Tetraphenylpentalenide organolanthanide complexes

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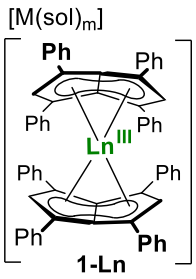
Supplementary Information

Contents

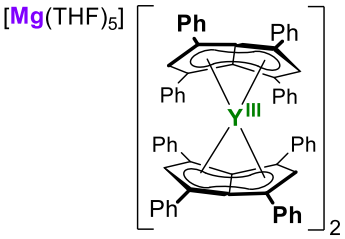
Compound Numbering Scheme

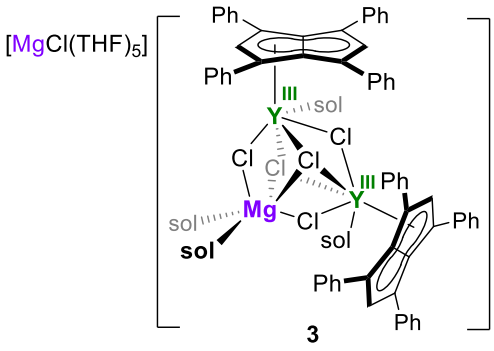
The THF-solvated $[Li/Na/K]_2[Ph_4Pn]$ and $[Mg][Ph_4Pn]$ were synthesised as previously reported.[1, 2]

The new DME solvates $[Li(DME)]_2[Ph_4Pn]$ and $[K(DME)_2]_2[Ph_4Pn]$ are reported here.



$[M(sol)_m][Ln^{III}(Ph_4Pn)_2]_2$ (1-Ln) for Ln = Y, La, Ce, Tb, Yb
Ln = Y, M = Li, n = 4, X = Cl, sol = THF, $M(sol)_m = Li(DME)_3$.
Ln = La, M = K n = 4, X=I, sol = DME, $M(sol)_m = K(DME)_4$.
Ln = Ce, M = K, n = 2, X = Br, sol = DME, $M(sol)_m = K(DME)_4$.
Ln = Tb, M = K, n = 4, X = I, sol = DME, $M(sol)_m = K(DME)_4$.
Ln = Yb, M = Na, n = 6, X = Cl, sol = THF, $M(sol)_m = Na(THF)_5$.





Scheme S1. $[M(sol)_m][Ln^{III}(Ph_4Pn)_2]_2$ for Ln = Y, La, Ce, Tb, Yb (**1-Ln**), $[Mg(THF)_5][Y^{III}(Ph_4Pn)_2]_2$ (**2**), and $[MgCl(THF)_5][(Y^{III}Ph_4Pn)_2(\mu\text{-}Cl)_5Mg(THF)_4]$ (**3**).

Experimental Section

1. General Considerations. All reactions were conducted under dinitrogen or argon using standard Schlenk techniques or a MBraun UniLab Plus glovebox unless stated otherwise. All glassware, cannula and Fisherbrand 1.2 µm retention glass microfiber filters were dried for at least 16 hours in a 160 °C oven prior to use. Molecular sieves were activated by heating to 250 ° under dynamic vacuum (10^{-3} mbar) for 16 hours and stored under argon prior to use. All commercially available materials were purchased from Sigma-Aldrich, Fisher, or Acros.

2. Solvents. Toluene was dried and distilled over sodium. THF, hexane, and pentane were dried and distilled over potassium, or collected from an MBraun Solvent Purification System packed with columns of activated alumina, degassed, and stored over activated 4 Å molecular sieves prior to use. 1,2-dimethoxyethane (DME) and benzene were distilled from potassium/benzophenone, degassed and stored over 4 Å molecular sieves. N-pentane was distilled from P_4O_{10} and stored over 4 Å molecular sieves. Deuterated solvents were purchased from Cambridge Isotope Laboratories. C_6D_6, THF-d_8, and pyridine-d_5 were refluxed over potassium, distilled, degassed, and stored on activated 4 Å molecular sieves prior to use. $CDCl_3$ was stirred over CaH_2, distilled and degassed prior to use.

3. Reagents. 1,3,4,6-Tetraphenyl-1,2-dihydropentalene Ph_4PnH_2, $[Mg(THF)_3][Ph_4Pn]$, and $[M_2(THF)_x][Ph_4Pn]$ (M = Li, Na, K) were prepared according to our previously reported procedures.[1,2] All commercial solid reagents were used as purchased from Sigma Aldrich, following rigorous drying under dynamic vacuum. KH was purchased as a dispersion in paraffin oil which was washed away with hexane prior to use.

4. Analyses. All NMR spectroscopic data were recorded at 298 K using a 500 MHz Bruker Avance III, Bruker AV-600, and AVQ-400 spectrometers, unless otherwise stated. ^1H and $^{13}C\{^1H\}$ spectra are referenced internally to the solvent ^1H and ^{13}C solvent resonances respectively. ^2H NMR spectra were referenced internally to the residual solvent. Resonances are reported in parts per million (ppm) relative to tetramethylsilane. Quantitative ^1H NMR data were acquired with a minimum of eight scans, with the delay time set to 5x the longest T1 value present. Chemical shifts are quoted in ppm and coupling constants in Hz. Structural assignments were performed using HSQC and HMBC NMR spectroscopic experiments when necessary. ATR-FTIR spectra were recorded on a Shimadzu IRSpirit FTIR spectrometer on neat

powders. Absorption bands are reported in wavenumbers (cm^{-1}) with a note on intensity: s – strong; m – medium; w – weak. UV-Vis spectra were recorded inside a MBraun UniLab Plus glove box using a fiber-optic AvaSpec-2048L photo spectrometer with an AvaLight-DH-S-BAL light source and 400 µm cables (Avantes), or on a Varian Cary 50 spectrometer using Schlenk-adapted quartz cuvettes with a 1 cm path length. Mass spectrometry was carried out at the Material and Chemical Characterization Facility at the University of Bath using a Bruker MaXis HD ESI-QTOF. Elemental analyses were carried out by the microanalytic services in the College of Chemistry at the University of California, Berkeley.

Single-crystal X-ray diffraction analyses for the new solvate $[K_2(DME)_4][Ph_4Pn]$, 1-Ce-THF, 1-Ce-DME, 1-La-DME, 1-Tb-DME were carried out using a RIGAKU Xtalab Synergy-S diffractometer fitted with a HyPix-6000HE photon counting detector using Mo Kα radiation (λ = 0.71073 Å) or Cu Kα radiation (λ = 1.54184 Å). X-ray crystallographic data for the new solvate $[Li_2(DME)_2][Ph_4Pn]$, 1-Y, 1-Yb, 2 and 3 were collected on a Rigaku SuperNova Dual, zero EoS2 diffractometer with Mo Kα radiation (λ = 0.71073 Å) or Cu Kα radiation (λ = 1.54184 Å). 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. Numerical absorption correction was based on a Gaussian integration over a multifaceted crystal model. Solvent accessible voids were treated using the Olex2 solvent mask function, and the final output of the mask was appended to the cif file and described in the additional details below.

5. Syntheses and Characterization

$[Li(DME)]_2[Ph_4Pn]$: The new solvate was isolated during the reaction of $[Li(THF)_2]_2[Ph_4Pn]$ with YCl_3 in DME as single crystals which were analysed by XRD.

$CeBr_3(THF)_{2.64}$: By adaptation of a literature method for $LaBr_3$.<Deacon, 2001 #419> In a 250 mL teflon tapped ampoule, 1.50 g (10.7 mmol) of freshly shaved cerium metal was added to 60 mL THF. The mixture was cooled in an ice bath and a solution of 4.50 g (23.9 mmol, 2.23 eq) of 1,2-dibromoethane in 15 mL THF was added slowly via cannula with vigorous stirring. After a 5-minute induction period the mixture became turbid and gas evolution began. The reaction

mixture was removed from the cooling bath and allowed to stir under nitrogen until the metal shavings are visibly consumed (40 hours). At this point 20 mL of hexane was added to the beige suspension to precipitate dissolved $CeBr_3$. The solids were washed twice with 20 mL of ether and dried for 4 hours under reduced pressure to yield $CeBr_3(THF)_{2.64}$. THF content was determined by elemental analysis. Yield: 5.46 g (89.4%).

Anal. Calcd for: $C_{10.6}H_{21.1}O_{2.64}Br_3Ce$: C 22.24%, H 3.73%. Found: C 22.25%, H 3.75%.

$[K(DME)_2]_2[Ph_4Pn]$: In a 20mL vial 98.6 mg (0.241 mmol) of H_2Ph_4Pn and 104.7 mg (0.525 mmol, 2.2 eq) of KHMDS were combined in 1 mL of DME, yielding a dark red solution and rapid crystallization. After gentle agitation the mixture is layered with 1 mL hexane and allowed to stand undisturbed for 16 hours to yield bright red, x-ray quality crystals. Following removal of the mother liquor the crystals are washed thrice with 1 mL cold pentane then dried to constant weight under reduced pressure. Yield: 174.0 mg (0.206 mmol, 85%).

^{1}H NMR (400 MHz, THF-d_8) δ: 7.75 – 6.00 (b, 22H), 3.47 (s, 16H, DME-*CH_2*), 3.27 (s, 24H, DME-*CH_3*).

ATR-FTIR (cm^{-1}): 3052 (w), 3017 (w), 2986 (w), 2926 (w), 2892 (w), 2819 (w), 1581 (s), 1487 (s), 1450 (s), 1405 (s), 1282 (w), 1267 (w), 1244 (w), 1171 (s), 1148 (w), 1128 (m), 1087 (s), 1065 (m), 1034 (w), 1017 (w), 986 (s), 964 (w), 937 (m), 893 (w), 856 (m), 771 (w), 762 (w), 741 (s), 733 (s), 696 (s), 680 (w), 658 (w), 627 (w), 614 (w), 508 (s).

UV-vis-NIR (DME): λ_{max} (ε) = 302 nm (17,000 M^{-1} cm^{-1}), 424 nm (26,000 M^{-1} cm^{-1}), 520 nm (55,000 M^{-1} cm^{-1}), 756 nm (150 M^{-1} cm^{-1}).

Anal. Calcd for: $C_{48}H_{62}O_8K_2$: C 68.21%, H 7.39%. Found: C 67.95%, H 7.33%.

$[M(sol)_m][Ln^{III}(Ph_4Pn)_2]_2$ (1-Ln) for Ln = Y, La, Ce, Tb, Yb

A) for Ln = Y: $[Li(DME)_3][Y(Ph_4Pn)_2]$ (1-Y): In 1mL DME solution of $[Li_2(THF)_4][Ph_4Pn]$ (20 mg, 0.028 mmol) half equivalent of YCl_3 (5.5 mg, 0.028 mmol) was added and allowed the solution to stir overnight. During the reaction formation of crystals of $[Li(DME)_3][Y(Ph_4Pn)_2]$ **1-Y** were seen on the wall of the vial. Crystals were taken out and dissolved in $CDCl_3$ to record the spectroscopic data. Yield: 19 mg (0.028 mmol, 56 %).

^{1}H NMR (500 MHz, $CDCl_3$) δ: 6.95 (m, 10H), 6.78 (t, *J* = 7.9 Hz, 2 H), 6.68 (d, *J* = 9.0 Hz, 2H), 6.48 (m, 5H), 6.40 (s, $1H_w$)*.

^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ: 143.4, 141.0, 140.7, 140.3, 136.5, 134.7, 130.1, 128.7, 127.9, 127.1, 126. 6, 126.1, 125.2, 124.5, 123.0, 121.10*, 71.6, 59.2 ppm.

*Found by ^{1}H-^{13}C HSQC.

The reactions of YCl_3 with group 1 pentalenides $M_2[Ph_4Pn]$ (M = Li, Na, K) in THF produce crude materials whose NMR spectra contain a H_w resonance at 6.32 ppm characteristic of the η^5 binding mode observed for the $Y^{III}(Ph_4Pn)$ group in **3**.

B) For Ln = La: $[K(DME)_4][La(Ph_4Pn)_2]$ (1-La): In a 20 mL vial 35.8 mg (58.8 µmol) $LaI_3(Et_2O)_{1.2}$ and 99.2 mg (117 µmol, 2 eq) $[K_2(DME)_4][Ph_4Pn]$ were dissolved in 7 mL THF and the resulting bright red solution was stirred for 16 hours. The orange mixture was filtered, and the volatiles removed under reduced pressure to give an orange solid. Recrystallization from hot DME cooled to -35 °C yields a crop of bright orange x-ray quality crystals of $[K(DME)_4][La(Ph_4Pn)_2]$ **1-La-DME** which were washed with cold pentane and dried briefly under vacuum (48.9 mg). Evaporation of the mother liquor and recrystallization of the solid residue from hot DME cooled to -35 °C yielded a second crop of crystals, which were washed with cold pentane and dried briefly under vacuum (11.1 mg). Yield: 60.0 mg (76 %).

^{1}H NMR (600 MHz, THF-d_8) δ: 6.83 – 6.75 (m, 24H, *m-,p*-Ph), 6.68 (dd, *J* = 7.8, 2.1 Hz, 16H, *o*-Ph), 6.39 (s, 4H, Pn-H_w), 3.43 (s, 12H, DME-CH_2), 3.27 (s, 18H, DME-CH_3).

^{13}C{^{1}H} NMR (600 MHz, THF-d_8) δ: 139.5 (*ipso*-Ph), 133.5(Pn-C7/8), 128.3 (*o*-Ph), 127.6 (*m*-Ph), 123.3 (*p*-Ph), 122.5 (Pn-C2/5), 114.4 (Pn-C1/3/4/6), 73.0 (DME-CH_2), 59.1 (DME-CH_3).

ATR-FTIR (cm^{-1}): 3054 (w), 3018 (w), 2982(w), 2928(w), 2893(w), 1592 (s), 1569 (w), 1501 (s), 1447 (m), 1405 (m), 1369 (w), 1244 (w), 1177 (s), 1127 (m), 1085 (s), 1030 (w), 1017 (m), 995 (m), 945 (w), 902 (m), 855 (m), 830 (m), 753 (s), 724 (s), 697 (s), 660 (w), 649 (w), 545 (w), 512 (m).

UV-vis-NIR (DME): λ_{max} (ε) = 277 nm (59,000 M^{-1} cm^{-1}), 378 nm (65,000 M^{-1} cm^{-1}), 743 nm (360 M^{-1} cm^{-1}).

Anal. Calcd. for: $C_{80}H_{84}O_8KLa$: C 71.09 %, H 6.26 %. Found: C 70.91 %, H 5.97 %.

C) For Ln = Ce: [K(DME)$_4$][Ce(Ph$_4$Pn)$_2$] (1-Ce): In a 20 mL vial 31.7 mg (55.6 µmol) $CeBr_3(THF)_{2.64}$ and 102.0 mg (121 µmol, 2.2 eq) $[K_2(DME)_4][Ph_4Pn]$ were dissolved in 8 mL THF, and the resulting dark red solution was stirred for 16 hours. The dark brown mixture was then filtered, and the volatiles were removed under reduced pressure to give an ochre solid. Recrystallization from hot DME cooled to -35 °C yielded a crop of rust-orange, x-ray quality crystals of $[K(DME)_4][Ce(Ph_4Pn)_2]$ **1-Ce-DME** which were washed with cold pentane and dried briefly under vacuum (43.9 mg). Evaporation of the mother liquor and recrystallization of the solid residue from hot DME cooled to -35 °C gave a second crop of crystals, which were washed with cold pentane and dried briefly under vacuum (24.5 mg). Yield: 68.4 mg (87.4 %). Crystals of the THF solvate, **1-Ce-THF**, can be grown by vapor diffusion of hexane into a THF solution of **1-Ce**.

^{1}H NMR (400 MHz, Pyridine-d_5): 3.52 (12H, s, DME-*CH$_2$*), 3.28 (18H, s, DME-*Me*), 2.17 (s, 8H, *p*-Ph)*, 1.38 (s, 16H, *m*-Ph)*, -1.65 (b, 3H, Pn-*H$_w$*)*, -7.24 (14H, b, *o*-Ph)*.

ATR-FTIR (cm^{-1}): 3052 (w), 3022 (w), 2982 (w), 2894 (w), 2822 (w), 1594 (s), 1501 (s), 1447 (w), 1404 (m), 1244 (w), 1178 (s), 1157 (w), 1127 (w), 1086 (s), 1017 (m), 995 (m), 945 (m), 905 (w), 854 (m), 837 (m), 754 (s), 724 (s), 698 (s).

UV-vis-NIR (DME): λ_{max} (ε) = 274 nm (35,000 M^{-1} cm^{-1}), 378 nm (36,000 M^{-1} cm^{-1}), 734 nm (240 M^{-1} cm^{-1}).

Anal. Calcd. for: $C_{80}H_{84}O_8KCe$: C 71.03 %, H 6.26 %. Found: C 70.81 %, H 5.98 %.

*Paramagnetic line-broadening make peak integration unreliable (assignments tentative).

D) For Ln=Tb: $K(DME)_4][Tb(Ph_4Pn)_2]$ (1-Tb): In a 20 mL vial 44.3 mg (58.9 µmol) $TbI_3(THF)_{2.9}$ and 99.4 mg (118 µmol, 2 eq) $[K_2(DME)_4][Ph_4Pn]$ were dissolved in 7 mL THF and the resulting dark red solution was stirred for 16 hours. The brown mixture was then filtered, and the volatiles removed under reduced pressure to give a burgundy solid. Recrystallization from hot DME cooled to -35 °C yields a first crop of dark red needles of $[K(DME)_4][Tb(Ph_4Pn)_2]$ **1-Tb-DME** which were washed with cold pentane and dried briefly under vacuum (48.5 mg). Evaporation of the mother liquor and recrystallization of the solid residue from hot DME yielded a second crop of crystals, which were washed with cold pentane and dried briefly under vacuum (12.6 mg). Yield: 62.1 mg (77 %)

^{1}H NMR (400 MHz, Pyridine-d5)*: -59.33 (8H), -81.89 (16H).

ATR-FTIR (cm^{-1}): 3055 (w), 3022 (w), 2982 (w), 2928 (w), 2892 (w), 2822 (w), 1592 (s), 1570 (w), 1507 (s), 1499 (s), 1470 (w), 1447 (w), 1399 (m), 1369 (w), 1244 (w), 1177 (s), 1125 (m), 1082 (s), 1030 (m), 1017 (w), 995 (m), 945 (m), 901 (w), 852 (s), 837 (s), 785 (m), 754 (s), 724 (m), 697 (s), 660 (w), 544 (w), 512 (m).

UV-vis-NIR (DME): λ_{max} (ε) = 275 nm (26,000 M^{-1} cm^{-1}), 383 nm (53,000 M^{-1} cm^{-1}).

Anal. Calcd. for: $C_{80}H_{84}O_8KTb$: C 70.06 %, H 6.17 %. Found: C 69.99 %, H 6.07 %.

*No other non-solvent resonances are observed within the scan range of -300 to 300 ppm due to the highly paramagnetic nature of Tb(III).

E) For Ln=Yb: $[Na(THF)_5][Yb(Ph_4Pn)_2]$ (1-Yb): A solution of $[Na_2(THF)_3][Ph_4Pn]$ (20mg, 0.022 mmol) was prepared in THF (1 mL) followed by the addition of $YbCl_3$ (12.6 mg, 0.044 mmol). Immediate colour changes from orange to light greenish were noticed with the formation of off-white precipitate. After 15 minutes the reaction mixture was filtered; a few single crystals were obtained from standing a THF solution at -35 ^oC.

F) $[Mg(THF)_5][Y(Ph_4Pn)_2]_2$ (2): A solution of $[Mg(THF)_3][Ph_4Pn]$ (20 mg, 0.032 mmol) was prepared in 1 mL of THF to which solid $Y(HMDS)_3$ (18 mg, 0.032 mmol) was added at room temperature. The mixture was stirred for 48 hours resulting in a colour change to yellow. The

solvent was removed under reduced pressure and the remaining residue washed with *n*-hexane (2×3 mL) to afford the product $[Mg(THF)_5][Y(Ph_4Pn)_2]_2$ (**2**) as a yellow powder that was dried under vacuum (22 mg, 40 % yield). Single crystals were obtained from storing a THF solution at -35 ^oC.

^{1}H NMR (500 MHz, THF-H_8) δ: 7.29 (d, *J* = 8.0 Hz, 4H), 7.20 (s, 2H)*, 7.11 (t, *J* = 8.3 Hz, 4H), 6.98 (d, *J* = 7.3 Hz, 2 H).

^{13}C{^{1}H} NMR (126 MHz, THF-H_8) δ: 138.7, 129.0, 127.6, 124.9*, 124.3,111.3.

*Found by ^{1}H-^{13}C HSQC.

ESI-MS (-) m/z expected for [M-$Mg(THF)_5$] = 901.2507, found 901.2242.

UV–vis (THF): λ_{max} (ε) = 347 nm (16,300 $M^{-1}\,cm^{-1}$).

G) $[MgCl(THF)_5][(YPh_4Pn)_2(\mu\text{-}Cl)_5Mg(THF)_4]$ (3): A solution of $[Mg(THF)_3][Ph_4Pn]$ (20 mg, 0.032 mmol) was prepared in 1 mL of THF to which YCl_3 (6 mg, 0.032 mmol) was added at room temperature. The mixture was stirred for 5 hours resulting in a colour change to orange-red. The solvent was removed under reduced pressure and the remaining residue washed with (2×3 mL) to afford the product $[MgCl(THF)_5][(YPh_4Pn)_2(\mu\text{-}Cl)_5Mg(THF)_4]$ (**3**) as yellow powder that was dried under vacuum (16 mg, 35 % yield). Single crystals were obtained from standing a THF solution at -35 ^oC.

^{1}H NMR (500 MHz, THF-H_8) δ: 6.79 (m, 6H), 6.70 (d, *J* = 7.16 Hz, 2 H), 6.32 (s, 1H_w)*.

^{13}C{^{1}H} NMR (126 MHz, THF-H_8) δ: 139.3, 129.1, 127.1, 123.1, 122.9*, 110.6 ppm.

*Found by ^{1}H-^{13}C HSQC.

ESI-MS (-) m/z expected for [M-$Y(THF)_5$] = 1207.106, found 1207. 019.

UV–vis (THF): λ_{max} = 355 nm (ε) (20,600 $M^{-1}\,cm^{-1}$).

Spectroscopic Data

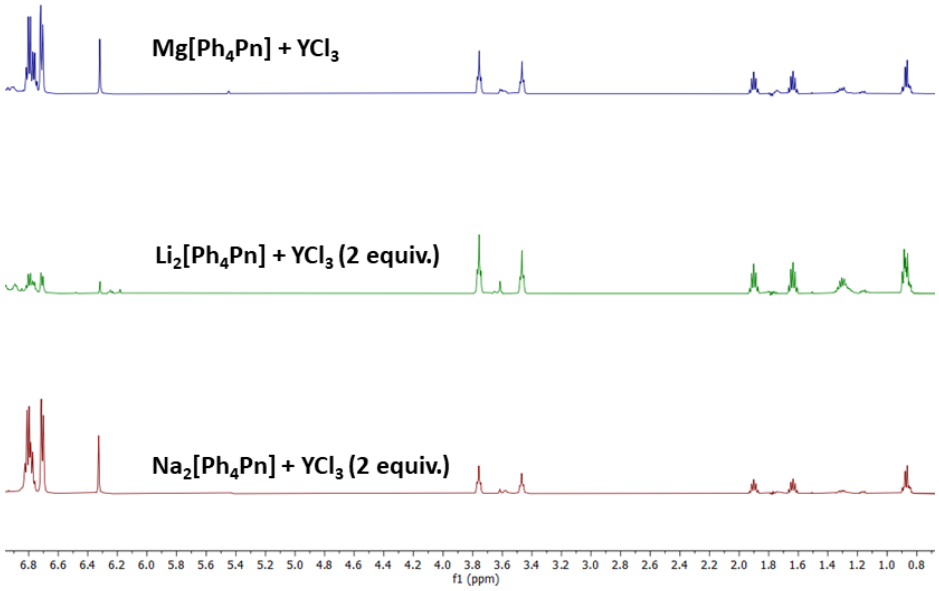


Figure S1. Comparison of ^{1}H NMR spectrum (500 MHz) spectra from reacting Mg[Ph_4Pn], Li_2[Ph_4Pn] and Na_2[Ph_4Pn] with YCl_3 in THF-H_8.

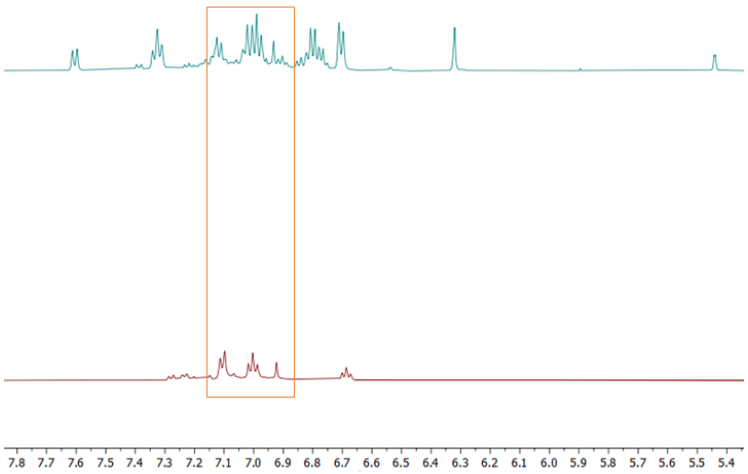
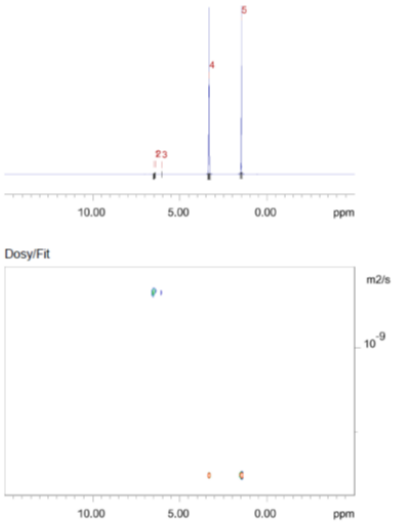


Figure S2. ^{1}H NMR spectra of [Mg(THF)$_5$][Y(Ph_4Pn)$_2$]$_2$ (**2**) (bottom) and after addition of dioxane into [MgCl(THF)$_5$][(Ph_4Pn)$_2$Y(μ-Cl)$_5$Mg(THF)$_4$] (**3**) (upper) in THF-H_8.



Peak name	F2 [ppm]	Io	error	D [m2/s]	error	fitInfo
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2	6.411	1.73e+07	5.326e+04	6.32e-10	4.196e-12	Done
3	6.024	4.11e+06	2.118e+04	6.33e-10	7.022e-12	Done
4	3.320	3.28e+09	6.520e+06	2.83e-09	1.087e-11	Done
5	1.473	3.25e+09	7.615e+06	2.83e-09	1.280e-11	Done

Figure S3. 500 MHz ^{1}H DOSY NMR Spectrum (top) and experimentally determined diffusion coefficients (bottom) of $[MgCl(THF)_5][(YPh_4Pn)_2(\mu\text{-}Cl)_5Mg(THF)_4]$ (**3**) in THF-H_8.

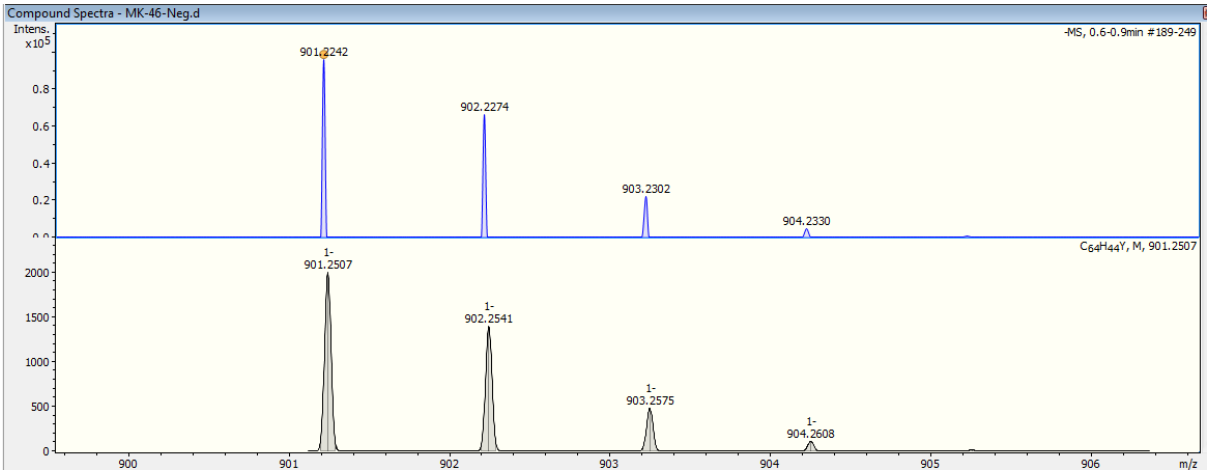

Figure S4. ESI-MS (-) of **2**. m/z expected for $[M\text{-}Mg(THF)_5]$ = 901.2507, found 901.2242.

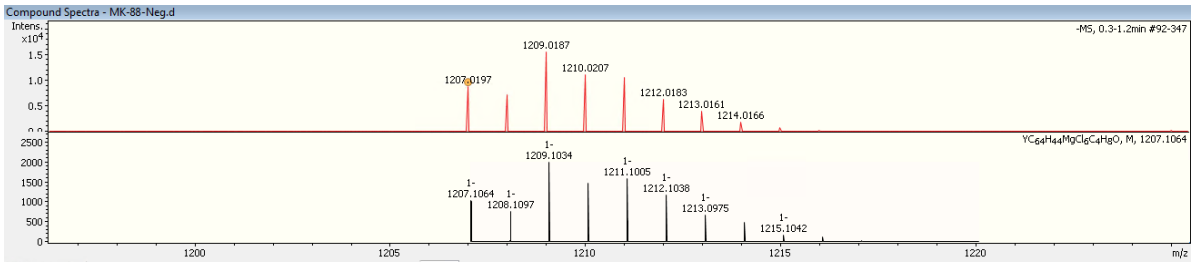

Figure S5. ESI-MS (-) of **3**. m/z expected for [M-Y(THF)$_5$] = 1207.1064, found 1207.0197.

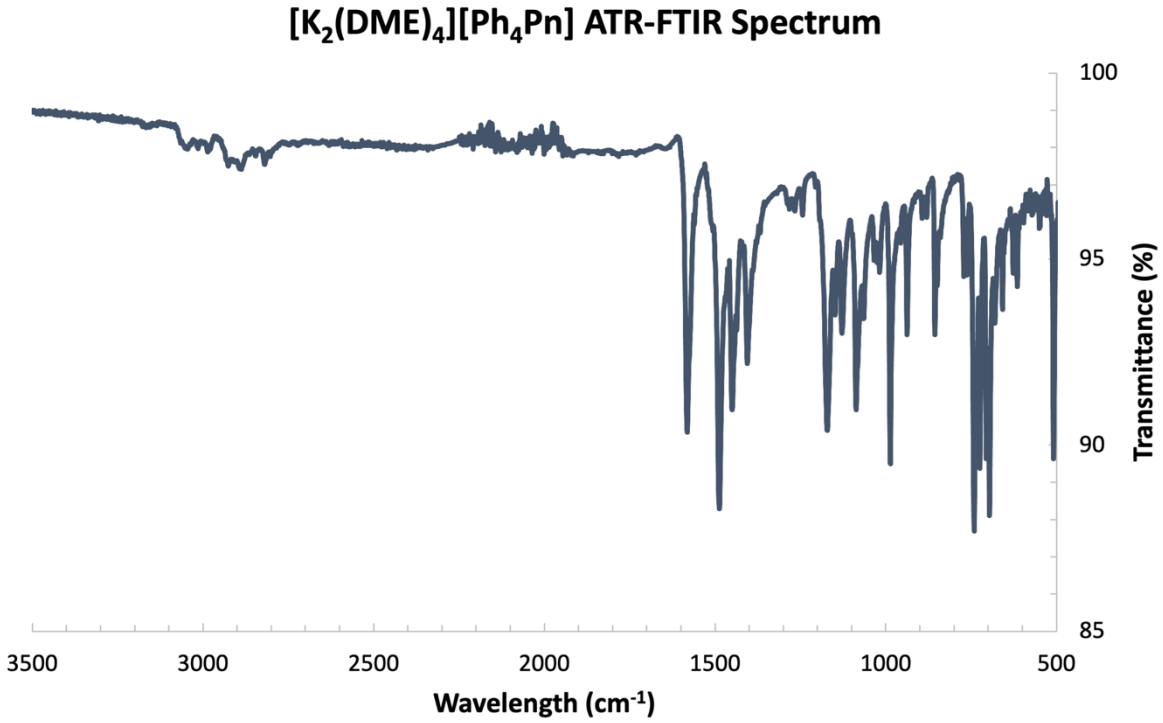

Figure S6. ATR-FTIR spectrum of [K_2(DME)$_4$][Ph_4Pn] as a neat powder.

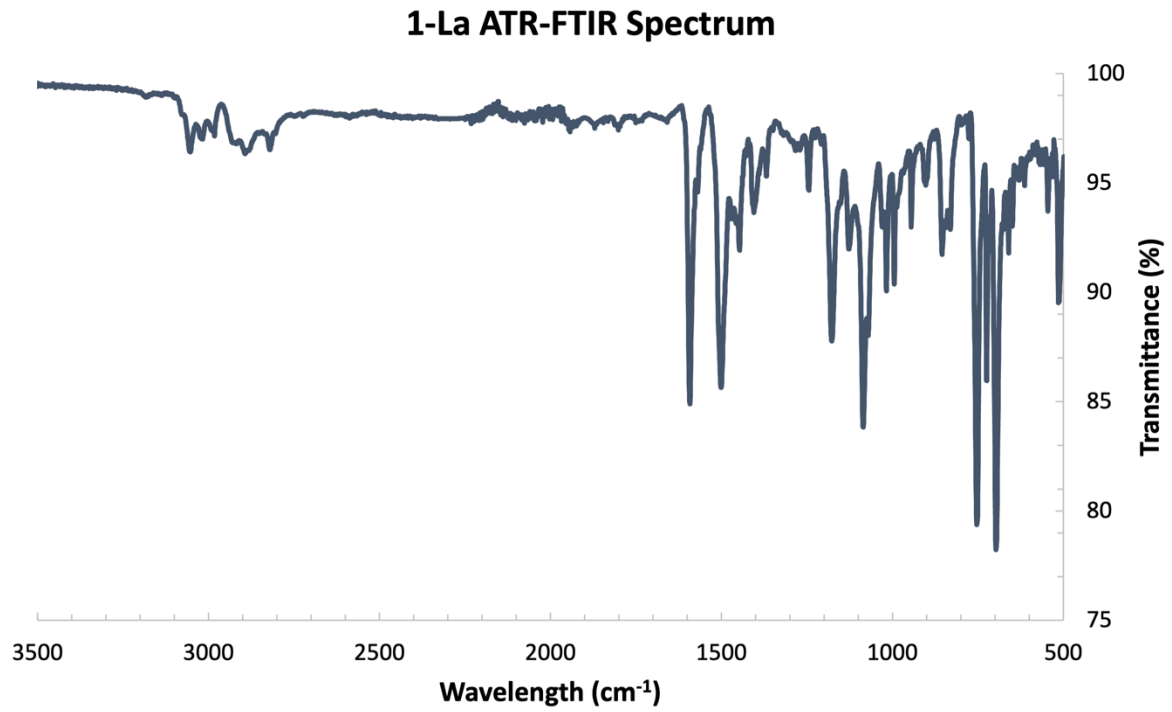

Figure S7. ATR-FTIR spectrum of **1-La** as a neat powder.

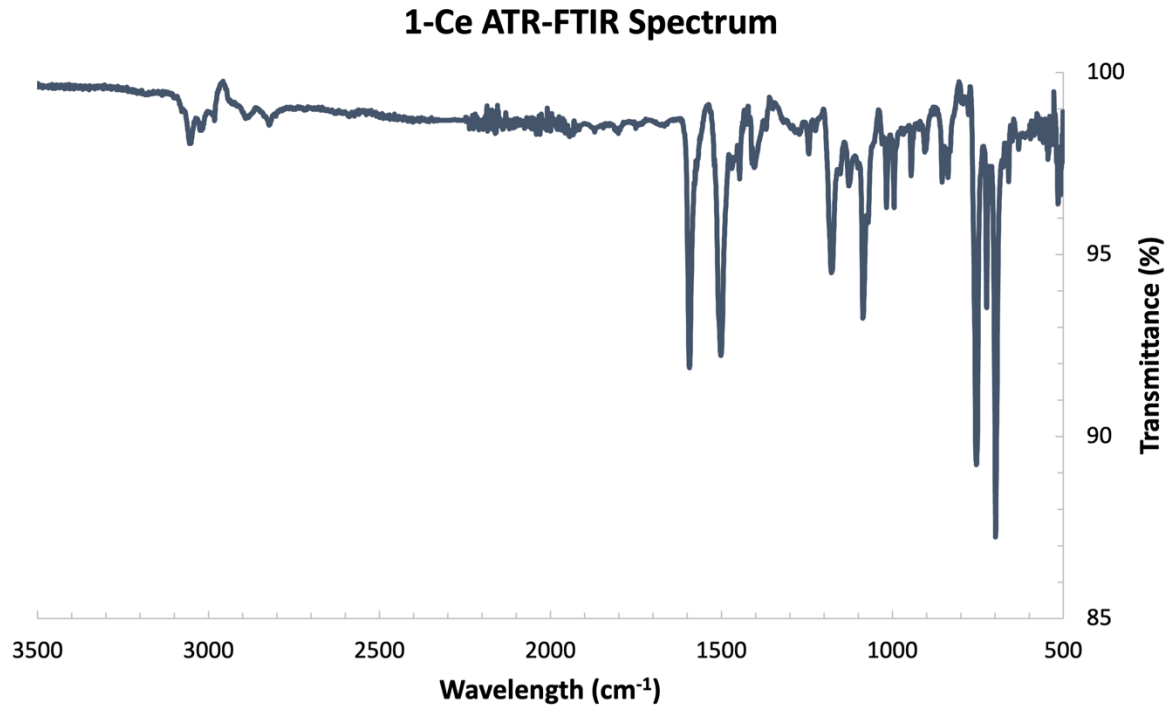

Figure S8. ATR-FTIR spectrum of **1-Ce** as a neat powder.

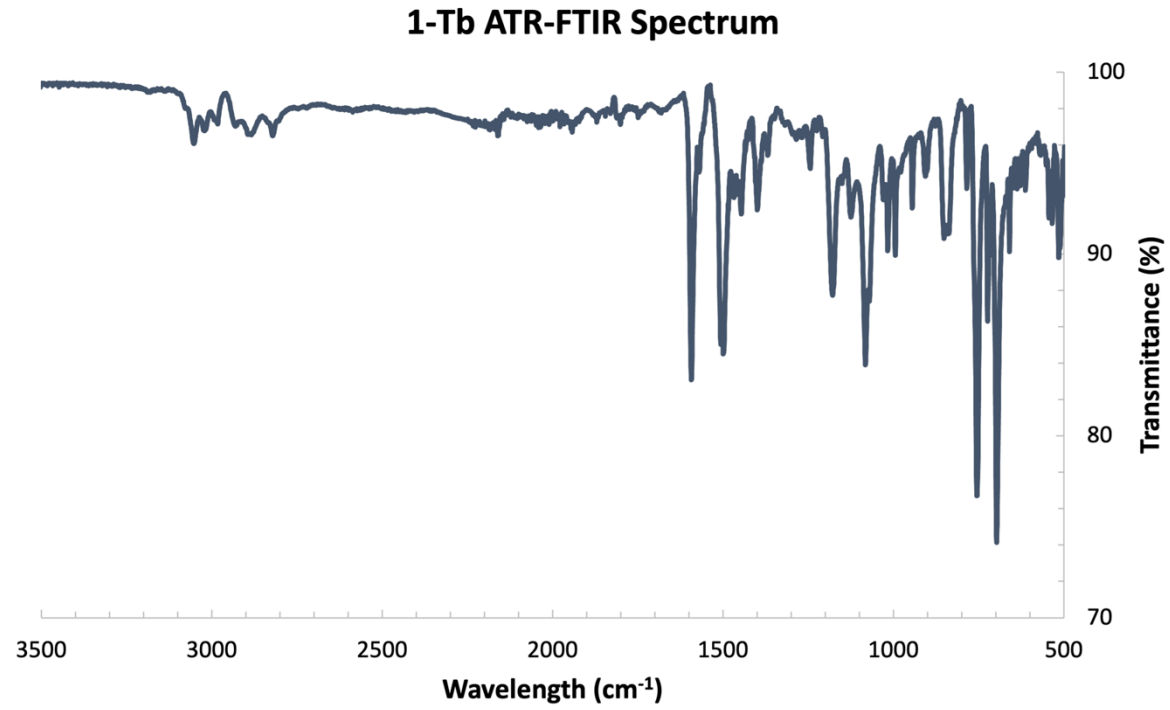

Figure S9. ATR-FTIR spectrum of **1-Tb** as a neat powder.

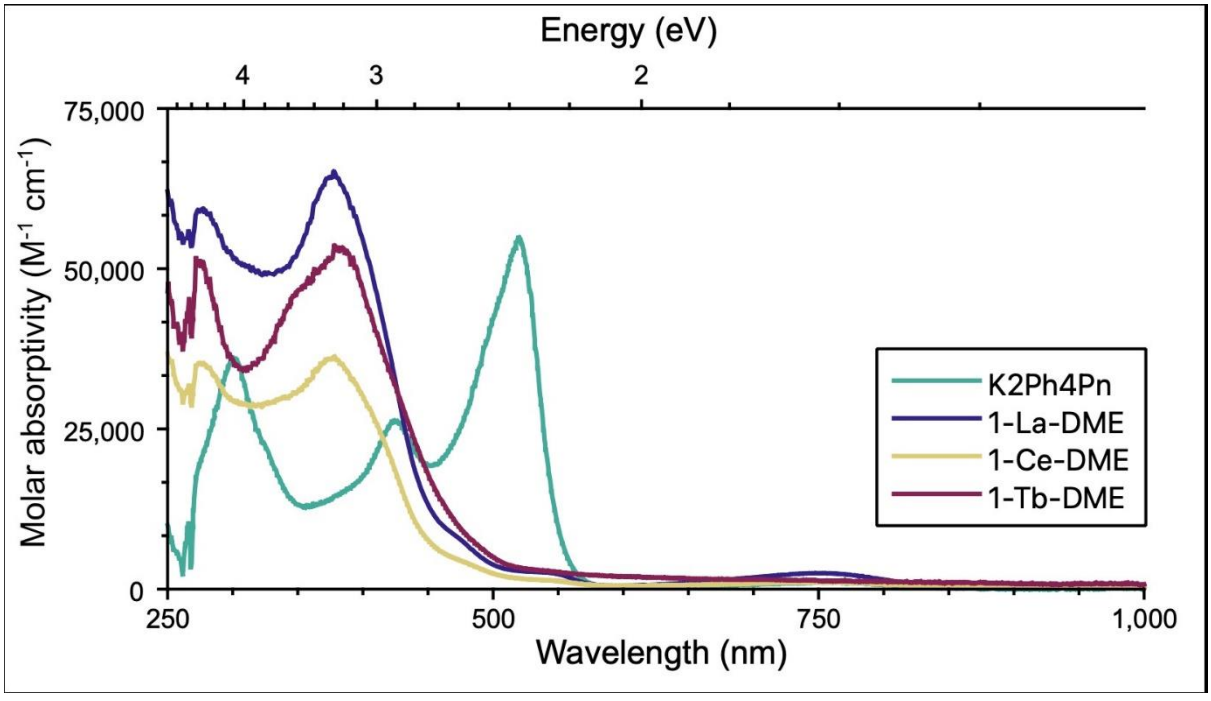

Figure S10. UV-Vis spectra of complexes **1-Ln-DME** (Ln = La, Ce, Tb) and K_2Ph_4Pn.

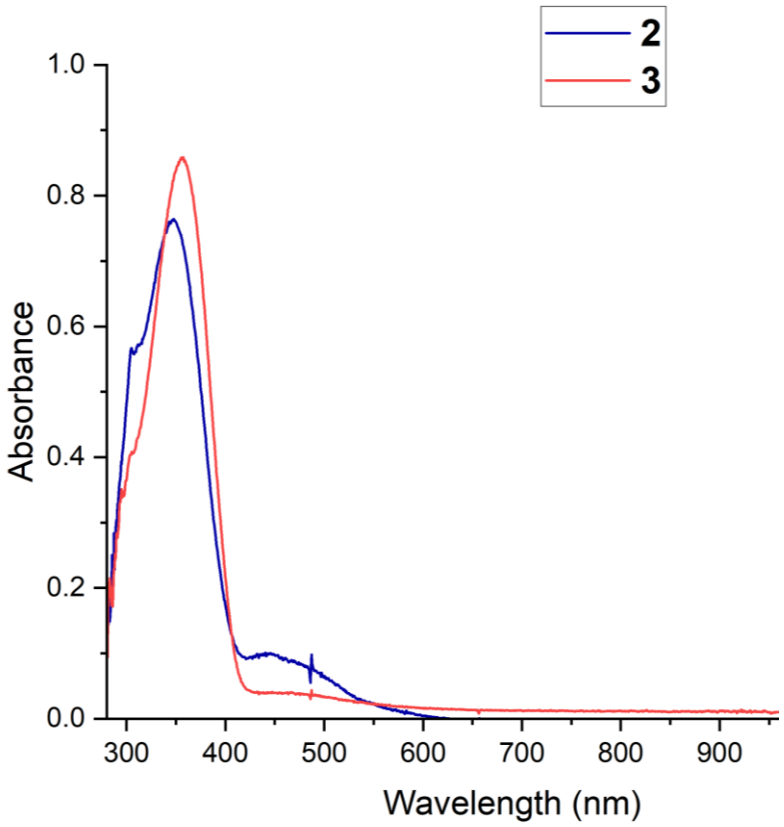

Figure S11. UV-Vis spectra of complexes **2** and **3** in THF.

Crystallographic Data

Compound	**Li_2Ph_4Pn-DME**	**Na_2Ph_4Pn-DME**	**K_2Ph_4Pn-DME**
CCDC Deposition Number	2332849	2357824	2357825
Identification Code	e23uh11	PLA23075	PLA23074
Chemical formula	C_{40} H_{42} Li_2 O_4	$C_{48}H_{62}K_2O_8$	$C_{48}H_{62}K_2O_8$
Formula weight	600.61	812.95	845.17
Temperature (K)	149.9(7)	200.0(1)	200.0(1)
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$
a (Å)	10.8476(4)	11.0913(1)	11.1442(1)
b (Å)	10.0967(4)	13.2818(1)	13.0688(1)
c (Å)	15.5113(5)	15.8392(1)	16.7460(1)
α (°)	90	90	90
β (°)	94.807(3)	105.146(1)	106.828(1)
γ (°)	90	90	90
Volume ($Å^3$)	1692.90(11)	2252.26(3)	2334.47(3)
Z	2	2	2
μ (mm^{-1})	0.073	0.81	2.19
ρ_{calc} (g cm^{-3})	1.178	1.199	1.202
F(000)	640	872	904
Crystal size (mm)	0.70 x 0.55 x 0.38	0.330x0.160x0.110	0.24 x 0.17 x 0.16
Radiation	MoKα (λ = 0.7173 Å)	CuKα (λ = 1.54184 Å)	CuKα (λ = 1.54184 Å)
2Θ range for data collection (°)	[2.990, 29.541]	[4.364, 79.687]	[8.288, 160.156]
Index ranges	$-14 \le h \le 14$ $-13 \le k \le 12$ $-21 \le l \le 20$	$-14 \le h \le 13$ $-16 \le k \le 16$ $-20 \le l \le 20$	$-14 \le h \le 13$ $-16 \le k \le 16$ $-21 \le l \le 21$
Reflections collected	15817	50957	51712
Independent reflections	4135 [R_{int} = 0.0257]	49719 [R_{int} = 0.0344, R_{sigma} = 0.0191]	5064 [R_{int} = 0.0363, R_{sigma} = 0.0177]
Data/restraints/parameters	4135 / 12 / 220	4901 / 0 / 271	5064 / 10 / 299
Goodness of fit on F^2	1.027	1.050	1.103
Final R indexes ($I \ge 2\sigma$)	R_1 = 0.0557, wR_2 = 0.1275	R_1 = 0.0432 wR_2 = 0.1110	R_1 = 0.0347, wR_2 = 0.0995
Final R indexes (all data)	R_1 = 0.0752 wR_2 = 0.1384	R_1 = 0.0460 wR_2 = 0.1511	R_1 = 0.0362, wR_2 = 0.1020
Largest diff. peak/hole (e $Å^{-3}$)	0.626 / -0.369	0.610 -0.420	0.580 / -0.190

Compound	**1-La-DME**	**1-Ce-DME**	**1-Tb-DME**
CCDC Deposition Number	2357829	2357826	2357823
Identification Code	PLA23116	PLA23085	PLA23115
Chemical formula	$C_{80}H_{84}LaKO_8$	$C_{80}H_{84}CeKO_8$	$C_{80}H_{84}KO_8Tb$
Formula weight	1351.48	1352.69	1371.49
Temperature (K)	100.0(1)	100.0(1)	100.0(1)
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	P2/n	P2/n	P2/n
a (Å)	15.9186(1)	15.8469(1)	15.6241(1)
b (Å)	10.1537(1)	10.1787(1)	10.2214(1)
c (Å)	21.3582(2)	21.4308(1)	21.5624(2)
α (°)	90	90	90
β (°)	93.633(1)	94.056(1)	94.643(1)
γ (°)	90	90	90
Volume ($Å^3$)	3445.25(5)	3448.15(5)	3432.22(5)
Z	2	2	2
μ (mm^{-1})	5.769	6.077	6.05
ρ_{calc} (g cm^{-3})	1.303	1.303	1.327
F(000)	1408	1410	1424
Crystal size (mm)	0.21 x 0.14 x 0.04	0.60 x 0.07 x 0.03	0.19 x 0.08 x 0.05
Radiation	CuKα (λ = 1.54184 Å)	CuKα (λ = 1.54184 Å)	CuKα (λ = 1.54184 Å)
2Θ range for data collection (°)	[6.690, 159.912]	[6.716, 159.920]	[6.734, 160.382]
Index ranges	$-20 \le h \le 20$ $-9 \le k \le 12$ $-27 \le l \le 27$	$-20 \le h \le 20$ $-10 \le k \le 12$ $-27 \le l \le 27$	$-19 \le h \le 19$ $-10 \le k \le 12$ $-27 \le l \le 27$
Reflections collected	80267	75093	82493
Independent reflections	7512 [R_{int} = 0.0571, R_{sigma} = 0.0289]	7501 [R_{int} = 0.0666, R_{sigma} = 0.0279]	7273 [R_{int} = 0.0700, R_{sigma} = 0.0290]
Data/restraints/parameters	7503 / 0 / 411	7501 / 0 / 411	7466 / 0 / 411
Goodness of fit on F^2	1.135	1.073	1.051
Final R indexes ($I \ge 2\sigma$)	R_1 = 0.0307, wR_2 = 0.0836	R_1 = 0.0334, wR_2 = 0.0796	R_1 = 0.0325, wR_2 = 0.0820
Final R indexes (all data)	R_1 = 0.0317, wR_2 = 0.0844	R_1 = 0.0348, wR_2 = 0.0803	R_1 = 0.0336, wR_2 = 0.0827
Largest diff. peak/hole (e $Å^{-3}$)	0.524 / -0.859	0.403 / -0.974	0.735 / -0.662

Compound	**1-Y**	**1-Yb**	**2**
CCDC Deposition Number	2357831	2357831	2357832
Identification Code	s23uh45	s23uh27	s22uh30
Chemical formula	C_{76} H_{74} Li O_6 Y	C_{96} H_{108} Na O_8 Yb	C_{176} H_{184} Mg O_{12} Y_2
Formula weight	1179.20	1585.85	2693.35
Temperature (K)	150.00(10)	150.00(10) K	150(2) K
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	P2/n	$P2_1/n$
a (Å)	10.33655(9)	20.18090(11)	17.52153(8)
b (Å)	25.4845(2)	15.78844(8)	19.2375(8)
c (Å)	23.3833(2)	25.03591(11)	21.05544(8)
α (°)	90	90	90
β (°)	96.3298(8)	90.51	92.9279
γ (°)	90	90	90
Volume (Å^3)	6122.12(9)	7976.74(7)	7087.9(3)
Z	4	4	2
μ (mm^{-1})	1.765	1.321	1.631
ρ_{calc} (g cm^{-3})	1.279	2.671	1.262
F(000)	2480	3316	2852
Crystal size (mm)	0.443x0.159x 0.078	0.391x0.227x 0.217	0.478x0.097x 0.054
Radiation	CuKα (λ = 1.54184 Å)	CuKα (λ = 1.54184 Å)	CuKα (λ = 1.54184 Å)
2Θ range for data collection (°)	[3.469, 72.997]	[3.531, 72.952]	[3.367, 72.896]
Index ranges	-12 ≤ *h* ≤ 12 -28 ≤ *k* ≤ 31 -28 ≤ *l* ≤ 28	-24 ≤ *h* ≤ 24 -19 ≤ *k* ≤ 19 -26 ≤ *l* ≤ 30	-21 ≤ *h* ≤ 21 -21 ≤ *k* ≤ 23 -26 ≤ *l* ≤ 26
Reflections collected	61832	85179	166010
Independent reflections	12165 [R_{int} = 0.0576]	15866 [R_{int} = 0.0355]	14135 [R_{int} = 0.0420]
Data/restraints/parameters	12165 / 0 / 937	15866 / 0 / 1033	14135 / 101 / 1017
Goodness of fit on F^2	1.058	1.046	1.017
Final R indexes ($I \geq 2\sigma$)	R_1 = 0.0413 wR_2 = 0.1057	R_1 = 0.0265 wR_2 = 0.0666	R_1 = 0.0307 wR_2 = 0.0769
Final R indexes (all data)	R_1 = 0.0455 wR_2 = 0.1096	R_1 = 0.0299 wR_2 = 0.0691	R_1 = 0.0352 wR_2 = 0.0802
Largest diff. peak/hole (*e* Å^{-3})	1.322 / -0.511	0.385 / -0.686	0.440 / -0.487

Compound	**3**	**1-Ce-THF**	
CCDC Deposition Number	2357830	2357828	
Identification Code	s23uh16_sq	PLA23069	
Chemical formula	C_{100} H_{116} Cl_6 Mg_2 O_9 Y_2	$C_{83.7}H_{83.7}CeKO_{4.7}$	
Formula weight	1901.06	1344.02	
Temperature (K)	150.00(10)	100	
Crystal system	Orthorhombic	Triclinic	
Space group	Pbcm	P-1	
a (Å)	14.8775(4)	10.2856(1)	
b (Å)	21.4215(8)	13.0071(2)	
c (Å)	37.4724(11)	25.7130(3)	
α (°)	90	80.814(1)	
β (°)	90	88.212(1)	
γ (°)	90	78.113(1)	
Volume (Å^3)	11942.4(7)	3323.09(7)	
Z	4	2	
μ (mm^{-1})	2.983	6.27	
ρ_{calc} (g cm^{-3})	1.057	1.343	
F(000)	3968	1401	
Crystal size (mm)	0.080x0.080x 0.020	0.41 x 0.03 x 0.02	
Radiation	CuKα (λ = 1.54184 Å)	CuKα (λ = 1.54184 Å)	
2Θ range for data collection (°)	[3.617, 68.250]	[6.964, 160.596]	
Index ranges	-15 ≤ *h* ≤ 17 -25 ≤ *k* ≤ 25 -45 ≤ *l* ≤ 32	-10 ≤ *h* ≤ 13 -16 ≤ *k* ≤ 16 -32 ≤ *l* ≤ 32	
Reflections collected	76884	82410	
Independent reflections	11118 [R_{int} = 0.1021]	14324 [R_{int} = 0.0673, R_{sigma} = 0.0390]	
Data/restraints/parameters	11118 / 175 / 670	14324 / 29 / 879	
Goodness of fit on F^2	1.029	1.0480	
Final R indexes ($I \geq 2\sigma$)	R_1 = 0.0555 wR2 = 0.1358	R_1 = 0.0449, wR_2 = 0.1089	
Final R indexes (all data)	R_1 = 0.0868 wR_2 = 0.1511	R_1 = 0.0476, wR_2 = 0.1102	
Largest diff. peak/hole (*e* Å^{-3})	0.505 / -0.622	1.500 / -1.850	

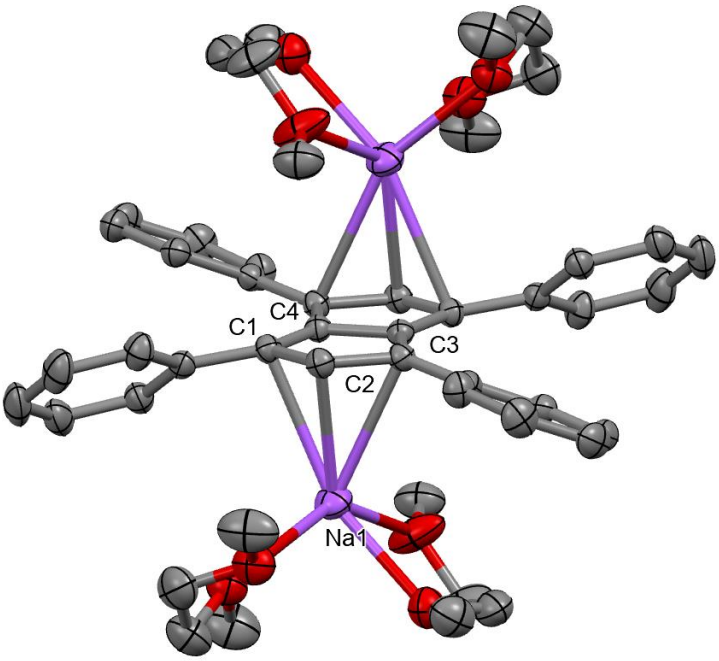

Figure S12: Molecular structure of **Na_2Ph_4Pn-DME** with thermal ellipsoids at 50% probability with hydrogen atoms omitted for clarity. Na: purple, C: grey, O: red.

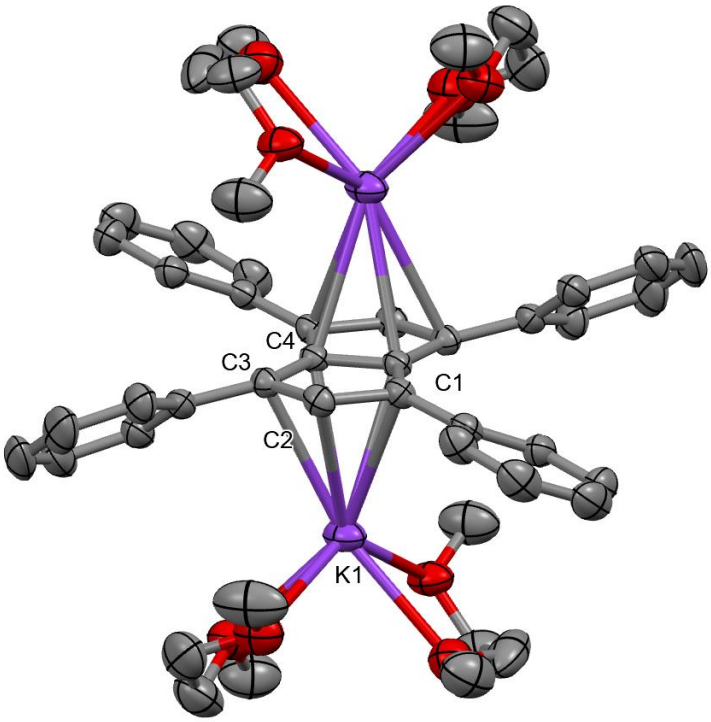

Figure S13: Molecular structure of **K_2Ph_4Pn-DME** with thermal ellipsoids at 50% probability with hydrogen atoms and minor component of disordered DME omitted for clarity. K: purple, C: grey, O: red.

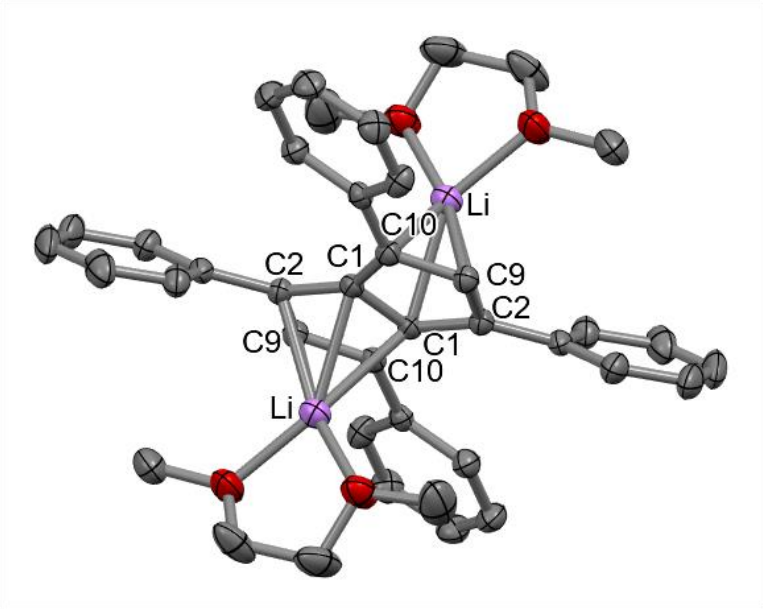

Figure S14: Molecular structure of **Li_2Ph_4Pn-DME** with thermal ellipsoids at 50% probability with hydrogen atoms are omitted for the clarity. Li: purple, C: grey, O: red.

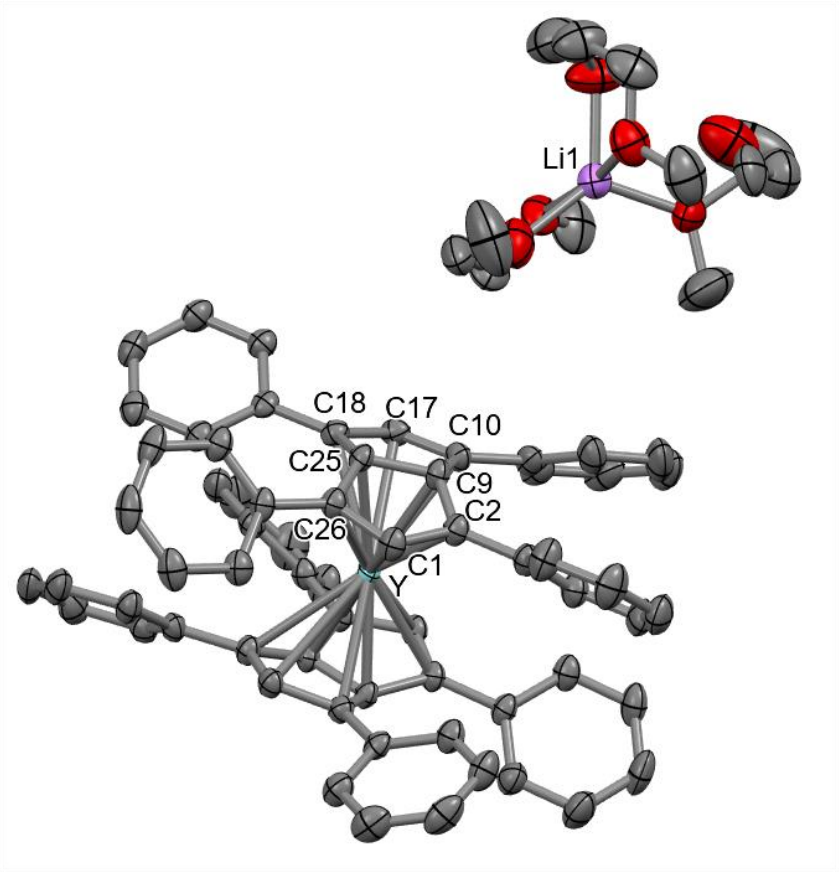

Figure S15: Molecular structure of **1-Y-DME** with thermal ellipsoids at 50% probability with hydrogen atoms and minor component of disordered DME omitted for clarity. Y: Cyan, Li: purple, C: grey, O: red.

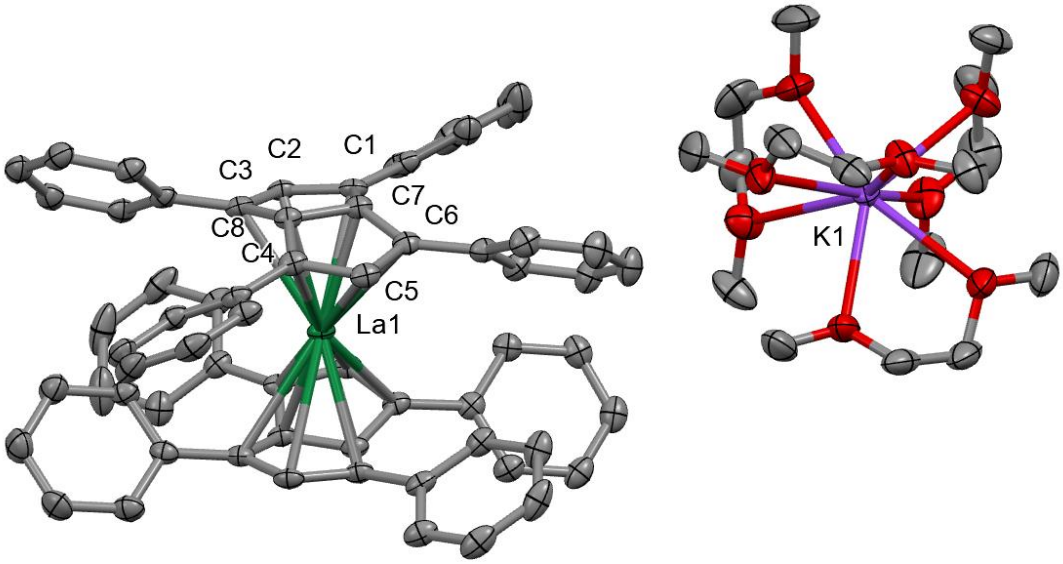

Figure S16: Molecular structure of **1-La-DME** with thermal ellipsoids at 50% probability with hydrogen atoms omitted for clarity. La: teal, K: purple, C: grey, O: red.

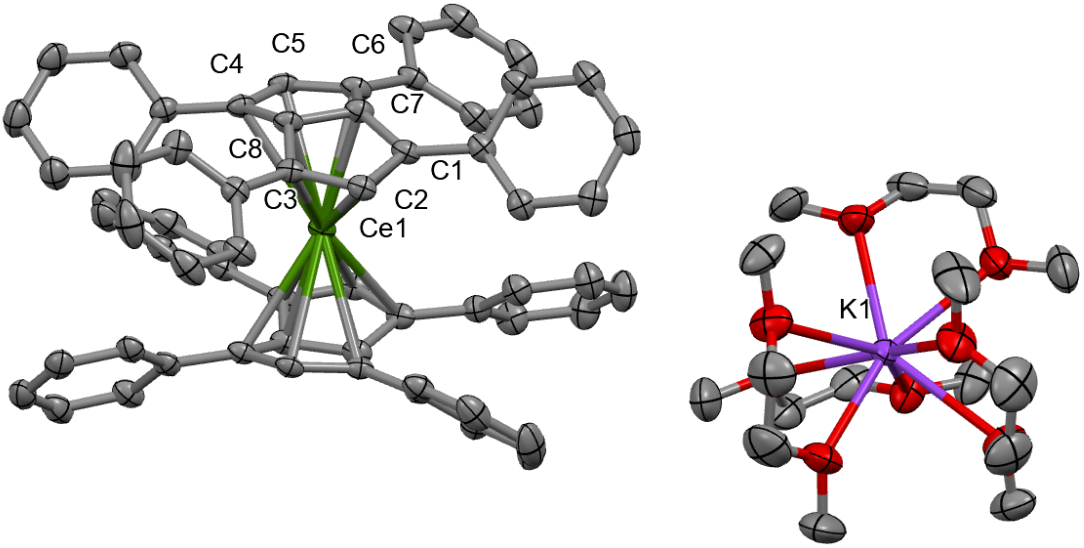

Figure S17: Molecular structure of **1-Ce-DME** with thermal ellipsoids at 50% probability with hydrogen atoms omitted for clarity. Ce: green, K: purple, C: grey, O: red.

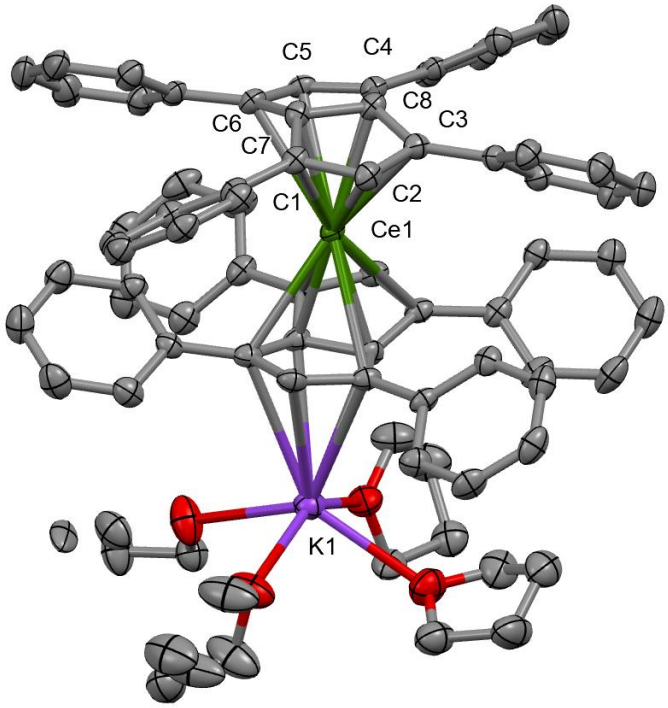

Figure S18: Molecular structure of **1-Ce-THF** with thermal ellipsoids at 50% probability with hydrogen atoms and disordered lattice solvent omitted for clarity. Ce: green, K: purple, C: grey, O: red.

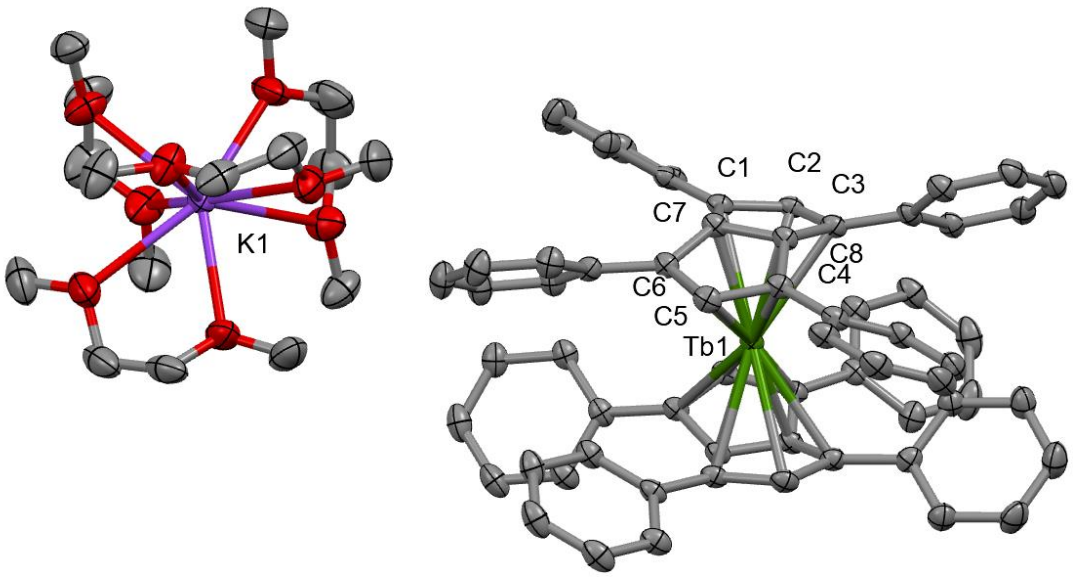

Figure S19: Molecular structure of **1-Tb-DME** with thermal ellipsoids at 50% probability with hydrogen atoms omitted for clarity. Tb: green, K: purple, C: grey, O: red.

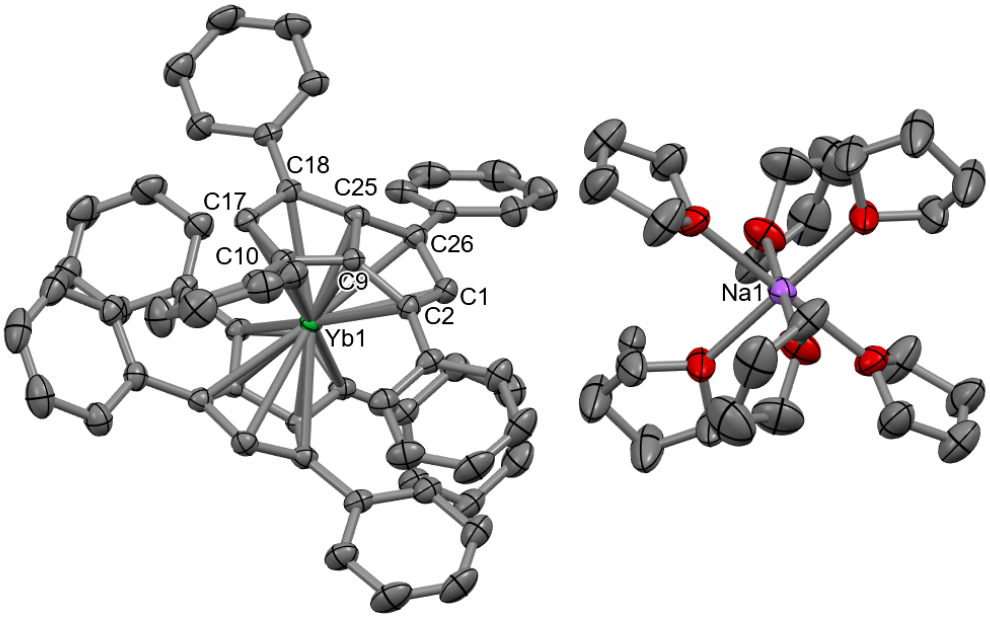

Figure S20: Molecular structure of **1-Yb-THF** with thermal ellipsoids at 50% probability with hydrogen atoms and disordered lattice solvent omitted for clarity. Yb: green, Na: purple, C: grey, O: red.

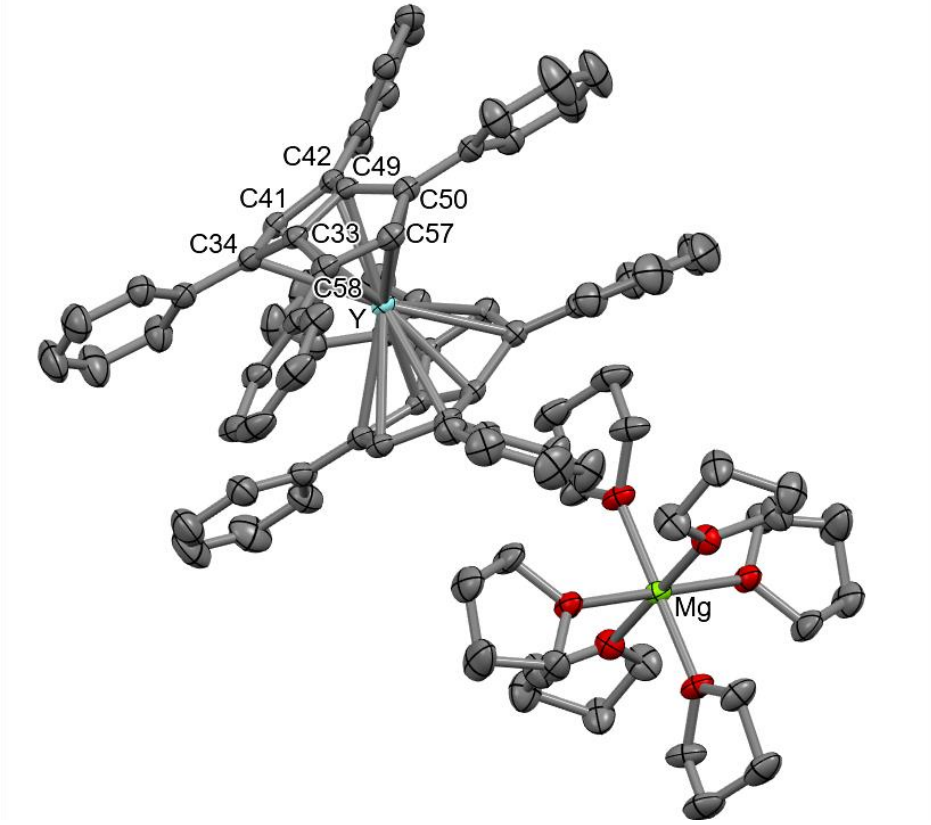

Figure S21: Molecular structure of **2** with thermal ellipsoids at 50% probability with hydrogen atoms are omitted for clarity. Y: Cyan, Mg: light green, C: grey, O: red.

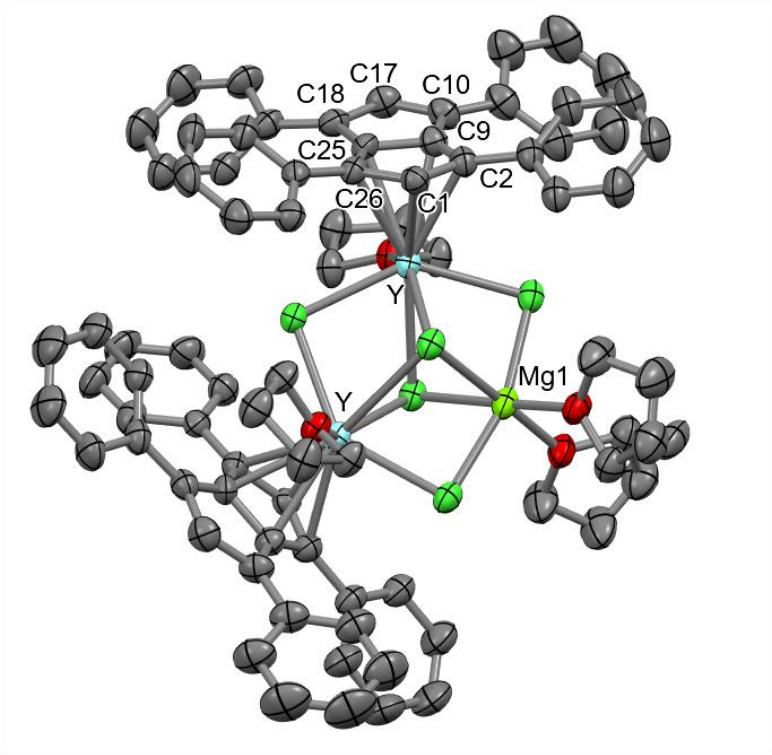

Figure S22: Molecular structure of **3** with thermal ellipsoids at 50% probability with hydrogen atoms and disordered cationic [$MgCl(THF)_5$] molecule are omitted for clarity. Y: Cyan, Mg: light green, C: grey, O: red.

Computational Methodology

Kohn-Sham density functional theory (DFT) calculations were performed, starting with the X-ray crystal structures of $[Ln(\eta^8\text{-}Ph_4Pn)_2]^-$ (Ln = La, Ce, Tb), using the 2023 release of the Amsterdam Density Functional (ADF) suite.[3] Both restrained (only hydrogen positions were optimised) and full geometry optimisations along with electronic structure analyses were performed employing the PBE0 hybrid functional[4] with 25% exact exchange, in conjunction with all-electron Slater-type orbital (STO) basis sets from the ADF basis set library. The basis sets were of triple-zeta doubly-polarized (TZ2P) quality for the metal (La, Ce, and Tb) and of double-zeta singly-polarized (DZP) quality for other atoms.[5] Relativistic effects were incorporated via the scalar-relativistic Zeroth-Order Regular Approximation (ZORA) Hamiltonian.[6] Dispersion corrections via the D3 model were used in a subset of the calculations to understand the impact of dispersion on the Ln-C distances. The calculations showed that the incorporation of these interactions made little difference regarding the optimized structures. The PBE0-optimized structures were retained for further analysis. To assess the chemical bond compositions, an analysis of the bonding in each system was performed using natural localized molecular orbitals (NLMOs) and natural population analysis (NPA)[7] as generated by the NBO program (version 6.0)[8] interfaced with ADF. For the interested reader, for selected canonical molecular orbitals (MOs), a breakdown in terms of fragment orbitals (FOs, in the form of `symmetrized FOs' (SFOs) generated by the ADF calculations) are provided in Figures S40-S42.

Additional geometry optimisations followed by harmonic vibrational frequency calculations were performed with Gaussian 2016 (G16) revision A.03.[9] Optimized minimum molecular structures were confirmed by means of real-positive vibrational frequencies. For this set of calculations, the hybrid B3LYP functional was employed along with the segmented ECP28MWB valence Gaussian-type orbital (GTO) basis sets in conjunction with matching relativistic pseudopotentials[10,11] for the metal centres, and the GTO basis SVP for other atoms.[12,13] Electronic excitation spectra were calculated with G16 using the same functional and basis set combination, employing the Tamm-Dancoff approximation (TDA).[14] Without TDA, the spectrum for the Ce complex afforded three negative excitation energies even though a wavefunction stability analysis did not indicate instability and the remainder of the spectrum was very similar to the TDA calculation. To understand the solvent effect on the electronic

spectra we also performed TDDFT calculations on the $[La(\eta^8\text{-}Ph_4Pn)_2]^-$ complex employing the SMD solvation model[15] with the solvent DME used experimentally in the spectral measurements. A total of 150 excited states were calculated for each system. Selected excitations were analysed via natural transition orbitals (NTOs).[16]

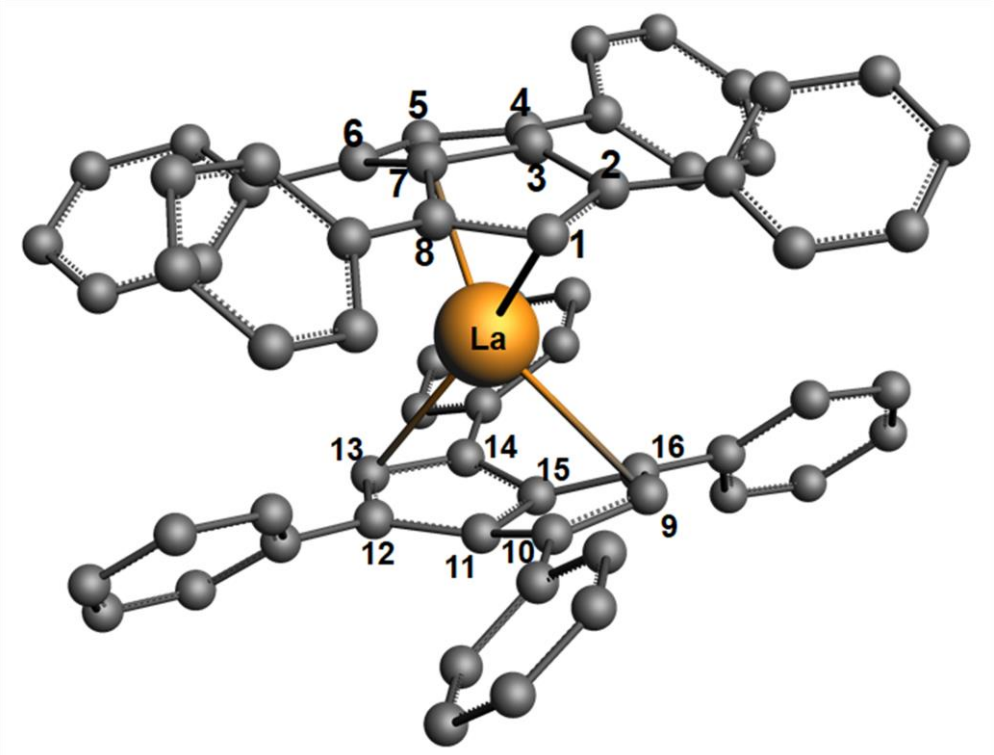

Figure S23. DFT optimised geometry of $[La(\eta^8\text{-}Ph_4Pn)_2]^-$ with numbering of selected carbon centres.

Table S1. Kohn-Sham DFT computed bond parameters of only hydrogen optimised X-ray structure and a fully optimised structure of **1-Ln**. Wiberg Bond Indices (WBIs) from NBO calculation. The numbering of the carbon centres corresponds to that in Figure S11.				
La-Pentalenide	**XRD structure (Å)**	**WBI (XRD)**	**Full optimisation (Å) (without D3)**	**Full optimisation (Å) (with D3)**
La-C1	2.964	0.093	2.979	2.951
La-C2	2.869	0.104	2.871	2.856
La-C3	2.592	0.138	2.588	2.587
La-C4	2.855	0.100	2.836	2.836
La-C5	2.964	0.086	2.953	2.759
La-C6	2.803	0.107	2.793	2.934
La-C7	2.578	0.141	2.571	2.557
La-C8	2.850	0.110	2.842	2.814
La-C9	2.964	0.093	2.979	2.951
La-C10	2.869	0.104	2.871	2.856
La-C11	2.592	0.138	2.588	2.587
La-C12	2.855	0.100	2.836	2.836
La-C13	2.964	0.086	2.953	2.759
La-C14	2.803	0.107	2.793	2.934
La-C15	2.578	0.141	2.571	2.557
La-C16	2.850	0.110	2.842	2.814

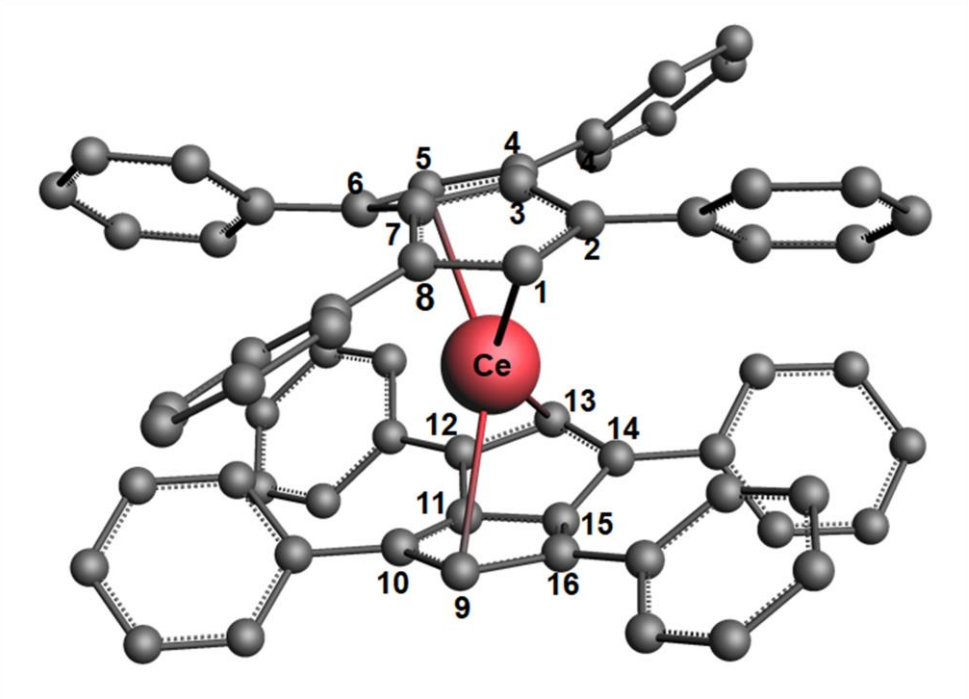

Figure S24. DFT optimised geometry of $[Ce(\eta^8\text{-}Ph_4Pn)_2]^-$ with numbering of selected carbon centres.

Table S2. Kohn-Sham DFT computed bond parameters of only hydrogen-optimised X-ray structure and a fully optimised structure of **1-Ce**. Wiberg Bond Indices (WBIs) from NBO calculation. The numbering of the carbon centres corresponds to Figure S12.				
Ce-Pentalenide	**XRD structure (Å)**	**WBI (XRD)**	**Full optimisation (Å) (without D3)**	**Full optimisation (Å) (with D3)**
Ce-C1	2.940	0.089	2.928	2.909
Ce-C2	2.829	0.106	2.807	2.809
Ce-C3	2.561	0.145	2.560	2.560
Ce-C4	2.839	0.111	2.843	2.829
Ce-C5	2.931	0.100	2.949	2.923
Ce-C6	2.820	0.115	2.811	2.784
Ce-C7	2.549	0.146	2.543	2.530
Ce-C8	2.779	0.113	2.771	2.736
Ce-C9	2.940	0.089	2.928	2.909
Ce-C10	2.829	0.106	2.807	2.809
Ce-C11	2.561	0.145	2.560	2.560
Ce-C12	2.839	0.111	2.843	2.829
Ce-C13	2.931	0.100	2.949	2.923
Ce-C14	2.820	0.115	2.811	2.784
Ce-C15	2.549	0.146	2.543	2.530
Ce-C16	2.779	0.113	2.771	2.736

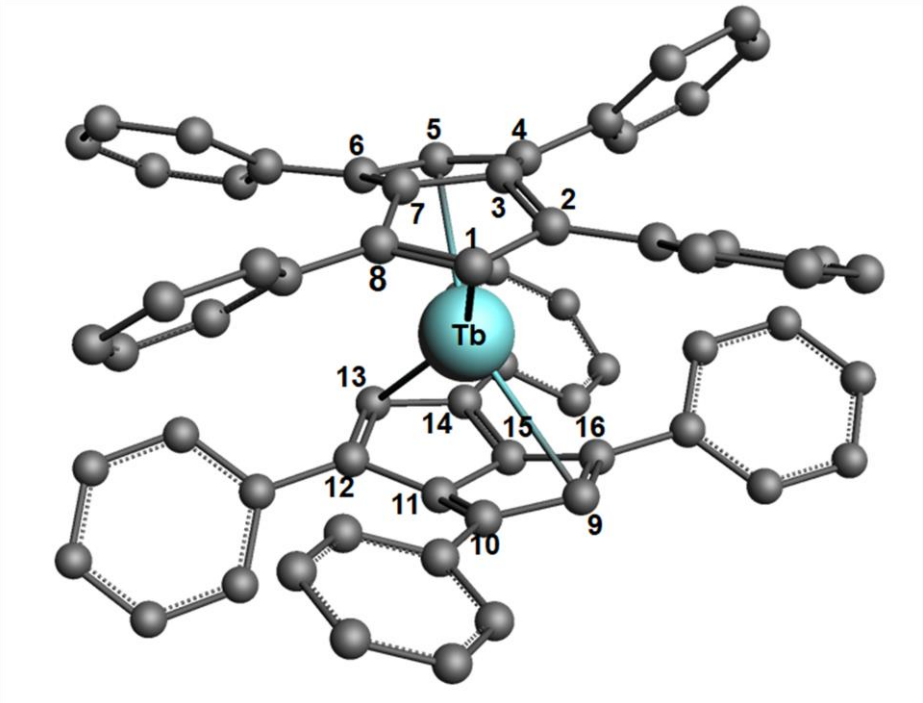

Figure S25. DFT optimised geometry of $[Tb(\eta^8\text{-}Ph_4Pn)_2]^-$ with numbering of selected carbon centres.

Table S3. Kohn-Sham DFT computed bond parameters of only hydrogen-optimised X-ray structure and a fully optimised structure of **1-Tb**. Wiberg Bond Indices (WBIs) from NBO calculation. The numbering of the carbon centres corresponds to Figure S13.

Tb-Pentalenide	**H-optimisation (Å)**	**WBI (H-opt)**	**Full optimisation (Å)**
Tb-C1	2.854	0.089	2.813
Tb-C2	2.686	0.104	2.667
Tb-C3	2.440	0.117	2.441
Tb-C4	2.713	0.114	2.715
Tb-C5	2.838	0.083	2.852
Tb-C6	2.745	0.107	2.744
Tb-C7	2.459	0.120	2.457
Tb-C8	2.725	0.128	2.697
Tb-C9	2.854	0.089	2.813
Tb-C10	2.686	0.104	2.667
Tb-C11	2.440	0.117	2.441
Tb-C12	2.713	0.114	2.715
Tb-C13	2.838	0.083	2.852
Tb-C14	2.745	0.107	2.744
Tb-C15	2.459	0.120	2.457
Tb-C16	2.725	0.128	2.697

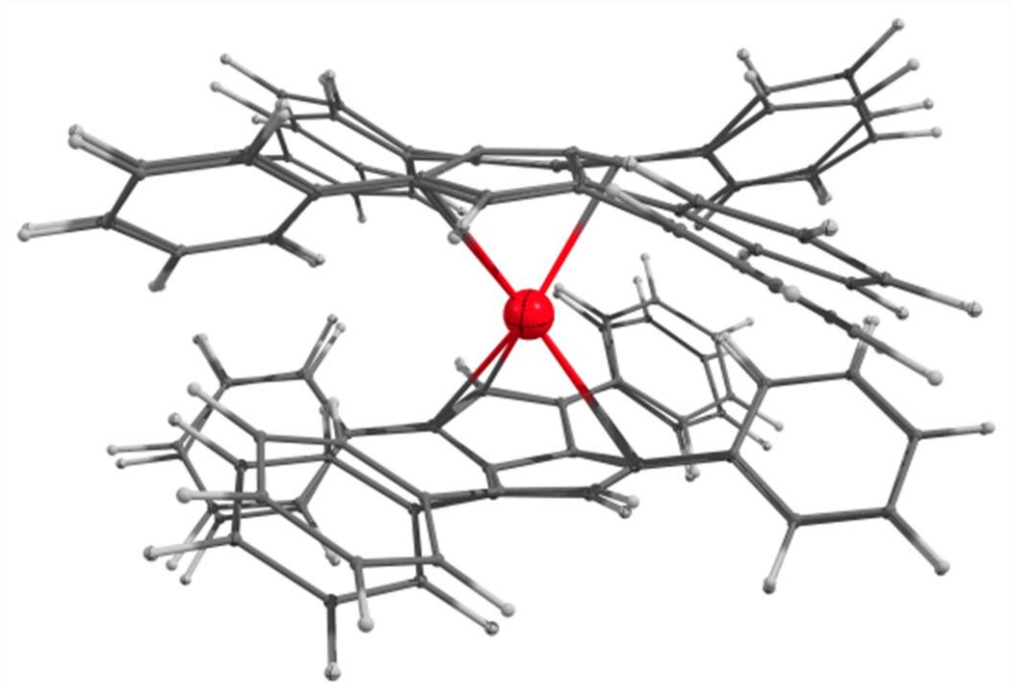

Figure S26. Superimposition of the X-ray crystal structure of $[La(\eta^8\text{-}Ph_4Pn)_2]^-$and the DFT (ZORA/PBE0/TZ2P/DZP) optimised geometry.

Table S4. Comparison between optimized and XRD crystal structures of [La(η^8- $Ph_4Pn)_2]^-$, [Ce(η^8-$Ph_4Pn)_2]^-$ and [Tb(η^8-$Ph_4Pn)_2]^-$ in terms of total and individual displacement RMSD (Å).			
La	**C**	**H**	Displacement RMSD
	0.133	0.221	0.175
Ce	**C**	**H**	Displacement RMSD
	0.134	0.219	0.174
Tb	**C**	**H**	Displacement RMSD
	0.152	0.238	0.192

Table S5. Natural charge and electronic configuration on Ln in fully optimised [Ln(η^8-$Ph_4Pn)_2]^-$(Ln = La, Ce, Tb, optimized molecular geometries) from Natural Population Analysis (NPA).		
1-Ln	Natural Charge on Ln	Electronic Configuration of Ln
La	1.85	$6s^{0.10}\ 4f^{0.24}\ 5d^{0.57}\ 6p^{0.04}\ 7s^{0.03}\ 5f^{0.01}\ 6d^{0.15}\ 8s^{0.01}$
Ce	1.82	$6s^{0.1}\ 4f^{1.22}\ 5d^{0.57}\ 6p^{0.04}\ 7s^{0.03}\ 5f^{0.05}\ 6d^{0.14}\ 8s^{0.01}$
Tb	1.89	$6s^{0.13}\ 4f^{8.04}\ 5d^{0.72}\ 6p^{0.04}\ 7s^{0.03}\ 5f^{0.02}\ 6d^{0.12}\ 8s^{0.01}$

Table S6. Natural charge and electronic configuration of Ln in fully optimised, parent [Ln(η^8-$Pn)_2]^-$ (Ln = La, Ce, Tb, Pn is unsubstituted pentalenide ligand: molecular geometries optimized analogously to **1-Ln**) from Natural Population Analysis (NPA).		
1-Ln	Natural Charge on Ln	Electronic Configuration of Ln
La	1.32	$6s^{0.08}\ 4f^{0.24}\ 5d^{1.28}\ 6p^{0.02}\ 7s^{0.02}\ 5f^{0.01}\ 6d^{0.02}\ 8s^{0.01}$
Ce	1.24	$6s^{0.08}\ 4f^{1.20}\ 5d^{1.34}\ 6p^{0.02}\ 7s^{0.02}\ 5f^{0.05}\ 6d^{0.02}\ 8s^{0.01}$
Tb	1.21	$6s^{0.11}\ 4f^{8.07}\ 5d^{1.48}\ 6p^{0.03}\ 7s^{0.02}\ 5f^{0.02}\ 6d^{0.03}\ 8s^{0.01}$

Table S7. Natural Charges on the metal, individual pentalenide cores, phenyl groups, phenyl-pentalenide ligand, and the residual charge on the overall system in fully optimised [Ln(η^8-$Ph_4Pn)_2]^-$ complexes from Natural Population Analysis (NPA).	
[La(η^8-$Ph_4Pn)_2]^-$	**Natural Charge**
Natural Charge on metal	1.84877
Natural charge on pentalenide core (unit 1)	-1.17996
Natural charge on pentalenide core (unit 2)	-1.17996
Sum of natural charges on phenyl rings (unit 1)	-0.24442
Sum of natural charges on phenyl rings (unit 2)	-0.24442
Total natural charges on each phenyl-pentalenide system	-1.42438
Residual charge on the system	-0.99999
[Ce(η^8-$Ph_4Pn)_2]^-$	**Natural Charge**
Natural Charge on metal	1.82502
Natural charge on pentalenide core (unit 1)	-1.17445
Sum of natural charges on phenyl rings (unit 2)	-1.17445
Sum of natural charges on phenyl rings (unit 1)	-0.23807
Sum of natural charges on phenyl rings (unit 2)	-0.23807
Total natural charges on each phenyl-pentalenide system	-1.41252
Residual charge on the system	-1.00002

$[Tb(\eta^8\text{-}Ph_4Pn)_2]^-$	**Natural Charge**
Natural Charge on metal	1.8882
Natural charge on pentalenide core (unit 1)	-1.20912
Sum of natural charges on phenyl rings (unit 2)	-1.20912
Sum of natural charges on phenyl rings (unit 1)	-0.23498
Sum of natural charges on phenyl rings (unit 2)	-0.23498
Total natural charges on each phenyl-pentalenide system	-1.4441
Residual charge on the system	-1.000

Table S8. Natural charge and electronic configuration of Ln in fully optimised $[Ln(COT)_2]^-$ (Ln = La, Ce, Tb, molecular geometries optimized analogously to **1-Ln**) from Natural Population Analysis (NPA).

$[Ln(COT)_2]^-$	Natural Charge on Ln	Electronic Configuration of Ln
La	1.54	$6s^{0.05}\ 4f^{0.25}\ 5d^{0.55}\ 6p^{0.03}\ 7s^{0.01}\ 5f^{0.01}\ 6d^{0.03}$
Ce	1.42	$6s^{0.05}\ 4f^{1.24}\ 5d^{1.15}\ 6p^{0.05}\ 7s^{0.01}\ 5f^{0.04}\ 6d^{0.04}$
Tb	1.46	$6s^{0.07}\ 4f^{8.10}\ 5d^{1.21}\ 6p^{0.06}\ 7s^{0.01}\ 5f^{0.03}\ 6d^{0.04}$

Table S9. Twist angles (°) between the phenyl rings and the pentalenide core in the fully optimised $[La(\eta^8\text{-}Ph_4Pn)_2]^-$ complex (see Figure S18 for C-centres)

C-centre	**Twist Angle**
3-4-17-19	44
3-2-20-21	26
7-6-23-25	-34
7-8-26-27	-21
11-10-20-31	26
11-12-32-34	44
15-14-35-37	-34
15-16-38-39	-21
3-4-17-18	-139
3-2-20-22	-155
7-6-23-24	150
7-8-26-28	161
11-10-29-30	-155
11-12-32-33	-139
15-14-35-36	150
15-16-38-40	161

Table S10. Twist angles (°) between the phenyl rings and the pentalenide core in the fully optimised $[Ce(\eta^8\text{-}Ph_4Pn)_2]^-$ complex (see Figure S18 for C-centres)

C-centre	**Twist Angle**
3-4-17-19	-26
3-2-20-21	-45
7-6-23-25	21
7-8-26-27	35
11-10-20-31	35
11-12-32-34	-45

15-14-35-37	-26
15-16-38-39	21
3-4-17-18	155
3-2-20-22	138
7-6-23-24	-161
7-8-26-28	-149
11-10-29-30	-149
11-12-32-33	138
15-14-35-36	155
15-16-38-40	-161

Table S11. Twist angles (°) between the phenyl rings and the pentalenide core in the fully optimised $[Tb(\eta^8\text{-}Ph_4Pn)_2]^-$ complex (see Figure S18 for C-centres)

C-centre	**Twist Angle**
3-4-17-19	-19
3-2-20-21	-36
7-6-23-25	26
7-8-26-27	49
11-10-20-31	-36
11-12-32-34	-19
15-14-35-37	26
15-16-38-39	49
3-4-17-18	164
3-2-20-22	147
7-6-23-24	-155
7-8-26-28	-134
11-10-29-30	147
11-12-32-33	164
15-14-35-36	-155
15-16-38-40	-134

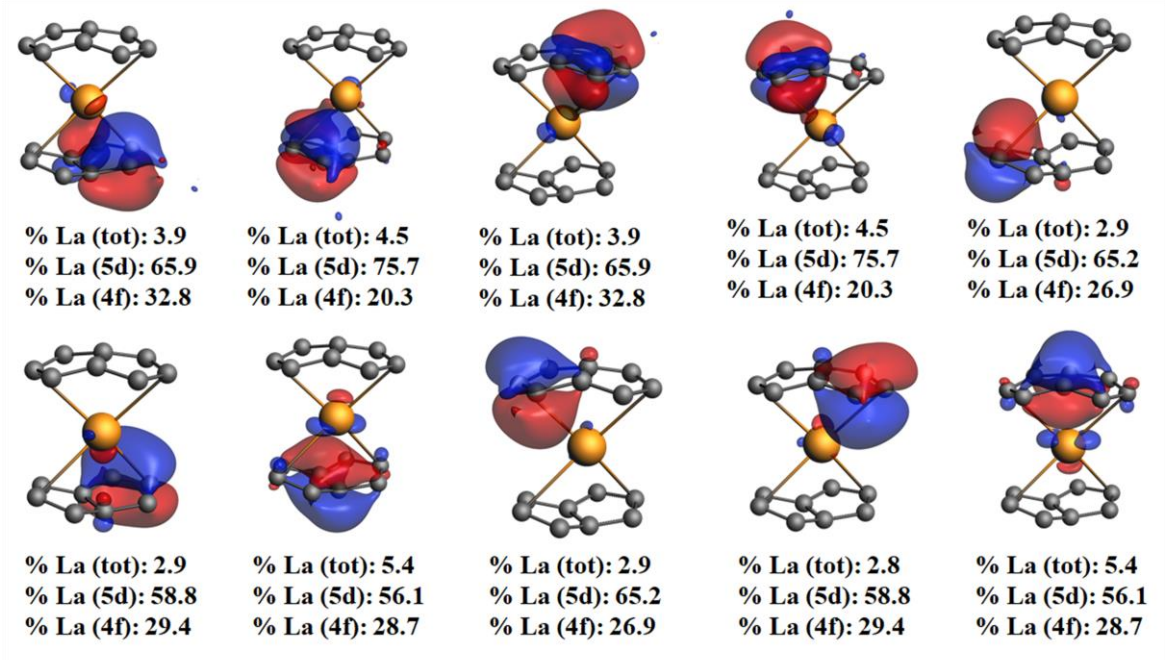

Figure S27. π-NLMOs in the pentalenide cores of $[La(\eta^8\text{-}Ph_4Pn)_2]^-$ showing electron donation to the metal. Weight-% metal character and relative 5d vs. 4f contribution at the metal is given. The phenyl groups of the **Ph_4Pn^{2-}** ligands are omitted from the graphics for clarity. Isosurfaces at ±0.04 a.u. Colour code for atoms: La yellow, C dark gray.

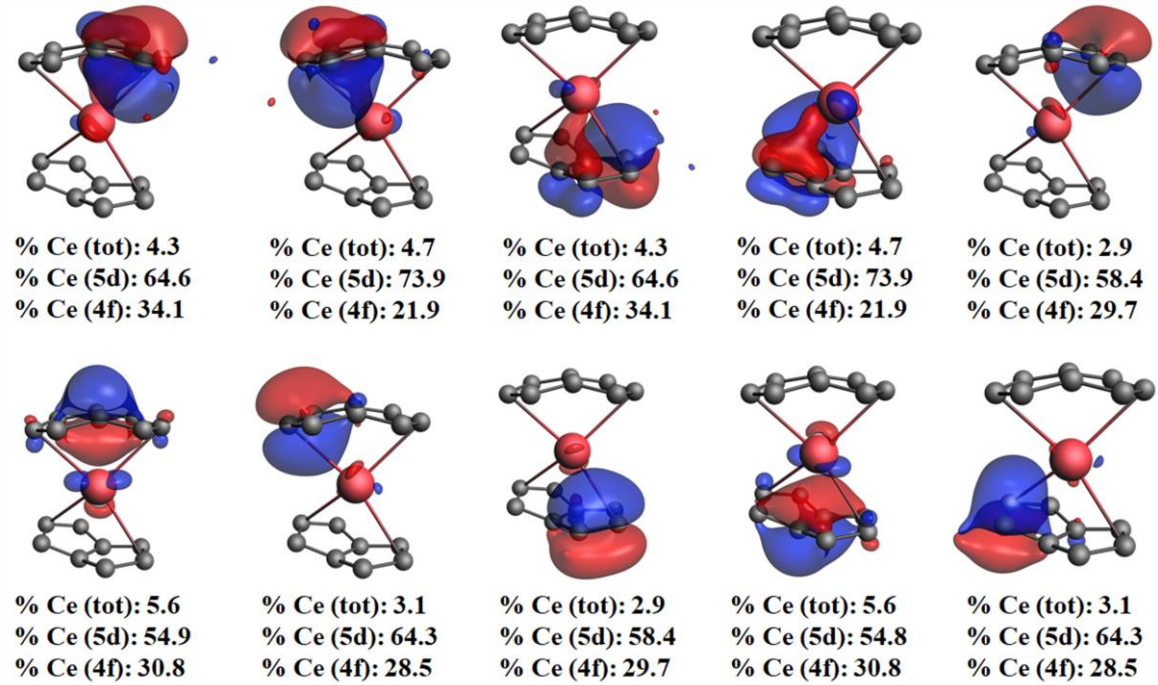

Figure S28. π-NLMOs in the pentalenide cores of $[Ce(\eta^8\text{-}Ph_4Pn)_2]^-$ showing electron donation to the metal. Weight-% metal character and relative 5d vs. 4f contribution at the metal is given. Here the α-spin NLMOs are shown but contributions in each case are averaged over equivalent α and β-spin NLMOs. The phenyl groups of the $\mathbf{Ph_4Pn^{2-}}$ ligands are omitted from the graphics for clarity. Isosurfaces at ±0.04 a.u. Colour code for atoms: Ce pink, C dark gray.

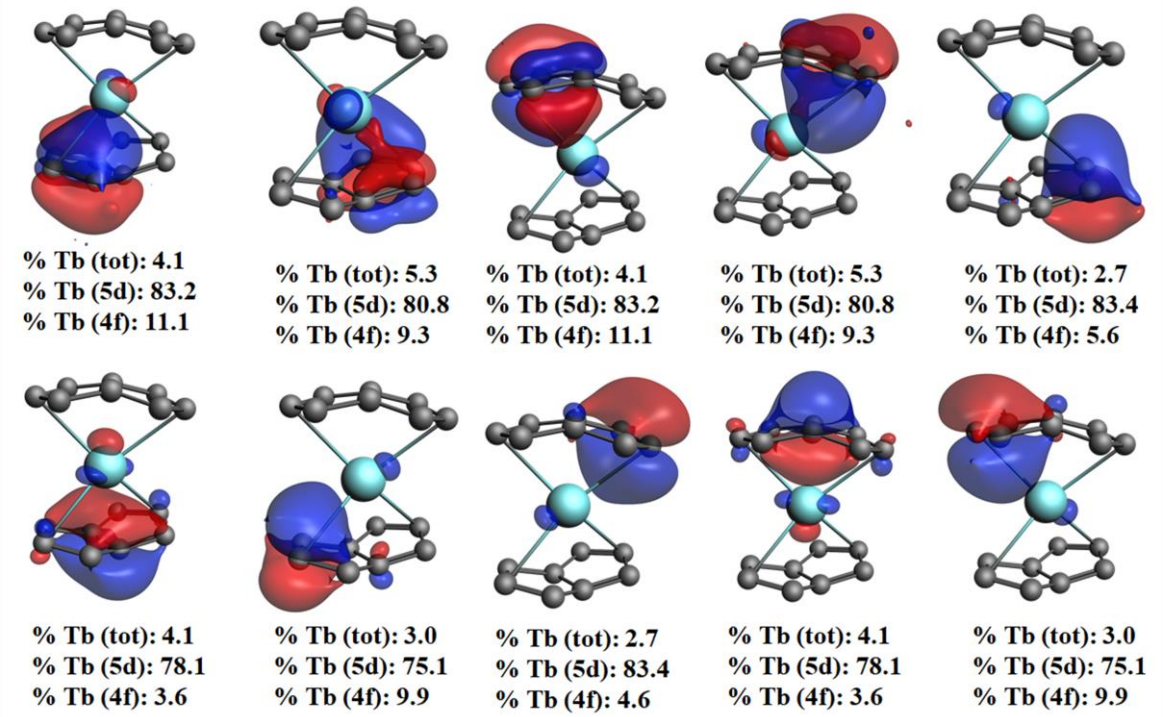

Figure S29. π-NLMOs in the pentalene cores of $[Tb(\eta^8\text{-}Ph_4Pn)_2]^-$ showing electron donation to the metal. Weight-% metal character and relative 5d vs. 4f contribution at the metal is given. Here the α-spin NLMOs are shown but contributions in each case are averaged over equivalent α and β-spin NLMOs. The phenyl groups of the **Ph_4Pn** ligands are omitted from the graphics for clarity. Isosurfaces at ±0.04 a.u. Colour code for atoms: Ce blue, C dark gray.

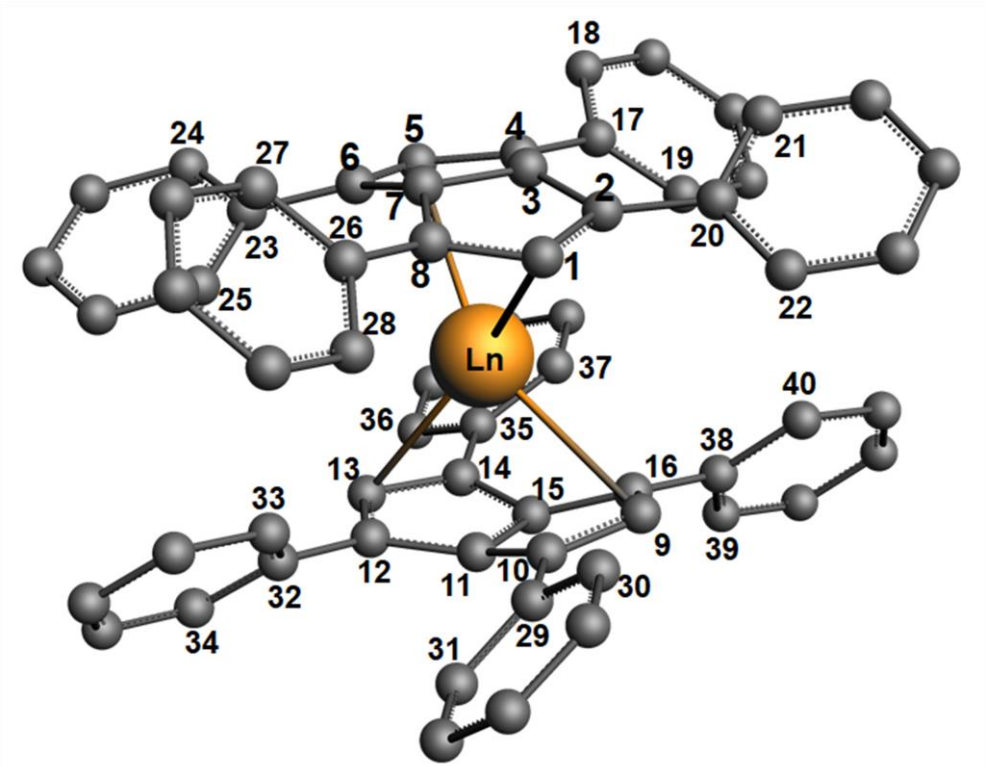

Figure S30. Representation of the fully optimised $[Ln(\eta^8\text{-}Ph_4Pn)_2]^-$ complex showing the numbering of the selected C-atoms involved in the twist angle between phenyl rings and the pentalenide core.

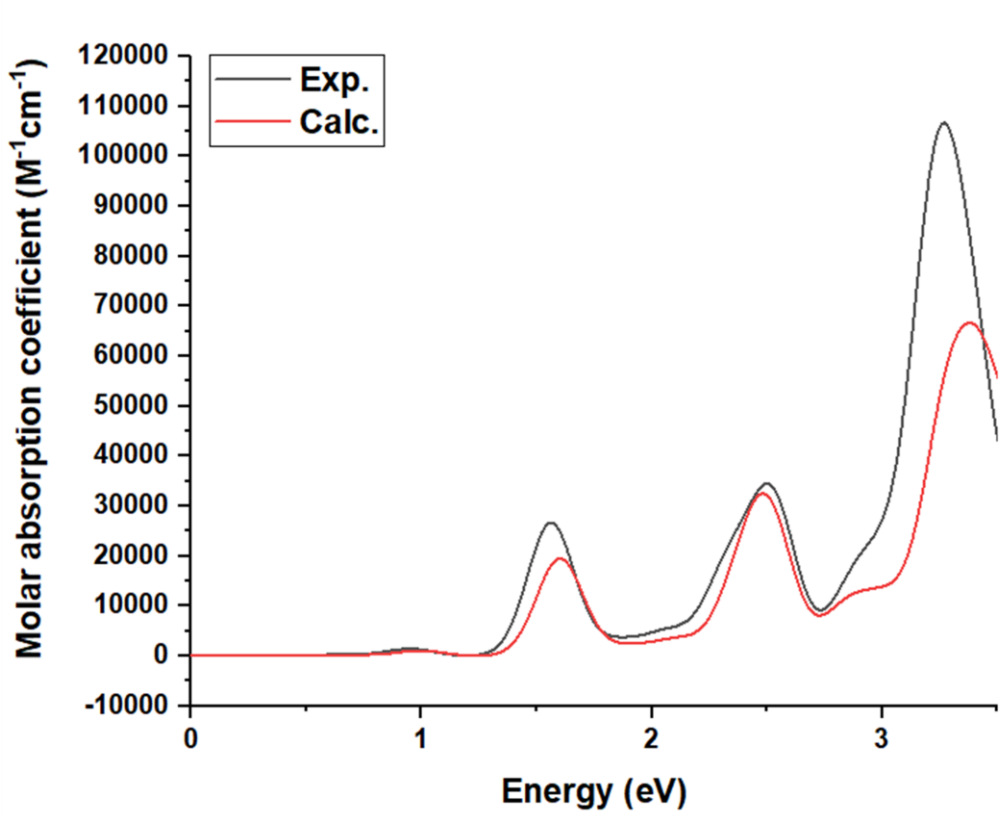

Figure S31. Overlay of TDA/uB3LYP computed gas-phase (gray) and solvent phase (red) UV-Vis spectrum of $[La(\eta^8\text{-}Ph_4Pn)_2]^-$. The Gaussian broadening parameter for the calculated spectra was σ = 0.1 eV.

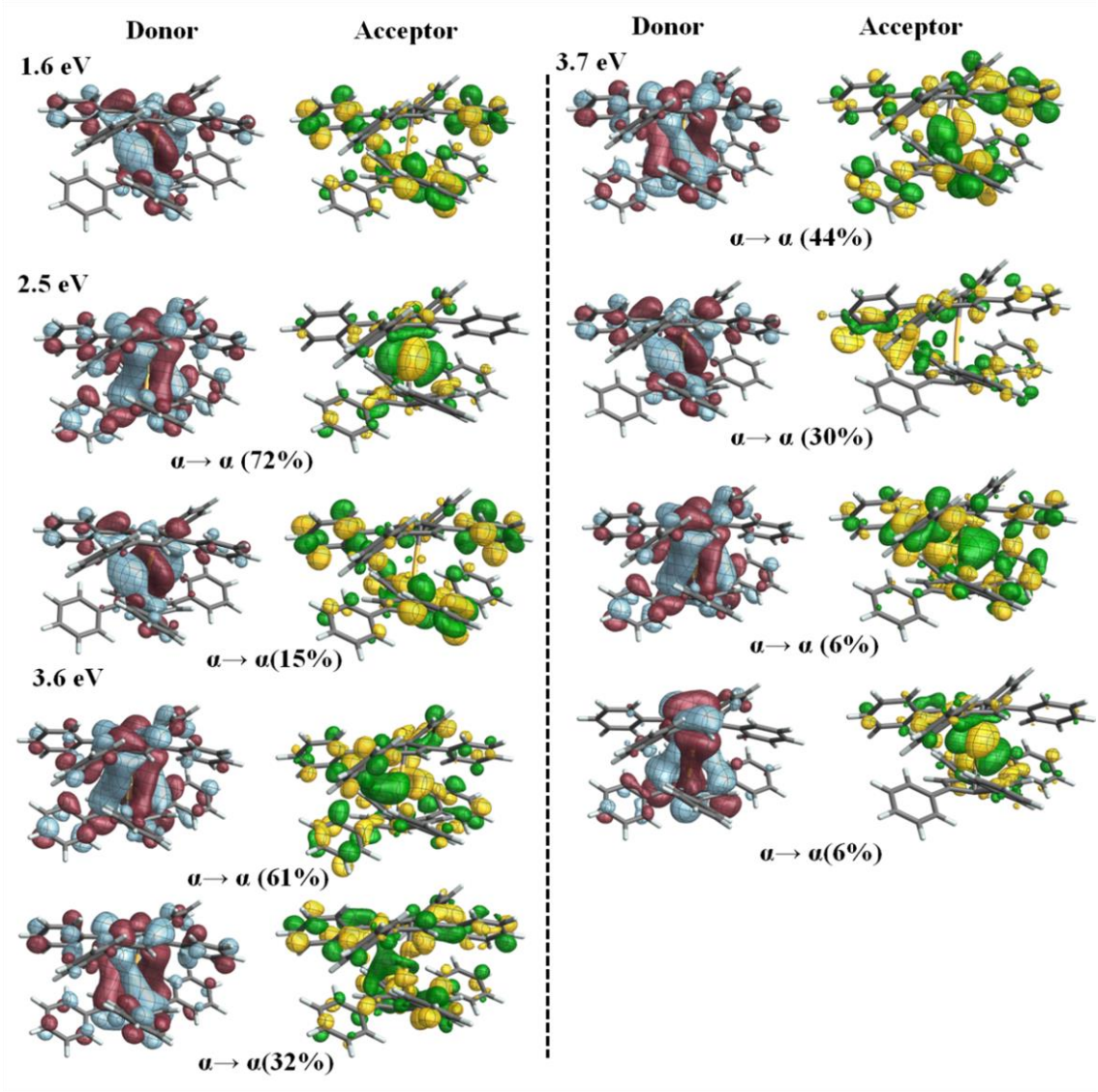

Figure S32: NTOs corresponding to the important transitions in UV-Vis spectrum of $[La(\eta^8\text{-}Ph_4Pn)_2]^-$. Isosurfaces at ±0.017 a.u for the donors and ±0.025 a.u. for the acceptors.

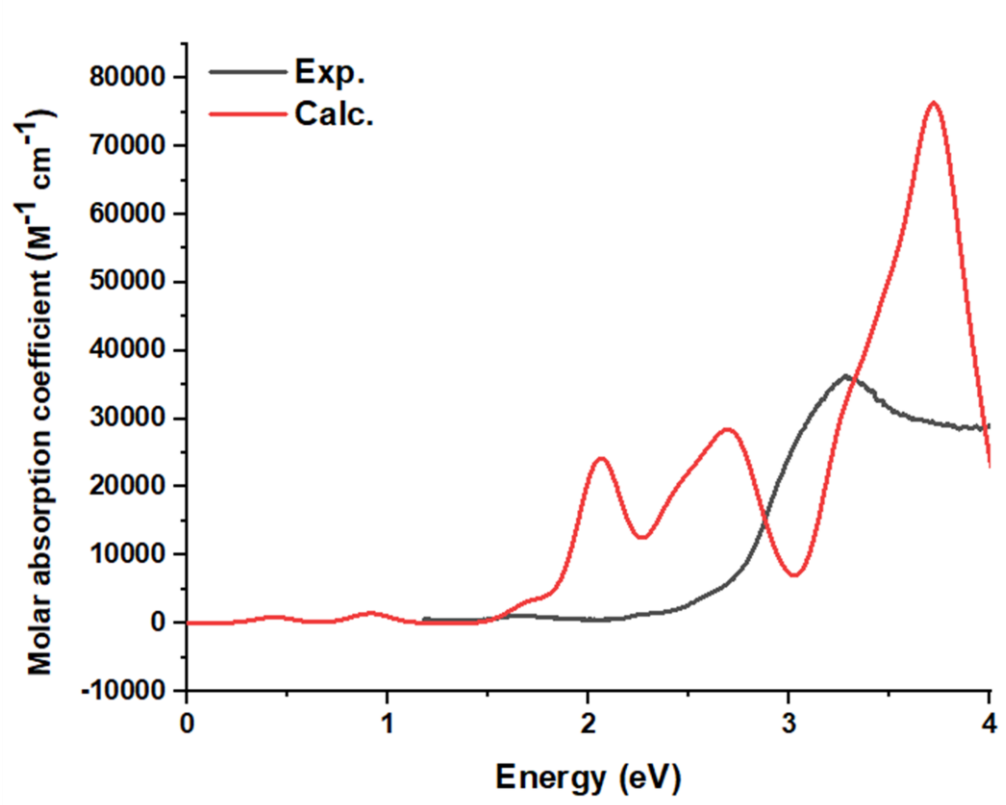

Figure S33. Overlay of experimentally recorded (gray) and TDA/uB3LYP computed (red) UV-Vis spectrum of $[Ce(\eta^8\text{-}Ph_4Pn)_2]^-$. The Gaussian broadening parameter for the calculated spectra was σ = 0.1 eV.

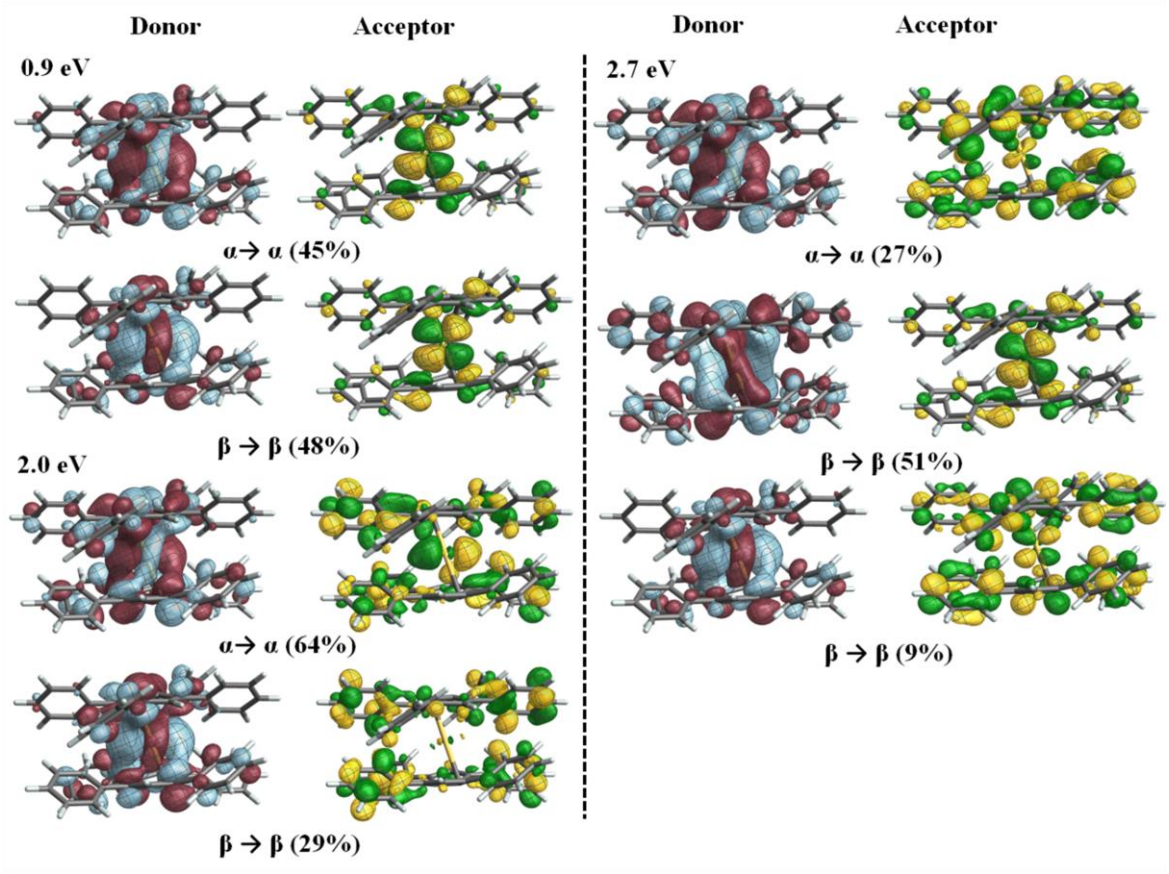

Figure S34. NTOs corresponding to the important transitions in UV-Vis spectrum of [Ce(η^8-$Ph_4Pn)_2]^-$ up to 3 eV. Weight-% of the NTOs corresponding to α→α and β→β transitions are shown. Isosurfaces at ±0.017 a.u for the donors and ±0.025 a.u. for the acceptors.

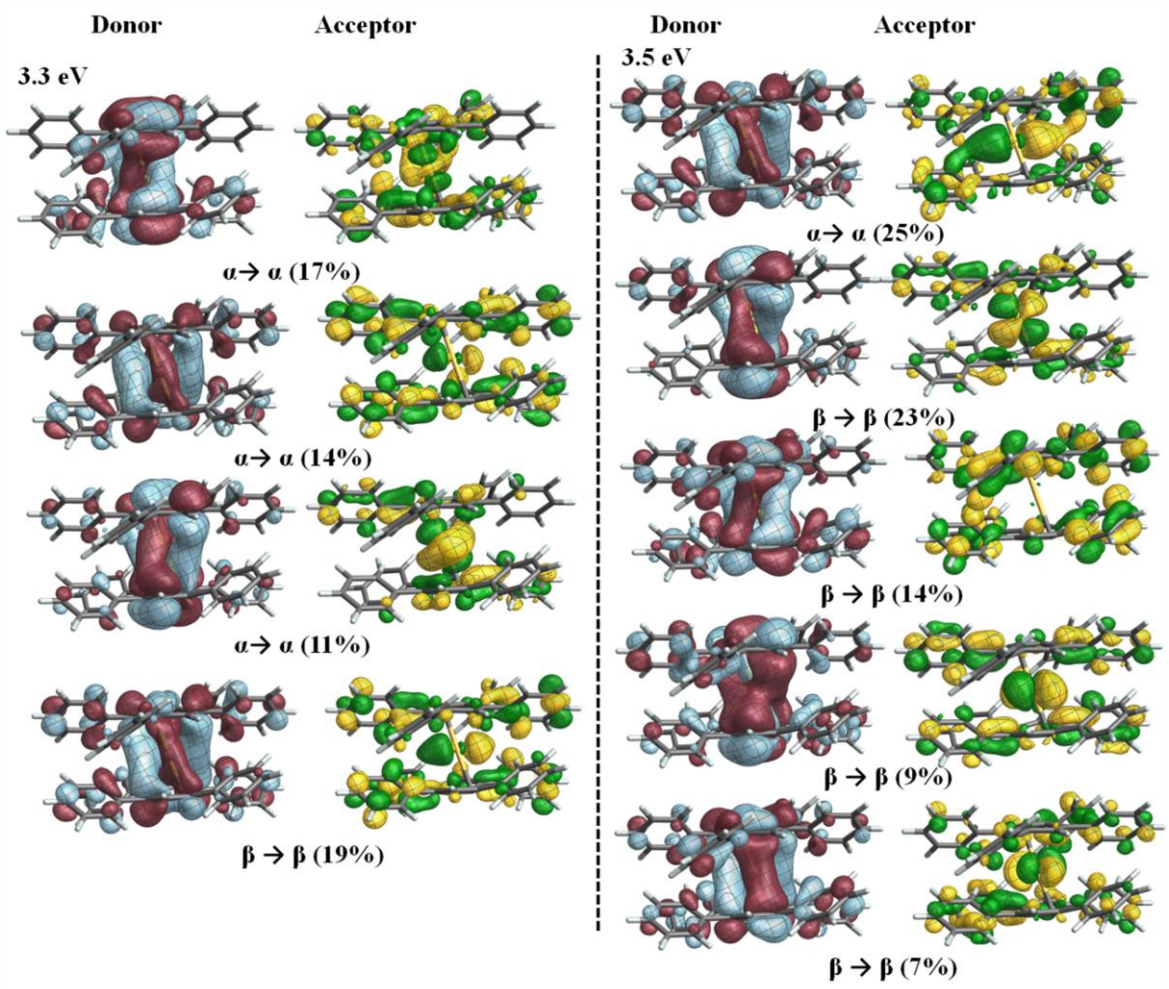

Figure S35. NTOs corresponding to the important transitions in UV-Vis spectrum of $[Ce(\eta^8\text{-}Ph_4Pn)_2]^-$ up to 4 eV. Weight-% of the NTOs corresponding to α→α and β→β transitions are shown. Isosurfaces at ±0.017 a.u for the donors and ±0.025 a.u. for the acceptors.

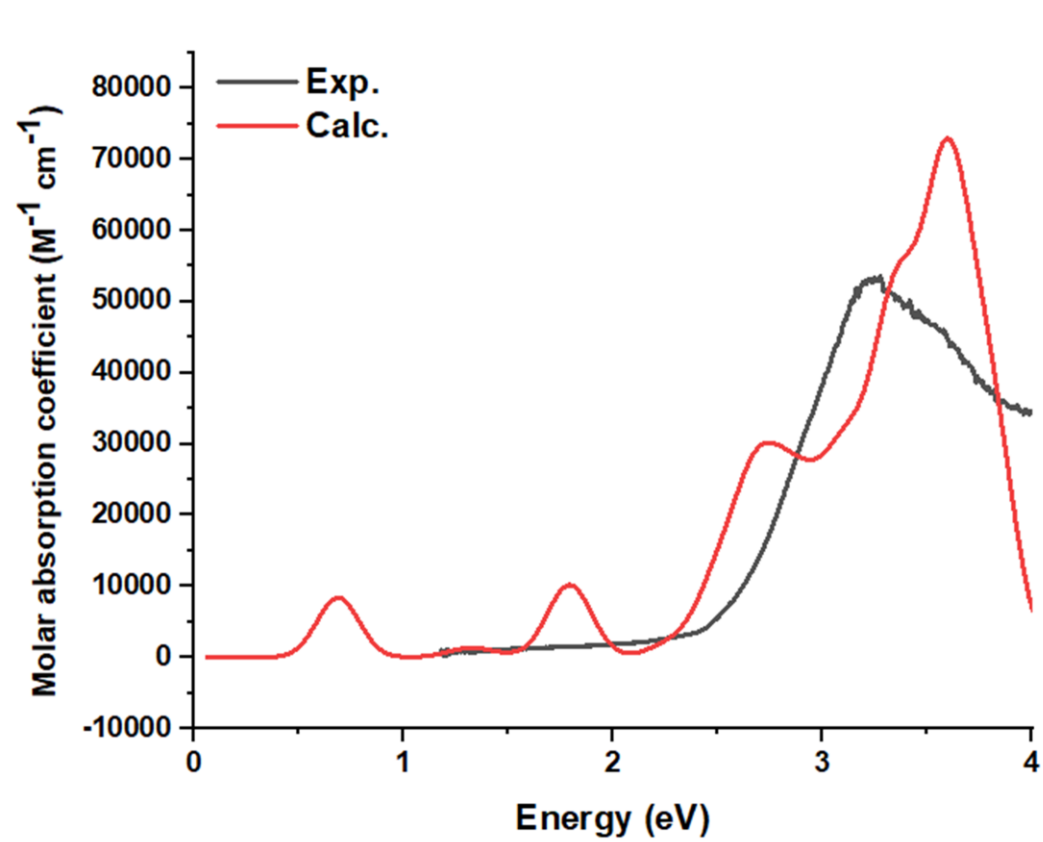

Figure S36. Overlay of experimentally recorded (gray) and TDA/uB3LYP computed (red) UV-Vis spectrum of $[Tb(\eta^8\text{-}Ph_4Pn)_2]^-$. The Gaussian broadening parameter for the calculated spectra was σ = 0.1 eV.

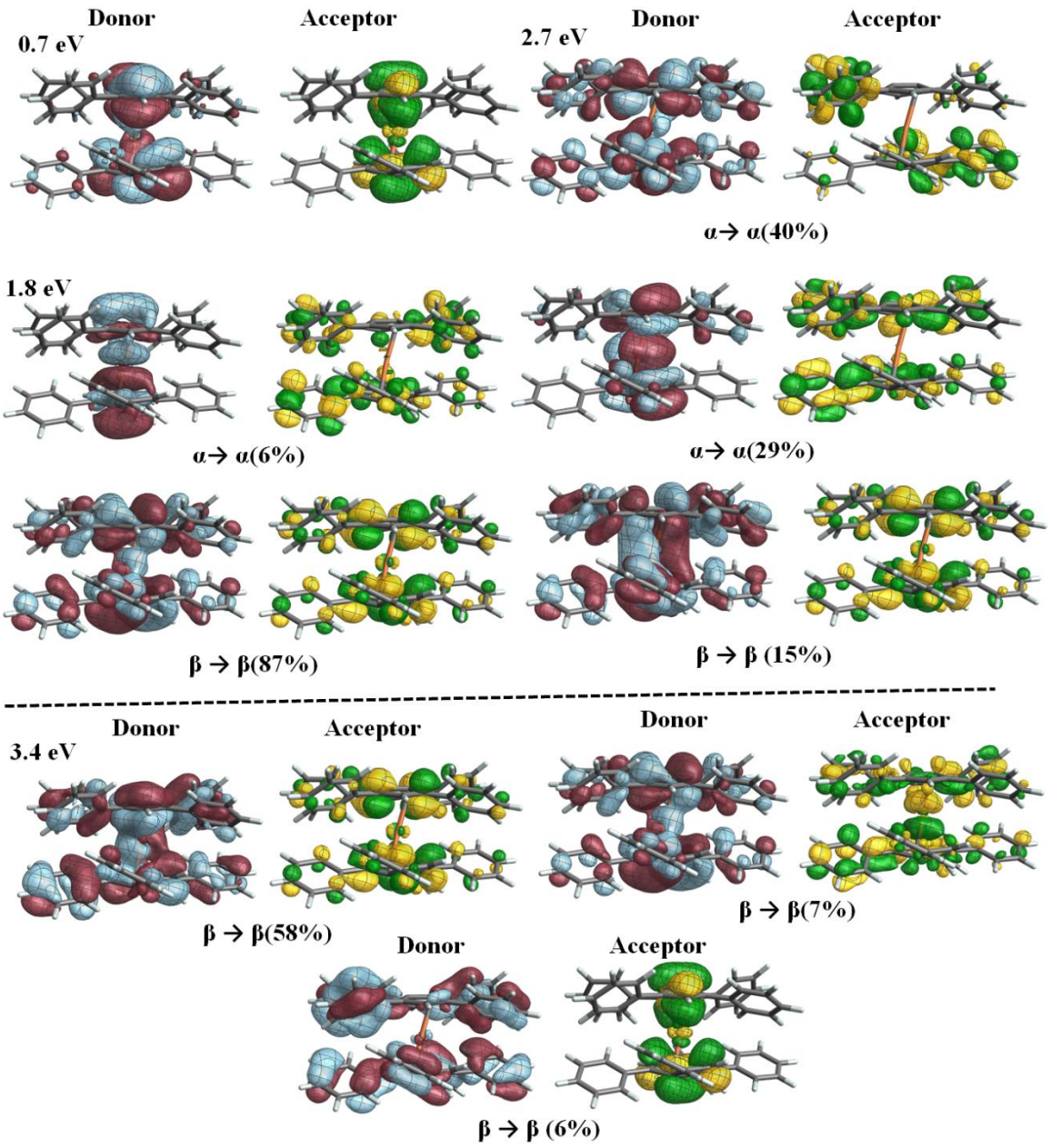

Figure S37. NTOs corresponding to the important transitions in UV-Vis spectrum of [Tb(η^8-$Ph_4Pn)_2]^-$. Weight-% of the NTOs corresponding to α→α and β→β transitions are shown. Isosurfaces at ±0.017 a.u for the donors and ±0.025 a.u. for the acceptors.

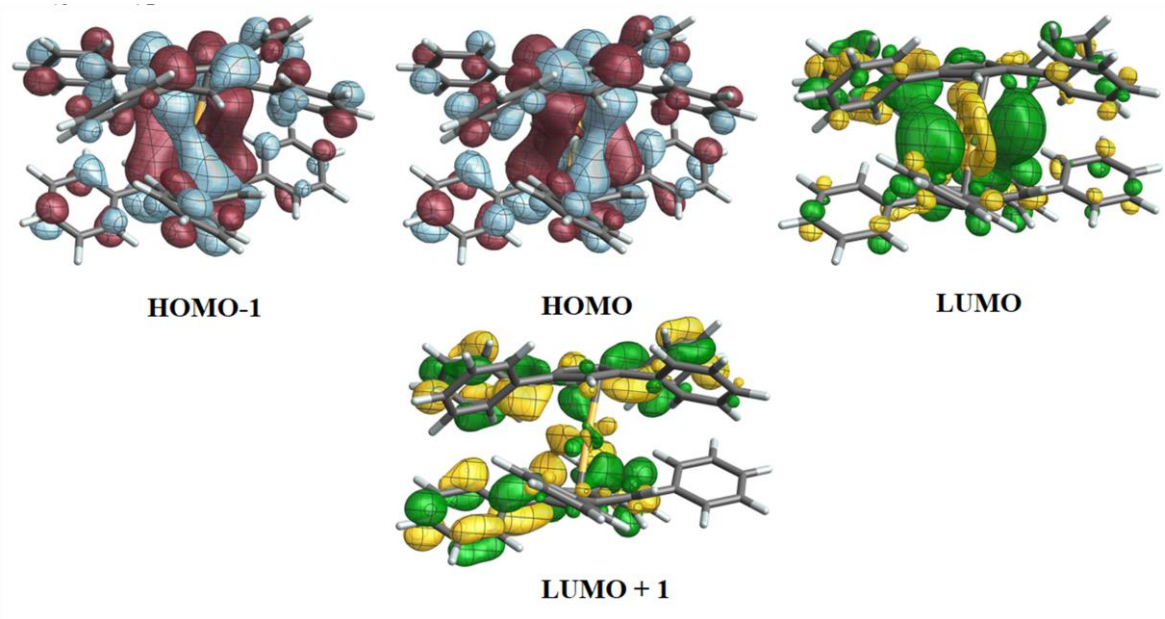

Figure S38. Important frontier molecular orbitals of $[La(\eta^8\text{-}Ph_4Pn)_2]^-$ complex. Isosurfaces at ±0.017 a.u for the donors and ±0.025 a.u. for the acceptors.

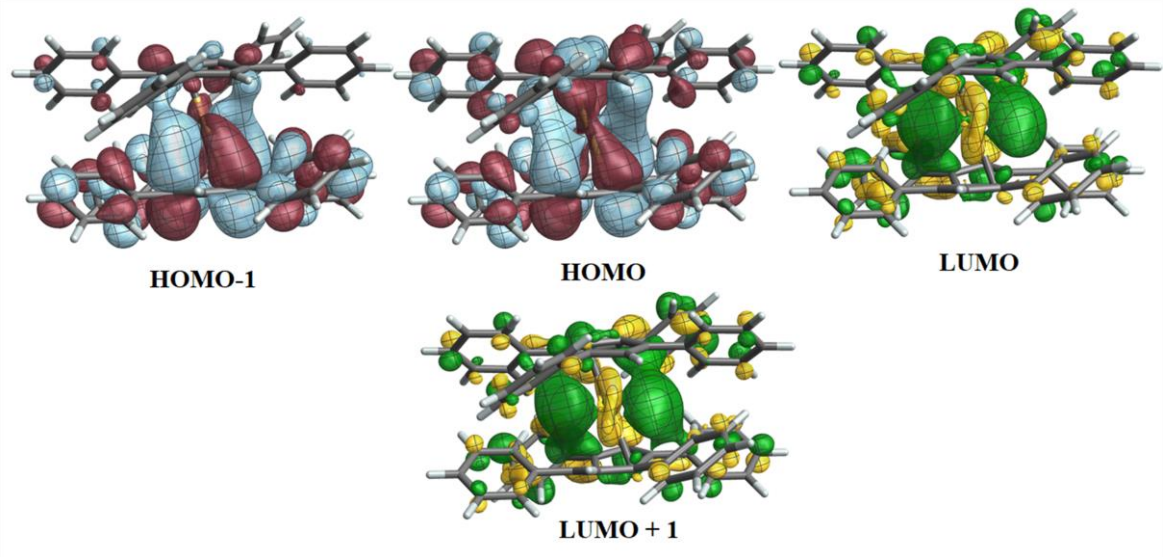

Figure S39. Important frontier molecular orbitals of $[Ce(\eta^8\text{-}Ph_4Pn)_2]^-$ complex. Isosurfaces at ±0.017 a.u for the donors and ±0.025 a.u. for the acceptors.

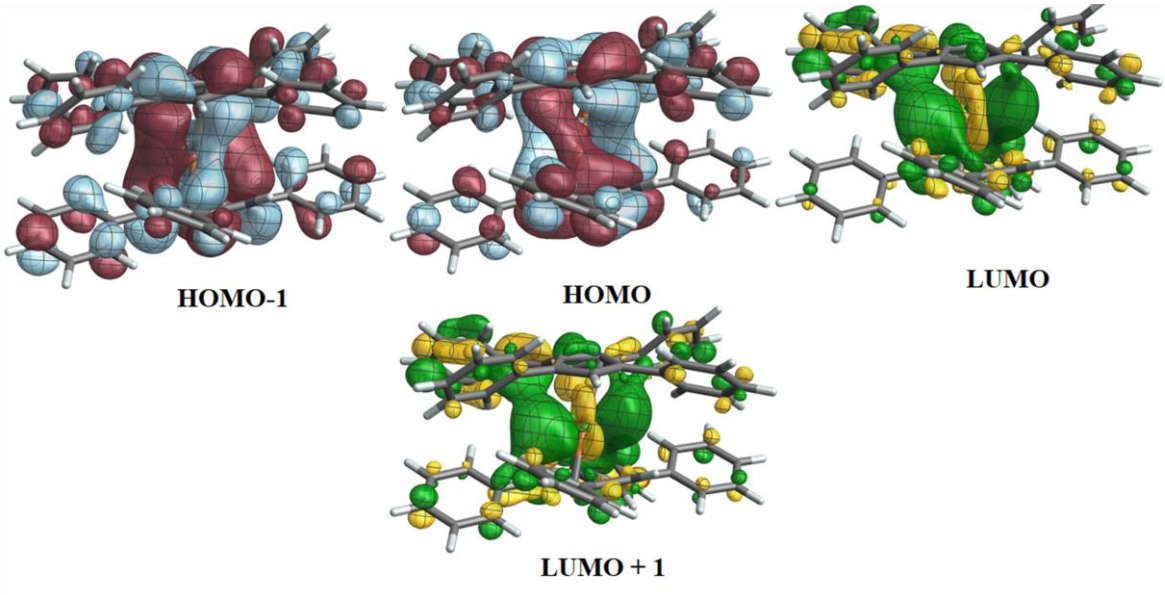

Figure S40. Important frontier molecular orbitals of $[Tb(\eta^8\text{-}Ph_4Pn)_2]^-$ complex. Isosurfaces at ±0.017 a.u for the donors and ±0.025 a.u. for the acceptors.

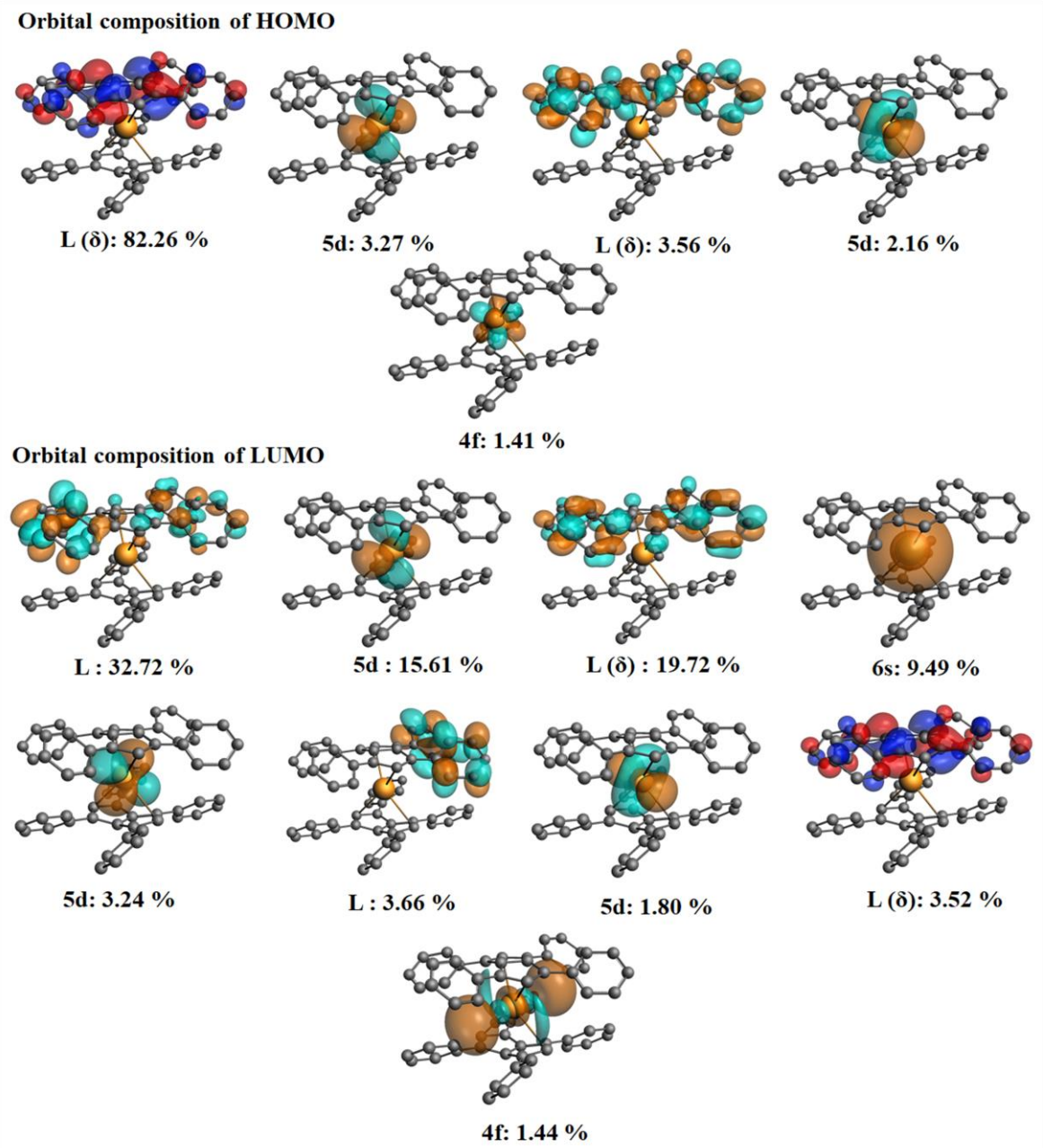

Figure S41. Weight-% of fragment orbitals (FOs) in the frontier molecular orbitals of [La(η^8-$Ph_4Pn)_2$]$^-$ complex. Isosurfaces at ±0.03 a.u.

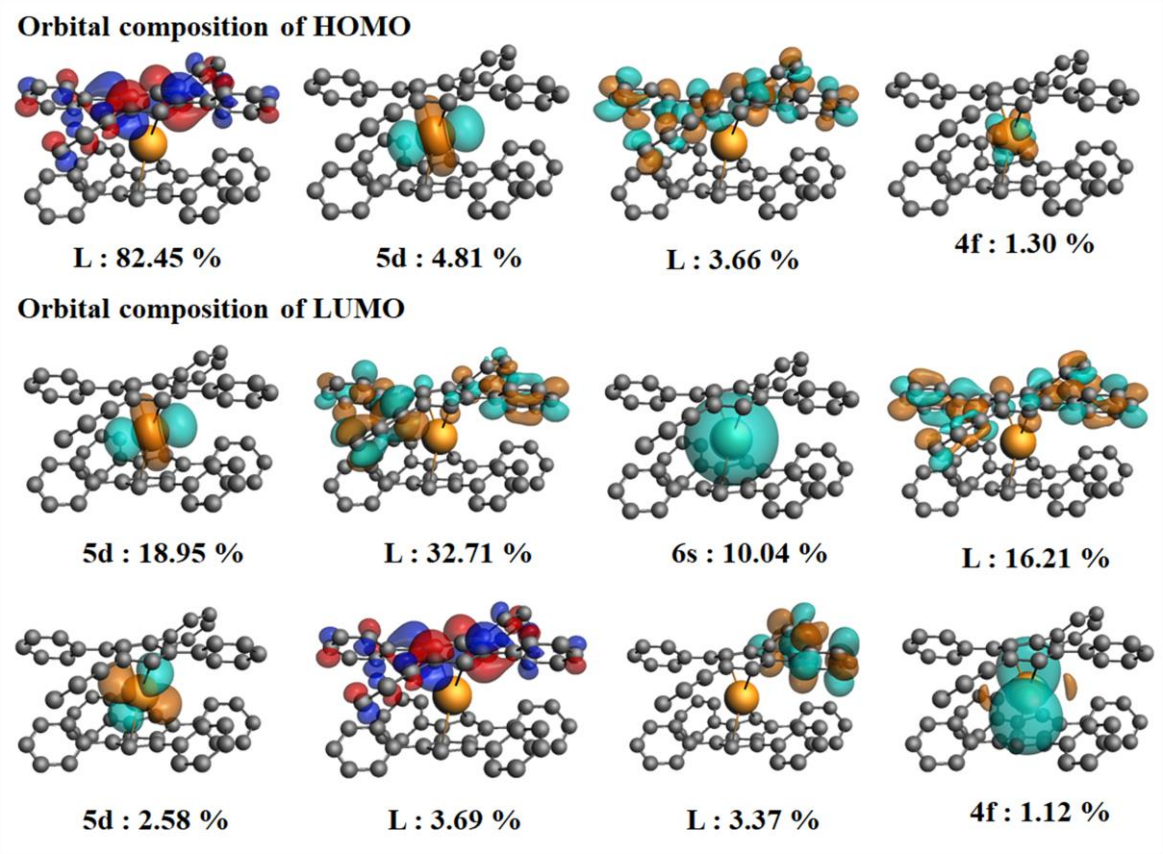

Figure S42. Weight-% of fragment orbitals (FOs) in the frontier molecular orbitals of [Ce(η^8-$Ph_4Pn)_2]^-$ complex. Isosurfaces at ±0.03 a.u.

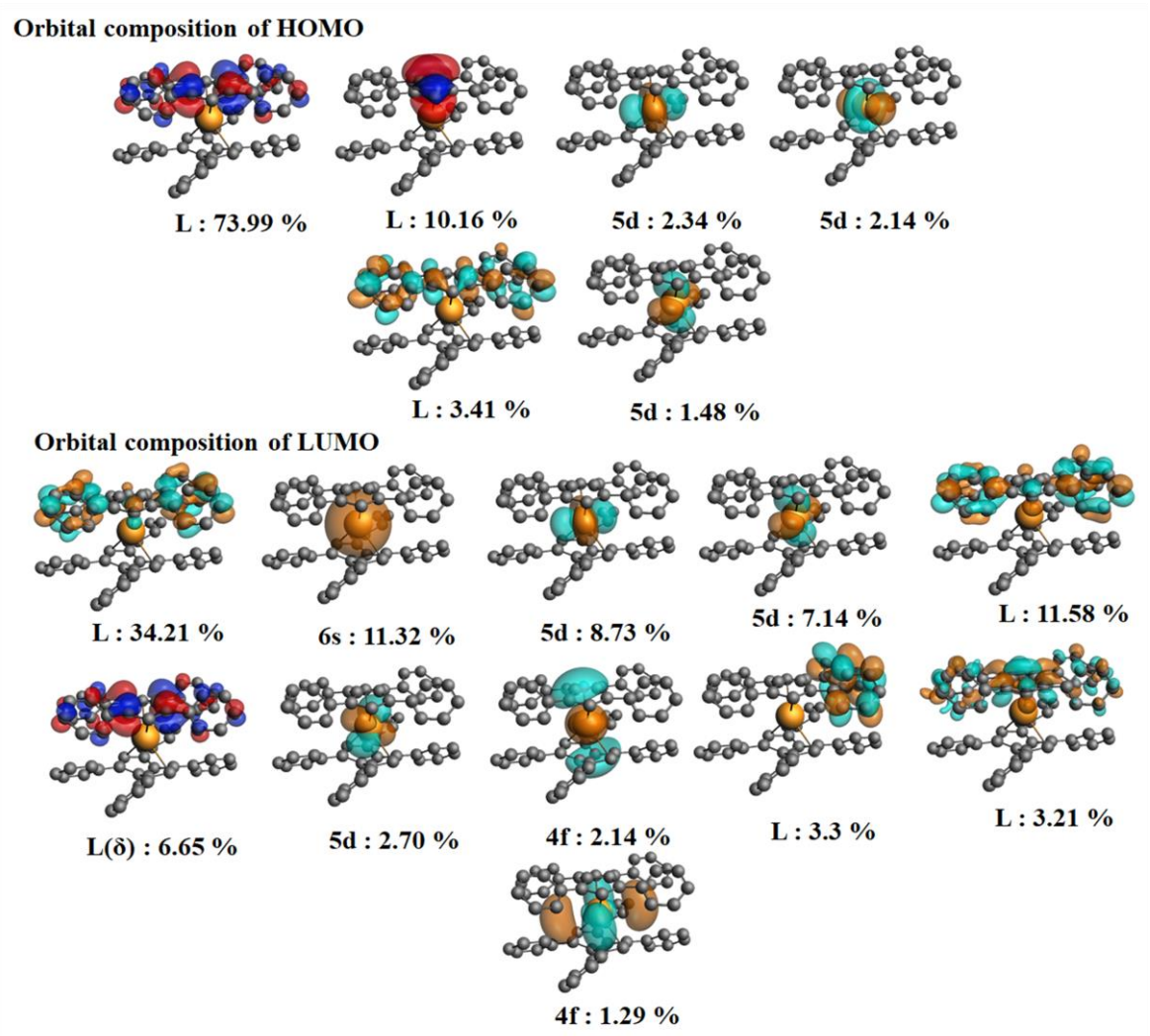

Figure S43. Weight-% of fragment orbitals (FOs) in the frontier molecular orbitals of [Tb(η^8-$Ph_4Pn)_2]^-$ complex. Isosurfaces at ±0.03 a.u.

Coordinates

1-La (full-optimisation)

La	0.00000000000000	0.00000000000000	-6.02054544565159
C	2.02445464736841	1.01617935321007	-7.78513338682681
C	1.61013046988718	3.31823598560069	-5.16888987337410
C	1.96154753043658	1.89945010249061	-5.25312648510264
C	2.32179112136902	1.08596421719912	-6.37933032250023
C	2.25051201788660	-1.38695779746262	-3.54626113956893
C	2.73280625830389	-2.56604812353196	-7.13783073101326
C	2.10043632325676	4.08993092148256	-4.11078871641317
H	2.78696649044038	3.63482454318585	-3.40776338522434
C	2.16476782429954	-3.37238231241249	-8.13239468931323
H	1.41834979067244	-2.95826876823811	-8.80033220674902
C	2.06976689561907	-0.34336532237170	-8.13522837929933
H	2.01398843613562	-0.70865081975561	-9.15143560389879
C	1.86944378454474	2.10855836666578	-8.73262825141293
C	2.00539506633530	1.05402868357534	-4.12651764881371
H	1.74315994043847	1.37016602073213	-3.12488963411549
C	3.66476579075241	-3.15401889649931	-6.27747105921672
H	4.12549449246341	-2.54715749302184	-5.50857842701831
C	2.31889971081420	-0.27116997830064	-4.48782685772723
C	2.55473792576586	-0.26063616973021	-5.90643835867071
C	0.75047296643806	3.93997672103881	-6.07658771766803
H	0.33588519049690	3.38022906686133	-6.90490880289893
C	2.62448995602165	-1.20650408467299	-2.20980648640398
H	3.05418802820613	-0.25952577418960	-1.90803674873485
C	1.10485997769322	1.96472329566529	-9.89591985071377
H	0.59388252071319	1.02810660225257	-10.08014147914994
C	1.73604231561133	-2.63293112148781	-3.91027697963031
H	1.43839345236177	-2.82493194206832	-4.93130768235967
C	2.51739329189256	-4.70235722201480	-8.26093838627124
H	2.05549533176672	-5.29991873415639	-9.03835566923329
C	2.39482930420761	-1.15440308166640	-7.02525003337080
C	1.74277968941422	5.41834386989177	-3.96511819973578
H	2.14315795633765	5.99240923142369	-3.13754173448522
C	4.00268031349474	-4.49018757880179	-6.39922131328176
H	4.71974049794233	-4.92098517757113	-5.71059526674968
C	2.46764323238614	-2.21844991739814	-1.28111505518439
H	2.76749459235240	-2.05156816587133	-0.25307224183012
C	1.57167987094057	-3.64425055831406	-2.98028890642681
H	1.14189155139427	-4.58632457942456	-3.29728257492400
C	2.49926551625752	3.33825761321178	-8.51787399113522
H	3.10827395723416	3.46805691625288	-7.63267443335920
C	0.38507074403157	5.26608025569046	-5.92819082395884
H	-0.30982035550144	5.70403080644629	-6.63383350024754
C	1.93557978442446	-3.44369666637984	-1.65885755427884
H	1.80801097970286	-4.23374283146912	-0.92905297239052
C	0.88173116181234	6.01592825617527	-4.87331981895562
H	0.59704064230939	7.05476036078330	-4.75798466085562
C	0.96788668109362	3.00437019833120	-10.79653358300216
H	0.36249017883354	2.86658682669492	-11.68479899794064
C	3.43672761536578	-5.27433660099812	-7.39235724994763
H	3.70560497446949	-6.31927176016696	-7.48661452422990
C	2.35058605995768	4.38122859410831	-9.41389009398976
H	2.83906225389718	5.32722772933068	-9.21303740754343
C	1.58408058557153	4.22509964961323	-10.55848478675267
H	1.46723981422166	5.04389208665540	-11.25756809592215

C	-2.02445464736841	-1.01617935321007	-7.78513338682681
C	-1.61013046988718	-3.31823598560069	-5.16888987337410
C	-1.96154753043658	-1.89945010249061	-5.25312648510264
C	-2.32179112136902	-1.08596421719912	-6.37933032250023
C	-2.25051201788660	1.38695779746262	-3.54626113956893
C	-2.73280625830389	2.56604812353196	-7.13783073101326
C	-2.10043632325676	-4.08993092148256	-4.11078871641317
H	-2.78696649044038	-3.63482454318585	-3.40776338522434
C	-2.16476782429954	3.37238231241249	-8.13239468931323
H	-1.41834979067244	2.95826876823811	-8.80033220674902
C	-2.06976689561907	0.34336532237170	-8.13522837929933
H	-2.01398843613562	0.70865081975561	-9.15143560389879
C	-1.86944378454474	-2.10855836666578	-8.73262825141293
C	-2.00539506633530	-1.05402868357534	-4.12651764881371
H	-1.74315994043847	-1.37016602073213	-3.12488963411549
C	-3.66476579075241	3.15401889649931	-6.27747105921672
H	-4.12549449246341	2.54715749302184	-5.50857842701831
C	-2.31889971081420	0.27116997830064	-4.48782685772723
C	-2.55473792576586	0.26063616973021	-5.90643835867071
C	-0.75047296643806	-3.93997672103881	-6.07658771766803
H	-0.33588519049690	-3.38022906686133	-6.90490880289893
C	-2.62448995602165	1.20650408467299	-2.20980648640398
H	-3.05418802820613	0.25952577418960	-1.90803674873485
C	-1.10485997769322	-1.96472329566529	-9.89591985071377
H	-0.59388252071319	-1.02810660225257	-10.08014147914994
C	-1.73604231561133	2.63293112148781	-3.91027697963031
H	-1.43839345236177	2.82493194206832	-4.93130768235967
C	-2.51739329189256	4.70235722201480	-8.26093838627124
H	-2.05549533176672	5.29991873415639	-9.03835566923329
C	-2.39482930420761	1.15440308166640	-7.02525003337080
C	-1.74277968941422	-5.41834386989177	-3.96511819973578
H	-2.14315795633765	-5.99240923142369	-3.13754173448522
C	-4.00268031349474	4.49018757880179	-6.39922131328176
H	-4.71974049794233	4.92098517757113	-5.71059526674968
C	-2.46764323238614	2.21844991739814	-1.28111505518439
H	-2.76749459235240	2.05156816587133	-0.25307224183012
C	-1.57167987094057	3.64425055831406	-2.98028890642681
H	-1.14189155139427	4.58632457942456	-3.29728257492400
C	-2.49926551625752	-3.33825761321178	-8.51787399113522
H	-3.10827395723416	-3.46805691625288	-7.63267443335920
C	-0.38507074403157	-5.26608025569046	-5.92819082395884
H	0.30982035550144	-5.70403080644629	-6.63383350024754
C	-1.93557978442446	3.44369666637984	-1.65885755427884
H	-1.80801097970286	4.23374283146912	-0.92905297239052
C	-0.88173116181234	-6.01592825617527	-4.87331981895562
H	-0.59704064230939	-7.05476036078330	-4.75798466085562
C	-0.96788668109362	-3.00437019833120	-10.79653358300216
H	-0.36249017883354	-2.86658682669492	-11.68479899794064
C	-3.43672761536578	5.27433660099812	-7.39235724994763
H	-3.70560497446949	6.31927176016696	-7.48661452422990
C	-2.35058605995768	-4.38122859410831	-9.41389009398976
H	-2.83906225389718	-5.32722772933068	-9.21303740754343
C	-1.58408058557153	-4.22509964961323	-10.55848478675267
H	-1.46723981422166	-5.04389208665540	-11.25756809592215

1-La (H-optimisation)

La	0.00000000000007	-0.00000000000007	-5.91839829563437
C	1.98458073117391	1.00653275469736	-7.72991929563417
C	1.64708480288319	3.31692769359082	-5.09554229563551
C	2.00670361404630	1.88791766572230	-5.17007029563537
C	2.32655683970741	1.07108590258707	-6.31703229563459
C	2.29422841887273	-1.45967405033041	-3.50394929563603
C	2.73574738020966	-2.59113082497145	-7.13410029563386
C	2.20962848071729	4.14326797825591	-4.11499929563608
H	2.94672107785398	3.72652343514629	-3.43963130736195
C	2.09003515000793	-3.43387624160997	-8.05534529563332
H	1.24425529117422	-3.06623268322242	-8.62589769519720
C	1.99936953289796	-0.35913865049732	-8.07666829563387
H	1.91167115375750	-0.72604789457423	-9.09041769681866
C	1.85382741691723	2.09724812939937	-8.68568729563336
C	2.05369482805205	1.02869421630828	-4.04524329563630
H	1.82066098200817	1.34698685768719	-3.03693581281308
C	3.81189494228448	-3.12432813550907	-6.40770429563467
H	4.32118861980067	-2.48943607745582	-5.69337690689049
C	2.34970257264968	-0.30588329325935	-4.42021929563558
C	2.56144992689173	-0.28629332537514	-5.85564829563442
C	0.71606014804114	3.88613377504322	-5.96916629563538
H	0.25786124925469	3.28120246803643	-6.74131086591613
C	2.64462520198342	-1.32456869875676	-2.15025829563724
H	3.02430642224563	-0.37474211473114	-1.79517265430733
C	1.17173345330728	1.93382465766780	-9.91073129563297
H	0.67384858724659	0.99747069466916	-10.12533289183046
C	1.82963825307935	-2.70870560370710	-3.92512529563610
H	1.54578010083355	-2.86221391415967	-4.95598021247595
C	2.52018261219151	-4.74501944126245	-8.24654029563306
H	2.00250061339054	-5.37017350961212	-8.96465496669881
C	2.36262714927172	-1.18769801992545	-6.98260729563445
C	1.85506168002843	5.48254052778113	-4.01955429563588
H	2.31200917847961	6.10326686411890	-3.25784301089406
C	4.23641322714111	-4.43206030260209	-6.60367129563446
H	5.07263269874960	-4.81153489100577	-6.02910134649662
C	2.55331044897488	-2.40012906480413	-1.27907129563766
H	2.84812880137113	-2.27389275563578	-0.24390250619398
C	1.71281030268213	-3.78106605608281	-3.04886029563577
H	1.32051316303726	-4.72144064924008	-3.41484349771599
C	2.47769178726027	3.32729361467165	-8.44555229563318
H	3.02999353622090	3.46333229343252	-7.52510250666443
C	0.34672652891665	5.22732622158108	-5.86854329563477
H	-0.39838618887382	5.62473369109964	-6.54602266423361
C	2.08492267463806	-3.63445225884503	-1.72278729563690
H	2.00817414973446	-4.46761872082174	-1.03502722359975
C	0.92683448848589	6.03021784448524	-4.89784929563581
H	0.65229351021717	7.07527673866030	-4.81758375567910
C	1.12334105701381	2.97081724043511	-10.83471829563217
H	0.58908903725156	2.82516185063468	-11.76646182073396
C	3.59470207810430	-5.24752209763788	-7.52562729563346
H	3.92621820076676	-6.26741746473943	-7.67820240587066
C	2.41668345156998	4.36492739096353	-9.37360029563306
H	2.90237132742308	5.30805946956047	-9.15723458759575
C	1.72958695129445	4.17997589239695	-10.57173729563276
H	1.67784283574758	4.98355281019283	-11.29660955854388
C	-1.98458073117382	-1.00653275469776	-7.72991929563398

C	-1.64708480288304	-3.31692769359085	-5.09554229563499
C	-2.00670361404615	-1.88791766572234	-5.17007029563505
C	-2.32655683970729	-1.07108590258727	-6.31703229563437
C	-2.29422841887253	1.45967405033061	-3.50394929563618
C	-2.73574738020957	2.59113082497113	-7.13410029563416
C	-2.20962848071711	-4.14326797825579	-4.11499929563543
H	-2.94672107785937	-3.72652343514745	-3.43963130736475
C	-2.09003515000785	3.43387624160952	-8.05534529563376
H	-1.24425529116978	3.06623268321614	-8.62589769518888
C	-1.99936953289788	0.35913865049686	-8.07666829563387
H	-1.91167115375591	0.72604789457356	-9.09041769681807
C	-1.85382741691718	-2.09724812939991	-8.68568729563301
C	-2.05369482805187	-1.02869421630816	-4.04524329563610
H	-1.82066098200885	-1.34698685768738	-3.03693581281161
C	-3.81189494228436	3.12432813550886	-6.40770429563501
H	-4.32118861979830	2.48943607745731	-5.69337690688747
C	-2.34970257264951	0.30588329325942	-4.42021929563557
C	-2.56144992689160	0.28629332537500	-5.85564829563439
C	-0.71606014804101	-3.88613377504338	-5.96916629563481
H	-0.25786124925675	-3.28120246803141	-6.74131086591526
C	-2.64462520198319	1.32456869875715	-2.15025829563736
H	-3.02430642224330	0.37474211472897	-1.79517265430554
C	-1.17173345330726	-1.93382465766851	-9.91073129563267
H	-0.67384858724912	-0.99747069466867	-10.12533289183181
C	-1.82963825307917	2.70870560370725	-3.92512529563644
H	-1.54578010084272	2.86221391416209	-4.95598021247859
C	-2.52018261219144	4.74501944126197	-8.24654029563368
H	-2.00250061338694	5.37017350961363	-8.96465496669659
C	-2.36262714927162	1.18769801992515	-6.98260729563456
C	-1.85506168002825	-5.48254052778101	-4.01955429563504
H	-2.31200917848193	-6.10326686412092	-3.25784301089550
C	-4.23641322714100	4.43206030260185	-6.60367129563499
H	-5.07263269874794	4.81153489100352	-6.02910134649636
C	-2.55331044897463	2.40012906480465	-1.27907129563794
H	-2.84812880136861	2.27389275563623	-0.24390250619369
C	-1.71281030268193	3.78106605608307	-3.04886029563627
H	-1.32051316304165	4.72144064923951	-3.41484349771449
C	-2.47769178726020	-3.32729361467215	-8.44555229563264
H	-3.02999353622233	-3.46333229342673	-7.52510250666041
C	-0.34672652891652	-5.22732622158122	-5.86854329563402
H	0.39838618887377	-5.62473369109908	-6.54602266423294
C	-2.08492267463782	3.63445225884549	-1.72278729563736
H	-2.00817414973614	4.46761872082391	-1.03502722360143
C	-0.92683448848573	-6.03021784448524	-4.89784929563492
H	-0.65229351021889	-7.07527673866147	-4.81758375567628
C	-1.12334105701381	-2.97081724043596	-10.83471829563171
H	-0.58908903724985	-2.82516185063485	-11.76646182073579
C	-3.59470207810421	5.24752209763751	-7.52562729563411
H	-3.92621820075973	6.26741746474217	-7.67820240586416
C	-2.41668345156994	-4.36492739096417	-9.37360029563238
H	-2.90237132742272	-5.30805946956274	-9.15723458759730
C	-1.72958695129444	-4.17997589239776	-10.57173729563212
H	-1.67784283574781	-4.98355281019075	-11.29660955854241

1-Ce (full-optimisation)

Ce	0.00000000000000	-0.00000000000000	-4.14238726739067
C	2.72908630111215	-2.54692765537959	-3.04873783857978
C	1.90135202161815	1.90575647265676	-4.93620401840863
C	2.17469510757027	-3.35557287402336	-2.04852992955270
H	1.42662003319851	-2.94725806923984	-1.37889937378111
C	1.55217411195482	3.32539268752061	-5.02091653630491
C	2.28782009236447	1.09982812661171	-3.81284240029342
C	2.22496200939546	-1.37606925057036	-6.64622460954847
C	1.94156871570573	1.05825980935104	-6.06206165828515
H	1.66395618390464	1.36925626779912	-7.06100904982290
C	2.00015733770203	1.03024963633946	-2.40446273174817
C	1.84343276749333	2.12316600143545	-1.45790055063738
C	2.05452919969615	-0.32741038982174	-2.05289828963283
H	2.00543423305721	-0.69212313429084	-1.03619433337641
C	2.03840705702888	4.09314234510295	-6.08354381359435
H	2.71690520876738	3.63376795453096	-6.79157905335531
C	1.08713948881022	1.97583842711905	-0.28973871027731
H	0.58252355895575	1.03650946053209	-0.10186629245249
C	2.27508566608929	-0.26094618056167	-5.70248441092188
C	2.54263665587649	-4.68105449640710	-1.91654144771097
H	2.09083021882640	-5.28084034173455	-1.13491261543818
C	0.70240894326578	3.95198295985456	-4.10774644072736
H	0.29030237157528	3.39415222294718	-3.27712307174216
C	2.52726153978078	-0.24572099872629	-4.28560629434831
C	2.37616651587634	-1.13895159633163	-3.16428125726938
C	3.66463229528943	-3.12733494348974	-3.91020705477005
H	4.11580710023202	-2.51803867599697	-4.68283460470373
C	1.73911013603821	-2.63345696379054	-6.28409595945381
H	1.44421827578583	-2.83220876224997	-5.26394466238633
C	1.68671998682220	5.42333935719371	-6.22790824507883
H	2.08371191731714	5.99445403894503	-7.05915258268137
C	0.95019302151179	3.01543013319959	0.61094748202692
H	0.35129270240418	2.87506034024032	1.50321100790797
C	2.59389307300876	-1.18448007697058	-7.98240116018397
H	3.00193756026216	-0.22756183087529	-8.28283080511340
C	4.01789398625421	-4.45921403954783	-3.78507901612262
H	4.73716645379818	-4.88442991129296	-4.47487326935327
C	2.46494037898014	3.35604912680926	-1.67783481285675
H	3.06753114716825	3.48844562270889	-2.56704440563932
C	0.34250076966980	5.27971904325461	-4.25488069389613
H	-0.34506692698870	5.72187939141311	-3.54469677680465
C	2.46004750485805	-2.19806906710339	-8.91299802478140
H	2.75540977620232	-2.02244119683629	-9.94088725030558
C	0.83539098015843	6.02603712321711	-5.31401327378884
H	0.55503228531547	7.06618705632839	-5.42832974197505
C	2.31612212981344	4.39898009661282	-0.78176151680094
H	2.79787867263212	5.34758312317259	-0.98653250087223
C	1.59879535881124	-3.64704100679296	-7.21551894815475
H	1.19159916079390	-4.59947883729465	-6.89974235646226
C	1.95736042102652	-3.43605409115633	-8.53680051363529
H	1.84835118106034	-4.22787810316870	-9.26774494953585
C	1.55804547745006	4.23935324267883	0.36792660968794
H	1.44115257593909	5.05805175348390	1.06713153688494
C	3.46456607450496	-5.24597964953001	-2.78693919082762
H	3.74549845225750	-6.28750096906175	-2.68990368211638
C	-2.72908630111215	2.54692765537959	-3.04873783857978
C	-1.90135202161815	-1.90575647265676	-4.93620401840863

C	-2.17469510757027	3.35557287402336	-2.04852992955270
H	-1.42662003319851	2.94725806923984	-1.37889937378111
C	-1.55217411195482	-3.32539268752061	-5.02091653630491
C	-2.28782009236447	-1.09982812661171	-3.81284240029342
C	-2.22496200939546	1.37606925057036	-6.64622460954847
C	-1.94156871570573	-1.05825980935104	-6.06206165828515
H	-1.66395618390464	-1.36925626779912	-7.06100904982290
C	-2.00015733770203	-1.03024963633946	-2.40446273174817
C	-1.84343276749333	-2.12316600143545	-1.45790055063738
C	-2.05452919969615	0.32741038982174	-2.05289828963283
H	-2.00543423305721	0.69212313429084	-1.03619433337641
C	-2.03840705702888	-4.09314234510295	-6.08354381359435
H	-2.71690520876738	-3.63376795453096	-6.79157905335531
C	-1.08713948881022	-1.97583842711905	-0.28973871027731
H	-0.58252355895575	-1.03650946053209	-0.10186629245249
C	-2.27508566608929	0.26094618056167	-5.70248441092188
C	-2.54263665587649	4.68105449640710	-1.91654144771097
H	-2.09083021882640	5.28084034173455	-1.13491261543818
C	-0.70240894326578	-3.95198295985456	-4.10774644072736
H	-0.29030237157528	-3.39415222294718	-3.27712307174216
C	-2.52726153978078	0.24572099872629	-4.28560629434831
C	-2.37616651587634	1.13895159633163	-3.16428125726938
C	-3.66463229528943	3.12733494348974	-3.91020705477005
H	-4.11580710023202	2.51803867599697	-4.68283460470373
C	-1.73911013603821	2.63345696379054	-6.28409595945381
H	-1.44421827578583	2.83220876224997	-5.26394466238633
C	-1.68671998682220	-5.42333935719371	-6.22790824507883
H	-2.08371191731714	-5.99445403894503	-7.05915258268137
C	-0.95019302151179	-3.01543013319959	0.61094748202692
H	-0.35129270240418	-2.87506034024032	1.50321100790797
C	-2.59389307300876	1.18448007697058	-7.98240116018397
H	-3.00193756026216	0.22756183087529	-8.28283080511340
C	-4.01789398625421	4.45921403954783	-3.78507901612262
H	-4.73716645379818	4.88442991129296	-4.47487326935327
C	-2.46494037898014	-3.35604912680926	-1.67783481285675
H	-3.06753114716825	-3.48844562270889	-2.56704440563932
C	-0.34250076966980	-5.27971904325461	-4.25488069389613
H	0.34506692698870	-5.72187939141311	-3.54469677680465
C	-2.46004750485805	2.19806906710339	-8.91299802478140
H	-2.75540977620232	2.02244119683629	-9.94088725030558
C	-0.83539098015843	-6.02603712321711	-5.31401327378884
H	-0.55503228531547	-7.06618705632839	-5.42832974197505
C	-2.31612212981344	-4.39898009661282	-0.78176151680094
H	-2.79787867263212	-5.34758312317259	-0.98653250087223
C	-1.59879535881124	3.64704100679296	-7.21551894815475
H	-1.19159916079390	4.59947883729465	-6.89974235646226
C	-1.95736042102652	3.43605409115633	-8.53680051363529
H	-1.84835118106034	4.22787810316870	-9.26774494953585
C	-1.55804547745006	-4.23935324267883	0.36792660968794
H	-1.44115257593909	-5.05805175348390	1.06713153688494
C	-3.46456607450496	5.24597964953001	-2.78693919082762
H	-3.74549845225750	6.28750096906175	-2.68990368211638

1-Ce (H-optimisation)

Ce	0.00000000000015	-0.00000000000020	-4.24749057598814
C	2.73279192384425	-2.57835562173558	-3.05078157598826
C	1.95209359215003	1.89659585050670	-5.01832357598805
C	2.10227609802531	-3.42247526766372	-2.12248357598832
H	1.25620041516636	-3.06127071142106	-1.54825796687964
C	1.60038793752829	3.32312719938204	-5.09059257598800
C	2.29344853844859	1.07503854479224	-3.87016657598799
C	2.27498126056778	-1.45045261224603	-6.68864857598808
C	2.00255446446507	1.02953477549229	-6.13798057598803
H	1.75771826993779	1.34317461557447	-7.14523280519265
C	1.95706268176262	1.01179634671302	-2.45736257598818
C	1.82504921473322	2.10182961778864	-1.49649357598819
C	1.97824956761369	-0.35270778917223	-2.11332257598823
H	1.89481061361233	-0.72245997806432	-1.10023558412343
C	2.15220325628386	4.13732575349826	-6.08505157598781
H	2.88022230440021	3.71525955260313	-6.76665986746499
C	1.14373465618767	1.93708007987774	-0.27504957598824
H	0.65159534812464	0.99669986432781	-0.06317765001564
C	2.30699385033845	-0.30015282327182	-5.76747657598808
C	2.54326580314130	-4.72908958777609	-1.93214157598836
H	2.03488605216791	-5.35749727519507	-1.21020214460617
C	0.67492841379281	3.90510519851623	-4.21217057598803
H	0.22103965109633	3.30502791517883	-3.43397582285113
C	2.53223346988940	-0.27409545668316	-4.33838657598814
C	2.34272658421570	-1.17854241836433	-3.21058657598821
C	3.81139620367861	-3.10305900956238	-3.78059357598824
H	4.31072572661326	-2.46552016139598	-4.49958819182080
C	1.84100854555348	-2.71144601020975	-6.26623257598813
H	1.55716430703729	-2.87306339050647	-5.23711060325462
C	1.80492102473520	5.48347865747345	-6.17767757598790
H	2.25738909896384	6.09822670394915	-6.94701605278299
C	1.08302313106961	2.96682218576580	0.64917642401175
H	0.54807227869861	2.81993406958521	1.57998239994325
C	2.61664731709779	-1.30063344431855	-8.03834457598797
H	2.96845520056850	-0.33981044117794	-8.39221414632245
C	4.25036979547687	-4.40582512706314	-3.58210957598815
H	5.08811750415246	-4.77802527851454	-4.15936013512345
C	2.43863313622014	3.33501396710900	-1.73671057598814
H	2.98884687931056	3.47486909506365	-2.65797872737397
C	0.31347665117338	5.24099802628632	-4.31904757598794
H	-0.42565714040047	5.64550792916163	-3.63880733999826
C	2.55651003107978	-2.37824790677326	-8.91371257598802
H	2.84710295338896	-2.23742588903027	-9.94837981514119
C	0.88470455812535	6.03617012960327	-5.29925557598792
H	0.61338319058825	7.08194439062613	-5.38178634582133
C	2.37038945480396	4.36817682989441	-0.81248457598801
H	2.85034387787849	5.31396570174114	-1.03183931998903
C	1.75884371078086	-3.78456875917033	-7.14770757598813
H	1.39414074279589	-4.73820603595148	-6.78765725592178
C	2.13260022787099	-3.62021631582780	-8.47704557598807
H	2.08276028224435	-4.45504015847129	-9.16548267211619
C	1.68908580676276	4.18760929080729	0.38147642401180
H	1.63180166553489	4.99204532170394	1.10485623417270
C	3.62044500452761	-5.22471883225495	-2.65788357598835
H	3.96090206864861	-6.24151619861607	-2.50419719101013
C	-2.73279192384395	2.57835562173511	-3.05078157598812
C	-1.95209359214972	-1.89659585050705	-5.01832357598817

C	-2.10227609802502	3.42247526766320	-2.12248357598813
H	-1.25620041516634	3.06127071142048	-1.54825796687902
C	-1.60038793752798	-3.32312719938239	-5.09059257598820
C	-2.29344853844829	-1.07503854479266	-3.87016657598806
C	-2.27498126056746	1.45045261224577	-6.68864857598800
C	-2.00255446446475	-1.02953477549258	-6.13798057598810
H	-1.75771826993323	-1.34317461557454	-7.14523280519439
C	-1.95706268176232	-1.01179634671352	-2.45736257598824
C	-1.82504921473293	-2.10182961778920	-1.49649357598831
C	-1.97824956761340	0.35270778917171	-2.11332257598822
H	-1.89481061361853	0.72245997806250	-1.10023558412287
C	-2.15220325628354	-4.13732575349855	-6.08505157598806
H	-2.88022230440116	-3.71525955260726	-6.76665986746506
C	-1.14373465618739	-1.93708007987836	-0.27504957598836
H	-0.65159534810247	-0.99669986433712	-0.06317765002647
C	-2.30699385033814	0.30015282327151	-5.76747657598807
C	-2.54326580314101	4.72908958777556	-1.93214157598810
H	-2.03488605216850	5.35749727519199	-1.21020214460418
C	-0.67492841379250	-3.90510519851663	-4.21217057598825
H	-0.22103965108960	-3.30502791517887	-3.43397582285409
C	-2.53223346988910	0.27409545668277	-4.33838657598813
C	-2.34272658421540	1.17854241836387	-3.21058657598815
C	-3.81139620367831	3.10305900956195	-3.78059357598808
H	-4.31072572660992	2.46552016139519	-4.49958819182014
C	-1.84100854555317	2.71144601020946	-6.26623257598798
H	-1.55716430704657	2.87306339050729	-5.23711060325109
C	-1.80492102473488	-5.48347865747374	-6.17767757598822
H	-2.25738909895792	-6.09822670394631	-6.94701605278835
C	-1.08302313106933	-2.96682218576648	0.64917642401158
H	-0.54807227869476	-2.81993406958807	1.57998239994431
C	-2.61664731709747	1.30063344431837	-8.03834457598791
H	-2.96845520055444	0.33981044117630	-8.39221414632622
C	-4.25036979547656	4.40582512706270	-3.58210957598791
H	-5.08811750415119	4.77802527851932	-4.15936013512252
C	-2.43863313621985	-3.33501396710954	-1.73671057598834
H	-2.98884687935315	-3.47486909504501	-2.65797872735331
C	-0.31347665117307	-5.24099802628671	-4.31904757598824
H	0.42565714041157	-5.64550792916045	-3.63880734000635
C	-2.55651003107945	2.37824790677313	-8.91371257598789
H	-2.84710295339095	2.23742588903858	-9.94837981514135
C	-0.88470455812504	-6.03617012960361	-5.29925557598827
H	-0.61338319059484	-7.08194439063199	-5.38178634580634
C	-2.37038945480368	-4.36817682989501	-0.81248457598827
H	-2.85034387790153	-5.31396570173201	-1.03183931997741
C	-1.75884371078054	3.78456875917010	-7.14770757598792
H	-1.39414074280179	4.73820603595291	-6.78765725591899
C	-2.13260022787066	3.62021631582765	-8.47704557598787
H	-2.08276028223550	4.45504015846999	-9.16548267211776
C	-1.68908580676248	-4.18760929080796	0.38147642401155
H	-1.63180166552820	-4.99204532170557	1.10485623416805
C	-3.62044500452731	5.22471883225446	-2.65788357598806
H	-3.96090206865005	6.24151619861521	-2.50419719101009

1-Tb (full-optimisation)

Tb	-0.00000000000000	-0.00000000000000	-6.06098990080564
C	-2.10186107144325	1.33680215676350	-3.47046054424948
C	-1.90520211452815	-1.01480754648639	-7.75463254233209
C	-2.17591267033833	-1.10488499227378	-6.34292963893329
C	-1.40216395225155	-3.34206576511995	-5.16665757567485
C	-1.71782957515542	-1.91248179663142	-5.24504555223737
C	-2.20109282300326	3.36061801762995	-8.09336719569796
H	-1.45620529350622	2.97657469901472	-8.78085215238731
C	-2.69529161751445	2.53838366959328	-7.07278503802657
C	-1.97543037437132	0.34642006065573	-8.08886927494166
H	-1.94709079977785	0.72287107484015	-9.10211379111306
C	-1.89226646948083	-4.09372188881559	-4.09496705562396
H	-2.54397148957086	-3.61452832033383	-3.37498451121806
C	-1.75587581637515	-2.09699262414388	-8.71475050751517
C	-1.71263138147690	2.63336730216655	-3.80755721929702
H	-1.43779757927265	2.87143916849149	-4.82397012518797
C	-1.72272001897061	-1.07145796659089	-4.11255900431181
H	-1.40330945362200	-1.38874602427885	-3.12795262665524
C	-2.10596198228373	0.24219891681612	-4.44191192320895
C	-2.43536088060722	1.08737063635501	-2.13485756753851
H	-2.76865942585402	0.09709155542452	-1.85111079996513
C	-0.58661897854388	-3.99222021115699	-6.09267748532152
H	-0.17010052646440	-3.44144685627908	-6.92471161564873
C	-3.63128486637640	3.08749758839927	-6.19198576372533
H	-4.04074438194890	2.46636537068185	-5.40572167522949
C	-2.42080088192518	0.23356122932876	-5.84930632510902
C	-2.29076424302385	1.14346540514005	-6.96329610893338
C	-1.02289962819298	-1.93284768408610	-9.89509753344599
H	-0.52962465785984	-0.98812835358308	-10.08343224554799
C	-0.89532022398735	-2.96210474888877	-10.80888802105156
H	-0.31445106593216	-2.80803164377839	-11.71074637451845
C	-2.36165345694186	2.08554808374014	-1.18052711643365
H	-2.62677909843654	1.86368389317613	-0.15335462326596
C	-1.57424700083393	-5.43296689261160	-3.95265450719783
H	-1.97131554648583	-5.99109059865114	-3.11269720391131
C	-1.63734542424890	3.63312504378908	-2.85414242931533
H	-1.30641838290768	4.62019286562994	-3.15262458040409
C	-2.62353121089278	4.66968337219004	-8.22318829680674
H	-2.21781071756992	5.28063420100195	-9.02128644828807
C	-1.95952080158268	3.36603838841362	-1.53336311518970
H	-1.89920808689615	4.14678642550256	-0.78495647928371
C	-2.36551697096216	-3.33595192664816	-8.49669136287731
H	-2.95130097920081	-3.48186404770844	-7.59848553740594
C	-4.03874250881888	4.40425583219367	-6.31485769364190
H	-4.75651643789865	4.80534916946638	-5.60922263470901
C	-3.54269958198044	5.20511929582005	-7.33136087517906
H	-3.86644328359872	6.23424055149957	-7.42714139576312
C	-0.26072376577665	-5.32882171482873	-5.94871496605712
H	0.40324534424938	-5.79073222962652	-6.66869603201858
C	-2.22598966844511	-4.36888308285580	-9.40575589042051
H	-2.69782238046865	-5.32263692770051	-9.20181258517267
C	-0.75468049981848	-6.05942192776533	-4.87893838811180
H	-0.49873981893548	-7.10603277587909	-4.76579886787655
C	-1.48995244442941	-4.19273724875721	-10.56728880516484
H	-1.38056399211263	-5.00345349112625	-11.27691982045543
C	2.10186107144325	-1.33680215676350	-3.47046054424948
C	1.90520211452815	1.01480754648639	-7.75463254233209

C	2.17591267033833	1.10488499227378	-6.34292963893329
C	1.40216395225155	3.34206576511995	-5.16665757567485
C	1.71782957515542	1.91248179663142	-5.24504555223737
C	2.20109282300326	-3.36061801762995	-8.09336719569796
H	1.45620529350622	-2.97657469901472	-8.78085215238731
C	2.69529161751445	-2.53838366959328	-7.07278503802657
C	1.97543037437132	-0.34642006065573	-8.08886927494166
H	1.94709079977785	-0.72287107484015	-9.10211379111306
C	1.89226646948083	4.09372188881559	-4.09496705562396
H	2.54397148957086	3.61452832033383	-3.37498451121806
C	1.75587581637515	2.09699262414388	-8.71475050751517
C	1.71263138147690	-2.63336730216655	-3.80755721929702
H	1.43779757927265	-2.87143916849149	-4.82397012518797
C	1.72272001897061	1.07145796659089	-4.11255900431181
H	1.40330945362200	1.38874602427885	-3.12795262665524
C	2.10596198228373	-0.24219891681612	-4.44191192320895
C	2.43536088060722	-1.08737063635501	-2.13485756753851
H	2.76865942585402	-0.09709155542452	-1.85111079996513
C	0.58661897854388	3.99222021115699	-6.09267748532152
H	0.17010052646440	3.44144685627908	-6.92471161564873
C	3.63128486637640	-3.08749758839927	-6.19198576372533
H	4.04074438194890	-2.46636537068185	-5.40572167522949
C	2.42080088192518	-0.23356122932876	-5.84930632510902
C	2.29076424302385	-1.14346540514005	-6.96329610893338
C	1.02289962819298	1.93284768408610	-9.89509753344599
H	0.52962465785984	0.98812835358308	-10.08343224554799
C	0.89532022398735	2.96210474888877	-10.80888802105156
H	0.31445106593216	2.80803164377839	-11.71074637451845
C	2.36165345694186	-2.08554808374014	-1.18052711643365
H	2.62677909843654	-1.86368389317613	-0.15335462326596
C	1.57424700083393	5.43296689261160	-3.95265450719783
H	1.97131554648583	5.99109059865114	-3.11269720391131
C	1.63734542424890	-3.63312504378908	-2.85414242931533
H	1.30641838290768	-4.62019286562994	-3.15262458040409
C	2.62353121089278	-4.66968337219004	-8.22318829680674
H	2.21781071756992	-5.28063420100195	-9.02128644828807
C	1.95952080158268	-3.36603838841362	-1.53336311518970
H	1.89920808689615	-4.14678642550256	-0.78495647928371
C	2.36551697096216	3.33595192664816	-8.49669136287731
H	2.95130097920081	3.48186404770844	-7.59848553740594
C	4.03874250881888	-4.40425583219367	-6.31485769364190
H	4.75651643789865	-4.80534916946638	-5.60922263470901
C	3.54269958198044	-5.20511929582005	-7.33136087517906
H	3.86644328359872	-6.23424055149957	-7.42714139576312
C	0.26072376577665	5.32882171482873	-5.94871496605712
H	-0.40324534424938	5.79073222962652	-6.66869603201858
C	2.22598966844511	4.36888308285580	-9.40575589042051
H	2.69782238046865	5.32263692770051	-9.20181258517267
C	0.75468049981848	6.05942192776533	-4.87893838811180
H	0.49873981893548	7.10603277587909	-4.76579886787655
C	1.48995244442941	4.19273724875721	-10.56728880516484
H	1.38056399211263	5.00345349112625	-11.27691982045543

1-Tb (H-optimisation)

Tb	-0.00000000000046	-0.00000000000011	-5.96567772268109
C	-2.18349801629711	1.41702256061830	-3.44702272268403
C	-1.86324666805400	-1.02017251575350	-7.70423572268009
C	-2.18063764214378	-1.09062234658882	-6.28857172268131
C	-1.45518901606213	-3.33982039567559	-5.07120372268187
C	-1.77343627546543	-1.90241659776679	-5.15297472268236
C	-2.09445337942845	3.40778110751451	-8.04971972268036
H	-1.24993558511339	3.06367807673881	-8.63637423148257
C	-2.68383182000883	2.55657683541205	-7.10423972268078
C	-1.89817038939069	0.33939319165084	-8.04747072267931
H	-1.83371035865954	0.70978622895963	-9.06181974700080
C	-2.00667130916042	-4.13042376195969	-4.05008572268323
H	-2.70586169437375	-3.67919717686639	-3.35693948793267
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C	-1.84599394663306	2.71550219856156	-3.85281272268317
H	-1.56229952573009	2.90702049004695	-4.87591726704832
C	-1.80602256669850	-1.03801820907933	-4.02759872268290
H	-1.53186459223037	-1.35108222955969	-3.02798847535868
C	-2.15400752365136	0.28634358572140	-4.38739172268263
C	-2.51810825711045	1.22557704363472	-2.10188672268518
H	-2.79792889173825	0.23600197635179	-1.76279702996812
C	-0.56979214979535	-3.95825393334572	-5.95944272268144
H	-0.11303534294953	-3.37703771472500	-6.74884336003518
C	-3.76445664482801	3.04888061824071	-6.36523272268195
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C	-2.42167510403800	0.25972957050687	-5.81225472268135
C	-2.24541585848383	1.16901738256471	-6.94202672268079
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C	-1.01896734623640	-2.98526703778148	-10.81971872267665
H	-0.49094108987459	-2.83699645716155	-11.75428172827325
C	-2.54834137998882	2.28834261775656	-1.20955872268559
H	-2.83146794890244	2.11167994045622	-0.17860368475998
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C	-2.56617273581597	4.70314603681181	-8.23370472267931
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C	-2.29475626485360	-4.37925803428603	-9.34477072267896
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H	-1.56646763082724	-5.01202950084122	-11.26607882425457
C	2.18349801629596	-1.41702256061837	-3.44702272268373
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H	1.56229952572837	-2.90702049004077	-4.87591726705034
C	1.80602256669740	1.03801820907923	-4.02759872268279
H	1.53186459223091	1.35108222955904	-3.02798847535688
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H	2.79792889173821	-0.23600197635187	-1.76279702997092
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H	0.11303534296398	3.37703771473234	-6.74884336005439
C	3.76445664482714	-3.04888061824096	-6.36523272268140
H	4.23874387404643	-2.40239375474967	-5.63758334796365
C	2.42167510403707	-0.25972957050709	-5.81225472268111
C	2.24541585848302	-1.16901738256499	-6.94202672268050
C	1.07450360936574	1.94957706216890	-9.89468172267850
H	0.58523408612117	1.00983175915173	-10.11467466361229
C	1.01896734623595	2.98526703778096	-10.81971872267675
H	0.49094108987646	2.83699645716018	-11.75428172827726
C	2.54834137998746	-2.28834261775649	-1.20955872268520
H	2.83146794890021	-2.11167994045649	-0.17860368476070
C	1.69200940573938	5.48121557707319	-3.94276072268352
H	2.14046166888986	6.07168022280542	-3.15241388219011
C	1.85678516515827	-3.78127415895576	-2.95741772268456
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C	2.56617273581527	-4.70314603681217	-8.23370472267877
H	2.08418260798422	-5.34065778669309	-8.96576724334511
C	2.22048568828521	-3.57285405269414	-1.63170272268523
H	2.24100258823126	-4.39981774101316	-0.93242275563823
C	2.35525708574681	3.34399739124605	-8.41871172267938
H	2.89685930621156	3.48492942182867	-7.49253385086526
C	4.23785955900832	-4.34381577387062	-6.56148372268073
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H	4.00445412314350	-6.18466693124789	-7.63993393897593
C	0.24192135079243	5.30238502419279	-5.84189672268231
H	-0.47039235604652	5.73561053220850	-6.53297253733888
C	2.29475626485301	4.37925803428560	-9.34477072267901
H	2.77404985576641	5.32397079842538	-9.11939132818104
C	0.80934702327733	6.06977524685138	-4.83508872268227
H	0.56078955532475	7.12044972803979	-4.74323684959957
C	1.61833778080108	4.20462196989420	-10.54578572267795
H	1.56646763082477	5.01202950084222	-11.26607882425355

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