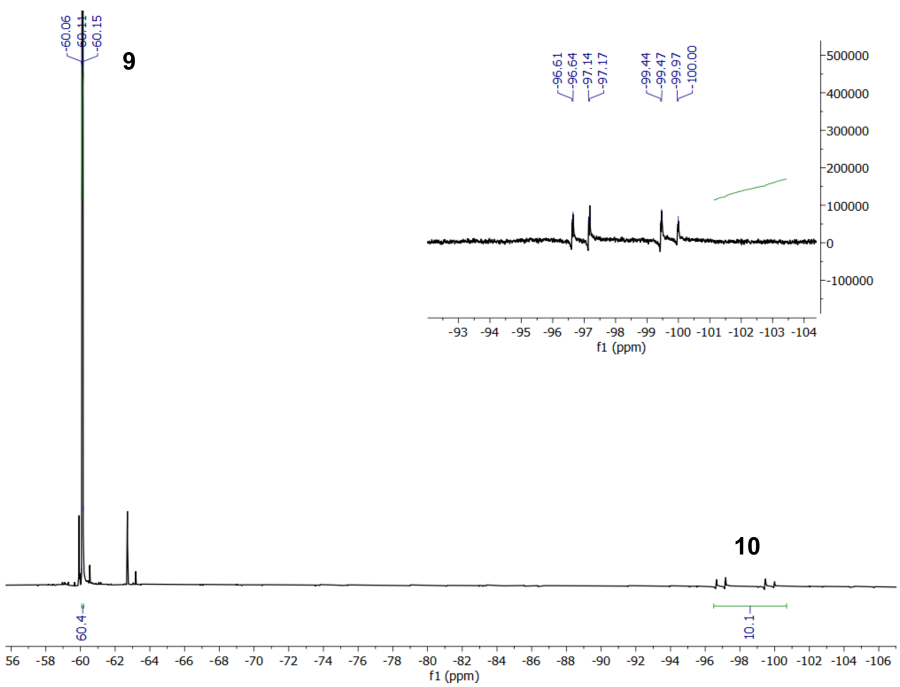


Figure S102.[19]F NMR in THF-H_8 of **1-La** with 5 equiv. **9**, following 7 days irradiation with a 40 W Kessil A160WE Tuna Blue lamp at room temperature.

S8.3 Formation of **7-Mg** via addition of $MgBn_2(THF)_2$ to **1-Ce** and **1-La**

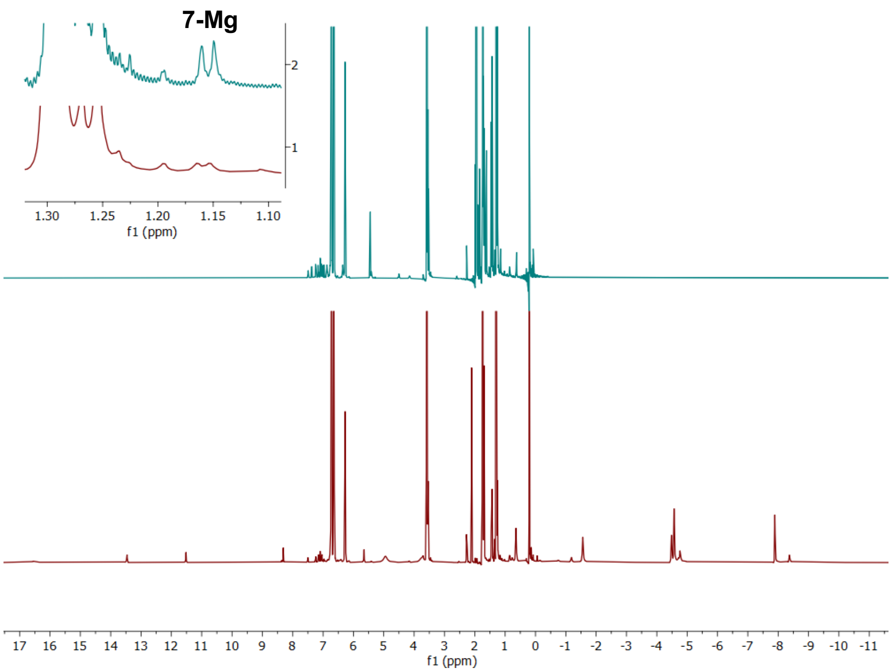


Figure S103. [1]H NMR in THF-D_8 of **1-La** (top spectrum, blue) and **1-Ce** (bottom spectrum, red) with 5 equiv. $MgBn_2(THF)_2$ and 1 equiv. after 24 hours, to monitor the formation of **7-Mg**. A single iPr resonance of **7-Mg** is highlighted and integrated relative to a $Si(SiMe_3)_4$ internal standard, demonstrating the higher conversion of **1-La** to **7-Mg** in comparison to **1-Ce**.

S8.4 Testing catalyst stability under a 40 W Kessil A160WE Tuna Blue lamp

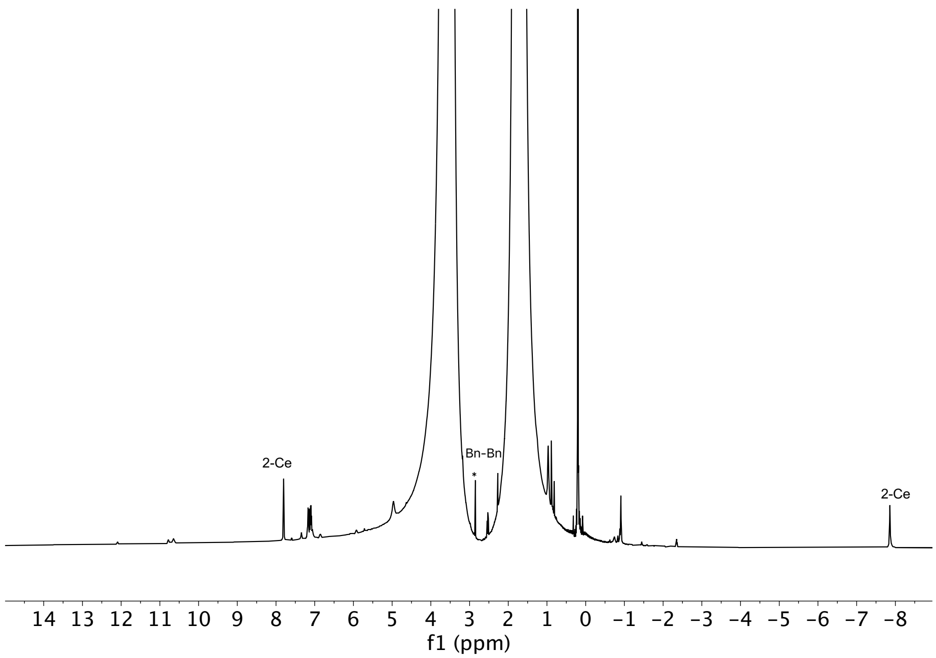


Figure S104. ^{1}H NMR in THF-H_8 **6-Ce** following 72 hours of irradiation under a 40 W Kessil A160WE Tuna Blue lamp. The complete consumption of **6-Ce** to form **2-Ce** and bibenzyl (Bn-Bn) was observed after this period.

S8.5 Irradiation wavelength dependence of catalysis

S8.5.1 Table of results

Table S6. Defluoroalkylative coupling of $PhCF_3$ with dibenzyl magnesium mediated by 20 mol% catalyst loading of **1-Ce** followed by 42 hours irradiation with a variety of wavelengths of light, with yields determined by ^{19}F NMR spectroscopy.

Irradiation wavelength (nm)	Conversion to $PhCF_2CH_2Ph$ and $PhCF_2H$ (%)
390	46
467	51
525	25

S8.5.2 ^{19}F NMR spectra

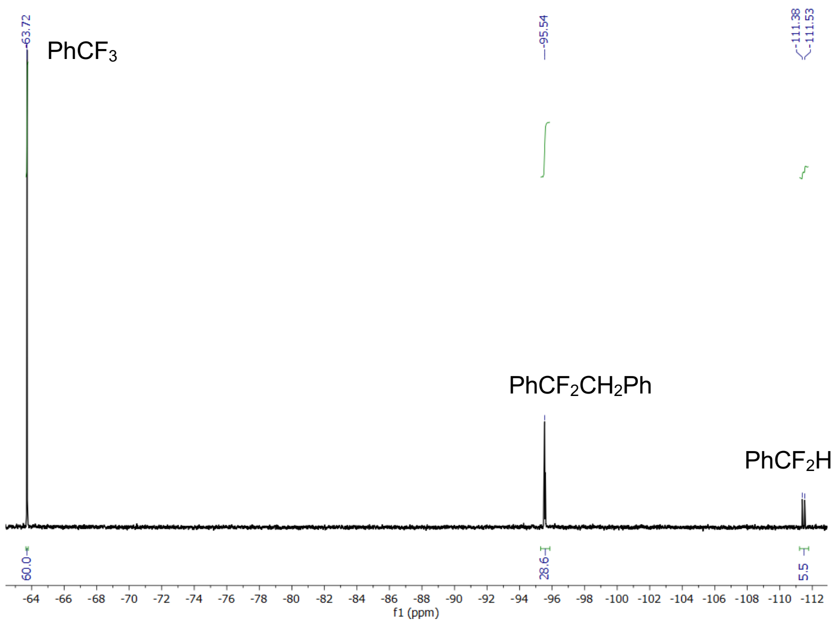


Figure S105. ^{19}F NMR in THF-H_8 20 mol% **1-Ce** with $MgBn_2(THF)_2$ and $PhCF_3$ following 80 hours of irradiation under a 52 W Kessil PR160L 390 nm lamp.

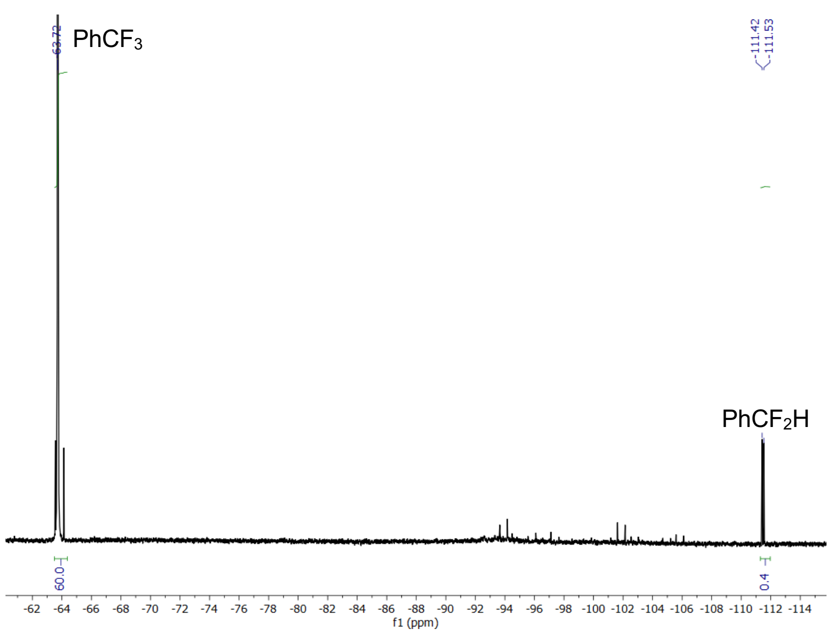


Figure S106. ^{19}F NMR in THF-H_8 20 mol% **1-La** with $MgBn_2(THF)_2$ and $PhCF_3$ following 48 hours of irradiation under a 52 W Kessil PR160L 390 nm lamp. Just 1% conversion to $PhCF_2H$ was observed alongside the generation of multiple other unidentified fluorine-containing species. The decomposition of **1-La** was also seen by ^{1}H NMR.

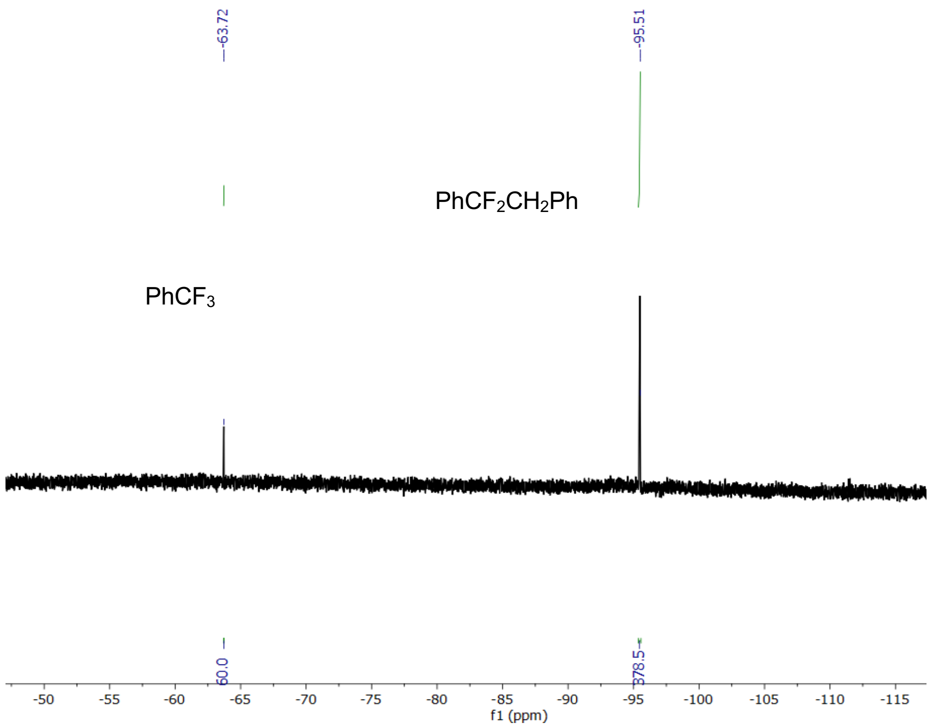


Figure S107. [19]F NMR in THF-H_8 20 mol% **1-Ce** with $MgBn_2(THF)_2$ and $PhCF_3$ following 80 hours of irradiation under a 40 W Kessil A160WE Tuna blue lamp

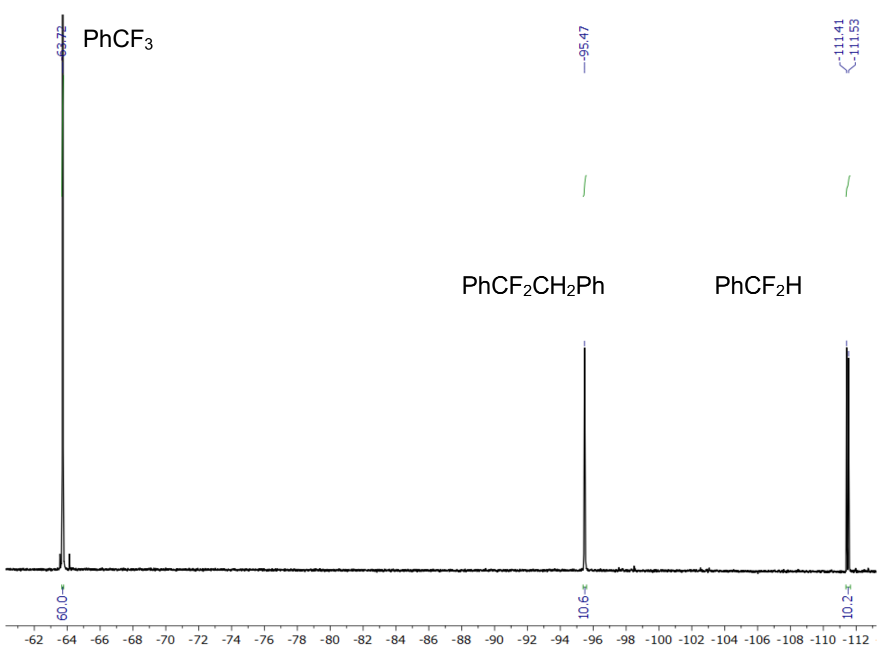


Figure S108. [19]F NMR in THF-H_8 20 mol% **1-Ce** with $MgBn_2(THF)_2$ and $PhCF_3$ following 80 hours of irradiation under a 44 W Kessil PR160L 467 nm lamp.

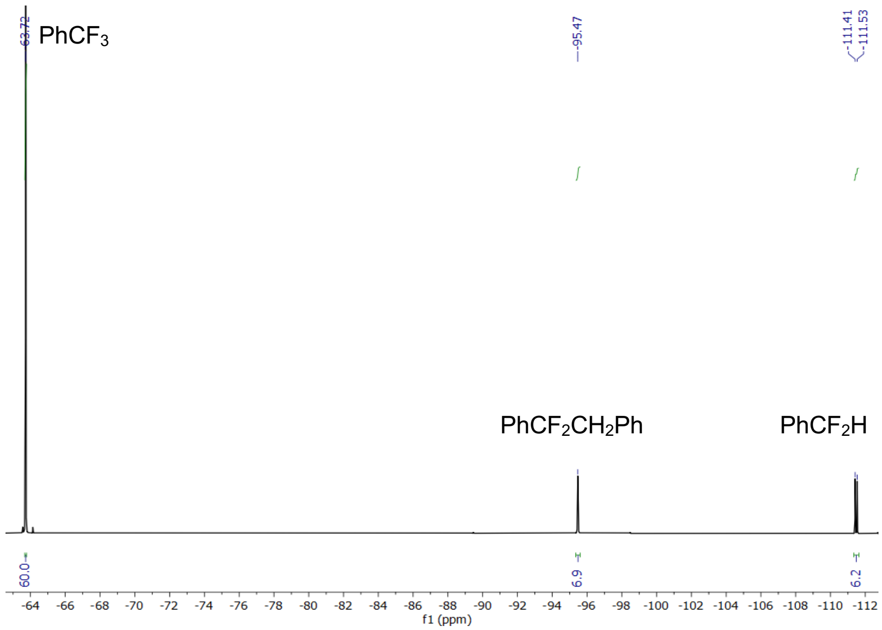


Figure S109. [19]F NMR in THF-H_8 20 mol% **1-Ce** with $MgBn_2(THF)_2$ and $PhCF_3$ following 80 hours of irradiation under a 52 W Kessil PR160L 525 nm lamp.

S8.6 Defluorination selectivity

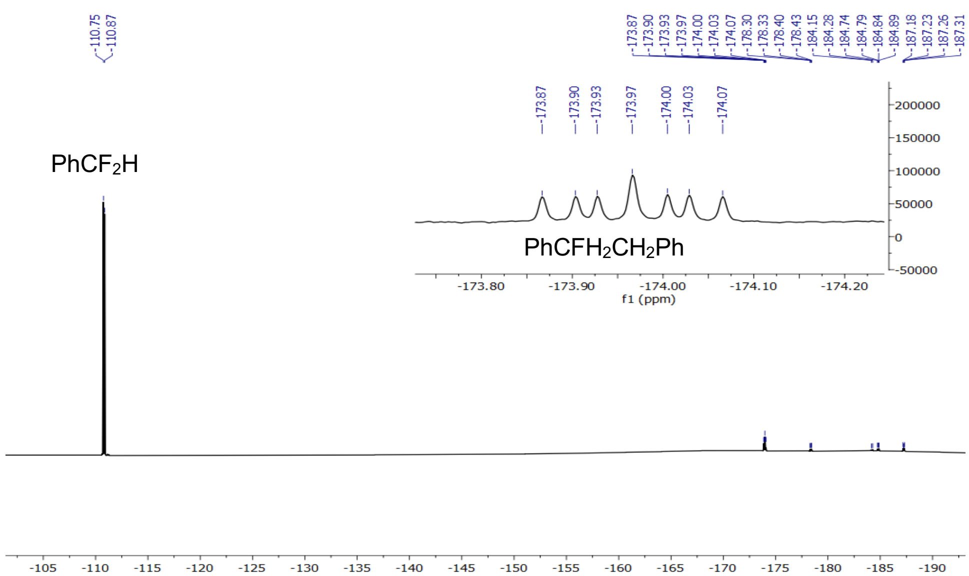


Figure S110.[19]F NMR in THF-H_8 20 mol% **1-Ce** with $MgBn_2(THF)_2$ and $PhCF_2H$ following 110 hours of irradiation under a 40 W Kessil A160WE Tuna Blue lamp. 47% conversion to $PhCFH_2CH_2Ph$ was observed alongside multiple other unidentified fluorine-containing compounds.[17] The negligible amount of the target compound in catalysis with $MgBn_2(THF)_2$ and $PhCF_3$ suggest no significant initial defluorination of $PhCF_2CH_2Ph$ and $PhCF_2H$ prior to the addition of catalyst.

S8.7 Evidence of formation of metal fluoride complex in defluoroalkylation reactions

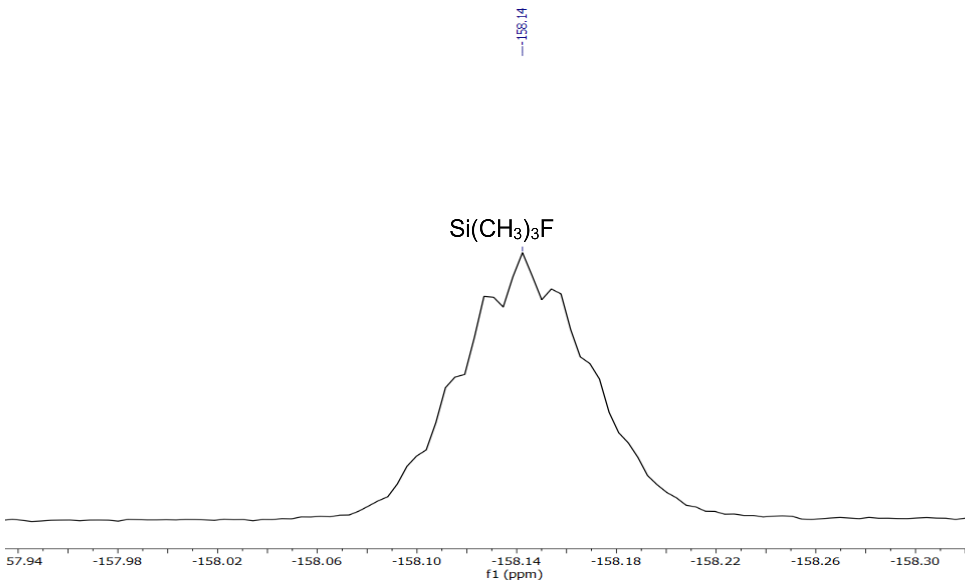


Figure S111.[19]F NMR in THF-H_8 following the addition of an excess of chlorotrimethylsilane to a reaction mixture containing 1 mol% **1-Ce** with $MgBn_2(THF)_2$ and $PhCF_2H$ following 63 hours of irradiation under a 40 W Kessil A160WE Tuna Blue lamp. The generation of fluorotrimethylsilane was observed.

S8.9. Variable temperature NMR experiments with **1-Ce**

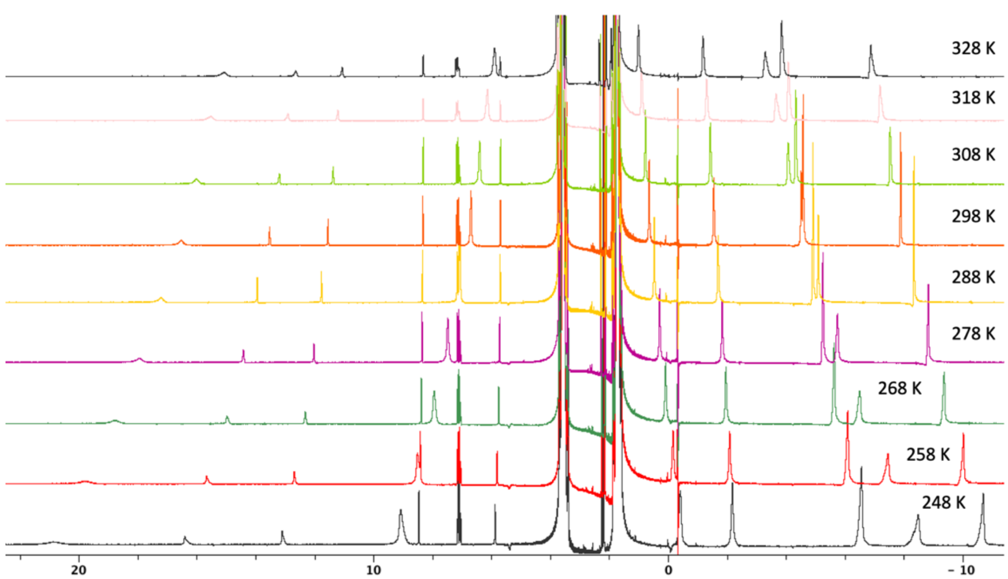


Figure S112. Variable temperature NoD ^{1}H NMR of **1-Ce** in THF-H_8 with 1 equivalent $MgBn_2(THF)_2$. No evidence of NHC lability was observed.

S8.10 Ligand exchange of Ce and Mg complexes

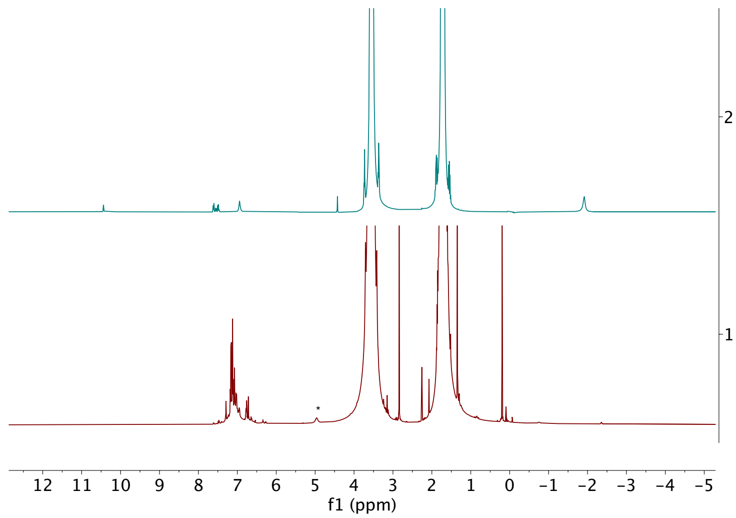


Figure S113. NoD ^{1}H NMR of 20 mol% **4-Ce** in THF-H_8 with 5 equivalent $MgBn_2(THF)_2$ and $PhCF_3$ before (top spectrum) and following (bottom spectrum) 80 hours irradiation with a 40 W Kessil A160WE Tuna Blue lamp. Generation of **6-Ce** is observed (marked *), indicating that bidentate aryloxy-NHC ligand **L** contributes to the robustness of **1-Ce** over **4-Ce** in reaction mixtures.

S8.11 Reaction to Target a Ce(III) Fluoride Adduct

To a 20 mL vial was added **6-Ce** (61.1 mg, 0.112 mmol, 1.00 equiv.) dissolved in THF (5 mL), resulting in a yellow-green solution. This solution was chilled in a freezer (–30 °C) for 15 minutes. With stirring, a similarly chilled solution of BF_3OEt_2 (5.1 mg, 0.0.036 mmol, 0.32 equiv.) in THF (2 mL) was added dropwise, resulting in a rapid color change to bright yellow. The solution was warmed to room temperature with stirring for 1 hour, during which time the reaction mixture became turbid, then lightened to a brighter yellow and became homogeneous. The volatiles were then removed *in vacuo*, resulting in a yellow-green residue. Extracting with hexanes (2 x 3 mL) gave a bright green solution, which ^{1}H NMR spectroscopy revealed to be **2-Ce**. The remaining yellow-orange residue was extracted with toluene and filtered to give a yellow-orange filtrate. Solvent was removed *in vacuo*, giving a yellow residue, which was recrystallized from a layered toluene/hexane solution stored at 30 °C overnight.

Crystals formed were suitable for X-ray diffraction and identified as **[$(Cp^{Me4})_2$Ce(BF_4)(THF)]$_2$** (see S9), indicating successful abstraction of the benzyl group for a fluoride, which is subsequently capped by an additional BF_3.

S8.11 Control reactions

S8.11.1 Reactions in the dark

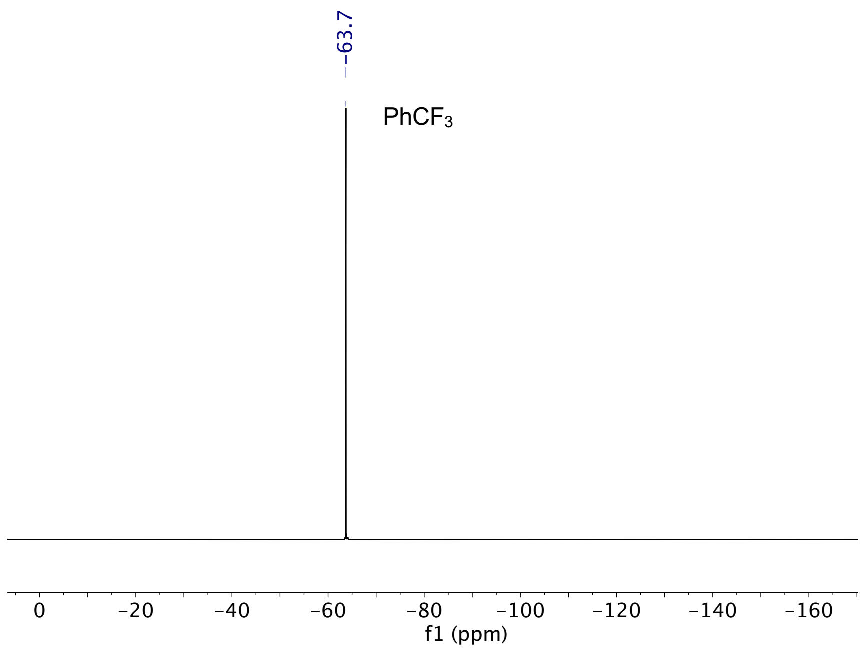


Figure S114. ^{19}F NMR in THF-H_8 20 mol% **1-Ce** with $MgBn_2(THF)_2$ and $PhCF_3$ after 72 hours with no irradiation. No $PhCF_2CH_2Ph$, $PhCF_2H$ or any other evidence of C-F activation was observed in this time period.

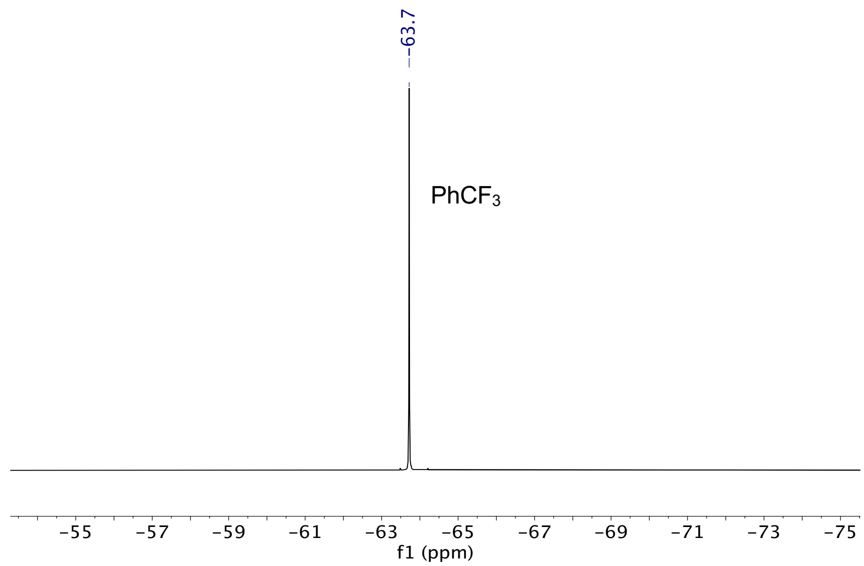


Figure S115. [19]F NMR in THF-H_8 20 mol% **1-La** with $MgBn_2(THF)_2$ and $PhCF_3$ after 72 hours with no irradiation. No $PhCF_2CF_2Ph$, $PhCF_2H$ or any other evidence of C-F activation was observed in this time period.

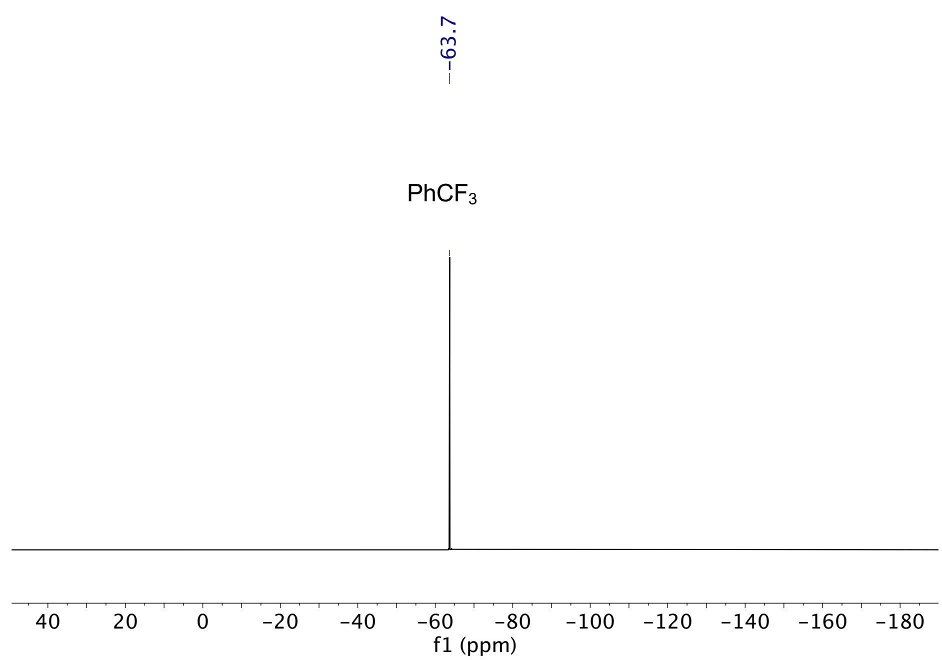


Figure S116. [19]F NMR in THF-H_8 of **2-La** with 5 equiv. $PhCF_3$ after 72 hours with no irradiation. No $PhCF_2CH_2Ph$, $PhCF_2H$ or any other evidence of C–F activation was observed in this time period, though **2-La** did gradually decompose in the presence of $PhCF_3$.

S8.11.2 Reactions of $MgBn_2(THF)_2$ and $PhCF_3$ without the addition of catalyst

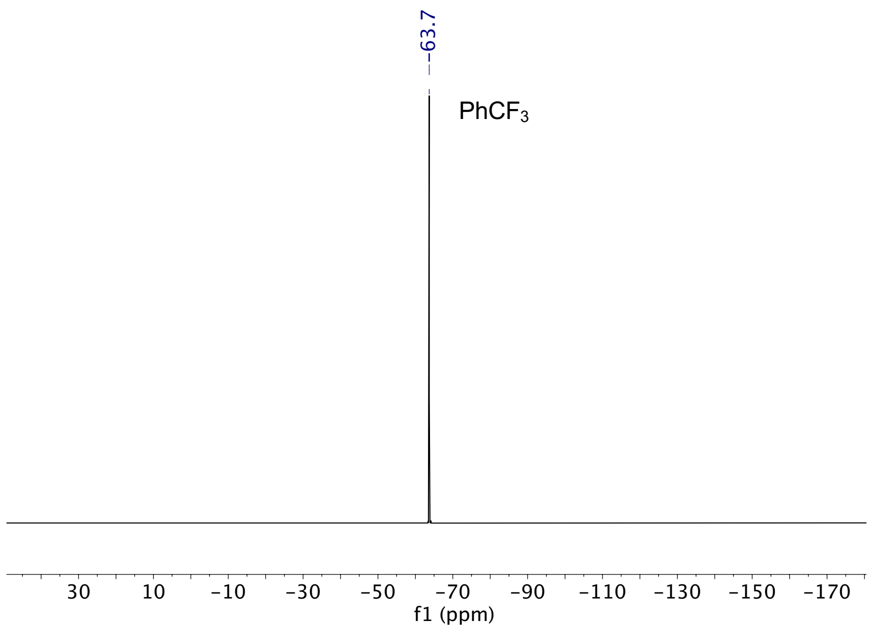


Figure S117. [19]F NMR in THF-H_8 $PhCF_3$ after 72 hours irradiation. No $PhCF_2H$ or any other evidence of C–F activation was observed in this time period.

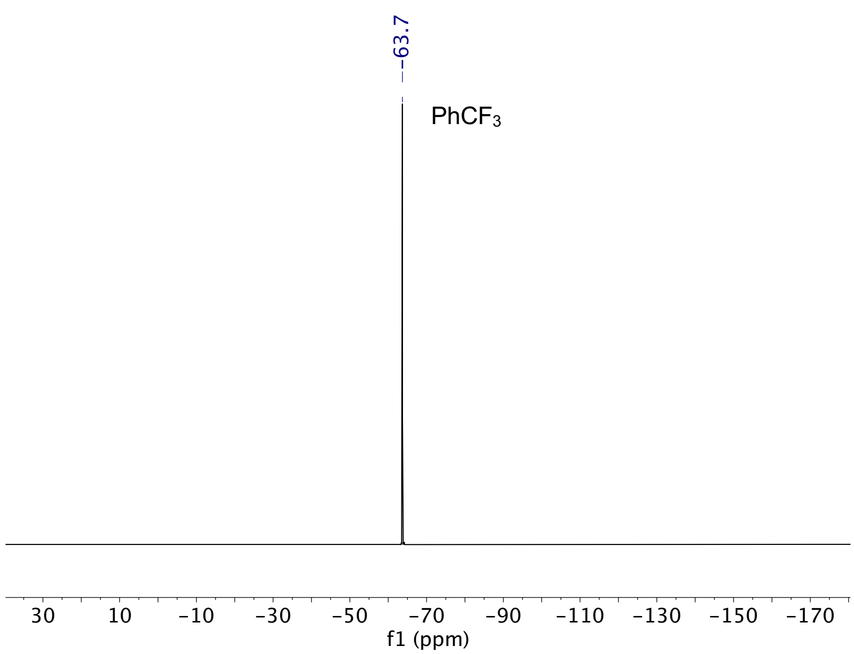


Figure S118. [19]F NMR in THF-H_8 20 mol% $MgBn_2(THF)_2$ and $PhCF_3$ after 72 hours with no irradiation. No $PhCF_2CH_2Ph$, $PhCF_2H$ or any other evidence of C–F activation was observed in this time period.

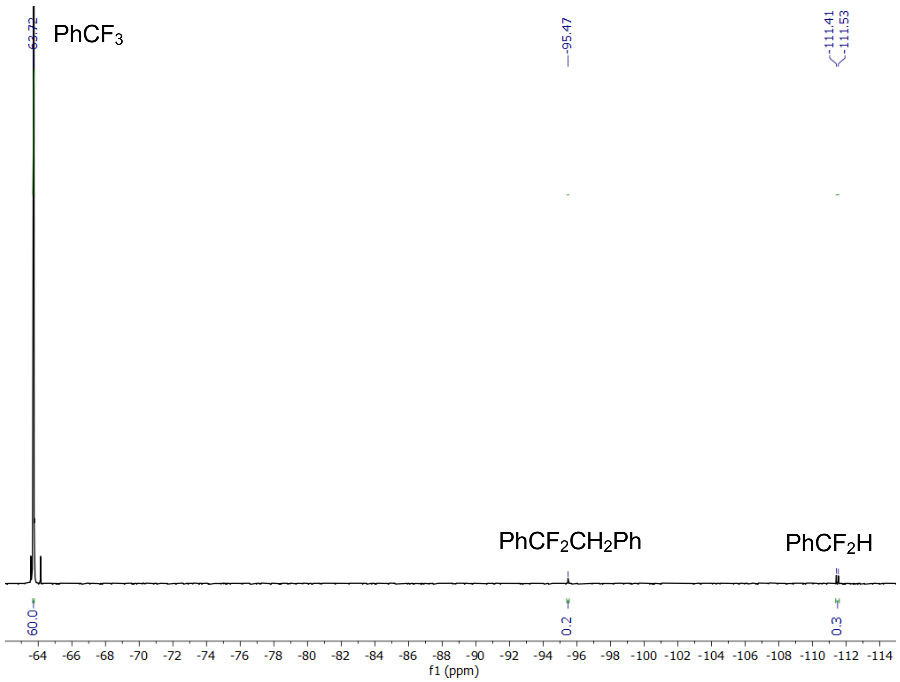


Figure S119. [19]F NMR in THF-H_8 $MgBn_2(THF)_2$ and 1 equiv. $PhCF_3$ after 48 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp. Just 1% total conversion to $PhCF_2CH_2Ph$ and $PhCF_2H$ was observed.

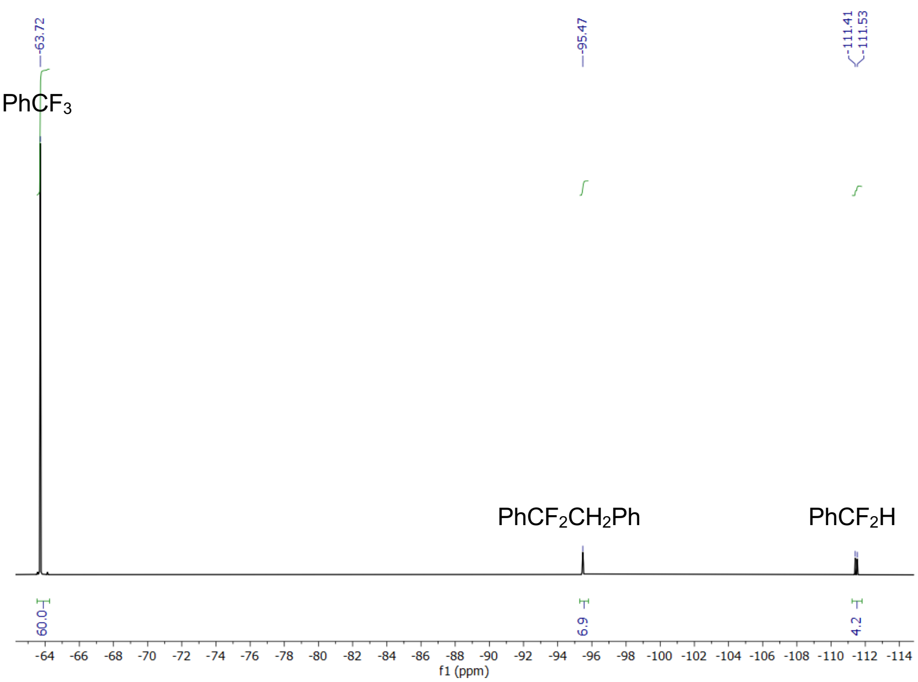


Figure S120. [19]F NMR in THF-H_8 $MgBn_2(THF)_2$ and 1 equiv. $PhCF_3$ after 260 hours irradiation under a 40 W Kessil A160WE Tuna Blue lamp. Just 22% total conversion to $PhCF_2CH_2Ph$ and $PhCF_2H$ was observed.

S9 Crystallography

S9.1 Crystal Structures

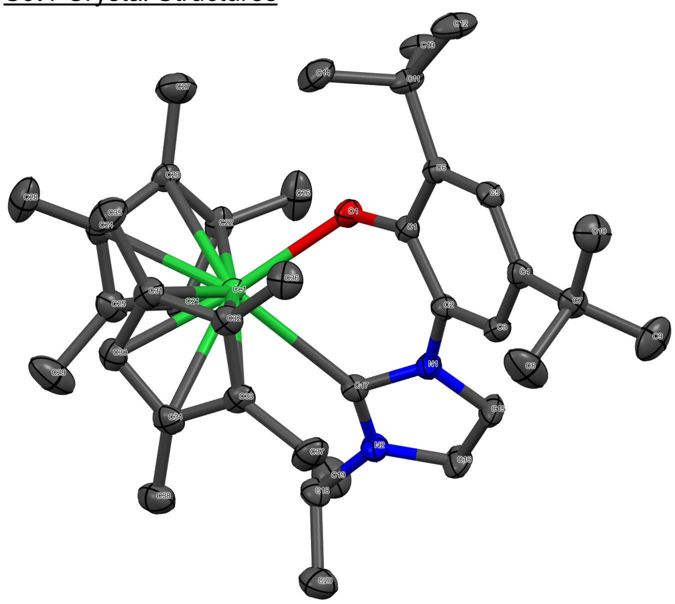


Figure S121. ORTEP diagram of **1-Ce**. Ellipsoids shown at 50% probability, lattice solvent, disorder and hydrogen atoms have been omitted for clarity.

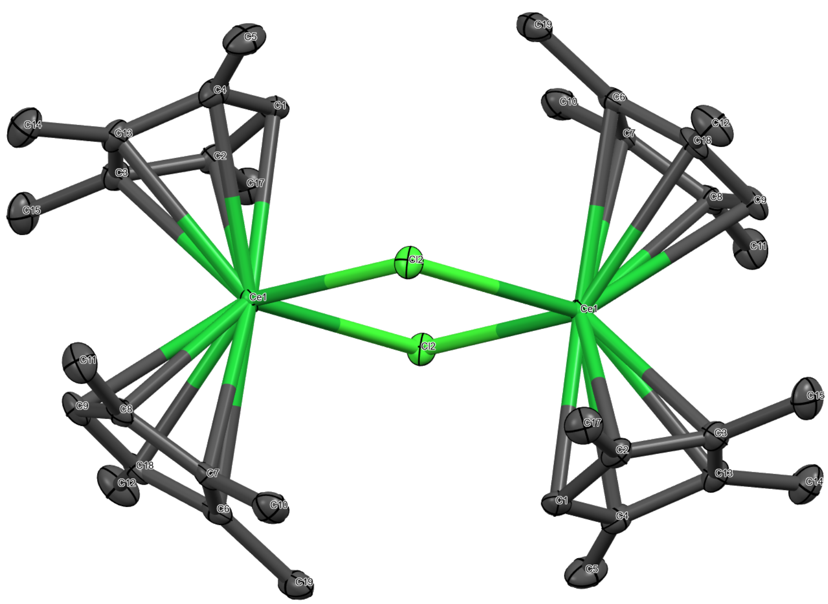


Figure S122. ORTEP diagram of **3-Ce**. Ellipsoids shown at 50% probability, lattice solvent, disorder and hydrogen atoms have been omitted for clarity.

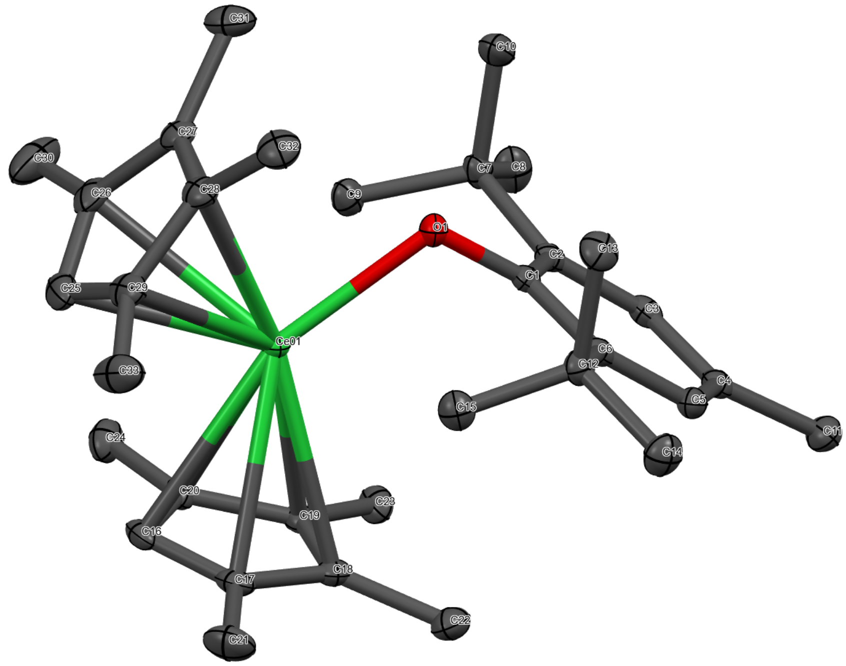


Figure S123. ORTEP diagram of **4-Ce**. Ellipsoids shown at 50% probability, lattice solvent, disorder and hydrogen atoms have been omitted for clarity.

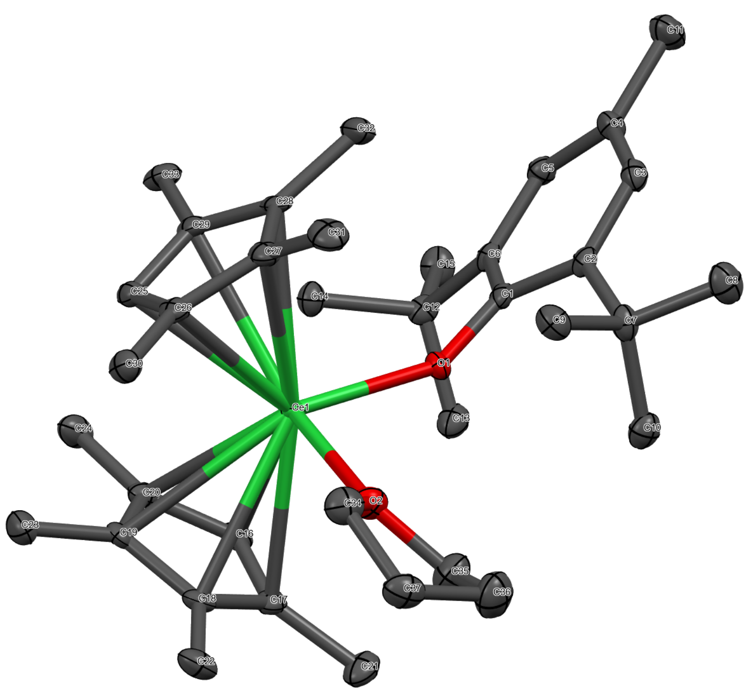


Figure S124. ORTEP diagram of **4-Ce(THF)**. Ellipsoids shown at 50% probability, lattice solvent, disorder and hydrogen atoms have been omitted for clarity.

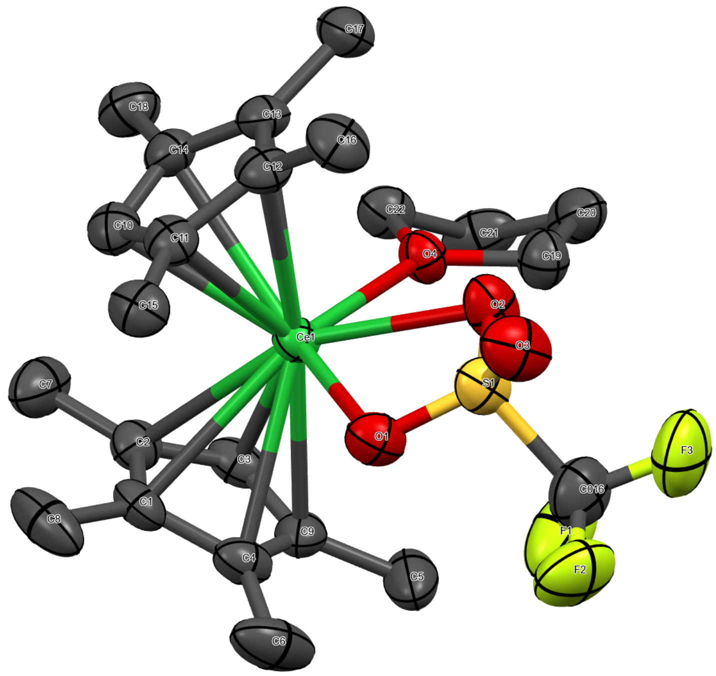


Figure S125. ORTEP diagram of **5-Ce**. Ellipsoids shown at 50% probability, lattice solvent, disorder and hydrogen atoms have been omitted for clarity.

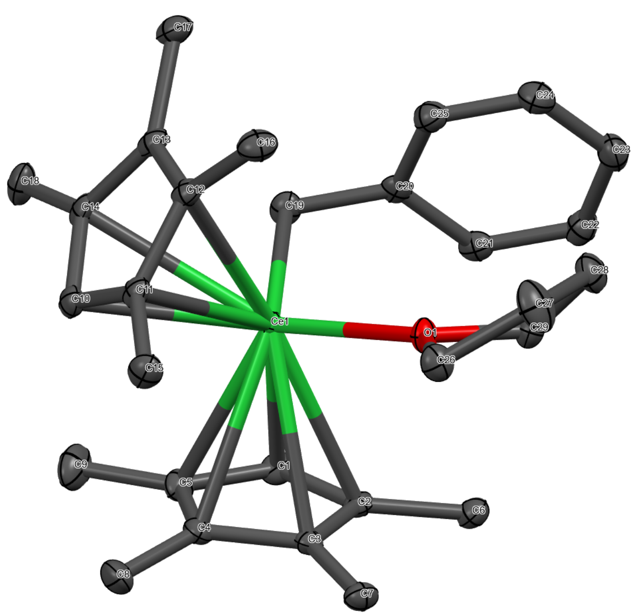


Figure S126. ORTEP diagram of **6-Ce**. Ellipsoids shown at 50% probability, lattice solvent, disorder and hydrogen atoms have been omitted for clarity.

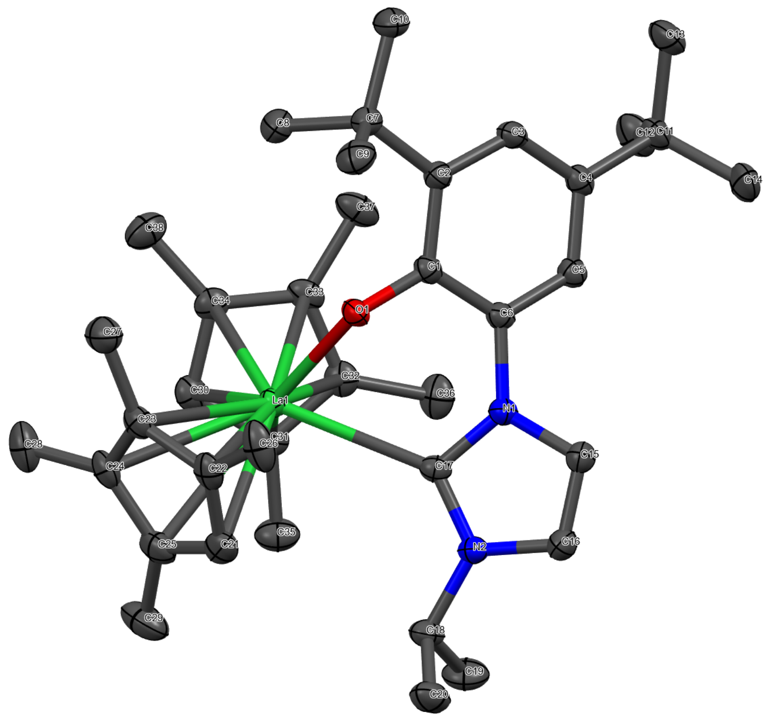


Figure S127. ORTEP diagram of **1-La**. Ellipsoids shown at 50% probability, lattice solvent, disorder and hydrogen atoms have been omitted for clarity.

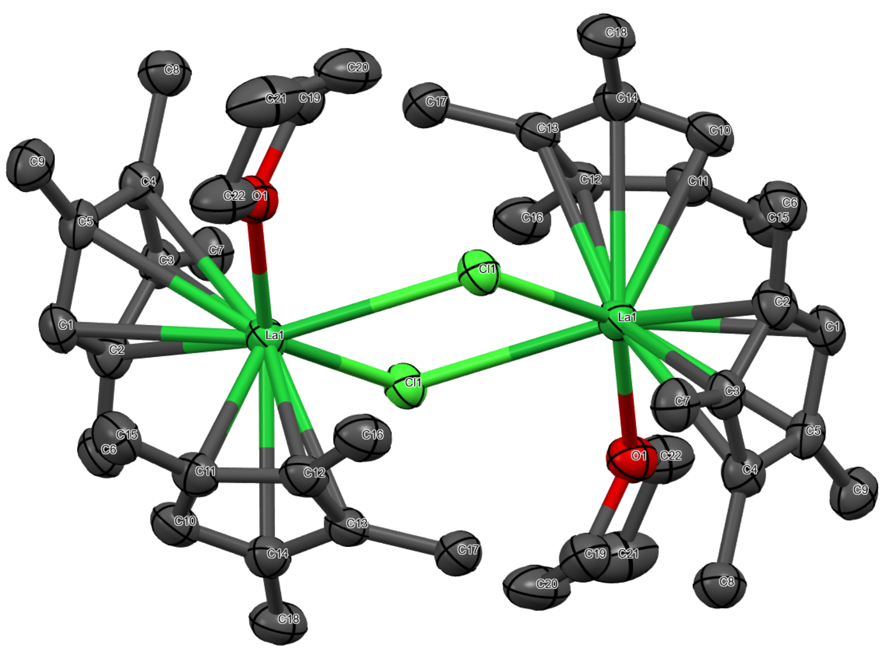


Figure S128. ORTEP diagram of **3-La**. Ellipsoids shown at 50% probability, lattice solvent, disorder and hydrogen atoms have been omitted for clarity.

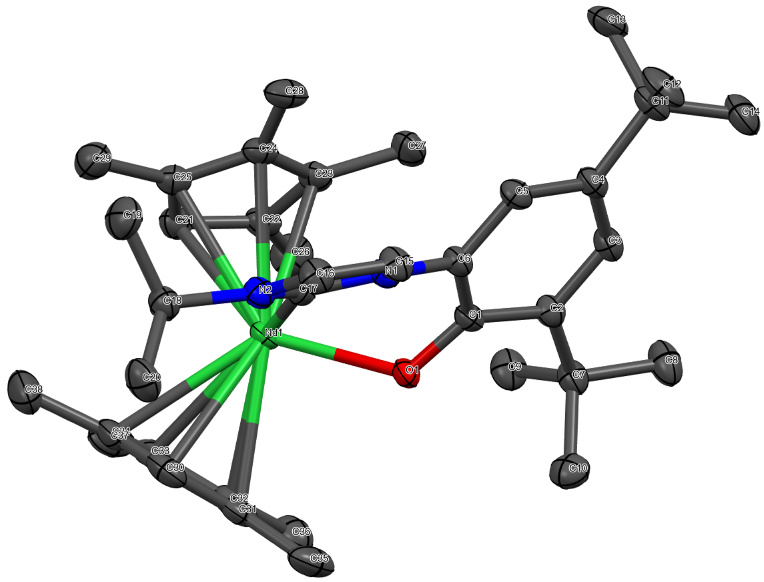


Figure S129. ORTEP diagram of **1-Nd**. Ellipsoids shown at 50% probability, lattice solvent, disorder and hydrogen atoms have been omitted for clarity.

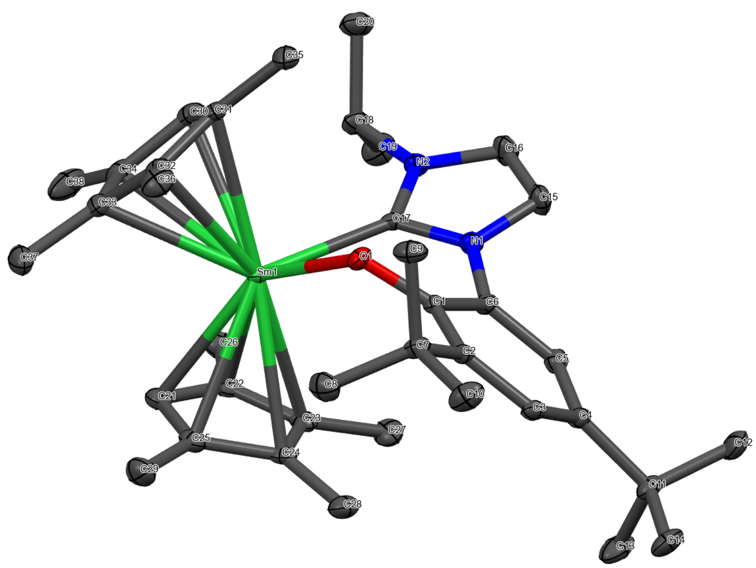


Figure S130. ORTEP diagram of **1-Sm**. Ellipsoids shown at 50% probability, lattice solvent, disorder and hydrogen atoms have been omitted for clarity.

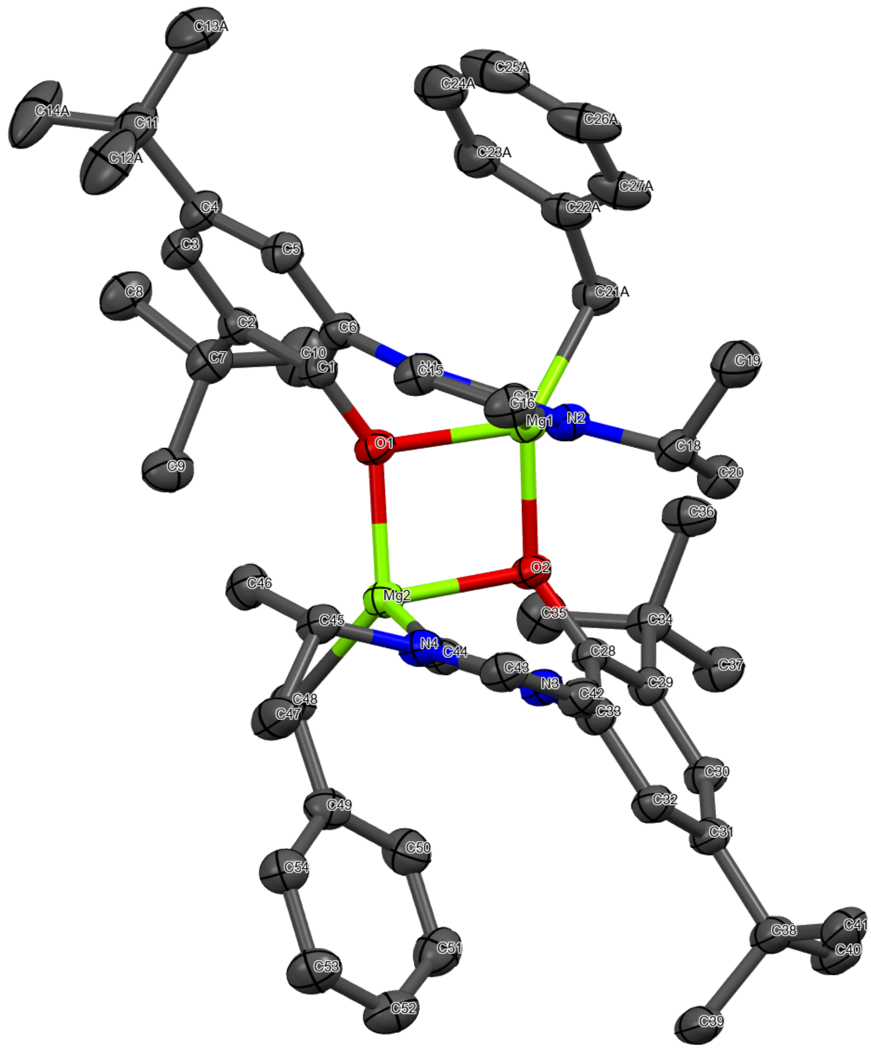


Figure 131. ORTEP diagram of **7-Mg**. Ellipsoids shown at 50% probability, lattice solvent, disorder and hydrogen atoms have been omitted for clarity.

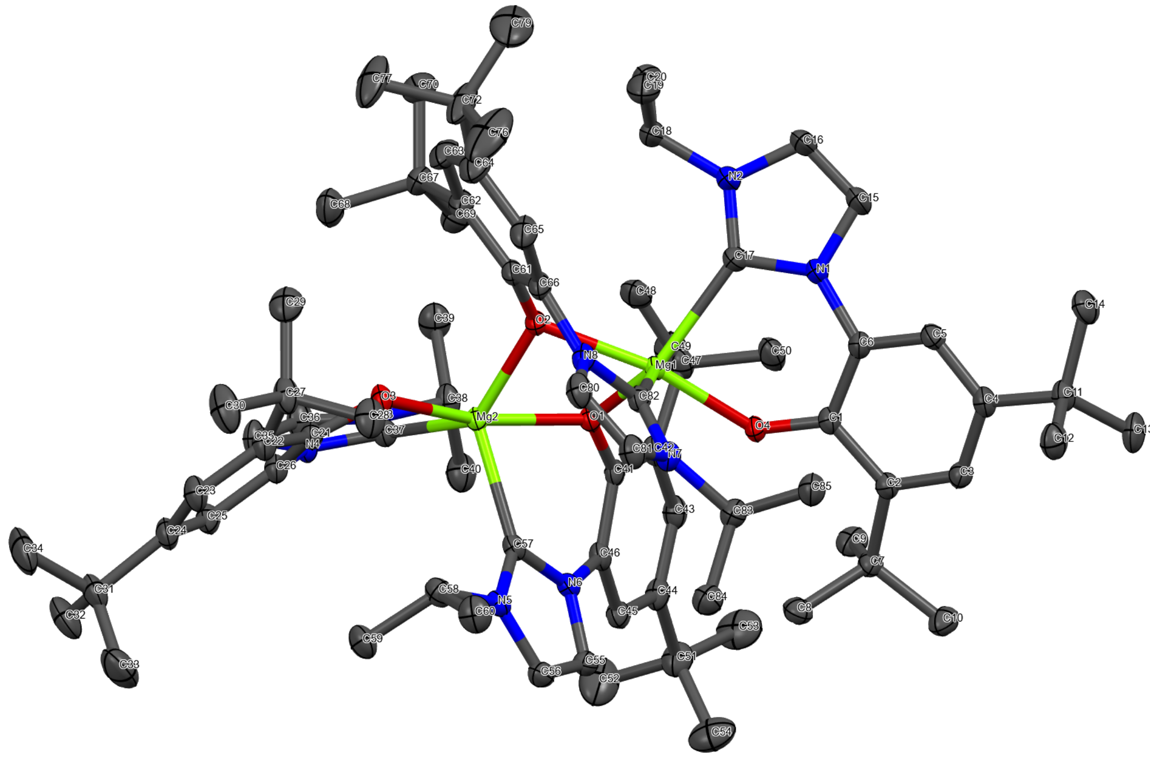


Figure S132. ORTEP diagram of **8-Mg**. Ellipsoids shown at 50% probability, lattice solvent, disorder and hydrogen atoms have been omitted for clarity.

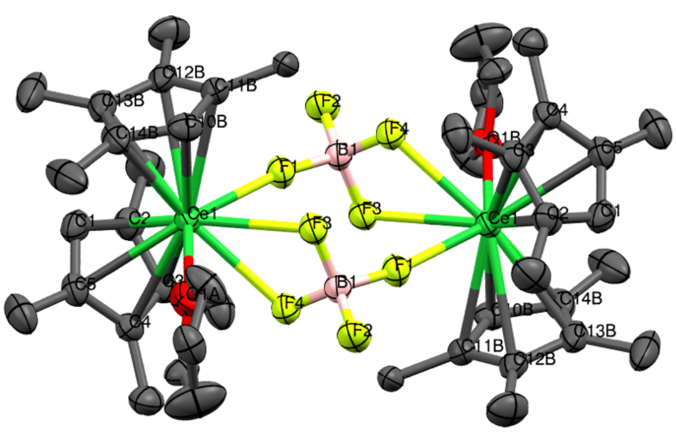


Figure S133. ORTEP diagram of $[(Cp^{Me4})_2Ce(BF_4)(THF)]_2$. Ellipsoids shown at 50% probability, lattice solvent, disorder and hydrogen atoms have been omitted for clarity.

S9.2 Crystallographic data tables

Table S7. Crystal data and structure refinement for **1-Ce**, **3-Ce**, **4-Ce**.

	1-Ce	**3-Ce**	**4-Ce**
Empirical formula	$C_{38}H_{55}CeN_2O$	$C_{36}H_{52}Ce_2Cl_2$	$C_{33}H_{49}CeO$
Formula weight	1391.91	417.96	601.84
Temperature/K	293(2)	100	100.00(10)
Crystal system	monoclinic	monoclinic	triclinic
Space group	$P2_1/n$	$P2_1/n$	P-1
a/Å	10.66730(10)	8.5165(4)	9.63360(10)
b/Å	17.46410(10)	10.4652(4)	10.07670(10)
c/Å	19.30400(10)	19.4321(8)	16.3047(2)
α/°	90	90	93.2430(10)
β/°	89.9070(10)	92.0320(10)	90.3960(10)
γ/°	90	90	107.6780(10)
Volume/$Å^3$	3596.23(4)	1730.83(13)	1505.14(3)
Z	4	2	2
$\rho_{calc}g/cm^3$	1.285	1.604	1.328
μ/mm^{-1}	1.295	2.943	1.534
F(000)	1452.0	836.0	626.0
Crystal size/mm^3	0.351 × 0.251 × 0.164	0.07 × 0.055 × 0.03	0.21 × 0.1 × 0.07
Radiation	Mo Kα (λ = 0.71073)	synchrotron (λ = 0.7288)	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	6.748 to 52.744	4.302 to 55.738	4.25 to 62.182
Index ranges	-13 ≤ h ≤ 13, -21 ≤ k ≤ 21, -24 ≤ l ≤ 24	-10 ≤ h ≤ 10, -13 ≤ k ≤ 13, -24 ≤ l ≤ 24	-13 ≤ h ≤ 13, -14 ≤ k ≤ 14, -22 ≤ l ≤ 23
Reflections collected	72839	22581	67296
Independent reflections	7352 [R_{int} = 0.0362, R_{sigma} = 0.0180]	3819 [R_{int} = 0.1107, R_{sigma} = 0.0729]	8291 [R_{int} = 0.0451, R_{sigma} = 0.0277]
Data/restraints/parameters	7352/0/395	3819/0/190	8291/0/331
Goodness-of-fit on F^2	1.061	1.068	1.052
Final R indexes [I>=2σ (I)]	R_1 = 0.0190, wR_2 = 0.0434	R_1 = 0.0490, wR_2 = 0.1212	R_1 = 0.0205, wR_2 = 0.0438
Final R indexes [all data]	R_1 = 0.0232, wR_2 = 0.0453	R_1 = 0.0514, wR_2 = 0.1239	R_1 = 0.0240, wR_2 = 0.0447
Largest diff. peak/hole / e $Å^{-3}$	0.34/-0.34	1.16/-1.38	0.91/-0.50

Table S7 Continued. Crystal data and structure refinement for **5-Ce**, **6-Ce**, **1-La**.

	5-Ce	**6-Ce**	**1-La**
Empirical formula	$C_{23}H_{34}CeF_3OS$	$C_{29}H_{41}CeO$	$C_{45}H_{63}LaN_2O$
Formula weight	150.92	545.74	786.88
Temperature/K	99.99(11)	293(2)	100.01(10)
Crystal system	monoclinic	monoclinic	monoclinic
Space group	Ia	$P2_1/c$	$P2_1/c$
a/Å	17.5622(3)	16.2557(2)	13.30050(10)
b/Å	9.40990(10)	8.82900(10)	22.02780(10)
c/Å	16.2878(3)	18.3743(2)	15.63480(10)
α/°	90	90	90
β/°	108.821(2)	105.1410(10)	113.5670(10)
γ/°	90	90	90
Volume/Å^3	2547.78(8)	2545.56(5)	4198.63(5)
Z	4	4	4
ρ_{calc}g/cm^3	1.574	1.424	1.245
μ/mm^{-1}	1.916	1.806	8.101
F(000)	1220.0	1124.0	1648.0
Crystal size/mm^3	0.374 × 0.263 × 0.203	0.306 × 0.217 × 0.096	0.154 × 0.133 × 0.093
Radiation	Mo Kα (λ = 0.71073)	MoKα (λ = 0.71073)	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	4.9 to 61.74	4.594 to 61.904	7.252 to 154.87
Index ranges	-22 ≤ h ≤ 24, -13 ≤ k ≤ 13, -23 ≤ l ≤ 22	-22 ≤ h ≤ 22, -12 ≤ k ≤ 12, -24 ≤ l ≤ 26	-16 ≤ h ≤ 15, -27 ≤ k ≤ 27, -19 ≤ l ≤ 19
Reflections collected	28412	57712	163711
Independent reflections	6338 [R_{int} = 0.0752, R_{sigma} = 0.0465]	7165 [R_{int} = 0.0350, R_{sigma} = 0.0217]	8870 [R_{int} = 0.0535, R_{sigma} = 0.0171]
Data/restraints/parameters	6338/2/297	7165/0/288	8870/289/524
Goodness-of-fit on F^2	0.928	1.057	1.069
Final R indexes [I>=2σ (I)]	R_1 = 0.0413, wR_2 = 0.1179	R_1 = 0.0183, wR_2 = 0.0399	R_1 = 0.0214, wR_2 = 0.0545
Final R indexes [all data]	R_1 = 0.0432, wR_2 = 0.1200	R_1 = 0.0216, wR_2 = 0.0407	R_1 = 0.0226, wR_2 = 0.0551
Largest diff. peak/hole / e Å^{-3}	0.91/-1.34	0.49/-0.36	0.43/-0.53

Table S7 Continued. Crystal data and structure refinement for **3-La**, **1-Nd**, **1-Sm**.

	3-La	**1-Nd**	**1-Sm**
Empirical formula	$C_{44}H_{68}Cl_2LaO_2$	$C_{45}H_{63}N_2NdO$	$C_{38}H_{55}N_2OSm$
Formula weight	244.42	792.21	706.19
Temperature/K	99.99(14)	100.00(13)	100.00(11)
Crystal system	monoclinic	monoclinic	monoclinic
Space group	$P2_1/n$	$P2_1/c$	$P2_1/n$
a/Å	11.3760(4)	13.1816(2)	10.68690(5)
b/Å	15.3980(7)	22.1050(2)	17.26346(8)
c/Å	12.4103(4)	15.5529(2)	19.16251(8)
α/°	90	90	90
β/°	91.155(3)	112.9380(10)	90.4636(4)
γ/°	90	90	90
Volume/Å^3	2173.44(14)	4173.45(10)	3535.23(3)
Z	2	4	4
ρ_{calc}g/cm^3	1.494	1.261	1.327
μ/mm^{-1}	16.351	9.732	12.684
F(000)	992.0	1660.0	1468.0
Crystal size/mm^3	0.104 × 0.07 × 0.031	0.096 × 0.08 × 0.027	0.2 × 0.11 × 0.07
Radiation	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	9.154 to 148.996	7.282 to 155.594	6.892 to 148.996
Index ranges	-14 ≤ h ≤ 14, -19 ≤ k ≤ 18, -15 ≤ l ≤ 15	-16 ≤ h ≤ 16, -27 ≤ k ≤ 26, -18 ≤ l ≤ 19	-13 ≤ h ≤ 13, -21 ≤ k ≤ 20, -23 ≤ l ≤ 23
Reflections collected	40521	85278	136174
Independent reflections	4453 [R_{int} = 0.1585, R_{sigma} = 0.0559]	8821 [R_{int} = 0.0540, R_{sigma} = 0.0253]	7240 [R_{int} = 0.0781, R_{sigma} = 0.0211]
Data/restraints/parameters	4453/0/234	8821/105/524	7240/0/395
Goodness-of-fit on F^2	1.131	1.103	1.055
Final R indexes [I>=2σ (I)]	R_1 = 0.0559, wR_2 = 0.1350	R_1 = 0.0334, wR_2 = 0.0779	R_1 = 0.0225, wR_2 = 0.0559
Final R indexes [all data]	R_1 = 0.0712, wR_2 = 0.1428	R_1 = 0.0369, wR_2 = 0.0795	R_1 = 0.0232, wR_2 = 0.0563
Largest diff. peak/hole / e Å^{-3}	1.06/-1.55	0.59/-1.31	0.53/-0.96

Table S7 Continued. Crystal data and structure refinement for **7-Mg**, **8-Mg** and $[(Cp^{Me4})_2Ce(BF_4)(THF)]_2$.

	7-Mg	**8-Mg**	$\mathbf{[(Cp^{Me4})_2Ce(BF_4)(THF)]_2}$
Empirical formula	$C_{57.5}H_{76}Mg_2N_4O_2$	$C_{92}H_{142}Mg_2N_8O_4$	$C_{51}H_{76}B_2Ce_2F_8O_2$
Formula weight	903.84	1472.75	1174.97
Temperature/K	99.99(13)	100.00(11)	100.01 (11)
Crystal system	monoclinic	triclinic	triclinic
Space group	$P2_1/n$	P-1	P-1
a/Å	13.1713(2)	13.91760(10)	8.8809(2)
b/Å	18.0503(2)	17.0140(3)	10.2164(2)
c/Å	23.2076(4)	19.2571(3)	15.0376(3)
α/°	90	99.0740(10)	94.808(2)
β/°	104.996(2)	98.3570(10)	103.253(2)
γ/°	90	91.4750(10)	105.252(2)
Volume/Å^3	5329.61(14)	4449.56(11)	1266.08(5)
Z	4	2	1
ρ_{calc}g/cm^3	1.126	1.099	1.541
μ/mm^{-1}	0.731	0.638	1.842
F(000)	1956.0	1612.0	596.0
Crystal size/mm^3	0.2 × 0.18 × 0.14	0.164 × 0.149 × 0.09	0.312 × 0.209 × 0.188
Radiation	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	6.286 to 154.828	5.266 to 148.996	4.182 to 62.112
Index ranges	-16 ≤ h ≤ 16, -22 ≤ k ≤ 15, -29 ≤ l ≤ 29	-17 ≤ h ≤ 15, -21 ≤ k ≤ 21, -23 ≤ l ≤ 24	-12 ≤ h ≤ 12, -13 ≤ k ≤ 14, -19 ≤ l ≤ 20
Reflections collected	104258	91809	268653
Independent reflections	11176 [R_{int} = 0.0709, R_{sigma} = 0.0316]	18131 [R_{int} = 0.0443, R_{sigma} = 0.0330]	6635 [R_{int} = 0.0920, R_{sigma} = 0.0632]
Data/restraints/parameters	11176/524/699	18131/284/1077	6635/646/454
Goodness-of-fit on F^2	1.022	1.045	0.978
Final R indexes [I>=2σ (I)]	R_1 = 0.0598, wR_2 = 0.1611	R_1 = 0.0494, wR_2 = 0.1188	R_1 = 0.0337, wR_2 = 0.0712
Final R indexes [all data]	R_1 = 0.0708, wR_2 = 0.1696	R_1 = 0.0585, wR_2 = 0.1238	R_1 = 0.0396, wR_2 = 0.0746
Largest diff. peak/hole / e Å^{-3}	0.84/-0.41	0.50/-0.34	0.60/-1.01

S10 Computational Details

All the structures reported in this study were fully optimized with the Becke's 3-parameter hybrid functional[18] combined with the non-local correlation functional provided by Perdew/Wang (denoted as B3PW91).[19] The basis set used for lanthanum and cerium atom were the Stuttgart-Dresden small core ECP in combination with its adapted basis set.[20] For the Mg atom a 6-311++G(d,p) basis set was used whereas for all the other atoms a 6-31G(d,p) basis set was set.[21] In all computations no constraints were imposed on the geometry. All stationary points have been identified for minimum (number of imaginary frequencies Nimag=0). The vibrational modes and the corresponding frequencies are based on a harmonic force field. Gibbs Free energies were obtained at T=298.15K within the harmonic approximation. GAUSSIAN09 program suite was used in all calculations.[22] The UV-Visible spectra were simulated at the TDDFT level using the same functional.

The computational strategy and especially the use of the B3PW91 functional was chosen because of its long history in lanthanide computational chemistry. See, for example, *Do f electrons play a role in the lanthanide-ligand bonds? A DFT study of Ln(NR2)3; R = H, SiH3.*[23] This methodology has also previously been successfully applied in C-F activation reactions of both alkanes and alkenes.[24,25]

S10.1 Atomic Orbital Compositions

Table S8. Atomic orbital composition of **1-Ce** LUMO+1.

Orbital: 170 Energy(a.u.): -0.01306916 Occ: 0.00000000 Type: Alpha

Atom	1(Ce) :	80.486521%	Atom	26(C) :	0.702710%	Atom	51(H) :	0.026905%	Atom	76(H) :	0.000981%
Atom	2(O) :	0.767145%	Atom	27(H) :	0.490512%	Atom	52(C) :	0.008751%	Atom	77(H) :	0.001556%
Atom	3(N) :	0.659114%	Atom	28(C) :	0.224297%	Atom	53(H) :	0.001165%	Atom	78(C) :	0.000613%
Atom	4(N) :	0.593343%	Atom	29(H) :	0.033465%	Atom	54(H) :	0.001267%	Atom	79(H) :	0.000099%
Atom	5(C) :	1.245663%	Atom	30(H) :	0.233137%	Atom	55(H) :	0.000557%	Atom	80(H) :	0.000197%
Atom	6(C) :	0.514240%	Atom	31(H) :	0.045209%	Atom	56(C) :	0.116490%	Atom	81(H) :	0.000085%
Atom	7(C) :	0.542150%	Atom	32(C) :	0.772335%	Atom	57(H) :	0.011128%	Atom	82(C) :	0.227500%
Atom	8(C) :	0.241415%	Atom	33(H) :	0.136632%	Atom	58(C) :	0.086611%	Atom	83(H) :	0.014968%
Atom	9(C) :	1.617072%	Atom	34(H) :	0.801274%	Atom	59(H) :	0.012194%	Atom	84(H) :	0.140785%
Atom	10(C) :	0.344298%	Atom	35(H) :	0.037615%	Atom	60(H) :	0.058862%	Atom	85(H) :	0.082953%
Atom	11(C) :	0.396588%	Atom	36(C) :	0.049397%	Atom	61(H) :	0.033495%	Atom	86(C) :	0.111446%
Atom	12(H) :	0.057794%	Atom	37(H) :	0.004426%	Atom	62(C) :	0.262270%	Atom	87(H) :	0.035052%
Atom	13(C) :	1.009403%	Atom	38(H) :	0.011096%	Atom	63(H) :	0.018164%	Atom	88(H) :	0.106065%
Atom	14(H) :	0.067040%	Atom	39(H) :	0.035610%	Atom	64(H) :	0.311691%	Atom	89(H) :	0.007843%
Atom	15(C) :	1.269144%	Atom	40(C) :	0.025513%	Atom	65(H) :	0.055524%	Atom	90(C) :	0.008234%
Atom	16(C) :	2.279342%	Atom	41(C) :	0.011697%	Atom	66(C) :	0.096658%	Atom	91(H) :	0.000420%
Atom	17(C) :	0.304977%	Atom	42(C) :	0.079666%	Atom	67(H) :	0.039190%	Atom	92(H) :	0.004256%
Atom	18(C) :	0.355731%	Atom	43(H) :	0.019720%	Atom	68(H) :	0.008397%	Atom	93(H) :	0.000222%
Atom	19(C) :	0.413715%	Atom	44(H) :	0.023290%	Atom	69(H) :	0.007724%	Atom	94(C) :	0.008339%
Atom	20(C) :	0.041871%	Atom	45(H) :	0.023605%	Atom	70(C) :	0.167600%	Atom	95(H) :	0.000407%
Atom	21(H) :	0.010021%	Atom	46(C) :	0.136056%	Atom	71(H) :	0.010707%	Atom	96(H) :	0.002005%
Atom	22(C) :	0.126799%	Atom	47(H) :	0.010299%	Atom	72(H) :	0.010239%	Atom	97(H) :	0.000461%
Atom	23(H) :	0.004141%	Atom	48(H) :	0.043220%	Atom	73(H) :	0.095720%			
Atom	24(C) :	0.060878%	Atom	49(H) :	0.060438%	Atom	74(C) :	0.012501%			
Atom	25(C) :	0.143835%	Atom	50(C) :	0.222430%	Atom	75(H) :	0.005814%			

Table S9. Atomic orbital composition of **1-La** HOMO.

Orbital: 167 Energy(a.u.): -0.18025753 Occ: 2.00000000 Type: Alpha&Beta

Atom	1(O) :	5.815632%	Atom	26(H) :	0.047942%	Atom	51(C) :	0.244483%	Atom	76(H) :	0.010591%
Atom	2(N) :	0.426904%	Atom	27(C) :	0.565444%	Atom	52(H) :	0.099074%	Atom	77(C) :	0.034744%
Atom	3(N) :	0.083989%	Atom	28(H) :	0.151739%	Atom	53(H) :	0.027834%	Atom	78(H) :	0.011502%
Atom	4(C) :	9.832815%	Atom	29(H) :	0.352462%	Atom	54(H) :	0.031353%	Atom	79(H) :	0.002170%
Atom	5(C) :	7.166953%	Atom	30(H) :	0.088810%	Atom	55(C) :	0.172370%	Atom	80(H) :	0.010346%
Atom	6(C) :	2.228082%	Atom	31(C) :	1.040018%	Atom	56(H) :	0.017066%	Atom	81(C) :	1.729080%
Atom	7(C) :	2.584318%	Atom	32(H) :	0.331449%	Atom	57(C) :	0.014375%	Atom	82(H) :	0.493959%
Atom	8(C) :	0.295536%	Atom	33(H) :	0.657356%	Atom	58(H) :	0.010392%	Atom	83(H) :	1.117699%
Atom	9(C) :	2.496012%	Atom	34(H) :	0.152509%	Atom	59(H) :	0.002835%	Atom	84(H) :	0.254054%
Atom	10(C) :	4.235121%	Atom	35(C) :	0.885466%	Atom	60(H) :	0.006641%	Atom	85(C) :	0.119659%
Atom	11(H) :	0.279294%	Atom	36(H) :	0.057118%	Atom	61(C) :	1.399757%	Atom	86(H) :	0.029781%
Atom	12(C) :	1.467337%	Atom	37(H) :	0.445901%	Atom	62(H) :	0.203484%	Atom	87(H) :	0.024498%
Atom	13(H) :	0.071606%	Atom	38(H) :	0.438995%	Atom	63(H) :	0.880601%	Atom	88(H) :	0.018286%
Atom	14(C) :	4.216625%	Atom	39(C) :	0.246398%	Atom	64(H) :	0.400919%	Atom	89(C) :	0.249113%
Atom	15(C) :	6.815857%	Atom	40(C) :	0.382772%	Atom	65(C) :	0.009134%	Atom	90(H) :	0.020511%
Atom	16(C) :	11.073421%	Atom	41(C) :	0.253230%	Atom	66(H) :	0.001142%	Atom	91(H) :	0.065595%
Atom	17(C) :	6.606805%	Atom	42(H) :	0.031106%	Atom	67(H) :	0.001649%	Atom	92(H) :	0.032192%
Atom	18(C) :	2.653574%	Atom	43(H) :	0.101332%	Atom	68(H) :	0.002538%	Atom	93(C) :	0.251025%
Atom	19(C) :	1.063290%	Atom	44(H) :	0.146283%	Atom	69(C) :	0.146306%	Atom	94(H) :	0.034423%
Atom	20(H) :	0.056100%	Atom	45(C) :	1.027641%	Atom	70(H) :	0.022964%	Atom	95(H) :	0.066393%
Atom	21(C) :	0.928902%	Atom	46(H) :	0.111828%	Atom	71(H) :	0.027643%	Atom	96(H) :	0.019558%
Atom	22(H) :	0.051445%	Atom	47(H) :	0.641569%	Atom	72(H) :	0.041729%	Atom	97(La) :	6.581608%
Atom	23(C) :	2.441680%	Atom	48(H) :	0.347475%	Atom	73(C) :	0.023341%			
Atom	24(C) :	3.496737%	Atom	49(C) :	0.098350%	Atom	74(H) :	0.006157%			
Atom	25(C) :	0.028353%	Atom	50(H) :	0.007857%	Atom	75(H) :	0.001985%			

Table S10. Atomic orbital composition of **1-La** LUMO.

Orbital: 168 Energy(a.u.): -0.01300708 Occ: 0.00000000 Type: Alpha&Beta

Atom	1(O) :	1.394519%	Atom	26(H) :	0.353756%	Atom	51(C) :	0.380251%	Atom	76(H) :	0.020972%
Atom	2(N) :	7.824972%	Atom	27(C) :	0.498541%	Atom	52(H) :	0.047768%	Atom	77(C) :	0.155468%
Atom	3(N) :	6.399520%	Atom	28(H) :	0.158328%	Atom	53(H) :	0.132532%	Atom	78(H) :	0.078599%
Atom	4(C) :	0.199331%	Atom	29(H) :	0.091341%	Atom	54(H) :	0.058553%	Atom	79(H) :	0.019507%
Atom	5(C) :	0.290379%	Atom	30(H) :	0.436529%	Atom	55(C) :	1.511509%	Atom	80(H) :	0.077643%

Atom 6(C) :	0.392803%	Atom 31(C) :	0.299174%	Atom 56(H) :	0.105796%	Atom 81(C) :	0.083804%
Atom 7(C) :	6.782737%	Atom 32(H) :	0.286754%	Atom 57(C) :	0.396703%	Atom 82(H) :	0.016107%
Atom 8(C) :	19.122107%	Atom 33(H) :	0.075515%	Atom 58(H) :	0.174866%	Atom 83(H) :	0.042520%
Atom 9(C) :	0.203806%	Atom 34(H) :	0.040112%	Atom 59(H) :	0.101510%	Atom 84(H) :	0.054469%
Atom 10(C) :	0.285315%	Atom 35(C) :	0.176494%	Atom 60(H) :	0.045236%	Atom 85(C) :	0.071487%
Atom 11(H) :	0.050556%	Atom 36(H) :	0.071912%	Atom 61(C) :	0.068117%	Atom 86(H) :	0.027107%
Atom 12(C) :	0.158494%	Atom 37(H) :	0.051202%	Atom 62(H) :	0.012809%	Atom 87(H) :	0.040427%
Atom 13(H) :	0.015327%	Atom 38(H) :	0.080033%	Atom 63(H) :	0.034908%	Atom 88(H) :	0.012317%
Atom 14(C) :	0.549680%	Atom 39(C) :	0.635866%	Atom 64(H) :	0.029865%	Atom 89(C) :	0.154230%
Atom 15(C) :	0.332750%	Atom 40(C) :	0.231285%	Atom 65(C) :	0.292330%	Atom 90(H) :	0.134661%
Atom 16(C) :	0.268716%	Atom 41(C) :	0.064082%	Atom 66(H) :	0.045241%	Atom 91(H) :	0.027156%
Atom 17(C) :	0.819851%	Atom 42(H) :	0.023560%	Atom 67(H) :	0.141484%	Atom 92(H) :	0.036707%
Atom 18(C) :	2.392169%	Atom 43(H) :	0.016841%	Atom 68(H) :	0.055749%	Atom 93(C) :	0.133389%
Atom 19(C) :	8.380959%	Atom 44(H) :	0.085510%	Atom 69(C) :	0.375602%	Atom 94(H) :	0.041100%
Atom 20(H) :	1.053745%	Atom 45(C) :	0.157409%	Atom 70(H) :	0.064757%	Atom 95(H) :	0.015491%
Atom 21(C) :	7.097858%	Atom 46(H) :	0.015974%	Atom 71(H) :	0.114463%	Atom 96(H) :	0.090734%
Atom 22(H) :	0.778957%	Atom 47(H) :	0.124029%	Atom 72(H) :	0.069470%	Atom 97(La) :	10.556532%
Atom 23(C) :	6.052621%	Atom 48(H) :	0.041844%	Atom 73(C) :	0.061581%		
Atom 24(C) :	2.405474%	Atom 49(C) :	4.965394%	Atom 74(H) :	0.041922%		
Atom 25(C) :	0.778369%	Atom 50(H) :	0.727921%	Atom 75(H) :	0.006129%		

Table S11. Atomic orbital composition of **1-La** LUMO+1.

Orbital: 169 Energy(a.u.): -0.00954429 Occ: 0.00000000 Type: Alpha&Beta

Atom 1(O) :	2.222657%	Atom 26(H) :	2.749823%	Atom 51(C) :	0.041628%	Atom 76(H) :	0.018384%
Atom 2(N) :	1.301125%	Atom 27(C) :	0.270996%	Atom 52(H) :	0.043870%	Atom 77(C) :	0.007122%
Atom 3(N) :	0.931956%	Atom 28(H) :	0.082265%	Atom 53(H) :	0.007112%	Atom 78(H) :	0.004065%
Atom 4(C) :	2.651875%	Atom 29(H) :	0.111316%	Atom 54(H) :	0.014405%	Atom 79(H) :	0.000791%
Atom 5(C) :	2.171454%	Atom 30(H) :	0.124062%	Atom 55(C) :	0.235206%	Atom 80(H) :	0.001735%
Atom 6(C) :	0.851756%	Atom 31(C) :	1.537281%	Atom 56(H) :	0.024478%	Atom 81(C) :	0.433850%
Atom 7(C) :	1.071948%	Atom 32(H) :	0.707878%	Atom 57(C) :	0.285040%	Atom 82(H) :	0.054578%
Atom 8(C) :	4.526794%	Atom 33(H) :	0.883305%	Atom 58(H) :	0.100207%	Atom 83(H) :	0.071192%
Atom 9(C) :	0.796186%	Atom 34(H) :	0.274023%	Atom 59(H) :	0.161670%	Atom 84(H) :	0.469738%
Atom 10(C) :	1.917369%	Atom 35(C) :	0.329690%	Atom 60(H) :	0.076903%	Atom 85(C) :	0.216950%

Atom	11(H) :	0.620363%	Atom	36(H) :	0.068224%	Atom	61(C) :	1.115239%	Atom	86(H) :	0.214347%
Atom	12(C) :	2.178319%	Atom	37(H) :	0.120551%	Atom	62(H) :	0.150081%	Atom	87(H) :	0.050674%
Atom	13(H) :	0.311961%	Atom	38(H) :	0.175192%	Atom	63(H) :	0.666369%	Atom	88(H) :	0.034596%
Atom	14(C) :	1.222469%	Atom	39(C) :	0.112427%	Atom	64(H) :	0.598299%	Atom	89(C) :	0.053090%
Atom	15(C) :	2.835052%	Atom	40(C) :	0.094220%	Atom	65(C) :	0.232150%	Atom	90(H) :	0.006479%
Atom	16(C) :	1.062440%	Atom	41(C) :	0.209943%	Atom	66(H) :	0.081637%	Atom	91(H) :	0.021093%
Atom	17(C) :	1.683707%	Atom	42(H) :	0.114071%	Atom	67(H) :	0.054467%	Atom	92(H) :	0.007861%
Atom	18(C) :	1.544879%	Atom	43(H) :	0.042615%	Atom	68(H) :	0.063926%	Atom	93(C) :	0.054788%
Atom	19(C) :	0.273493%	Atom	44(H) :	0.057266%	Atom	69(C) :	0.595920%	Atom	94(H) :	0.012237%
Atom	20(H) :	0.052909%	Atom	45(C) :	1.033217%	Atom	70(H) :	0.088903%	Atom	95(H) :	0.015251%
Atom	21(C) :	0.665069%	Atom	46(H) :	0.157251%	Atom	71(H) :	0.070751%	Atom	96(H) :	0.006707%
Atom	22(H) :	0.071330%	Atom	47(H) :	0.479095%	Atom	72(H) :	1.360706%	Atom	97(La) :	46.979059%
Atom	23(C) :	0.364142%	Atom	48(H) :	0.659988%	Atom	73(C) :	0.053086%			
Atom	24(C) :	0.770150%	Atom	49(C) :	0.691785%	Atom	74(H) :	0.026349%			
Atom	25(C) :	1.774141%	Atom	50(H) :	0.149378%	Atom	75(H) :	0.007606%			

S10.2 Excitation energies and orbitals

S10.2.1 **1-Ce**

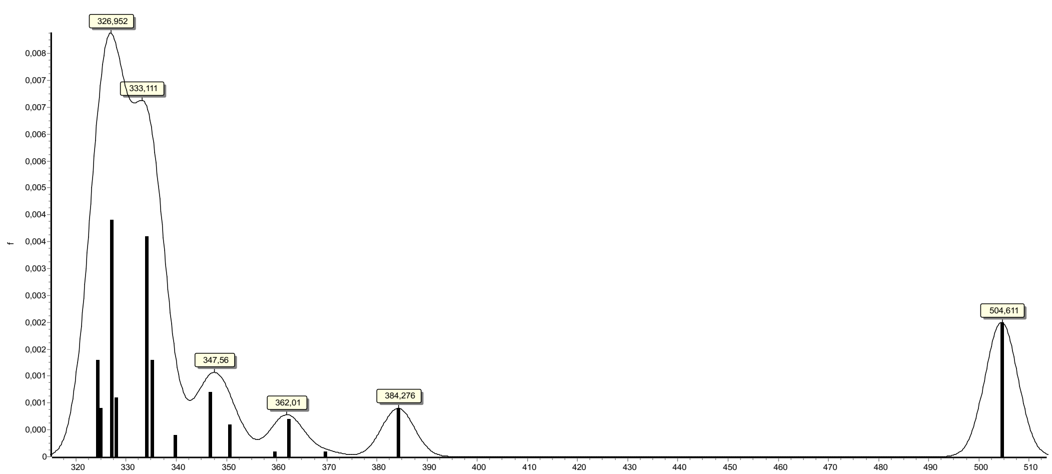


Figure S134. Computed UV-Vis spectrum of **1-Ce** using TD-DFT.

Excited State 20: ?Spin -?Sym 3.8240 eV 324.22 nm f=0.0018

163A ->171A 0.16714

164A ->171A 0.11612

166A ->169A 0.16813

166A ->170A 0.28457

166A ->171A 0.20839

166A ->172A -0.11409

166A ->174A -0.11111

167A ->169A 0.16496

167A ->170A 0.40351

167A ->171A 0.16418

167A ->172A -0.30275

167A ->173A -0.20816

167A ->174A -0.18486

165B ->168B 0.13047

166B ->168B -0.21173

167B ->168B -0.21318

167B ->169B 0.38086

167B ->170B -0.12316

Excited State 18: ?Spin -?Sym 3.7911 eV 327.04 nm f=0.0044

165A ->171A 0.12028

167A ->170A 0.24950

167A ->172A 0.51973

167A ->173A -0.10849

168A ->169A 0.11586

168A ->170A 0.16291

168A ->171A -0.13306

168A ->173A 0.26813

168A ->174A 0.23434

168A ->176A -0.37917

168A ->177A 0.11200

168A ->178A 0.16192

168A ->179A -0.16447

168A ->181A -0.12607

168A ->182A -0.16052

168A ->183A 0.11297

167B ->168B -0.13469

167B ->169B 0.20933

Excited State 16: ?Spin -?Sym 3.7126 eV 333.96 nm f=0.0041

164A ->169A -0.11337

164A ->170A 0.10118

165A ->169A 0.24929

165A ->171A -0.12914

166A ->169A -0.16606

166A ->171A -0.35772

167A ->169A -0.35650

167A ->170A -0.15837

167A ->172A -0.20857

167A ->174A 0.18640

164B ->169B -0.12331

166B ->168B 0.10911

166B ->169B 0.19163

167B ->169B 0.59378

Excited State 8: ?Spin -?Sym 3.2271 eV 384.19 nm f=0.0009

168A ->169A 0.60932

168A ->170A 0.55120

168A ->171A 0.13697

168A ->172A -0.10436

168A ->174A 0.14699

168A ->175A -0.17407

168A ->176A 0.31305

168A ->177A -0.10204

168A ->179A 0.15739

168A ->180A -0.24127

168A ->184A -0.10283

Excited State 7: ?Spin -?Sym 2.4575 eV 504.50 nm f=0.0025

168A ->169A -0.39569

168A ->170A 0.62899

168A ->171A 0.23498

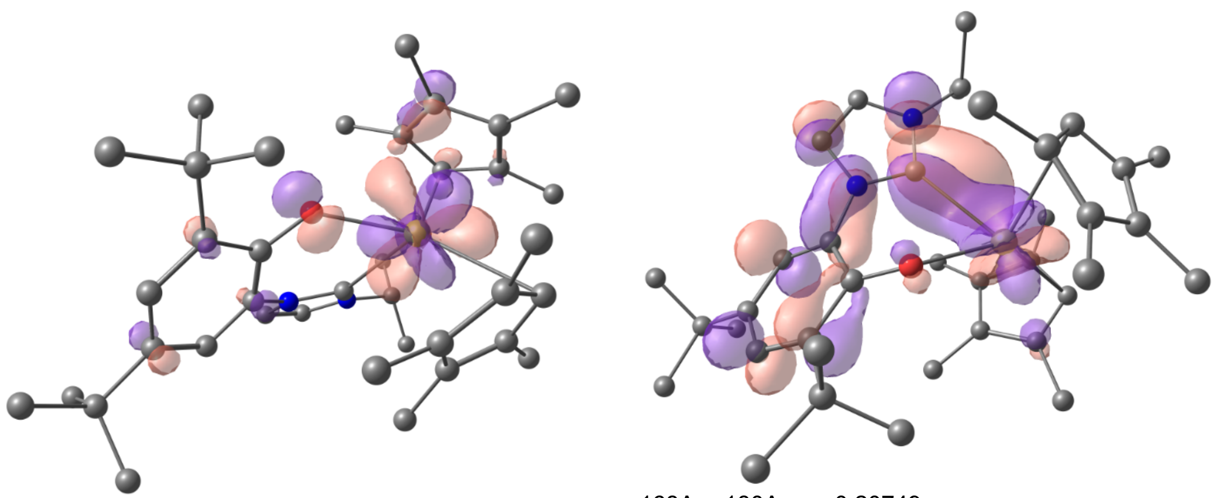
168A ->172A 0.23179

168A ->174A -0.44046

168A ->175A 0.15675

168A ->176A -0.20171

168A ->178A 0.12712



168A ->180A -0.20749

Figure S135. Depictions of the TD-DFT-calculated Alpha 168 HOMO (left) and Alpha 169 LUMO (right) orbitals of **1-Ce.**

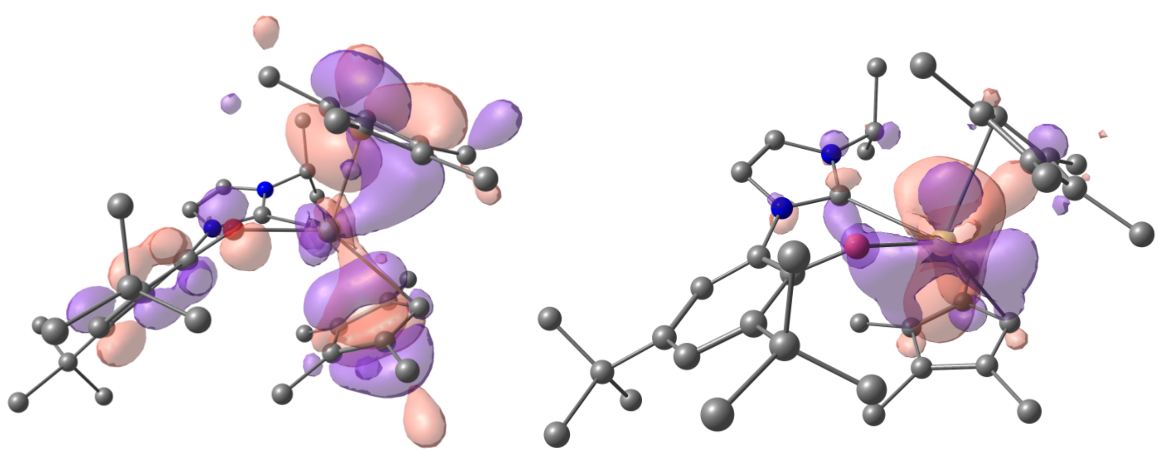


Figure S136. Depictions of the TD-DFT-calculated Alpha 167 HOMO-1 (left) and Alpha 170 LUMO+1 (right) orbitals of **1-Ce.**

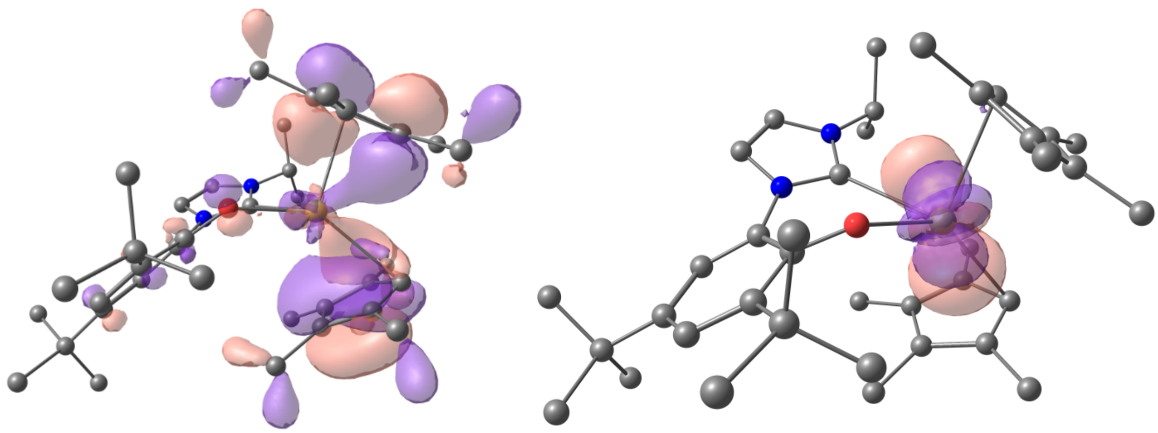


Figure S137. Depictions of the TD-DFT-calculated Alpha 166 HOMO-2 (left) and Alpha 171 LUMO+2 (right) orbitals of **1-Ce.**

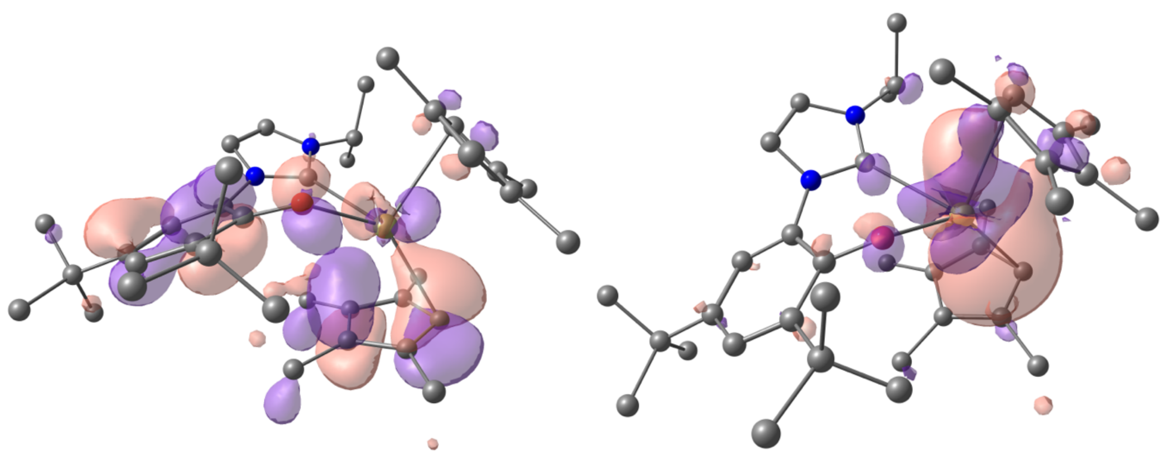


Figure S138. Depictions of the TD-DFT-calculated Alpha 165 HOMO-3 (left) and Alpha 172 LUMO+3 (right) orbitals of **1-Ce.**

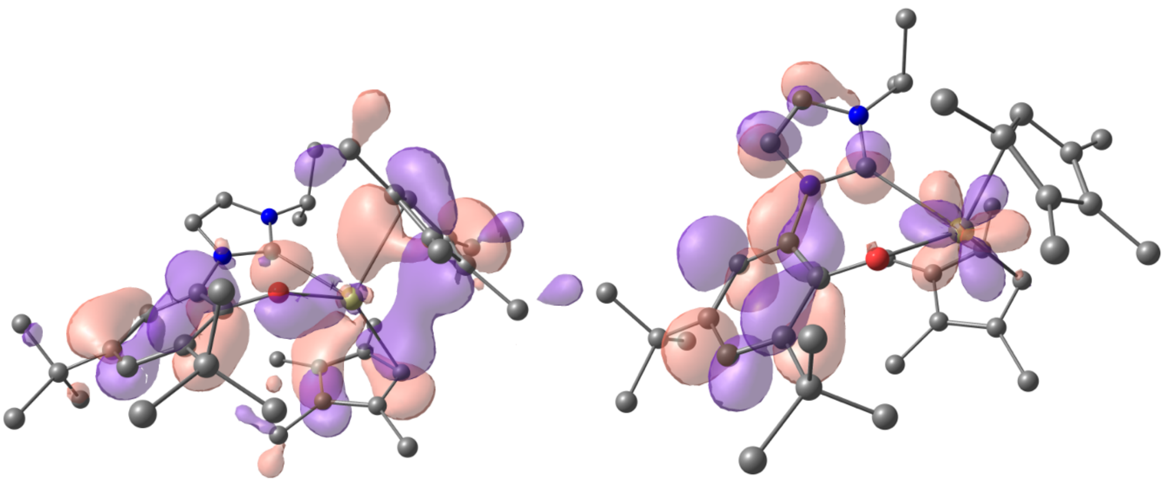


Figure S139. Depictions of the TD-DFT-calculated Alpha 164 HOMO-4 (left) and Alpha 173 LUMO+4 (right) orbitals of **1-Ce.**

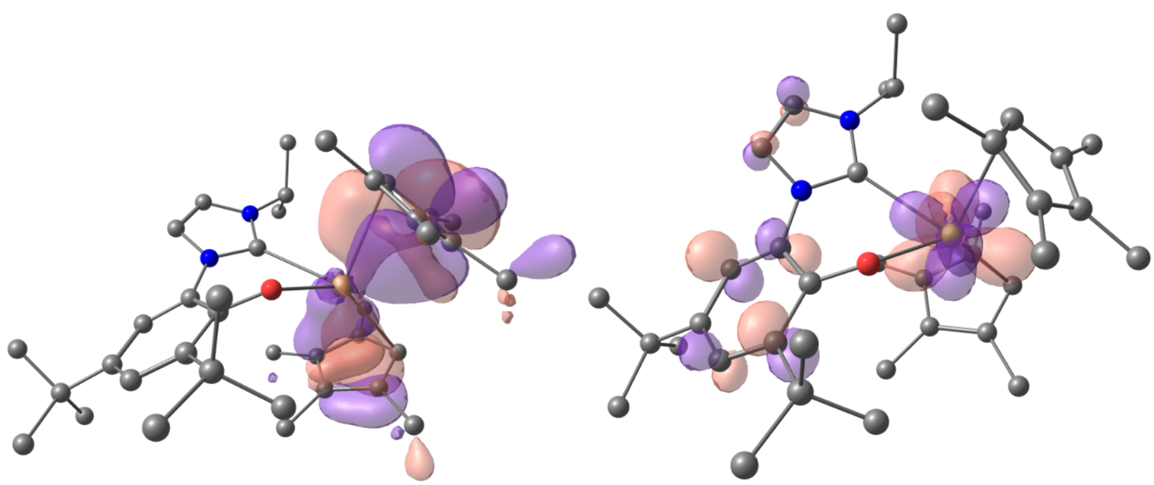


Figure S140. Depictions of the TD-DFT-calculated Alpha 163 HOMO-5 (left) and Alpha 174 LUMO+5 (right) orbitals of **1-Ce.**

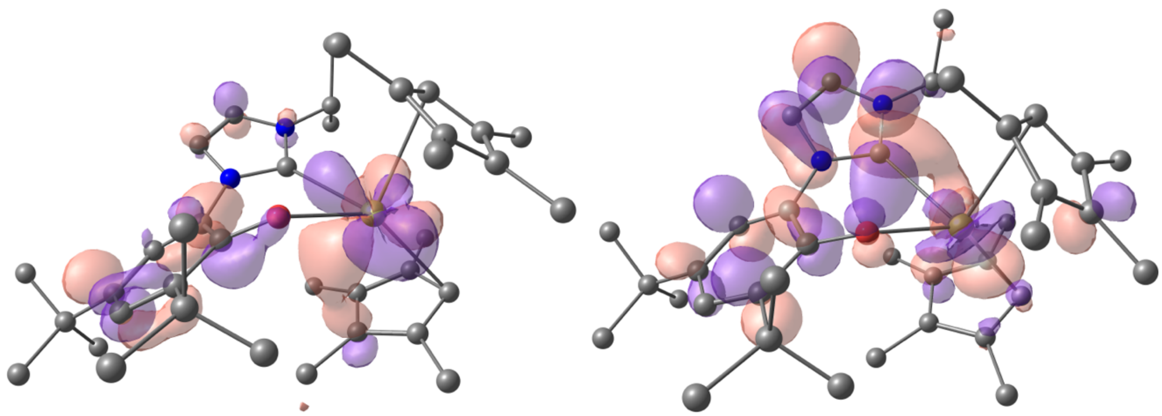


Figure S141. Depictions of the TD-DFT-calculated Alpha 175 LUMO+6 (left) and Alpha 176 LUMO+7 (right) orbitals of **1-Ce.**

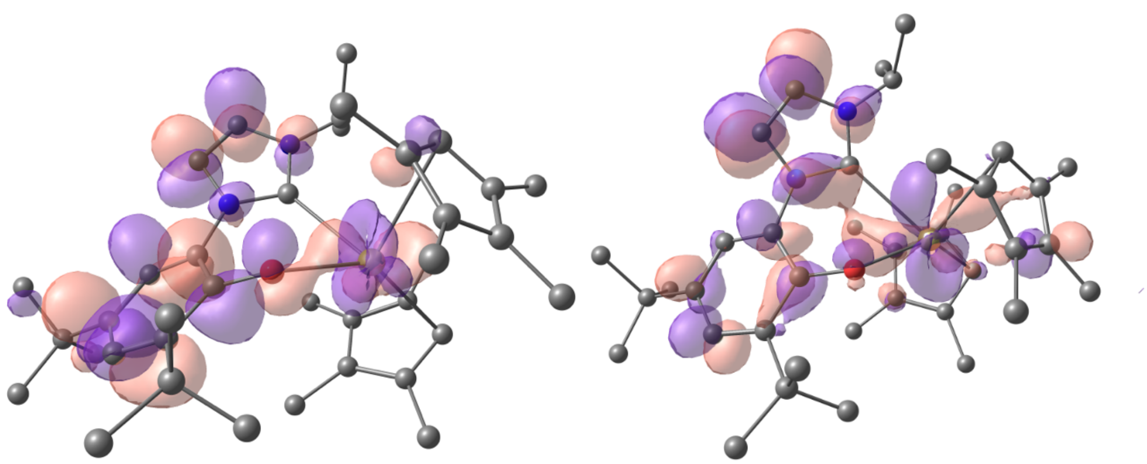


Figure S142. Depictions of the TD-DFT-calculated Alpha 177 LUMO+8 (left) and Alpha 178 LUMO+9 (right) orbitals of **1-Ce.**

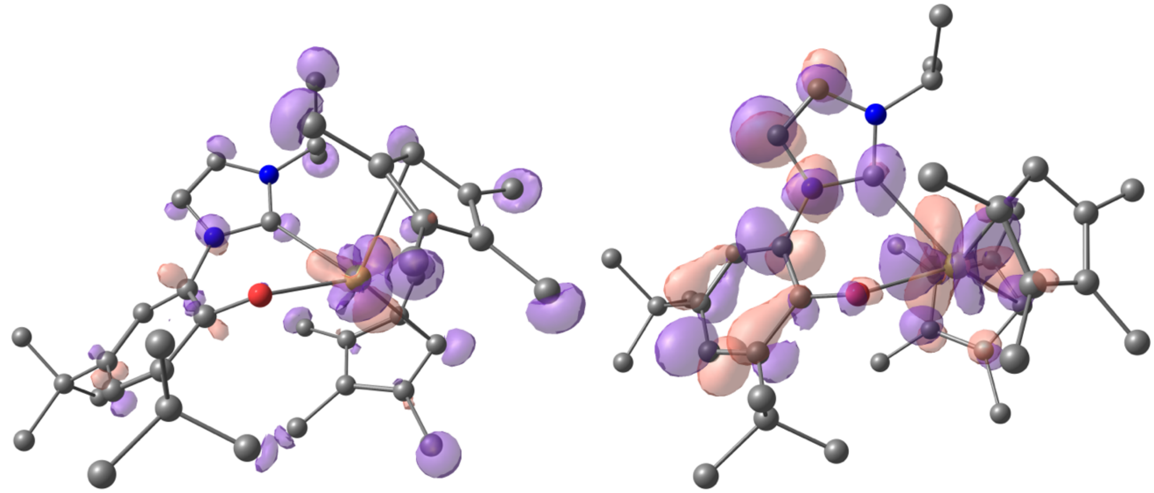


Figure S143. Depictions of the TD-DFT-calculated Alpha 179 LUMO+10 (left) and Alpha 180 LUMO+11 (right) orbitals of **1-Ce.**

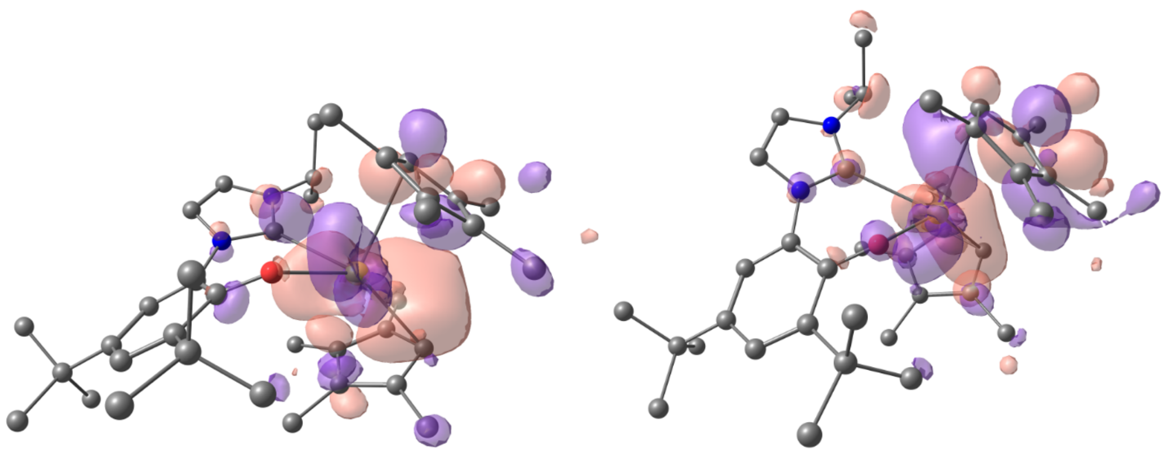


Figure S144. Depictions of the TD-DFT-calculated Alpha 181 LUMO+12 (left) and Alpha 182 LUMO+13 (right) orbitals of **1-Ce.**

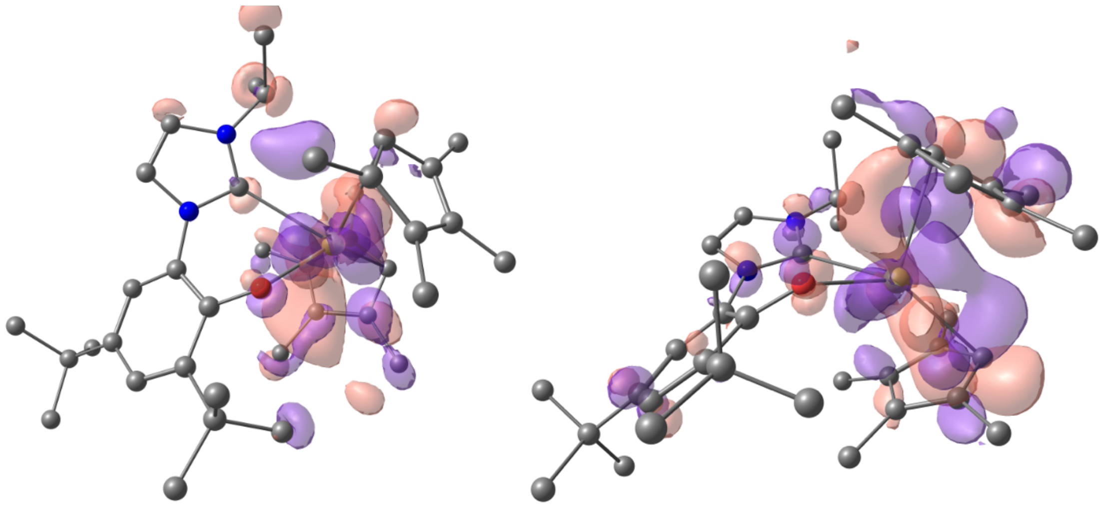


Figure S145. Depictions of the TD-DFT-calculated Alpha 183 LUMO+14 (left) and Alpha 184 LUMO+15 (right) orbitals of **1-Ce.**

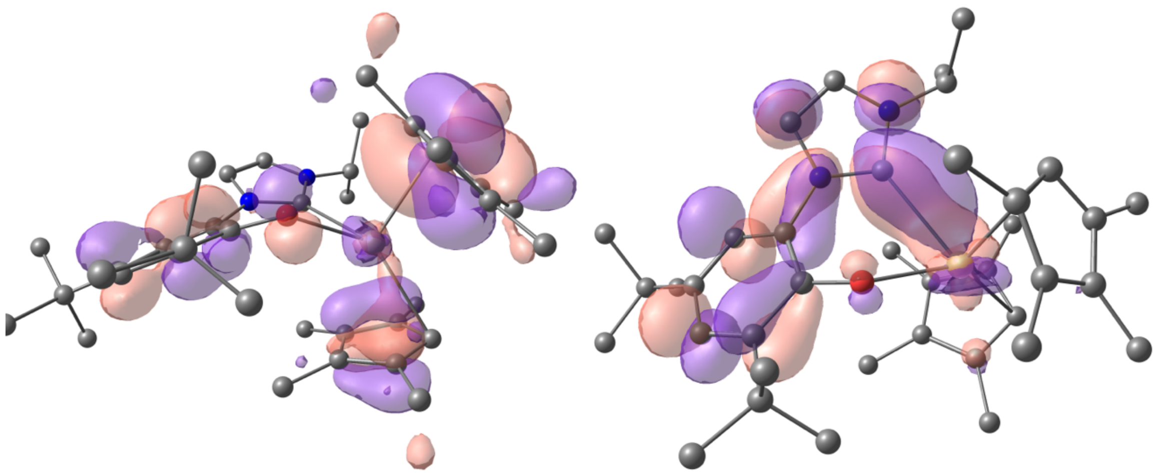


Figure S146. Depictions of the TD-DFT-calculated Beta 167 HOMO (left) and Beta 168 LUMO (right) orbitals of **1-Ce.**

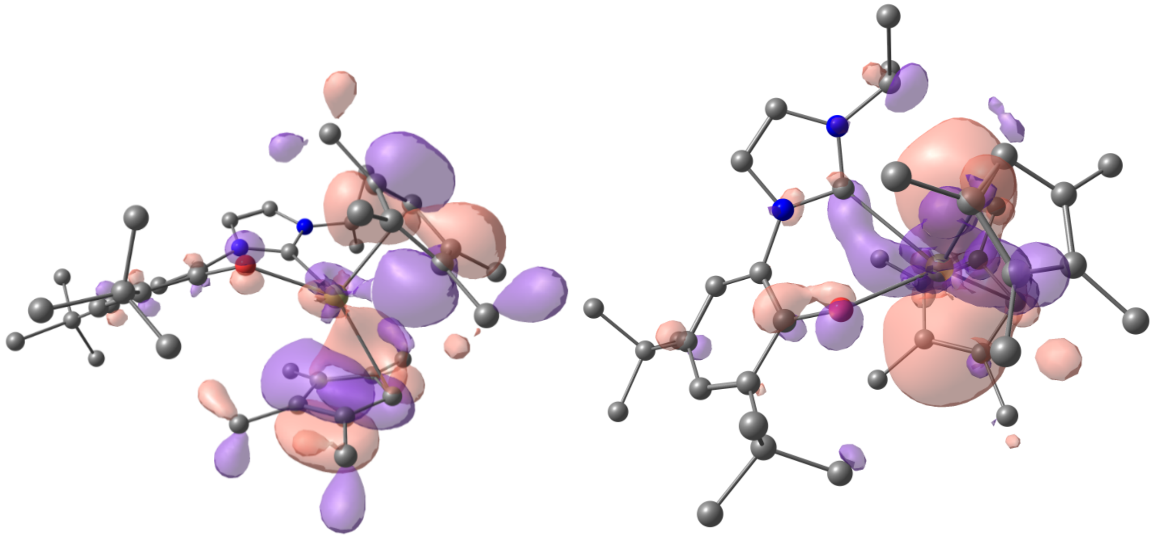


Figure S147. Depictions of the TD-DFT-calculated Beta 166 HOMO-1 (left) and Beta 169 LUMO+1 (right) orbitals of **1-Ce.**

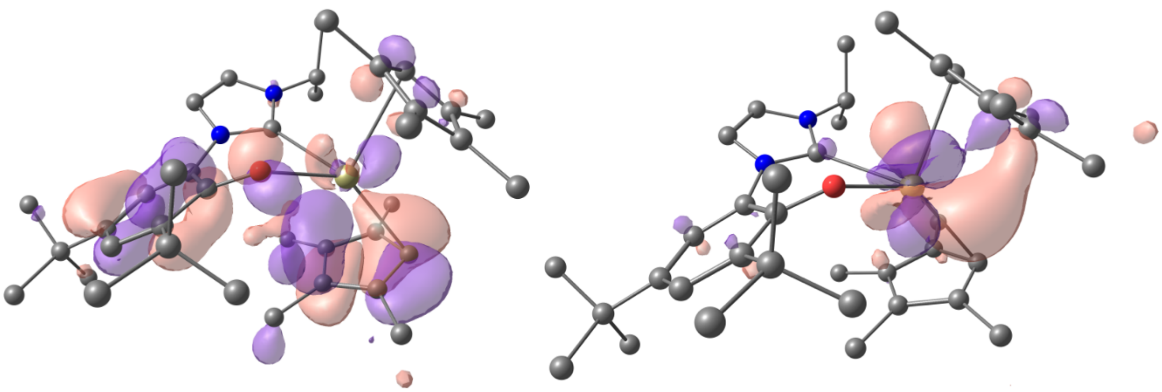


Figure S148. Depictions of the TD-DFT-calculated Beta 165 HOMO-2 (left) and Beta 170 LUMO+2 (right) orbitals of **1-Ce.**

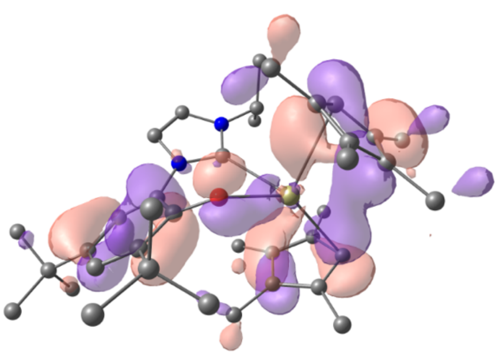


Figure S149. Depictions of the TD-DFT-calculated Beta 164 HOMO-3 orbitals of **1-Ce.**

S9.2.2 **1-La**

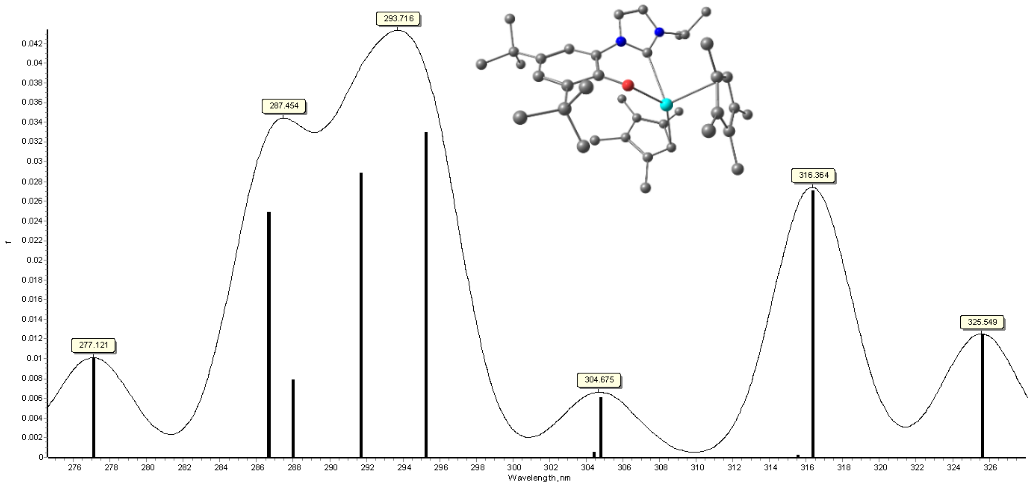


Figure S150. Computed UV-Vis spectrum of **1-La** using TD-DFT with a representation of TS1.

Excited State 1: 3.8083 eV 325.56 nm f=0.0125

167 ->168 0.24967

167 ->169 0.63192

Excited State 2: 3.9194 eV 316.34 nm f=0.0271

166 ->168 0.16778

166 ->169 0.35055

167 ->168 0.54096

167 ->169 -0.15789

167 ->170 0.10181

Excited State 3: 3.9299 eV 315.49 nm f=0.0003

166 ->168 0.14446

166 ->169 0.53723

167 ->168 -0.33182

167 ->169 0.21312

Excited State 4: 4.0684 eV 304.75 nm f=0.0061

164 ->169 -0.20393

165 ->168 0.19937

165 ->169 0.47323

166 ->168 -0.39603

Excited State 5: 4.0732 eV 304.39 nm f=0.0005

164 ->169 -0.15933

165 ->168 0.17720

165 ->169 0.31526

166 ->168 0.51268

166 ->169 -0.21637

Excited State 6: 4.1997 eV 295.22 nm f=0.0330

165 ->168 0.62632

165 ->169 -0.26908

Excited State 7: 4.2510 eV 291.66 nm f=0.0289

163 ->169 0.34726

164 ->168 0.39379

164 ->169 0.35431

165 ->169 0.19998

167 ->171 0.10110

Excited State 8: 4.3056 eV 287.96 nm f=0.0079

163 ->169 -0.20079

164 ->168 -0.34585

164 ->169 0.52202

165 ->169 0.16524

Excited State 9: 4.3256 eV 286.63 nm f=0.0249

163 ->168 0.20584

163 ->169 0.48449

164 ->168 -0.40830

Excited State 10: 4.4742 eV 277.11 nm f=0.0101

163 ->168 -0.39319

164 ->168 -0.11248

167 ->170 0.40637

167 ->171 0.31071

167 ->172 -0.15003

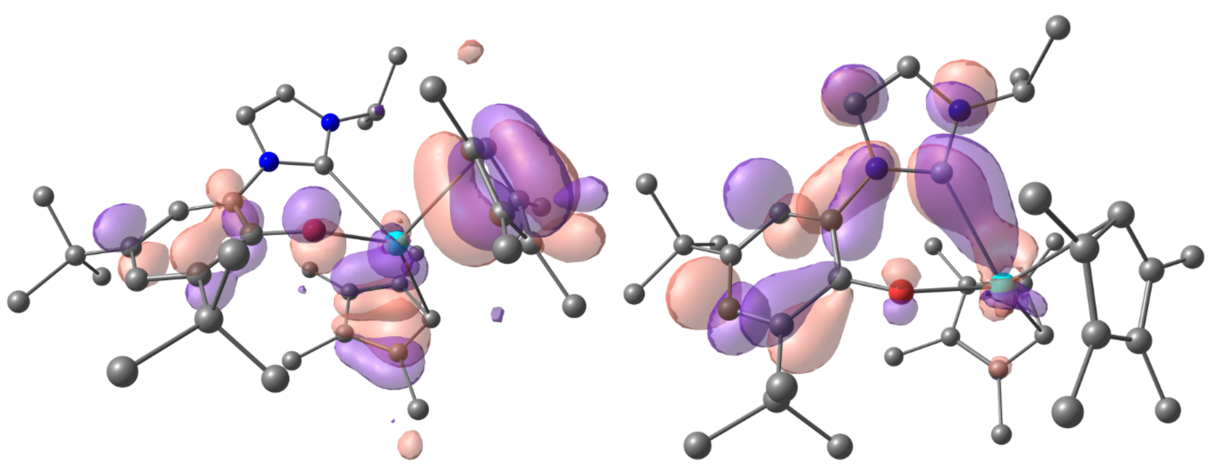


Figure S151. Depictions of the TD-DFT-calculated 167 HOMO (left) and 168 LUMO (right) orbitals of **1-La.**

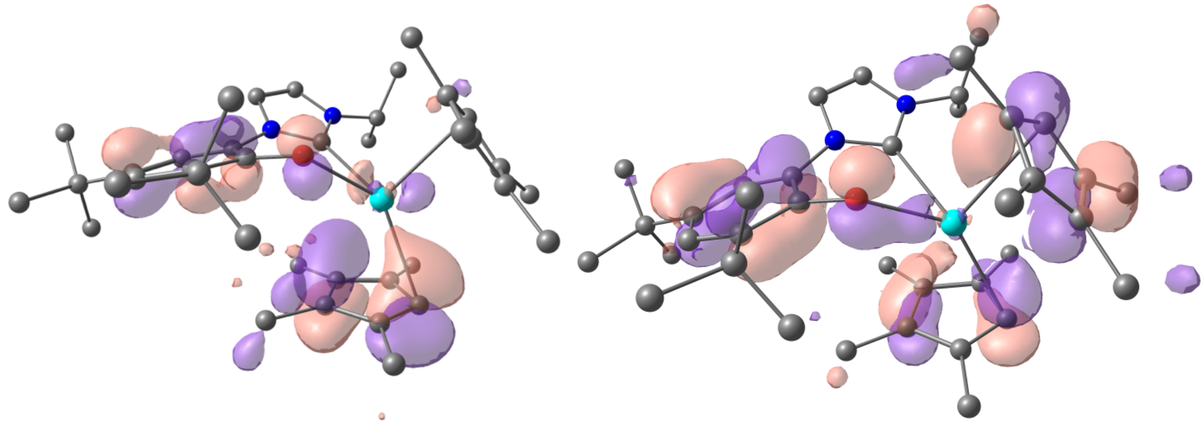


Figure S152. Depictions of the TD-DFT-calculated 165 HOMO-2 (left) and 164 HOMO-3 (right) orbitals of **1-La.**

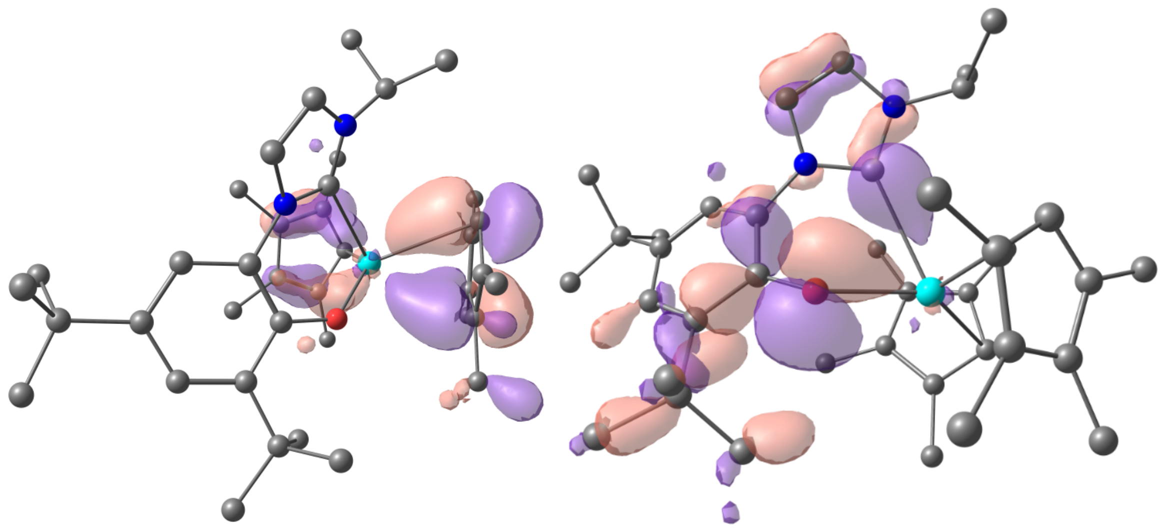


Figure S153. Depictions of the TD-DFT-calculated 163 HOMO-4 (left) and 161 HOMO-6 (right) orbitals of **1-La.**

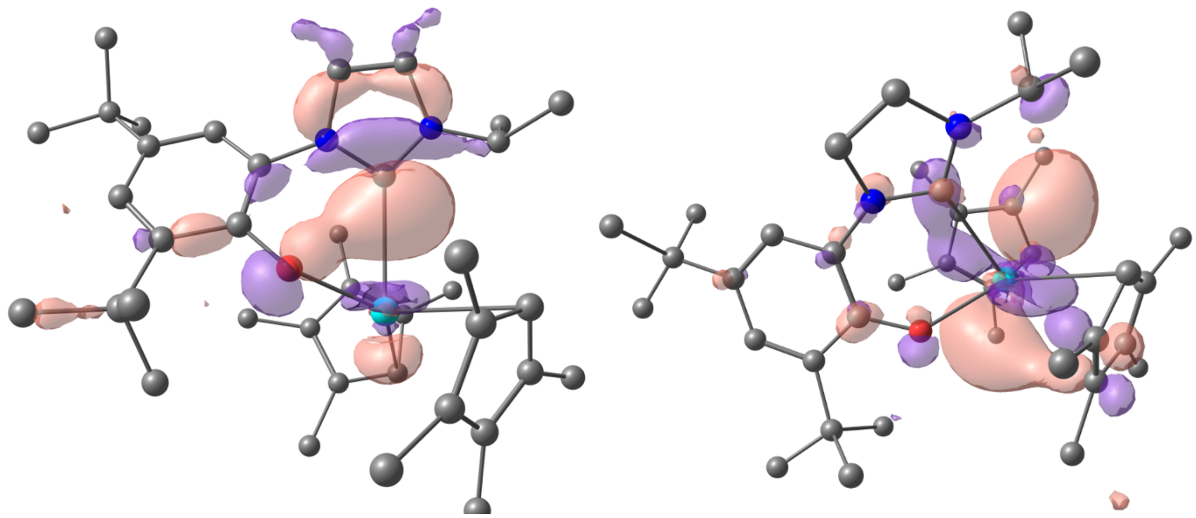


Figure S154. Depictions of the TD-DFT-calculated 159 HOMO-8 (left) and 169 LUMO+1 (right) orbitals of **1-La.**

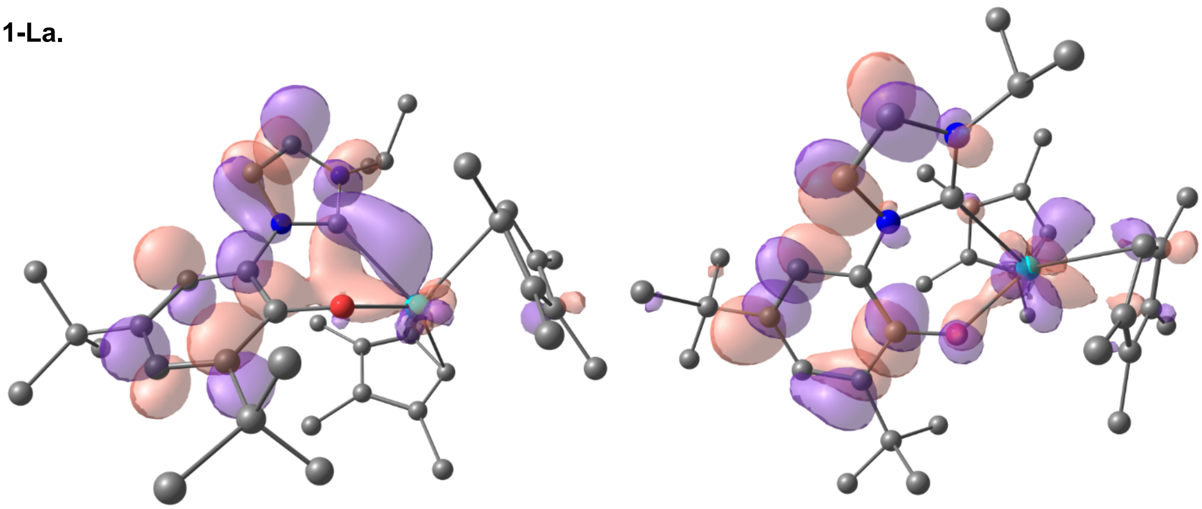


Figure S155. Depictions of the TD-DFT-calculated 170 LUMO+2 (left) and 172 LUMO+4 (right) orbitals of **1-La.**

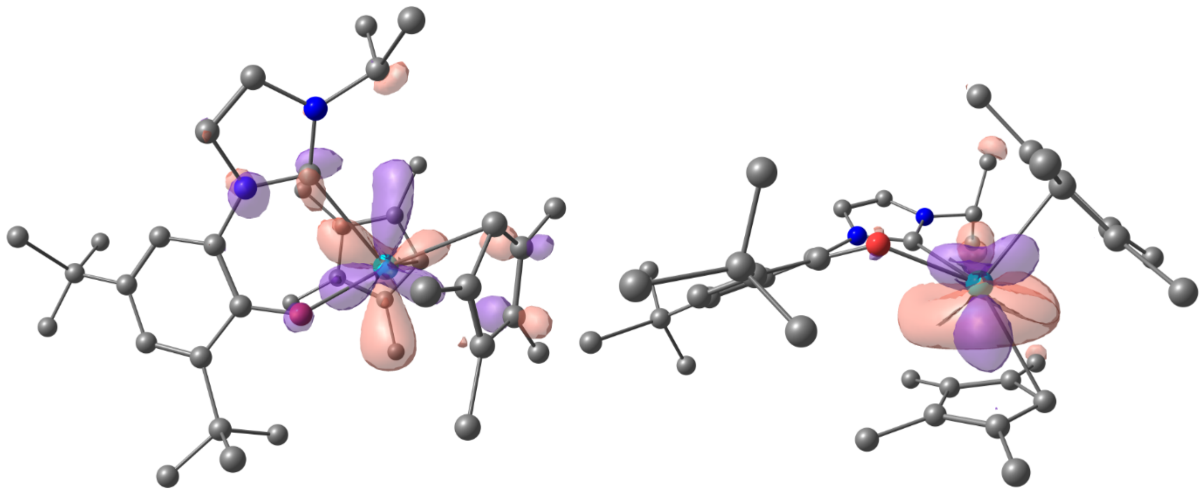
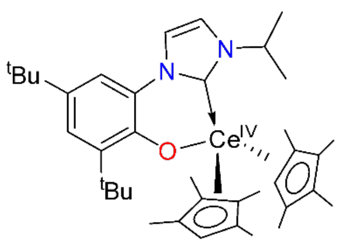


Figure S156. Depictions of the TD-DFT-calculated 176 LUMO+8 (left) and 177 LUMO+9 (right) orbitals of **1-La.**

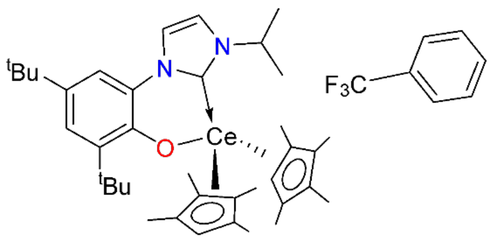
S10.3 Cartesian coordinates



Ce	5.41357300	7.74712400	14.46932900	C	6.78955600	7.80806900	9.84777100
O	4.03990400	7.01425600	12.79992800	H	6.53937200	7.39812700	8.88320700
N	6.23794100	7.32431200	11.02592600	C	1.17352400	6.44897200	11.93818700
N	7.49501100	8.97968700	11.55697200	H	1.77103300	7.28518300	12.30420600
C	3.35547800	9.49306800	15.24469600	H	0.19335700	6.47711000	12.42881200
C	4.00371300	10.15301700	14.16803100	H	1.01639400	6.58041800	10.86201800
C	4.24037900	9.49042400	16.36521100	C	7.58829900	8.84707600	10.18465300
C	5.36412100	6.18628700	11.00739600	H	8.18811800	9.49549600	9.56591400
C	6.65941800	8.05460200	12.10511300	C	9.74436000	9.70111600	12.26254200
C	6.29616400	5.09727100	15.06287900	H	9.96893000	8.68238900	12.58894500
C	5.28838000	10.54029500	14.62543800	H	10.28369700	10.39841000	12.91054800

H	6.00385000	11.12712400	14.05952700	H	10.12935900	9.82611200	11.24489000
C	6.70398500	6.67668300	16.66813800	C	1.94179200	8.98633700	15.24233300
H	6.62407000	7.26835800	17.57426900	H	1.59545000	8.76814600	14.22861800
C	7.48556000	5.79542700	14.70749300	H	1.25045700	9.72537200	15.67035300
C	7.74259200	6.77297900	15.70931300	H	1.82399400	8.07003500	15.83227600
C	5.44021000	10.14725000	15.98046300	C	7.90407800	11.39555600	11.85685700
C	5.80831900	5.64643400	16.27995700	H	8.26976500	11.57997300	10.84116500
C	4.20733600	6.13528700	11.83127800	H	8.37752800	12.12998600	12.51511900
C	5.65830300	5.17543500	10.09295300	H	6.82472700	11.56626900	11.86783200
H	6.59837800	5.22904300	9.55046400	C	2.00242700	4.89801900	13.74464800
C	3.58630500	4.13261800	10.60052900	H	2.46252000	3.92930500	13.96598100
H	2.86799200	3.34441500	10.41791500	H	1.01104500	4.91433200	14.21328100
C	3.25684700	5.10834800	11.54497100	H	2.60843000	5.68362700	14.19712700
C	4.78772200	4.10879900	9.88236400	C	0.96211900	3.99103400	11.68894900
C	8.24325800	9.98139900	12.32526300	H	0.79589200	4.07729200	10.60972300
H	7.89628900	9.85635900	13.35532300	H	-0.01493800	4.06305000	12.17867200
C	8.39781800	5.42944000	13.57286200	H	1.35820900	2.99130500	11.89885700
H	7.84264400	5.07452700	12.69894400	C	4.06971700	1.92097500	8.78999300
H	9.08902500	4.62551400	13.86320000	H	3.88920900	1.43342600	9.75378000
H	9.00918400	6.27800600	13.25070800	H	4.38162200	1.14652400	8.08110900
C	8.96444700	7.64020200	15.81412500	H	3.12073800	2.33332500	8.43082200
H	9.24947700	8.08682700	14.85439800	C	6.58156700	10.52463200	16.88000400
H	9.83432800	7.06567000	16.16022600	H	6.82760700	9.73892000	17.60202100
H	8.81450600	8.45584800	16.52784600	H	6.34884400	11.42722500	17.46134400
C	3.41818800	10.43951600	12.81469000	H	7.48924900	10.74096300	16.30648900
H	4.15478400	10.92619800	12.16787600	C	3.88846400	9.03223900	17.75122800
H	2.55355800	11.11143100	12.88626900	H	3.23950500	8.14962100	17.74532100
H	3.08707000	9.52921400	12.30306200	H	3.34917700	9.81382000	18.30426600
C	1.87498600	5.10571300	12.22418800	H	4.77779400	8.78297900	18.33813900
C	5.15895900	2.99773500	8.89101200	C	6.46452900	2.31664900	9.34725300
C	5.74996500	3.89272500	14.35236300	H	7.29551200	3.02715800	9.40244900

H	4.73718600	3.65510400	14.68825400	H	6.75134700	1.52364900	8.64637100
H	6.36926300	3.00627800	14.54676900	H	6.34465700	1.86813700	10.33885000
H	5.70880100	4.02406300	13.26602300	C	5.36591100	3.60052800	7.48740300
C	4.63567900	5.15328500	17.08040100	H	4.45161100	4.08752500	7.13237000
H	4.33837700	5.88700100	17.83585500	H	5.63779900	2.81931800	6.76773600
H	4.87829600	4.22403900	17.61278200	H	6.16654100	4.34728100	7.48067500
H	3.75666300	4.93855100	16.46150000				

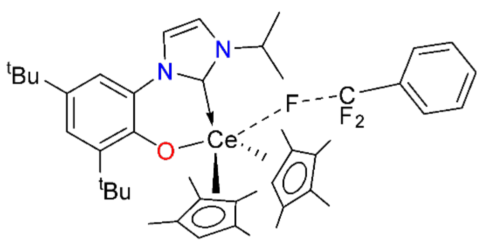


IRC reverse

Ce	-0.50915500	-0.18846500	0.94067400	H	1.07564800	-0.10461200	-4.75573600
O	-2.37862800	-0.92182300	-0.13866800	C	3.29492600	0.38460700	-2.47988900
N	-0.70622200	-1.45774000	-2.38137400	H	3.41111100	-0.50813000	-1.86038600
N	0.85419200	0.00003100	-2.60071700	H	4.05210800	1.11511000	-2.18063900
C	-1.95370200	2.14861100	1.54782400	H	3.48433100	0.10710900	-3.52235700
C	-1.23843000	2.47548300	0.36344000	C	-3.44854700	2.06883000	1.67582000
C	-1.01588200	2.03351800	2.62056500	H	-3.92444900	1.84807400	0.71655100
C	-1.71142400	-2.36559500	-1.90846600	H	-3.86812100	3.01800600	2.03768000
C	0.07281400	-0.59394100	-1.65697900	H	-3.76789700	1.29469700	2.38218900
C	0.07924700	-2.86342300	1.77868600	C	1.71975500	2.23586000	-3.18098000
C	0.13515000	2.54382500	0.70969800	H	1.93958900	2.02923300	-4.23359200
H	0.93628300	2.86510500	0.05111700	H	2.40129500	3.02092000	-2.84931000
C	1.05467200	-1.17202500	2.98132800	H	0.69894100	2.61982300	-3.11151700
H	1.27998100	-0.47302600	3.77920200	C	-4.41997700	-2.27365500	1.71324800
C	1.24658000	-2.44308000	1.08893600	H	-4.07552200	-3.24392500	2.08842600
C	1.85660300	-1.39362800	1.83691300	H	-5.24522200	-1.94033300	2.35462500
C	0.27694600	2.29359800	2.10024200	H	-3.60378400	-1.55653700	1.80092800
C	-0.04751500	-2.07039800	2.95631300	C	-6.07403000	-3.37556200	0.23883800

C	-2.60752700	-1.99612200	-0.86795800	H	-6.49073900	-3.50148600	-0.76617300
C	-1.82097000	-3.58983500	-2.56791600	H	-6.87289000	-2.98739500	0.87995100
H	-1.05743500	-3.85447300	-3.29424300	H	-5.79787700	-4.36307900	0.62487800
C	-3.82667000	-4.03621100	-1.37884400	C	-4.17731300	-6.63417800	-2.59793700
H	-4.68087100	-4.67403300	-1.19450600	H	-4.17443700	-6.85090800	-1.52459400
C	-3.74803700	-2.83265500	-0.67380500	H	-4.18901100	-7.59217900	-3.12876700
C	-2.86786800	-4.46951700	-2.30189000	H	-5.10876400	-6.11135600	-2.84011400
C	1.90225700	0.99081700	-2.31545900	C	1.54482000	2.47540800	2.88371700
H	1.75271200	1.26417800	-1.26706100	H	1.62625600	1.78574200	3.73025000
C	1.83006700	-3.12111500	-0.11503200	H	1.61171400	3.49048400	3.29974100
H	1.05593300	-3.47740600	-0.80149900	H	2.42764400	2.33283700	2.25353200
H	2.42997600	-3.99569600	0.17469000	C	-1.37079700	1.81037000	4.06314100
H	2.48771900	-2.45229700	-0.67778200	H	-2.19654100	1.10043600	4.18112100
C	3.18313900	-0.74638900	1.55083300	H	-1.69015000	2.74209900	4.54965300
H	3.23771000	-0.28215800	0.55809100	H	-0.52247400	1.42438900	4.63667300
H	3.99991100	-1.47836300	1.59827300	C	-1.68793400	-6.65517400	-2.68089600
H	3.40367300	0.03410800	2.28450600	H	-0.77082300	-6.14874800	-2.99839900
C	-1.84980000	2.75781300	-0.97787900	H	-1.72155600	-7.62929700	-3.18347100
H	-2.44994100	1.91957800	-1.35165700	H	-1.61489900	-6.83047800	-1.60263900
H	-1.07662400	2.97045000	-1.72078300	C	-3.01212000	-5.61110400	-4.54382600
H	-2.50941700	3.63387700	-0.93667600	H	-3.89312500	-5.02036400	-4.81606900
C	-4.89438300	-2.39010700	0.25354400	H	-3.07063100	-6.57274600	-5.06719700
C	-2.94356900	-5.82636100	-3.01841000	H	-2.12901100	-5.08631000	-4.92059300
C	-0.77794700	-4.04485200	1.41900800	C	5.76003900	6.96431800	2.43199800
H	-1.76893300	-3.97995200	1.87692200	C	6.59986300	6.39395200	1.47723800
H	-0.32314200	-4.98174100	1.77006500	C	6.07116700	5.57558400	0.48132700
H	-0.92704400	-4.14448200	0.33913300	C	4.69838000	5.33328700	0.44521500
C	-1.06856000	-2.23809300	4.04323400	C	3.85259500	5.90297400	1.40001900
H	-2.09143300	-2.33577600	3.65935800	C	4.38726500	6.71832500	2.39265000
H	-1.05290200	-1.38752800	4.73184300	H	6.17414800	7.60369500	3.20652600
H	-0.87249200	-3.14002500	4.63881800	H	7.66821200	6.58682800	1.50488900

C	-0.41407300	-1.37767300	-3.73629400	H	6.71813700	5.13106300	-0.26751300
H	-0.95911400	-1.93803700	-4.47765200	H	2.78454700	5.71288800	1.36031300
C	-5.42706200	-1.02710000	-0.23288100	H	3.73174200	7.16432800	3.13477200
H	-4.63430600	-0.27747100	-0.23174400	C	4.11457700	4.41873100	-0.59230500
H	-6.23834200	-0.68150600	0.41856800	F	4.93870300	4.24049900	-1.64369300
H	-5.82389000	-1.11185700	-1.25063400	F	2.94335000	4.88759200	-1.07010100
C	0.57550000	-0.46513300	-3.87122200	F	3.85536800	3.19321200	-0.08160700

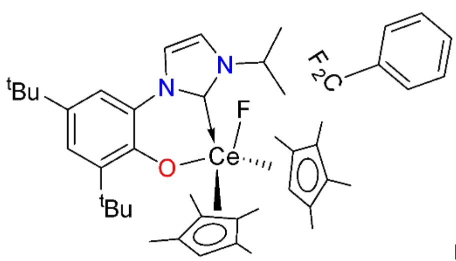


TS :

Ce	5.10278400	8.28669900	13.25446700	H	5.63399500	7.81764500	7.33808600
O	3.15859800	7.24752700	12.54455700	C	8.10294500	8.68839000	8.89596800
N	4.42276800	6.59346700	10.10503500	H	8.46038000	7.82238300	9.45950700
N	5.78305400	8.12164500	9.47886900	H	8.86179900	9.47300500	8.95584100
C	2.98025200	10.21699200	13.80848500	H	8.00602900	8.39766800	7.84409300
C	4.09596300	10.87450500	13.21503400	C	1.61740300	10.14757600	13.19412600
C	3.34502100	9.82453000	15.12122600	H	1.64870000	9.79323800	12.15876600
C	3.59450100	5.67647900	10.82070300	H	1.14313000	11.13873000	13.18370400
C	5.23327900	7.57875000	10.60412500	H	0.95687800	9.47857800	13.74808900
C	5.59342800	5.58112200	14.18656900	C	6.25564600	10.41261600	8.69745500
C	5.12972100	10.90232100	14.18323200	H	6.13028900	10.19757000	7.63040700
H	6.11243400	11.32649900	14.04862000	H	6.96544600	11.23984800	8.78618000
C	6.78109900	7.26468700	15.17950400	H	5.29363400	10.74402000	9.09630600
H	7.11462700	8.00564800	15.89772300	C	1.26830100	6.15325800	14.68658500
C	6.71303000	5.88276200	13.35792900	H	1.68987300	5.29080800	15.21491500
C	7.46506400	6.90321600	13.99323700	H	0.47654000	6.57057000	15.32056800
C	4.69036000	10.24996700	15.35092700	H	2.04910000	6.90204900	14.55891800

C	5.62611400	6.44895000	15.31064100	C	-0.37619800	4.65522200	13.61076600
C	2.85504300	6.10815000	11.95396600	H	-0.89696700	4.33567400	12.70176000
C	3.47724600	4.38968600	10.29709400	H	-1.12957700	5.07409000	14.28701300
H	4.14452100	4.10104900	9.48924100	H	0.04467400	3.76916100	14.09894700
C	1.69239900	3.97159900	11.79624400	C	1.38579000	1.22198200	10.93729300
H	0.90977300	3.31849700	12.15856100	H	1.57103600	1.13651500	12.01323800
C	1.78468000	5.24592000	12.36307800	H	1.37707600	0.20908500	10.52057900
C	2.54552400	3.48516800	10.79984200	H	0.38576100	1.64506500	10.79452000
C	6.77858100	9.19843000	9.46333600	C	5.41289500	10.23293000	16.66539900
H	6.91253400	9.45330300	10.51344100	H	5.29299200	9.28964300	17.20674000
C	7.14968800	5.10803200	12.14946000	H	5.03623600	11.02453000	17.32849300
H	6.30020100	4.68722500	11.60414500	H	6.48469400	10.40779800	16.53159600
H	7.80216500	4.26925600	12.43090700	C	2.42758800	9.30021900	16.18574000
H	7.71329800	5.73431600	11.45122200	H	1.51924300	8.86118800	15.76780200
C	8.81633800	7.38590200	13.57337600	H	2.11386800	10.11053400	16.85907200
H	8.84902500	7.68090700	12.52133400	H	2.90267500	8.53793900	16.81077500
H	9.57255800	6.60366700	13.72399700	C	3.82165000	1.35265500	10.43569600
H	9.11202800	8.24955900	14.17269400	H	4.63251000	1.88108900	9.92436600
C	4.10029000	11.55076800	11.87584700	H	3.78584500	0.33215800	10.03615300
H	3.56096000	10.97129600	11.11689100	H	4.08092800	1.29423300	11.49782000
H	5.12003800	11.71054300	11.51710400	C	2.13536400	2.11010600	8.73454600
H	3.61217700	12.53476500	11.92086700	H	1.17425300	2.60591000	8.56237500
C	0.68896700	5.72690400	13.32912800	H	2.07639500	1.09762200	8.31764500
C	2.46615000	2.05965200	10.23935400	H	2.89895600	2.65528800	8.17023900
C	4.70159000	4.38795500	14.04456400	C	9.90824600	12.52081700	15.88292200
H	3.70473000	4.56556400	14.45282500	C	10.50443400	11.38739500	15.32091400
H	5.12726100	3.53258100	14.58948900	C	10.01762800	10.85041600	14.13982200
H	4.57772500	4.08000000	13.00382600	C	8.90836800	11.44792400	13.49967700
C	4.75346800	6.33116400	16.52603200	C	8.32134600	12.60478700	14.06136000
H	3.68654800	6.29589400	16.28578000	C	8.82245900	13.12716200	15.24334800
H	4.91512700	7.16426400	17.21515200	H	10.29303300	12.93453400	16.81020900

H	4.98390100	5.41068600	17.07970400	H	11.35831300	10.92495600	15.80714100
C	4.46193900	6.55282700	8.71847300	H	10.49022600	9.98259100	13.69466100
H	3.84742600	5.88011200	8.14375200	H	7.48891900	13.08583000	13.55974100
C	-0.02423300	6.91614200	12.65663600	H	8.36765000	14.01629100	15.66966400
H	0.68789900	7.70265200	12.40752600	C	8.40472000	10.90045000	12.28551700
H	-0.79002700	7.33465100	13.32147000	F	9.16960200	10.10022400	11.57831800
H	-0.51768800	6.59260100	11.73359200	F	7.63768900	11.64361500	11.51705200
C	5.32668300	7.51453000	8.32630500	F	7.02503900	9.50865200	12.57962100



IRC forward :

Ce	-0.12357100	0.30721300	0.64351700	H	0.49963600	-0.08013100	-5.22368300
O	-1.98897300	-0.80408700	-0.02110500	C	3.00457200	0.53268400	-3.60791300
N	-0.81962100	-1.34965900	-2.53094200	H	3.27420200	-0.37385600	-3.05967000
N	0.63427900	0.12926400	-3.07305400	H	3.81899700	1.25337000	-3.49572700
C	-2.09001500	2.32038100	0.92795000	H	2.92379100	0.27859800	-4.67109300
C	-0.84202600	2.94690100	0.64603300	C	-3.27759800	2.34550600	0.01004700
C	-2.03143500	1.79966500	2.24869900	H	-3.15899300	1.68319300	-0.85554000
C	-1.67744200	-2.27159600	-1.85932400	H	-3.44597900	3.35822200	-0.37505600
C	0.03346400	-0.42925300	-1.97884600	H	-4.18944500	2.03912800	0.52764700
C	0.68224900	-2.28746400	1.47123000	C	1.29212400	2.38199600	-3.84541000
C	-0.02896400	2.81449000	1.79492500	H	1.19861800	2.18474500	-4.91946100
H	0.98618900	3.18106200	1.89191500	H	2.04699700	3.16193200	-3.71518700
C	1.44355200	-0.52982400	2.72273300	H	0.33814100	2.77292900	-3.48293900
H	1.56932700	0.17355600	3.53685400	C	-3.70817000	-2.21923900	2.19624000
C	1.81964200	-1.72290600	0.81557500	H	-3.31662500	-3.19369100	2.50894400
C	2.31236400	-0.65869300	1.61831200	H	-4.40901800	-1.87898100	2.96803100
C	-0.74949500	2.11666400	2.78931100	H	-2.88208600	-1.51149700	2.14210300
C	0.44614200	-1.54460500	2.65568200	C	-5.56811700	-3.34385700	1.01431600
C	-2.35552200	-1.89841000	-0.67114700	H	-6.13841600	-3.48558400	0.09004200

C	-1.86316600	-3.51589600	-2.45941200
H	-1.23655600	-3.77645000	-3.30772600
C	-3.59072500	-3.98233700	-0.90839500
H	-4.37690700	-4.63508700	-0.55364000
C	-3.42336300	-2.75609800	-0.25705800
C	-2.80601000	-4.42031900	-1.97892600
C	1.71006200	1.13703800	-3.06497400
H	1.84579900	1.39529600	-2.01633300
C	2.50811000	-2.27912900	-0.39440800
H	1.80736500	-2.74761400	-1.09064100
H	3.24622100	-3.04273400	-0.11102200
H	3.04512400	-1.49646400	-0.93718000
C	3.56826500	0.12183700	1.38681200
H	3.58803800	0.58108400	0.39557300
H	4.45037600	-0.52405800	1.48385200
H	3.66554700	0.92605400	2.12164600
C	-0.50580900	3.71352500	-0.59603400
H	-0.95795000	3.26647600	-1.48833600
H	0.57380100	3.75549800	-0.74865400
H	-0.88091300	4.74452300	-0.53575000
C	-4.41752200	-2.33983300	0.83967800
C	-2.95994500	-5.80005100	-2.63058300
C	0.00048300	-3.56020000	1.07109600
H	-1.04512700	-3.59031400	1.38584400
H	0.50610800	-4.42467800	1.52333700
H	0.01210700	-3.70973500	-0.01155900
C	-0.49946100	-1.90590700	3.76349300
H	-1.19609300	-2.68945600	3.46136700
H	-1.09399300	-1.05706400	4.11694700
H	0.05814300	-2.28357700	4.63046200
C	-0.76178700	-1.33465900	-3.91720100
H	-1.40247000	-1.94571600	-4.53061900
C	-5.04790700	-0.99270900	0.44111000
H	-4.27966700	-0.23410600	0.29370000
H	-5.74092300	-0.64919200	1.21887400

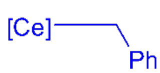
H	-6.25999000	-2.96033500	1.77205600
H	-5.21959200	-4.32300700	1.36084500
C	-4.05140100	-6.64186900	-1.95514600
H	-3.83331600	-6.81597100	-0.89616900
H	-4.11827100	-7.61964700	-2.44394400
H	-5.03636900	-6.16875400	-2.02907400
C	-0.34296300	1.98076700	4.22634700
H	-0.55016000	0.99152000	4.64579300
H	-0.88630400	2.70632500	4.84663800
H	0.72401300	2.18405000	4.35552300
C	-3.17787800	1.24771000	3.04032500
H	-3.92958400	0.77602900	2.40510800
H	-3.67873300	2.04670200	3.60526800
H	-2.85465200	0.50118300	3.77233900
C	-1.62785900	-6.56845300	-2.52464800
H	-0.81153900	-6.03526500	-3.02217300
H	-1.71430100	-7.55606700	-2.99318000
H	-1.34205000	-6.71175500	-1.47745700
C	-3.33314200	-5.63586400	-4.11720400
H	-4.27855000	-5.09413600	-4.22576400
H	-3.44413300	-6.61558300	-4.59652300
H	-2.56590000	-5.08385100	-4.66961300
C	5.58998600	5.44169900	2.88513300
C	6.15104300	4.27179000	2.35652900
C	5.66475800	3.71664500	1.18672700
C	4.57841700	4.33465400	0.50400800
C	4.01430300	5.52429900	1.04704100
C	4.52120200	6.05579100	2.21932300
H	5.97981900	5.86883600	3.80390100
H	6.97910000	3.78979000	2.86904200
H	6.10246700	2.81086000	0.78133200
H	3.18660000	6.00373400	0.53543800
H	4.08013900	6.96192300	2.62560700
C	4.09612800	3.80008900	-0.68703500
F	4.53601400	2.67173500	-1.22332500

H	-5.61379700	-1.09439900	-0.49149100	F	3.07208600	4.30139800	-1.36213800
C	0.16038700	-0.40632900	-4.25350800	F	1.48457200	1.40256900	-0.16364400

[Ce]-F :

Ce	5.06163300	8.24830500	13.23941000	C	4.29870900	6.50478300	8.73260900
O	3.18558000	7.11010500	12.65651200	H	3.64704900	5.87390000	8.15176800
N	4.28139400	6.52035100	10.12001700	C	0.14571600	6.92540500	13.20844500
N	5.70123900	8.00303000	9.50225500	H	0.90665200	7.68166700	13.01533600
C	3.11294700	10.27876900	13.51732400	H	-0.52157700	7.28677300	14.00044800
C	4.35889500	10.89529800	13.20436200	H	-0.45101600	6.79916300	12.29833700
C	3.18991400	9.78434600	14.84797100	C	5.19990300	7.43500800	8.34842300
C	3.44852900	5.60920200	10.83656700	H	5.50636600	7.74157100	7.36115100
C	5.13965300	7.46204800	10.62609400	C	8.05749900	8.41635800	8.91732800
C	5.89850400	5.68739700	14.11944900	H	8.35818500	7.54669100	9.50729400
C	5.18942700	10.77886900	14.34224700	H	8.86186300	9.15671100	8.96609000
H	6.20795000	11.14190200	14.41542400	H	7.95675000	8.10285900	7.87190000
C	6.68833400	7.48186300	15.29812600	C	1.90744400	10.29570200	12.62284900
H	6.83508700	8.20901900	16.08730600	H	2.02992400	9.67228200	11.72941000
C	7.01781100	6.23405900	13.41831400	H	1.69553200	11.31572900	12.27996400
C	7.52921100	7.32144400	14.17642400	H	1.01745000	9.93745400	13.14455600
C	4.48135500	10.10492300	15.36184900	C	6.31708100	10.23522600	8.64053300
C	5.69197100	6.46361700	15.28791200	H	6.19286500	9.99533600	7.57840000
C	2.80473300	6.00335400	12.03709800	H	7.07352600	11.02254800	8.71128100
C	3.24814900	4.35255500	10.26727200	H	5.37281100	10.63859400	9.01461000
H	3.84908500	4.07539000	9.40589400	C	1.54846100	5.74348400	14.94723200
C	1.56794900	3.91305200	11.87770200	H	1.94380600	4.77552300	15.27492900
H	0.79371900	3.26660500	12.26793100	H	0.87657000	6.11145000	15.73182200
C	1.75250400	5.15158500	12.49966500	H	2.37851200	6.44139500	14.84570300
C	2.32184400	3.45624100	10.79285400	C	-0.34684700	4.58650500	13.85448800
C	6.76344600	9.02421900	9.45809500	H	-0.94898200	4.42447100	12.95402600
H	6.91125700	9.31988700	10.49561100	H	-1.01270900	4.98356400	14.62834400

C	7.67443600	5.63832800	12.20924900	H	0.01716300	3.61545600	14.20772300
H	6.95121300	5.18548700	11.52550300	C	1.07563700	1.23643900	10.88577900
H	8.38739600	4.85256000	12.49619900	H	1.31637400	1.08246700	11.94294800
H	8.23440700	6.39347300	11.65071000	H	0.99783700	0.24947800	10.41748600
C	8.77376200	8.10171200	13.88629200	H	0.08938600	1.70866600	10.82386700
H	8.74247200	8.56112600	12.89473700	C	4.90914100	9.99307100	16.79476400
H	9.66063300	7.45804900	13.94036600	H	4.69853300	9.01429700	17.23679400
H	8.90496500	8.90584200	14.61621700	H	4.38287200	10.73634600	17.40874900
C	4.68301200	11.63949100	11.94528600	H	5.97995600	10.18785300	16.90428300
H	4.17646700	11.20978100	11.07419000	C	2.05480900	9.25682400	15.67239100
H	5.75821200	11.62635600	11.75340400	H	1.28525500	8.77984500	15.06328000
H	4.36236500	12.68792900	12.01313600	H	1.57281000	10.07059800	16.23253200
C	0.79352800	5.58975800	13.61856200	H	2.38712300	8.52147100	16.41181800
C	2.15242800	2.06435300	10.17099400	C	3.48627600	1.29705800	10.26223500
C	5.20905100	4.40409600	13.76867500	H	4.29147800	1.81891600	9.73536500
H	4.18645300	4.36307900	14.15020900	H	3.38846100	0.30014300	9.81643700
H	5.75382800	3.54810600	14.19055200	H	3.79577000	1.17509700	11.30536900
H	5.15227500	4.24878000	12.68806700	C	1.74638200	2.20100700	8.69023000
C	4.76175100	6.14958200	16.42310800	H	0.80050300	2.74397700	8.59237600
H	4.14364200	5.27678200	16.20570500	H	1.62118100	1.21269500	8.23253800
H	4.08415400	6.97441100	16.66859300	H	2.50261800	2.73910400	8.10957800
H	5.33292500	5.92692200	17.33303500	F	6.63481800	9.32962900	12.35560900



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Ce	4.98880200	8.16593400	13.53152000	H	5.99004600	8.01105800	7.55791800
O	3.15129600	7.21920000	12.56222100	C	8.49107500	8.38111600	9.07008900
N	4.58207200	6.70674400	10.18822400	H	8.71422400	7.40355800	9.50651000
N	6.12551200	8.11345000	9.71787800	H	9.36764400	9.02203400	9.20288600
C	2.78851800	9.91857200	13.99885400	H	8.33644400	8.24961000	7.99375400

C	3.80488100	10.63528400	13.31478800	C	1.39568400	9.74244400	13.48886200
C	3.24774200	9.64387000	15.31776200	H	1.38257600	9.53692600	12.41558200
C	3.69177200	5.75746100	10.78147500	H	0.81549200	10.66243000	13.65028500
C	5.48100900	7.55171900	10.79115900	H	0.86545600	8.93291900	13.99141500
C	5.12324800	5.59393700	14.83378900	C	6.92769000	10.38056400	9.15087900
C	4.87221300	10.82454600	14.22438600	H	6.70273100	10.30627700	8.08126000
H	5.75455600	11.42140700	14.05366300	H	7.77043500	11.06835600	9.26654600
C	6.85026700	7.04920100	15.21335500	H	6.05859600	10.81552800	9.65173000
H	7.48885800	7.77850700	15.69662900	C	0.93668900	6.17372100	14.40483100
C	6.04705800	5.47471800	13.76126800	H	1.24027700	5.34029800	15.04418800
C	7.12776600	6.36307200	14.00560500	H	0.06520100	6.64720800	14.87310400
C	4.54735200	10.21208700	15.45576500	H	1.75305200	6.89302100	14.36234800
C	5.62187800	6.56941000	15.73985000	C	-0.46794200	4.54913700	13.19741200
C	2.88352200	6.11061400	11.88960100	H	-0.89861800	4.20252400	12.25235500
C	3.60409000	4.51512200	10.15548100	H	-1.29320700	4.93391600	13.80637900
H	4.31956400	4.28538300	9.37072400	H	-0.04586400	3.68646800	13.72485800
C	1.74467800	3.99001500	11.52081600	C	1.48751200	1.31293200	10.44097000
H	0.94232100	3.31507800	11.78560800	H	1.59310600	1.15079300	11.51886700
C	1.78645800	5.22881900	12.17068800	H	1.50939000	0.33153900	9.95536600
C	2.65506700	3.57468700	10.54386200	H	0.50045600	1.74959700	10.25493700
C	7.28267100	9.02227500	9.75236800	C	5.35973800	10.36690200	16.70806300
H	7.51933900	9.15568900	10.80550000	H	5.01588600	9.71242900	17.51177100
C	6.04339000	4.40532900	12.71231700	H	5.28796300	11.39617300	17.08264100
H	5.04793300	3.98669500	12.55443200	H	6.42177400	10.16792000	16.53304300
H	6.70431900	3.57888600	13.01105900	C	2.39771700	9.09549000	16.42677100
H	6.40482700	4.77146100	11.74669600	H	1.90256600	8.15571700	16.16395800
C	8.40537300	6.35720900	13.21851900	H	1.60424900	9.80797900	16.68899200
H	8.23168100	6.45109200	12.14018600	H	2.98071700	8.92167600	17.33400000
H	8.93657600	5.40809200	13.37038000	C	3.95394300	1.46560900	10.13211900
H	9.08438900	7.15762300	13.52031800	H	4.80119200	2.02698700	9.72577900
C	3.69603600	11.21322100	11.93282100	H	3.95025100	0.47745200	9.65705400

H	3.41324800	10.46673600	11.18012700
H	4.64335600	11.66353000	11.62089500
H	2.93485500	12.00351200	11.89169900
C	0.56608400	5.67080200	13.00160100
C	2.61660400	2.19068000	9.88376900
C	3.98875500	4.65577000	15.10565100
H	3.31601000	5.05049000	15.87049200
H	4.37108400	3.69531800	15.47863600
H	3.39490000	4.44229100	14.21260800
C	5.11478600	6.79449000	17.13364500
H	4.02905300	6.91450300	17.18260800
H	5.57527900	7.67424200	17.58731200
H	5.36854500	5.93517500	17.76899000
C	4.64688300	6.78210400	8.80494200
H	3.97755000	6.22797300	8.16802100
C	-0.12457200	6.78847500	12.19162000
H	0.56171100	7.61173900	11.99250200
H	-0.99039200	7.18405600	12.73653200
H	-0.47677900	6.39836600	11.23059300
C	5.62389400	7.66560600	8.51137700
H	4.13002100	1.32694400	11.20384400
C	2.39870100	2.34494100	8.36554200
H	1.45448900	2.85850000	8.15608300
H	2.36771700	1.36282600	7.87938100
H	3.20371600	2.91934000	7.89584700
C	7.12307800	9.50574900	13.07025300
H	7.59781100	8.59084300	12.70692800
H	6.61805100	10.02937000	12.24880500
C	8.06637200	10.39308300	13.75977500
C	9.04111900	9.91477300	14.66398300
C	8.05970000	11.78919400	13.53645400
C	9.92390800	10.77070000	15.31394200
H	9.11102400	8.84878000	14.85505500
C	8.93716600	12.64760900	14.19207100
H	7.36384400	12.20225900	12.80846300
C	9.87637800	12.14782700	15.09288400
H	10.65828500	10.35630700	16.00076100
H	8.89368000	13.71459100	13.98638600
H	10.56459800	12.81503700	15.60374700

$(PhCH_2)_2Mg(THF)_2$:

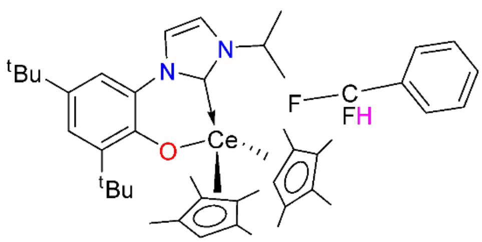
Mg	-0.75509500	0.47775600	-0.37826200
C	-2.69637600	-0.37885400	0.13198500
H	-3.52224700	0.09273200	-0.41504100
H	-2.62377500	-1.42067000	-0.20841700
C	0.94926000	-0.64789300	-1.14610000
H	1.85346700	-0.51826600	-0.53841700
H	0.63469300	-1.69640900	-1.05485500
H	1.75450100	0.76365600	-6.31472100
C	-2.08947000	2.04368900	-2.68852000
O	-1.11130500	2.13787400	-1.62053100
C	-0.09745800	3.11942700	-1.95782100
C	-0.37207500	3.50721900	-3.40452300
C	-1.88475200	3.30189800	-3.51691400
H	-1.87750000	1.14149200	-3.27375000

C	-2.91536800	-0.31459600	1.58957000
C	-2.28137000	-1.21454200	2.47792900
C	-3.72949100	0.67383200	2.18666700
C	-2.43798200	-1.12322200	3.85781400
H	-1.66769600	-2.01280400	2.06201800
C	-3.88505000	0.76837800	3.56806100
H	-4.26790700	1.36647300	1.54079800
C	-3.23677600	-0.12559600	4.42238000
H	-1.94038200	-1.84699400	4.50024500
H	-4.53359400	1.53881800	3.98062200
H	-3.36687100	-0.06005300	5.49889200
C	1.19854100	-0.29386600	-2.55666400
C	0.38173400	-0.78414600	-3.60237900
C	2.23272300	0.58859700	-2.94107800
C	0.57573000	-0.40890900	-4.92843200
H	-0.41027500	-1.49117000	-3.35813300
C	2.42647400	0.96754400	-4.26788300
H	2.91096300	0.96283300	-2.17510900
C	1.59692300	0.47805900	-5.27852400
H	-0.07029100	-0.82301000	-5.70001100
H	3.24552800	1.63951200	-4.51687100
H	-3.07583300	1.95815300	-2.22731400
H	-0.21237400	3.96783800	-1.27235200
H	0.88429700	2.66081800	-1.81813300
H	-0.05699900	4.53113500	-3.62282200
H	0.15969500	2.82808500	-4.07859300
H	-2.42799500	4.14593800	-3.07696800
H	-2.22590200	3.17422900	-4.54737200
C	0.82044500	1.05918100	2.21875100
O	-0.06436600	1.64618400	1.22945400
C	-0.82341200	2.73196100	1.82099100
C	-0.51411700	2.68027400	3.31128100
C	0.89833500	2.09069800	3.33268100
H	0.37255800	0.12332800	2.57235300
H	1.77240400	0.84752700	1.72688600
H	-0.48401800	3.66709100	1.35933000
H	-1.88121800	2.57200600	1.59959200
H	-0.57836200	3.66636800	3.77906400
H	-1.21861200	2.00989300	3.81392300
H	1.64587400	2.85675500	3.09732000
H	1.16098700	1.63863900	4.29246800

-(PhCH$_2$)MgF :

Mg	-1.26663500	1.47703700	-0.06615100
C	-0.39540400	-0.48841300	-0.17451400
H	0.19224700	-0.72365400	0.72214300
H	-1.23504700	-1.19514100	-0.20900300
C	0.42991300	-0.58207500	-1.39800600
C	-0.13254700	-0.91796300	-2.64953100
C	1.80822300	-0.27518400	-1.39891200
H	-3.03003000	3.31229000	-1.35560000
H	0.56405700	3.24463100	-2.11351500
H	0.24604300	1.87135400	-3.20591500
H	-0.03038500	4.50967700	-4.08008200
H	-1.09624800	3.22756700	-4.67287900
H	-1.64258000	5.11451800	-2.31737900
H	-2.71202700	4.78489800	-3.69294300

C	0.62420300	-0.93171000	-3.81782100	C	1.21465600	2.37515300	1.66977100
H	-1.18862100	-1.17890000	-2.69378400	O	0.01113600	2.78782900	0.97792700
C	2.56677600	-0.28614500	-2.56651100	C	-0.68908500	3.79737400	1.75592800
H	2.29187400	-0.03612600	-0.45281500	C	-0.21499400	3.56379100	3.17902000
C	1.98309200	-0.60912200	-3.79238000	C	1.25532200	3.18974300	2.96380400
H	0.14957000	-1.20583800	-4.75787000	H	1.13776000	1.29912400	1.85494200
H	3.62774600	-0.04939000	-2.51682600	H	2.07319300	2.55703500	1.01619900
H	2.57511000	-0.62412000	-4.70315100	H	-0.39125500	4.78850200	1.38873800
C	-2.49349700	3.12703400	-2.28857000	H	-1.75305800	3.61890400	1.57753900
O	-1.30311100	2.38091200	-1.92881300	H	-0.34493600	4.44391000	3.81426700
C	-0.18346500	2.77210100	-2.76102600	H	-0.76839000	2.73171700	3.62781300
C	-0.76195400	3.75713100	-3.77418200	H	1.85980400	4.09345900	2.83012100
C	-1.96494000	4.34443300	-3.02738100	H	1.68366100	2.61989200	3.79247300
H	-3.11027800	2.49806300	-2.94335100	F	-2.81369700	2.14809500	0.55211400

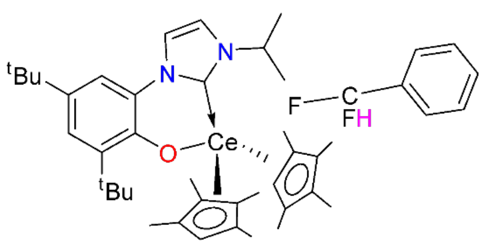


IRC reverse :

Ce	-0.37225200	-0.12644300	0.91973000	H	1.18137400	0.04054800	-4.76094700
O	-2.25330100	-0.86150700	-0.14286800	C	3.42864500	0.40584600	-2.60742500
N	-0.61693200	-1.35010900	-2.41954200	H	3.55202200	-0.56514800	-2.12023300
N	0.98388200	0.06774800	-2.60109600	H	4.21531800	1.07564900	-2.25146400
C	-1.84292500	2.13297700	1.73354200	H	3.56045700	0.26610900	-3.68596600
C	-1.39913800	2.44203400	0.42189000	C	-3.27170800	1.95482600	2.16051900
C	-0.70755500	2.13139000	2.60050600	H	-3.90972900	1.67081900	1.31949100
C	-1.63240400	-2.25696900	-1.96623100	H	-3.68251900	2.88297400	2.58157600
C	0.19456200	-0.53798200	-1.67230400	H	-3.38747200	1.18449400	2.93175300
C	0.17896200	-2.76663000	1.86455600	C	1.84893300	2.34776600	-2.99512300
C	0.00737600	2.61535700	0.48515100	H	1.94334800	2.24467600	-4.08158100
H	0.63915000	2.92387300	-0.34107900	H	2.60351700	3.06433900	-2.66318200

C	1.24263300	-1.05958600	2.95795900
H	1.50099600	-0.31960700	3.70856600
C	1.33435300	-2.41105800	1.11406100
C	1.99873600	-1.35271500	1.79648200
C	0.44113800	2.44149400	1.82467600
C	0.11733700	-1.92365500	3.00828900
C	-2.50637900	-1.90974100	-0.90035600
C	-1.77194200	-3.45447900	-2.66744700
H	-1.02235300	-3.70569200	-3.41286300
C	-3.76520700	-3.91356900	-1.46185400
H	-4.62593900	-4.54431700	-1.28443400
C	-3.65517900	-2.73824500	-0.71478300
C	-2.82870100	-4.32653700	-2.41680700
C	2.06352000	1.01231400	-2.28664800
H	1.99056800	1.17029100	-1.20704400
C	1.85172300	-3.15637800	-0.08165100
H	1.04120500	-3.51377400	-0.72450600
H	2.43412300	-4.03783900	0.22214300
H	2.50904100	-2.53429900	-0.69663600
C	3.33180400	-0.76043900	1.43688000
H	3.43313200	-0.56464900	0.36324000
H	4.15455400	-1.43544400	1.70936800
H	3.50407800	0.18460500	1.96041300
C	-2.26192300	2.61737800	-0.79506000
H	-2.90497200	1.75001800	-0.97983900
H	-1.64819000	2.76268400	-1.68955300
H	-2.91395500	3.49555900	-0.70190200
C	-4.77841600	-2.31758700	0.25039500
C	-2.93017100	-5.65362800	-3.18079500
C	-0.71581700	-3.93688200	1.57737200
H	-1.64506300	-3.88240000	2.15044400
H	0.85805300	2.75441000	-2.77602400
C	-4.27477500	-2.27312000	1.70488900
H	-3.94428200	-3.26496500	2.03090900
H	-5.08055500	-1.94963700	2.37481400
H	-3.44133500	-1.57731900	1.80675100
C	-5.97472000	-3.28210500	0.21288600
H	-6.41292800	-3.35613400	-0.78822700
H	-6.75448400	-2.91052200	0.88644400
H	-5.70753000	-4.29015000	0.54884600
C	-4.17812200	-6.45629500	-2.78832900
H	-4.17933200	-6.71177100	-1.72344500
H	-4.20594000	-7.39440500	-3.35293400
H	-5.10077500	-5.90973900	-3.01096300
C	1.82603500	2.70557800	2.34159900
H	2.14480800	1.97170300	3.09011900
H	1.88944800	3.69204000	2.82037500
H	2.56364900	2.69910500	1.53391100
C	-0.75407700	2.00531300	4.09585800
H	-1.53245300	1.31064700	4.42977000
H	-0.97219700	2.97191500	4.57140600
H	0.19821400	1.65640900	4.50666700
C	-1.69003800	-6.51706500	-2.87550700
H	-0.76352500	-6.01458800	-3.17144500
H	-1.73981800	-7.46960700	-3.41663800
H	-1.62160500	-6.73615900	-1.80491400
C	-2.99663900	-5.38175900	-4.69670800
H	-3.87077500	-4.77151300	-4.94699100
H	-3.06701100	-6.32341300	-5.25387900
H	-2.10678300	-4.85401700	-5.05471800
C	4.40780100	7.03965600	2.40970900
C	5.56962900	6.26986900	2.39191200

H	-0.22588100	-4.88203400	1.84985800
H	-0.98974000	-4.01012600	0.51996700
C	-0.86828700	-2.02055600	4.13928300
H	-1.90222300	-2.14136700	3.79577700
H	-0.83132500	-1.12941300	4.77355800
H	-0.65025500	-2.88226100	4.78423700
C	-0.33769100	-1.22508500	-3.77341400
H	-0.90402600	-1.74413400	-4.52894000
C	-5.29811400	-0.92588000	-0.16330000
H	-4.49159700	-0.19112300	-0.14912200
H	-6.08644700	-0.59489700	0.52347300
H	-5.72109600	-0.95682700	-1.17344300
C	0.67712900	-0.33679700	-3.88555100
C	5.78414000	5.36064000	1.35824800
C	4.83708500	5.21882000	0.34306800
C	3.67410500	5.99283500	0.36036900
C	3.46191200	6.90113400	1.39317000
H	4.24003400	7.75056800	3.21386500
H	6.30950300	6.37909600	3.17951400
H	6.69144000	4.76088600	1.34203400
H	2.94603800	5.88744100	-0.43737200
H	2.55765800	7.50263100	1.40509600
C	5.06018600	4.20485400	-0.73699000
F	4.52733300	4.62426300	-1.92303500
F	4.43202400	3.01959800	-0.43061300
H	6.12033600	3.97862400	-0.90021500



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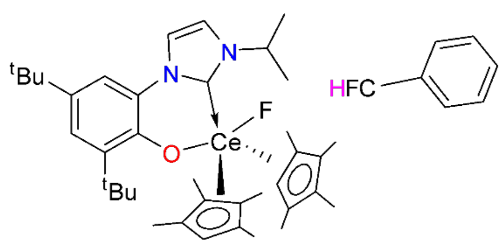
Ce	5.24956000	8.21025400	13.28754100
O	3.25168200	7.19437400	12.69410700
N	4.34958100	6.63737900	10.13921900
N	5.70517900	8.16396000	9.49066000
C	3.23451700	10.27979900	13.58487500
C	4.47899500	10.89896400	13.27193900
C	3.31721200	9.77312200	14.90661500
C	3.54365900	5.70663900	10.86646900
C	5.20448200	7.59195400	10.62469500
C	5.77488900	5.49052700	14.17842700
C	5.31593200	10.77237500	14.40838200
H	5.43990800	7.93085200	7.35210100
C	8.04779500	8.66688400	8.92964000
H	8.37267100	7.80116100	9.51365300
H	8.82236100	9.43703400	8.99224600
H	7.96628100	8.35901900	7.88113000
C	2.02641600	10.29792100	12.69326900
H	2.10420600	9.58660100	11.86293900
H	1.87376500	11.29453400	12.26213800
H	1.11920600	10.04598100	13.24799900
C	6.24518700	10.42408400	8.65544200
H	6.15289300	10.19383700	7.58813900

H	6.32447500	11.15170800	14.49467300	H	6.96619300	11.24046500	8.75423700
C	7.12571900	7.14042400	15.01172500	H	5.27689100	10.78012100	9.01582900
H	7.56338800	7.87190800	15.68432800	C	1.53723100	5.82069100	14.95638300
C	6.79546300	5.75414900	13.22267400	H	1.88544400	4.84744200	15.31826200
C	7.64865800	6.75509600	13.75547900	H	0.84116700	6.22270400	15.70233600
C	4.61493000	10.08500500	15.41849400	H	2.39072300	6.49404400	14.87942900
C	5.96922200	6.35765300	15.28523000	C	-0.31639500	4.67156500	13.78868200
C	2.88847500	6.09475700	12.06682400	H	-0.88528400	4.51402400	12.86599300
C	3.36386700	4.44782700	10.29392100	H	-1.00881500	5.06946600	14.53870600
H	3.97394800	4.18221200	9.43461400	H	0.03028500	3.69817100	14.15304400
C	1.66467300	3.99447000	11.88020200	C	1.22595200	1.30426600	10.89906100
H	0.88949900	3.34115500	12.25806600	H	1.46339800	1.15824000	11.95809900
C	1.82712700	5.23450200	12.50380500	H	1.16557400	0.31460400	10.43359700
C	2.44170600	3.54069200	10.80883800	H	0.23321500	1.76171900	10.83055800
C	6.72496100	9.21856000	9.46147500	C	5.06276500	9.93262500	16.84164500
H	6.85496500	9.50383300	10.50427600	H	4.67658600	9.02391600	17.31178900
C	7.06500600	4.95515500	11.98169900	H	4.71026500	10.77625000	17.45182700
H	6.14385900	4.55846100	11.54634800	H	6.15428600	9.91552600	16.91935700
H	7.71766500	4.09654500	12.19630200	C	2.18646000	9.22969200	15.72622400
H	7.56224300	5.55347400	11.21187600	H	1.41320200	8.77053200	15.10793200
C	8.95466500	7.17209300	13.15216600	H	1.70883400	10.02888300	16.31120500
H	8.84134900	7.57518200	12.13961200	H	2.52077200	8.47372600	16.44424900
H	9.64388500	6.32043300	13.08434400	C	3.63696200	1.39600700	10.28283800
H	9.44792900	7.92850500	13.76978600	H	4.43743400	1.93100800	9.76207600
C	4.77483500	11.67690900	12.02529200	H	3.55543700	0.39893200	9.83344800
H	4.20803000	11.29941600	11.16750000	H	3.94284000	1.27555200	11.32719900
H	5.83647700	11.63105100	11.77190000	C	1.89100000	2.27502900	8.70486200
H	4.50501000	12.73645900	12.13964200	H	0.93701300	2.80309300	8.60381000
C	0.83586500	5.67068100	13.59662300	H	1.78320300	1.28454400	8.24697700
C	2.29395100	2.14634500	10.18736700	H	2.64069700	2.82532600	8.12707700
C	4.83928900	4.32172200	14.14067400	C	8.93231800	13.11444100	15.85804300

H	3.95801300	4.48568300	14.76230800	C	9.37396900	11.78839100	15.92508900
H	5.34209700	3.42085000	14.52158700	C	9.29590400	10.97038300	14.80957500
H	4.48956700	4.09369200	13.13074200	C	8.76849300	11.47060400	13.59701200
C	5.23693900	6.28476200	16.59511600	C	8.32592100	12.81250500	13.53891300
H	4.15616700	6.44026400	16.50044500	C	8.41262800	13.61966200	14.66206500
H	5.62085800	7.02763400	17.29870000	H	8.99373000	13.75162300	16.73526300
H	5.37153600	5.29986300	17.06116100	H	9.78067100	11.39747500	16.85307000
C	4.31672600	6.64321500	8.75166100	H	9.63672300	9.94086700	14.86305500
H	3.65819900	6.00400100	8.18769300	H	7.92345700	13.20160200	12.61037900
C	0.20636900	7.01057800	13.17166600	H	8.07171000	14.64951600	14.61154000
H	0.97598300	7.76527500	13.01328000	C	8.69660400	10.62019500	12.46199700
H	-0.48906500	7.36841200	13.94094900	F	8.41425100	11.19088600	11.29758000
H	-0.35642500	6.89134500	12.23911600	F	7.07752000	9.49899300	12.53284100
C	5.17958800	7.60106900	8.34525200	H	9.27093400	9.70903000	12.37613100



IRC forward :

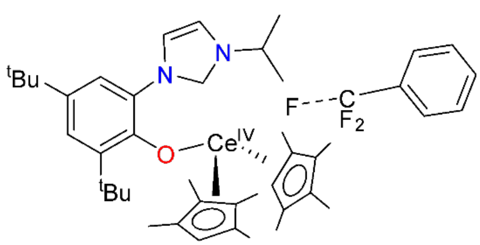
Ce	-0.21399300	0.31803300	0.84092300	H	0.48323600	0.44355000	-5.02096300
O	-2.00025100	-0.84021800	0.06752200	C	2.86185600	1.27190400	-3.16393000
N	-0.75401500	-1.12656800	-2.44949700	H	3.21341800	0.43143400	-2.55985700
N	0.52900900	0.54269700	-2.85915300	H	3.55114500	2.10889800	-3.01866400
C	-2.29936900	2.18502700	1.26024700	H	2.90634400	0.97922300	-4.21925200
C	-1.09644000	2.90295800	0.99779100	C	-3.50283800	2.20592000	0.36454900
C	-2.18735100	1.59496000	2.54725600	H	-3.34874600	1.65049800	-0.56776700
C	-1.55314800	-2.15130300	-1.85884300	H	-3.75745900	3.23677900	0.08969100
C	-0.02838900	-0.14832600	-1.82020300	H	-4.37771100	1.77614600	0.85682600
C	0.62799300	-2.31996400	1.53279300	C	0.94537800	2.87791400	-3.56370000

C	-0.26085500	2.76092900	2.12889500
H	0.72736000	3.19171600	2.23663300
C	1.39560000	-0.60419800	2.83821800
H	1.52593400	0.07350300	3.67355700
C	1.74276100	-1.71491200	0.87475800
C	2.24354500	-0.68248400	1.71270000
C	-0.91730200	1.96048500	3.08939900
C	0.40761500	-1.62759400	2.74966800
C	-2.28336600	-1.90449300	-0.66777900
C	-1.64036100	-3.36416100	-2.54025400
H	-0.97894600	-3.53100700	-3.38545800
C	-3.37657700	-4.03855000	-1.07558000
H	-4.12840000	-4.76046500	-0.78788500
C	-3.30574100	-2.85014600	-0.34215800
C	-2.53509300	-4.35536700	-2.14590500
C	1.45089000	1.68786800	-2.75065200
H	1.45578500	1.94194900	-1.69270100
C	2.40643100	-2.22407800	-0.37010800
H	1.69089300	-2.67648900	-1.06212200
H	3.15523900	-2.99191600	-0.13000600
H	2.92560300	-1.42408400	-0.90512300
C	3.49673600	0.10471100	1.49392000
H	3.54329400	0.52664800	0.48673000
H	4.38247700	-0.52688300	1.63935300
H	3.56156400	0.93326000	2.20530600
C	-0.84006000	3.75898600	-0.20478100
H	-1.17339000	3.27910000	-1.13207400
H	0.21956200	3.99666600	-0.31071300
H	-1.38801200	4.70849900	-0.13123000
C	-4.35125600	-2.56867600	0.75084900
C	-2.57788500	-5.69675300	-2.88917700

H	1.01667100	2.70424800	-4.64345100
H	1.55359500	3.75398000	-3.32541200
H	-0.09456900	3.11220600	-3.32094000
C	-3.68914900	-2.50545300	2.13535500
H	-3.25970000	-3.47824000	2.39951400
H	-4.42895100	-2.24974400	2.90330400
H	-2.89852200	-1.75645100	2.15504800
C	-5.44787000	-3.64429900	0.81670600
H	-5.98218300	-3.74953600	-0.13356900
H	-6.18157200	-3.35421100	1.57651100
H	-5.05530500	-4.62589000	1.10430700
C	-3.64495700	-6.64203800	-2.32085300
H	-3.46280600	-6.87318100	-1.26603200
H	-3.63204400	-7.58768000	-2.87313600
H	-4.65237000	-6.22195500	-2.41116500
C	-0.47738400	1.76933400	4.51038700
H	-0.63382000	0.75232200	4.88268400
H	-1.03888600	2.43832900	5.17642200
H	0.58230600	2.01217100	4.63242500
C	-3.28370400	0.92356500	3.31800700
H	-4.04819200	0.50116000	2.66301100
H	-3.78206900	1.64024900	3.98572400
H	-2.91301200	0.11112600	3.95089600
C	-1.20749700	-6.39212100	-2.76726000
H	-0.40397900	-5.78292200	-3.19329700
H	-1.21415300	-7.35171000	-3.29762500
H	-0.95927800	-6.58424100	-1.71828600
C	-2.89439400	-5.45853000	-4.37895700
H	-3.86379900	-4.96380600	-4.49937300
H	-2.92715600	-6.41049500	-4.92149700
H	-2.13685400	-4.83188000	-4.86069000

C	-0.03099000	-3.59482200	1.10354200
H	-1.05663800	-3.67673600	1.46813600
H	0.52621600	-4.45928900	1.49053000
H	-0.06896000	-3.69606600	0.01605500
C	-0.52419900	-2.03395900	3.85333800
H	-1.18250100	-2.84862700	3.54681900
H	-1.16040300	-1.21392700	4.20124000
H	0.04486800	-2.38473500	4.72367000
C	-0.65542500	-1.02495100	-3.83001700
H	-1.20324600	-1.66607800	-4.49982000
C	-5.04389800	-1.23113200	0.43204900
H	-4.31459700	-0.42368000	0.37372100
H	-5.78049900	-0.98798300	1.20756000
H	-5.57131500	-1.28873000	-0.52645400
C	0.15958200	0.02284900	-4.08247000

C	7.10369900	5.70997900	0.97352300
C	6.66139600	4.49456400	1.51196900
C	5.43925500	3.96259700	1.14015000
C	4.61061800	4.64114400	0.20388000
C	5.07265800	5.87357500	-0.33455500
C	6.29869400	6.38914100	0.05094500
H	8.06357400	6.12236200	1.26989100
H	7.28165900	3.96243900	2.22832100
H	5.10245400	3.01856600	1.55984900
H	4.45014100	6.40263800	-1.04837900
H	6.63736400	7.33282900	-0.36879500
C	3.37661900	4.08693000	-0.16177900
F	2.60428800	4.73869700	-1.05678600
F	1.39592000	1.53678900	0.17894400
H	2.93269200	3.16354400	0.19291700



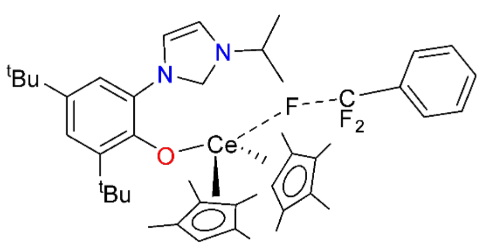
IRC reverse :

Ce	0.11064900	-0.37722400	1.16346500
O	-1.75049700	-1.35016800	0.44707400
N	-1.21694500	-0.64582600	-2.16563300
N	0.39003900	0.29557700	-3.20465400
C	-1.51863700	1.64661500	2.30897400
C	-0.50655500	2.36960100	1.62246600
C	-0.90689500	0.96327900	3.40171200
C	-2.28734300	-1.53787400	-1.84601600
C	-0.38256500	-0.83595500	-3.23558200
C	1.22459700	-2.94992300	0.93474500

H	0.53485300	2.10517100	-2.00460700
C	0.80094800	1.59269200	-5.25271400
H	-0.15629000	1.24531500	-5.65089100
H	1.49264800	1.73627900	-6.08867000
H	0.64397200	2.56610800	-4.77495700
C	-2.99095200	1.70040300	2.01884900
H	-3.19173900	2.03066300	0.99453700
H	-3.50470600	2.40610900	2.68551100
H	-3.47610400	0.72751600	2.14412200
C	2.72024300	1.00596000	-3.70106800

C	0.72347600	2.11953900	2.28792700	H	2.67012000	1.97720100	-3.20016700
H	1.68054200	2.55697200	2.02014200	H	3.44255600	1.09812700	-4.51783400
C	2.38269900	-1.48357000	2.25736300	H	3.10394700	0.27003100	-2.99006300
H	2.78705600	-0.98288600	3.12877500	C	-3.26627100	-2.72601300	2.34650600
C	2.04281600	-2.14421800	0.09396300	H	-2.23378200	-3.07472700	2.27842000
C	2.76117700	-1.22983600	0.91806100	H	-3.69971700	-3.11816100	3.27456600
C	0.48335600	1.27710500	3.39992500	H	-3.24704400	-1.63754400	2.40896600
C	1.43301400	-2.53918200	2.28035500	C	-4.10706200	-4.75727300	1.21873100
C	-2.54419900	-1.86859000	-0.48676300	H	-4.76808800	-5.20717600	0.47266200
C	-3.02647700	-2.05393800	-2.89754600	H	-4.44310700	-5.09839300	2.20509400
H	-2.73725800	-1.75693200	-3.90057700	H	-3.09910500	-5.14970800	1.04901400
C	-4.35389400	-3.23734100	-1.32847100	C	-6.00052600	-4.45402700	-3.38259600
H	-5.18209200	-3.90352300	-1.11480200	H	-5.60233800	-5.31519000	-2.83524600
C	-3.62896700	-2.74593000	-0.22943100	H	-6.53858000	-4.83828900	-4.25586300
C	-4.08448100	-2.93456800	-2.66181500	H	-6.73124000	-3.94822000	-2.74216200
C	1.36879200	0.57529500	-4.26279300	C	1.45802700	0.97062400	4.49993800
H	1.47664100	-0.38862200	-4.76837200	H	1.36565000	-0.05074000	4.88419300
C	2.23301900	-2.35366000	-1.38077500	H	1.30035400	1.64379700	5.35362400
H	1.32473200	-2.20139000	-1.97782200	H	2.49135600	1.10947700	4.16812300
H	2.57195600	-3.37771000	-1.58306200	C	-3.93742600	-4.28918600	-4.76803200
H	2.99968000	-1.68083800	-1.77582000	H	-3.13346300	-3.65590000	-5.15476700
C	3.80527000	-0.24133200	0.47613400	H	-4.48779700	-4.69389700	-5.62585700
H	3.44129900	0.48578800	-0.26049000	H	-3.47345000	-5.12546700	-4.23476000
H	4.66698600	-0.74591900	0.02039800	C	-5.53011000	-2.35006800	-4.63106800
H	4.17984800	0.32903800	1.33144800	H	-6.21946500	-1.77997800	-3.99923300
C	-0.71480600	3.39763000	0.54574100	H	-6.09409300	-2.73921200	-5.48720400
H	-1.44679000	3.10084700	-0.21317500	H	-4.77804400	-1.65442900	-5.01581700
H	0.22167900	3.63477400	0.03488200	C	6.31513800	5.67449300	1.67815600
H	-1.08637200	4.33619400	0.97826500	C	6.64239100	5.00685200	0.49861600
C	-4.11066400	-3.21449200	1.16182100	C	5.64353000	4.65970000	-0.40715400
C	-4.88504600	-3.50441700	-3.83934600	C	4.31533200	4.98507800	-0.12809100

C	0.39389900	-4.11093700	0.47312000	C	3.98344000	5.65442500	1.05136500
H	-0.34154300	-4.40682900	1.22665600	C	4.98681100	5.99783300	1.95329000
H	1.02195900	-4.99032500	0.27393500	H	7.09628900	5.94572500	2.38259700
H	-0.15226800	-3.88884400	-0.44871200	H	7.67692600	4.75838800	0.28113500
C	0.87457900	-3.19180000	3.51390800	H	5.89217000	4.14644600	-1.33023100
H	-0.19608400	-3.41186500	3.43484100	H	2.94903800	5.91062400	1.25615700
H	1.01742600	-2.55934800	4.39580000	H	4.73099600	6.52138200	2.86964300
H	1.37665900	-4.14616600	3.71997700	C	3.22939000	4.57143500	-1.07687100
C	-0.97515300	0.55684600	-1.50757700	F	3.66725200	4.47199800	-2.34618300
H	-1.62242100	0.93869100	-0.73149500	F	2.19113000	5.42685900	-1.07002200
C	-5.54944300	-2.70285600	1.38742800	F	2.72033300	3.35144600	-0.75293200
H	-5.58064400	-1.60833200	1.36514900	C	-1.62516800	0.20121900	4.47932900
H	-5.92341300	-3.03361700	2.36397700	H	-1.85614900	0.84890800	5.33628400
H	-6.24156100	-3.06965800	0.62380200	H	-2.57480000	-0.21054300	4.12677100
C	0.05471000	1.15359800	-2.17665800	H	-1.02968800	-0.63284800	4.86609200

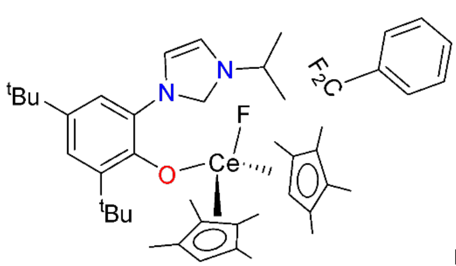


TS :

Ce	4.71730000	8.66346200	13.49150000	H	4.82619200	11.15699700	8.68254400
O	3.06414600	7.99629700	12.18841700	C	5.12232300	10.06777700	5.76442100
N	3.40007900	8.32586300	9.42042700	H	4.11462200	9.74963300	5.48311900
N	4.78970700	9.08656600	8.00111400	H	5.75643400	10.03792200	4.87262500
C	2.82030200	10.17193600	15.08148300	H	5.07070300	11.10921900	6.10139000
C	3.65905700	11.08394400	14.38097900	C	1.32784700	10.11117000	14.92797100
C	3.61195400	9.50027500	16.05295300	H	1.01532900	9.95633500	13.88902100
C	2.39195900	7.48066900	9.97169200	H	0.86933000	11.05109600	15.26259900
C	4.15921000	7.92713600	8.34439300	H	0.88584700	9.31138000	15.52678100

C	5.56887700	5.95375300	13.22671500	C	7.10556400	9.55596600	7.26359400
C	4.95414200	10.99334600	14.94891800	H	7.13345200	10.57306100	7.66851200
H	5.82023500	11.56984400	14.64619200	H	7.77404000	9.52427300	6.39727300
C	6.79050300	7.24559900	14.66834000	H	7.49425300	8.87368100	8.02418200
H	7.21153000	7.64512900	15.58389800	C	1.83141600	6.60715300	14.32747100
C	6.48314900	6.73980600	12.46098000	H	2.81823900	6.17609000	14.14418500
C	7.26035700	7.51560800	13.36355400	H	1.50140100	6.27375100	15.31853700
C	4.93872400	10.02496900	15.97824800	H	1.91953400	7.69213700	14.34964900
C	5.75979100	6.26625500	14.59760000	C	0.67865200	4.61033800	13.47587900
C	2.23570300	7.33001700	11.37839300	H	-0.12683100	4.17288600	12.88068400
C	1.58361200	6.82240700	9.05711600	H	0.45646800	4.39209800	14.52703600
H	1.79791900	6.99203000	8.00717700	H	1.60691000	4.09529400	13.20993800
C	0.39557300	5.83537400	10.84661300	C	-1.39117800	4.37763800	9.08664900
H	-0.40625200	5.19977700	11.20285200	H	-0.93953100	3.58803800	9.69696600
C	1.19803700	6.45824300	11.81732500	H	-1.99132600	3.89142000	8.30995400
C	0.55669700	5.97505700	9.47170300	H	-2.07586700	4.95196700	9.72019700
C	5.69051000	9.15488600	6.85133000	C	6.04281300	9.77271300	16.96238600
H	5.70506000	8.12566300	6.48024300	H	6.04181100	8.74533600	17.33899300
C	6.66511000	6.65887900	10.97465200	H	5.94026600	10.42986000	17.83699700
H	5.71864900	6.53587700	10.43925200	H	7.02700700	9.96922800	16.52565200
H	7.30470000	5.80874800	10.69895000	C	0.55235900	4.38969900	7.52757100
H	7.14098300	7.56218200	10.58223500	H	1.31849200	4.97632600	7.01182300
C	8.44677400	8.35956600	13.01478300	H	-0.06056500	3.89336500	6.76570600
H	8.32050500	8.85183900	12.04787700	H	1.06378300	3.61695200	8.11089500
H	9.35673100	7.74761000	12.95485800	C	-1.04688900	6.32798900	7.57434800
H	8.62327500	9.13408700	13.76750800	H	-1.68828400	6.96506100	8.19265500
C	3.19344700	12.05814100	13.33812600	H	-1.67471100	5.84385800	6.81676400
H	2.34744100	11.66655300	12.76336900	H	-0.33590200	6.97659800	7.05367300
H	3.98513800	12.30591600	12.62755100	C	9.27147400	13.59608900	14.15991100
H	2.85341800	12.99820100	13.79476400	C	9.80779300	12.53149300	13.42887500
C	0.81755600	6.13723200	13.27990800	C	9.03044000	11.85154300	12.50474500

C	-0.32718800	5.27156300	8.43577400	C	7.68656100	12.23736900	12.30017500
C	4.70267500	4.86737800	12.66082900	C	7.15026400	13.31784200	13.03715000
H	4.11776400	4.37408400	13.44220900	C	7.94359000	13.98546200	13.95634100
H	5.31843300	4.09321000	12.18512500	H	9.88681800	14.12267600	14.88315700
H	4.00401800	5.23162700	11.90012200	H	10.84138500	12.23492300	13.58003900
C	5.17985100	5.54699400	15.78220100	H	9.44847700	11.03265700	11.93106000
H	4.10382800	5.36593600	15.70221600	H	6.12228400	13.62272900	12.87623600
H	5.35249600	6.10903500	16.70512100	H	7.52811800	14.81614900	14.51870300
H	5.65829400	4.56709300	15.91226200	C	6.88054600	11.54990500	11.35225700
C	3.55072000	9.67519700	9.71306500	F	7.43487300	10.78039200	10.45333600
H	3.01575400	10.16321200	10.51152500	F	5.77548400	12.10339600	10.91822400
C	-0.53794300	6.80298500	13.59623600	F	5.94967000	10.01578200	12.22590000
H	-0.47383000	7.89060700	13.49209200	C	3.11228500	8.58369100	17.13150600
H	-0.84816300	6.57639800	14.62396400	H	2.88895200	9.14159900	18.05119400
H	-1.32503500	6.45067600	12.92241400	H	2.19612600	8.06382000	16.84051400
C	4.43378600	10.16030200	8.80648800	H	3.84992200	7.81968200	17.39434600

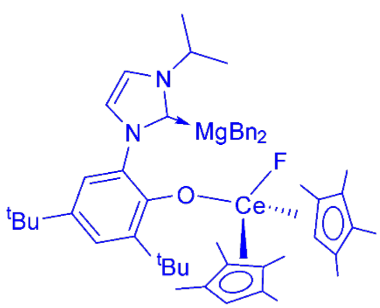


IRC forward :

Ce	0.22057000	-0.17526000	0.87701400	H	-0.88492300	2.59832700	-3.47569200
O	-1.68795800	-1.01660900	0.24879900	C	0.76396500	1.16690800	-5.81902000
N	-1.57258000	-0.41409400	-2.45292200	H	0.15157700	0.37371400	-6.25728900
N	-0.07003000	0.58209400	-3.57560000	H	1.66837900	1.28134200	-6.42515500
C	-1.22217900	1.83391300	2.14466000	H	0.20243300	2.10615200	-5.87740000
C	-0.12249000	2.47160600	1.50065500	C	-2.66459500	2.05507300	1.79765700
C	-0.71360400	1.08305600	3.24549500	H	-2.80487900	2.19075300	0.72096500
C	-2.43902400	-1.43343400	-1.95424600	H	-3.05075600	2.95874000	2.28831100

C	-0.40571100	-0.66282300	-3.12936800	H	-3.30021400	1.22194300	2.10792000
C	1.17825500	-2.72917200	0.38133000	C	2.01540700	1.89484000	-3.72778200
C	1.05000000	2.09675700	2.19585000	H	1.55650000	2.88815400	-3.78925600
H	2.05437500	2.42643400	1.95250700	H	2.97902500	1.94733100	-4.24416400
C	2.11522700	-1.65042900	2.16962300	H	2.18234900	1.66116500	-2.67522700
H	2.36874800	-1.37411800	3.18535800	C	-3.18500800	-2.05280000	2.39545200
C	2.18901300	-1.84873300	-0.10744700	H	-2.11797900	-2.27539000	2.41181400
C	2.77044900	-1.18145100	1.00281800	H	-3.59423300	-2.28398900	3.38599900
C	0.69866600	1.25408100	3.28008000	H	-3.30108500	-0.98282200	2.21661600
C	1.14492700	-2.61631100	1.79998700	C	-3.70165900	-4.36886200	1.65780500
C	-2.53977000	-1.65986200	-0.55671900	H	-4.28988200	-5.02482400	1.00940800
C	-3.18195600	-2.14532200	-2.88042200	H	-3.98523900	-4.58541000	2.69446900
H	-3.01467700	-1.92242000	-3.92996800	H	-2.64863000	-4.64055300	1.53188900
C	-4.25474800	-3.27726300	-1.09950000	C	-5.86089500	-4.91618500	-2.87454000
H	-4.98723400	-3.99636800	-0.75066300	H	-5.33621800	-5.65088800	-2.25445300
C	-3.53081100	-2.57814200	-0.11795400	H	-6.39420100	-5.46606400	-3.65732300
C	-4.10190400	-3.11542900	-2.47419600	H	-6.61216100	-4.41612000	-2.25361500
C	1.13238700	0.83007700	-4.37424500	C	1.59759800	0.85172800	4.41053600
H	1.65641400	-0.12985500	-4.35819100	H	1.34105900	-0.12693100	4.82801100
C	2.61057700	-1.72237000	-1.53850400	H	1.51931800	1.57615800	5.23257200
H	1.74784900	-1.66254800	-2.21336200	H	2.64739300	0.82757200	4.10510200
H	3.21424800	-2.58953700	-1.83875600	C	-3.90646000	-4.69870700	-4.40634300
H	3.21842700	-0.82738700	-1.69211200	H	-3.20561400	-4.03191800	-4.91745500
C	3.90840600	-0.20598100	0.95155700	H	-4.44781700	-5.26716400	-5.17185400
H	3.74419000	0.58168100	0.20954500	H	-3.31794800	-5.40396300	-3.81033800
H	4.84541000	-0.71088200	0.68346000	C	-5.71067200	-2.94825200	-4.39477600
H	4.06410100	0.27207700	1.92310600	H	-6.42289200	-2.37754200	-3.78949800
C	-0.19891700	3.41991000	0.34240300	H	-6.27579200	-3.50326900	-5.15280100
H	-0.82180900	3.03438700	-0.47151800	H	-5.06847500	-2.23280800	-4.91724800
H	0.79292600	3.60668400	-0.07308800	C	5.99203000	5.59646000	2.71942400
H	-0.62454200	4.38262300	0.65436900	C	6.53276500	4.43908600	2.14467800

C	-3.93250800	-2.87661600	1.34267700
C	-4.89167300	-3.91500000	-3.51683500
C	0.38705800	-3.67527600	-0.47026900
H	-0.56044100	-3.95610500	-0.00296700
H	0.95097400	-4.60046000	-0.65113100
H	0.15579800	-3.23736900	-1.44654300
C	0.37300900	-3.47873200	2.75371900
H	-0.54169400	-3.87537100	2.30655300
H	0.09529500	-2.94066800	3.66649800
H	0.97510000	-4.34289900	3.06474100
C	-1.94570000	0.92555200	-2.49387300
H	-2.85525000	1.29217300	-2.04328000
C	-5.43359900	-2.55428000	1.51871300
H	-5.63035800	-1.49704900	1.31188300
H	-5.74423600	-2.76233100	2.54947400
H	-6.07011800	-3.14663100	0.85571000
C	-0.98220000	1.55750100	-3.20715300
C	5.95828700	3.86820100	1.02291600
C	4.80099200	4.45691500	0.43974300
C	4.25877700	5.63380100	1.02854000
C	4.85399600	6.18230100	2.15047500
H	6.45174800	6.03612200	3.59915600
H	7.41462900	3.97927600	2.58239200
H	6.38096700	2.97260100	0.58019500
H	3.37711000	6.09043600	0.59174500
H	4.42830300	7.07845000	2.59349500
C	4.22987900	3.91227700	-0.71052400
F	4.61966200	2.76805500	-1.25190600
F	3.10595000	4.35863000	-1.25197700
F	1.06164200	0.84651400	-0.69830700
C	-1.51776500	0.40307600	4.31435600
H	-1.56019400	1.02300700	5.22021600
H	-2.54756500	0.22172400	4.00077000
H	-0.88492300	2.59832700	-3.47569201



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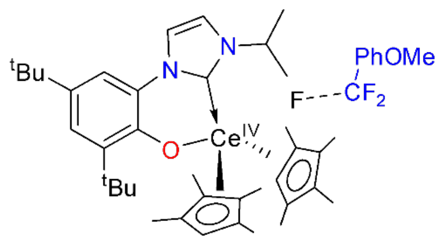
Ce	0.13468600	-0.18153600	1.20502600
O	-1.39865900	-1.03362600	-0.08265100
N	-1.36434900	-0.51081400	-2.82702300
N	0.02170200	0.31158400	-4.24143100
C	-1.76088400	1.50215000	2.40242400
C	-0.75533300	2.33253600	1.82845300
C	-1.19050600	0.83318700	3.52749000
H	-3.72311400	0.59114400	2.36578400
C	2.37670600	0.04535100	-4.93658100
H	2.74807100	0.72043000	-4.15768900
H	3.05477900	0.10321400	-5.79286200
H	2.40513600	-0.97851800	-4.55441100
C	-2.40707500	-2.45530300	2.10192800
H	-1.39528000	-2.75378800	1.81664500

C	-2.32639100	-1.38888100	-2.24082900	H	-2.60452800	-2.86000600	3.10077400
C	-0.65297900	-0.82554800	-3.95102300	H	-2.45837900	-1.36666700	2.17234300
C	1.44259300	-2.63445000	1.05642000	C	-3.35176500	-4.54806500	1.19689700
C	0.42416400	2.15851800	2.59282800	H	-4.12751900	-5.04541100	0.60910100
H	1.36932700	2.65848600	2.40930500	H	-3.46218700	-4.88201800	2.23510800
C	2.33869900	-1.12784700	2.52892000	H	-2.38220600	-4.89621700	0.82728100
H	2.62899000	-0.64347500	3.45259700	C	-6.31973500	-4.29121000	-2.81766200
C	2.23109700	-1.69889900	0.32092800	H	-5.88043700	-5.14157900	-2.28526800
C	2.80677600	-0.78022100	1.24103200	H	-7.04190500	-4.69551600	-3.53421400
C	0.16332300	1.25527800	3.65107200	H	-6.87519200	-3.68083200	-2.09707000
C	1.50602200	-2.27533200	2.43172100	C	1.05034000	0.99574300	4.83175900
C	-2.31096300	-1.64787400	-0.84150400	H	1.03210900	-0.04811100	5.16094200
C	-3.26037200	-1.96266300	-3.09505000	H	0.72549300	1.60212200	5.68787700
H	-3.23649200	-1.67196700	-4.14257800	H	2.08835600	1.26806700	4.62185900
C	-4.20029400	-3.10817700	-1.24910900	C	-4.53272700	-4.40688800	-4.55272500
H	-4.94349800	-3.78523200	-0.84553500	H	-3.79024900	-3.86921100	-5.15032800
C	-3.28202900	-2.55430900	-0.34239200	H	-5.24870100	-4.86167100	-5.24684400
C	-4.23201400	-2.84679300	-2.61564900	H	-4.01717400	-5.21277100	-4.01993100
C	0.96554100	0.43428000	-5.37138100	C	-5.98371900	-2.36184500	-4.35421600
H	0.60769800	-0.27425400	-6.12491300	H	-6.50519200	-1.67532800	-3.67882400
C	2.47959400	-1.71862000	-1.15556300	H	-6.72451400	-2.80178800	-5.03101200
H	1.69445500	-2.25603100	-1.69377200	H	-5.29318300	-1.77346700	-4.96566100
H	3.43127400	-2.21519800	-1.38646800	F	0.95500000	1.03309700	-0.23793100
H	2.52853700	-0.70434500	-1.56104900	C	-1.91693500	0.01680100	4.55675700
C	3.76488400	0.32221800	0.90594300	H	-2.06793300	0.60266100	5.47318300
H	3.37623200	0.96520400	0.11043200	H	-2.90458800	-0.30007000	4.21447300
H	4.72464700	-0.08537700	0.56541100	H	-1.36414500	-0.88382600	4.84567600
H	3.96638500	0.94772300	1.78059200	Mg	-0.73783000	-2.82386000	-4.96884500
C	-0.92442500	3.29686800	0.69306900	C	-1.67141800	-2.80944100	-6.92884700
H	-1.80814900	3.06821900	0.08931600	H	-2.74912400	-2.60818800	-6.90435100
H	-0.05153700	3.28860000	0.03529800	H	-1.52882300	-3.83244400	-7.30074800

H	-1.05568300	4.31931300	1.06925500
C	-3.44958300	-3.00846000	1.12373300
C	-5.25973800	-3.47143600	-3.56671100
C	0.79078700	-3.85413000	0.47453500
H	0.19418600	-4.38713500	1.21954800
H	1.54873400	-4.55722800	0.10814300
H	0.13806100	-3.62120200	-0.37296600
C	0.97728800	-3.05602600	3.59984100
H	0.03941800	-3.57315400	3.37978700
H	0.80655500	-2.41238400	4.46860200
H	1.69937000	-3.82286200	3.90904500
C	-1.13610300	0.79470000	-2.43753500
H	-1.61656600	1.23494500	-1.58171400
C	-4.83692700	-2.56425600	1.63426000
H	-4.94025000	-1.47511000	1.59058800
H	-4.97719500	-2.87989200	2.67477100
H	-5.65059000	-2.99650400	1.04533000
C	-0.25340900	1.31100800	-3.32623700
H	0.19218500	2.29067400	-3.37188800
C	0.91230400	1.83137700	-5.98001900
H	-0.11412800	2.11945900	-6.22028400
H	1.48231200	1.82934800	-6.91159500
H	1.35283800	2.58619300	-5.31890300
C	-3.20264900	1.47402200	1.98583800
H	-3.32294900	1.47797200	0.89807100
H	-3.73708200	2.35177500	2.37172700
C	0.28005000	-4.49513700	-4.04051800
H	-0.41650500	-5.34310700	-4.02960400
H	0.56992400	-4.28064700	-3.00546300
C	-0.96838100	-1.83069300	-7.78522500
C	0.31386100	-2.09997000	-8.31754100
C	-1.51379400	-0.56146700	-8.07817100
C	0.99672800	-1.16652900	-9.09216600
H	0.77084800	-3.06861900	-8.12098200
C	-0.83118300	0.37107600	-8.85574700
H	-2.50678600	-0.31989000	-7.70254500
C	0.43334100	0.08110500	-9.37089200
H	1.97688200	-1.42112500	-9.48977900
H	-1.29837600	1.32984100	-9.07242800
H	0.96151000	0.80405400	-9.98662000
C	1.45861100	-4.77829300	-4.89021600
C	1.35688800	-5.55549100	-6.06544000
C	2.73335800	-4.24177500	-4.60611000
C	2.45012400	-5.77490100	-6.89845700
H	0.39522200	-5.99921200	-6.31744700
C	3.82714200	-4.45937100	-5.43993700
H	2.86347100	-3.65700100	-3.69694300
C	3.69816900	-5.22644500	-6.59783600
H	2.32678800	-6.38605600	-7.79006500
H	4.79300800	-4.03271300	-5.17662100
H	4.55139300	-5.39912500	-7.24772700

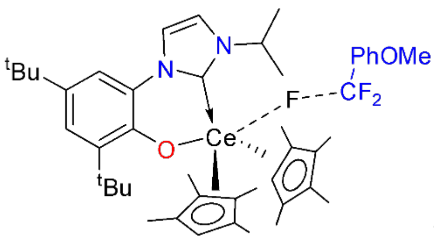


IRC reverse :

Ce	-0.93141	-0.31164	0.79326	H	3.11289	-0.57822	-2.21092
O	-2.74157	-1.16102	-0.31207	H	3.68918	1.08967	-2.38865
N	-1.00962	-1.59693	-2.52496	H	3.05144	0.22033	-3.79195
N	0.51061	-0.09267	-2.70004	C	-4.01536	1.60368	1.84926
C	-2.57789	1.86259	1.50105	H	-4.58239	1.25492	0.98224
C	-2.07906	2.18330	0.21184	H	-4.50876	2.51464	2.21568
C	-1.49625	1.94016	2.43032	H	-4.12733	0.84928	2.63652
C	-1.97544	-2.55865	-2.07631	C	1.24540	2.23254	-3.09091
C	-0.26033	-0.72865	-1.77599	H	1.35994	2.14190	-4.17649
C	-0.25976	-2.90170	1.79987	H	1.94446	2.99775	-2.74523
C	-0.69164	2.44382	0.35157	H	0.22796	2.57328	-2.88196
H	-0.03235	2.77829	-0.44269	C	-4.73702	-2.64312	1.50990
C	0.66755	-1.11592	2.89168	H	-4.35855	-3.60068	1.88301
H	0.85759	-0.34940	3.63596	H	-5.58673	-2.35025	2.13838
C	0.89543	-2.49085	1.07725	H	-3.95413	-1.89185	1.61752
C	1.47451	-1.38280	1.75832	C	-6.30935	-3.81187	-0.00363
C	-0.32599	2.31160	1.71603	H	-6.70717	-3.94621	-1.01529
C	-0.40522	-2.04505	2.92564	H	-7.13489	-3.47356	0.63189
C	-2.90258	-2.24376	-1.04631	H	-5.98700	-4.78871	0.37375
C	-2.01344	-3.77928	-2.74968	C	-4.20294	-6.94373	-2.84484
H	-1.22679	-3.99554	-3.46772	H	-4.20617	-7.16987	-1.77334
C	-4.00731	-4.34101	-1.58901	H	-4.15181	-7.89610	-3.38339
H	-4.82888	-5.02452	-1.42012	H	-5.15856	-6.47260	-3.09856
C	-3.99992	-3.14180	-0.87214	C	1.00418	2.67621	2.30941
C	-3.01685	-4.71415	-2.50533	H	1.32066	1.98516	3.09835
C	1.53698	0.90983	-2.38487	H	0.97390	3.67673	2.76280

H	1.46006	1.06228	-1.30466
C	1.49217	-3.22172	-0.09018
H	0.72403	-3.64688	-0.74364
H	2.12638	-4.05452	0.24543
H	2.11980	-2.56785	-0.70326
C	2.77604	-0.71193	1.42234
H	2.90010	-0.54343	0.34639
H	3.63322	-1.31962	1.74299
H	2.86637	0.25841	1.91935
C	-2.88047	2.28518	-1.05455
H	-3.45123	1.37302	-1.26010
H	-2.22786	2.46113	-1.91534
H	-3.59449	3.11783	-1.01250
C	-5.18186	-2.76838	0.04104
C	-3.00897	-6.06271	-3.23753
C	-1.07798	-4.12556	1.50791
H	-2.04504	-4.09397	2.01647
H	-0.56375	-5.03395	1.85161
H	-1.27751	-4.25340	0.43922
C	-1.41760	-2.17841	4.02869
H	-2.42982	-2.37593	3.65735
H	-1.45909	-1.27038	4.63817
H	-1.16467	-3.00693	4.70377
C	-0.71387	-1.47552	-3.87542
H	-1.23522	-2.03867	-4.63182
C	-5.77687	-1.42895	-0.43889
H	-5.02131	-0.64198	-0.42467
H	-6.60879	-1.12820	0.20925
H	-6.16105	-1.52239	-1.46058
C	0.25008	-0.53194	-3.98361
H	0.74795	-0.13901	-4.85578
H	1.79064	2.69423	1.54973
C	-1.61882	1.82608	3.92236
H	-2.37532	1.09258	4.22175
H	-1.91536	2.78357	4.37329
H	-0.67319	1.53380	4.38954
C	-1.71601	-6.82759	-2.89194
H	-0.82262	-6.26672	-3.18445
H	-1.68786	-7.79302	-3.41121
H	-1.65126	-7.01738	-1.81555
C	-3.06831	-5.83000	-4.76025
H	-3.97857	-5.28808	-5.03757
H	-3.06339	-6.78595	-5.29723
H	-2.21158	-5.24842	-5.11587
C	6.34506	5.90182	2.50419
C	6.96515	4.78564	1.92174
C	6.36147	4.12695	0.86489
C	5.13041	4.57131	0.36810
C	4.51565	5.67932	0.94564
C	5.11462	6.34930	2.00964
H	7.92108	4.45912	2.31769
H	6.84873	3.26789	0.41504
H	3.56369	6.03058	0.56106
H	4.61869	7.21160	2.43965
C	4.45556	3.82277	-0.73635
F	5.33781	3.27458	-1.59706
F	3.62549	4.60764	-1.45473
F	3.69938	2.79428	-0.27176
O	7.01516	6.47494	3.53012
C	6.43760	7.60161	4.16315
H	5.46581	7.35861	4.61076
H	7.13277	7.89192	4.95176

C	2.93005	0.37502	-2.71435
H	6.31567	8.43871	3.46431

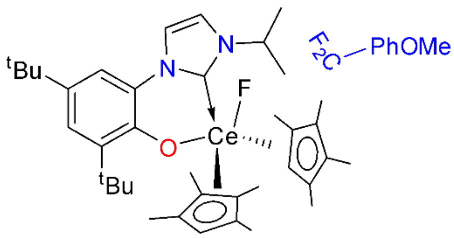


TS :

Ce	5.18201	8.31051	13.20472
O	3.19727	7.27636	12.54741
N	4.40010	6.58963	10.08322
N	5.77433	8.08701	9.41516
C	3.07509	10.25356	13.78193
C	4.15423	10.89717	13.11247
C	3.50788	9.90212	15.08674
C	3.57756	5.68850	10.82552
C	5.23959	7.56276	10.55680
C	5.64445	5.59920	14.16880
C	5.23311	10.96010	14.02530
H	6.20580	11.38060	13.82378
C	6.88994	7.27221	15.10836
H	7.25994	8.01327	15.80878
C	6.74995	5.86341	13.31083
C	7.53975	6.87511	13.91371
C	4.85823	10.33937	15.23479
C	5.72244	6.48355	15.27933
C	2.86883	6.13879	11.97222
C	3.43587	4.39842	10.31652
H	4.08182	4.09571	9.49649
C	1.67943	4.01261	11.85708
H	0.89750	3.37098	12.24040
C	1.79705	5.29076	12.41024
H	8.44176	7.71553	9.36156
H	8.88038	9.34872	8.83231
H	7.98006	8.28379	7.74576
C	1.68263	10.15794	13.24323
H	1.66831	9.82478	12.20064
H	1.18119	11.13551	13.27834
H	1.07118	9.45999	13.81774
C	6.29769	10.35668	8.60270
H	6.15240	10.13543	7.53939
H	7.03072	11.16531	8.67394
H	5.35032	10.71764	9.01086
C	1.32302	6.25909	14.72202
H	1.75957	5.41326	15.26483
H	0.53989	6.68768	15.35950
H	2.09714	7.00802	14.55919
C	-0.33567	4.72757	13.71859
H	-0.87866	4.38711	12.83052
H	-1.07239	5.16010	14.40448
H	0.10008	3.85316	14.21484
C	1.31543	1.26236	11.01644
H	1.50947	1.18227	12.09122
H	1.28766	0.24639	10.60791
H	0.32045	1.69934	10.87986
C	5.65355	10.35224	16.50722

C	2.50622	3.50798	10.84755
C	6.79780	9.13604	9.37345
H	6.95598	9.39655	10.41908
C	7.13932	5.06397	12.10210
H	6.26634	4.66234	11.58002
H	7.77437	4.20968	12.37720
H	7.70398	5.66756	11.38486
C	8.89195	7.32028	13.45668
H	8.90086	7.62993	12.40815
H	9.62814	6.51349	13.57338
H	9.23393	8.16590	14.05793
C	4.09181	11.52970	11.75250
H	3.57250	10.89869	11.02100
H	5.09462	11.73356	11.36764
H	3.55129	12.48655	11.77715
C	0.72070	5.79398	13.38721
C	2.40160	2.07829	10.30198
C	4.72119	4.42613	14.06472
H	3.74083	4.63244	14.49901
H	5.14088	3.56551	14.60623
H	4.55952	4.11095	13.03121
C	4.87431	6.40988	16.51523
H	3.80214	6.37873	16.29821
H	5.05821	7.26241	17.17510
H	5.10721	5.50428	17.09229
C	4.40615	6.53905	8.69641
H	3.76590	5.87376	8.14137
C	-0.00908	6.96336	12.69678
H	0.69547	7.74373	12.40896
H	-0.76075	7.40115	13.36551
H	-0.52195	6.61311	11.79425
H	5.54677	9.42833	17.08420
H	5.33159	11.17183	17.16564
H	6.71981	10.49740	16.30753
C	2.64118	9.41265	16.20934
H	1.75610	8.88342	15.84944
H	2.28519	10.25412	16.82090
H	3.17496	8.73665	16.88372
C	3.74843	1.35384	10.49492
H	4.56323	1.86846	9.97580
H	3.69670	0.33111	10.10245
H	4.01296	1.29904	11.55595
C	2.05925	2.11733	8.79933
H	1.10482	2.62664	8.62937
H	1.98085	1.10134	8.39424
H	2.82650	2.64382	8.22241
C	10.06267	12.45530	15.75217
C	10.64095	11.31077	15.16886
C	10.13825	10.79606	13.99568
C	9.02974	11.41105	13.36037
C	8.47035	12.57057	13.94154
C	8.97774	13.08657	15.12152
H	11.48918	10.85201	15.66594
H	10.59548	9.92162	13.54759
H	7.63988	13.06995	13.45501
H	8.52884	13.97778	15.54389
C	8.50808	10.88146	12.15731
F	9.23467	10.06270	11.43601
F	7.70273	11.60787	11.41683
F	7.10411	9.42651	12.48093
O	10.62633	12.87017	16.90285
C	10.08238	14.00539	17.55621

C	5.28010	7.48112	8.27731
H	5.57029	7.77120	7.28000
C	8.09972	8.58423	8.79263
H	9.03368	13.84341	17.83217
H	10.67629	14.14196	18.46020
H	10.16234	14.90357	16.93199



IRC forward :

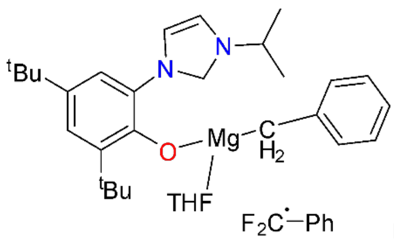
Ce	-0.25279	0.06936	0.50340
O	-2.16116	-1.00049	-0.11397
N	-1.06960	-1.55039	-2.66158
N	0.39125	-0.08886	-3.23355
C	-2.16132	2.13426	0.83046
C	-0.90275	2.72825	0.52430
C	-2.09057	1.61174	2.15015
C	-1.92957	-2.45784	-1.97320
C	-0.18918	-0.64490	-2.12731
C	0.49706	-2.54079	1.32171
C	-0.07110	2.57300	1.65671
H	0.95554	2.91165	1.73202
C	1.34006	-0.80292	2.54729
H	1.50813	-0.10124	3.35512
C	1.63488	-2.01212	0.63681
C	2.17912	-0.96206	1.42411
C	-0.78999	1.89317	2.66488
C	0.31183	-1.78831	2.50906
C	-2.56813	-2.07929	-0.76458
C	-2.16083	-3.69285	-2.57700
H	-1.56349	-3.96252	-3.44323
C	-3.85964	-4.13089	-0.98575
H	-4.65254	-4.76684	-0.61628
H	3.02275	-0.62658	-3.21920
H	3.58965	0.98323	-3.68711
H	2.67537	-0.00082	-4.84226
C	-3.36781	2.19775	-0.06031
H	-3.27204	1.56942	-0.95355
H	-3.53974	3.22520	-0.40339
H	-4.26998	1.87539	0.46420
C	1.07683	2.14075	-4.05047
H	0.98233	1.92773	-5.12146
H	1.84141	2.91258	-3.93154
H	0.12703	2.54928	-3.69590
C	-3.84354	-2.38589	2.13317
H	-3.47615	-3.37286	2.43579
H	-4.50860	-2.02124	2.92515
H	-2.99456	-1.70815	2.05347
C	-5.76434	-3.46105	1.00183
H	-6.36691	-3.58155	0.09513
H	-6.42248	-3.06799	1.78433
H	-5.42805	-4.45113	1.32877
C	-4.41973	-6.76466	-2.05377
H	-4.18843	-6.95426	-1.00028
H	-4.52213	-7.73581	-2.54963
H	-5.39239	-6.26397	-2.10650

C	-3.64475	-2.91515	-0.32942
C	-3.11340	-4.57788	-2.07987
C	1.48060	0.90493	-3.24846
H	1.62760	1.18095	-2.20594
C	2.27530	-2.59577	-0.58676
H	1.53986	-3.00938	-1.28224
H	2.96460	-3.40933	-0.31991
H	2.85737	-1.84290	-1.12529
C	3.45067	-0.21758	1.15954
H	3.44188	0.27633	0.18485
H	4.31272	-0.89586	1.19395
H	3.60941	0.55640	1.91589
C	-0.56882	3.48461	-0.72494
H	-1.03514	3.03929	-1.61087
H	0.50978	3.51217	-0.88929
H	-0.93116	4.52038	-0.66645
C	-4.59647	-2.48271	0.79805
C	-3.31736	-5.94694	-2.74075
C	-0.23083	-3.79310	0.93819
H	-1.25733	-3.80883	1.31095
H	0.28239	-4.67526	1.34559
H	-0.28365	-3.92340	-0.14590
C	-0.62874	-2.10335	3.63537
H	-1.28281	-2.94180	3.38993
H	-1.27086	-1.26012	3.91177
H	-0.06568	-2.38113	4.53529
C	-1.04563	-1.52968	-4.04879
H	-1.71067	-2.12749	-4.64909
C	-5.20622	-1.11896	0.42405
H	-4.42407	-0.37833	0.25764
H	-5.86831	-0.76318	1.22299

C	-0.35813	1.73994	4.09278
H	-0.59142	0.75727	4.51438
H	-0.86221	2.48239	4.72634
H	0.71800	1.90463	4.19983
C	-3.23402	1.09100	2.96738
H	-4.01925	0.65179	2.34979
H	-3.69151	1.90058	3.55367
H	-2.91710	0.32633	3.68354
C	-2.00528	-6.75254	-2.66533
H	-1.18375	-6.23836	-3.17422
H	-2.12776	-7.73388	-3.13882
H	-1.70422	-6.91131	-1.62468
C	-3.71234	-5.75844	-4.21884
H	-4.64264	-5.18733	-4.30535
H	-3.86207	-6.72988	-4.70450
H	-2.93904	-5.22510	-4.78110
C	5.20601	5.12982	2.70406
C	5.83729	3.97206	2.21453
C	5.46802	3.42785	1.00312
C	4.43744	4.02385	0.22941
C	3.81233	5.18901	0.73007
C	4.18920	5.73188	1.95061
H	6.61855	3.51835	2.81616
H	5.96076	2.53348	0.63724
H	3.02245	5.65988	0.15465
H	3.68273	6.62109	2.30884
C	4.10679	3.51525	-1.04276
F	4.48734	2.30009	-1.43357
F	3.01160	3.91323	-1.69102
F	1.35689	1.12662	-0.33603
O	5.65062	5.57927	3.90500

H	-5.80061	-1.20231	-0.49253
C	-0.11868	-0.61315	-4.40378
H	0.20104	-0.28788	-5.38078
C	2.76462	0.27271	-3.78451

C	5.04684	6.73585	4.44829
H	3.97385	6.58742	4.62602
H	5.54516	6.91729	5.40168
H	5.18617	7.60923	3.79800

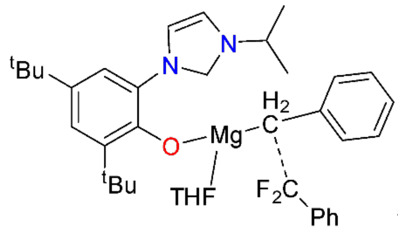


IRC reverse:

O	-1.65685	-0.79675	-0.03127
N	-0.43365	-2.45590	-2.01494
N	1.22815	-1.44804	-2.93858
C	-1.39948	-2.93954	-1.06769
C	0.48779	-1.47014	-1.80272
C	-2.00654	-2.05858	-0.12510
C	-1.71862	-4.29547	-1.12343
H	-1.16584	-4.93037	-1.81056
C	-3.33159	-3.97731	0.58963
H	-4.09881	-4.38044	1.23754
C	-3.02475	-2.62093	0.70769
C	-2.69489	-4.85048	-0.30085
C	2.34397	-0.51387	-3.15692
H	2.56406	-0.10328	-2.16683
C	-3.75769	-1.73621	1.73166
C	-3.01174	-6.34973	-0.38542
C	-0.27401	-3.00916	-3.27625
H	-0.92315	-3.77927	-3.65880
C	-4.45528	-0.56386	1.01311

H	-1.40644	-6.93997	0.97468
C	-3.46912	-6.70500	-1.81400
H	-4.36843	-6.14294	-2.08702
H	-3.69778	-7.77463	-1.89257
H	-2.69620	-6.47765	-2.55540
C	1.11010	5.50556	5.67108
C	0.09814	6.31160	5.13707
C	-0.01013	6.49776	3.76929
C	0.91018	5.86478	2.89335
C	1.93669	5.05183	3.44140
C	2.02168	4.88005	4.81305
H	1.18623	5.36469	6.74491
H	-0.61473	6.79571	5.79878
H	-0.79672	7.12127	3.35745
H	2.64437	4.56131	2.78160
H	2.80444	4.24715	5.22125
C	0.84110	6.09146	1.50870
F	1.54970	5.38718	0.62978
F	-0.20873	6.66730	0.92895

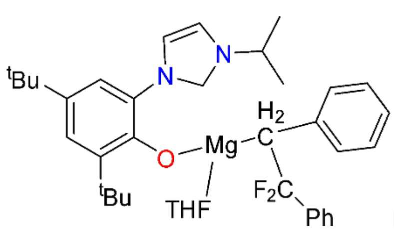
H	-3.72584	0.04247	0.47466	C	1.54426	0.59698	1.28726
H	-4.97497	0.07129	1.74108	H	1.53653	-0.19829	2.04438
H	-5.19872	-0.93539	0.29875	H	1.24729	1.52872	1.78406
C	0.77640	-2.37539	-3.85575	C	2.87441	0.71624	0.65695
H	1.21967	-2.50943	-4.82959	C	3.69859	-0.41312	0.44468
C	3.58550	-1.25219	-3.64840	C	3.37830	1.94918	0.18385
H	3.83796	-2.07760	-2.97800	C	4.93154	-0.31638	-0.19384
H	4.43205	-0.56115	-3.66614	H	3.35814	-1.38196	0.80601
H	3.45394	-1.64889	-4.66126	C	4.60823	2.04502	-0.46295
C	1.92225	0.61760	-4.09241	H	2.79436	2.85235	0.35018
H	1.67386	0.23951	-5.09030	C	5.39992	0.91326	-0.66259
H	2.73828	1.33874	-4.19632	H	5.53832	-1.21093	-0.31915
H	1.04934	1.14022	-3.69202	H	4.95868	3.01834	-0.80095
C	-2.75388	-1.18983	2.76713	H	6.36556	0.98969	-1.15463
H	-2.27528	-2.01109	3.31199	Mg	0.10236	-0.01720	-0.20394
H	-3.27002	-0.55582	3.49865	C	-0.07590	3.04532	-0.92272
H	-1.97698	-0.59839	2.28084	O	-0.51105	1.70298	-1.25860
C	-4.83988	-2.50632	2.50452	C	-1.80658	1.74660	-1.90818
H	-5.61174	-2.91253	1.84127	C	-2.38741	3.09305	-1.50944
H	-5.33445	-1.82419	3.20465	C	-1.13868	3.97940	-1.49414
H	-4.42193	-3.33062	3.09285	H	-0.00876	3.11128	0.16692
C	-4.12649	-6.76364	0.58521	H	0.92070	3.19999	-1.34275
H	-3.84993	-6.57327	1.62756	H	-1.65440	1.67903	-2.99327
H	-4.32262	-7.83683	0.48674	H	-2.36485	0.87584	-1.55957
H	-5.06351	-6.23579	0.37796	H	-3.15450	3.43923	-2.20715
C	-1.75027	-7.16571	-0.04003	H	-2.83382	3.03245	-0.51096
H	-0.92537	-6.94699	-0.72568	H	-0.87670	4.28235	-2.51398
H	-1.95639	-8.24122	-0.09991	H	-1.24672	4.88397	-0.89176



TS:

O	2.78690	7.34007	12.49284
N	3.97107	6.72992	9.96031
N	4.75692	8.52619	9.07039
C	3.50997	5.72677	10.87914
C	4.43150	7.97761	10.26902
C	2.85042	6.09055	12.08930
C	3.69761	4.39510	10.50995
H	4.28933	4.17956	9.62444
C	2.42951	3.70982	12.39555
H	1.98204	2.91891	12.98279
C	2.24360	5.02457	12.82527
C	3.17236	3.35040	11.26390
C	5.31498	9.87697	8.91148
H	5.28100	10.30764	9.91624
C	1.39203	5.32732	14.07119
C	3.42091	1.89546	10.84366
C	4.00423	6.52456	8.58940
H	3.64004	5.62118	8.12954
C	0.23423	6.27116	13.68878
H	0.62261	7.20681	13.28425
H	-0.37842	6.49530	14.57068
H	-0.41407	5.80710	12.93691
C	4.50849	7.65307	8.03147
H	4.68935	7.89783	6.99691
C	6.77066	9.81230	8.45426
H	7.37110	9.21529	9.14512
H	5.35135	1.75612	11.85853
C	2.87292	1.66137	9.42205
H	1.79607	1.85622	9.38138
H	3.04438	0.62500	9.10772
H	3.35798	2.31229	8.68731
C	8.17996	14.25547	15.50821
C	7.92417	14.44057	14.14583
C	7.96291	13.36968	13.26372
C	8.26955	12.06900	13.72844
C	8.52465	11.88972	15.10815
C	8.48193	12.97117	15.97573
H	8.14890	15.09762	16.19352
H	7.70106	15.43562	13.76745
H	7.77783	13.52406	12.20508
H	8.75965	10.89672	15.47710
H	8.69231	12.81532	17.03116
C	8.18535	10.94065	12.84948
F	8.87883	9.83859	13.19112
F	8.36683	11.19317	11.52555
C	6.13060	10.08217	12.72131
H	5.69750	11.06931	12.84169
H	6.44464	9.78366	11.72611
C	5.97258	9.08654	13.73887
C	5.48790	9.39712	15.05377
C	6.33371	7.71314	13.51558
C	5.38891	8.42766	16.03768

H	7.19665	10.81877	8.42141
H	6.85462	9.37550	7.45326
C	4.44262	10.72216	7.98546
H	4.45819	10.34538	6.95733
H	4.81596	11.75006	7.96435
H	3.40434	10.73926	8.32899
C	2.25636	5.98013	15.16569
H	3.06087	5.30655	15.47755
H	1.64337	6.20511	16.04756
H	2.71135	6.90434	14.80987
C	0.76462	4.06069	14.67459
H	0.11335	3.54097	13.96297
H	0.15088	4.34181	15.53730
H	1.52106	3.35305	15.03119
C	2.73773	0.89418	11.78536
H	3.10867	0.98273	12.81186
H	2.94124	-0.12787	11.44811
H	1.65060	1.02635	11.80145
C	4.93531	1.60779	10.85668
H	5.47889	2.26602	10.17132
H	5.13522	0.57309	10.55341
H	5.26082	10.43394	15.29100
C	6.22024	6.75866	14.52018
H	6.76648	7.43526	12.55596
C	5.74936	7.09484	15.79157
H	5.03709	8.71565	17.02606
H	6.51785	5.73509	14.30581
H	5.66761	6.34475	16.57106
Mg	4.13725	8.70166	12.30270
C	2.76804	11.35614	13.38695
O	2.75687	10.26591	12.42696
C	1.41019	10.06023	11.92423
C	0.51235	10.68152	12.97890
C	1.33908	11.89302	13.41869
H	3.07804	10.94517	14.35280
H	3.50423	12.09665	13.06383
H	1.31868	10.57668	10.95990
H	1.28702	8.98464	11.78799
H	-0.47026	10.95152	12.58337
H	0.36963	9.98352	13.81034
H	1.22062	12.71462	12.70394
H	1.06724	12.26700	14.40893

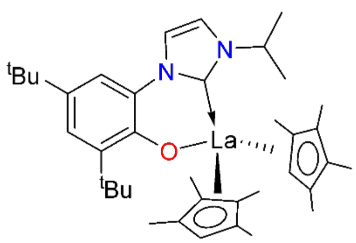


IRC forward:

O	-2.44437	-0.94289	0.34445
N	-0.91466	-1.14018	-2.06136
N	-0.28765	0.80781	-2.72733
C	-1.27120	-2.27740	-1.25878
H	1.24125	-5.89364	-0.39328
C	-1.05731	-6.28218	-2.97295
H	-2.14852	-6.28937	-3.06524
H	-0.67748	-7.24426	-3.33694

C	-0.66002	0.12558	-1.61637
C	-2.07779	-2.12698	-0.09386
C	-0.80984	-3.52298	-1.68174
H	-0.13117	-3.56484	-2.52922
C	-2.01660	-4.55699	0.08281
H	-2.32157	-5.45345	0.60648
C	-2.47704	-3.33093	0.56549
C	-1.16996	-4.69567	-1.02390
C	0.07462	2.23203	-2.71876
H	0.18337	2.48271	-1.65840
C	-3.39527	-3.26621	1.79884
C	-0.63072	-6.04767	-1.51034
C	-0.72281	-1.22189	-3.43212
H	-0.90547	-2.12518	-3.99008
C	-4.71972	-2.56766	1.43070
H	-4.52996	-1.55750	1.06510
H	-5.37440	-2.50949	2.30903
H	-5.24940	-3.12853	0.65238
C	-0.32344	0.00503	-3.84998
H	-0.07509	0.35751	-4.83833
C	1.41982	2.45481	-3.40493
H	2.19143	1.81848	-2.96472
H	1.72492	3.49813	-3.28364
H	1.36977	2.25052	-4.47998
C	-1.04289	3.07701	-3.32802
H	-1.20303	2.82788	-4.38263
H	-0.78487	4.13887	-3.26941
H	-1.98102	2.92066	-2.78880
C	-2.69773	-2.49369	2.93656
H	-1.77001	-2.99572	3.23243
H	-3.34972	-2.44443	3.81749
H	-0.67141	-5.50277	-3.63810
C	5.23007	5.21414	3.14196
C	5.91686	5.04749	1.94016
C	5.81269	3.84951	1.23611
C	5.02121	2.81116	1.73156
C	4.33473	2.97815	2.93724
C	4.44015	4.17758	3.63786
H	5.31269	6.14785	3.69198
H	6.54067	5.84852	1.55247
H	6.35530	3.71011	0.30667
H	3.72130	2.16966	3.31992
H	3.90456	4.30095	4.57517
C	4.87170	1.52850	0.95152
F	4.86173	0.46554	1.82138
F	5.97924	1.35426	0.14860
C	3.63599	1.43421	0.04738
H	3.72752	2.24541	-0.68454
H	3.76220	0.48990	-0.50079
C	2.30815	1.49112	0.74049
C	1.53161	2.68500	0.77437
C	1.81090	0.37841	1.48364
C	0.31543	2.75336	1.41301
H	1.93567	3.58378	0.30847
C	0.60948	0.42324	2.14893
H	2.42319	-0.51746	1.55557
C	-0.29500	1.57610	2.04203
H	-0.20759	3.70738	1.45850
H	0.29935	-0.43195	2.74663
H	-0.94228	1.76336	2.90457
Mg	-1.39167	0.67114	0.35886
C	-3.32580	3.14297	0.74271

H	-2.45722	-1.47677	2.62351	O	-2.98832	1.99055	-0.06977
C	-3.74910	-4.65993	2.34085	C	-4.18238	1.46033	-0.70256
H	-4.27156	-5.27210	1.59734	C	-5.32860	1.99170	0.14054
H	-4.41568	-4.55084	3.20329	C	-4.81742	3.38392	0.52200
H	-2.86437	-5.20966	2.68023	H	-3.09416	2.89789	1.78436
C	-1.15707	-7.21930	-0.66992	H	-2.69665	3.98161	0.43194
H	-0.85570	-7.13501	0.37948	H	-4.22832	1.83896	-1.73181
H	-0.75149	-8.16124	-1.05468	H	-4.07889	0.37364	-0.70853
H	-2.24944	-7.28967	-0.70803	H	-6.27413	2.01492	-0.40748
C	0.90840	-6.05103	-1.42434	H	-5.46271	1.36866	1.03119
H	1.35114	-5.26096	-2.03924	H	-4.97645	4.08635	-0.30354
H	1.31304	-7.00920	-1.77190	H	-5.30134	3.79543	1.41150

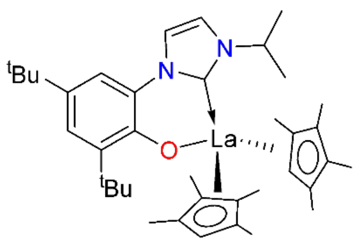


singlet :

O	4.02387	7.02154	12.77356	H	6.50640	7.42257	8.86096
N	6.23001	7.33573	11.00612	C	1.16537	6.43595	11.91418
N	7.48857	8.99139	11.53261	H	1.75725	7.27600	12.28076
C	3.34377	9.52446	15.26572	H	0.18429	6.45784	12.40338
C	3.99063	10.18314	14.18879	H	1.00877	6.56592	10.83776
C	4.23220	9.51775	16.38532	C	7.56627	8.86781	10.15838
C	5.36058	6.19355	10.98940	H	8.15730	9.52144	9.53664
C	6.66289	8.05994	12.08469	C	9.74506	9.69854	12.22816
C	6.29109	5.07280	15.10067	H	9.96525	8.67743	12.55022
C	5.27931	10.56163	14.64285	H	10.29239	10.39082	12.87483
H	5.99749	11.14314	14.07410	H	10.12410	9.82415	11.20837
C	6.73022	6.65601	16.69544	C	1.92871	9.02091	15.26606

H	6.66461	7.25382	17.59899
C	7.48366	5.75613	14.73101
C	7.75876	6.73734	15.72527
C	5.43269	10.16997	15.99852
C	5.81927	5.63503	16.31971
C	4.20081	6.14012	11.80968
C	5.66200	5.18224	10.07782
H	6.60280	5.24038	9.53692
C	3.59480	4.12911	10.58367
H	2.88152	3.33611	10.40200
C	3.25751	5.10592	11.52418
C	4.79782	4.11024	9.86788
C	8.24585	9.98647	12.30069
H	7.90528	9.85836	13.33264
C	8.38039	5.37872	13.58743
H	7.81286	5.01892	12.72345
H	9.07348	4.57511	13.87421
H	8.98974	6.22317	13.25048
C	8.98454	7.60156	15.80878
H	9.25517	8.04539	14.84339
H	9.85888	7.02643	16.14229
H	8.84703	8.41932	16.52282
C	3.40447	10.47093	12.83582
H	4.14070	10.95941	12.18987
H	2.53913	11.14184	12.90786
H	3.07440	9.56115	12.32223
C	1.87467	5.09702	12.20160
C	5.17750	2.99854	8.88043
C	5.72437	3.87123	14.40018
H	4.72124	3.63297	14.76380
H	6.34754	2.98315	14.57311
H	1.57859	8.80719	14.25249
H	1.23983	9.75936	15.69905
H	1.81044	8.10272	15.85327
C	7.90977	11.40445	11.84200
H	8.26837	11.59246	10.82448
H	8.39188	12.13319	12.50026
H	6.83132	11.58012	11.86251
C	2.00160	4.89178	13.72254
H	2.47253	3.92886	13.94586
H	1.00934	4.89793	14.18957
H	2.59754	5.68515	14.17509
C	0.96889	3.97629	11.66686
H	0.80439	4.05975	10.58716
H	-0.00952	4.04375	12.15452
H	1.37009	2.97912	11.87926
C	4.09524	1.91465	8.78087
H	3.91624	1.42885	9.74583
H	4.41321	1.14006	8.07483
H	3.14423	2.31986	8.41895
C	6.58170	10.53709	16.89297
H	6.82852	9.74618	17.60919
H	6.35842	11.43804	17.48050
H	7.48688	10.75112	16.31448
C	3.88268	9.05778	17.77155
H	3.23571	8.17348	17.76687
H	3.34219	9.83741	18.32619
H	4.77363	8.81039	18.35687
C	6.48649	2.32693	9.34092
H	7.31303	3.04270	9.39482
H	6.77923	1.53314	8.64335
H	6.36777	1.88126	10.33395

H	5.65245	4.00675	13.31564
C	4.64831	5.15931	17.13375
H	4.36835	5.89981	17.88925
H	4.88344	4.22864	17.66697
H	3.75963	4.95383	16.52518
C	6.76643	7.82836	9.82475
C	5.38306	3.59838	7.47536
H	4.46633	4.07868	7.11747
H	5.66091	2.81677	6.75838
H	6.17908	4.35003	7.46778
La	5.40619	7.73965	14.47758



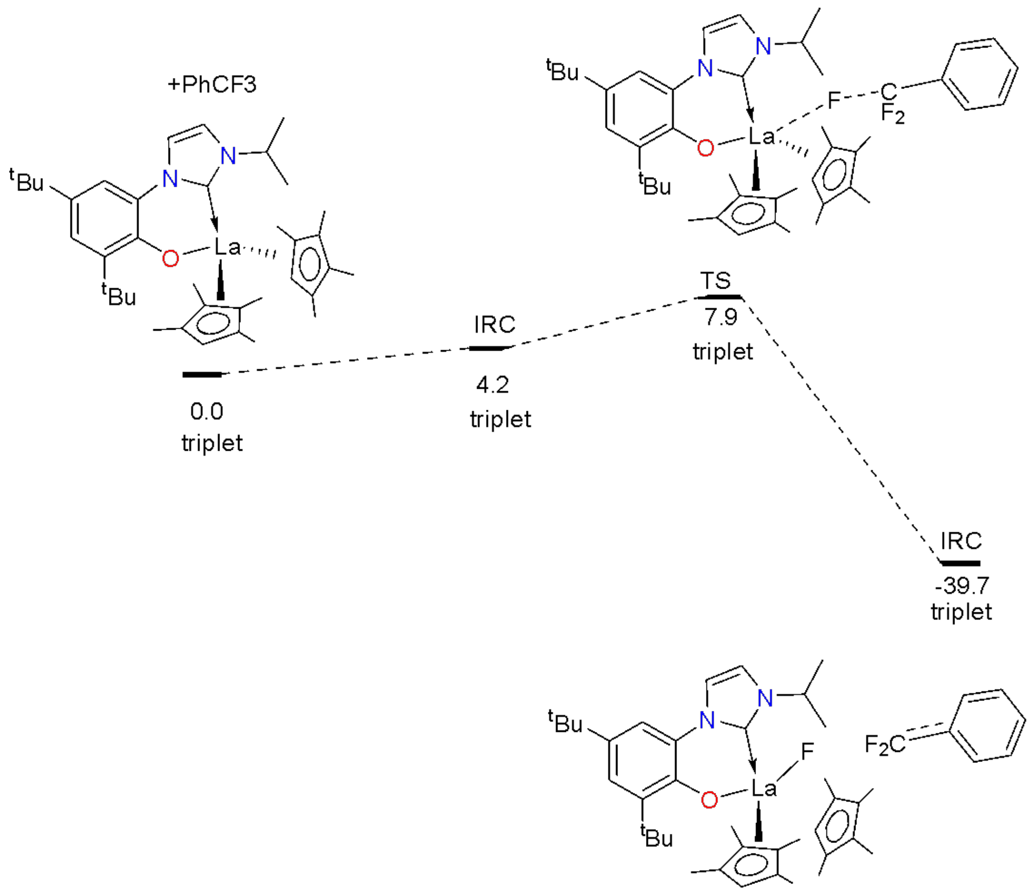
triplet :

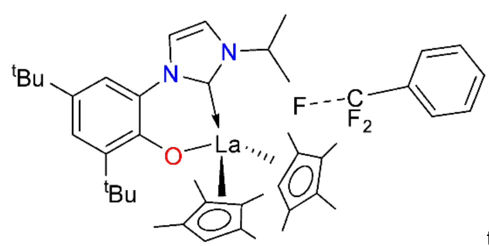
O	4.02387	7.02154	12.77356
N	6.23001	7.33573	11.00612
N	7.48857	8.99139	11.53261
C	3.34377	9.52446	15.26572
C	3.99063	10.18314	14.18879
C	4.23220	9.51775	16.38532
C	5.36058	6.19355	10.98940
C	6.66289	8.05994	12.08469
C	6.29109	5.07280	15.10067
C	5.27931	10.56163	14.64285
H	5.99749	11.14314	14.07410
C	6.73022	6.65601	16.69544
H	6.66461	7.25382	17.59899
C	7.48366	5.75613	14.73101
C	7.75876	6.73734	15.72527
C	5.43269	10.16997	15.99852
C	5.81927	5.63503	16.31971
H	6.50640	7.42257	8.86096
C	1.16537	6.43595	11.91418
H	1.75725	7.27600	12.28076
H	0.18429	6.45784	12.40338
H	1.00877	6.56592	10.83776
C	7.56627	8.86781	10.15838
H	8.15730	9.52144	9.53664
C	9.74506	9.69854	12.22816
H	9.96525	8.67743	12.55022
H	10.29239	10.39082	12.87483
H	10.12410	9.82415	11.20837
C	1.92871	9.02091	15.26606
H	1.57859	8.80719	14.25250
H	1.23983	9.75936	15.69905
H	1.81044	8.10272	15.85327
C	7.90977	11.40445	11.84200
H	8.26837	11.59246	10.82448

C	4.20081	6.14012	11.80968
C	5.66200	5.18224	10.07782
H	6.60280	5.24038	9.53692
C	3.59480	4.12911	10.58367
H	2.88152	3.33611	10.40200
C	3.25751	5.10592	11.52418
C	4.79782	4.11024	9.86788
C	8.24585	9.98647	12.30069
H	7.90528	9.85836	13.33264
C	8.38039	5.37872	13.58743
H	7.81286	5.01892	12.72345
H	9.07348	4.57511	13.87421
H	8.98974	6.22317	13.25048
C	8.98454	7.60156	15.80878
H	9.25517	8.04539	14.84339
H	9.85888	7.02643	16.14229
H	8.84703	8.41932	16.52282
C	3.40447	10.47093	12.83582
H	4.14070	10.95941	12.18987
H	2.53913	11.14184	12.90786
H	3.07440	9.56115	12.32223
C	1.87467	5.09702	12.20160
C	5.17750	2.99854	8.88043
C	5.72437	3.87123	14.40018
H	4.72124	3.63297	14.76380
H	6.34754	2.98315	14.57311
H	5.65245	4.00675	13.31564
C	4.64831	5.15931	17.13375
H	4.36835	5.89981	17.88925
H	4.88344	4.22864	17.66697
H	3.75963	4.95383	16.52518
H	8.39188	12.13319	12.50026
H	6.83132	11.58012	11.86251
C	2.00160	4.89178	13.72254
H	2.47253	3.92886	13.94586
H	1.00934	4.89793	14.18957
H	2.59754	5.68515	14.17509
C	0.96889	3.97629	11.66686
H	0.80439	4.05975	10.58716
H	-0.00952	4.04375	12.15452
H	1.37009	2.97912	11.87926
C	4.09524	1.91465	8.78087
H	3.91624	1.42885	9.74583
H	4.41321	1.14006	8.07483
H	3.14423	2.31986	8.41895
C	6.58170	10.53709	16.89297
H	6.82852	9.74618	17.60919
H	6.35842	11.43804	17.48051
H	7.48688	10.75112	16.31448
C	3.88268	9.05778	17.77156
H	3.23571	8.17348	17.76687
H	3.34219	9.83741	18.32619
H	4.77363	8.81039	18.35687
C	6.48649	2.32693	9.34092
H	7.31303	3.04270	9.39482
H	6.77923	1.53314	8.64335
H	6.36777	1.88126	10.33395
C	5.38306	3.59838	7.47536
H	4.46633	4.07868	7.11747
H	5.66091	2.81677	6.75838
H	6.17908	4.35003	7.46778
La	5.40619	7.73965	14.47758

C	6.76643	7.82836	9.82475

IRC for the reaction of 1-La with $PhCF_3$:





triplet IRC reverse :

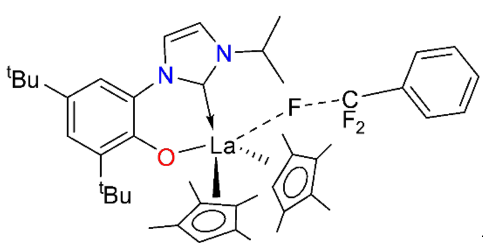
O	-2.60533500	-1.01522000	-0.19359600	C	3.12049800	0.56871600	-2.40539300
N	-0.80733800	-1.44081300	-2.35742000	H	3.29461300	-0.37505400	-1.88160100
N	0.70549600	0.07492500	-2.48832000	H	3.85448200	1.29989400	-2.05832900
C	-2.46100900	2.04190000	1.68222000	H	3.28933600	0.40198000	-3.47478900
C	-1.92133400	2.37551000	0.41341400	C	-3.91069300	1.79037900	1.98323600
C	-1.40565300	2.09267700	2.64426900	H	-4.45171700	1.44346600	1.09859500

C	-1.78228600	-2.40666400	-1.93746200
C	-0.08129500	-0.57304400	-1.58577700
C	-0.13983800	-2.78191100	2.02089300
C	-0.53522700	2.61635500	0.59678300
H	0.14971200	2.96344700	-0.17003100
C	0.78452700	-1.01227200	3.14095500
H	0.97003900	-0.25179300	3.89297400
C	1.02801700	-2.37260900	1.31769100
C	1.60493300	-1.27477700	2.01683500
C	-0.21163700	2.46086800	1.96980900
C	-0.29493000	-1.93307100	3.15221200
C	-2.74021800	-2.09692500	-0.93372100
C	-1.79621500	-3.62572900	-2.61442800
H	-0.98805400	-3.83649600	-3.30982100
C	-3.81883600	-4.19947400	-1.51123800
H	-4.64126600	-4.88725300	-1.36509700
C	-3.83594700	-3.00272700	-0.79041700
C	-2.80231600	-4.56532400	-2.40193900
C	1.70845100	1.08990600	-2.14222200
H	1.58348500	1.25251800	-1.06764600
C	1.63499000	-3.10061200	0.15339600
H	0.87217000	-3.50817100	-0.51738400
H	2.25041700	-3.94624400	0.49203900
H	2.28323500	-2.45083700	-0.44242900
C	2.91549800	-0.60865600	1.70624600
H	3.03583700	-0.38162800	0.64038700
H	3.76438700	-1.24724600	1.98583800
H	3.02500800	0.33063800	2.25622700
C	-2.68543400	2.50527100	-0.87322000
H	-3.30575000	1.62596100	-1.07831800
H	-2.00477300	2.62622000	-1.72167300

H	-4.41215000	2.70385000	2.33200900
H	-4.05215500	1.03797200	2.76766000
C	1.43376000	2.40242600	-2.87354500
H	1.57553200	2.29655700	-3.95442600
H	2.12474500	3.17222400	-2.52271000
H	0.41170000	2.74597300	-2.69367900
C	-4.61908200	-2.53614000	1.58038400
H	-4.24088300	-3.49673200	1.94566100
H	-5.48056400	-2.25625500	2.19855200
H	-3.84191300	-1.78252400	1.71241100
C	-6.16188200	-3.68652000	0.02171100
H	-6.53759500	-3.80937900	-0.99985700
H	-7.00134200	-3.35657700	0.64321400
H	-5.84671300	-4.66747100	0.39431100
C	-3.97053100	-6.79773100	-2.78239100
H	-4.00508400	-7.02751400	-1.71222200
H	-3.90087300	-7.74819800	-3.32228400
H	-4.91945000	-6.32824600	-3.06291200
C	1.10787300	2.79357700	2.60465000
H	1.37762700	2.09920000	3.40774300
H	1.09092600	3.79788600	3.05033400
H	1.91958700	2.78312400	1.87173800
C	-1.57045500	1.94466900	4.12949100
H	-2.33363100	1.20318800	4.39062600
H	-1.88047100	2.89064800	4.59510300
H	-0.63770400	1.64117800	4.61531100
C	-1.48363000	-6.67354700	-2.75481700
H	-0.58379800	-6.11029300	-3.02191400
H	-1.43852200	-7.63873500	-3.27323700
H	-1.44918100	-6.86336800	-1.67703300
C	-2.78348100	-5.67627500	-4.66014200

H	-3.34939100	3.37950900	-0.86119600
C	-5.03736700	-2.64189000	0.10188500
C	-2.76821800	-5.91201700	-3.13700700
C	-0.96408000	-3.99646500	1.70501000
H	-1.91123300	-3.99040100	2.25095100
H	-0.43567500	-4.91683200	1.98987500
H	-1.20365500	-4.07988300	0.63969100
C	-1.32509000	-2.06636900	4.23917800
H	-2.33790100	-2.23065000	3.85251600
H	-1.35186900	-1.17094900	4.86782900
H	-1.10157400	-2.91553100	4.89858500
C	-0.47974100	-1.31073000	-3.69974500
H	-0.97907700	-1.87330400	-4.47131600
C	-5.62608600	-1.29736300	-0.37138300
H	-4.87292600	-0.50896400	-0.33221300
H	-6.47171700	-1.00723800	0.26382700
H	-5.98986300	-1.37836700	-1.40159800
C	0.48003200	-0.36001700	-3.78011700
H	0.99611900	0.04035300	-4.63821300

H	-3.68739600	-5.13751300	-4.96318300
H	-2.75928200	-6.63134400	-5.19815600
H	-1.91887300	-5.09102800	-4.98950800
C	6.93220300	6.75630500	1.81712000
C	7.44102100	5.69934400	1.06142800
C	6.57549600	4.85405300	0.37486000
C	5.19700100	5.06963700	0.44578200
C	4.68428800	6.12401100	1.20044800
C	5.55661400	6.96771300	1.88526900
H	7.60981700	7.41591800	2.35173100
H	8.51304300	5.53501600	1.00556900
H	6.96581300	4.03357400	-0.21940500
H	3.61254500	6.28404400	1.24688300
H	5.15933100	7.79120200	2.47122400
C	4.27710100	4.12583000	-0.27204200
F	4.69738700	3.87797900	-1.53333600
F	3.01848500	4.59629500	-0.35829300
F	4.20744000	2.92365400	0.34378800
La	-0.81529800	-0.17273100	1.00020000



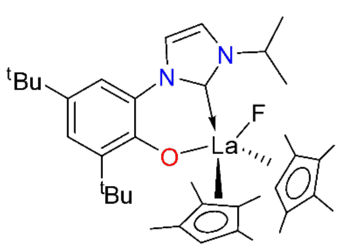
triplet TS :

O	3.20284700	7.18628300	12.63508600
N	4.29444300	6.57227600	10.07686800
N	5.73792100	8.00983800	9.41843500
C	3.22007700	10.40998300	13.55227200
C	4.44982100	11.01191400	13.20046400
C	3.33466900	9.93413600	14.88926400

C	8.09607400	8.35833100	8.80820800
H	8.36980700	7.45774800	9.36433200
H	8.92922900	9.06551700	8.87080300
H	7.96925500	8.08540400	7.75427100
C	1.98674200	10.38282800	12.69505900
H	2.03750000	9.61796500	11.91153100

C	3.46838800	5.67062100	10.81909700	H	1.82134100	11.35030600	12.20673900
C	5.21313300	7.46696200	10.55609400	H	1.09551900	10.16960900	13.29130500
C	5.95532700	5.46940900	14.12217200	C	6.41199400	10.24241700	8.62016000
C	5.32880400	10.89208800	14.32434200	H	6.24378300	10.03452900	7.55736900
H	6.35793700	11.22337100	14.35606900	H	7.20052300	10.99805100	8.68345900
C	7.06825800	7.14822200	15.21671100	H	5.49535300	10.66975900	9.03500100
H	7.37603600	7.85966800	15.97614500	C	1.57650800	5.84787100	14.93577900
C	7.06249900	5.84987000	13.32344100	H	1.97583700	4.88609400	15.27683800
C	7.77513200	6.86674500	14.01661700	H	0.90500900	6.22658600	15.71626000
C	4.65182200	10.24154900	15.36446700	H	2.40157000	6.54968000	14.81399900
C	5.95969900	6.28076200	15.30546100	C	-0.32213800	4.68395700	13.85492100
C	2.83305700	6.08416100	12.02501500	H	-0.92371200	4.51456600	12.95536900
C	3.26187300	4.41036500	10.25990400	H	-0.98777400	5.08969200	14.62494300
H	3.85553700	4.13192400	9.39276000	H	0.03976300	3.71515600	14.21676300
C	1.58935400	3.98526800	11.88026800	C	1.09347400	1.29714300	10.91378200
H	0.81598000	3.34210300	12.27927500	H	1.34331100	1.15207000	11.97013300
C	1.77661700	5.22897700	12.48927200	H	1.01202000	0.30647400	10.45334000
C	2.33790200	3.51698900	10.79514200	H	0.10677200	1.76919800	10.85749900
C	6.83046900	8.98980900	9.38889500	C	5.14685000	10.06243000	16.76903800
H	7.00489000	9.23799400	10.43903500	H	4.87775900	9.08959900	17.19312900
C	7.51706400	5.17309200	12.06369200	H	4.72443200	10.82368700	17.44003700
H	6.67301200	4.82884200	11.45905300	H	6.23606400	10.15746700	16.81897900
H	8.14158700	4.29440000	12.27983700	C	2.23085200	9.37890100	15.73266000
H	8.11251700	5.84685600	11.44004800	H	1.47851700	8.85895000	15.13602700
C	9.07380300	7.46993300	13.59575800	H	1.71525000	10.17841500	16.28574700
H	8.95245400	8.08475500	12.69701400	H	2.60377800	8.67228500	16.48158100
H	9.82575800	6.69978300	13.38262700	C	3.49718300	1.35264000	10.26705900
H	9.47328000	8.10838000	14.38999200	H	4.29748900	1.87385600	9.73219200
C	4.74533300	11.74142100	11.92816500	H	3.39711300	0.35325600	9.82610000
H	4.00979500	11.51138900	11.15118300	H	3.81521600	1.23618000	11.30833400
H	5.73508300	11.47570800	11.54532500	C	1.74346800	2.24520900	8.70599300

H	4.72805900	12.83217700	12.06921600	H	0.79468200	2.78428500	8.61417100
C	0.82137400	5.68024400	13.60755800	H	1.61804900	1.25356700	8.25468400
C	2.16349800	2.12117400	10.18417100	H	2.49196000	2.78400000	8.11597400
C	5.07000600	4.28617000	13.88760600	C	9.29901100	13.04609600	15.93877200
H	4.08188200	4.41720900	14.33431800	C	10.04899900	11.90329700	15.62403000
H	5.50884300	3.37905900	14.32918300	C	9.89963600	11.28351500	14.39997700
H	4.91959100	4.08686100	12.82308900	C	8.97397100	11.81110800	13.45602400
C	5.07964600	6.09229100	16.50431400	C	8.21325500	12.96943800	13.78256700
H	4.01135500	6.12395700	16.26759500	C	8.38767200	13.57132300	15.01445500
H	5.28050800	6.85533300	17.26178700	H	9.42445800	13.52482300	16.90507200
H	5.26404200	5.11638600	16.97423200	H	10.75219000	11.50120100	16.34678100
C	4.24449800	6.58513800	8.68976400	H	10.47370700	10.39890600	14.14950400
H	3.54270800	5.98682100	8.13256300	H	7.50310700	13.36631300	13.06621700
C	0.17950700	7.01888600	13.19677900	H	7.80579700	14.45215200	15.26678700
H	0.94658600	7.76902900	13.00406900	C	8.82906700	11.20604800	12.21223300
H	-0.48497800	7.38477000	13.98963800	F	9.56184200	10.21630800	11.81195600
H	-0.41870800	6.89509100	12.28716800	F	8.08445900	11.69567800	11.26881300
C	5.16290100	7.48761800	8.27594800	F	7.04917800	9.39259000	12.39246800
H	5.43291200	7.80226300	7.28029800	La	5.27783100	8.22434600	13.23497200

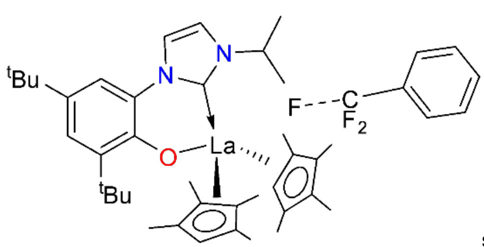


triplet :

O	-1.73559400	-0.68334200	-0.44455500	C	3.45740200	-0.18439700	-3.98172700
N	-0.54948400	-1.80022500	-2.75808700	H	3.74245900	-1.11462300	-3.48375400
N	1.09211500	-0.56360200	-3.37525100	H	4.28483700	0.52417800	-3.88209100
C	-2.56539600	2.94663900	1.75023800	H	3.32467200	-0.39133500	-5.04960500
C	-1.26432200	2.94974300	1.06664800	C	-3.83344100	3.39846800	1.10424700

C	-2.36995700	2.48104700	3.02552900	H	-4.10771000	2.75626100	0.25839900
C	-1.56789700	-2.47251800	-2.01037900	H	-3.74037400	4.41858900	0.71071900
C	0.44197600	-1.00048500	-2.26366600	H	-4.67150900	3.39126600	1.80553200
C	1.64964000	-2.68390700	0.84986500	C	1.76655200	1.70731300	-4.04386400
C	-0.29553200	2.45397400	1.95842100	H	1.58570100	1.56352100	-5.11504300
H	0.77560900	2.47111300	1.78784300	H	2.55003800	2.46059700	-3.93017500
C	1.56352100	-1.23025400	2.61312700	H	0.85485800	2.09853600	-3.58563200
H	1.27339300	-0.76528900	3.55067500	C	-3.54116700	-1.42905000	1.92481100
C	2.73049700	-1.75555500	0.72195800	H	-3.20883500	-2.36451000	2.38588000
C	2.68436800	-0.86564400	1.82408900	H	-4.20981800	-0.92334200	2.63197300
C	-0.94225600	2.18677400	3.18104800	H	-2.67247900	-0.79011300	1.76169900
C	0.93255100	-2.36182000	2.03025200	C	-5.54934500	-2.50082500	0.95456400
C	-2.21160000	-1.81726900	-0.92330900	H	-6.15823200	-2.71938000	0.07082200
C	-1.95389200	-3.73873600	-2.44312300	H	-6.16634700	-1.91102200	1.64106700
H	-1.37343200	-4.20947800	-3.23265900	H	-5.31618300	-3.44673500	1.45610900
C	-3.74324500	-3.70735200	-0.88195400	C	-4.64921500	-6.35944400	-1.61597800
H	-4.61934100	-4.17897200	-0.45629300	H	-4.48756200	-6.42706000	-0.53496600
C	-3.38720900	-2.44204000	-0.40568300	H	-4.87553900	-7.36763000	-1.97932800
C	-3.03884000	-4.40146700	-1.87288200	H	-5.53420400	-5.73868200	-1.79206100
C	2.19660600	0.41018900	-3.36020100	C	-0.30663000	1.75750100	4.45622100
H	2.36686300	0.63229900	-2.30466300	H	-0.72583700	0.80950200	4.81825800
C	3.80926900	-1.79405200	-0.32097700	H	-0.48900800	2.49428700	5.24985500
H	3.44968100	-2.22374300	-1.26127800	H	0.77343300	1.63579300	4.34869300
H	4.66191700	-2.40646800	0.00432500	C	-3.37602800	2.28526500	4.11253100
H	4.19959400	-0.79401800	-0.53834800	H	-4.37463100	2.60200600	3.80184200
C	3.65915200	0.24092600	2.10684100	H	-3.11531400	2.85475800	5.01377600
H	3.80806900	0.89039900	1.23693600	H	-3.44571900	1.23229700	4.41379500
H	4.64372100	-0.15144500	2.39346300	C	-2.23684900	-6.77226700	-2.07584000
H	3.31331000	0.87230800	2.93174300	H	-1.32775400	-6.45270200	-2.59485400
C	-1.02936300	3.46979900	-0.30837300	H	-2.47847500	-7.78564500	-2.41834300
H	-1.73642600	3.03353300	-1.02576000	H	-2.00886500	-6.81986800	-1.00588700

H	-0.01171300	3.25797700	-0.64190000
H	-1.19287800	4.55628700	-0.34251600
C	-4.28380800	-1.70267800	0.60376800
C	-3.41339200	-5.81296500	-2.34392300
C	1.41097500	-3.88242900	-0.02246200
H	0.35405900	-4.16434600	-0.05417000
H	1.96705900	-4.75732100	0.34244600
H	1.73026300	-3.70698500	-1.05447000
C	-0.20696700	-3.14217800	2.62040800
H	-0.91847900	-3.48573100	1.86135100
H	-0.76530600	-2.54419000	3.34804600
H	0.15214000	-4.03632300	3.14801900
C	-0.50699100	-1.85308000	-4.14378200
H	-1.22962800	-2.40487700	-4.72271500
C	-4.73707600	-0.36779500	-0.02188800
H	-3.87422500	0.24847800	-0.28159100
H	-5.36737100	0.18700100	0.68360500
H	-5.32358100	-0.54746900	-0.92964100
C	0.53156200	-1.07379200	-4.53079500
H	0.89677500	-0.83798800	-5.51790600
C	-3.71875000	-5.79531700	-3.85480500
H	-4.55488700	-5.12394200	-4.07687300
H	-3.98439300	-6.79938100	-4.20632700
H	-2.85667600	-5.45925000	-4.43994900
C	4.42177700	5.94547500	2.71831800
C	5.17590900	4.80963600	2.39491900
C	4.89552000	4.06899700	1.26101800
C	3.82623000	4.45611600	0.40255100
C	3.06568500	5.61351700	0.73824700
C	3.36919000	6.33429300	1.87885700
H	4.65100300	6.51935300	3.61092700
H	5.99482100	4.50279300	3.04006100
H	5.48492800	3.19233800	1.01498300
H	2.24969500	5.91968200	0.09246800
H	2.78035300	7.21450300	2.12292700
C	3.52981400	3.71972900	-0.73953600
F	4.21329000	2.65769000	-1.13017000
F	2.59426900	4.05981100	-1.61020400
F	1.57867100	1.50784800	-0.43076100
La	0.40846600	-0.16757100	0.28641000

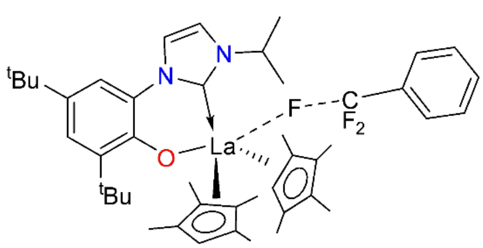


singlet IRC reverse :

O	-2.34936300	-0.84439500	-0.34985400
N	-0.73715100	-1.55903600	-2.55714800
N	0.87974600	-0.16969200	-2.79837300
C	-2.09937000	2.17810700	1.56237400
C	-0.90072400	2.75335100	0.94689600
C	3.30047700	0.34272800	-2.85548400
H	3.51830200	-0.58240100	-2.31558800
H	4.03877800	1.09576000	-2.56485800
H	3.42395500	0.14737900	-3.92701800
C	-3.45476800	2.22379600	0.93510800

C	-1.75886600	1.71106600	2.83218900	H	-3.43493700	1.87422900	-0.10245800
C	-1.75852800	-2.41369200	-2.04072300	H	-3.84698800	3.25009900	0.92432000
C	0.08831400	-0.73369100	-1.83676300	H	-4.17165200	1.60260000	1.47558400
C	0.55048600	-2.59248800	1.75266900	C	1.57655800	2.14137500	-3.29033700
C	0.15430500	2.61984900	1.84862700	H	1.66334400	2.00893000	-4.37451700
H	1.16277100	2.98415000	1.70214500	H	2.27469400	2.92879800	-2.99597500
C	1.40194000	-0.77234400	2.83260800	H	0.56134600	2.48054200	-3.06726400
H	1.61606000	-0.05582100	3.61393400	C	-4.19133300	-2.15737400	1.72089100
C	1.66907600	-2.08783600	0.98939200	H	-3.80512300	-3.11510300	2.08800000
C	2.18975800	-0.95378200	1.65262100	H	-4.95511200	-1.81190600	2.42924700
C	-0.35277100	2.02080000	3.03968100	H	-3.37122200	-1.43626700	1.70976800
C	0.39604500	-1.78432600	2.89734600	C	-5.97040000	-3.31476500	0.44546600
C	-2.60756900	-1.96388900	-0.98892300	H	-6.48348200	-3.47532500	-0.50906400
C	-1.92641100	-3.65471300	-2.65207200	H	-6.70625900	-2.91054000	1.14943600
H	-1.19919400	-3.96033000	-3.40038700	H	-5.64901800	-4.28804700	0.83286400
C	-3.87339200	-4.01799000	-1.34400200	C	-4.36317800	-6.63103100	-2.49922300
H	-4.72219100	-4.63710100	-1.08402400	H	-4.32849400	-6.82113500	-1.42129800
C	-3.73547000	-2.79286000	-0.68712100	H	-4.42177300	-7.60158000	-3.00380200
C	-2.98116500	-4.49811000	-2.31026500	H	-5.28718300	-6.08642900	-2.72111100
C	1.89841500	0.85287700	-2.53463500	C	0.32887000	2.03177400	4.36703800
H	1.81390700	1.04215700	-1.45313500	H	0.11568500	1.13825000	4.96182800
C	2.26577000	-2.79115600	-0.18936900	H	-0.01985900	2.89138200	4.95799000
H	1.50110900	-3.19775700	-0.85742100	H	1.41274700	2.13022700	4.26318400
H	2.89482900	-3.63202200	0.13667100	C	-2.69203600	1.21512300	3.89416100
H	2.89991600	-2.12408800	-0.77852400	H	-3.60137800	0.78986600	3.46220300
C	3.47192900	-0.23506000	1.34884300	H	-2.99923900	2.02650800	4.57079800
H	3.69979100	-0.23762000	0.27905700	H	-2.23483700	0.43799800	4.51287800
H	4.32624200	-0.70176000	1.86375700	C	-1.88075200	-6.72804300	-2.66814600
H	3.43228500	0.81017700	1.66705500	H	-0.95985100	-6.25230900	-3.02035700
C	-0.86832200	3.44118400	-0.37759700	H	-1.95524400	-7.70972500	-3.15164600
H	-1.26417100	2.81267800	-1.18519800	H	-1.78110900	-6.88598300	-1.58914500

H	0.14946300	3.73656500	-0.64088400
H	-1.49328900	4.34540600	-0.35903100
C	-4.80237700	-2.32439000	0.31688700
C	-3.12164300	-5.86940800	-2.98376600
C	-0.23060200	-3.82648900	1.41986500
H	-1.16443800	-3.87138600	1.98648600
H	0.34087700	-4.73501000	1.65701900
H	-0.49070500	-3.88144800	0.35689800
C	-0.51518000	-2.04729000	4.06016200
H	-1.52553600	-2.32879400	3.74628600
H	-0.60303100	-1.16452100	4.69991500
H	-0.13029300	-2.86072300	4.69138900
C	-0.46660100	-1.49038800	-3.91619400
H	-1.04099100	-2.03411300	-4.64844500
C	-5.39030100	-0.98378400	-0.16603600
H	-4.60156500	-0.24132300	-0.29001400
H	-6.12467600	-0.60507600	0.55604500
H	-5.90010500	-1.11304900	-1.12726900
C	0.55804100	-0.61772200	-4.06506800
H	1.06003200	-0.27857100	-4.95754900
C	-3.23792700	-5.69178000	-4.51063700
H	-4.11399200	-5.08696800	-4.76736500
H	-3.33664800	-6.66472300	-5.00696200
H	-2.35621500	-5.19603700	-4.92945000
C	6.20068300	6.58909100	2.18270700
C	6.68693000	5.38019500	1.68298500
C	5.91661000	4.62960200	0.80075800
C	4.65491600	5.09209500	0.41715100
C	4.16495700	6.29998600	0.91519900
C	4.94183600	7.04741100	1.79725200
H	6.80462500	7.17411300	2.87044900
H	7.66886900	5.02303700	1.97911400
H	6.29294400	3.69184500	0.40404900
H	3.18645300	6.65400400	0.60849900
H	4.56299400	7.98979300	2.18182700
C	3.81515100	4.24860500	-0.49557400
F	4.54569200	3.70525100	-1.49302200
F	2.81498100	4.94761100	-1.06825300
F	3.24052300	3.21403500	0.16130900
La	-0.40259200	-0.10850400	0.75299200



singlet TS :

O	3.00640700	7.09207400	12.39273800
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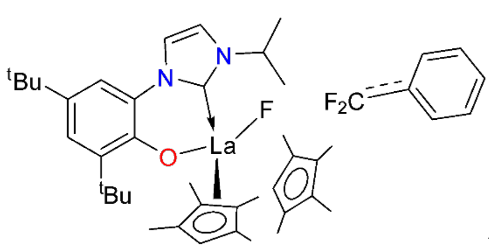
N	5.91888700	7.75486300	9.51414700
C	8.30958800	8.19277700	9.08451300
H	8.56738100	7.26502400	9.60260600
H	9.10691000	8.91824000	9.26310800

C	2.97490500	10.19459600	14.09263700	H	8.27405100	7.98570800	8.00889900
C	4.17238200	10.82158000	13.49427700	C	1.63296900	10.20753600	13.44029600
C	3.31094300	9.75721400	15.36137300	H	1.67248800	9.82343200	12.41583900
C	3.43789800	5.50000900	10.67968200	H	1.24102100	11.23211800	13.38492000
C	5.24351400	7.25313500	10.58702800	H	0.90804900	9.60497100	13.98986100
C	5.76195800	5.42950100	14.14762400	C	6.58566500	10.03977000	8.86872600
C	5.21367300	10.73979700	14.42083500	H	6.52041600	9.88914300	7.78533100
H	6.21369900	11.13316700	14.30024600	H	7.32773700	10.81790800	9.06039600
C	6.74084100	7.20768100	15.20693200	H	5.61668600	10.40187400	9.22392000
H	6.98708200	7.94919900	15.95880700	C	1.22865500	5.90651000	14.60379200
C	6.88145800	5.86219200	13.36610200	H	1.65867300	4.98861800	15.01977000
C	7.49298300	6.96161200	14.02902900	H	0.48101200	6.27483000	15.31711500
C	4.70707000	10.13153700	15.59583400	H	2.02020300	6.65115000	14.51104300
C	5.67922800	6.26117100	15.29272600	C	-0.56175000	4.61646400	13.48729900
C	2.68794100	5.95421400	11.79706000	H	-1.11356200	4.38188600	12.57094000
C	3.25829300	4.22836400	10.13698400	H	-1.27574900	5.04625500	14.19838500
H	3.92325900	3.91340700	9.33731400	H	-0.19500600	3.67920400	13.92009300
C	1.44660800	3.86827900	11.62454700	C	0.99092900	1.16679100	10.68754300
H	0.63917000	3.24152300	11.97922700	H	1.16091600	1.04122000	11.76215200
C	1.60025200	5.12632700	12.21402400	H	0.92932900	0.16750300	10.24362600
C	2.27315700	3.36685900	10.61298200	H	0.01747400	1.64910200	10.54852500
C	6.98777900	8.75884800	9.59700900	C	5.39823100	10.08167300	16.91228200
H	7.08133200	8.98016500	10.66239700	H	5.24875500	9.12811600	17.42856700
C	7.43218400	5.14031600	12.17315400	H	4.99095700	10.85969000	17.57422700
H	6.64302800	4.71142300	11.54915100	H	6.46945200	10.26814900	16.80883100
H	8.08592500	4.31386600	12.48572300	C	2.40734400	9.19191200	16.41047700
H	8.03175000	5.80296600	11.54306000	H	1.44888500	8.88022100	15.99047800
C	8.79861100	7.60844700	13.67322200	H	2.19876000	9.93607300	17.19108500
H	8.91489200	7.76637700	12.59719300	H	2.84712800	8.32218700	16.90861100
H	9.64214300	6.98567600	14.00273300	C	3.43593300	1.17579400	10.21572400
H	8.90387400	8.58293000	14.15657100	H	4.28045000	1.66802000	9.72303200

C	4.20029600	11.48973200	12.16208200
H	3.74075800	10.86962900	11.38146600
H	5.22016800	11.73284200	11.86195800
H	3.61629000	12.42080200	12.18857900
C	0.57023300	5.62653000	13.24174900
C	2.12323200	1.95993700	10.02034400
C	4.94319100	4.19988400	13.88978800
H	3.96730400	4.25166900	14.37970100
H	5.45203900	3.30483100	14.27428500
H	4.76091400	4.03549900	12.82387000
C	4.77377600	6.05341900	16.47187000
H	3.73668100	5.85609600	16.18203600
H	4.77687200	6.92442000	17.13405100
H	5.10517400	5.19768700	17.07545900
C	4.49212700	6.34335900	8.63771500
H	3.85486700	5.74420200	8.00844200
C	-0.07521900	6.91408000	12.69306000
H	0.68531800	7.66469900	12.47593600
H	-0.78453100	7.32910500	13.42009100
H	-0.62545300	6.70417600	11.76939300
C	5.47633600	7.21756400	8.32341000
H	5.87638000	7.50371800	7.36360400
H	3.34862200	0.16688800	9.79535900
H	3.68008600	1.08198600	11.27893000
C	1.81323500	2.06084900	8.51369900
H	0.88194200	2.61075000	8.34226300
H	1.70579500	1.06212300	8.07422800
H	2.61111000	2.57643800	7.96950500
C	9.77906900	12.75800200	15.90734600
C	10.44908500	11.69580700	15.27230400
C	10.03206200	11.22405100	14.04174600
C	8.91451600	11.81362300	13.38897100
C	8.24484000	12.89382700	14.02981200
C	8.67978700	13.34944900	15.26226400
H	10.11444800	13.12330000	16.87296700
H	11.31465700	11.24195500	15.74922600
H	10.56883900	10.41538800	13.55583900
H	7.40957000	13.37782400	13.53261600
H	8.16620000	14.18673700	15.72954000
C	8.38929700	11.24379800	12.17237000
F	9.28591700	10.59651900	11.40036100
F	7.70185900	12.10668800	11.38652700
F	7.36538100	10.17906700	12.40390200
La	4.98483100	7.97007400	13.18532500



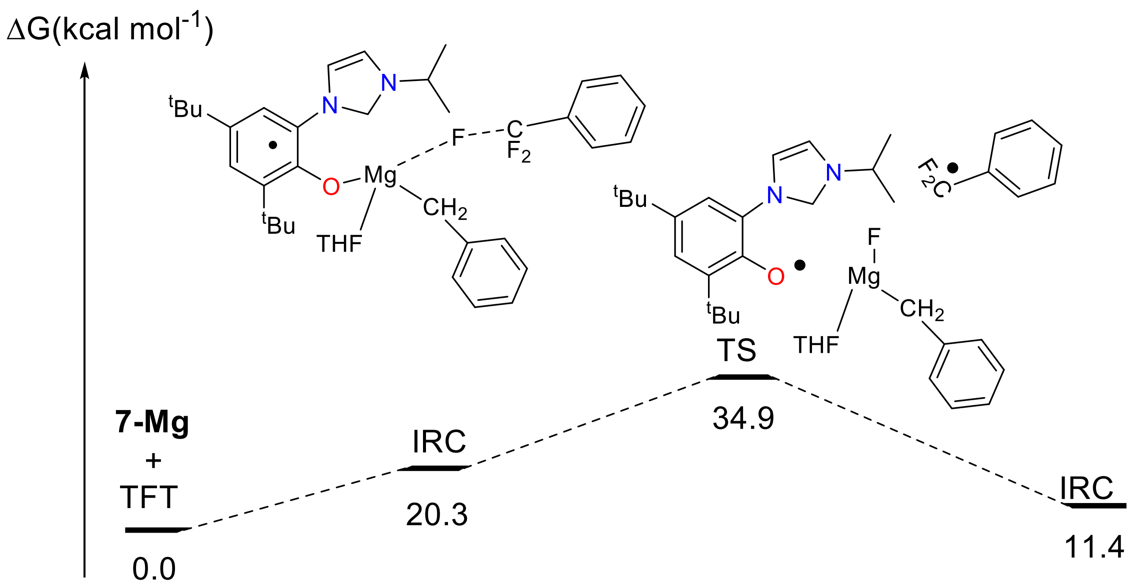
triplet IRC forward :

O	-1.78268300	-0.71320100	-0.31164400
N	-0.65972100	-1.70389100	-2.70830600
N	0.94260500	-0.41836700	-3.32693000
C	3.32304700	-0.08288100	-3.88451500
H	3.57493300	-1.01218700	-3.36657900
H	4.16150600	0.61009300	-3.77102100

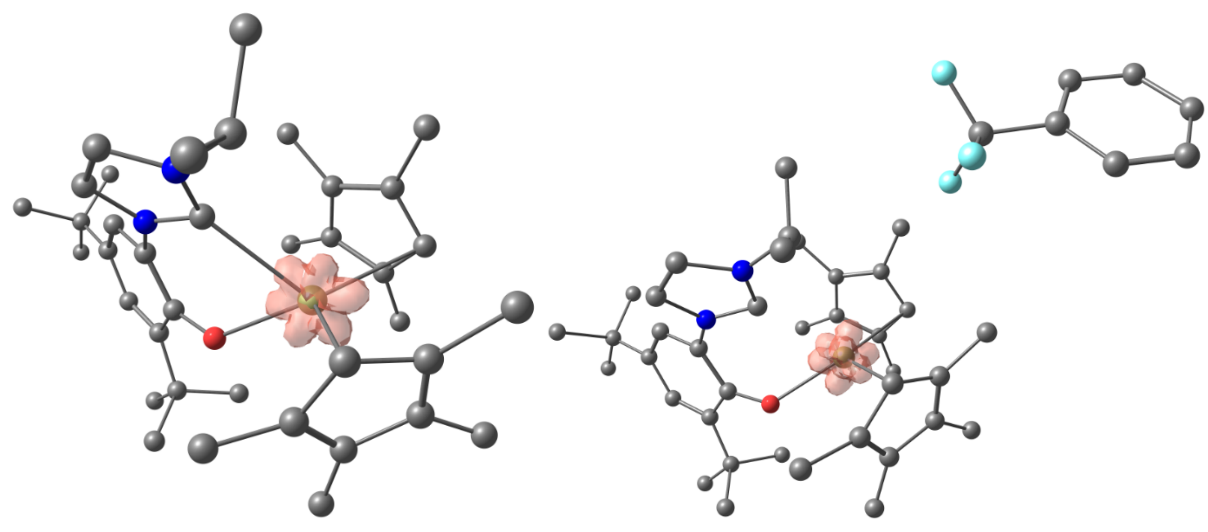
C	-2.73470100	2.96127500	1.63552900
C	-1.36287800	2.98956500	1.11293800
C	-2.69925000	2.39128100	2.88242200
C	-1.63745300	-2.42951600	-1.95643700
C	0.33090300	-0.90294000	-2.21354200
C	1.98290900	-2.45185700	0.68562300
C	-0.51448400	2.39378900	2.06767800
H	0.57011500	2.39906200	2.03116100
C	1.33438100	-1.45344600	2.63762700
H	0.81727400	-1.25580300	3.57255100
C	2.86165300	-1.35283600	0.93914400
C	2.46205800	-0.73901700	2.15205500
C	-1.30563600	2.04212700	3.17704900
C	1.04449100	-2.52084500	1.75110400
C	-2.25172800	-1.83753300	-0.81739700
C	-2.01445800	-3.68321600	-2.43218500
H	-1.45653400	-4.10594300	-3.26395900
C	-3.73754000	-3.76448300	-0.80000300
H	-4.58311800	-4.27603800	-0.35952600
C	-3.38432600	-2.51786600	-0.27508300
C	-3.06455700	-4.39345500	-1.85382200
C	2.05697300	0.54238200	-3.30457900
H	2.20588300	0.77870700	-2.24888100
C	4.05197700	-0.94630700	0.11891400
H	4.06171800	-1.44920600	-0.85263500
H	4.99356200	-1.20704900	0.62124500
H	4.07365200	0.13294500	-0.06912300
C	3.14796700	0.41645000	2.82285800
H	3.32697600	1.25604100	2.14102500
H	4.12690700	0.12242800	3.22470700
H	2.55946100	0.79280000	3.66599400
H	3.21264600	-0.30409600	-4.95218500
C	-3.91176300	3.48671700	0.88139000
H	-4.07270000	2.93235600	-0.05156300
H	-3.77441300	4.53974600	0.60479300
H	-4.83258300	3.41669800	1.46531700
C	1.66385900	1.83331700	-4.02084200
H	1.51746400	1.67840800	-5.09570700
H	2.45334500	2.57772100	-3.89200400
H	0.74209200	2.24296700	-3.59962300
C	-3.40126900	-1.69548200	2.12467200
H	-3.02849200	-2.66121300	2.48098600
H	-4.02531500	-1.26281700	2.91624400
H	-2.55114000	-1.03259000	1.95786800
C	-5.46144800	-2.71094800	1.20095400
H	-6.11952300	-2.87036500	0.34005800
H	-6.04225100	-2.18356600	1.96550700
H	-5.19004400	-3.68863600	1.61435000
C	-4.63088300	-6.39172000	-1.63416900
H	-4.42533900	-6.51212300	-0.56528200
H	-4.85604800	-7.38359800	-2.04057700
H	-5.53138200	-5.77796200	-1.74331300
C	-0.84032100	1.47216200	4.47049500
H	-1.33496800	0.51674100	4.68877100
H	-1.08723200	2.14207900	5.30486000
H	0.23920900	1.30729700	4.47568600
C	-3.82695100	2.14720900	3.83107000
H	-4.78067500	2.49195900	3.42451200
H	-3.66965200	2.66491500	4.78616100
H	-3.93542400	1.08079100	4.06448800
C	-2.23146700	-6.73611900	-2.20500500
H	-1.35025600	-6.37718200	-2.74606500

C	-0.96057500	3.62292600	-0.17236000	H	-2.47100200	-7.73676600	-2.58444900
H	-1.62666400	3.32036800	-0.99007400	H	-1.95785900	-6.82814800	-1.14878300
H	0.06633100	3.36588000	-0.43880800	C	-3.79692100	-5.70110900	-3.87554400
H	-1.04298000	4.71713000	-0.10199100	H	-4.65225700	-5.03553500	-4.03249200
C	-4.22814800	-1.86927300	0.83680900	H	-4.05882800	-6.69162100	-4.26610000
C	-3.43346600	-5.78697800	-2.37997700	H	-2.96343600	-5.32089500	-4.47495500
C	2.11737300	-3.46971900	-0.41105900	C	5.24812800	5.32790900	2.71280500
H	1.14679600	-3.88716000	-0.69726800	C	5.84516000	4.20179100	2.13094300
H	2.75049200	-4.31166400	-0.09776300	C	5.32932800	3.63965500	0.97718900
H	2.56623800	-3.04692800	-1.31478900	C	4.17401200	4.20489300	0.36377400
C	0.02018000	-3.59830600	1.96601900	C	3.57325200	5.34992500	0.96230400
H	-0.60110900	-3.78649700	1.08262500	C	4.11176600	5.89021700	2.11590500
H	-0.65184600	-3.33834600	2.78933100	H	5.66201800	5.76088700	3.61823600
H	0.49684700	-4.55250000	2.22787000	H	6.72676600	3.76057600	2.58805900
C	-0.65406500	-1.70967100	-4.09551300	H	5.79790900	2.76949500	0.53025900
H	-1.38477800	-2.25165100	-4.67348400	H	2.69400900	5.78996400	0.50410500
C	-4.73461100	-0.49573300	0.35226700	H	3.64373800	6.76384900	2.56168500
H	-3.89926900	0.15681400	0.09374800	C	3.64406600	3.65098800	-0.79630400
H	-5.32773400	-0.01253700	1.13794700	F	4.17616300	2.61502200	-1.42645600
H	-5.37409000	-0.61258700	-0.52969400	F	2.60806100	4.15025600	-1.44739600
C	0.36103200	-0.90064400	-4.48379700	F	1.52297800	1.56938500	-0.32130500
H	0.69540700	-0.62579700	-5.47170300	La	0.36077300	-0.13020700	0.35953900

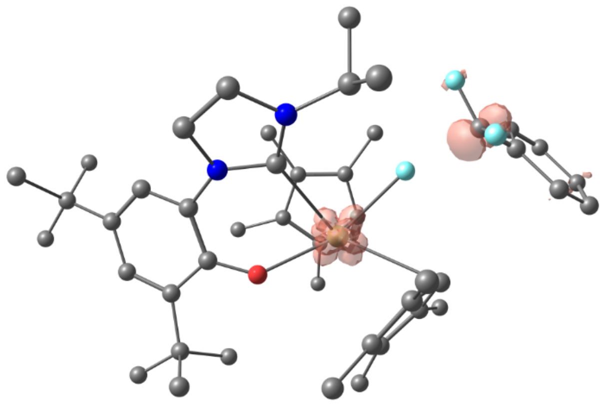
IRC for the reaction of 7-Mg with $PhCF_3$



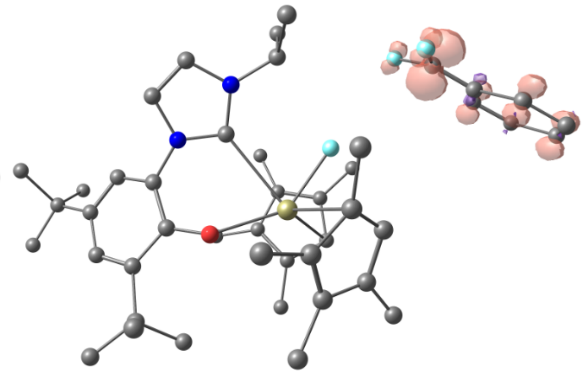
S10.4 Unpaired Spin Density Plots



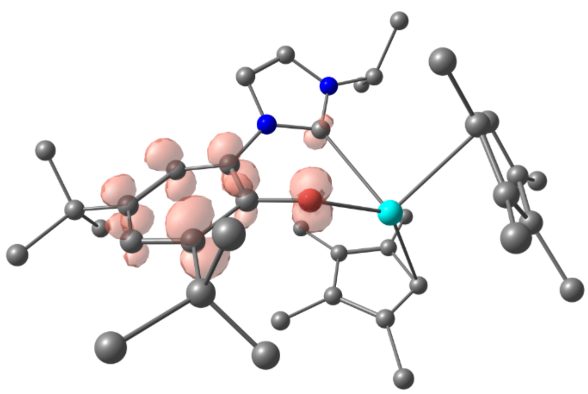
1-Ce **1-Ce***



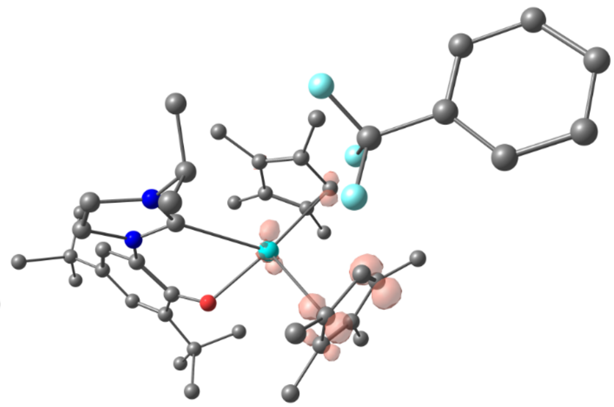
TS1



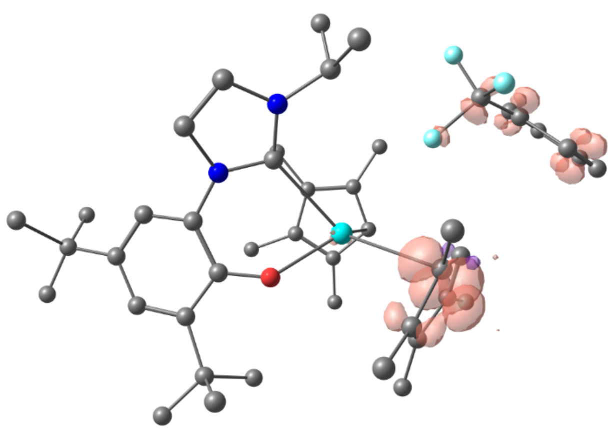
INT1



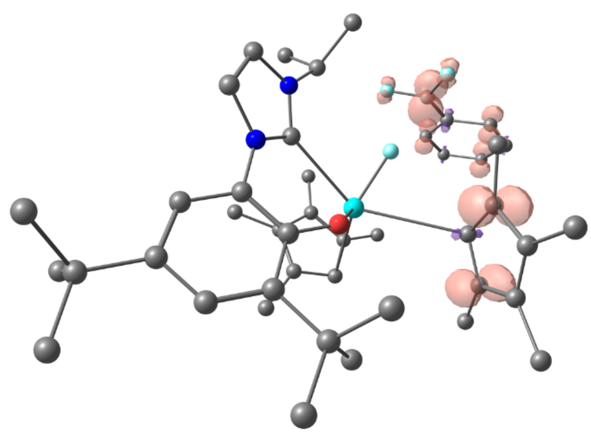
1-La*



INT6

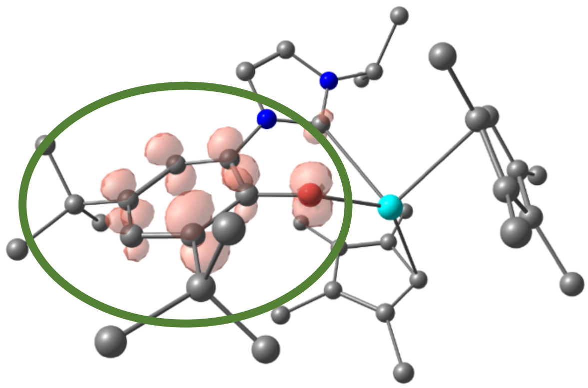


TS4

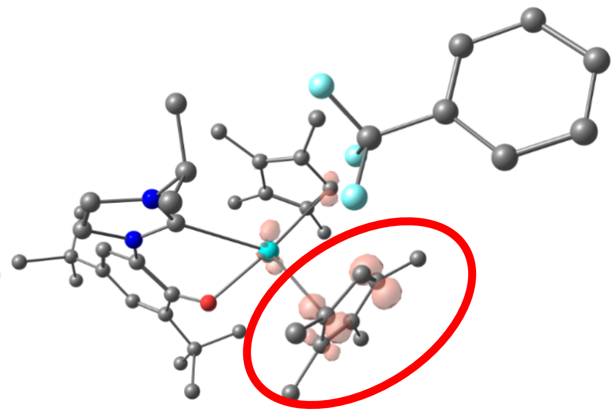


INT7

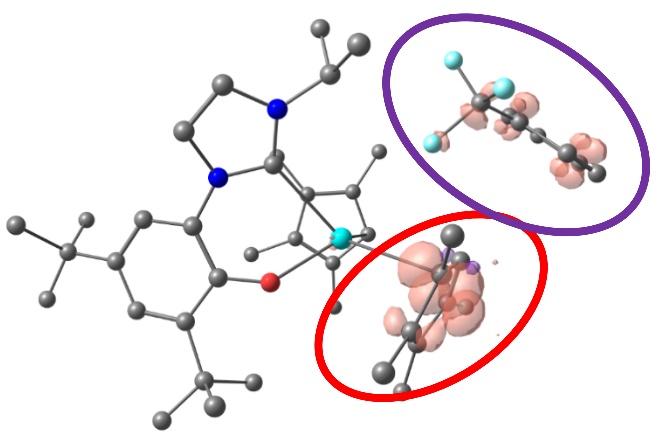
The unpaired spin density plot for photoexcited **1-La*** shows that the unpaired spin density is mainly located at the O-NHC ligand (green circle) which then relocalizes on the Cp ring in the intermediate (red circle, **INT6**). Then at **TS4**, the unpaired spin density is still mainly located at the Cp (red circle) and some spin density starts to develop at the $PhCF_3$ (purple circle) as expected for the C-F activation step. Finally, heading towards the product, in **INT7** unpaired spin density is located on both the $PhCF_2$• radical and the Cp ligand.



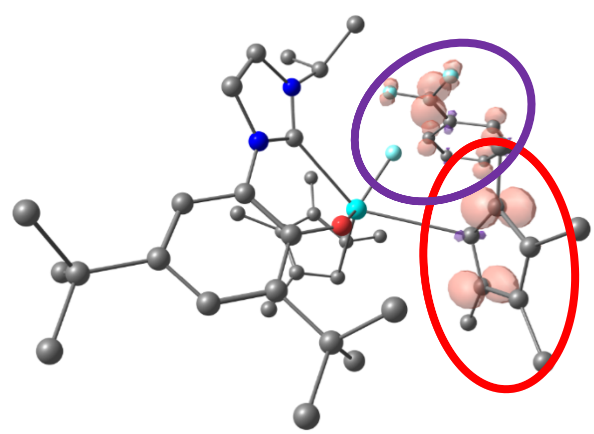
1-La*



INT6



TS4



INT7

S11 References

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