Electronic Supplementary Material (ESI) for Dalton Transactions.

Spectroscopic and Electrochemical Characterization of a Pr^{4+} Imidophosphorane Complex and the Redox Chemistry of Nd^{3+} and Dy^{3+} Complexes

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General Considerations

Unless otherwise noted, all reagents were obtained from commercial suppliers and the syntheses and manipulations were conducted under argon with exclusion of oxygen and water using Schlenk techniques or in an inert atmosphere box (Vigor) under a dinitrogen (<0.1 ppm O_2/H_2O) atmosphere. The glovebox is equipped with two -35 ˚C freezers. All glassware and cannulae were stored in an oven overnight (>8 h) at a temperature of ca. 160 ˚C. Celite and molecular sieves were dried under vacuum at a temperature >250 ˚C for a minimum of 24 h. C_6D_6 was stored over 3 Å molecular sieves and then vacuum-transferred from purple sodium/benzophenone prior to use. Diethyl ether, *n*-pentane, *n*-hexane, benzene, toluene, tetrahydrofuran, and 1,2-dimethoxyethane were purged with UHP-grade argon (Airgas) and passed through columns containing Q-5 and molecular sieves in a solvent purification system (JC Meyer Solvent Systems). All solvents in the glovebox were stored in bottles over 3 Å molecular sieves. Methanol was dried by refluxing over magnesium turnings activated with iodine for 12 h and then distilled and stored over 3 Å molecular sieves.

The starting materials $PrI_3(THF)_4$, $NdI_3(THF)_{3.5}$, $DyI_3(THF)_{3.5}$[1], $[(CH_2N^tBu)_2(Et_2N)P{=}NK]$[2], and potassium benzyl[3] were prepared according to literature procedures. Potassium *t*-butoxide was sublimed prior to use. Electrolyte, $[NBu_4][PF_6]$ was recrystallized from ethanol and solvent evacuated for 18 h prior to use. NMR spectra were obtained on a Bruker Avance III 400 MHz spectrometer at 298 K, unless otherwise noted. ^1H, ^{13}C, and ^{31}P NMR chemical shifts are reported in δ, parts per million. ^1H NMR are referenced to the residual ^1H resonances of the solvent. ^{13}C NMR are referenced to the ^{13}C resonance of the deuterated solvent.[4] Peak position is listed, followed by peak multiplicity, integration value, and proton assignment, where applicable. Multiplicity and shape are indicated by the following abbreviations: s (singlet); d (doublet); t (triplet); q (quartet); dd (doublet of doublets); td (triplet of doublets); m (multiplet); br (broad). Infrared (IR) samples were taken on a Bruker ALPHA FTIR spectrometer from 400 to 4000 cm^{-1}. IR samples were prepared as Nujol mulls sandwiched between two KBr plates. The peaks are listed in wavenumber [cm^{-1}] and intensity using the following abbreviations: vw (very weak); w (weak); m (medium); s (strong); vs (very strong); br (broad). UV/visible/NIR spectroscopy was performed in Teflon-valve sealed quartz cuvettes with a 1 cm path length on a Hitachi UH4150 UV-vis-NIR scanning spectrophotometer between 2400-200 nm. Elemental analyses were determined at Berkeley Microanalytical Facility (University of California Berkeley).

Synthetic Methods

Preparation of $[K][Pr(NP^*)_4]$, (1-Pr(NP*)).

Inside a glovebox, $PrI_3(THF)_4$ (0.372 g, 0.459 mmol) was added to a 20 mL scintillation vial charged with a Teflon stir bar and 1 mL diethyl ether. $[(CH_2N^tBu)_2(Et_2N)P{=}NK]$ (0.600 g, 1.84 mmol) was added as a solution in diethyl ether (6 mL) and the reaction mixture was stirred overnight. Then the mixture was filtered through a fine porosity frit packed with Celite. The filtrate was concentrated *in vacuo* to give a colorless solid. The residue was triturated three times with 1 mL *n*-pentane and then taken up in 10 mL hexanes and filtered through a pipet filter packed with Celite and glass fiber filter paper. The pale yellow

solution was concentrated *in vacuo* and placed into a -35° C freezer. Overnight pale green crystals formed which were isolated by decantation and residual volatiles were removed *in vacuo* to afford the title compound (48%, 0.293 g). ^{1}H NMR (400.13 MHz, C_6D_6): 5.54 (s, 8 H), 4.76 (s, 8 H), 2.50 (s, 72 H), -3.35 (s, 24 H), -5.88 (s, 16 H). ^{31}P NMR (161.98 MHz, C_6D_6): 343.87 (s). ^{13}C NMR (100.61 MHz, C_6D_6): 54.21 (s), 44.51 (s), 28.38 (s), 8.94 (s). Quaternary carbon not observed. IR: ν [cm^{-1}] = 1356(m), 1266 (m), 1249 (m), 1210 (s), 1196 (s) 1161 (s), 1095 (w), 1074 (m), 1054 (m), 1027 (m), 974 (m), 926 (m), 869 (m), 795 (m), 690 (m), 624 (w). Elemental analysis found(calculated): C, 50.87(50.59), H, 9.63(9.70), N, 16.82(16.85). XRD quality crystals were grown from *n*-hexane at -35 °C.

***In situ* preparation of [Pr(NP*)$_4$], (2-Pr(NP*)) for EPR (toluene), UV-vis-NIR (toluene and THF), and ^{31}P NMR (d_8-toluene).**

Inside a glovebox, **1-Pr(NP*)** (0.05 g, 0.04 mmol) was suspended in 2 mL solvent in a 20 mL scintillation vial. This suspension was chilled to -35 °C in a glovebox freezer. Excess AgI (4 eq.) was added to the scintillation vial as solid and the vial replaced in the freezer. The reaction mixture was kept in the freezer for 1 h for toluene and for 40 min. for THF with occasional manual agitation. Over this period, the color of the solution went from pale green to dark blue. The solution was filtered cold through a pipet filter packed with Celite and a glass fiber filter paper into a cold well (at 77 K). A fine grey powder was observed on the pipet filter.

Preparation of [K][Nd(NP*)$_4$], (1-Nd(NP*)).

Inside a glovebox, $NdI_3(THF)_{3.5}$ (0.179 g, 0.230 mmol) was added to a 20 mL scintillation vial charged with a glass stir bar and 1 mL diethyl ether. [$(CH_2N^tBu)_2(Et_2N)P$=NK] (0.300 g, 0.919 mmol) was added as a solution in diethyl ether (6 mL) and the reaction mixture was stirred overnight in the dark. Then the mixture was filtered through a fine porosity frit packed with Celite. The filtrate was concentrated *in vacuo* to give a blue solid. The residue was triturated three times with 1 mL *n*-pentane and then taken up in 12 mL hexanes and filtered through a pipet filter packed with Celite and glass fiber filter paper. The pale blue solution was concentrated *in vacuo* and placed into a -35° C freezer. Overnight pale green crystals formed which were isolated by decantation and residual volatiles were removed *in vacuo* to afford the title compound (46 %, 0.143 g). ^{1}H NMR (400.13 MHz, C_6D_6): 4.80 (s, 8 H), 4.62 (s, 8 H), 2.09 (s, 72 H), -1.55 (s, 24 H), -2.06 (s, br, 16H). ^{31}P NMR (161.98 MHz, C_6D_6): 525.93 (s). ^{13}C NMR (100.61 MHz, C_6D_6): 53.28 (s), 43.95 (s), 30.56 (s), 27.09 (s), 11.00 (s). IR: ν [cm^{-1}] = 1356 (m), 1266 (m), 1249 (m), 1210 (s), 1196 (s), 1164 (s), 1095 (w), 1054 (m), 1027 (m), 974 (m), 926 (m), 869 (m), 795 (m), 692 (m), 626 (w). Elemental analysis found(calculated) with ½ hexane molecule as identified by ^{1}H NMR. Amount of hexanes identified is dependent on absolute vacuum: C, 51.65(51.50), H, 10.19(9.89), N, 16.38(16.29). XRD quality crystals were grown from diethyl ether at -35 °C.

Preparation of [K][Dy(NP*)$_4$], (1-Dy(NP*)).

Inside a glovebox, $DyI_3(THF)_{3.5}$ (0.201 g, 0.252 mmol) was added to a 20 mL scintillation vial charged with a Teflon stir bar and 1 mL diethyl ether. [$(CH_2N^tBu)_2(Et_2N)P$=NK] (0.330 g, 1.01 mmol) was added as a solution in diethyl ether (6 mL) and the reaction mixture was stirred overnight. Then the mixture was filtered through a fine porosity frit packed

with Celite. The filtrate was concentrated *in vacuo* to give a colorless solid. The residue was triturated three times with 1 mL *n*-pentane and then taken up in 5 mL *n*-pentane and filtered through a pipet filter packed with Celite and glass fiber filter paper. The pale yellow solution was concentrated *in vacuo* and placed into a -35° C freezer. Over 2-3 days, crystals formed which were isolated by decantation and residual volatiles were removed *in vacuo* to afford the title compound (33%, 0.1141 g). ^{1}H NMR (400.13 MHz, C_6D_6): 27.24 (b), 11.24 (b), 8.02 (s). ^{31}P NMR (161.98 MHz, C_6D_6): 2335.74 (s). ^{13}C NMR (100.61 MHz, C_6D_6): No resonances were observed. IR: ν [cm^{-1}] = 1356(m), 1266 (m), 1251 (m), 1210 (s), 1196 (s), 1171 (s), 1151 (s), 1112 (w), 1095 (w), 1054 (m), 1029 (m), 976 (m), 926 (m), 869 (m), 797 (m), 692 (m), 626 (w). Elemental analysis found(calculated): C, 49.98(49.78), H, 9.45(9.55), N, 16.40(16.59). XRD quality crystals were grown from diethyl ether at -35 °C.

NMR Spectroscopy

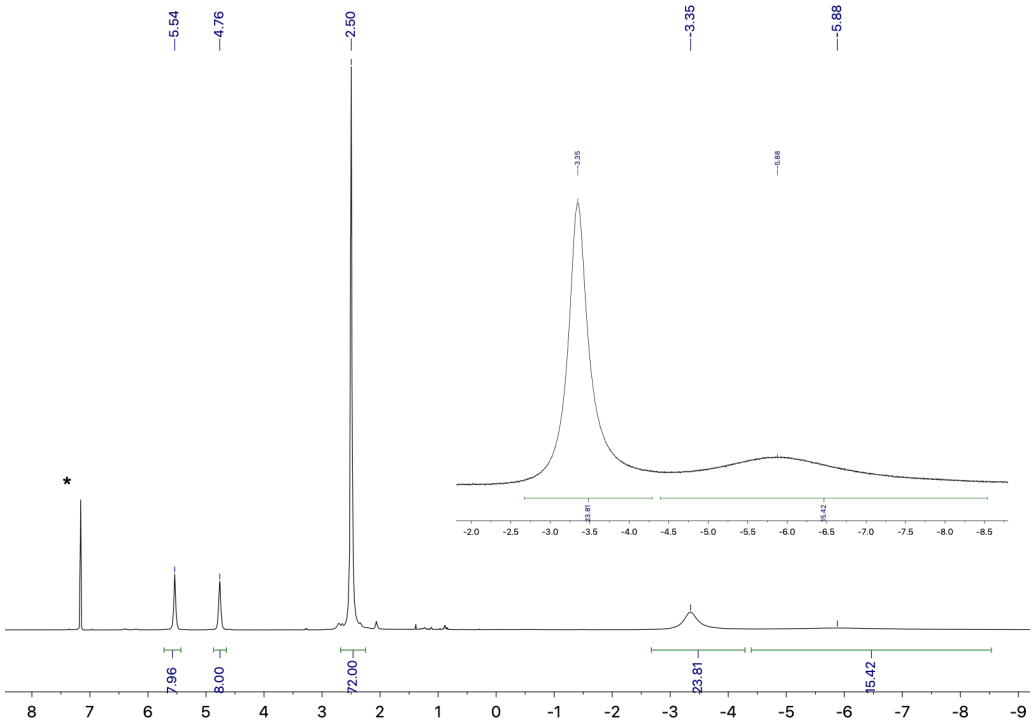


Figure S1. ^{1}H NMR of **1-Pr(NP*)** in C_6D_6. Peak of C_6D_5H is noted as *.

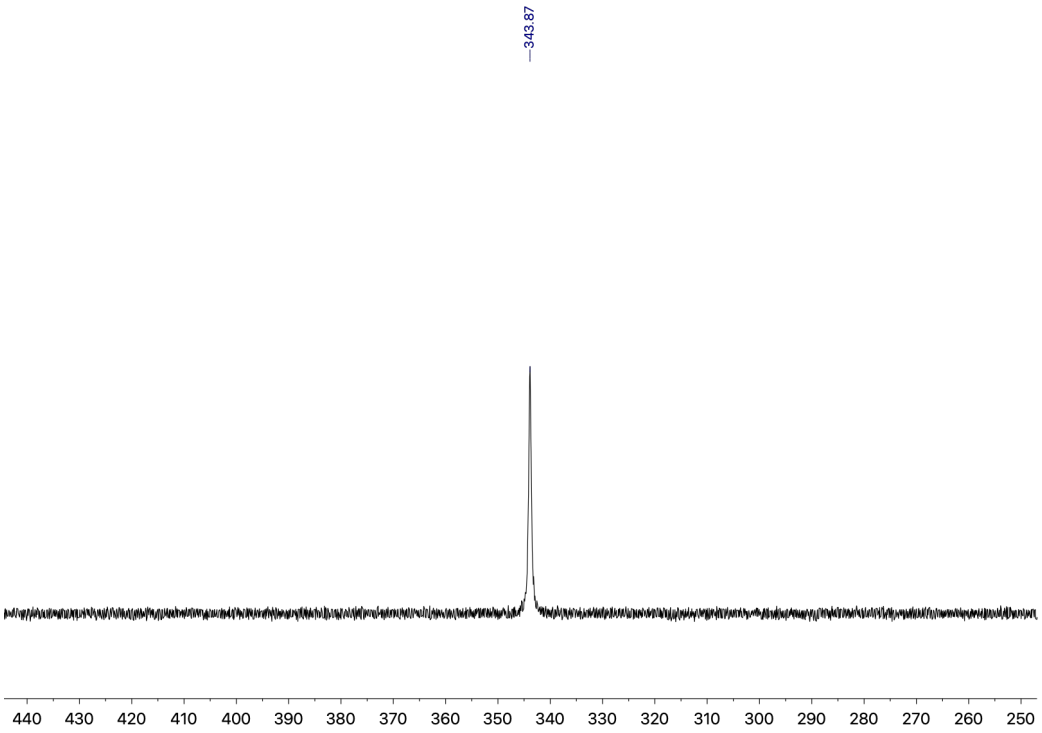


Figure S2. $^{31}P\{^{1}H\}$ NMR of **1-Pr(NP*)** in C_6D_6.

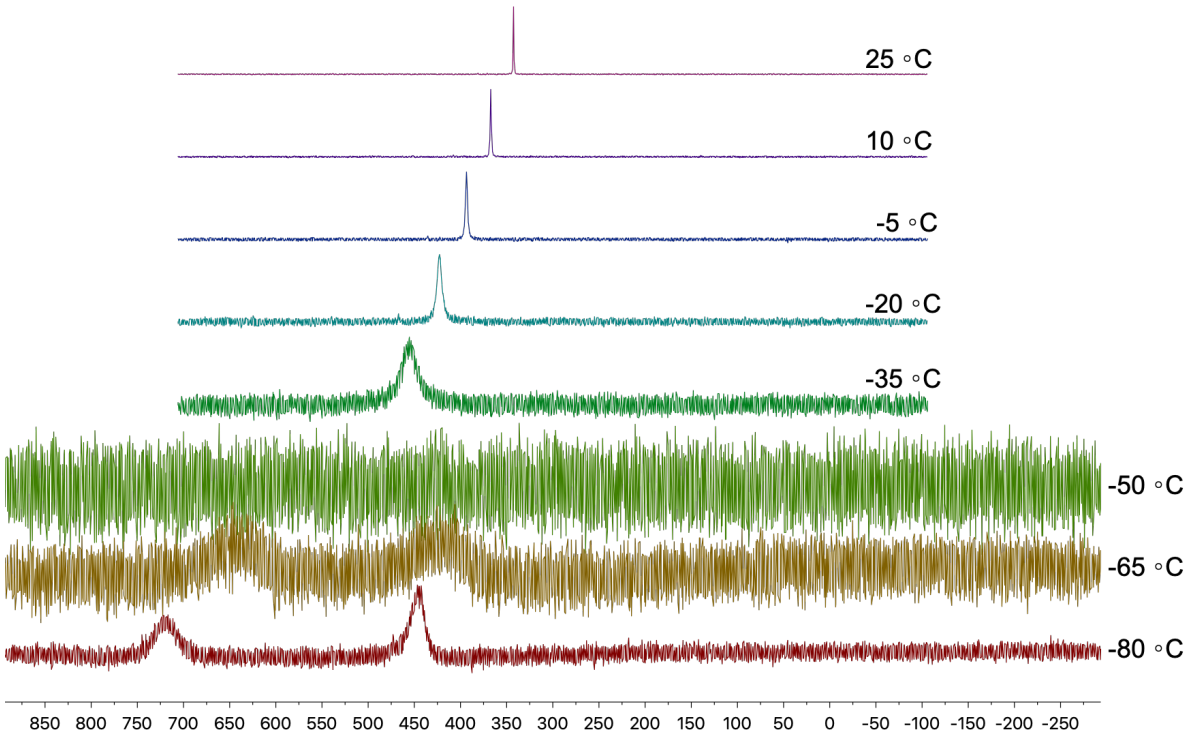


Figure S3. Variable temperature $^{31}P\{^{1}H\}$ NMR of **1-Pr(NP*)** in d_8-toluene.

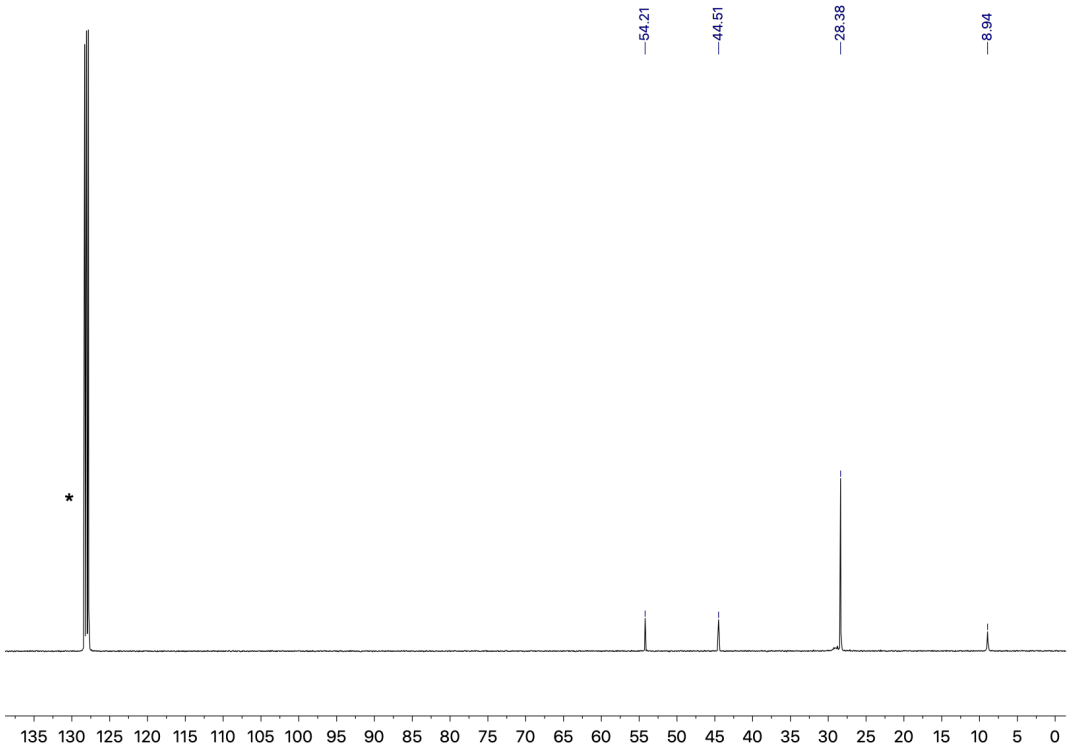


Figure S4. $^{13}C\{^{1}H\}$ NMR of **1-Pr(NP*)** in C_6D_6. Peak of C_6D_5H is noted as *.

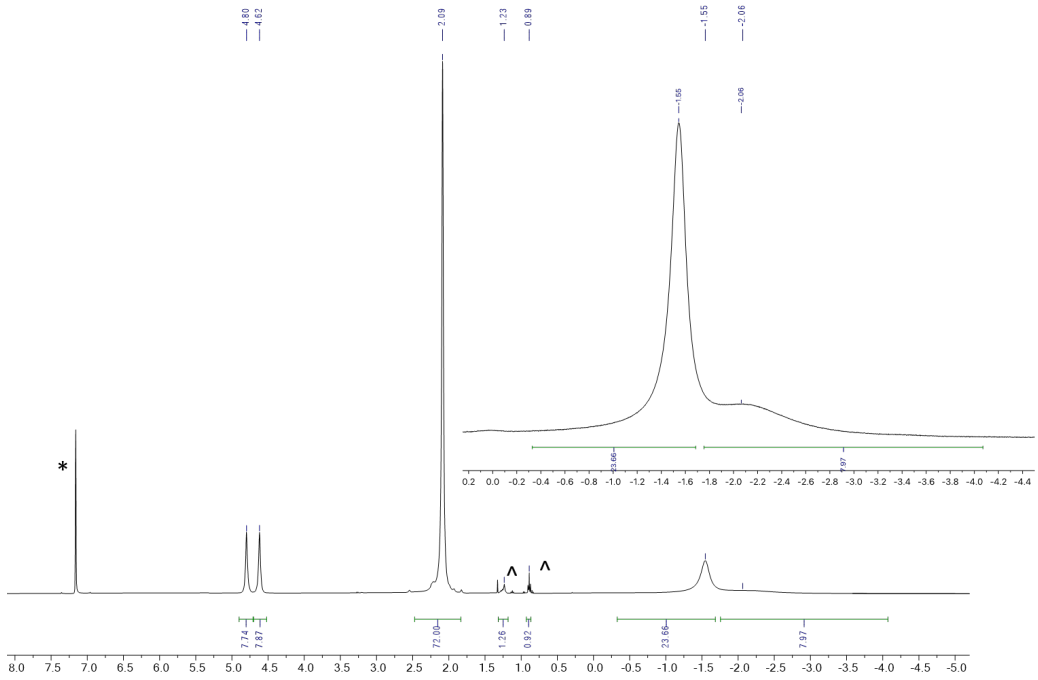


Figure S5. ^{1}H NMR of **1-Nd(NP*)** in C_6D_6. Peak of C_6D_5H is noted as *. Residual hexanes is denoted by ^.

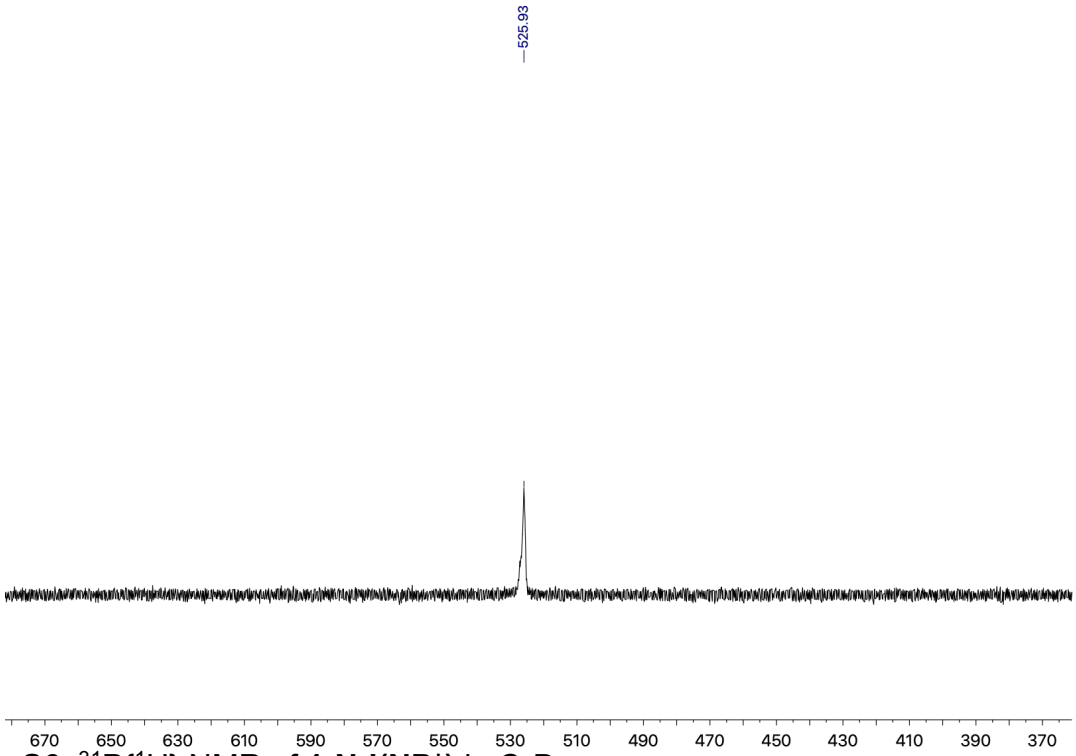


Figure S6. $^{31}P\{^{1}H\}$ NMR of **1-Nd(NP*)** in C_6D_6.

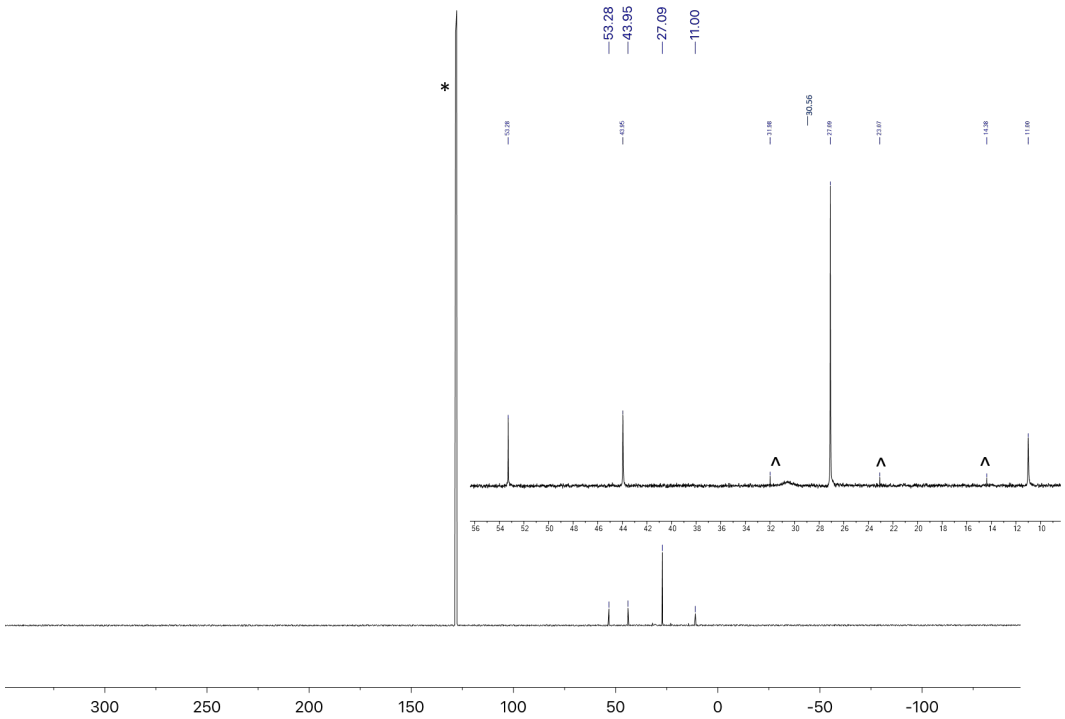


Figure S7. $^{13}C\{^{1}H\}$ NMR of **1-Nd(NP*)** in C_6D_6. Peak of C_6D_5H is noted as *. Residual hexanes is denoted by ^.

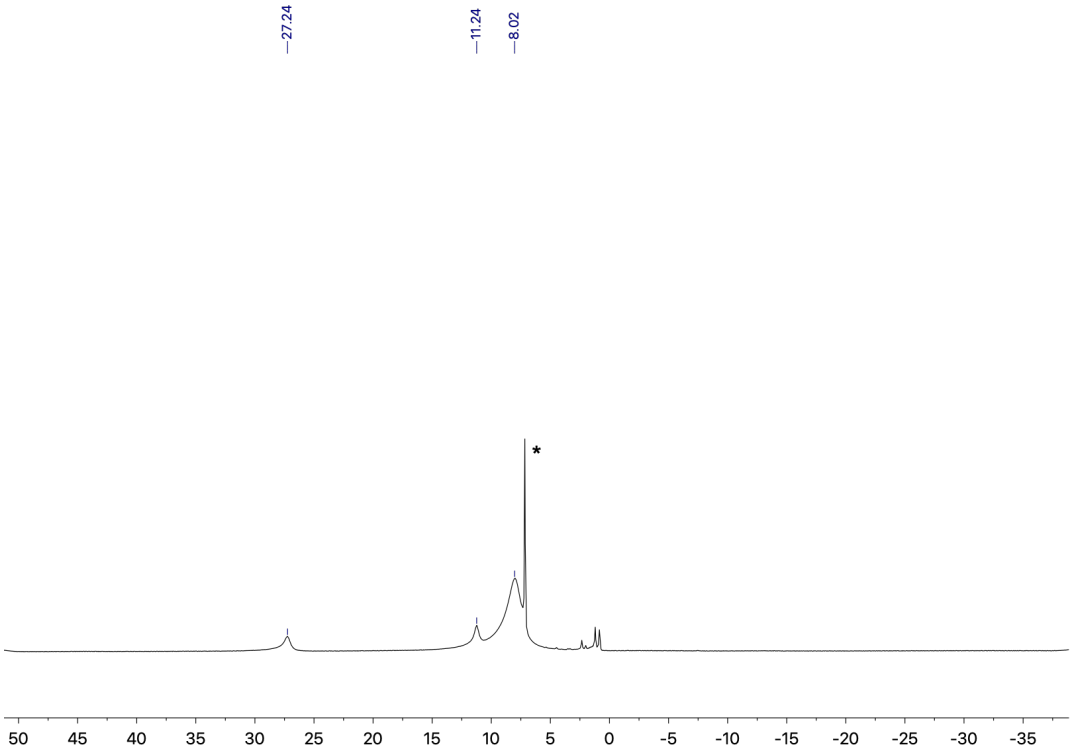


Figure S8. ^{1}H NMR of **1-Dy(NP*)** in C_6D_6. Peak of C_6D_5H is noted as *. No peaks were assigned as the spectrum is very paramagnetically broadened.

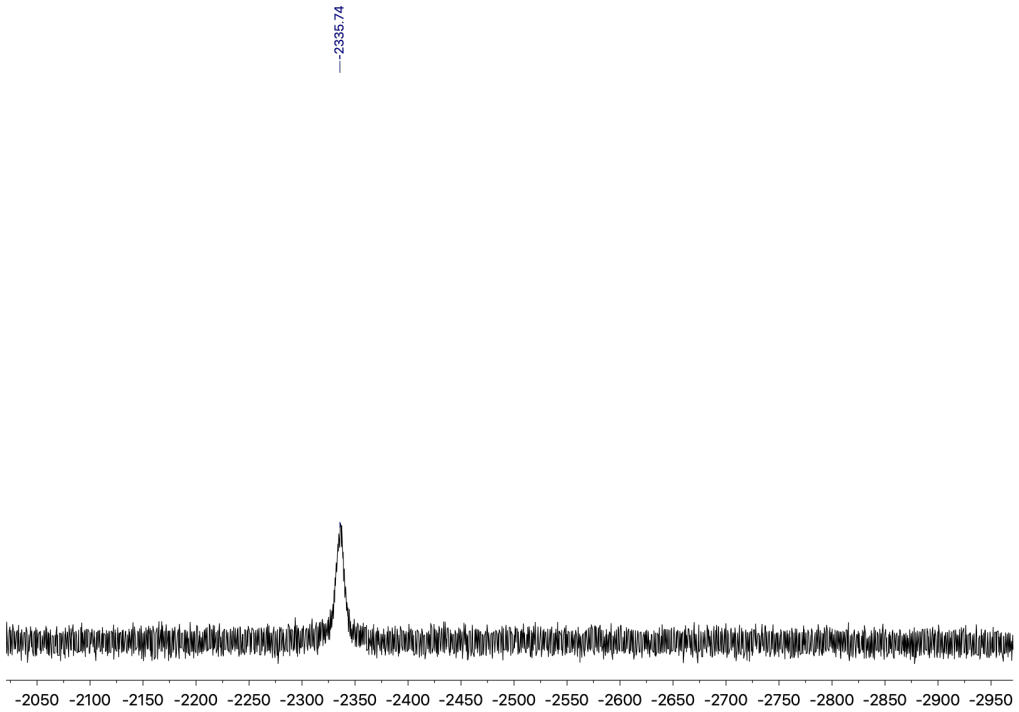


Figure S9. ^{31}P{^{1}H} NMR of **1-Dy(NP*)** in C_6D_6.

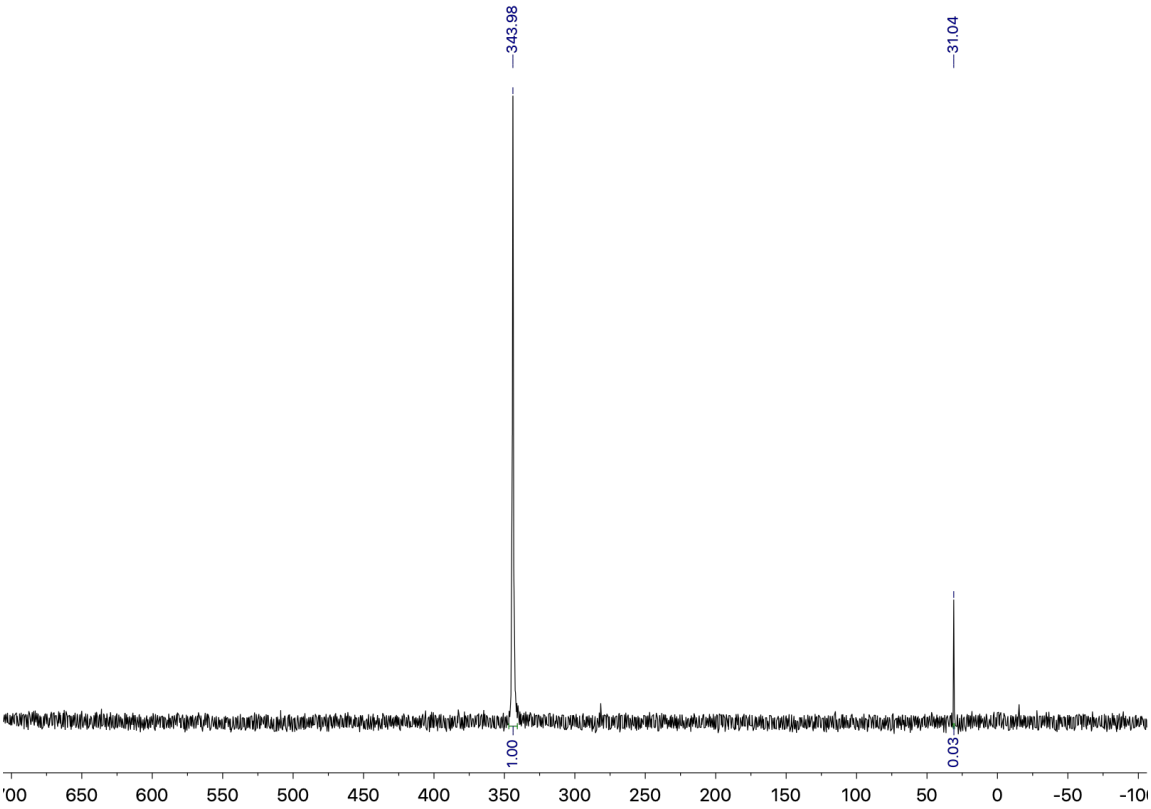


Figure S10. $^{31}P\{^{1}H\}$ NMR of reaction products of the reaction of **1-Pr(NP*)** and excess AgI in toluene at -35 °C for one hour. The blue solution was then warmed to room temperature (blue color of solution fades) and toluene evacuated. NMR was taken of the residual product. The major compound present is **1-Pr(NP*)** (~343 ppm) and the minor product is protonated ligand (~31 ppm).

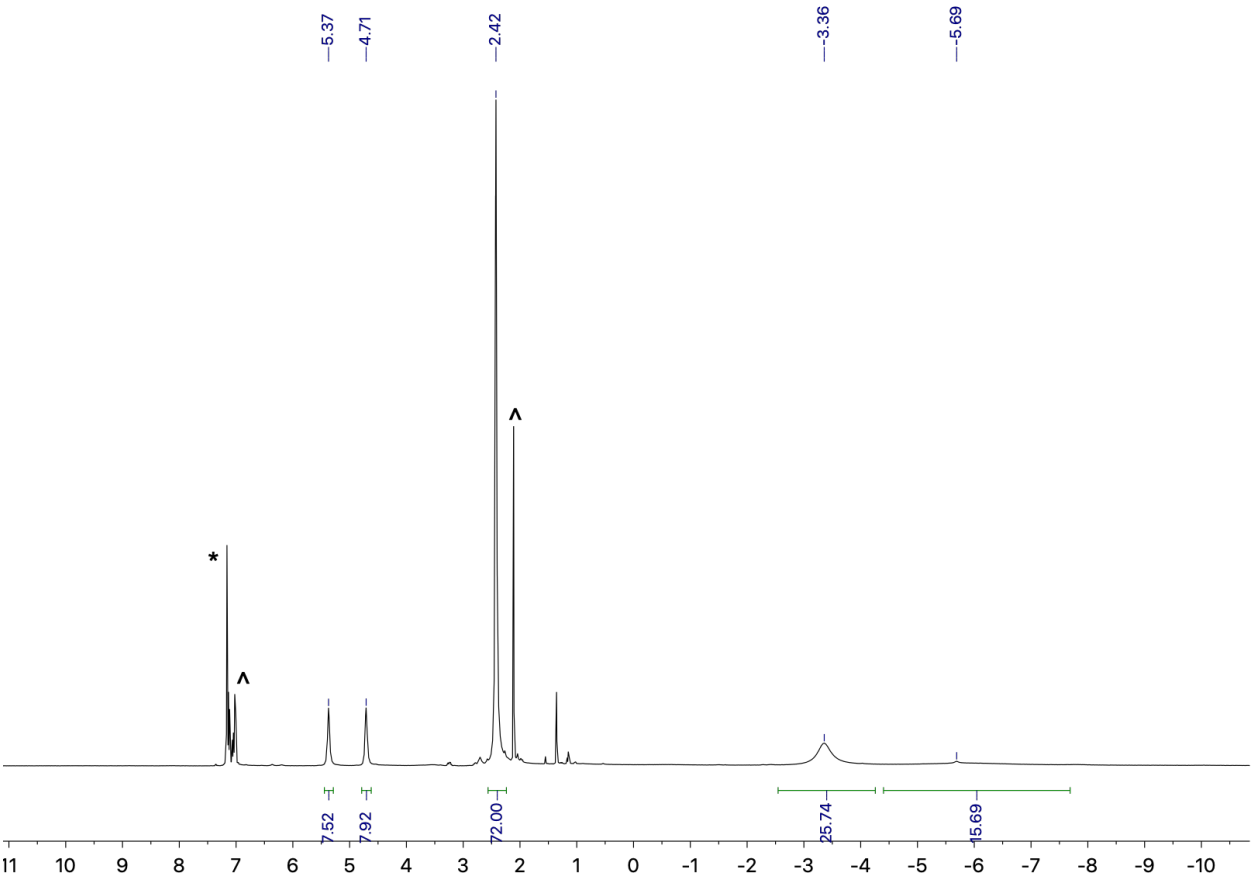


Figure S11. ^{1}H NMR of reaction products of the reaction of **1-Pr(NP*)** and excess AgI in toluene at -35 °C for one hour. The blue solution was then warmed to room temperature (blue color of solution fades) and toluene evacuated. NMR was taken of the residual product. Peak of C_6D_5H is noted as *. Peaks of residual toluene are denoted as ^. The labelled and integrated shifts are that of **1-Pr(NP*)**.

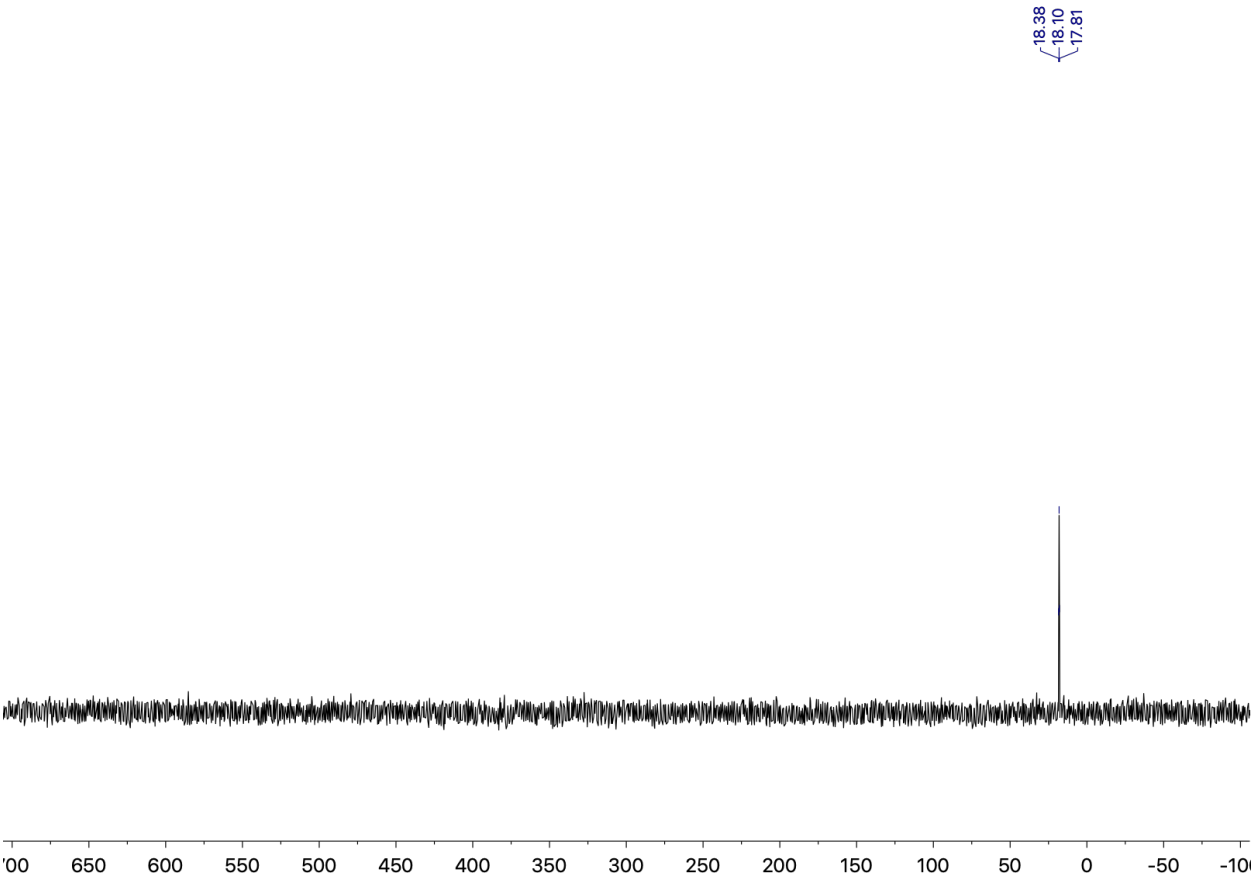


Figure S12. $^{31}P\{^{1}H\}$ NMR of reaction products of the reaction of **1-Pr(NP*)** and excess AgI in toluene at 25 °C for one hour. No darkening of the solution was observed. After one hour, the toluene was evacuated. NMR was taken of the residual product. Only **Ag(NP*)** is observed.

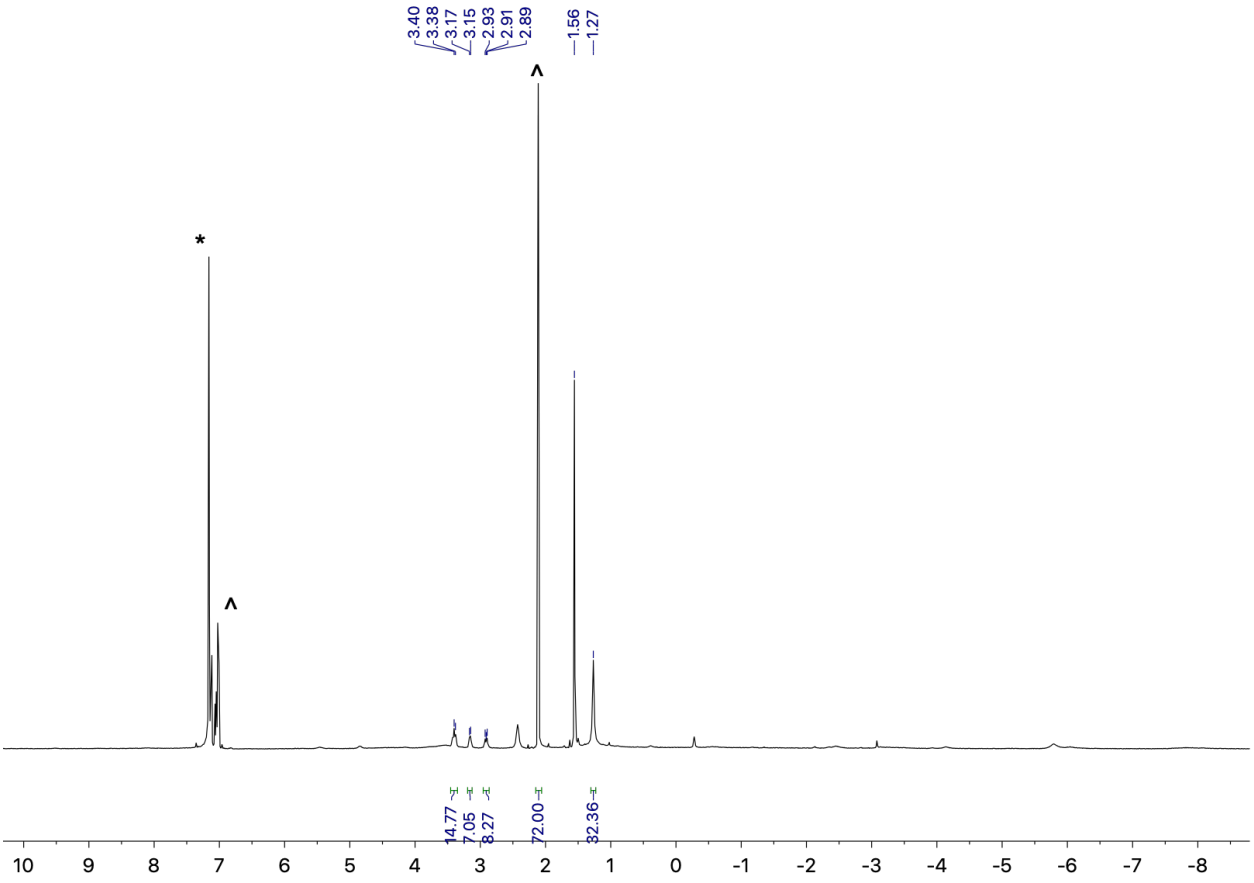


Figure S13. ^{1}H NMR of reaction products of the reaction of **1-Pr(NP*)** and excess AgI in toluene at 25 °C for one hour. No darkening of the solution was observed. After one hour, the toluene was evacuated. NMR was taken of the residual product. Peak of C_6D_5H is noted as *. Peaks of residual toluene are denoted as ^. The labelled and integrated peaks are those of **Ag(NP*)**.

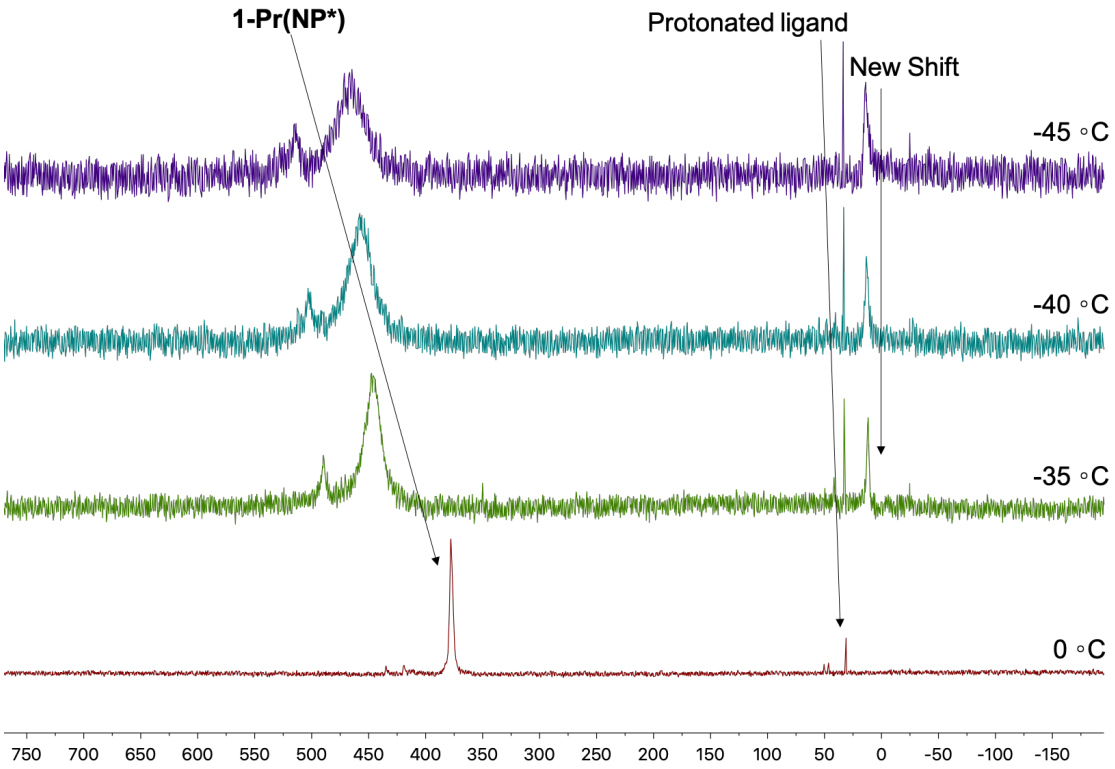


Figure S14. Variable temperature $^{31}P\{^{1}H\}$ NMR of reaction products of the reaction of **1-Pr(NP*)** and excess AgI in d_8-toluene at -35 °C for one hour.

Crystallographic Analyses

Crystals suitable for X-ray diffraction were covered in paratone oil in a glove box and transferred to the diffractometer in a 20 mL capped vial. Crystals were mounted on a loop with paratone oil on a Bruker D8 VENTURE diffractometer. The crystals were cooled and kept at T = 100(2) K during data collections. The structures were solved with the ShelXT structure solution program using the Intrinsic Phasing solution method and by using Olex2 as the graphical interface.[5-6] The model was refined with version 2014/7 of XL using Least Squares minimization.[7]

Table S1. Crystallographic Data

	1-Pr(NP*)	***1-Nd(NP*)***	***1-Dy(NP*)***
Empirical Formula	$C_{56}H_{128}KN_{16}P_4Pr$	$C_{64}H_{148}KN_{16}P_4NdO_2$	$C_{60}H_{138}KN_{16}OP_4Dy$
Formula Weight	1329.63	1481.20	1425.34
Temperature (K)	100(2)	100(1)	130(2)
Crystal System	triclinic	triclinic	monoclinic
Space Group	P-1	P1	*C*2/c
a/Å	13.0693(16)	13.798(3)	22.4405(10)
b/Å	13.9895(17)	13.807(3)	15.8568(7)
c/Å	23.626(3)	24.382(4)	25.4452(16)
α/°	75.191(4)	96.467(7)	90
β/°	81.487(4)	104.784(7)	114.536(2)
γ/°	65.497(4)	110.524(7)	90
Volume/Å3	3795.7(8)	4100.3(14)	8236.7(7)
Z	2	2	4
Z'	1	2	0.5
ρ(g/cm3)	1.163	1.200	1.079
μ(mm-1)	0.823	0.810	1.079
F(000)	1428.0	-	-
Crystal Size/mm3	0.41 x 0.24 x 0.10	0.41 x 0.25 x 0.21	0.40 x 0.29 x 0.28
Radiation	MoKα (λ=0.71073)	MoKα (λ=0.71073)	MoKα (λ=0.71073)
2θ range for data collection(°)	4.464 to 61.15	2.410 to 27.585	2.037 to 36.349
Index Ranges	*-18 ≤ h ≤ 18, -19 ≤ k ≤ 19, -33 ≤ l ≤ 33	*-17 ≤ h ≤ 17, -17 ≤ k ≤ 17, -30 ≤ l ≤ 31	*-37 ≤ h ≤ 37, -26 ≤ k ≤ 26, -37 ≤ l ≤ 42
Reflections Collected	81875	88316	167230
Independent Reflections	23153 [R_{int} = 0.0677, R_{sigma} = 0.0704]	32769 [R_{int} = 0.036, R_{sigma} = 0.0488]	19958 [R_{int} = 0.0486, R_{sigma} = 0.0277]
Data/Restraints/Parameters	23153/2032/1043	32769/1268/1660	19958/88/446
Goodness-of-Fit on F2	1.059	1.045	1.099
Final R Indexes [I>=2σ (I)]	R_1=0.0555, wR_2=0.1224	R_1=0.0363, wR_2=0.0786	R_1=0.0401, wR_2=0.1002
Final R Indexes [all data]	R_1=0.0658, wR_2=0.1271	R_1=0.0383, wR_2=0.0801	R_1=0.0438, wR_2=0.1019
Largest Diff. Peak/Hole/ (e Å3)	1.54/-1.36	1.377/-1.018	2.462/-1.519
Completeness to 2θ	99.9	99.9	99.8

Table S2. Important bond lengths and angles for **1-Pr(NP*)**, **1-Nd(NP*)**, and **1-Dy(NP*)**. Metrics are reported for both molecules in the asymmetric unit for **1-Nd(NP*)**.

	Ln-N K capped (Å)	*Ln-N terminal (Å)*	*N_{imido}-P average (Å)*	*Ln-N-P K capped (º)*	*Ln-N-P terminal (º)*	*N-Ln-N average (º)*
1-Pr(NP*)	2.348(5)	2.299(5)	1.533(5)	167.7(4)	165.3(3)	109.2(2)
1-Nd(NP*) 1	2.344(9)	2.286(9)	1.527(9),1.557(8)	162.5(5)	169.4(6)	109.4(3)
1-Nd(NP*) 2	2.33(1)	2.291(9)	1.52(1)	165.4(6)	172.1(6)	109.3(3)
1-Dy(NP*)	2.260(2)	2.222(2)	1.525(2)	167.7(1)	168.3(1)	109.4(7)

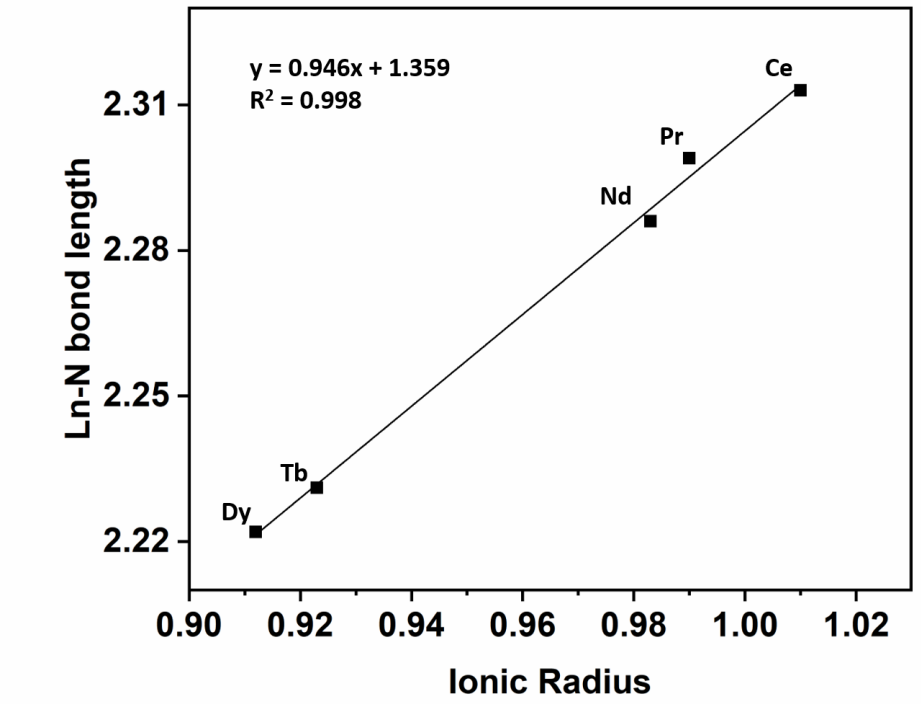


Table S15. Ln-N bond lengths comparison for terminal ligands for **1-Ln(NP*)** where Ln = Ce,[8] Pr, Nd, Tb,[2] and Dy. The ionic radius used is for 6-coordinate Ln ions.

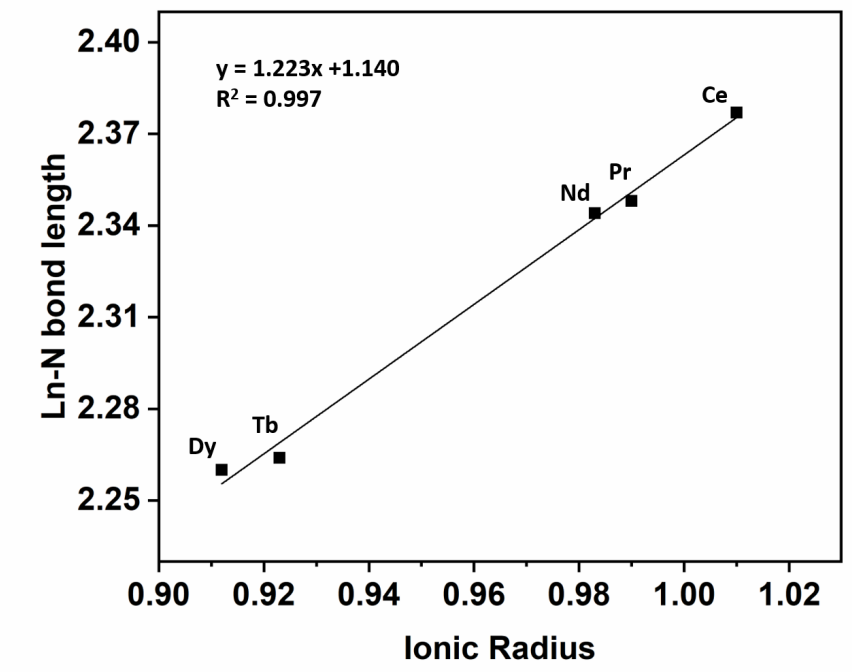


Table S16. Ln-N bond lengths comparison for potassium capped ligands for **1-Ln(NP*)** where Ln = Ce,[8] Pr, Nd, Tb,[2] and Dy. The ionic radius used is for 6-coordinate Ln ions.

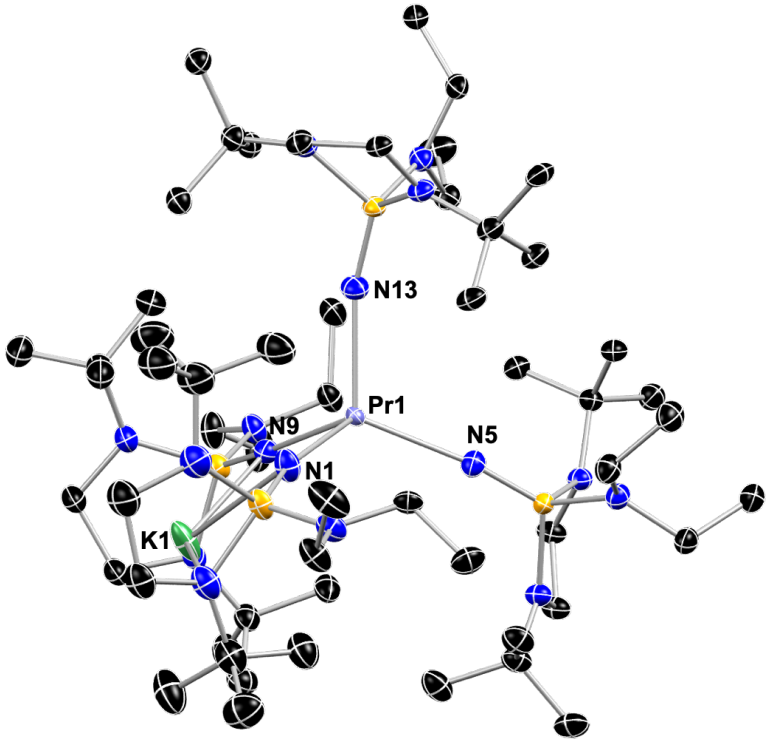


Figure S17. Molecular structure of **1-Pr(NP*)** at with thermal ellipsoids shown at 50% probability. H atoms are omitted for clarity.

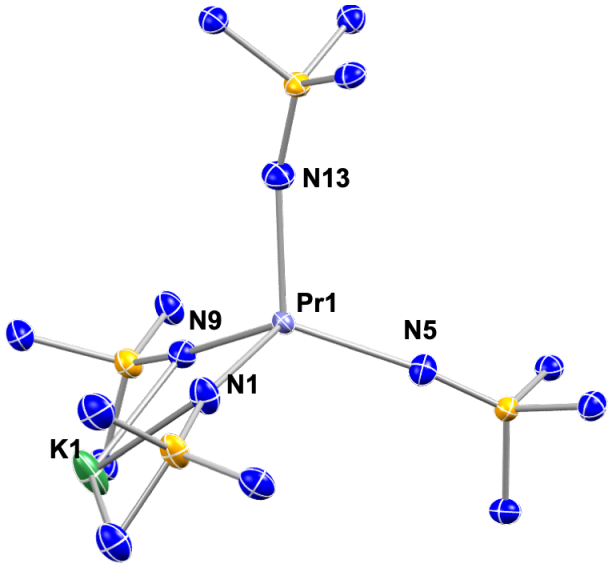


Figure S18. Molecular structure of **1-Pr(NP*)** at with thermal ellipsoids shown at 50% probability. H and C atoms are omitted for clarity.

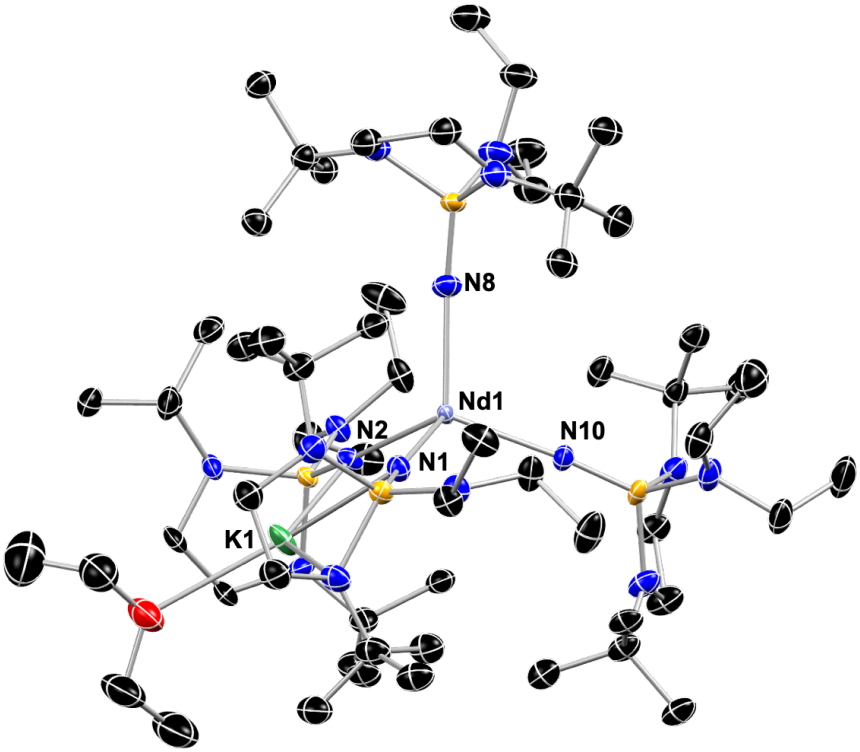


Figure S19. Molecular structure of **1-Nd(NP*)** at with thermal ellipsoids shown at 50% probability. H atoms are omitted for clarity.

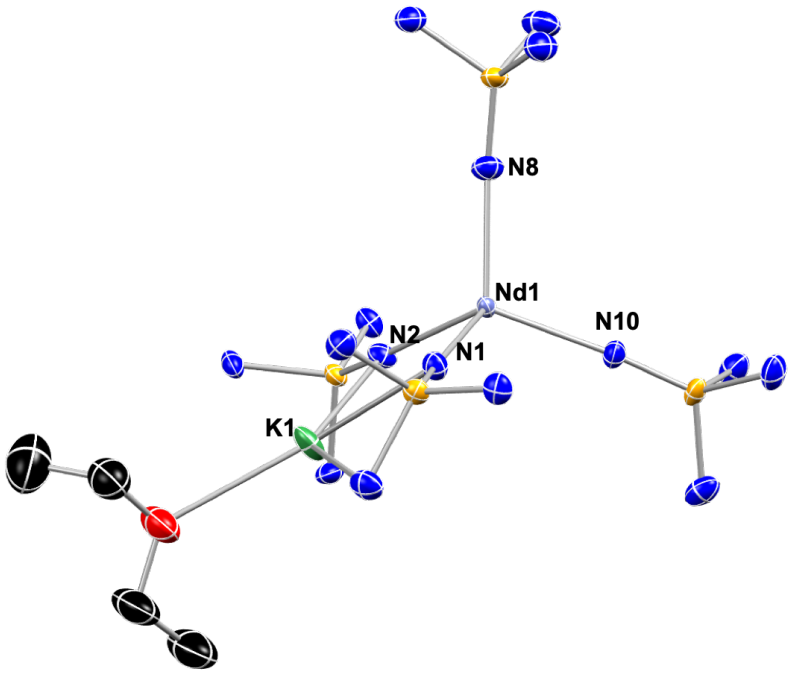


Figure S20. Molecular structure of **1-Nd(NP*)** at with thermal ellipsoids shown at 50% probability. H and C atoms are omitted for clarity.

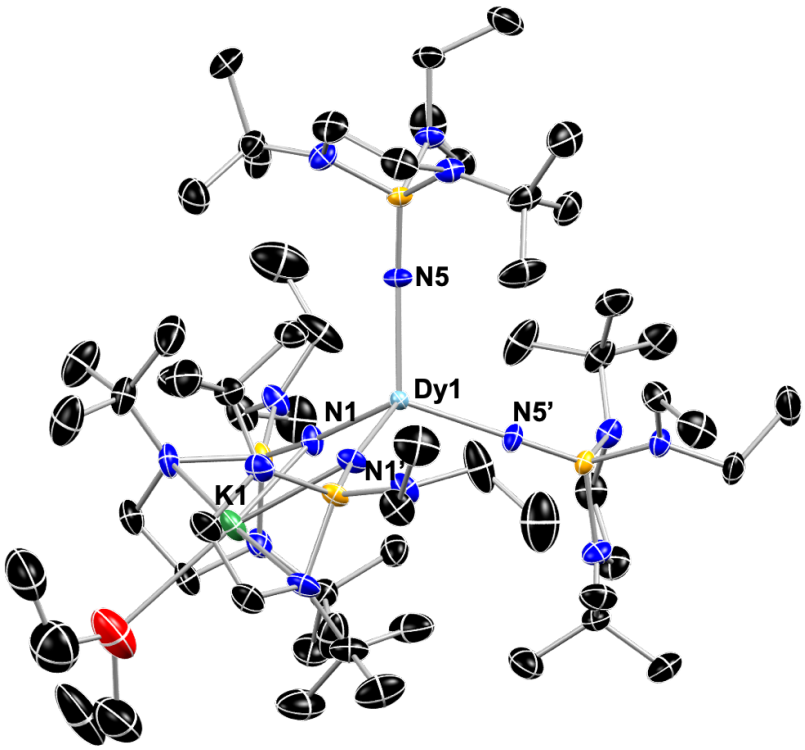


Figure S21. Molecular structure of **1-Dy(NP*)** at with thermal ellipsoids shown at 50% probability. H atoms are omitted for clarity.

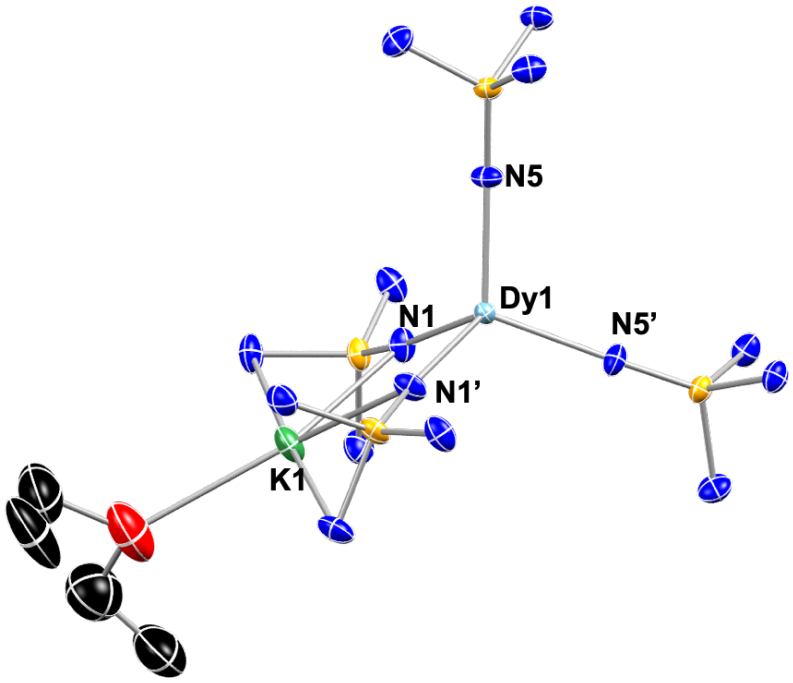


Figure S22. Molecular structure of **1-Dy(NP*)** at with thermal ellipsoids shown at 50% probability. H and C atoms are omitted for clarity.

Table S3. Bond Lengths in Å for **1-Pr(NP*)**.

Atom	Atom	Length/Å
Pr1	N1	2.362(3)
Pr1	N5	2.304(2)
Pr1	N9	2.335(3)
Pr1	N13	2.293(2)
P1	N1	1.532(3)
P1	N2	1.705(3)
P1	N3	1.711(3)
P1	N4	1.680(3)
P2	N5	1.531(2)
P2	N6	1.694(2)
P2	N7	1.719(2)
P2	N8	1.687(2)
P3	N9	1.535(3)
P3	N10	1.696(3)
P3	N11	1.710(3)
P3	N12	1.674(3)
P4	N13	1.531(3)
P4	N14	1.711(3)
P4	N15	1.703(3)
P4	N16	1.684(3)
N2	C1	1.441(4)
N2	C3	1.492(4)
N3	C2	1.456(4)
N3	C7	1.475(4)
N4	C11	1.459(3)
N4	C13	1.470(3)
N6	C15	1.439(3)
N6	C17	1.479(3)
N7	C16	1.466(3)
N7	C21	1.481(3)
N8	C25	1.459(3)
N8	C27	1.467(3)
N10	C29	1.425(4)
N10	C31	1.482(4)
N11	C30	1.439(4)
N11	C35	1.477(4)
N12	C39	1.457(3)
N12	C41	1.464(3)
N14	C43	1.447(4)
N14	C45	1.491(4)
N15	C44	1.447(4)
N15	C49	1.474(4)
N16	C53	1.459(3)
N16	C55	1.466(3)
C1	C2	1.505(4)
C3	C6	1.535(4)
C3	C4	1.522(4)
C3	C5	1.530(4)
C7	C8	1.527(4)
C7	C9	1.554(4)
C7	C10	1.524(4)
C11	C12	1.521(4)

Atom	Atom	Length/Å
C13	C14	1.505(4)
C15	C16	1.510(4)
C17	C18	1.523(4)
C17	C19	1.535(4)
C17	C20	1.536(4)
C21	C22	1.528(4)
C21	C23	1.545(4)
C21	C24	1.524(4)
C25	C26	1.518(4)
C27	C28	1.507(4)
C29	C30	1.495(4)
C31	C32	1.523(4)
C31	C33	1.534(4)
C31	C34	1.536(4)
C35	C36	1.524(4)
C35	C37	1.551(4)
C35	C38	1.525(4)
C39	C40	1.517(4)
C41	C42	1.501(4)
C43	C44	1.509(4)
C45	C46	1.523(4)
C45	C47	1.529(4)
C45	C48	1.537(4)
C49	C50	1.528(4)
C49	C51	1.548(4)
C49	C52	1.526(4)
C53	C54	1.521(4)
C55	C56	1.502(4)

Table S4. Bond Angles in º for **1-Pr(NP*)**.

Atom	Atom	Atom	Angle/˚
N5	Pr1	N1	118.33(16)
N5	Pr1	N9	113.1(2)
N9	Pr1	N1	95.1(2)
N13	Pr1	N1	107.7(2)
N13	Pr1	N5	112.4(2)
N13	Pr1	N9	108.6(3)
P1	N1	Pr1	166.9(3)
P2	N5	Pr1	167.75(18)
P3	N9	Pr1	168.5(4)
P4	N13	Pr1	162.9(4)
N1	P1	N2	119.8(2)
N1	P1	N3	117.7(2)
N1	P1	N4	113.7(2)
N2	P1	N3	91.56(16)
N4	P1	N2	104.9(2)
N4	P1	N3	106.3(2)
N5	P2	N6	120.12(15)
N5	P2	N7	120.34(14)
N5	P2	N8	113.10(14)

Atom	Atom	Atom	Angle/°
N6	P2	N7	90.69(11)
N8	P2	N6	106.19(13)
N8	P2	N7	103.16(13)
N9	P3	N10	118.8(2)
N9	P3	N11	118.2(2)
N9	P3	N12	113.6(2)
N10	P3	N11	91.34(15)
N12	P3	N10	106.9(2)
N12	P3	N11	105.2(2)
N13	P4	N14	120.4(2)
N13	P4	N15	119.6(2)
N13	P4	N16	113.4(2)
N15	P4	N14	90.96(15)
N16	P4	N14	103.4(2)
N16	P4	N15	105.9(2)
C1	N2	P1	112.2(3)
C1	N2	C3	117.2(3)
C3	N2	P1	122.4(2)
C2	N3	P1	112.5(2)
C2	N3	C7	117.6(3)
C7	N3	P1	126.0(3)
C11	N4	P1	121.1(3)
C11	N4	C13	116.2(3)
C13	N4	P1	120.5(3)
C15	N6	P2	114.15(18)
C15	N6	C17	118.6(2)
C17	N6	P2	127.21(19)
C16	N7	P2	108.48(18)
C16	N7	C21	116.6(2)
C21	N7	P2	123.37(18)
C25	N8	P2	120.15(19)
C25	N8	C27	116.2(2)
C27	N8	P2	120.4(2)
C29	N10	P3	114.3(2)
C29	N10	C31	120.1(3)
C31	N10	P3	125.4(2)
C30	N11	P3	114.2(2)
C30	N11	C35	119.6(3)
C35	N11	P3	124.0(3)
C39	N12	P3	121.4(3)
C39	N12	C41	116.8(3)
C41	N12	P3	121.7(3)
C43	N14	P4	109.8(2)
C43	N14	C45	117.8(3)
C45	N14	P4	121.6(2)
C44	N15	P4	113.8(2)
C44	N15	C49	119.4(3)
C49	N15	P4	125.7(2)
C53	N16	P4	120.7(3)
C53	N16	C55	116.3(3)
C55	N16	P4	120.4(3)
N2	C1	C2	105.8(3)
N2	C3	C6	109.5(3)
N2	C3	C4	110.7(3)

Atom	Atom	Atom	Angle/°
N2	C3	C5	108.9(3)
C4	C3	C6	109.3(3)
C4	C3	C5	109.0(3)
C5	C3	C6	109.4(3)
N3	C2	C1	105.7(3)
N3	C7	C8	110.2(3)
N3	C7	C9	110.0(3)
N3	C7	C10	111.4(3)
C8	C7	C9	108.2(3)
C10	C7	C8	109.4(3)
C10	C7	C9	107.7(3)
N4	C11	C12	114.0(4)
N4	C13	C14	115.9(4)
N6	C15	C16	106.2(2)
N6	C17	C18	111.1(2)
N6	C17	C19	109.2(2)
N6	C17	C20	109.7(3)
C18	C17	C19	108.5(3)
C18	C17	C20	109.3(3)
C19	C17	C20	109.0(3)
N7	C16	C15	104.1(2)
N7	C21	C22	109.4(2)
N7	C21	C23	110.6(2)
N7	C21	C24	110.8(2)
C22	C21	C23	109.3(2)
C24	C21	C22	108.9(2)
C24	C21	C23	107.8(2)
N8	C25	C26	114.2(3)
N8	C27	C28	116.3(3)
N10	C29	C30	108.7(3)
N10	C31	C32	110.8(3)
N10	C31	C33	109.2(3)
N10	C31	C34	110.0(3)
C32	C31	C33	108.7(3)
C32	C31	C34	109.0(3)
C33	C31	C34	109.1(3)
N11	C30	C29	108.3(3)
N11	C35	C36	110.0(3)
N11	C35	C37	109.8(3)
N11	C35	C38	110.5(3)
C36	C35	C37	109.2(3)
C36	C35	C38	109.4(3)
C38	C35	C37	107.9(3)
N12	C39	C40	114.6(4)
N12	C41	C42	115.6(4)
N14	C43	C44	105.8(3)
N14	C45	C46	110.7(3)
N14	C45	C47	109.3(3)
N14	C45	C48	109.4(3)
C46	C45	C47	108.8(3)
C46	C45	C48	109.1(3)
C47	C45	C48	109.4(3)
N15	C44	C43	106.7(3)
N15	C49	C50	110.1(3)

Atom	Atom	Atom	Angle/°
N15	C49	C51	110.3(3)
N15	C49	C52	110.3(3)
C50	C49	C51	109.3(3)
C52	C49	C50	108.7(3)
C52	C49	C51	108.2(3)
N16	C53	C54	114.0(3)
N16	C55	C56	116.7(4)

Table S5. Bond Lengths in Å for **1-Nd(NP*)**.

Atom	Atom	Length/Å
Nd1	N1	2.347(9)
Nd1	N2	2.340(8)
Nd1	N8	2.284(9)
Nd1	N10	2.288(9)
P1	N1	1.527(9)
P1	N3	1.695(9)
P1	N4	1.716(8)
P1	N5	1.744(8)
P1	K1	3.382(4)
P2	N2	1.557(8)
P2	N6	1.712(7)
P2	N7	1.684(7)
P2	N12	1.666(8)
P2	K1	3.555(4)
P3	N8	1.532(9)
P3	N9	1.703(8)
P3	N30	1.718(9)
P3	N35	1.690(8)
P4	N10	1.538(10)
P4	N11	1.677(9)
P4	N46	1.698(8)
P4	N51	1.678(8)
N1	K1	2.770(8)
N2	K1	2.762(9)
N3	C13	1.444(12)
N3	C3	1.440(12)
N4	C1	1.430(11)
N4	C8	1.486(11)
N5	C2	1.456(12)
N5	C121	1.469(12)
N5	K1	3.133(8)
N6	C18	1.455(9)
N6	C23	1.485(10)
N7	C19	1.463(10)
N7	C20	1.464(11)
N9	C27	1.461(12)
N9	C28	1.467(13)
N11	C41	1.503(11)
N11	C44	1.440(12)
N12	C4	1.449(10)

Atom	Atom	Length/Å
N12	C113	1.476(10)
C1	C2	1.487(13)
C4	C114	1.520(14)
C5	C121	1.563(13)
C6	C121	1.519(12)
C7	C121	1.514(13)
C8	C9	1.538(12)
C8	C10	1.525(12)
C8	C11	1.525(12)
C12	C41	1.546(12)
C13	C14	1.553(11)
C3	C16	1.517(13)
C18	C19	1.539(13)
C20	C21	1.558(12)
C20	C22	1.538(11)
C20	C37	1.537(11)
C23	C24	1.537(10)
C23	C25	1.536(11)
C23	C26	1.545(12)
C26	K1	3.457(9)
C27	C109	1.515(15)
C27	C119	1.521(13)
C27	C120	1.534(13)
C28	C29	1.518(13)
C29	N30	1.451(12)
N30	C31	1.509(10)
C31	C32	1.536(11)
C31	C33	1.522(12)
C31	C34	1.532(12)
N35	C36	1.432(12)
N35	C39	1.454(11)
C36	C38	1.461(14)
C39	C40	1.501(13)
C41	C42	1.513(12)
C41	C43	1.531(11)
C44	C45	1.503(12)
C45	N46	1.431(12)
N46	C47	1.498(11)
C47	C48	1.517(12)
C47	C49	1.562(12)
C47	C50	1.523(11)
N51	C52	1.476(11)
N51	C53	1.456(13)
C52	C115	1.562(13)
C53	C118	1.491(15)
C112	C113	1.541(13)
Nd2	N13	2.312(9)
Nd2	N19	2.286(9)
Nd2	N23	2.295(9)
Nd2	N27	2.346(10)
P5	N13	1.538(9)
P5	N14	1.696(9)
P5	N16	1.723(9)
P5	N18	1.679(9)

Atom	Atom	Length/Å
P5	K2	3.363(4)
P6	N19	1.553(9)
P6	N20	1.684(10)
P6	N21	1.721(9)
P6	N22	1.686(9)
P7	N23	1.518(9)
P7	N24	1.709(8)
P7	N25	1.692(9)
P7	N26	1.698(8)
P8	N27	1.510(10)
P8	N28	1.707(9)
P8	N29	1.692(8)
P8	N17	1.737(9)
P8	K2	3.384(4)
N13	K2	2.781(10)
N14	C54	1.462(12)
N14	C57	1.490(13)
C15	C54	1.531(14)
N16	C58	1.478(13)
N16	C59	1.513(13)
N16	K2	3.167(8)
N18	C62	1.500(12)
N18	C64	1.424(14)
N20	C66	1.442(12)
N20	C72	1.481(12)
N21	C67	1.471(12)
N21	C68	1.470(13)
N22	C76	1.456(12)
N22	C78	1.446(12)
N24	C80	1.462(12)
N24	C86	1.483(13)
N25	C81	1.449(12)
N25	C82	1.479(12)
N26	C90	1.447(11)
N26	C92	1.444(11)
N27	K2	2.804(10)
N28	C94	1.499(13)
N28	C98	1.456(13)
N29	C99	1.456(13)
N29	C101	1.459(13)
N17	C103	1.482(12)
N17	C111	1.453(12)
N17	K2	3.167(8)
C17	C59	1.545(14)
C54	C55	1.523(14)
C54	C56	1.548(16)
C57	C58	1.534(14)
C59	C60	1.507(13)
C59	C61	1.529(14)
C62	C63	1.517(16)
C64	C65	1.557(13)
C66	C67	1.470(13)
C68	C69	1.504(14)
C68	C70	1.540(14)

Atom	Atom	Length/Å
C68	C71	1.499(14)
C72	C73	1.529(14)
C72	C74	1.534(13)
C72	C75	1.523(12)
C76	C77	1.543(14)
C78	C79	1.529(12)
C80	C81	1.526(13)
C82	C83	1.547(13)
C82	C84	1.536(11)
C82	C85	1.518(12)
C86	C87	1.542(13)
C86	C88	1.550(12)
C86	C89	1.598(14)
C90	C91	1.507(12)
C92	C93	1.511(13)
C94	C95	1.500(14)
C94	C96	1.536(14)
C94	C97	1.555(14)
C98	C111	1.465(13)
C99	C100	1.543(12)
C101	C102	1.511(15)
C103	C104	1.480(13)
C103	C105	1.554(12)
C103	C106	1.567(12)
K1	O1S_4	2.811(5)
K2	O1S_1	2.937(9)
O1S_1	C2S_1	1.4213(12)
O1S_1	C4S_1	1.4210(12)
C2S_1	C3S_1	1.5206(13)
C4S_1	C5S_1	1.5197(13)
O1S_2	C2S_2	1.4199(12)
O1S_2	C4S_2	1.4199(12)
C2S_2	C3S_2	1.5206(12)
C4S_2	C5S_2	1.5205(12)
O1S_3	C2S_3	1.4201(12)
O1S_3	C4S_3	1.4204(12)
C2S_3	C3S_3	1.5195(12)
C4S_3	C5S_3	1.5198(12)
O1S_4	C2S_4	1.4202(12)
O1S_4	C4S_4	1.4207(12)
C2S_4	C3S_4	1.5198(12)
C4S_4	C5S_4	1.5197(12)

Table S6. Bond Angles in º for **1-Nd(NP*)**.

Atom	Atom	Atom	Angle/˚
N2	Nd1	N1	95.2(2)
N8	Nd1	N1	115.2(3)
N8	Nd1	N2	110.1(4)
N8	Nd1	N10	109.27(19)
N10	Nd1	N1	110.4(3)
N10	Nd1	N2	116.1(3)
N1	P1	N3	113.7(5)

Atom	Atom	Atom	Angle/°
N1	P1	N4	121.4(5)
N1	P1	N5	114.7(4)
N1	P1	K1	53.8(3)
N3	P1	N4	103.5(4)
N3	P1	N5	110.1(4)
N3	P1	K1	156.5(3)
N4	P1	N5	91.0(4)
N4	P1	K1	99.9(3)
N5	P1	K1	66.7(2)
N2	P2	N6	121.1(4)
N2	P2	N7	118.5(5)
N2	P2	N12	113.8(4)
N2	P2	K1	47.8(3)
N6	P2	K1	88.2(2)
N7	P2	N6	91.2(3)
N7	P2	K1	88.3(3)
N12	P2	N6	102.8(4)
N12	P2	N7	106.4(4)
N12	P2	K1	161.3(3)
N8	P3	N9	120.5(5)
N8	P3	N30	121.7(5)
N8	P3	N35	112.5(5)
N9	P3	N30	91.4(4)
N35	P3	N9	104.9(4)
N35	P3	N30	102.5(4)
N10	P4	N11	120.8(5)
N10	P4	N46	120.4(5)
N10	P4	N51	114.0(5)
N11	P4	N46	89.8(4)
N11	P4	N51	105.3(4)
N51	P4	N46	102.7(4)
Nd1	N1	K1	93.4(3)
P1	N1	Nd1	166.7(5)
P1	N1	K1	99.8(4)
Nd1	N2	K1	93.7(3)
P2	N2	Nd1	158.2(5)
P2	N2	K1	107.5(4)
C13	N3	P1	121.8(6)
C3	N3	P1	121.0(7)
C3	N3	C13	117.2(8)
C1	N4	P1	112.3(6)
C1	N4	C8	116.8(8)
C8	N4	P1	122.9(6)
P1	N5	K1	82.5(3)
C2	N5	P1	111.1(6)
C2	N5	C121	116.7(7)
C2	N5	K1	112.5(6)
C121	N5	P1	123.9(6)
C121	N5	K1	103.9(5)
C18	N6	P2	111.1(5)
C18	N6	C23	115.5(6)
C23	N6	P2	123.8(5)
C19	N7	P2	114.9(5)
C19	N7	C20	118.1(6)

Atom	Atom	Atom	Angle/°
C20	N7	P2	127.0(5)
P3	N8	Nd1	166.3(6)
C27	N9	P3	126.9(7)
C27	N9	C28	120.2(7)
C28	N9	P3	112.3(6)
P4	N10	Nd1	172.5(6)
C41	N11	P4	126.5(6)
C44	N11	P4	114.7(6)
C44	N11	C41	118.5(8)
C4	N12	P2	122.7(7)
C4	N12	C113	115.8(7)
C113	N12	P2	121.4(5)
N4	C1	C2	106.9(8)
N5	C2	C1	105.9(7)
N12	C4	C114	114.9(8)
N4	C8	C9	110.6(7)
N4	C8	C10	109.9(7)
N4	C8	C11	109.0(7)
C10	C8	C9	109.1(7)
C11	C8	C9	110.2(8)
C11	C8	C10	108.0(7)
N3	C13	C14	113.0(7)
N3	C3	C16	115.9(9)
N6	C18	C19	104.4(6)
N7	C19	C18	104.3(6)
N7	C20	C21	108.3(7)
N7	C20	C22	111.2(7)
N7	C20	C37	113.0(6)
C22	C20	C21	109.4(7)
C22	C20	C37	107.3(8)
C37	C20	C21	107.6(7)
N6	C23	C24	110.1(6)
N6	C23	C25	108.6(7)
N6	C23	C26	112.9(7)
C24	C23	C26	108.9(7)
C25	C23	C24	107.8(7)
C25	C23	C26	108.4(7)
C23	C26	K1	112.1(5)
N9	C27	C109	110.1(8)
N9	C27	C119	108.9(8)
N9	C27	C120	110.7(8)
C109	C27	C119	109.5(9)
C109	C27	C120	108.4(8)
C119	C27	C120	109.3(8)
N9	C28	C29	107.4(7)
N30	C29	C28	104.1(8)
C29	N30	P3	109.7(6)
C29	N30	C31	115.4(8)
C31	N30	P3	121.4(6)
N30	C31	C32	111.6(6)
N30	C31	C33	108.6(7)
N30	C31	C34	109.2(7)
C33	C31	C32	109.4(7)
C33	C31	C34	107.8(7)

Atom	Atom	Atom	Angle/°
C34	C31	C32	110.1(7)
C36	N35	P3	121.6(6)
C36	N35	C39	115.0(8)
C39	N35	P3	120.6(7)
N35	C36	C38	116.0(8)
N35	C39	C40	115.3(8)
N11	C41	C12	108.4(6)
N11	C41	C42	109.9(7)
N11	C41	C43	109.9(7)
C42	C41	C12	110.2(7)
C42	C41	C43	109.3(6)
C43	C41	C12	109.0(7)
N11	C44	C45	105.3(8)
N46	C45	C44	104.2(7)
C45	N46	P4	110.0(6)
C45	N46	C47	116.1(7)
C47	N46	P4	122.0(6)
N46	C47	C48	110.3(7)
N46	C47	C49	108.3(7)
N46	C47	C50	110.9(7)
C48	C47	C49	107.6(7)
C48	C47	C50	109.4(7)
C50	C47	C49	110.2(7)
C52	N51	P4	120.1(7)
C53	N51	P4	122.0(6)
C53	N51	C52	114.3(7)
N51	C52	C115	115.8(7)
N51	C53	C118	115.9(9)
N12	C113	C112	113.2(7)
N5	C121	C5	109.4(7)
N5	C121	C6	114.4(7)
N5	C121	C7	108.7(8)
C6	C121	C5	110.2(8)
C7	C121	C5	106.4(8)
C7	C121	C6	107.5(8)
N13	Nd2	N27	93.25(18)
N19	Nd2	N13	112.9(3)
N19	Nd2	N23	112.1(2)
N19	Nd2	N27	112.5(4)
N23	Nd2	N13	111.2(3)
N23	Nd2	N27	113.7(3)
N13	P5	N14	121.5(5)
N13	P5	N16	114.9(5)
N13	P5	N18	114.1(5)
N13	P5	K2	54.9(4)
N14	P5	N16	91.5(5)
N14	P5	K2	95.8(3)
N16	P5	K2	68.5(3)
N18	P5	N14	103.3(4)
N18	P5	N16	109.0(4)
N18	P5	K2	160.8(3)
N19	P6	N20	120.2(5)
N19	P6	N21	120.8(4)
N19	P6	N22	113.6(5)

Atom	Atom	Atom	Angle/°
N20	P6	N21	91.3(4)
N20	P6	N22	103.6(4)
N22	P6	N21	103.8(5)
N23	P7	N24	121.3(5)
N23	P7	N25	121.3(5)
N23	P7	N26	112.4(5)
N25	P7	N24	90.8(4)
N25	P7	N26	104.3(4)
N26	P7	N24	103.4(4)
N27	P8	N28	121.6(5)
N27	P8	N29	113.2(5)
N27	P8	N17	115.1(5)
N27	P8	K2	54.9(4)
N28	P8	N17	91.1(4)
N28	P8	K2	97.1(3)
N29	P8	N28	103.6(4)
N29	P8	N17	109.7(4)
N29	P8	K2	159.3(3)
N17	P8	K2	67.8(2)
Nd2	N13	K2	96.7(3)
P5	N13	Nd2	165.1(6)
P5	N13	K2	98.1(5)
C54	N14	P5	126.1(7)
C54	N14	C57	113.7(9)
C57	N14	P5	114.4(7)
P5	N16	K2	81.1(3)
C58	N16	P5	111.2(7)
C58	N16	C59	114.7(7)
C58	N16	K2	119.7(6)
C59	N16	P5	122.9(7)
C59	N16	K2	103.2(5)
C62	N18	P5	122.8(8)
C64	N18	P5	122.7(6)
C64	N18	C62	114.5(8)
P6	N19	Nd2	170.7(5)
C66	N20	P6	113.9(7)
C66	N20	C72	118.5(8)
C72	N20	P6	126.6(7)
C67	N21	P6	108.9(7)
C68	N21	P6	122.3(6)
C68	N21	C67	116.9(7)
C76	N22	P6	121.9(6)
C78	N22	P6	121.2(7)
C78	N22	C76	116.8(8)
P7	N23	Nd2	173.4(6)
C80	N24	P7	110.3(7)
C80	N24	C86	113.8(7)
C86	N24	P7	122.1(6)
C81	N25	P7	115.4(7)
C81	N25	C82	118.2(8)
C82	N25	P7	126.3(6)
C90	N26	P7	121.6(6)
C92	N26	P7	121.0(6)
C92	N26	C90	117.0(7)

Atom	Atom	Atom	Angle/°
Nd2	N27	K2	95.4(3)
P8	N27	Nd2	165.6(6)
P8	N27	K2	98.9(5)
C94	N28	P8	124.1(7)
C98	N28	P8	112.2(7)
C98	N28	C94	118.2(8)
C99	N29	P8	120.4(6)
C99	N29	C101	117.1(8)
C101	N29	P8	122.5(7)
P8	N17	K2	81.6(3)
C103	N17	P8	125.4(6)
C103	N17	K2	100.5(5)
C111	N17	P8	110.7(6)
C111	N17	C103	115.6(8)
C111	N17	K2	117.6(5)
N14	C54	C15	109.6(9)
N14	C54	C55	109.5(8)
N14	C54	C56	109.9(9)
C15	C54	C56	106.0(9)
C55	C54	C15	110.1(9)
C55	C54	C56	111.8(10)
N14	C57	C58	105.0(9)
N16	C58	C57	104.6(8)
N16	C59	C17	111.4(8)
N16	C59	C61	105.6(9)
C60	C59	N16	112.2(8)
C60	C59	C17	108.8(10)
C60	C59	C61	110.7(8)
C61	C59	C17	108.0(8)
N18	C62	C63	112.9(9)
N18	C64	C65	111.8(9)
N20	C66	C67	108.1(8)
C66	C67	N21	106.2(7)
N21	C68	C69	114.1(9)
N21	C68	C70	108.7(8)
N21	C68	C71	110.3(8)
C69	C68	C70	107.9(8)
C71	C68	C69	107.5(9)
C71	C68	C70	108.2(9)
N20	C72	C73	109.0(7)
N20	C72	C74	109.0(8)
N20	C72	C75	110.4(8)
C73	C72	C74	110.6(8)
C75	C72	C73	110.2(9)
C75	C72	C74	107.5(7)
N22	C76	C77	114.9(8)
N22	C78	C79	113.9(8)
N24	C80	C81	105.3(7)
N25	C81	C80	105.2(8)
N25	C82	C83	109.3(7)
N25	C82	C84	111.2(7)
N25	C82	C85	112.1(7)
C84	C82	C83	108.5(8)
C85	C82	C83	108.0(7)

Atom	Atom	Atom	Angle/°
C85	C82	C84	107.7(7)
N24	C86	C87	108.8(7)
N24	C86	C88	112.0(8)
N24	C86	C89	107.6(7)
C87	C86	C88	111.1(8)
C87	C86	C89	107.8(8)
C88	C86	C89	109.4(8)
N26	C90	C91	112.5(8)
N26	C92	C93	116.0(8)
N28	C94	C95	113.9(9)
N28	C94	C96	111.5(8)
N28	C94	C97	107.0(8)
C95	C94	C96	111.1(9)
C95	C94	C97	108.5(8)
C96	C94	C97	104.2(9)
N28	C98	C111	108.2(8)
N29	C99	C100	114.5(9)
N29	C101	C102	114.8(10)
N17	C103	C105	111.7(7)
N17	C103	C106	109.9(7)
C104	C103	N17	111.4(8)
C104	C103	C105	108.9(8)
C104	C103	C106	109.0(8)
C105	C103	C106	105.8(8)
N17	C111	C98	105.6(8)
P1	K1	Nd1	65.28(6)
P1	K1	P2	128.49(6)
P1	K1	C26	116.61(19)
P2	K1	Nd1	63.33(6)
N1	K1	Nd1	38.87(19)
N1	K1	P1	26.4(2)
N1	K1	P2	102.2(2)
N1	K1	N5	55.3(2)
N1	K1	C26	107.7(3)
N1	K1	O1S_4	143.7(3)
N2	K1	Nd1	38.72(18)
N2	K1	P1	103.81(18)
N2	K1	P2	24.68(18)
N2	K1	N1	77.50(16)
N2	K1	N5	131.4(2)
N2	K1	C26	66.7(3)
N2	K1	O1S_4	136.5(3)
N5	K1	Nd1	93.10(15)
N5	K1	P1	30.76(14)
N5	K1	P2	154.61(16)
N5	K1	C26	134.0(2)
C26	K1	Nd1	88.31(16)
C26	K1	P2	59.06(17)
O1S_4	K1	Nd1	170.92(19)
O1S_4	K1	P1	117.68(19)
O1S_4	K1	P2	112.59(19)
O1S_4	K1	N5	92.1(2)
O1S_4	K1	C26	82.7(2)
P5	K2	Nd2	63.87(6)

Atom	Atom	Atom	Angle/°
P5	K2	P8	127.70(5)
P8	K2	Nd2	63.83(6)
N13	K2	Nd2	36.95(19)
N13	K2	P5	26.9(2)
N13	K2	P8	100.8(2)
N13	K2	N16	54.6(3)
N13	K2	N27	74.64(15)
N13	K2	N17	126.3(3)
N13	K2	O1S_1	138.6(3)
N16	K2	Nd2	89.84(18)
N16	K2	P5	30.41(17)
N16	K2	P8	149.1(2)
N16	K2	N17	178.1(3)
N27	K2	Nd2	37.7(2)
N27	K2	P5	101.6(2)
N27	K2	P8	26.2(2)
N27	K2	N16	125.9(3)
N27	K2	N17	54.3(3)
N27	K2	O1S_1	145.4(3)
N17	K2	Nd2	90.70(17)
N17	K2	P5	150.93(18)
N17	K2	P8	30.52(16)
O1S_1	K2	Nd2	171.6(2)
O1S_1	K2	P5	112.1(2)
O1S_1	K2	P8	119.8(2)
O1S_1	K2	N16	88.6(3)
O1S_1	K2	N17	91.1(3)
C2S_1	O1S_1	K2	125.9(4)
C4S_1	O1S_1	K2	105.8(7)
C4S_1	O1S_1	C2S_1	113.0(2)
O1S_1	C2S_1	C3S_1	108.65(19)
O1S_1	C4S_1	C5S_1	108.88(19)
C4S_2	O1S_2	C2S_2	113.5(2)
O1S_2	C2S_2	C3S_2	108.76(18)
O1S_2	C4S_2	C5S_2	108.71(19)
C2S_3	O1S_3	C4S_3	113.4(2)
O1S_3	C2S_3	C3S_3	108.86(19)
O1S_3	C4S_3	C5S_3	108.89(19)
C2S_4	O1S_4	K1	133.5(4)
C2S_4	O1S_4	C4S_4	113.3(2)
C4S_4	O1S_4	K1	110.1(3)
O1S_4	C2S_4	C3S_4	108.88(18)
O1S_4	C4S_4	C5S_4	108.93(18)

Table S7. Bond Lengths in Å for **1-Dy(NP*)**.

Atom	Atom	Length/Å
C1	C2	1.505(4)
C1	N2	1.451(3)
C2	N3	1.446(3)
C3	C4	1.531(4)
C3	C5	1.519(3)
C3	C6	1.542(4)

Atom	Atom	Length/Å
C3	N2	1.479(3)
C7	C8	1.524(4)
C7	C9	1.519(4)
C7	C10	1.550(4)
C7	N3	1.480(3)
C11	C12	1.520(4)
C11	N4	1.459(3)
C13	C14	1.542(6)
C13	N4	1.455(3)
C15	C16	1.518(4)
C15	N6	1.447(3)
C16	N7	1.462(3)
C17	C19	1.544(4)
C17	N6	1.468(3)
C17	C18	1.527(4)
C17	C20	1.519(4)
C21	C22	1.525(4)
C21	C23	1.546(4)
C21	C24	1.540(4)
C21	N7	1.481(3)
C26	C25	1.525(3)
C27	C28	1.531(4)
C27	N8	1.463(3)
K1	N1[1]	2.8060(19)
K1	N1	2.8060(19)
K1	N3[1]	3.162(2)
K1	O1	2.907(5)
N1	P1	1.5235(16)
N1	Dy1	2.2597(15)
N2	P1	1.708(2)
N3	P1	1.7215(18)
N4	P1	1.6789(19)
N5	P2	1.5259(16)
N5	Dy1	2.2214(15)
N6	P2	1.6922(18)
N7	P2	1.7127(17)
N8	P2	1.6842(17)
N8	C25	1.446(3)
C30	C29	1.519(2)
C29	O1	1.442(8)
C31	C32	1.491(8)
C31	O1	1.436(7)

Table S8. Bond Angles in º for **1-Dy(NP*)**.

Atom	Atom	Atom	Angle/˚
N2	C1	C2	106.5(2)
N3	C2	C1	105.29(19)
C4	C3	C6	109.4(3)

Atom	Atom	Atom	Angle/°
C5	C3	C4	108.9(2)
C5	C3	C6	108.4(2)
N2	C3	C4	108.7(2)
N2	C3	C5	111.0(2)
N2	C3	C6	110.5(2)
C8	C7	C10	105.1(3)
C9	C7	C8	110.4(3)
C9	C7	C10	107.9(2)
N3	C7	C8	111.6(2)
N3	C7	C9	112.6(2)
N3	C7	C10	108.9(3)
N4	C11	C12	114.7(2)
N4	C13	C14	114.3(3)
N6	C15	C16	105.72(19)
N7	C16	C15	104.26(18)
N6	C17	C19	109.9(2)
N6	C17	C18	109.0(2)
N6	C17	C20	111.03(18)
C18	C17	C19	108.9(2)
C20	C17	C19	108.4(2)
C20	C17	C18	109.5(2)
C22	C21	C23	108.6(3)
C22	C21	C24	108.6(2)
C24	C21	C23	110.3(2)
N7	C21	C22	109.94(18)
N7	C21	C23	107.88(19)
N7	C21	C24	111.5(2)
N8	C27	C28	114.4(2)
N1[1]	K1	N1	72.98(6)
N1	K1	N3[1]	122.99(5)
N1[1]	K1	N3[1]	54.34(5)
N1	K1	O1	146.6(2)
N1[1]	K1	O1	139.51(18)
O1	K1	N3[1]	89.9(2)
P1	N1	K1	96.39(8)
P1	N1	Dy1	167.66(11)
Dy1	N1	K1	95.91(6)
C1	N2	C3	116.1(2)
C1	N2	P1	113.14(17)
C3	N2	P1	123.16(14)
C2	N3	C7	115.75(19)
C2	N3	K1	111.52(16)
C2	N3	P1	111.95(17)
C7	N3	K1	105.72(13)
C7	N3	P1	124.66(17)
P1	N3	K1	80.40(7)
C11	N4	P1	122.95(16)
C13	N4	C11	114.6(2)
C13	N4	P1	122.34(16)
P2	N5	Dy1	168.31(11)
C15	N6	C17	117.26(18)
C15	N6	P2	114.43(17)
C17	N6	P2	128.23(15)
C16	N7	C21	116.02(18)

Atom	Atom	Atom	Angle/°
C16	N7	P2	109.59(16)
C21	N7	P2	122.97(14)
C27	N8	P2	120.31(15)
C25	N8	C27	117.39(18)
C25	N8	P2	122.21(14)
N1	P1	N2	121.16(10)
N1	P1	N3	115.30(10)
N1	P1	N4	113.88(10)
N2	P1	N3	91.06(10)
N4	P1	N2	103.47(10)
N4	P1	N3	109.30(10)
N5	P2	N6	120.29(10)
N5	P2	N7	121.46(9)
N5	P2	N8	113.32(9)
N6	P2	N7	90.79(9)
N8	P2	N6	104.29(9)
N8	P2	N7	103.14(9)
N1[1]	Dy1	K1	47.60(5)
N1	Dy1	K1	47.60(5)
N1[1]	Dy1	N1	95.19(9)
N5[1]	Dy1	K1	125.10(5)
N5	Dy1	K1	125.10(5)
N5[1]	Dy1	N1[1]	112.62(7)
N5	Dy1	N1	112.61(7)
N5	Dy1	N1[1]	113.02(6)
N5[1]	Dy1	N1	113.02(6)
N5[1]	Dy1	N5	109.80(9)
N8	C25	C26	113.8(2)
O1	C29	C30	109.2(7)
O1	C31	C32	110.2(7)
C29	O1	K1	111.2(4)
C31	O1	K1	132.8(5)
C31	O1	C29	111.2(5)

Electrochemistry

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

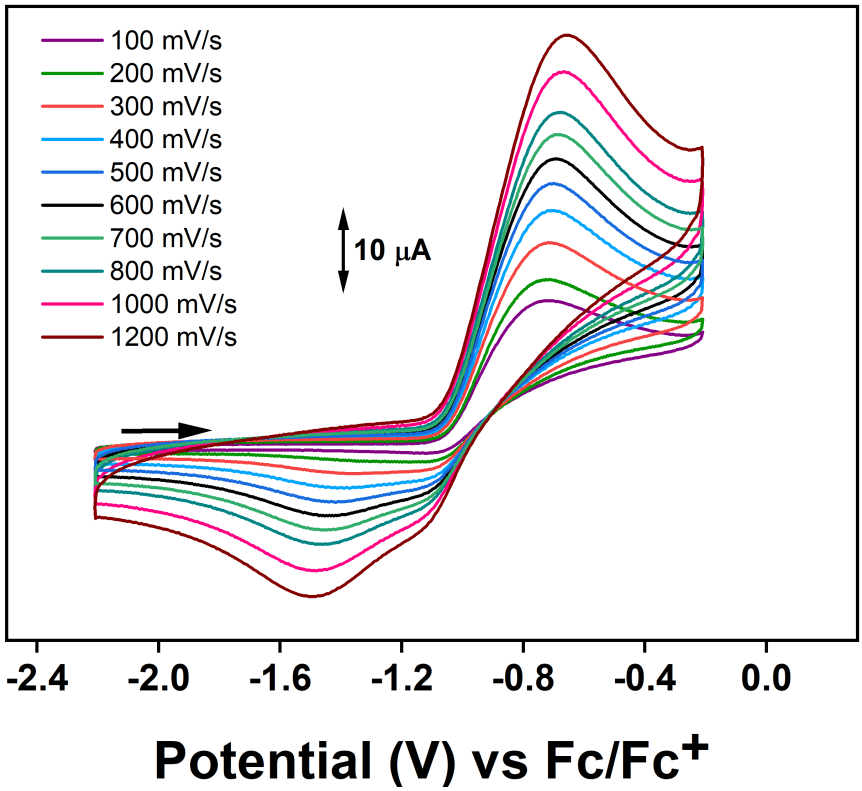


Figure S23. Scan rate dependence of **1-Pr(NP*)** (2.5 mM) vs. Fc/Fc^+ in 0.1 M $[^n(Bu)_4N][PF_6]$ in THF.

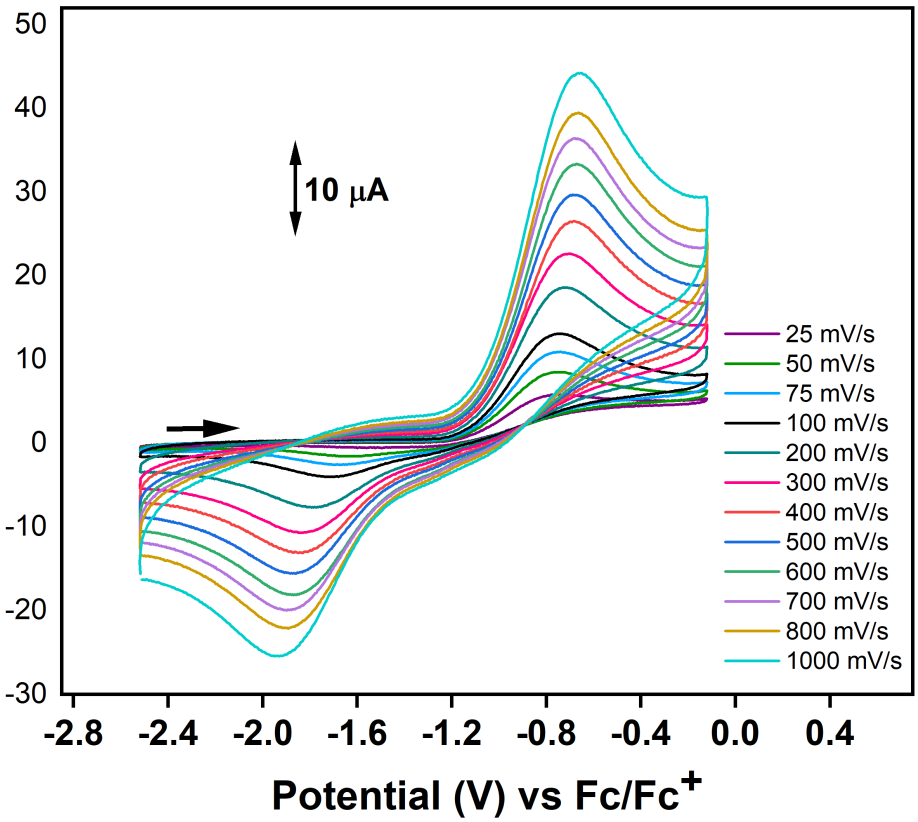


Figure S24. Scan rate dependence of **1-Tb(NP*)** (2.5 mM) vs. Fc/Fc^+ in 0.1 M $[^n(Bu)_4N][PF_6]$ in THF.

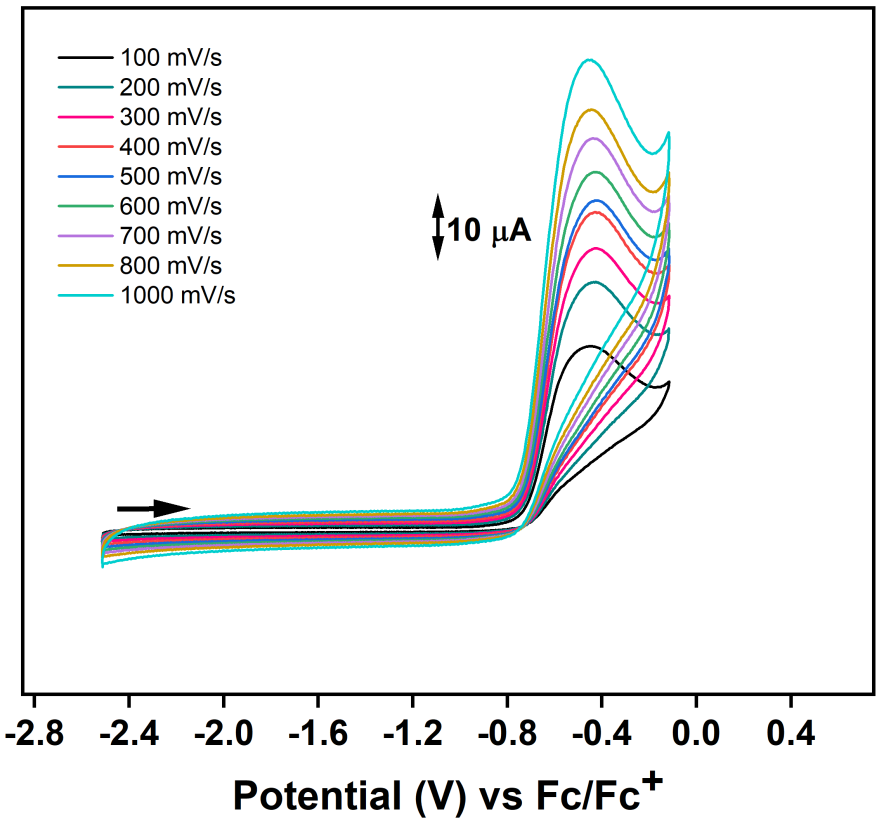


Figure S25. Scan rate dependence of **1-Nd(NP*)** (2.5 mM) vs. Fc/Fc^{+} in 0.1 M $[^{n}(Bu)_4N][PF_6]$ in THF.

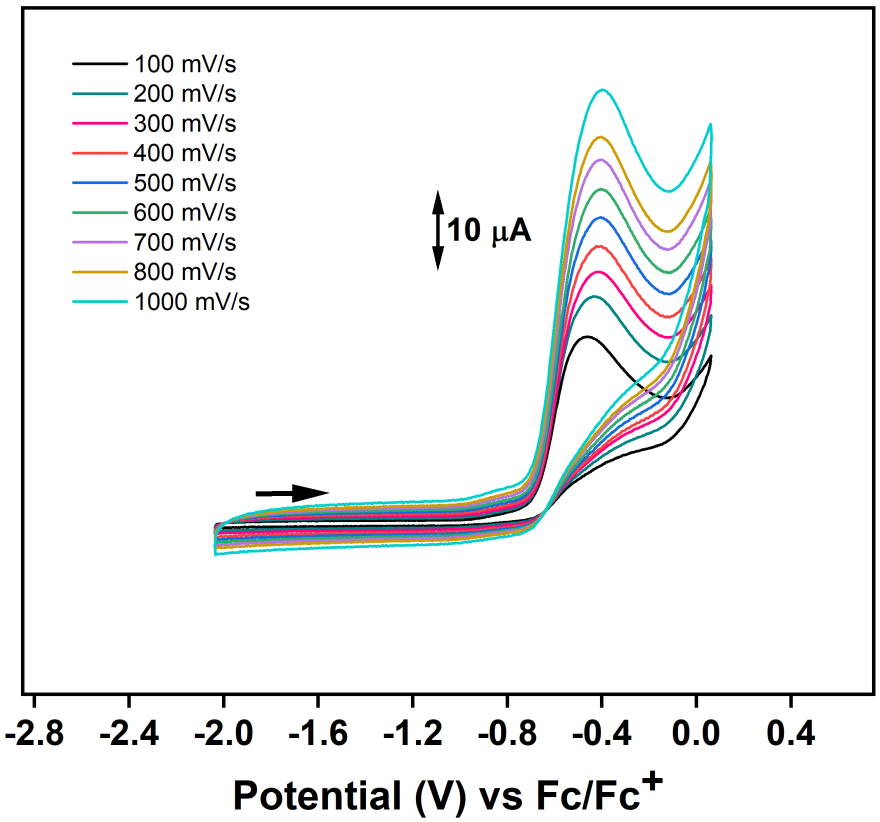


Figure S26. Scan rate dependence of **1-Dy(NP*)** (2.5 mM) vs. Fc/Fc^{+} in 0.1 M $[^{n}(Bu)_4N][PF_6]$ in THF.

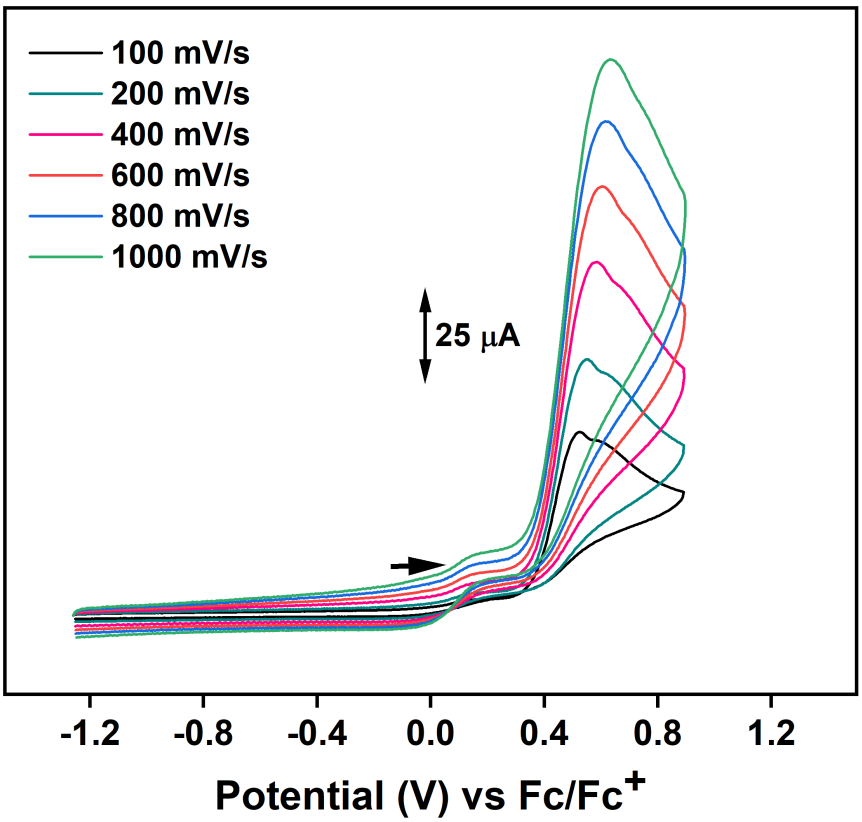


Figure S27. Scan rate dependence of [K][(NP(1,2-*bis*-^{t}Bu-diamidoethane)(NEt_2))] (2.5 mM) vs. Fc/Fc^+ in 0.1 M [$^{n}(Bu)_4N$][PF_6] in THF.

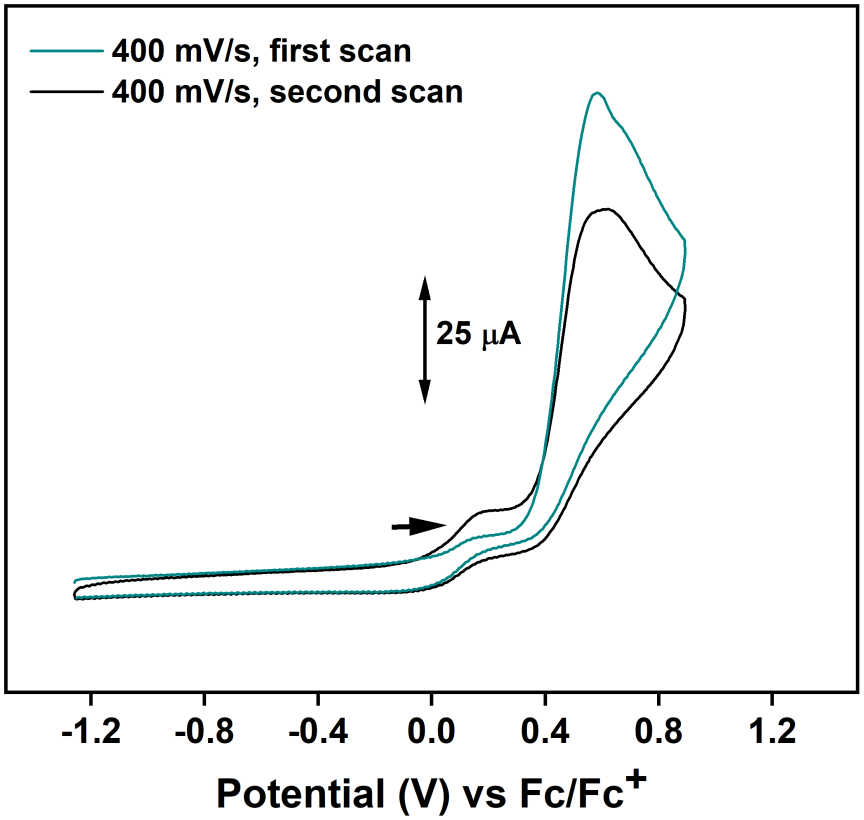


Figure S28. Difference between first and second scan of [K][(NP(1,2-*bis*-^{t}Bu-diamidoethane)(NEt_2))] (2.5 mM) vs. Fc/Fc^+ in 0.1 M [$^{n}(Bu)_4N][PF_6$] in THF. Note the decrease in intensity of the oxidation event and the in growth of a degradation feature on the second scan.

EPR Spectroscopy

X-band EPR measurements were performed on a Bruker E680 spectrometer (Billerica, MA) with a Bruker high sensitivity resonator (ER 4119HS) and an Oxford ESR-900 helium flow cryostat at 9.5 GHz on frozen solutions of **1-Pr(NP*)** and **2-Pr(NP*)** in toluene at 5K, 10, and 20, and 30 K and at room temperature. The EPR signal was attenuated at 20 K and higher. EPR simulations used the program Easy Spin.[9]

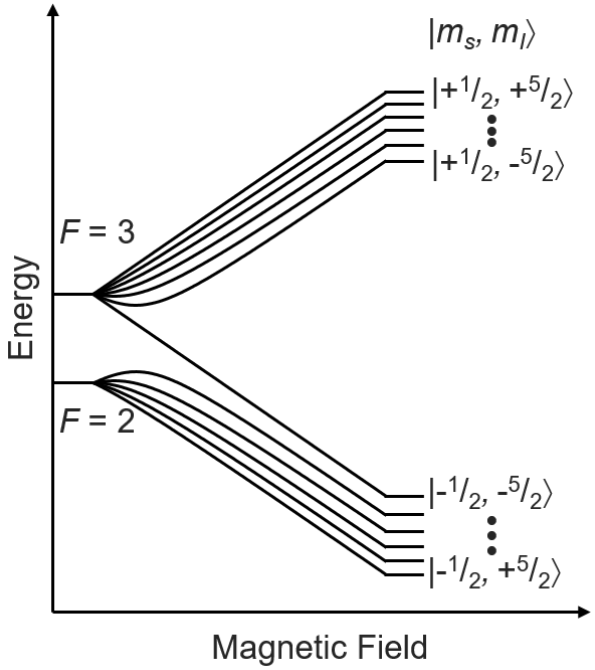


Figure S29. Pictorial representation of the energy levels for a system with $S = ½$ and $I = {}^5/_2$. At low magnetic fields the states are represented in the $|F,m_F\rangle$ basis while at high fields the $|S,I,m_S,m_I\rangle$ basis is used.

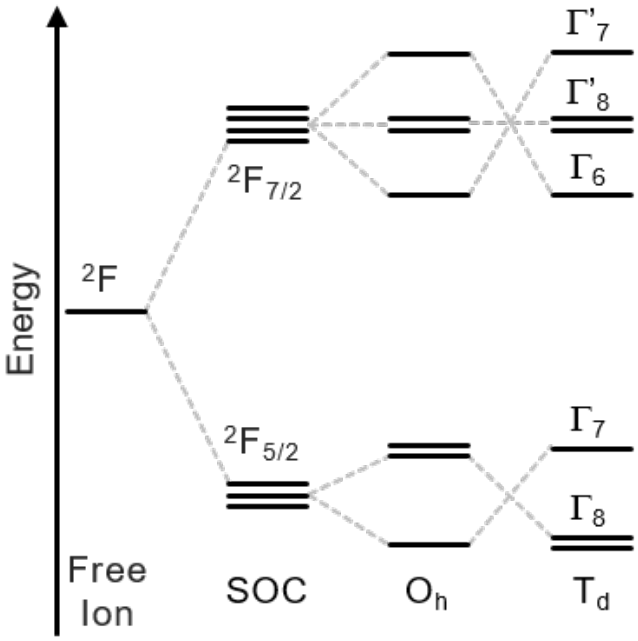
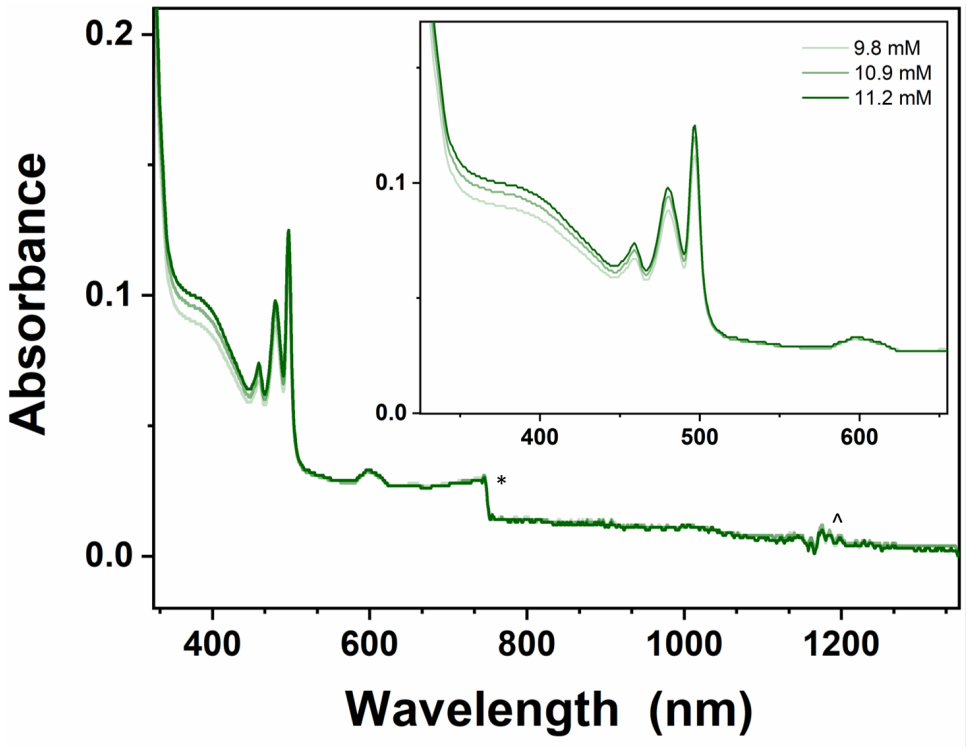


Figure S30. Representation of the energy levels in an f^1 system starting with the free ion, then including spin-orbit coupling (SOC), and finally the crystal field (octahedral, O_h and tetrahedral, T_d).

Electronic Absorption Spectroscopy



S31. Concentration dependent UV-vis-NIR spectra of **1-Pr(NP*)** in THF. Artifact is noted by ^ and grating change is denoted by *. Observable transitions and their molar absorptivities are reported in Table S9 below.

Table S9. Concentration, absorbance, and molar absorptivity values for observable transitions and transition assignments in concentrated samples of **1-Pr(NP*)**. Absorption features were assigned according to their proximity to known transitions.[10-11] Absorbance values for transition at 598 nm ($^3H_4 \rightarrow {}^1D_2$) were too low to provide a reliable extinction coefficient value.

Wavelength (nm)	*Concentration (M)*	*Absorbance*	*Molar absorptivity ($cm^{-1}M^{-1}$)*	*Transition Assignment*
497	9.84E-03	0.112	ε = <10	$^3H_4 \rightarrow 3P_0$
	1.09E-02	0.12		
	1.12E-02	0.125		
480	9.84E-03	0.088	ε = <10	$^3H_4 \rightarrow {}^3P_1$
	1.09E-02	0.094		
	1.12E-02	0.098		
460	9.84E-03	0.067	ε = <10	$^3H_4 \rightarrow {}^3P_2$
	1.09E-02	0.071		
	1.12E-02	0.074		

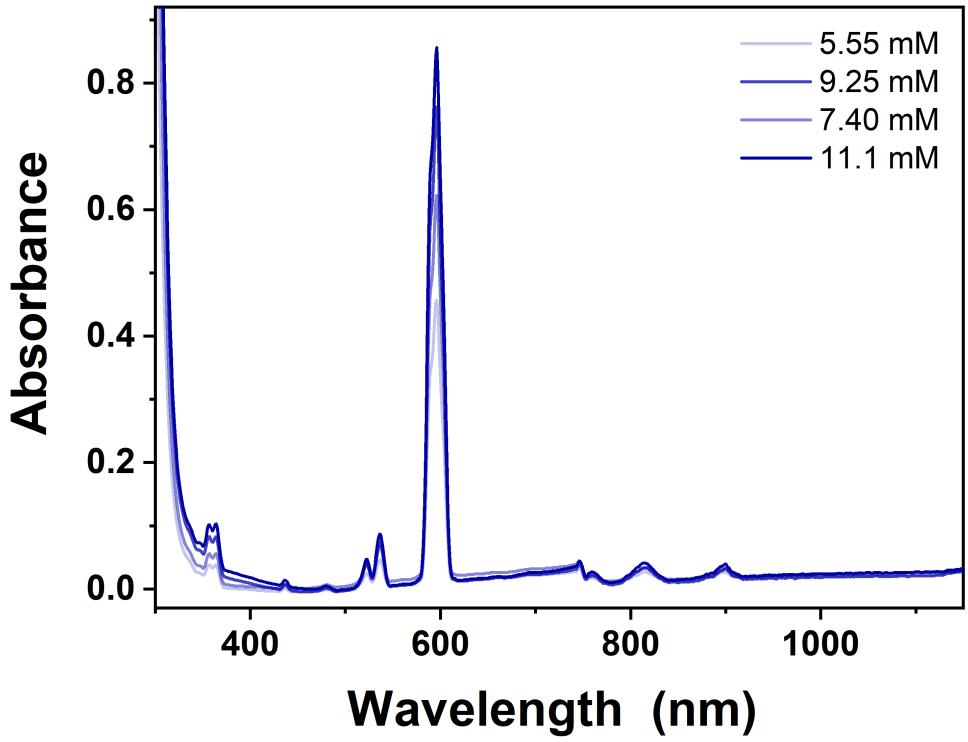
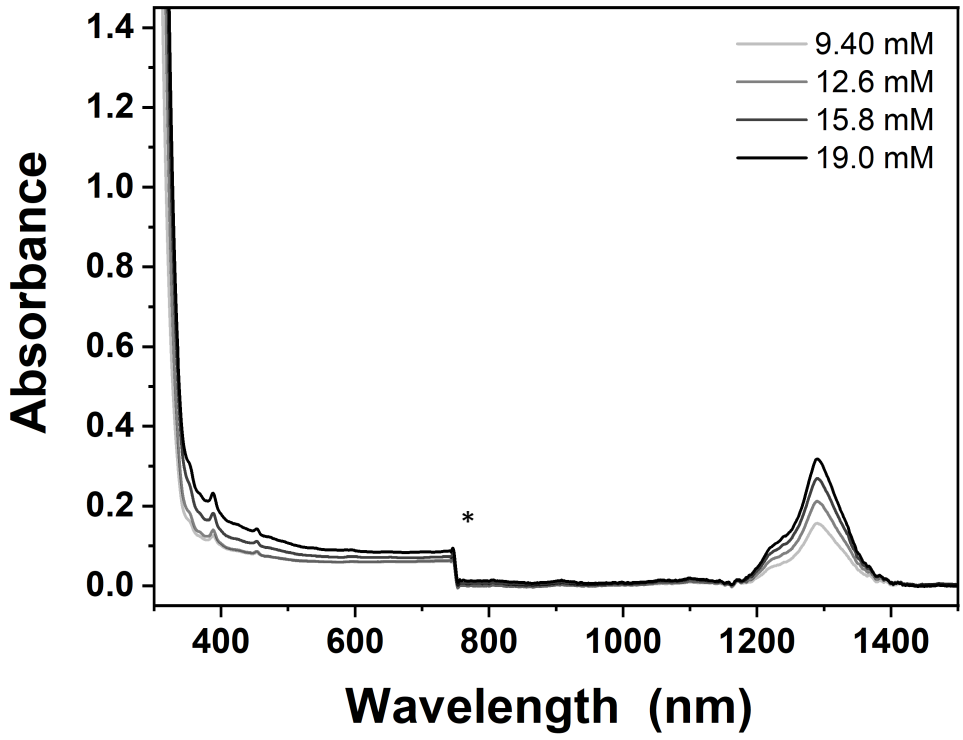


Figure S32. Concentration dependent UV-vis-NIR spectra of **1-Nd(NP*)** in THF. Artifact is noted by ^ and grating change is denoted by *. Absorption features were assigned according to their proximity to known transitions.[10-12] Observable transitions and their molar absorptivities are reported in Table S10 below.

Table S10. Concentration, absorbance, molar absorptivity values as available, and transition assignments for observable transitions in concentrated samples of **1-Nd(NP*)**. Absorbance values for transitions at 900 ($^4I_{9/2} \rightarrow {}^4F_{3/2}$), 815 ($^4I_{9/2} \rightarrow {}^2H_{9/2} + {}^4F_{5/2}$), 760 ($^4I_{9/2} \rightarrow {}^4S_{3/2} + {}^4F_{7/2}$), 523 ($^4I_{9/2} \rightarrow {}^4G_{9/2} + {}^2K_{13/2}$) and 480 ($^4I_{9/2} \rightarrow {}^2G_{9/2} + {}^2D_{3/2}$) nm were too low to provide a reliable extinction coefficient value.

Wavelength (nm)	*Concentration (mM)*	*Absorbance*	*Molar Absorptivity ($cm^{-1}M^{-1}$)*	*Transition Assignment*
596	5.6E-03	0.457	ε = 72	($^4I_{9/2} \rightarrow {}^4G_{7/2} + {}^4G_{5/2}$)
	7.4E-03	0.622		
	9.3E-03	0.762		
	1.1E-02	0.856		
536	5.6E-03	0.046	ε <10	($^4I_{9/2} \rightarrow {}^4G_{7/2}$)
	7.4E-03	0.067		
	9.3E-03	0.074		
	1.1E-02	0.087		

364	5.6E-03	0.038	ε = 12	($^4I_{9/2}$ → $^2D_{1/2}$ + $^2D_{3/2}$ + $^2D_{5/2}$ + $^2I_{11/2}$)
	7.4E-03	0.056		
	9.3E-03	0.083		
	1.1E-02	0.102		
357	5.6E-03	0.038	ε = 12	coupled with 364 nm
	7.4E-03	0.056		
	9.3E-03	0.083		
	1.1E-02	0.102		



S33. Concentration dependent UV-vis-NIR spectra of **1-Dy(NP*)** in THF. Grating change is denoted by *. Absorption features were assigned according to their proximity to known transitions.[11, 13-14] Observable transitions and their molar absorptivities are reported in Table S11 below.

Table S11. Concentration, absorbance, and molar absorptivity values for observable transitions in concentrated samples of **1-Dy(NP*)**. Absorbance values for transition at 453 ($^6H_{11/2} \rightarrow {}^4F_{9/2}$) and 388 ($^6H_{11/2} \rightarrow {}^4I_{15/2}$) nm were too low to provide a reliable extinction coefficient value.

Wavelength (nm)	*Concentration (M)*	*Absorbance*	*Molar Absorptivity ($cm^{-1}M^{-1}$)*	*Transition Assignment*
1290	9.40E-03	0.157	ε = 17	($^6H_{11/2} \rightarrow {}^6F_{11/2}$)
	1.26E-03	0.212		
	1.58E-03	0.269		
	1.90E-02	0.318		

Density Functional Theory

All DFT calculations were carried out with the PBE0[15] hybrid functional as implemented in the Gaussian 16 software package revision B.01.[16] ECP28MWB[17] small core quasi-relativistic pseudopotential and ECP28MWB_ANO[18] basis set were used to describe Ln atoms (Ln=Pr, Nd, Dy), and the remaining atoms were described with the all-electron Pople basis set 6-311G(d).[19] The geometrical structures of the trivalent complexes **1-Ln(NP*)** were optimized excluding the K^+ counter ion. Since there are no XRD data for **2-Ln(NP*)** (Pr, Nd, Dy), their initial structures for the geometry optimization were taken from the similar Ce^{4+} and Tb^{4+} complexes with the previously reported experimental crystal structures[2,8] All calculations for both **1-Ln(NP*)** and **2-Ln(NP*)** compounds were performed in gas phase without any constraints based on the XRD structures (if available). Harmonic frequency calculations were performed to confirm that the optimized structures were stationary points on the potential energy surface. The computed structural metrics of the **1-Ln(NP*)** complexes are in good agreement with the XRD data, with Ln−N and N−P bond distances, as well as Ln−N−P and N−Ln−N valence angles deviating by less than 1.1%, 0.5%, 4.1%, and 0.3% of the experimental parameters, respectively, providing confidence to the theoretical model (Table S12). In accordance with Hund's rules, the highest spin states of **1-Ln(NP*)** were considered for their electronic ground states: triplet for **1-Pr(NP*)**, quartet for **1-Nd(NP*)**, and sextet for **1-Dy(NP*)**. For the metal-oxidized **2-Pr(NP*)**, doublet spin state was considered. For the ligand-oxidized compounds, **2-Nd(NP*)** and **2-Dy(NP*)**, both high (quintet and septet, respectively) and low (triplet and quintet, respectively) spin states were considered to account for the ferromagnetic/antiferromagnetic spin coupling between Ln and ligands. In both **2-Nd(NP*)** and **2-Dy(NP*)**, the lower spin states were found to be slightly more stable than the high spin states, *i.e.* by 1.00 kcal/mol and 0.53 kcal/mol, respectively. Wave functions of all studied species are stable indicating that the calculations converged to the ground electronic state. Time-dependent DFT calculations (TD-DFT) of up to 200 excited states were carried out to simulate the UV-vis spectra. The computed spectra were plotted broadening the calculated excitation lines with Gaussian-type peaks using 0.1 eV half-width at half height. Natural transition orbitals (NTOs),[20] which most of the time can yield a single electron-hole representations of the electronic excitations, were employed to interpret the calculated excitation spectra. To gain more insight into electronic structure of these complexes, chemical bonding analyses were performed using Natural Bond Orbital[21-22] (NBO7) method. The IQMol[23] was used for molecular orbitals visualization of the NBO results. Chemissian 4.60[24] was used to plot molecular orbital energy level diagrams.

Table S12. Experimental (exp) vs. theoretical (theor) bond lengths (Å) and valence angles (º) of complexes **1-Ln(NP*)**, Ln=Pr, Nd, Dy.

Bond/complex	**1-Pr(NP*)** exp	**1-Pr(NP*)** theor	**1-Nd(NP*)** exp	**1-Nd(NP*)** theor	**1-Dy(NP*)** exp	**1-Dy(NP*)** theor
avg. Ln–N	2.324	2.332	2.313	2.318	2.241	2.217
avg. N_{imido}-P	1.533(5)	1.535	1.535	1.535	1.525	1.533
avg. Ln-N-P	166.5	173.29	167.35	172.78	168.00	171.84
avg. N-Ln-N	109.2(2)	109.48	109.35	109.47	109.4	109.47

Table S13. Theoretical bond lengths (Å) and valence angles (º) of complexes **2-Ln(NP*)**, Ln=Pr, Nd, Dy.

Bond/complex	**2-Pr(NP*)**	**2-Nd(NP*)**	**2-Dy(NP*)**
The longest Ln-N	2.194	2.474	2.357
Three shorter Ln-N, avg.	2.183	2.258	2.168
avg. Ln–N	2.185	2.312	2.215
N_{imido}-P (related to the longest Ln-N bond)	1.559	1.588	1.585
avg. N_{imido}-P (related to the 3 shorter Ln-N bonds)	1.558	1.546	1.543
avg. N_{imido}-P	1.558	1.557	1.554
avg. Ln-N-P	169.13	169.64	170.97
avg. N-Ln-N	109.47	109.33	109.32

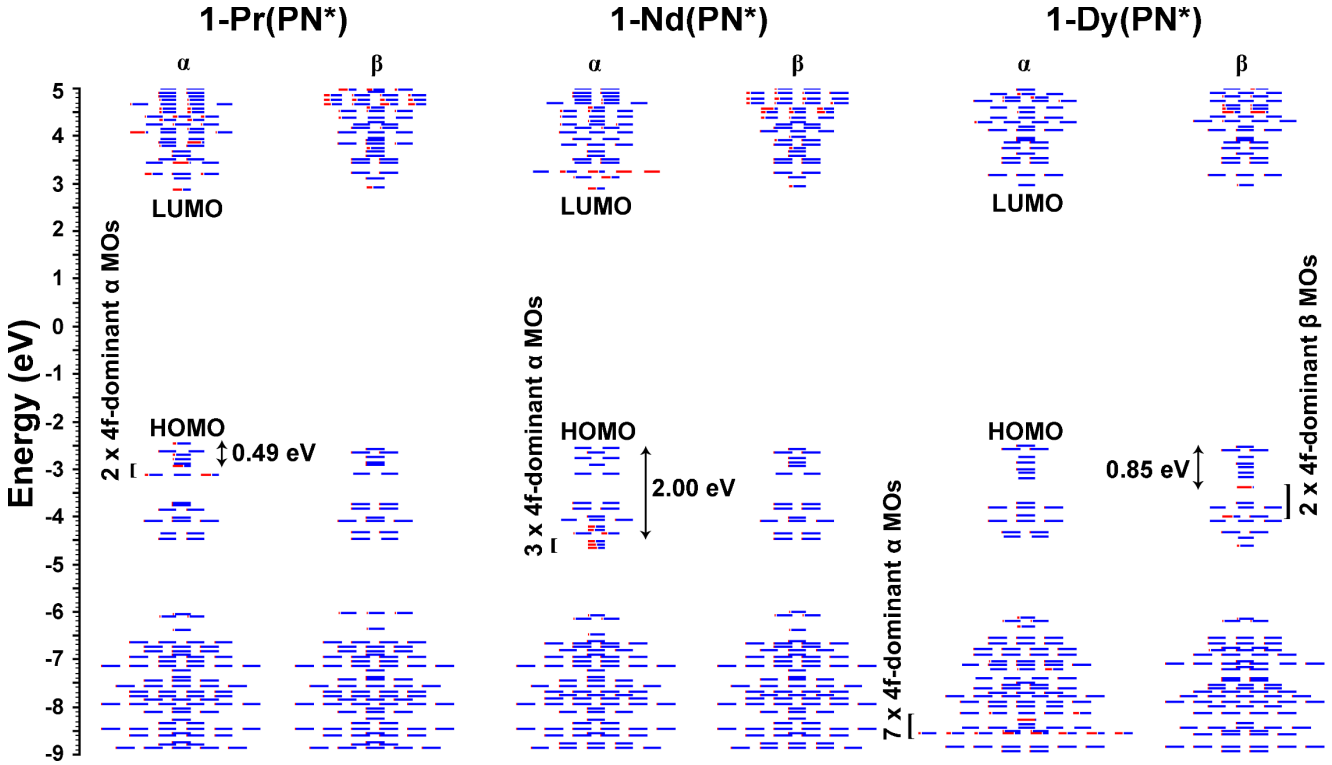


Figure S34. Combined (α+β) MO diagrams of **1-Ln(NP*)**, Ln=Pr, Nd, Dy. The red fraction of the MO lines represents the percentage of Ln AOs in the MOs, and the blue lines are the ligand fraction. The arrows reflect the energy difference between HOMO and the highest 4f-dominant MO of Ln. Degeneracy of the MO energy levels is set to 0.05 eV.

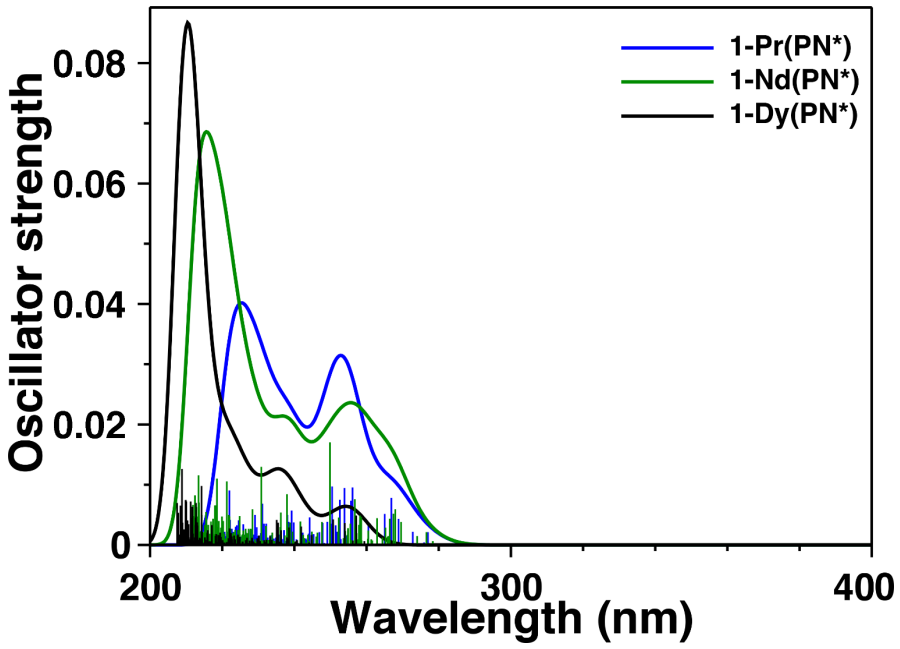


Figure S35. Computed TD-DFT spectra of **1-Ln(NP*)**, Ln=Pr, Nd, Dy. Vertical bars depict theoretical oscillator strength of single-electron excitations.

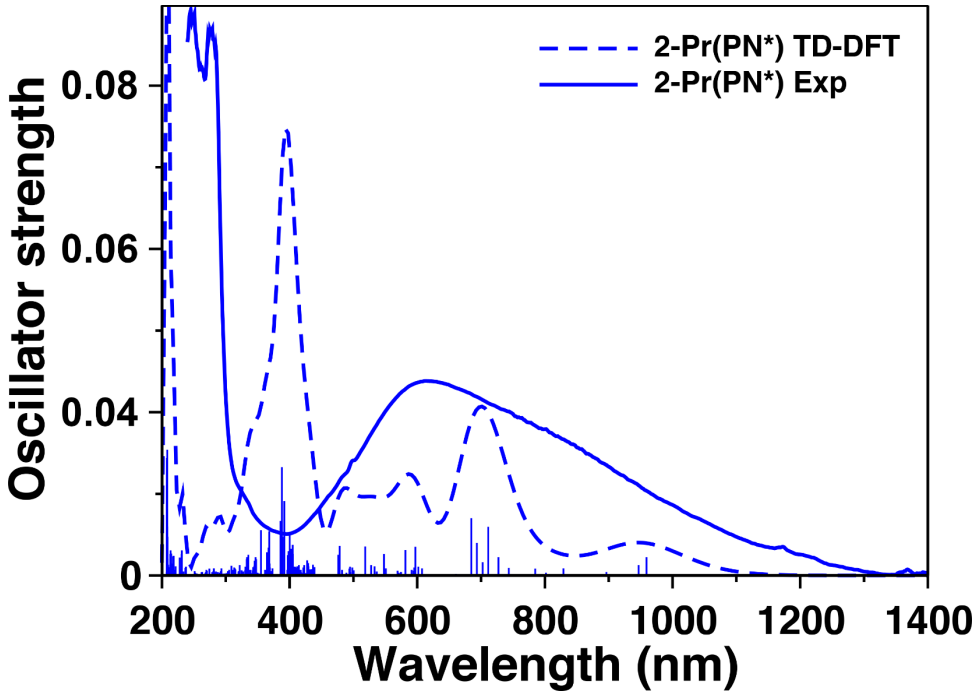


Figure S36. Experimental UV-Vis and computed TD-DFT spectra of **2-Pr(NP*)**. Vertical bars depict theoretical oscillator strength of single-electron excitations.

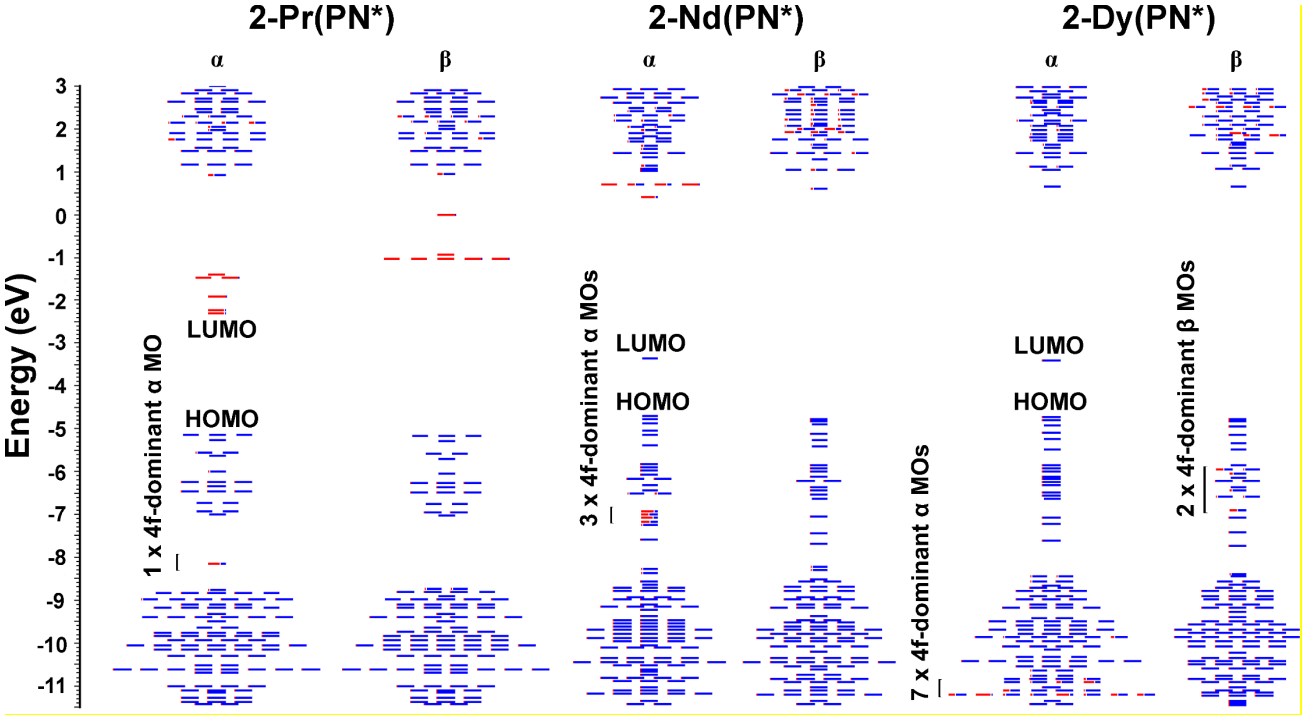


Figure S37. Combined (α+β) MO diagrams of **2-Ln(NP*)**, Ln=Pr, Nd, Dy. The red fraction of the MO lines represents the percentage of Ln AOs in the MOs, and the blue lines are the ligand fraction. Degeneracy of the MO energy levels is set to 0.05 eV.

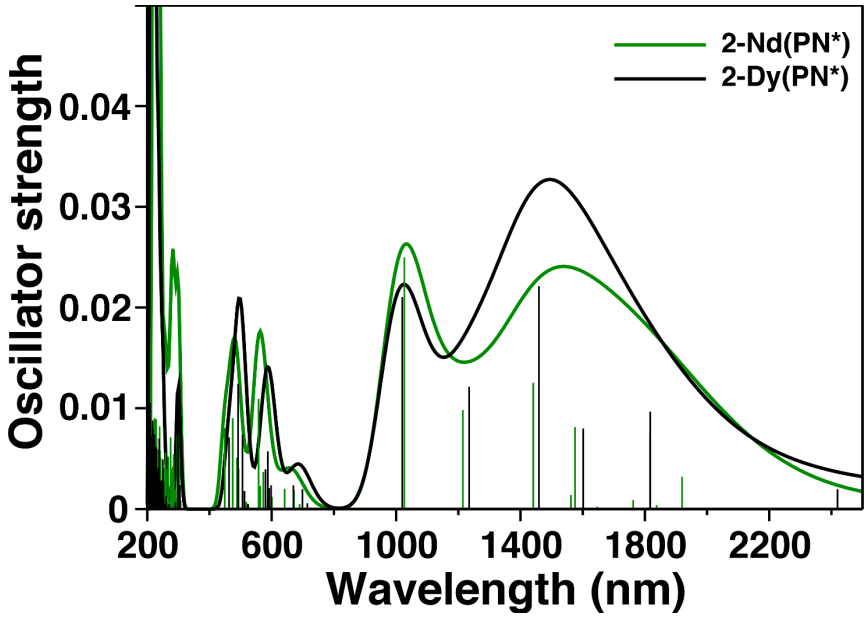


Figure S38. Computed TD-DFT spectra of **2-Nd(NP*)** and **2-Dy(NP*)**. Vertical bars depict theoretical oscillator strength of single-electron excitations.

Details of the TD-DFT and NTO analyses for 2-Dy(NP*).

Similar to the TD-DFT spectrum of **2-Nd(NP*)**, the broad band at ~840-2500nm in **2-Dy(NP*)** is attributed to the LLCT excitations arising from the frontier ligand-dominant MOs (primarily 2p orbitals of N atoms) to the LUMO, which is also ligand-dominant (98% orbitals of N, P, C and 2% 4f/5d orbitals of Dy). The band at the ~430-760nm range features similar LLCT excitations. As opposed to **2-Nd(NP*)**, NTO analysis shows no f-f or MLCT within these energy ranges, in accordance with the significantly lower MO levels of the seven 4f-dominant MOs (α spin density), residing at the [-10.8 eV; -11.3 eV] range. LMCT excitations originating from the ligand-dominant MOs to the Dy-dominant unoccupied MOs start appearing at ~230nm and higher in energy, in addition to the LLCT excitations. MLCT excitations originating from the 4f-dominant β-MOs to the ligand-dominant orbitals start appearing at ~210nm and higher in energy.

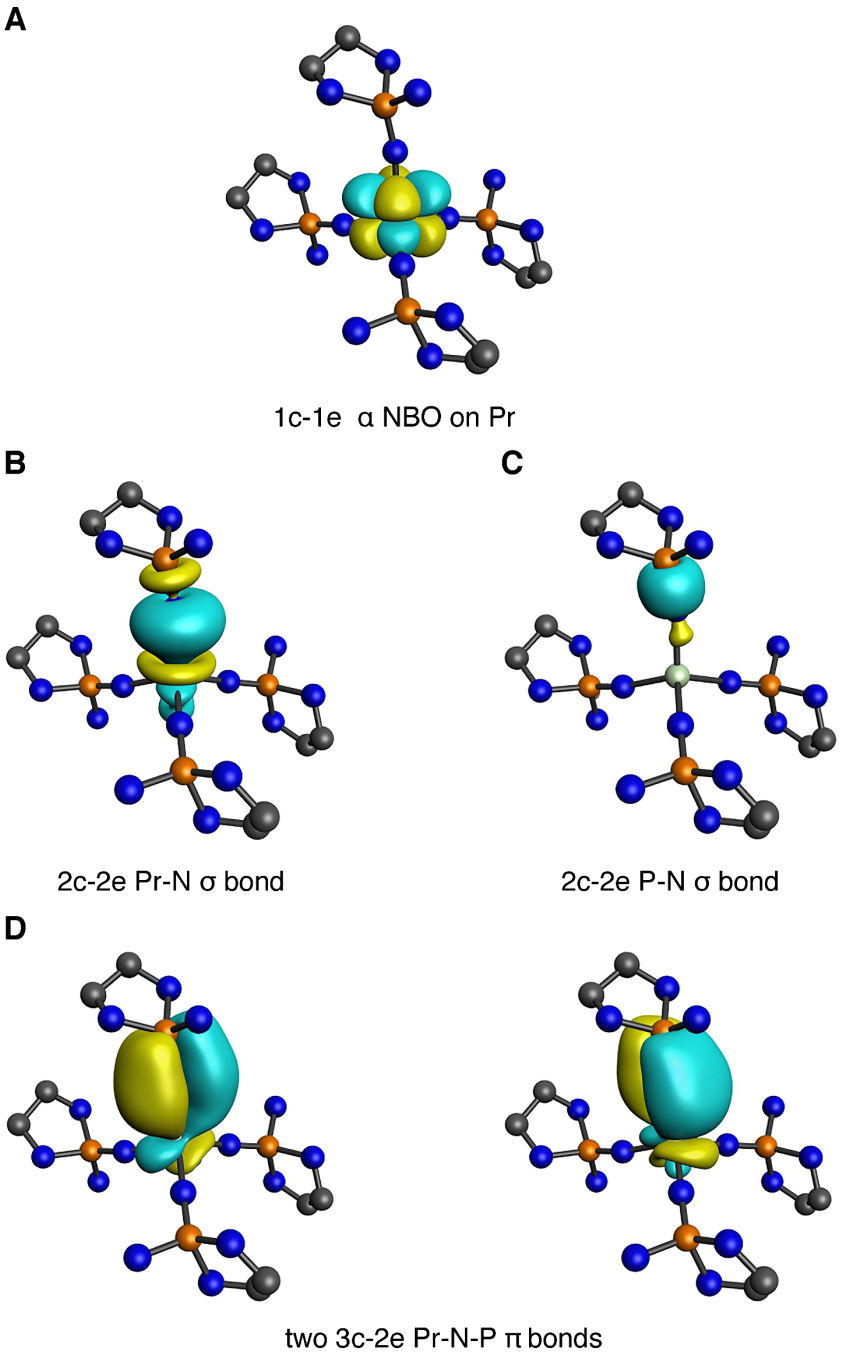
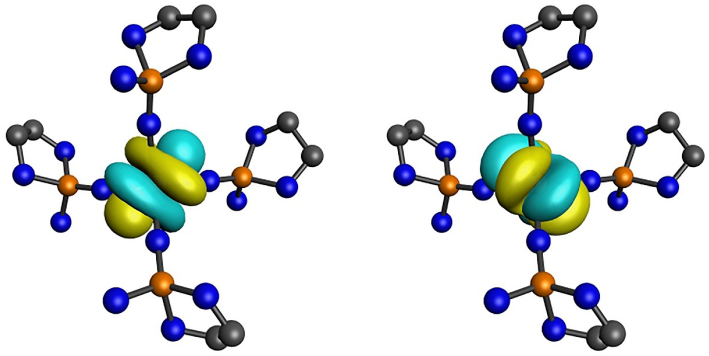


Figure S39. Bonding analysis of the Pr–N–P interactions in **2-Pr(NP*)**. (A) Unpaired Pr 4f electron identified as 1c-1e α NBO on Pr. (B) Two-center two-electron Pr–N σ bond. (C) Two-center two-electron P–N σ bond. (D) Two three-center two-electron Pr–N–P π bonds. ON denotes occupation number here and elsewhere. H atoms and side groups of the ligands (^{t}Bu, Et_2) are omitted for simplicity. An equivalent set of bonds is identified for other three ligands.

Table S14. ON values (|e|) of the Ln–N σ bonds, N–P σ bonds, Ln–N–P π bonds, and 1c-1e α NBOs (unpaired f electrons on Ln) in **1-Ln(NP*)**, Ln=Pr, Nd, Dy, and **2-Pr(NP*)**. ON values for the 1c-1e β NBOs are shown in italic.

Bond/complex	Pr–N σ	N–P σ	Pr–N–P π	1c-1e NBOs
1-Pr(NP*)	1.97	1.99	1.94	1.00; 1.00
1-Nd(NP*)	1.97	1.99	1.94	1.00; 1.00; 1.00
1-Dy(NP*)	1.97	1.99	1.94	1.00; 1.00; 1.00; 1.00; 1.00 *0.95; 1.00*
2-Pr(NP*)	1.98	1.98	1.95	1.00



two 1c-1e α NBOs

Figure S41. Two unpaired 4f electrons identified as two 1c-1e α NBOs on Pr in **1-Pr(NP*)**. Hydrogen and side groups of the ligands (^{t}Bu, Et_2) are omitted for simplicity.

Table S15. ON values (|e|) of the Ln–N σ bonds, N–P σ bonds, Ln–N–P π bonds, and 1c-1e α NBOs (unpaired f electrons on Ln) in **2-Nd(NP*)** and **2-Dy(NP*)**. ON values for the 1c-1e β NBOs are shown in italic.

Bond/ complex	Ln–N σ (longer bond)	Ln–N σ (3 shorter bonds)	N–P σ (longer & shorter bonds)	Ln–N–P π (longer bond)	Ln–N–P π (3 shorter bonds)	1c-1e NBOs
2-Nd(NP*)	1.98	1.97	1.99	1.98 (3c-2e) & 0.99 (3c-1e)	1.97	0.98; 1.00; 1.00
2-Dy(NP*)	1.97	1.96	1.99	1.97 (3c-2e) & 0.99 (3c-1e)	1.97	1.00; 1.00; 1.00; 1.00; 1.00 *0.95; 1.00*

Table S16. Bond polarization (%) of the Ln-based NBOs in **1-Ln(NP*)**, Ln=Pr, Nd, Dy, & **2-Pr(NP*)**.

Bond/ complex	Ln–N σ bond		Ln–N–P π bonds		
	Ln	N	Ln	N	P
1-Pr(NP*)	5.95	94.05	1.37	96.39	2.24
1-Nd(NP*)	5.61	94.39	1.13	96.63	2.24
1-Dy(NP*)	5.60	94.40	0.91	96.88	2.21
2-Pr(NP*)	10.38	89.62	4.70	93.58	1.73

Table S17. Bond polarization (%) of the Ln-based NBOs in **2-Nd(NP*)** and **2-Dy(NP*)**.

Bond/ complex	Ln–N σ (longer bond, avg.)		Ln–N σ (3 shorter bonds, avg.)		Ln–N–P π (longer bond, avg.)			Ln–N–P π (3 shorter bonds, avg.)		
	Ln	N	Ln	N	Ln	N	P	Ln	N	P
2-Nd(NP*)	4.08	95.92	6.49	93.51	0.60	97.65	1.75	1.68	96.34	1.98
2-Dy(NP*)	4.13	95.87	5.97	94.03	0.59	97.67	1.74	1.28	96.76	1.96

Table S18. Ln hybrids (%) of the Ln-based NBOs in **1-Ln(NP*)**, Ln=Pr, Nd, Dy, and **2-Pr(NP*)**. Ln hybrids for the 1c-1e β NBOs are shown in italic for each 1c-1e β NBO.

Bond character/ complex	Ln–N σ bond, avg.				Ln–N–P π bonds, avg.				1c-1e NBOs on Ln, avg.			
	s	p	d	f	s	p	d	f	s	p	d	f
1-Pr(NP*)	1.18	0.72	70.83	27.11	0.50	5.35	26.77	64.16	0.00	0.02	0.11	99.88
1-Nd(NP*)	1.96	0.50	71.32	26.03	1.57	11.42	28.77	53.00	0.00	0.00	0.04	99.95
1-Dy(NP*)	18.33	0.46	73.41	7.70	1.77	17.73	38.39	36.26	0.00	0.00	0.01	99.99
									0.00	*0.00*	*0.14*	*99.86*
									47.33	*0.00*	*0.01*	*52.65*
2-Pr(NP*)	0.36	0.47	66.03	33.03	0.03	3.06	26.70	67.31	0.00	0.02	0.08	99.91

Table S19. Ln hybrids (%) of the Ln-based NBOs in **2-Nd(NP*)** and **2-Dy(NP*)**.

Bond character/ complex	s	p	d	f	s	p	d	f
	Ln–N shorter σ bonds, avg.				Ln–N–P shorter π bonds, avg.			
2-Nd(NP*)	0.95	0.53	71.79	26.55	4.06	5.81	34.59	52.53
2-Dy(NP*)	16.62	0.57	74.60	8.10	1.94	13.20	41.26	39.88
	Ln–N longer σ bond				Ln–N–P longer π bond, avg.			
2-Nd(NP*)	1.16	0.27	70.09	28.33	4.31	4.05	39.36	49.04
2-Dy(NP*)	17.63	0.27	73.88	8.11	3.90	6.70	62.02	24.60

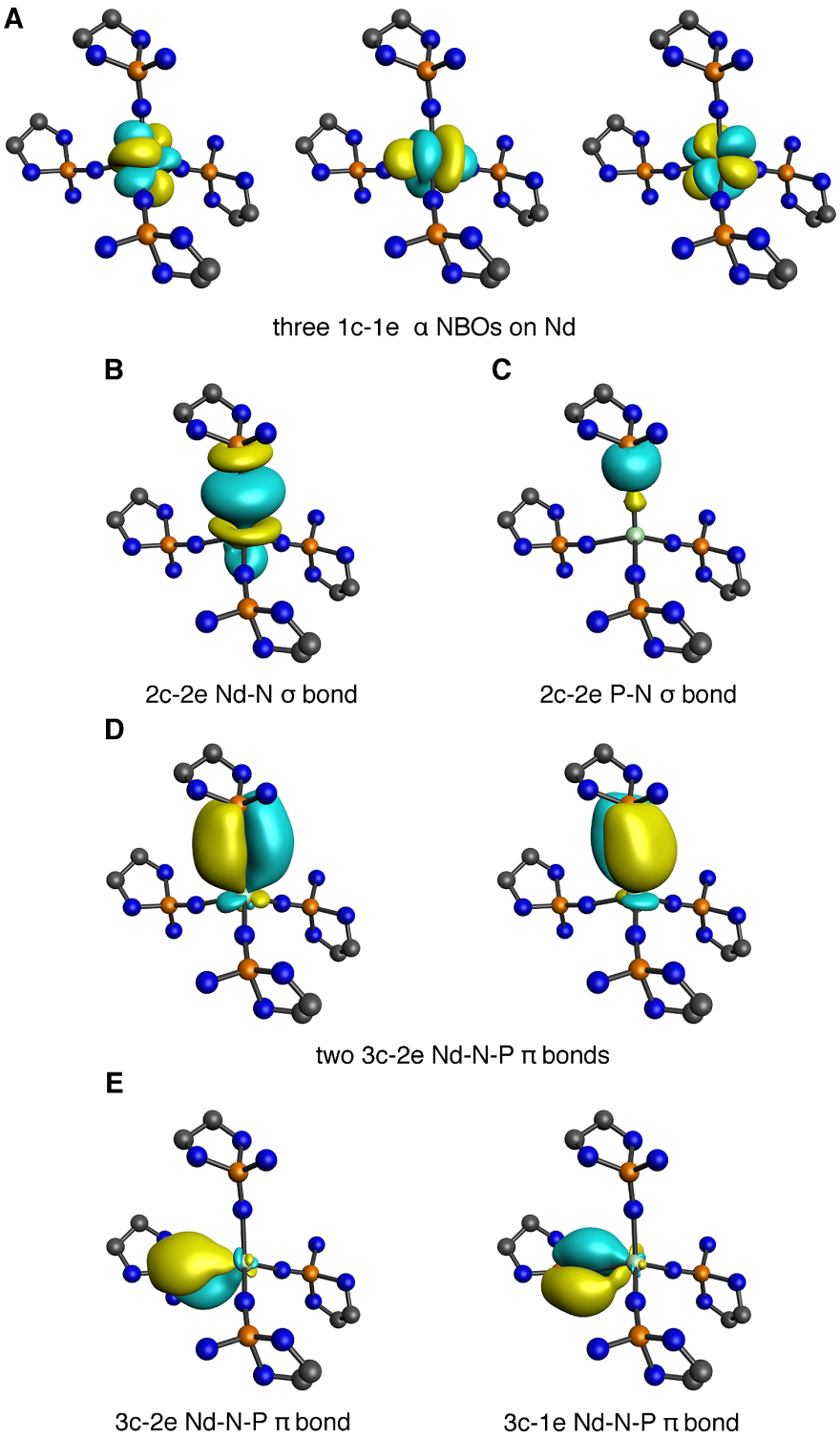


Figure S42. Bonding analysis of the Nd–N–P interactions in **2-Nd(NP*)**. (A) Unpaired Nd 4f electrons identified as 1c-1e α NBOs on Nd. (B) 2c-2e Nd–N σ bond. (C) 2c-2e P–N σ bond. (D) Two 3c-2e Nd–N–P π bonds identified for one of the three shorter Nd-N contacts. An equivalent set of bonds was found for other two ligands. (E) Two Nd–N–P π bonds identified for the longer Nd-N contact. An equivalent set of bonds shown in B and C was identified for other three ligands.

Multiconfiguration Pair-Density Functional Theory

All MC-PDFT[25-26] calculations were done in the OpenMolcas[27] program package using the extended multistate (XMS-PDFT)[28] version of MC-PDFT. The on-top ftLSDA[29] functional was used for all calculations on a truncated ligand of 61 atoms, cut from the full DFT optimized structure. The basis sets are as follows: ANO-RCC-VTZP[30] for Pr, ANO-RCC-VDZP[31] for C and P, ANO-RCC-MB[32] for H, and MG3S[19, 33-37] for N. Scalar relativity was accounted for by use of the DKH second order Hamiltonian[38] using the 'Expert' keyword and 'RELA=R02E00' in the Seward module. State averaged complete active space self-consistent field (SA-CASSCF) calculations were done to obtain the reference states for the XMS-PDFT calculations. The two SA-CASSCF calculations presented here used an active space of 7 electrons in 11 orbitals (7, 11) with 47 states for the spectrum in the main text and 43 states for the spectrum containing the high energy excitations (see Figs. S9 and S10) for the doublet spin state.

Active Spaces

The results of two calculations with slightly different active spaces and number of states for the SA-CASSCF calculations are presented because we could not get one SA-CASSCF calculation that included all the orbitals needed for the excitations from the low to high energy regions of the spectrum. The problem is that, formally, the lanthanide has only one electron in the f shell and everything else is empty. This means that the only way to get the necessary orbitals in the active space is by computing enough states to get the electrons to excite into those orbitals. The first problem was that there was a low lying Pr d shell that would come into the active space instead of the f orbitals, even though there were no excitations into these d orbitals. This made it hard to rotate in other f or ligand orbitals that were needed to get the correct states. The second problem was getting the right occupied ligand orbitals in the active space that excite into the f shell. One active space, (AS2 in main text) (Fig. S10) contains two ligand orbitals and one lanthanide p orbital. Removing this p orbital resulted in the ligand orbital L6, the orbital that is necessary for the high energy excitations, leaving the active space and we were unable to get it back in the active space without this p orbital. Attempts were made to get all 7 f orbitals in the active space, but this also resulted in L6 leaving the active space and we could not get L6 back by doing more states or enlarging the active space to a reasonable size.

The second active space (AS1 in main text) contains the same 4 f electrons, but with 3 ligand orbitals that excite into the f shell (Fig S9). By removing the p orbital, L6 was not in the active space and two different correlating orbitals, compared to those in Fig S10, came in the active space. The total number of states in the SA-CASSCF calculation was 47 for this active space and similarly to the first active space, we tried calculating more states and enlarging the active space to try and get L6 in the active space, but it did not work. Some on-going work suggests that p orbitals correlation is important for actinide oxides, even though these orbitals are mostly doubly occupied. This may also be the case with Pr and could be why L6 has trouble staying in the active space, however, more rigorous calculations would be necessary.

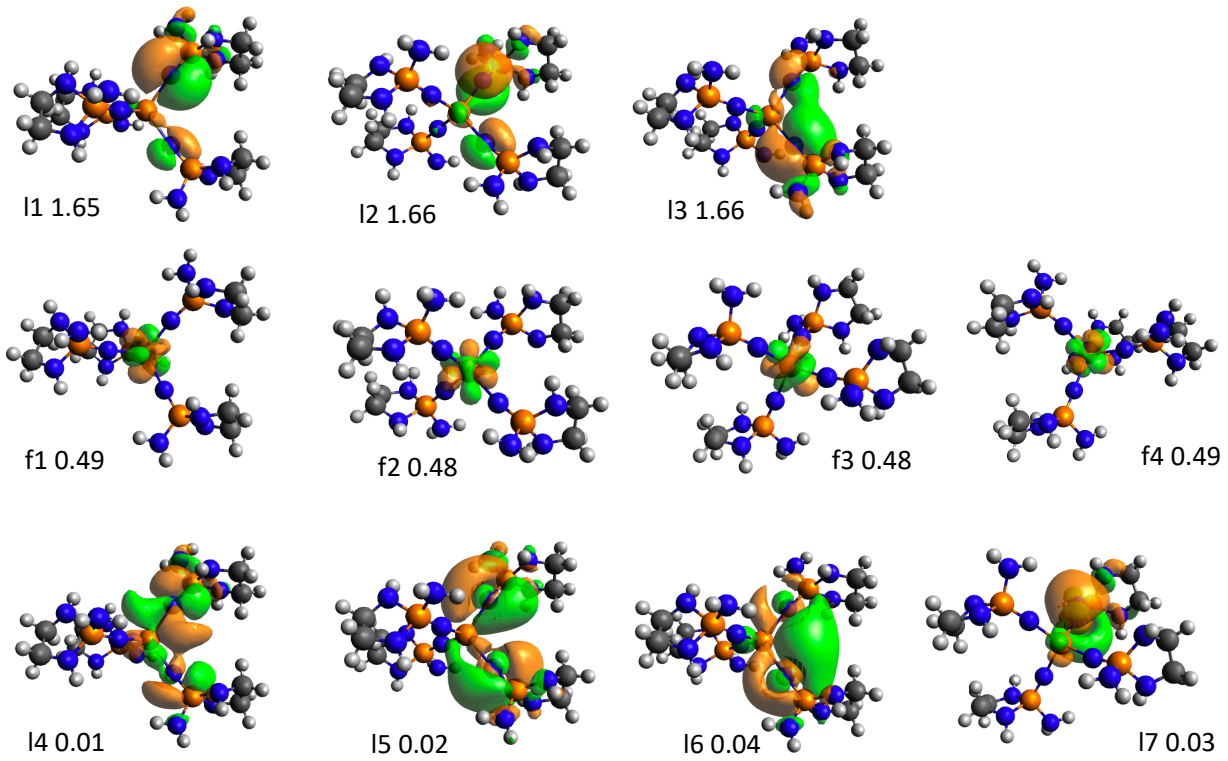


Figure S43. Orbitals from active space 1 (AS1) from a (7, 11) SA-CASSCF calculation, with the average natural orbital occupation numbers from the 47 SA-CASSCF calculation. Orbitals l4 and l7 are different correlating orbitals than in Fig. S10. Lowercase letters denote AS1

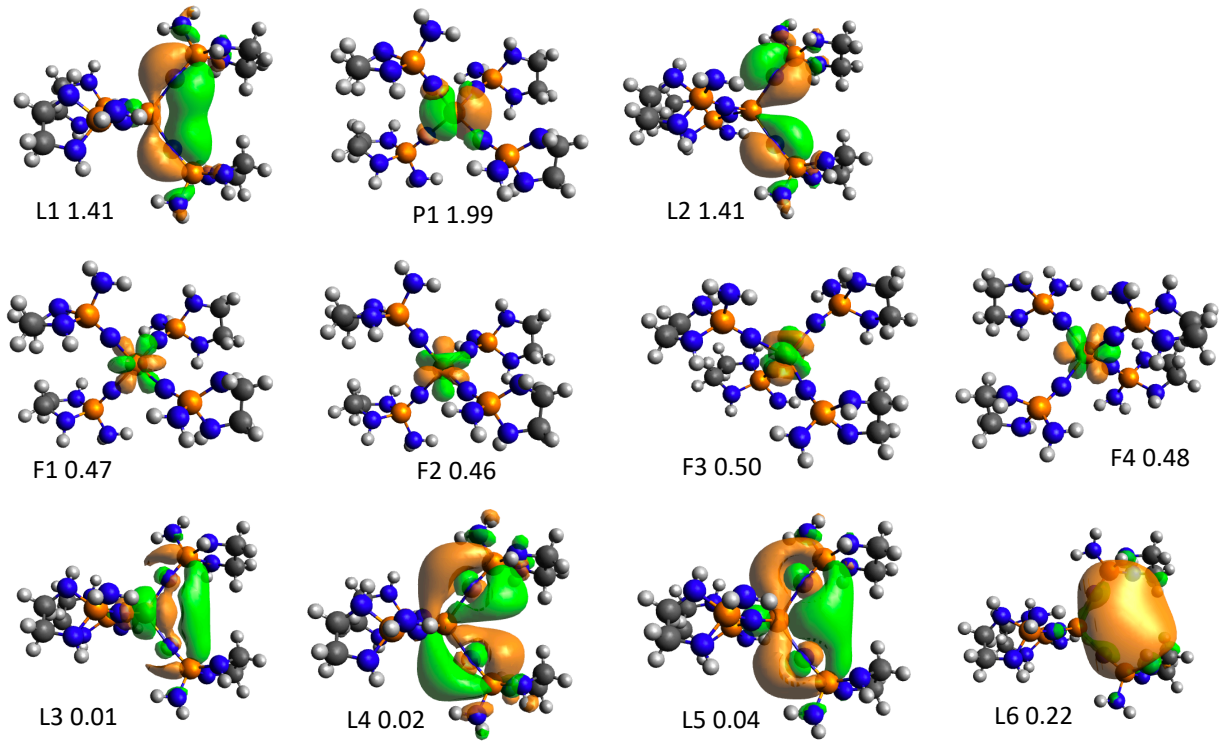


Figure S44. Orbitals from active space 2 from a (7, 11) SA-CASSCF calculation, with the average natural orbital occupation numbers from the 43 SA-CASSCF calculation. P1 is the lanthanide p orbital and L6 is the orbital that is necessary for the high energy excitations. Uppercase letters denote AS2 and are numbered independently of AS1 (ie l3 and L3 don't necessarily correspond)

Spectral Assignment for 300-1200 nm region using AS1

The energies and oscillator strengths for the spectrum in the main text can be found in Table S20. This was a challenging problem to analyze because there are so many configurations in each state and many XMS-PDFT states contained nearly equal contribution from many CASSCF reference states (Table S24). In Table S22, the CI coefficients for configurations with coefficients larger than 0.31 are listed and we attempted to use only these configurations to analyze the XMS-PDFT wave functions, but it seemed that in the XMS-PDFT wave function, nothing simplified to produce an easily digestible result. We decided to present a more qualitative approach at the CASSCF level, where we monitor the change in average natural orbital occupation numbers (NOON) from states CAS1 and CAS3, the two reference states that make up the 1st two XMS-PDFT states, in conjunction with analyzing the main configurations from those CAS wave functions. The changes in NOON for CAS1 are in Table S21 and Table S22 contains the main configurations and CI coefficients larger than 0.31. The assignment listed in Table S22 is based on analyzing the configurations and the change in NOON for each state. Most states have excitations between the ligand and f shell, which is also reflected in Table S23, where we analyze the net change in electrons between the ligand and f shells for each state. For nearly every state, there is a net loss of electrons from

the ligand shell and net gain in the f shell. While this indicates L-f transitions, since the net loss is usually around 0.3 electrons and the total number of electrons excited in each state is usually between 1-2 electrons, this indicates there are other types of transitions occurring (Table S23). These possibilities are listed in Table S22 for each CAS state and it's likely that some of these configurations get suppressed at the XMS-PDFT level, but this was difficult to determine exactly by only looking at configurations with coefficients above 0.31.

Spectral Assignment for 200-300 nm region using AS2

The XMS-PDFT spectrum for the 43 state calculation using active space 2 is shown in **Figure S45**. Similarly to the 47 state spectrum, excitations from the first two states were required for the best description of the experimental spectrum. The natural orbital occupation numbers for the higher energy states are listed in Table S26 and the main configurations are listed in Table S27. States 37 and 38 are comprised of linear combinations of configurations that give the open shell low spin configuration in the ligand shell. These are the first states that occupy L6 and also the first states to have 0.5 electrons in each f orbital. Comparing to the f orbital occupation of the lower energy states (Table S21), these lower energy states mostly occupy 2-3 f orbitals with at least one f orbital containing nearly a whole electron.

The spectrum is shifted 40 nm to match the experimental peak at 280 nm and due to lack of orbital l2, there are no transitions around 400 nm.

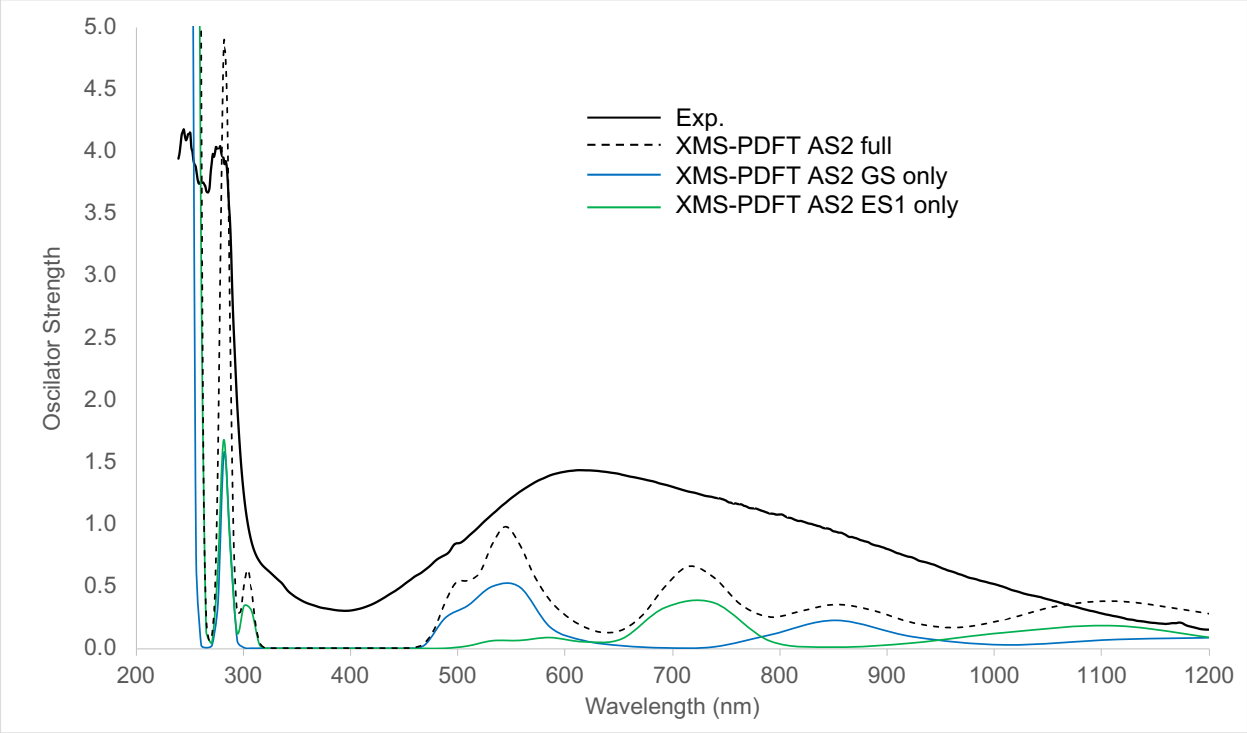


Figure S45. XMS-PDFT spectrum using the ftLSDA on-top functional for 43 state calculation, shifted 40 nm to match experimental peak at 280 nm and scaled to match experimental intensities. The dashed line is the total XMS-PDFT spectrum including

excitations from the ground state (GS) (blue) and 1st excited state (ES1) (green) using active space 2 (AS2).

Comparing the 47 state calculation with AS1 and 43 state calculation with AS2, it is clear that the additional ligand orbital l2, adds transitions that are missing in the 43 state calculation (Fig. S46). In Fig. S46, the XMS-PDFT energies for the 43 state calculation are not shifted to show that these l2 transitions fall nicely in the troughs of the 43 state spectrum. While the resultant 43 state spectrum is qualitatively a good description, this l2 orbital is necessary for a more accurate description of the states and the resulting XMS-PDFT spectrum. Since including l2 in the active space increased the accuracy of predicted XMS-PDFT energies compared to the experimental spectrum, we think that if we were able to get orbital L6 in active space 1, the higher energy transitions shown in the 43 state calculation would also become more accurate because the states and interaction between the states would be improved. Particularly for the 300-400nm region, the 43 state calculation with AS2 has zero states in that window because of the missing l2 orbital.

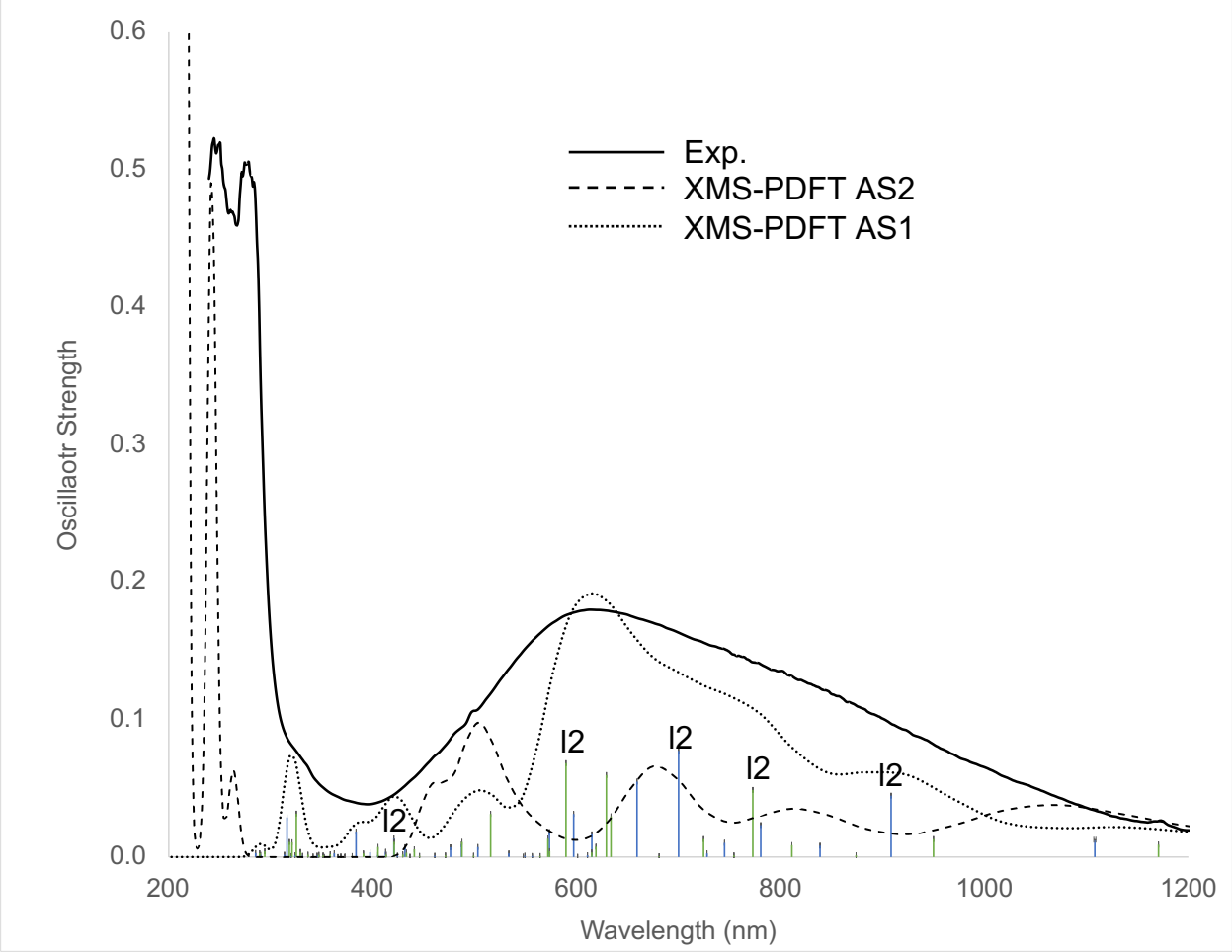


Figure S46. XMS-PDFT spectrum using the ftLSDA on-top functional for AS2 (dashed) and XMS-PDFT spectrum using the ftLSDA on-top functional for AS1 (dotted). The stick

intensities correspond to the oscillator strengths for transitions from the 1st XMS-PDFT state (blue) and 2nd XMS-PDFT state (green) for the 47 state calculation with AS1. The l2 labels correspond to transitions in the 47 state calculation that originate from orbital l2.

Comparison to TD-DFT

The TD-DFT computed spectrum is shown in Figure S47 with the XMS-PDFT spectrum of the 47 state calculation. By plotting only the stick spectrum for transitions from the ground XMS-PDFT state and the corresponding fitted spectrum (blue line in Fig S47), it seems that in the 500-1200nm range, the XMS-PDFT transitions from the ground state correspond well to the TD-DFT spectrum. The XMS-PDFT stick spectrum is clustered under the TD-DFT peaks in this region and the peak maxima of the fitted XMS-PDFT spectrum from the ground state align with the peak maxima of the TD-TDFT spectrum. This indicates that part of the TD-DFT spectrum is likely correct.

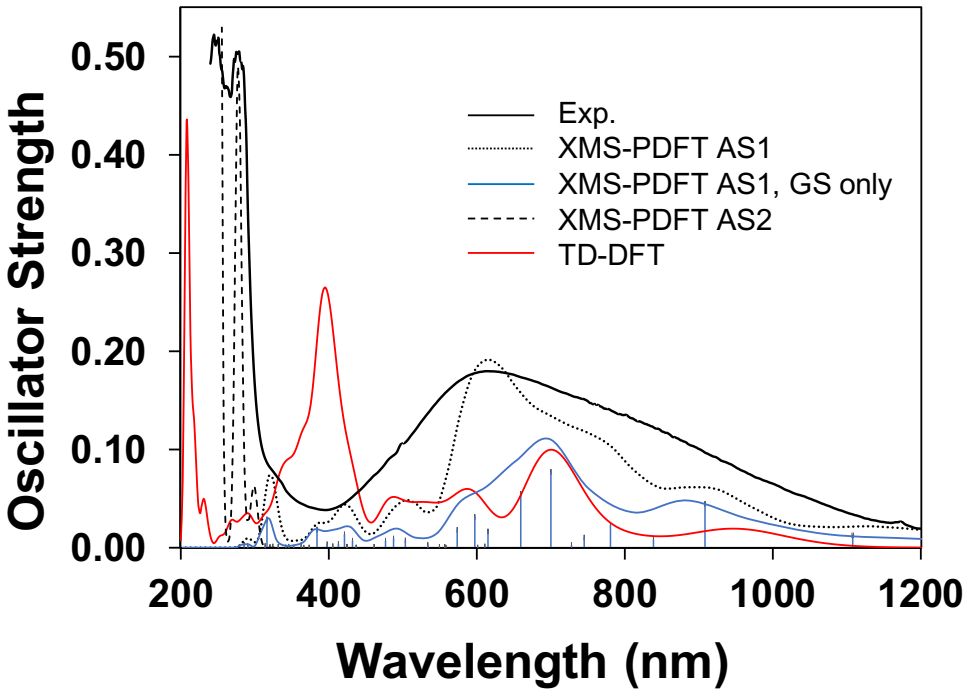


Figure S47. XMS-PDFT spectrum for AS1 (dotted), XMS-PDFT spectrum using ground state (GS) only of 47 state calculation (blue), and TD-DFT spectrum (red), where all are scaled to the XMS-PDFT intensities. The blue sticks are oscillator strengths for transitions from the ground XMS-PDFT state of the 47 state calculation. The dashed line corresponds to XMS-PDFT with AS2 for only the high energy region, shifted 35 nm.

Looking at Figure S48, the feature A_T clearly corresponds to A_x, where T and X refer for TD-DFT and XMS-PDFT, respectively. Looking at the M diagnostic,[39] which is a measure of multireference character in a wave function, the M value for the transitions in A_x at the CASSCF level are between 0.8-1.5 (Table S27). Significant multireference character corresponds to values of M > 0.1 and these states can therefore be challenging to describe correctly (right energy and character) with single reference methods, such as

TD-DFT. Not only are these excited states significantly multiconfigurational, the 1st and 2nd reference CASSCF states (states that contribute to ground XMS-PDFT states for AS2) also have large multireference character with an M value of about 0.6. Not only do the transitions in A_x have significant multireference character, there is also a substantial contribution from transitions from the 1st excited XMS-PDFT state (Fig S45). The region in the box B_x, in Fig. S48 is also dominated by transitions from the nearly degenerate XMS-PDFT state and this is the region where the TD-DFT intensity is the most inaccurate. Similarly to the A_X transitions, the M value for all the CASSCF reference states that make up the XMS-PDFT transitions in this region (states XMS 11-16) are significantly greater than 0.1, with many close to 1 or > 1 (Table S25). A hypothetical shifted TD-DFT spectrum is presented in Figure S49 and is in good much better agreement with XMS-PDFT.

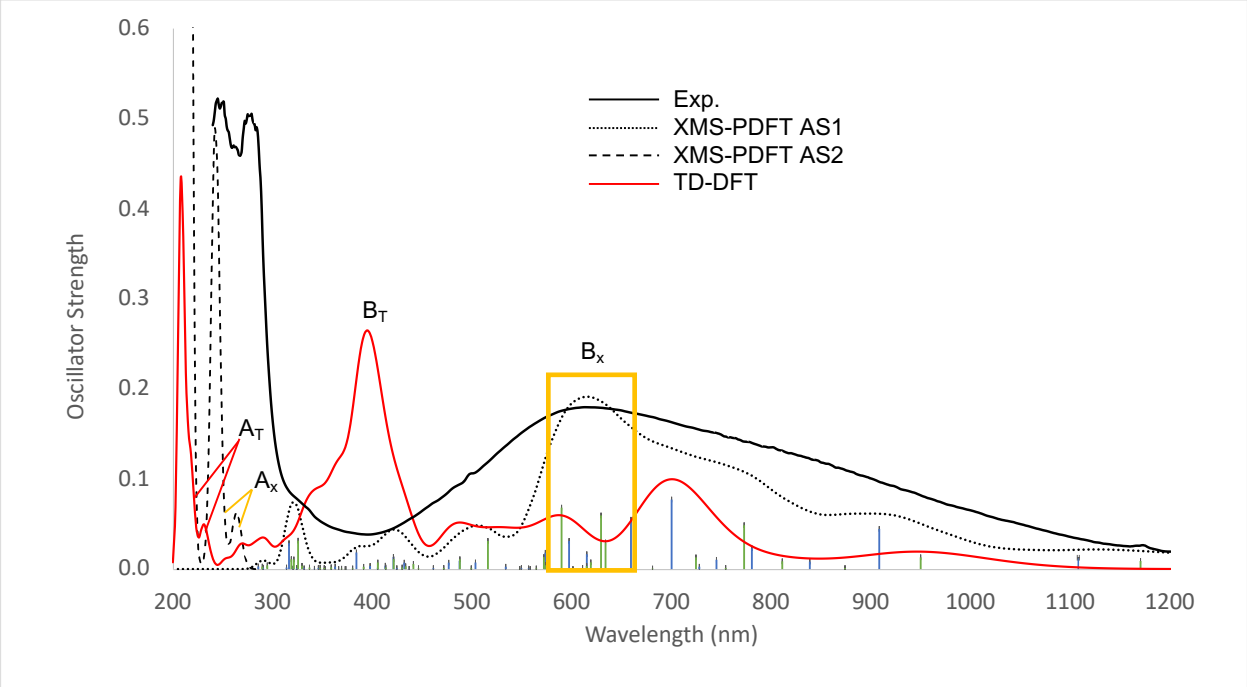


Figure S48. XMS-PDFT spectrum for AS1 (dotted), XMS-PDFT spectrum for AS2 at high energy (unshifted, dashed), and TD-DFT spectrum (red), where the intensities all are scaled to the XMS-PDFT intensities. The blue sticks are oscillator strengths for transitions from the ground XMS-PDFT state and the green are oscillator strengths for transitions from the 1st excited XMS-PDFT state of the 47 state calculation. A_T/B_T and A_x/B_x refer to groups of corresponding transitions between TD-DFT and XMS-PDFT, where T stands for TD-DFT and X stands for XMS-PDFT.

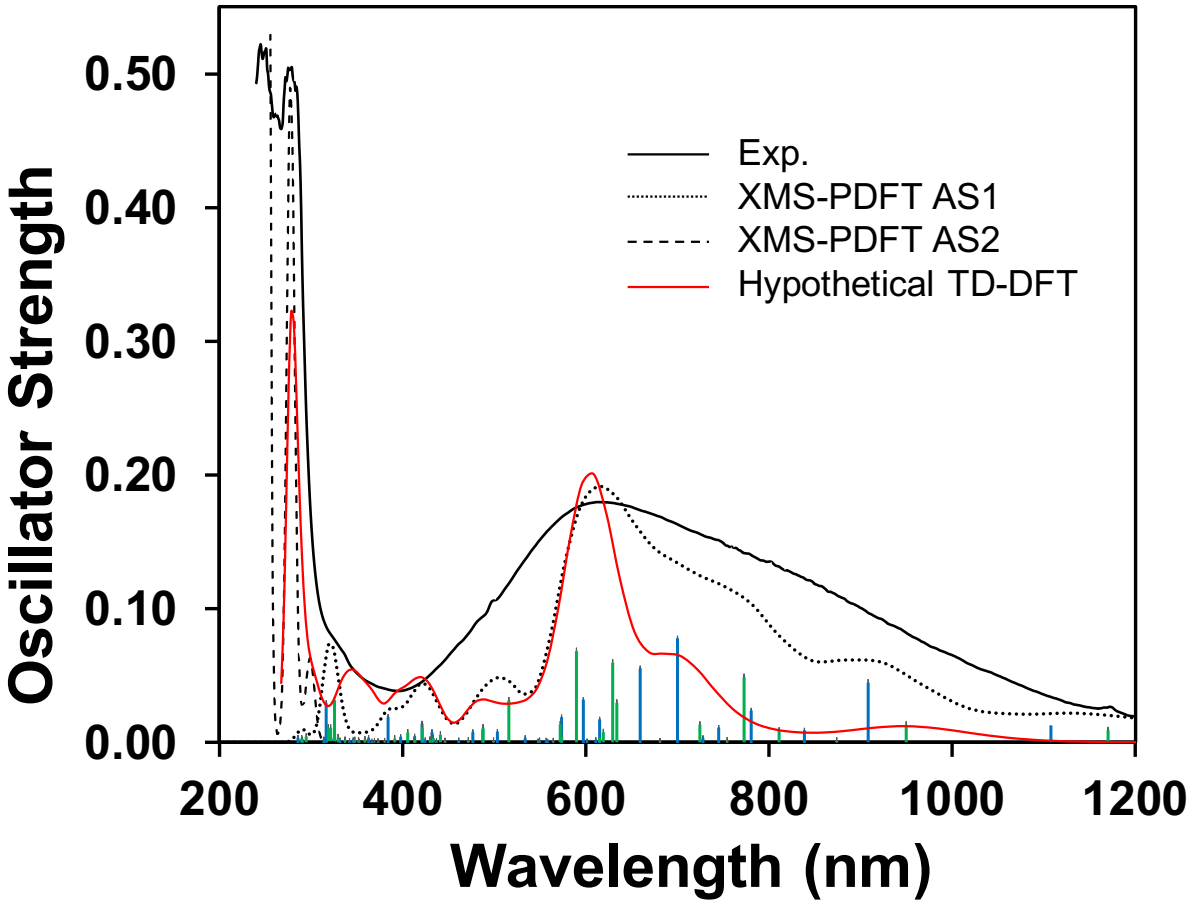


Figure S49. Hypothetical TDDFT spectrum, where the transitions around 200 nm in Fig 6 are red-shifted by 70 nm and those between 360-430 nm with oscillator strength > 0.01 are red-shifted by 215 nm.

Conclusions

The XMS-PDFT spectrum is in good agreement with the experimental spectrum for **2-Pr(NP*)** and there are two nearly degenerate states that contribute excitations to the spectrum. Each transition contains ligand to f transitions and the transitions in the 200-300 nm region also contain ligand to ligand transitions. We made a significant effort at the CASSCF level to get one active space that described the entire spectrum but could not get the orbital L6, in the same active space as the 47 state calculation. We think that if we were able to do so, the shift in energy found for XMS-PDFT for AS2 would be remediated. These states have very significant multireference character and regions of the spectrum that are dominated by excitations from the nearly degenerate XMS-PDFT state are the most poorly described by TD-DFT. The purpose of MC-PDFT was to be able to describe multiconfigurational wave functions accurately to do so at an affordable cost. This problem shows the promise of MC-PDFT for large applications and for the interested reader, the total time spent in the MC-PDFT module was ~24 hours and would be significantly greater for methods such as CASPT2.

Table S20. XMS-PDFT relative energies (cm^{-1}) and oscillator strengths from 47 state calculation for the ground state (state 1) and 1st excited state (state 2).

State	Rel. E (cm^{-1})	osc. strength	Rel. E (cm^{-1})	osc. strength
1	0.00			
2	497.0612	0.00001564	0.00	
3	7817.1305	0.00295011	7320.0693	0.0025437
4	9319.1379	0.01265071	8822.0767	0.0090081
5	11366.7996	0.04461763	10869.7384	0.0130847
6	12310.5694	0.00828895	11813.5082	0.0012369
7	13226.9964	0.02322543	12729.9352	0.0086705
8	13857.0355	0.01035117	13359.9743	0.0487863
9	14184.1369	0.00264888	13687.0757	0.0012203
10	14747.3796	0.07720792	14250.3184	0.0130833
11	15658.7706	0.05483312	15161.7094	0.0006018
12	16786.0691	0.01653620	16289.0079	0.0295390
13	16903.0374	0.00127735	16405.9762	0.0596087
14	17173.8213	0.00017004	16676.7601	0.0075350
15	17286.2758	0.03129714	16789.2146	0.0033811
16	18003.8487	0.01816191	17506.7875	0.0682376
17	18494.9765	0.00007877	17997.9153	0.0042779
18	18546.2144	0.00076773	18049.1532	0.0133637
19	18790.5202	0.00095160	18293.4590	0.0007419
20	19343.1975	0.00264995	18846.1363	0.0002158
21	20509.3819	0.00729930	20012.3207	0.0312989
22	21180.3642	0.00928975	20683.3030	0.0009573
23	21663.1896	0.00712442	21166.1284	0.0109815
24	22387.3168	0.00095261	21890.2556	0.0011809
25	23632.2601	0.00027110	23135.1989	0.0008205
26	23899.9978	0.00717943	23402.9366	0.0056483
27	24317.5109	0.00101888	23820.4497	0.0031564
28	24515.6581	0.01352048	24018.5969	0.0018383
29	24998.6361	0.00380037	24501.5749	0.0110812
30	25468.4676	0.00147563	24971.4064	0.0017309
31	25957.6836	0.00346055	25460.6224	0.0073351
32	26884.4883	0.01847093	26387.4271	0.0026104
33	27649.3634	0.00021229	27152.3022	0.0007212
34	28190.9820	0.00004435	27693.9208	0.0001538
35	28465.6360	0.00272362	27968.5748	0.0004711
36	29278.8905	0.00009975	28781.8293	0.0020107
37	29850.6982	0.00105246	29353.6370	0.0012196
38	30194.9555	0.00042019	29697.8943	0.0015911
39	31136.7367	0.00086462	30639.6755	0.0016932

40	31834.2306	0.00122305	31337.1694	0.0037089
41	32212.9149	0.00071355	31715.8537	0.0315884
42	32628.4823	0.02882238	32131.4211	0.0107686
43	32887.3302	0.00169618	32390.2690	0.0109694
44	35539.5975	0.00160865	35042.5363	0.0041996
45	36142.6517	0.00291741	35645.5905	0.0028041
46	53475.4369	0.00016567	52978.3757	0.0000935
47	54292.0501	0.00040032	53794.9889	0.0000497

Table S21. Natural orbital occupation numbers for 47 state calculation, labeled according to orbitals in Fig. S9, with difference from CAS state 1 in bold.

CAS ref.	l1	l2	l3	f1	f2	l4	l5	f3	l6	l7	f4
1	1.493	1.858	1.945	0.504	0.993	0.004	0.016	0.121	0.037	0.025	0.004
2	1.427	1.916	1.946	0.063	0.573	0.004	0.015	0.992	0.036	0.026	0.003
	-0.066	**0.058**	**0.001**	**-0.441**	**-0.420**	**-0.001**	**-0.001**	**0.871**	**-0.001**	**0.001**	**-0.001**
3	1.474	1.859	1.948	0.111	0.526	0.004	0.016	0.012	0.037	0.024	0.989
	-0.019	**0.001**	**0.003**	**-0.393**	**-0.467**	**0.000**	**0.000**	**-0.109**	**-0.001**	**0.000**	**0.985**
4	1.963	1.356	1.970	0.636	1.004	0.003	0.022	0.006	0.028	0.010	0.001
	0.470	**-0.501**	**0.025**	**0.132**	**0.011**	**-0.001**	**0.006**	**-0.115**	**-0.009**	**-0.015**	**-0.003**
5	1.067	1.969	1.959	0.006	0.934	0.002	0.010	0.996	0.031	0.026	0.001
	-0.426	**0.111**	**0.014**	**-0.499**	**-0.060**	**-0.002**	**-0.006**	**0.875**	**-0.006**	**0.001**	**-0.003**
6	1.892	1.170	1.965	0.045	0.832	0.002	0.023	0.101	0.029	0.011	0.932
	0.400	**-0.688**	**0.021**	**-0.460**	**-0.161**	**-0.002**	**0.007**	**-0.020**	**-0.009**	**-0.014**	**0.928**
7	1.677	1.308	1.967	0.291	0.694	0.002	0.019	0.927	0.028	0.015	0.072
	0.184	**-0.549**	**0.022**	**-0.214**	**-0.299**	**-0.002**	**0.003**	**0.806**	**-0.009**	**-0.010**	**0.068**
8	1.956	1.100	1.970	0.990	0.011	0.002	0.022	0.895	0.027	0.009	0.019
	0.463	**-0.758**	**0.026**	**0.485**	**-0.982**	**-0.003**	**0.006**	**0.774**	**-0.010**	**-0.016**	**0.015**
9	1.426	1.573	1.962	0.558	0.412	0.002	0.016	0.029	0.031	0.020	0.971
	-0.067	**-0.285**	**0.017**	**0.054**	**-0.581**	**-0.002**	**0.000**	**-0.092**	**-0.007**	**-0.005**	**0.967**
10	1.336	1.886	1.727	0.119	0.306	0.004	0.020	0.832	0.037	0.027	0.704
	-0.157	**0.029**	**-0.218**	**-0.385**	**-0.687**	**0.000**	**0.004**	**0.712**	**0.000**	**0.003**	**0.700**
11	1.683	1.909	1.326	0.144	0.699	0.005	0.025	0.852	0.039	0.030	0.289
	0.190	**0.051**	**-0.619**	**-0.361**	**-0.294**	**0.000**	**0.009**	**0.731**	**0.002**	**0.005**	**0.285**
12	1.746	1.809	1.388	0.188	0.640	0.005	0.025	0.832	0.039	0.028	0.299
	0.253	**-0.048**	**-0.557**	**-0.317**	**-0.354**	**0.001**	**0.009**	**0.712**	**0.002**	**0.004**	**0.295**
13	1.757	1.509	1.648	0.211	0.343	0.005	0.024	0.783	0.039	0.023	0.657
	0.264	**-0.349**	**-0.296**	**-0.293**	**-0.650**	**0.001**	**0.008**	**0.662**	**0.001**	**-0.002**	**0.653**
14	1.944	1.893	1.081	0.017	0.917	0.004	0.021	0.069	0.032	0.030	0.991
	0.451	**0.036**	**-0.864**	**-0.487**	**-0.077**	**0.000**	**0.005**	**-0.051**	**-0.005**	**0.005**	**0.987**
15	1.873	1.959	1.134	0.883	0.074	0.004	0.021	0.951	0.033	0.030	0.037
	0.381	**0.101**	**-0.811**	**0.379**	**-0.919**	**0.000**	**0.005**	**0.830**	**-0.005**	**0.005**	**0.033**
16	1.408	1.626	1.903	0.599	0.828	0.004	0.018	0.058	0.034	0.022	0.499
	-0.084	**-0.231**	**-0.042**	**0.094**	**-0.165**	**-0.001**	**0.002**	**-0.062**	**-0.003**	**-0.002**	**0.495**
17	1.662	1.346	1.923	0.753	0.404	0.003	0.020	0.078	0.031	0.017	0.764
	0.169	**-0.511**	**-0.021**	**0.249**	**-0.589**	**-0.001**	**0.003**	**-0.043**	**-0.007**	**-0.008**	**0.760**
18	1.944	1.017	1.970	0.293	1.356	0.003	0.022	0.091	0.028	0.010	0.267
	0.451	**-0.841**	**0.025**	**-0.212**	**0.363**	**-0.002**	**0.006**	**-0.030**	**-0.009**	**-0.015**	**0.263**
19	1.117	1.945	1.904	0.972	0.045	0.003	0.015	0.899	0.035	0.027	0.037

	-0.376	**0.087**	**-0.040**	**0.468**	**-0.948**	**-0.001**	**-0.001**	**0.778**	**-0.002**	**0.002**	**0.033**
20	1.910	1.968	1.061	0.041	0.011	0.004	0.016	0.947	0.031	0.029	0.982
	0.417	**0.110**	**-0.884**	**-0.464**	**-0.982**	**0.000**	**0.000**	**0.826**	**-0.006**	**0.004**	**0.978**
21	1.228	1.952	1.776	0.977	0.089	0.004	0.018	0.559	0.037	0.028	0.332
	-0.265	**0.095**	**-0.169**	**0.473**	**-0.905**	**-0.001**	**0.002**	**0.438**	**0.000**	**0.003**	**0.328**
22	1.792	1.838	1.307	0.918	0.047	0.005	0.025	0.223	0.038	0.029	0.777
	0.299	**-0.019**	**-0.637**	**0.413**	**-0.946**	**0.001**	**0.009**	**0.102**	**0.001**	**0.004**	**0.773**
23	1.890	1.253	1.844	0.582	0.070	0.005	0.023	1.058	0.033	0.016	0.227
	0.397	**-0.604**	**-0.101**	**0.077**	**-0.923**	**0.000**	**0.007**	**0.937**	**-0.004**	**-0.009**	**0.223**
24	1.917	1.340	1.665	0.164	0.415	0.005	0.026	0.637	0.038	0.021	0.774
	0.424	**-0.518**	**-0.280**	**-0.341**	**-0.579**	**0.001**	**0.009**	**0.516**	**0.000**	**-0.004**	**0.770**
25	1.934	1.602	1.377	0.366	0.876	0.006	0.025	0.209	0.040	0.027	0.537
	0.441	**-0.256**	**-0.568**	**-0.138**	**-0.117**	**0.002**	**0.009**	**0.088**	**0.002**	**0.002**	**0.533**
26	1.139	1.884	1.923	0.518	0.171	0.003	0.014	0.051	0.034	0.026	1.238
	-0.354	**0.026**	**-0.022**	**0.013**	**-0.822**	**-0.001**	**-0.002**	**-0.070**	**-0.003**	**0.001**	**1.234**
27	1.965	1.017	1.958	0.474	0.125	0.002	0.022	0.005	0.028	0.009	1.396
	0.472	**-0.841**	**0.013**	**-0.030**	**-0.868**	**-0.002**	**0.006**	**-0.116**	**-0.010**	**-0.015**	**1.392**
28	1.929	1.958	1.261	0.671	0.078	0.004	0.018	1.011	0.032	0.029	0.008
	0.436	**0.101**	**-0.684**	**0.167**	**-0.915**	**0.000**	**0.002**	**0.890**	**-0.005**	**0.005**	**0.004**
29	1.933	1.961	1.001	0.151	0.050	0.004	0.017	0.701	0.031	0.029	1.120
	0.440	**0.104**	**-0.943**	**-0.354**	**-0.943**	**0.000**	**0.001**	**0.580**	**-0.006**	**0.005**	**1.116**
30	1.457	1.891	1.847	0.387	0.819	0.006	0.020	0.202	0.038	0.028	0.305
	-0.036	**0.034**	**-0.098**	**-0.117**	**-0.174**	**0.002**	**0.004**	**0.081**	**0.001**	**0.003**	**0.301**
31	1.844	1.935	1.261	0.497	0.154	0.005	0.022	0.097	0.035	0.029	1.122
	0.351	**0.078**	**-0.684**	**-0.008**	**-0.839**	**0.001**	**0.005**	**-0.024**	**-0.002**	**0.005**	**1.118**
32	1.401	1.801	1.878	0.892	0.163	0.005	0.020	0.578	0.039	0.026	0.197
	-0.092	**-0.057**	**-0.066**	**0.388**	**-0.831**	**0.001**	**0.004**	**0.457**	**0.002**	**0.001**	**0.193**
33	1.317	1.836	1.946	0.560	0.121	0.005	0.017	0.918	0.035	0.025	0.220
	-0.176	**-0.022**	**0.002**	**0.055**	**-0.872**	**0.000**	**0.001**	**0.797**	**-0.002**	**0.001**	**0.216**
34	1.283	1.808	1.934	0.915	0.167	0.004	0.016	0.247	0.033	0.024	0.567
	-0.210	**-0.050**	**-0.010**	**0.411**	**-0.826**	**0.000**	**0.000**	**0.126**	**-0.004**	**0.000**	**0.563**
35	1.196	1.819	1.951	1.037	0.076	0.003	0.014	0.623	0.032	0.024	0.225
	-0.297	**-0.038**	**0.006**	**0.532**	**-0.917**	**-0.002**	**-0.002**	**0.502**	**-0.005**	**0.000**	**0.221**
36	1.231	1.744	1.958	0.164	0.194	0.002	0.014	0.707	0.031	0.023	0.932
	-0.262	**-0.114**	**0.013**	**-0.341**	**-0.799**	**-0.002**	**-0.002**	**0.586**	**-0.006**	**-0.002**	**0.928**
37	1.869	1.296	1.968	0.111	0.054	0.002	0.021	1.071	0.028	0.011	0.567
	0.376	**-0.561**	**0.023**	**-0.394**	**-0.939**	**-0.002**	**0.005**	**0.950**	**-0.009**	**-0.013**	**0.563**
38	1.867	1.153	1.966	0.956	0.157	0.002	0.021	0.612	0.028	0.012	0.225
	0.374	**-0.704**	**0.021**	**0.452**	**-0.837**	**-0.002**	**0.005**	**0.491**	**-0.009**	**-0.013**	**0.220**
39	1.908	1.121	1.968	0.960	0.836	0.003	0.021	0.056	0.028	0.011	0.087
	0.415	**-0.736**	**0.024**	**0.455**	**-0.157**	**-0.001**	**0.005**	**-0.065**	**-0.010**	**-0.014**	**0.083**
40	1.935	1.066	1.971	0.031	1.077	0.002	0.021	0.050	0.026	0.010	0.812
	0.442	**-0.791**	**0.026**	**-0.474**	**0.084**	**-0.002**	**0.005**	**-0.071**	**-0.011**	**-0.015**	**0.808**
41	1.938	1.884	1.168	0.075	0.944	0.005	0.025	0.869	0.037	0.030	0.026
	0.445	**0.026**	**-0.777**	**-0.429**	**-0.049**	**0.001**	**0.009**	**0.748**	**-0.001**	**0.005**	**0.022**
42	1.918	1.950	1.119	0.352	0.039	0.005	0.020	1.046	0.033	0.030	0.490
	0.425	**0.092**	**-0.826**	**-0.152**	**-0.955**	**0.000**	**0.004**	**0.925**	**-0.005**	**0.005**	**0.486**
43	1.898	1.939	1.250	0.182	0.927	0.005	0.024	0.127	0.036	0.030	0.581
	0.405	**0.081**	**-0.694**	**-0.322**	**-0.067**	**0.001**	**0.008**	**0.007**	**-0.001**	**0.005**	**0.577**
44	1.953	1.923	1.162	0.056	0.801	0.005	0.020	0.986	0.034	0.030	0.032

	0.460	**0.065**	**-0.783**	**-0.449**	**-0.193**	**0.000**	**0.004**	**0.865**	**-0.004**	**0.005**	**0.028**
45	1.910	1.950	1.154	0.999	0.120	0.005	0.022	0.033	0.034	0.030	0.744
	0.417	**0.093**	**-0.791**	**0.495**	**-0.873**	**0.000**	**0.005**	**-0.087**	**-0.003**	**0.005**	**0.740**
46	1.946	1.834	1.859	0.935	0.167	0.009	0.023	0.108	0.045	0.027	0.048
	0.453	**-0.024**	**-0.086**	**0.431**	**-0.827**	**0.005**	**0.007**	**-0.013**	**0.008**	**0.002**	**0.044**
47	1.915	1.940	1.639	0.414	0.861	0.007	0.026	0.105	0.043	0.029	0.020

Table S22. Configurations with CI coefficient above 0.31 for 47 CASSCF reference states and types of transitions at the CASSCF level, relative to CAS state 1

state	Transition	Config. 1	CI coef.	Config. 2	CI coef.	Config. 3	CI coef.
1		u22du000000	0.5498	u22ud000000	-0.3571		
2	f-f	u220d00u000	0.5009	u22du000000	0.3805	2220000u000	-0.3333
3		u220d00000u	-0.6298	2220000000u	0.3822		
4	L-L	2u2du000000	0.7214	2u2ud000000	-0.3939		
5	f-f, L-f	u220d00u000	-0.4854	u22d000u000	-0.4707		
6	L-L, f-f, L-f	2u20d00000u	-0.4881	u220d00000u	-0.4254	u22d000000u	-0.3167
7	L-f, f-f	2u20d00u000	-0.5664	u22d000u000	0.4096	2u20u00d000	0.3258
8	f-L, L-f, f-f	2u2d000u000	0.62622	2u2u000d000	-0.3721		
9	f-f, L-f	u22d000000u	-0.5714	2u20d00000u	0.4342		
10	f-f, L-f	u220000d00u	0.5975	u220000u00d	-0.3332		
11	L-f, f-f	22udu000000	-0.4681	22u0d00u000	0.3478		
12	L-f, f-f	22u0d00u000	-0.3718	22udu000000	-0.3568		
13	L-f, f-f	2u20000d00u	-0.4678	22u0d00u000	0.3799		
14	f-L, L-f, f-f	22u0d00000u	-0.6790				
15	f-L, L-f, f-f	22ud000u000	0.6791				
16	f-f, L-f	u2202000000	-0.4125	u22ud000000	-0.3767	2u2d000000u	0.3774
17	f-L, L-f, f-f	2u2d000000u	0.4714	2u20000d00u	0.3528		
18	f-L, L-f, f-f	2u202000000	-0.5418	2u2ud000000	-0.5268		
19	f-f, L-f	u220u00d000	-0.4393	u22u000d000	0.4126	u220000u00d	-0.4106
20	f-L, L-f, f-f	22u0000d00u	-0.5356	22ud000000u	0.4552	22u0000u00d	0.3201
21	f-f, L-f	u22u000000d	-0.4984	u2200002000	0.3827		
22	f-L, L-f, f-f	22ud000000u	0.4966				
23	f-L, L-f, f-f	2u20000u00d	-0.4080	2u20u00d000	-0.3789		
24	f-L, L-f, f-f	2u200002000	-0.3313	2u2u000000d	0.3284		
25	f-L, L-f or L-L and f-f	22u02000000	0.4328	22uud000000	0.3408		
26	f-f, L-f	u22u000000d	0.3196	u2200000002	-0.5549		
27	f-L, L-f, f-f	2u200000002	-0.5470	2u2u000000d	0.4514		
28	f-L, L-f, f-f	22uu000d000	0.4356	22u0000u00d	-0.3958		
29	f-L, L-f, f-f	22u00002000	-0.4825	22uu000000d	0.4466		
30	f-f	u22u000000d	-0.3972	u2202000000	0.3481	2220u000000	-0.3672
31	f-L, L-f, f-f	22u00000002	-0.5287	22uu000000d	0.3726		
32	f-f	u2220000000	0.3773	u220000u00d	-0.3401		
33	f-f	u22u000d000	0.3786	u220000u00d	0.3727		
34	f-f	u220u00000d	-0.4085				
35	f-f, L-f	u220u00d000	0.4568	u22u000d000	0.3998	u2220000000	-0.3229
36	f-f , L-f	u220u00000d	0.4040	u220u00d000	-0.3720		
37	f-L, L-f, f-f	2u20000u00d	0.4070	2u20u00000d	-0.3863		
38	f-L, L-f, f-f	2u220000000	0.4244	u2220000000	-0.3752	2u20u00d000	-0.3333
39	f-L, L-f, f-f	2u202000000	-0.4851				

40	L-f, f-L	2u20u00000d	-0.5464	2u20000u00d	-0.3676		
41	L-f, f-L	22u00002000	-0.4274	22uud000000	-0.3303	22u02000000	0.3262
42	f-L, L-f, f-f	22uu000d000	-0.4380	22u0000u00d	-0.4353		
43	f-L, L-f, f-f or L-L, f-f	22u0u00000d	-0.4944				
44	f-L, L-f,	22u0u00d000	0.5712	22uu000d000	0.3884		
45	f-f, f-L	22u20000000	-0.4721	22u00000002	0.3526		
46	f-L, f-f	222u0000000	0.6591				
47	f-L	2220u000000	-0.5730				

Table S23. Sum of the change in electrons for the f shell and ligand shells, relative to CAS 1 and CAS 3, along with the net total number of electrons excited in each CAS state.

	Relative to CAS 1			Relative to CAS 3		
state	sum f	sum L	tot	sum f	sum L	tot
1						
2	0.01	-0.01	-0.93			
3	0.02	-0.01	-0.99			
4	0.03	-0.01	-0.64	0.01	0.01	-1.52
5	0.31	-0.30	-1.00	0.30	-0.29	-1.51
6	0.29	-0.27	-1.35	0.27	-0.25	-0.84
7	0.36	-0.34	-1.08	0.35	-0.33	-1.49
8	0.29	-0.27	-1.77	0.28	-0.26	-2.27
9	0.35	-0.33	-1.04	0.33	-0.32	-0.48
10	0.34	-0.35	-1.45	0.32	-0.33	-0.86
11	0.36	-0.38	-1.27	0.35	-0.36	-1.32
12	0.34	-0.35	-1.28	0.32	-0.34	-1.30
13	0.37	-0.38	-1.59	0.36	-0.37	-1.17
14	0.37	-0.38	-1.48	0.36	-0.36	-0.97
15	0.32	-0.33	-1.73	0.31	-0.31	-2.22
16	0.36	-0.36	-0.59	0.35	-0.34	-0.84
17	0.38	-0.36	-1.18	0.36	-0.35	-0.90
18	0.38	-0.36	-1.11	0.37	-0.35	-1.59
19	0.33	-0.33	-1.37	0.32	-0.31	-1.84
20	0.36	-0.36	-2.34	0.34	-0.34	-1.48
21	0.34	-0.34	-1.34	0.32	-0.33	-1.51
22	0.34	-0.36	-1.60	0.33	-0.34	-1.35
23	0.31	-0.31	-1.64	0.30	-0.29	-1.94
24	0.37	-0.37	-1.72	0.35	-0.36	-1.13
25	0.37	-0.38	-1.08	0.35	-0.37	-1.28
26	0.36	-0.35	-1.27	0.34	-0.34	-0.72
27	0.38	-0.36	-1.88	0.36	-0.34	-1.28
28	0.15	-0.15	-1.60	0.13	-0.13	-2.12
29	0.40	-0.40	-2.25	0.38	-0.38	-1.43
30	0.09	-0.10	-0.43	0.08	-0.09	-0.80

31	0.25	-0.26	-1.56	0.23	-0.24	-1.06
32	0.21	-0.22	-1.05	0.19	-0.20	-1.36
33	0.20	-0.20	-1.07	0.18	-0.18	-1.36
34	0.27	-0.27	-1.10	0.26	-0.25	-1.04
35	0.34	-0.33	-1.26	0.32	-0.31	-1.54
36	0.37	-0.36	-1.53	0.36	-0.35	-0.76
37	0.18	-0.16	-1.92	0.17	-0.15	-1.48
38	0.33	-0.31	-1.56	0.31	-0.29	-1.86
39	0.32	-0.30	-0.98	0.30	-0.28	-1.66
40	0.32	-0.30	-0.98	0.33	-0.31	-1.08
41	0.29	-0.31	-1.26	0.28	-0.29	-1.78
42	0.30	-0.31	-1.94	0.29	-0.29	-1.82
43	0.20	-0.21	-1.08	0.18	-0.19	-1.11
44	0.25	-0.26	-1.43	0.24	-0.24	-1.80
45	0.27	-0.28	-1.75	0.26	-0.27	-1.45
46	-0.36	0.34	-0.95	-0.38	0.36	-1.41
47	-0.22	0.20	-0.54	-0.24	0.21	-1.28

Table S24. Selected XMS-PDFT eigenvectors (columns) with coefficients of reference states larger than 0.31 (rows) for 47 state calculation

CAS Ref.	XMS-PDFT State																			
	1	2	4	5	7	8	10	11	12	13	15	16	21	23	28	29	32	41	42	43
1	0.60	-0.59																		
2		0.36																		
3	0.60	0.55																		
4			0.83																	
5			-0.33		-0.77															
6				0.90																
7					-0.34															
8						-0.34	0.48													
9						-0.68														
10						-0.35	-0.50		-0.31											
11							0.33			-0.45	-0.34									
12									-0.33	0.36										
13										0.38		0.37								
14												-0.47								
15								0.44		0.40										
16								0.53			-0.43	-0.35								
17											-0.54									
18											0.35			-0.34						
19												-0.39								
20								-0.33	-0.59	-0.41										
21														-0.62						
25													-0.86							
26																0.45				

28																-0.58				
29															-0.62					
30															-0.62					
31																0.40				
34																	-0.38			
35																	-0.73			
40																			0.32	
41																			-0.62	0.32
42																				0.67
43																		0.74		
44																			-0.39	-0.42

Table S25. M diagnostic values for the main CAS reference wave functions (rows) that contribute to the XMS-PDFT states (columns)

CAS Ref.	XMS-PDFT State																			
	1	2	4	5	7	8	10	11	12	13	15	16	21	23	28	29	32	41	42	43
1	0.63	0.50																		
2		0.50																		
3	0.61	0.61																		
4			0.39																	
5			0.39		0.31															
6				0.11																
7					0.65															
8						0.14	0.14													
9						0.87														
10						0.69	0.69		0.69											
11							1.33			1.33	1.33									
12									0.23	0.23										
13										0.88		0.88								
14												0.17								
15								0.25		0.25										
16								1.09			1.09	1.09								
17											0.79									
18											0.48			0.48						
19												1.12								
20								0.13	0.13	0.13										
21														0.85						
25													0.57							
26																0.57				
28																0.37				
29															1.21					
30															1.37					
31																0.82				
34																	1.33			
35																	1.36			
40																			0.22	
41																			1.12	1.12
42																				0.69
43																		1.12		

44																		0.25	0.25

Table S26. Selected Natural Orbital occupations for states from 43 SA-CASSCF calculation

CAS ref.	L1	P1	L2	F1	F2	L3	L4	L5	L6	F3	F4
1	1.922	1.992	1.325	0.147	0.853	0.008	0.016	0.050	0.000	0.532	0.154
2	1.923	1.992	1.268	0.780	0.220	0.008	0.016	0.050	0.000	0.516	0.226
37	1.082	1.992	1.004	0.438	0.563	0.009	0.003	0.001	0.930	0.543	0.436
38	1.080	1.992	1.001	0.587	0.410	0.009	0.004	0.001	0.934	0.571	0.413
39	1.158	1.992	1.055	0.621	0.353	0.009	0.002	0.002	0.845	0.581	0.382
40	1.159	1.992	1.048	0.592	0.389	0.009	0.003	0.001	0.842	0.557	0.409

Table S27. Selected Configurations from 43 SA-CASSCF calculation with CI coefficients above 0.31, and M diagnostic values

state	Transition	Config. 1	CI coef.	Config. 2	CI coef.	Config. 3	CI coef.	M
1		22u0d0000u0	-0.6769					0.58
2		22u02000000	-0.4311	2220u000000	0.4243			0.64
37	L-F, L-f	0220u000du0	-0.4084	2200u000du0	0.4067	220u0000d0u	-0.3974	1.52
38	L-F, L-f	220u0000du0	-0.4365	022u0000du0	0.4387	2200u000d0u	-0.3665	1.49
39	L-F, L-f	u2u0d000du0	-0.4448	u2ud0000du0	0.4004	u2ud0000d0u	0.3756	1.03
40	L-F, L-f	u2ud0000du0	0.4397	u2u0d000du0	0.4081	u2u0d000d0u	0.3773	0.82

Table S28. XMS-PDFT total energies (hartees) for 47 state and 43 state calculations

State	Energy (hartrees)	Energy (hartrees)
1	-11788.047708	-11788.016297
2	-11788.045444	-11788.009104
3	-11788.012091	-11788.004201
4	-11788.005247	-11788.003882
5	-11787.995917	-11788.000009
6	-11787.991617	-11787.996431
7	-11787.987442	-11787.995249
8	-11787.984571	-11787.993850
9	-11787.983081	-11787.990595
10	-11787.980514	-11787.990170
11	-11787.976362	-11787.984791
12	-11787.971225	-11787.983211
13	-11787.970693	-11787.977845
14	-11787.969459	-11787.976346
15	-11787.968946	-11787.971466
16	-11787.965677	-11787.965159
17	-11787.963439	-11787.963514
18	-11787.963206	-11787.959236
19	-11787.962093	-11787.955712

20	-11787.959574	-11787.955113
21	-11787.954261	-11787.940402
22	-11787.951204	-11787.938066
23	-11787.949004	-11787.932953
24	-11787.945704	-11787.927580
25	-11787.940032	-11787.926503
26	-11787.938812	-11787.923041
27	-11787.936910	-11787.922871
28	-11787.936007	-11787.920308
29	-11787.933806	-11787.914573
30	-11787.931666	-11787.913363
31	-11787.929437	-11787.830828
32	-11787.925214	-11787.822648
33	-11787.921729	-11787.816279
34	-11787.919261	-11787.813407
35	-11787.918009	-11787.800379
36	-11787.914304	-11787.799099
37	-11787.911699	-11787.791346
38	-11787.910130	-11787.791232
39	-11787.905839	-11787.790362
40	-11787.902661	-11787.789582
41	-11787.900936	-11787.789310
42	-11787.899042	-11787.783047
43	-11787.897863	-11787.781664
44	-11787.885778	
45	-11787.883030	
46	-11787.804056	
47	-11787.800336	

Table S29. Cartesian coordinates of the computed **1-Ln(NP*)** and **2-Ln(NP*)**, Ln=Pr, Nd, Dy, complexes at the DFT level.

1-Pr(NP*)				**2-Pr(NP*)**			
Pr	0.02207800	-0.03618300	-0.00959200	Pr	-0.01104900	0.00112100	0.00141000
P	0.50414500	2.80784000	-2.58774900	P	1.10840700	0.03480800	-3.54860800
P	3.26601600	-2.13702600	0.17806100	N	2.73671500	-0.34878400	-3.76475400
P	-0.74661400	1.68284200	3.35107000	N	0.78622900	1.31662300	-4.62160400
P	-3.01238700	-2.25541700	-0.83386700	N	0.73342000	0.17294300	-2.04263900
N	-0.50537700	0.90701100	2.04793300	N	0.24592400	-1.06424400	-4.55221900
N	0.32737300	1.65089900	-1.59285800	C	3.60075700	-0.69812200	-2.65293700
N	3.20159500	-3.54957600	1.14758100	H	3.83347200	-1.77342300	-2.67265300
N	-0.28289900	0.82466300	4.74964100	H	3.02240600	-0.52640000	-1.74286300
N	1.96612800	-1.32118600	0.19393700	C	4.90135500	0.09156000	-2.60435200
N	-1.72385700	-1.44275200	-0.65131500	H	5.48362400	-0.20659500	-1.72794600
N	3.94868500	-2.74676900	-1.30571000	H	4.71397200	1.16501900	-2.53392300
N	0.16747500	2.37727600	-4.20228300	H	5.53041400	-0.08418800	-3.48235800
C	3.07624800	-3.26958300	-2.37902200	C	1.28148300	2.70064400	-4.55831200

N	1.99215200	3.67600400	-2.67362500	C	1.79359500	3.13179300	-5.93706900
N	-2.32451500	2.31683000	3.75426500	H	2.57453500	2.45414500	-6.29322400
N	-2.94866100	-3.31961300	-2.17790300	H	2.21951900	4.13757100	-5.87797400
N	-3.65444200	-3.25100700	0.44785500	H	0.99722300	3.15978200	-6.68597900
N	4.77900400	-1.41403400	0.58070100	C	-0.08138000	-2.45114400	-4.16514000
N	-0.36487100	4.30850800	-2.43258500	C	2.43068300	2.82306600	-3.56360100
N	-0.05552600	3.23327200	3.60877300	H	2.14576600	2.45212000	-2.57740900
C	5.01373800	-1.85363700	-1.72520300	H	2.71241600	3.87521200	-3.46429600
H	4.63214200	-0.92827700	-2.18331400	H	3.30631400	2.26788400	-3.90196800
H	5.67466400	-2.34065300	-2.44857500	C	-0.76544000	-0.33321100	-5.29423800
C	3.32504300	3.06778200	-2.61756300	H	-1.64914000	-0.10243500	-4.67993700
C	-4.40893000	-4.51441800	-3.82403900	H	-1.09994400	-0.90147300	-6.16637900
H	-4.68654900	-3.57759000	-4.31556700	C	0.14990700	3.63311100	-4.11898800
H	-5.26755800	-5.19344600	-3.87288700	H	-0.70601200	3.57998900	-4.79826100
H	-3.60093200	-4.97065400	-4.40246700	H	0.48844200	4.67421200	-4.09715000
C	-0.03348600	-0.60068000	4.68611100	H	-0.19136000	3.35470700	-3.12126700
H	0.02190000	-0.85274800	3.62467000	C	-0.08221000	0.94998700	-5.72032500
H	-0.88154600	-1.17186500	5.10050500	H	0.48801100	0.78493800	-6.64854400
C	4.41323900	-4.28503900	1.45743800	H	-0.82456200	1.72983100	-5.92249300
H	4.40327000	-4.53505600	2.52965600	C	-0.10335100	-3.31342600	-5.43197300
H	5.27237000	-3.62256100	1.31453200	H	-0.88310300	-3.00291800	-6.13293500
C	2.00548600	-4.17729300	-1.77658100	H	-0.30000000	-4.35850400	-5.17434400
H	2.45562500	-4.99629700	-1.21302900	H	0.85801200	-3.26134000	-5.94937300
H	1.39286800	-4.59990500	-2.57866800	C	3.30380800	-0.39230500	-5.10128000
H	1.34879400	-3.61876100	-1.10674500	H	4.06298400	0.39762100	-5.20863100
N	-4.54290000	-1.49469000	-1.00831400	H	2.51020900	-0.14525400	-5.80826900
C	2.39488000	-2.14863900	-3.17183000	C	0.98635100	-3.01406500	-3.23097700
H	1.80777800	-1.51732700	-2.50250600	H	1.02428200	-2.46637800	-2.28715500
H	1.72802200	-2.56575700	-3.93237800	H	1.97689700	-2.98086400	-3.68683800
H	3.12131600	-1.51460700	-3.68864200	H	0.75170000	-4.05768600	-3.00635300
C	5.10303900	-0.66614500	1.79840900	C	3.91641400	-1.72887300	-5.49481900
C	5.77371600	-1.51502900	-0.45767100	H	4.72822000	-2.02741700	-4.82552200
H	6.51691800	-2.30250100	-0.24047300	H	4.33381100	-1.66495900	-6.50435200
H	6.32333100	-0.57416500	-0.58908200	H	3.16674600	-2.52325000	-5.49187500
C	3.29921800	1.66750800	-3.22799800	C	-1.44082300	-2.53791700	-3.46758100
H	2.62987600	1.00993300	-2.67049300	H	-1.47730100	-1.89079100	-2.58692500
H	4.30638600	1.24022100	-3.19727200	H	-1.63374800	-3.56542700	-3.14774400
H	2.97014300	1.69276800	-4.26909600	H	-2.25881200	-2.25115100	-4.13581700
C	0.23472600	3.35612700	-5.26557500	P	1.08782000	3.06046200	1.82120200
H	0.34360500	4.33768700	-4.80126400	N	0.97127200	4.47856500	0.91543100
H	-0.72921100	3.38977600	-5.79807600	N	0.53937200	3.46079400	3.38218100
C	-4.01258900	-4.28167600	-2.37171300	N	0.47303000	1.83752100	1.07653500
H	-4.88370700	-3.93144900	-1.81535300	N	2.71592100	3.00487900	2.37137200
H	-3.74188700	-5.25458400	-1.92225500	C	0.53500400	4.47629100	-0.46839000
C	2.08513900	-3.74673400	2.04869100	H	1.38301600	4.69032900	-1.13610000
H	1.28069200	-3.09458400	1.70251100	H	0.21793600	3.45605900	-0.69304500
H	2.34540400	-3.40884700	3.06838400	C	-0.59330100	5.45371000	-0.76727400
C	-5.51727200	-1.90264400	-0.02516000	H	-0.87955900	5.37873200	-1.82008900
H	-6.23265700	-2.63825600	-0.43338900	H	-1.47721900	5.23958600	-0.16293500
H	-6.10121100	-1.05137200	0.34517000	H	-0.30464400	6.49366200	-0.58658200
C	-0.03033200	0.99112900	-4.57246000	C	-0.82673800	3.80811300	3.80475600
H	-0.18415900	0.44190300	-3.64047900	C	-0.79352200	5.05884300	4.69004300
H	0.87994100	0.56845700	-5.03093800	H	-0.32432700	5.89603300	4.16581300
C	-2.54396300	3.27020700	-2.86592300	H	-1.81270200	5.35416500	4.95557400
H	-2.40847000	3.41739300	-3.94000000	H	-0.24982100	4.89189600	5.62407500
H	-3.61181500	3.33027100	-2.63699600	C	3.84606600	2.51844000	1.55483000
H	-2.19874900	2.26807300	-2.60715100	C	-1.71323800	4.10102200	2.59910500
C	-2.78578200	-4.08046900	1.29909100	H	-1.70909600	3.27139200	1.88961800
C	-1.32619800	0.98855100	7.03134400	H	-2.74196700	4.25651800	2.93632000
H	-2.32324400	1.24715700	6.66876800	H	-1.38717000	5.00216000	2.07860000
H	-1.18395700	1.46869700	8.00609000	C	2.72660300	2.66023900	3.78183200
H	-1.28996700	-0.09391100	7.19088500	H	2.56709800	1.58435400	3.95038500

C	-1.79410500	4.33604400	-2.07184800	H	3.67693500	2.93697700	4.24617700
C	1.86510200	5.08650300	-2.38966900	C	-1.43533100	2.64323300	4.58950500
H	1.96149200	5.69285200	-3.30630200	H	-0.83273800	2.38494300	5.46518000
H	2.63415500	5.43384400	-1.68913300	H	-2.44013000	2.89501900	4.94428600
C	2.25202700	2.39222500	3.50187000	H	-1.50015900	1.76155400	3.95074400
H	2.21696800	2.02682000	4.53089500	C	1.58477600	3.45356400	4.38376200
H	3.28117200	2.67963000	3.26913700	H	1.92015400	4.47501500	4.62493500
H	1.96615600	1.57339400	2.83915400	H	1.24491900	2.98837800	5.31551900
C	-2.11791200	-3.26718200	2.41278400	C	5.10593900	3.28799000	1.96630400
H	-1.56655100	-2.42718200	1.98466100	H	5.38510700	3.10255400	3.00720500
H	-1.42123200	-3.88920100	2.98438700	H	5.95456400	2.98289900	1.34654300
H	-2.85268900	-2.86828000	3.11805500	H	4.95753000	4.36364700	1.84148400
C	1.24450000	-1.04066800	5.38595600	C	1.36495300	5.74962500	1.49788800
H	1.20113900	-0.89847000	6.47115900	H	0.48541900	6.40548200	1.58796500
H	2.10932800	-0.49264600	5.00516200	H	1.70354000	5.55809300	2.51742400
H	1.41697400	-2.10605800	5.20484200	C	3.59214100	2.78690100	0.07383500
C	-1.66152500	-3.64921500	-2.76385200	H	2.72671700	2.23120100	-0.29296700
H	-1.56498700	-4.74526000	-2.82011700	H	3.42653600	3.84771400	-0.11971900
H	-0.88226000	-3.29272900	-2.08765900	H	4.46531600	2.46972700	-0.50210200
C	4.63571800	-5.54913000	0.63511400	C	2.46179500	6.48848700	0.74455700
H	3.81500800	-6.26204600	0.74667800	H	2.17540500	6.72040500	-0.28512300
H	5.56294300	-6.04871100	0.94138000	H	2.68182900	7.43770200	1.24268000
H	4.72037200	-5.28788100	-0.42131800	H	3.38395300	5.90367100	0.71547300
C	3.92476600	-4.11752500	-3.33343300	C	4.07899100	1.01842200	1.74942500
H	4.65300200	-3.51951100	-3.88871300	H	3.17965400	0.44312200	1.51286200
H	3.27901800	-4.60351700	-4.07140500	H	4.88752400	0.67684600	1.09749500
H	4.46482000	-4.89525900	-2.78555700	H	4.37476900	0.78393100	2.77673400
C	-3.54756900	1.52928600	3.51008600	P	-3.73288300	-0.28683400	-0.17408500
C	6.49780800	-1.05929400	2.30270000	N	-4.52837500	0.18804100	1.23573400
H	6.55796800	-2.13381500	2.49858700	N	-4.53428000	-1.68959000	-0.70990600
H	6.71722500	-0.53332500	3.23711800	N	-2.18409900	-0.29776200	0.00298600
H	7.28416000	-0.79841900	1.58808400	N	-4.44638400	0.64249000	-1.43377700
C	1.33505200	3.59836800	3.31844600	C	-3.81407100	0.70980700	2.38581500
C	-4.94001800	-0.49871700	-2.00973000	H	-3.99134500	1.79106900	2.48756100
C	4.09485000	-0.97628900	2.90149500	H	-2.75015400	0.59219900	2.17090700
H	3.07264300	-0.78278300	2.56901500	C	-4.16165500	0.02237300	3.69892400
H	4.30043600	-0.34452100	3.77070100	H	-3.56768000	0.45161400	4.51061500
H	4.16180300	-2.02015400	3.21790800	H	-3.94945100	-1.04804800	3.65699300
C	-2.36536300	3.71141500	3.35520100	H	-5.21424200	0.14741800	3.97082700
H	-2.48908100	3.83647900	2.26833600	C	-4.55037600	-3.02175100	-0.08524100
H	-3.18531300	4.24081500	3.85043600	C	-5.98746300	-3.55165200	-0.03241500
C	0.49016700	5.27744400	-1.77362300	H	-6.63868100	-2.86106400	0.51062300
H	0.54665400	5.11821600	-0.68599800	H	-6.01027800	-4.51536200	0.48447500
H	0.13426100	6.29798300	-1.94571700	H	-6.40913000	-3.70734600	-1.02925900
C	-3.88314200	-0.36743000	-3.10189900	C	-4.06068300	2.03253800	-1.75067400
H	-2.90752200	-0.12105000	-2.67800500	C	-4.01142200	-2.96219900	1.33998700
H	-4.17560800	0.42941900	-3.79194900	H	-3.01525300	-2.51703900	1.37159900
H	-3.77759500	-1.29593900	-3.66383600	H	-3.94496900	-3.97630100	1.74403100
C	4.30857600	3.92346500	-3.42396200	H	-4.66989900	-2.38154700	1.98701200
H	3.97511400	4.02951800	-4.46032800	C	-4.73670200	-0.23021500	-2.55746000
H	5.29670800	3.45270200	-3.42956800	H	-3.83869700	-0.46083000	-3.15078300
H	4.42682100	4.92638100	-3.00321700	H	-5.47499200	0.22188000	-3.22509800
C	-1.02781000	4.28739000	3.78457800	C	-3.68053200	-3.98307400	-0.89925300
H	-0.78904800	5.16721100	3.17521300	H	-4.02105800	-4.05937500	-1.93595700
H	-1.07592400	4.61950600	4.83592900	H	-3.70529500	-4.99004700	-0.46990900
C	-3.63020100	-5.20048300	1.91830200	H	-2.64837500	-3.63101800	-0.90655100
H	-4.37751400	-4.82020800	2.62058500	C	-5.28373900	-1.49772100	-1.93368800
H	-2.98790700	-5.89039100	2.47476400	H	-6.36159900	-1.38643000	-1.73414600
H	-4.14833200	-5.76337400	1.13636600	H	-5.15962800	-2.34484000	-2.61717900
C	5.07920200	0.83766500	1.51181000	C	-5.29269800	2.76279900	-2.29628800
H	5.78318600	1.10271200	0.71705300	H	-5.65098400	2.33034900	-3.23457400
H	5.35400700	1.41447100	2.40175900	H	-5.05240400	3.81120200	-2.49667100

H	4.08110500	1.14007400	1.19402600	H	-6.11145400	2.72931900	-1.57286500
C	-0.25901100	1.45856500	6.04989600	C	-5.97837700	0.13745600	1.30673600
H	-0.36078900	2.53392500	5.89303600	H	-6.28727600	-0.59968200	2.06357300
H	0.73339400	1.31707900	6.50585800	H	-6.34567900	-0.24035500	0.35120700
C	1.35004500	3.13760800	-6.28086900	C	-3.59996800	2.76245800	-0.49156500
H	1.30800100	3.90392300	-7.06292600	H	-2.69543200	2.31427600	-0.07547700
H	1.27398600	2.16290600	-6.77298600	H	-4.37134200	2.75873500	0.27999000
H	2.32999900	3.19613200	-5.80249900	H	-3.37622600	3.80262100	-0.74214800
C	-5.12336800	0.87206100	-1.34788700	C	-6.65351100	1.46884800	1.60350900
H	-5.87639900	0.84639700	-0.55478500	H	-6.33123000	1.89481000	2.55783700
H	-5.44869700	1.61560500	-2.08331900	H	-7.73809100	1.33327200	1.65748800
H	-4.18190100	1.20719700	-0.90966900	H	-6.44597300	2.20041900	0.81938200
C	-6.25996600	-0.92476600	-2.66565600	C	-2.93717800	2.08517400	-2.78840600
H	-6.16334100	-1.91577800	-3.11861400	H	-2.05979400	1.52610000	-2.45199100
H	-6.53829100	-0.21554300	-3.45165900	H	-2.63784800	3.12156300	-2.96543300
H	-7.08489400	-0.95810400	-1.94719500	H	-3.25523600	1.67431200	-3.75161300
C	-1.70594600	-4.73493500	0.44167100	P	1.53778800	-2.80350500	1.90042900
H	-2.14814200	-5.29852900	-0.38375000	N	0.82224200	-4.30486000	1.61641600
H	-1.12290500	-5.42808900	1.05266800	N	3.21518000	-3.08917400	1.95146000
H	-1.02232900	-3.98870500	0.03254300	N	0.96882400	-1.69735200	0.96248400
C	-2.01752100	4.09805100	-0.57408300	N	1.48828400	-2.59606300	3.60767700
H	-1.56717600	3.15223400	-0.26507700	C	-0.32374900	-4.46033200	0.74033200
H	-3.08835800	4.06950900	-0.34596600	H	-1.23061900	-4.66495600	1.32914000
H	-1.57549000	4.89706900	0.02973200	H	-0.48200800	-3.49272200	0.26014300
C	-3.32381900	0.08418900	3.94919700	C	-0.15915200	-5.54698500	-0.31304400
H	-2.55708800	-0.39398400	3.33707000	H	-1.04780700	-5.58366300	-0.94939600
H	-4.25367800	-0.48036400	3.82933300	H	0.70464800	-5.35497000	-0.95287200
H	-3.02126100	0.02619500	4.99596600	H	-0.03836500	-6.54151100	0.12707900
C	1.46262600	4.11493300	1.88162400	C	4.10434800	-3.48799400	0.84871800
H	1.14146100	3.34714900	1.17373600	C	4.99500200	-4.65300200	1.29443500
H	2.49620900	4.39460700	1.65023800	H	4.39115500	-5.50030500	1.63092900
H	0.83933100	5.00191200	1.72554700	H	5.61364800	-4.98971800	0.45751300
C	-2.37538400	5.69965800	-2.46354500	H	5.67178100	-4.37131300	2.10591300
H	-1.97075900	6.51649300	-1.85910100	C	0.30290700	-2.11344700	4.34420900
H	-3.45999500	5.69811900	-2.31681200	C	3.29919100	-3.94002100	-0.36454400
H	-2.16946600	5.91503200	-3.51626300	H	2.58657800	-3.17500200	-0.67788000
C	3.80359300	2.95920400	-1.16743900	H	3.97995000	-4.13450800	-1.19820700
H	3.84535800	3.93981900	-0.68203700	H	2.74953900	-4.85822000	-0.15402500
H	4.80478500	2.52007400	-1.11130200	C	2.78269400	-2.12080800	4.06231100
H	3.11423800	2.32724500	-0.60511500	H	2.92533100	-1.04649900	3.86930400
C	-4.72519100	-2.52848000	1.10527200	H	2.90909200	-2.29067000	5.13497800
H	-4.35262400	-1.74179100	1.77920600	C	4.98182800	-2.30163100	0.44113000
H	-5.35982800	-3.20240600	1.68928400	H	5.58084400	-1.93298200	1.27888200
C	1.78734700	4.68324800	4.30269900	H	5.67402300	-2.58527100	-0.35846800
H	1.21605700	5.60963400	4.19239200	H	4.35428700	-1.48290600	0.08709900
H	2.84083800	4.92622500	4.13258000	C	3.79110300	-2.92667200	3.26973000
H	1.67930800	4.33674100	5.33508500	H	3.96493300	-3.89906600	3.75769900
C	1.60701400	-5.18920000	2.12638300	H	4.75173700	-2.40187000	3.22607100
H	0.73488800	-5.25990700	2.78451500	C	0.30473500	-2.75545100	5.73587500
H	2.37418100	-5.85530700	2.53456200	H	1.17041000	-2.45373100	6.33202200
H	1.32226200	-5.56336200	1.13979700	H	-0.58867600	-2.45525900	6.29176200
C	-1.41295800	-3.02687600	-4.13177900	H	0.31094700	-3.84558500	5.65675300
H	-2.19322600	-3.27418700	-4.85606300	C	1.31248500	-5.48661400	2.30413100
H	-0.45494900	-3.36839500	-4.53965700	H	1.73881500	-6.19081200	1.57324000
H	-1.36831800	-1.94012400	-4.03952100	H	2.14091200	-5.17937700	2.94471400
C	-1.20563600	0.76861800	-5.51467500	C	-0.98015100	-2.53449000	3.63261100
H	-2.13359100	1.15419200	-5.08598600	H	-1.06093400	-2.07602000	2.64499200
H	-1.33913400	-0.30099600	-5.69937800	H	-1.03698400	-3.61743500	3.51361600
H	-1.05815500	1.24835200	-6.48811400	H	-1.84071500	-2.21288200	4.22484700
C	-3.95776000	1.52751800	2.03460100	C	0.27796700	-6.21400000	3.15112400
H	-4.18626700	2.53447000	1.67232400	H	-0.57765300	-6.55458500	2.56119600
H	-4.85511800	0.91784800	1.88757800	H	0.72850900	-7.09868100	3.61139400

H	-3.15329400	1.11191300	1.42437300	H	-0.09747300	-5.57400800	3.95272500
C	-4.68355700	2.11101600	4.35876400	C	0.30778000	-0.58988800	4.48747100
H	-4.38741100	2.16862600	5.41042900	H	0.35888800	-0.09913100	3.51162100
H	-5.57068300	1.47414600	4.28390900	H	-0.60307500	-0.25788200	4.99277500
H	-4.97808700	3.11207600	4.03089600	H	1.15316800	-0.24191400	5.08909900
1-Nd(NP*)				**2-Nd(NP*)**			
Nd	0.01880800	-0.02324700	-0.02759000	Nd	-0.07456200	0.02113600	0.08233300
P	0.24501400	3.45863300	-1.65769200	P	1.92104300	0.84786800	3.19570500
P	3.32094600	-1.91934300	-0.62754100	N	3.41827000	0.06820200	3.35854900
P	-0.55869400	0.53097100	3.72944400	N	1.21714300	0.78067100	4.74824300
P	-2.99921600	-1.99998700	-1.32145400	N	1.14240800	0.36413500	1.94897300
N	-0.38956500	0.21494200	2.23665400	N	2.28949600	2.52540000	3.41285400
N	0.16651700	2.03929800	-1.07647700	C	3.93626900	-0.79733500	2.32010800
N	3.36663100	-3.55621200	-0.12032600	H	4.80044300	-0.32743400	1.82235100
N	0.00718100	-0.70351100	4.76055900	H	3.14747000	-0.87565400	1.56866400
N	2.00078500	-1.21019300	-0.29796800	C	4.33500200	-2.18662700	2.80002200
N	-1.72386600	-1.22616500	-0.96322400	H	4.69380100	-2.78462200	1.95667800
N	3.92022700	-2.03132000	-2.26078100	H	3.48596000	-2.71020000	3.24466800
N	-0.25222800	3.56264000	-3.28451400	H	5.14049400	-2.15906400	3.54051400
C	2.99742000	-2.26852600	-3.39154000	C	0.63566500	-0.39055700	5.41858900
N	1.72161700	4.34877100	-1.59905300	C	1.06350800	-0.40474000	6.89021600
N	-2.11815100	0.94723800	4.39955200	H	2.15379700	-0.40431000	6.97759400
N	-2.99354000	-2.58603100	-2.93401000	H	0.68401500	-1.30589700	7.38071700
N	-3.52316800	-3.37748100	-0.38670800	H	0.67602600	0.45509400	7.44379600
N	4.83534500	-1.27093000	-0.11445300	C	2.76519400	3.38763200	2.31367600
N	-0.59745600	4.80511500	-0.94652200	C	1.12248500	-1.68325800	4.77132700
N	0.11896900	1.94769200	4.42442900	H	0.90656400	-1.69833900	3.70128900
C	4.91815400	-0.99477100	-2.45509400	H	0.61612900	-2.53459300	5.23536200
H	4.47033000	0.00205100	-2.58849500	H	2.19758000	-1.80977000	4.90899600
H	5.54079200	-1.20521000	-3.32985700	C	1.30430900	3.10151500	4.31062200
C	3.04682300	3.77857600	-1.86317700	H	0.34072500	3.28966600	3.81157800
C	-4.52122300	-3.28506900	-4.79055300	H	1.65746700	4.04776200	4.73001800
H	-4.85953500	-2.25733700	-4.95040300	C	-0.89177800	-0.33631000	5.32756400
H	-5.35975600	-3.95780900	-5.00284100	H	-1.29107800	0.57737500	5.77783000
H	-3.73940400	-3.49926900	-5.52436300	H	-1.34613400	-1.18604400	5.84773400
C	0.28494000	-2.02566800	4.23832900	H	-1.19986800	-0.36035600	4.28120100
H	0.29129200	-1.92818600	3.15029800	C	1.12125500	2.06707800	5.40308000
H	-0.52759400	-2.72991000	4.48533400	H	1.89959000	2.18741400	6.17417700
C	4.61767500	-4.29051900	-0.11180600	H	0.14966000	2.19923400	5.89216100
H	4.68977000	-4.84325500	0.83780200	C	3.60462000	4.52027800	2.91504000
H	5.44466300	-3.57413400	-0.10293000	H	3.01482700	5.17603000	3.56124800
C	1.99679000	-3.36194500	-3.02205400	H	4.02326900	5.14500200	2.11986800
H	2.50725100	-4.28554200	-2.74415000	H	4.42978800	4.11402300	3.50601200
H	1.34747700	-3.56552800	-3.87896800	C	4.23585800	0.27985100	4.53773800
H	1.36727000	-3.05179200	-2.18580800	H	4.32956100	-0.66156100	5.10164600
N	-4.55911700	-1.29838800	-1.16197000	H	3.70061100	0.96891500	5.19282400
C	2.23065200	-1.00328600	-3.79109500	C	3.66300900	2.59386600	1.36608400
H	1.66923400	-0.61714700	-2.93834700	H	3.10737600	1.79036300	0.87810400
H	1.52839300	-1.21941400	-4.60167600	H	4.51040400	2.15330900	1.89359600
H	2.90140800	-0.21455100	-4.14384300	H	4.05186300	3.26460700	0.59456200
C	5.22945700	-0.91753200	1.25206300	C	5.62649400	0.83663500	4.26590700
C	5.75628400	-1.00816200	-1.19194600	H	6.21551200	0.18388200	3.61480600
H	6.53714000	-1.78566900	-1.26512100	H	6.17828000	0.94236100	5.20520000
H	6.26527200	-0.04369200	-1.06758400	H	5.57068000	1.82200600	3.79742800
C	2.95299200	2.69095000	-2.93188500	C	1.60612400	3.98454000	1.50976500
H	2.31162100	1.87284600	-2.59965100	H	0.95203500	3.20129200	1.11770700
H	3.95118900	2.28662600	-3.12726100	H	1.98998900	4.56954600	0.66872400
H	2.55463600	3.08504500	-3.86904900	H	0.99724300	4.66050900	2.11788200
C	-0.29520900	4.83468500	-3.97280300	P	-1.72369200	-3.39691200	0.20793800
H	-0.17859300	5.61698100	-3.22082100	N	-2.42741000	-3.70414800	1.71740800
H	-1.29893000	4.98603200	-4.40064400	N	-2.85925900	-3.98037300	-0.92848600

C	-4.03747400	-3.49327600	-3.36119600	N	-1.15115200	-1.96651300	0.07767200
H	-4.88053700	-3.37674300	-2.67812900	N	-0.70564400	-4.77084200	-0.08057800
H	-3.70735800	-4.54255700	-3.25237600	C	-2.29299000	-2.77637900	2.82243500
C	2.31850600	-4.06636600	0.73885900	H	-1.62025100	-3.18588400	3.59186400
H	1.47460100	-3.37920200	0.64947800	H	-1.79632500	-1.88990900	2.42314200
H	2.63629100	-4.03639700	1.79691400	C	-3.61292400	-2.38365600	3.47172100
C	-5.45491700	-2.04504400	-0.31213400	H	-3.43326000	-1.65800500	4.27002000
H	-6.17017400	-2.65064500	-0.89640800	H	-4.29053500	-1.92633100	2.74738600
H	-6.04190300	-1.38513600	0.33798100	H	-4.12722300	-3.23791900	3.92303200
C	-0.46280300	2.36248400	-4.06731700	C	-4.15702900	-3.38781300	-1.28107500
H	-0.53428700	1.53792500	-3.35371800	C	-5.21874600	-4.48856500	-1.38199700
H	0.41156100	2.14300400	-4.70370800	H	-5.28790300	-5.04885300	-0.44531900
C	-2.81233500	3.89956300	-1.49502600	H	-6.19805600	-4.04504000	-1.58418600
H	-2.77563900	4.37346200	-2.47862000	H	-5.00900900	-5.19650900	-2.18889200
H	-3.85469200	3.85943100	-1.16560600	C	0.67135300	-4.86619800	0.44000200
H	-2.44811200	2.87550600	-1.59058400	C	-4.60793100	-2.38970700	-0.21897700
C	-2.57497100	-4.38664300	0.11316600	H	-3.85458900	-1.61700700	-0.05413900
C	-0.89038600	-1.31069400	7.02953300	H	-5.53093200	-1.90324500	-0.54760200
H	-1.91562200	-0.99680700	6.82275100	H	-4.80485200	-2.88824900	0.73113300
H	-0.69655800	-1.15563700	8.09690300	C	-0.92950400	-5.24605300	-1.43156400
H	-0.81589900	-2.38555200	6.83569100	H	-0.42235900	-4.62292700	-2.18726800
C	-1.99044400	4.68703700	-0.47827300	H	-0.57685000	-6.27416700	-1.55426800
C	1.63626400	5.57354900	-0.83735500	C	-4.04524500	-2.65797500	-2.62305100
H	1.66329700	6.45846600	-1.49519500	H	-3.70511500	-3.32811400	-3.41883500
H	2.46569600	5.67272800	-0.12625900	H	-5.01311200	-2.24709100	-2.92899700
C	2.43092300	1.25796200	3.95724500	H	-3.32988600	-1.83867200	-2.53549000
H	2.45710200	0.59029000	4.82154500	C	-2.43038300	-5.16821300	-1.63081200
H	3.44105200	1.63679600	3.77905200	H	-2.91157500	-6.07577900	-1.23032200
H	2.12413700	0.67671800	3.08580700	H	-2.67045800	-5.11508000	-2.69927800
C	-1.86514800	-3.93089100	1.39216900	C	1.02616400	-6.34688500	0.61368900
H	-1.36922200	-2.97231600	1.22458800	H	1.04352300	-6.88643600	-0.33750400
H	-1.11419300	-4.66472700	1.70264600	H	2.02039800	-6.44766300	1.05966300
H	-2.56661800	-3.81106900	2.22286500	H	0.30334200	-6.83889000	1.26959100
C	1.60640400	-2.61584800	4.70958700	C	-3.13692800	-4.94559900	1.96229900
H	1.61640400	-2.82072400	5.78552300	H	-4.19643300	-4.73355800	2.17475200
H	2.43950700	-1.94662600	4.48287100	H	-3.12741000	-5.52289000	1.03653600
H	1.79041200	-3.56495500	4.19700500	C	0.77278300	-4.19471900	1.80796900
C	-1.73974600	-2.65207600	-3.66399300	H	0.57266100	-3.12355300	1.74259200
H	-1.61469900	-3.67003600	-4.06643800	H	0.07135200	-4.63263500	2.51961800
H	-0.92708200	-2.48542400	-2.95444300	H	1.78438900	-4.32737000	2.20152700
C	4.82111500	-5.24668800	-1.28148900	C	-2.56664600	-5.80236100	3.08413400
H	4.03136600	-5.99973300	-1.34001600	H	-2.55668800	-5.27728100	4.04363600
H	5.78115900	-5.76887800	-1.18799900	H	-3.17337400	-6.70422500	3.21287900
H	4.82730100	-4.68418200	-2.21685500	H	-1.54446200	-6.11464200	2.85827300
C	3.80962100	-2.76518000	-4.59315800	C	1.68418400	-4.20837100	-0.50303700
H	4.48446300	-1.99966300	-4.98665700	H	1.41524200	-3.16469000	-0.68565400
H	3.13401200	-3.04651600	-5.40692800	H	2.68575000	-4.23862800	-0.06431400
H	4.40506400	-3.64224700	-4.32341500	H	1.73642800	-4.72891000	-1.46518000
C	-3.34011800	0.22992700	3.99028800	P	-2.53201100	2.83920200	-0.45535300
C	6.66475300	-1.38641100	1.52588600	N	-3.82852400	2.46365500	-1.48319100
H	6.76296800	-2.46574800	1.37809400	N	-2.13085900	4.45311800	-0.85939700
H	6.93768300	-1.16195000	2.56178900	N	-1.44482200	1.74201400	-0.43500100
H	7.39268400	-0.88613300	0.88018400	N	-3.28543000	3.37920400	1.00729800
C	1.48531800	2.43055000	4.19995200	C	-3.97128800	1.14632400	-2.06713600
C	-5.05561100	-0.06504600	-1.78260800	H	-4.82064200	0.61092800	-1.61497700
C	4.30822700	-1.59155300	2.26519200	H	-3.07407400	0.58832000	-1.79047200
H	3.26080900	-1.35495700	2.06571900	C	-4.13793700	1.15109800	-3.58124100
H	4.55525100	-1.24145200	3.27185300	H	-4.20720600	0.12434500	-3.95282600
H	4.42481400	-2.67789100	2.24612600	H	-3.28876700	1.63387600	-4.07115400
C	-2.21074500	2.39400100	4.46170400	H	-5.04736900	1.66994700	-3.90018600
H	-2.40899400	2.84702700	3.47827800	C	-1.41744500	4.91850800	-2.05298900
H	-3.00557400	2.71051200	5.14431700	C	-2.05391200	6.21668300	-2.56135200

C	0.32085900	5.51858000	-0.07885400	H	-3.11618800	6.06846300	-2.77518900
H	0.47070200	5.00788200	0.88419200	H	-1.56300200	6.53958400	-3.48440700
H	-0.04073400	6.53007700	0.13068800	H	-1.96209700	7.03364900	-1.84036900
C	-4.07283200	0.45849400	-2.82489900	C	-3.74145500	2.45514100	2.06398500
H	-3.08334000	0.61496500	-2.39040100	C	-1.49889700	3.88327500	-3.17151000
H	-4.43791300	1.41275000	-3.21551900	H	-1.11823800	2.91500600	-2.83984400
H	-3.96597400	-0.24112600	-3.65443100	H	-0.90090800	4.22146700	-4.02359100
C	3.97851000	4.87892300	-2.38297100	H	-2.52820700	3.75003400	-3.50822000
H	3.56583400	5.34804700	-3.28099700	C	-2.62553900	4.59463400	1.44703800
H	4.95363100	4.45235100	-2.63814800	H	-1.65021800	4.39593400	1.91940100
H	4.14965800	5.66348700	-1.64011800	H	-3.24238900	5.14110400	2.16604900
C	-0.85860900	2.85895500	4.97268700	C	0.05643200	5.16481000	-1.71520500
H	-0.67632200	3.89241100	4.65406400	H	0.16910100	5.90656500	-0.91901500
H	-0.84411600	2.84856700	6.07619600	H	0.60491300	5.53402800	-2.58895500
C	-3.34085400	-5.68634300	0.38721400	H	0.51198200	4.23383100	-1.37299800
H	-4.05445500	-5.58486600	1.20988600	C	-2.42602100	5.40960700	0.18445100
H	-2.64197600	-6.48197400	0.66419800	H	-3.33649600	5.98855000	-0.04187700
H	-3.88841200	-6.00127300	-0.50593700	H	-1.60726900	6.12541300	0.32170200
C	5.15636400	0.59990200	1.44523600	C	-4.90853500	3.11043800	2.81104600
H	5.79683200	1.12390800	0.72939700	H	-4.60889200	4.02482700	3.33061300
H	5.48442600	0.88512200	2.45087500	H	-5.30573500	2.42616700	3.56710000
H	4.13302500	0.94691300	1.30020500	H	-5.71438000	3.36297100	2.11690400
C	0.09742300	-0.50793100	6.19124100	C	-4.86682600	3.43949600	-1.75337500
H	-0.04443600	0.55640300	6.38692400	H	-4.86249000	3.70385200	-2.82296700
H	1.12075700	-0.73843300	6.52686900	H	-4.60871000	4.35471400	-1.21857300
C	0.74170900	5.01751700	-5.07462900	C	-4.25287200	1.15330200	1.45068500
H	0.60307800	5.98487700	-5.57040300	H	-3.45851300	0.61470400	0.93009700
H	0.66728500	4.24175200	-5.84327700	H	-5.06099800	1.33724200	0.74102600
H	1.75357600	4.98963300	-4.66519100	H	-4.63691900	0.50698600	2.24443300
C	-5.25216000	1.02025500	-0.71764600	C	-6.27275800	3.01303800	-1.35399500
H	-5.95633200	0.70905600	0.05960100	H	-6.59263000	2.10152100	-1.86740600
H	-5.64753600	1.93658600	-1.16888400	H	-6.99011600	3.79932100	-1.60953000
H	-4.30018700	1.25333600	-0.23811900	H	-6.33804100	2.83598400	-0.27804800
C	-6.39541200	-0.33946300	-2.47821000	C	-2.62363400	2.12866200	3.05903600
H	-6.28831500	-1.13379900	-3.22257700	H	-1.74522600	1.72540500	2.54818900
H	-6.74823800	0.56205800	-2.98919300	H	-2.96823800	1.39031100	3.78839300
H	-7.17333000	-0.64006100	-1.76946700	H	-2.30972000	3.01403000	3.62078600
C	-1.53058700	-4.68212800	-0.95994700	P	2.45303100	-0.26629100	-3.06596200
H	-2.00516100	-4.98205500	-1.89770800	N	2.91469800	1.21644300	-3.66541900
H	-0.88582700	-5.49960400	-0.62849400	N	3.82666700	-1.23597700	-3.11284300
H	-0.90110700	-3.81015800	-1.14665400	N	1.59153500	-0.10716400	-1.74194900
C	-2.08555800	3.99509300	0.88605700	N	1.64063000	-1.20386200	-4.21156400
H	-1.61371900	3.01059500	0.85230300	C	2.33091200	2.46784600	-3.18774400
H	-3.13339800	3.87198300	1.17980100	H	1.73560700	2.92683600	-3.98746400
H	-1.59295200	4.58010000	1.66925600	H	1.63262900	2.21438500	-2.38949200
C	-3.06124300	-1.27016600	3.93562000	C	3.36491600	3.46082700	-2.68279500
H	-2.32990100	-1.50155700	3.15921000	H	2.86068300	4.35111900	-2.30022300
H	-3.98704500	-1.80356000	3.69890300	H	3.95757700	3.03572700	-1.87003500
H	-2.68663900	-1.64283900	4.89020800	H	4.04939400	3.79034500	-3.47014600
C	1.52815100	3.36989000	2.99006900	C	4.98587000	-1.17349100	-2.19976100
H	1.18603400	2.84599900	2.09447400	C	6.26605500	-1.39353900	-3.00892700
H	2.54281700	3.74304900	2.81194100	H	6.36765800	-0.63890800	-3.79388900
H	0.88000800	4.23924800	3.14359500	H	7.13949200	-1.32223800	-2.35518700
C	-2.59724700	6.09180900	-0.38047200	H	6.29171000	-2.38081100	-3.47846800
H	-2.13115900	6.69522100	0.40374700	C	0.27189200	-0.99084800	-4.73440000
H	-3.66317400	6.02207900	-0.14166800	C	5.06379000	0.19319400	-1.52672600
H	-2.49023100	6.62143600	-1.33173400	H	4.16413100	0.41286500	-0.94546500
C	3.63182500	3.16098400	-0.59067000	H	5.90683800	0.20245000	-0.83140800
H	3.71232600	3.89780500	0.21554100	H	5.21611300	0.99336100	-2.25274000
H	4.63340400	2.75675700	-0.77050800	C	2.18184900	-2.55613100	-4.21789500
H	2.98589200	2.34894700	-0.25177100	H	1.72953200	-3.17181000	-3.43071500
C	-4.57183200	-2.95330300	0.51954400	H	1.98940600	-3.03743000	-5.17925800

H	-4.18179900	-2.40030200	1.38770000	C	4.85931800	-2.24442200	-1.11428000
H	-5.14543100	-3.80792400	0.89187400	H	4.81847800	-3.25353600	-1.53376000
C	1.97084300	3.17221100	5.45079500	H	5.71923400	-2.20796100	-0.43900700
H	1.37977300	4.06890100	5.65881900	H	3.95262900	-2.08222600	-0.52915400
H	3.00987600	3.48871400	5.31728200	C	3.67413800	-2.39347300	-3.97982000
H	1.92261200	2.52055600	6.32862600	H	4.20305600	-2.24231200	-4.93206800
C	1.88756400	-5.48722300	0.40540500	H	4.08110300	-3.29358600	-3.51238000
H	1.06070300	-5.79044700	1.05593300	C	0.29683000	-1.22909100	-6.24863500
H	2.69745700	-6.20863800	0.55544900	H	0.56661400	-2.25666300	-6.50604400
H	1.55224100	-5.56391200	-0.63191000	H	-0.69509300	-1.04333400	-6.66891500
C	-1.60454700	-1.62386400	-4.77968400	H	1.00658800	-0.55627700	-6.73677800
H	-2.42745200	-1.66981600	-5.49760900	C	3.88078900	1.30811700	-4.75469900
H	-0.66938200	-1.77613200	-5.33008700	H	4.76429700	1.86257700	-4.41158900
H	-1.58131900	-0.61887800	-4.35426800	H	4.22736500	0.29801300	-4.97854000
C	-1.70795200	2.41227700	-4.94215600	C	-0.18497900	0.44193400	-4.48546700
H	-2.59964800	2.62192600	-4.34685500	H	-0.25822800	0.67007900	-3.42002400
H	-1.85398600	1.44920800	-5.43935600	H	0.48612400	1.16602900	-4.95200000
H	-1.63814800	3.17355600	-5.72643300	H	-1.17718900	0.57832000	-4.92090900
C	-3.84844300	0.67613200	2.61629300	C	3.33332000	1.95226500	-6.01888400
H	-4.12269300	1.73545000	2.60554800	H	3.03482100	2.99172500	-5.86063100
H	-4.74015500	0.10681400	2.33480800	H	4.10095200	1.95011100	-6.79790600
H	-3.07789500	0.50758700	1.86122800	H	2.46708300	1.40407900	-6.39747000
C	-4.42694400	0.47115200	5.04374300	C	-0.70912800	-1.95709100	-4.07252800
H	-4.06244400	0.20512200	6.04040600	H	-0.71848000	-1.84014600	-2.98495100
H	-5.30598700	-0.14232900	4.82202400	H	-1.72002300	-1.77125500	-4.44316400
H	-4.75988300	1.51275400	5.06800400	H	-0.46935000	-3.00001300	-4.30058200
1-Dy(NP*)				**2-Dy(NP*)**			
Dy	-0.00000700	0.03667200	0.00123300	Dy	-0.03749100	-0.07643200	0.06322800
P	-3.00592100	2.16341900	-0.62282300	P	-2.11527700	1.73787800	2.52582200
N	-1.72197100	1.33652800	-0.49506300	N	-1.57856500	3.27927800	2.98212500
N	-2.89813000	3.40681300	-1.78637000	N	-2.56346800	0.97439500	3.98421300
N	-3.71012900	2.96453100	0.75683600	N	-1.14519100	1.05283100	1.53810900
N	-4.52183300	1.43514800	-0.97663600	N	-3.77744200	1.98324600	2.12418900
C	-4.81048500	2.15700700	1.24829600	C	-0.39286300	3.86964500	2.39825200
H	-5.47506200	2.74145700	1.89248200	H	-0.66658000	4.70179600	1.72936300
H	-4.46702600	1.28075600	1.81751100	H	0.04916700	3.09313500	1.77139100
C	-5.54472200	1.69755400	0.00433000	C	0.63248500	4.36926200	3.40793400
H	-6.13974700	0.80181000	0.22263600	H	1.49305500	4.79465700	2.88309900
H	-6.24601000	2.48313700	-0.32989900	H	0.99744700	3.55869200	4.04145000
C	-4.86068400	0.61836200	-2.14641900	H	0.23361800	5.15340100	4.05889100
C	-6.16889400	1.11410400	-2.77621600	C	-1.67669200	0.47710800	5.04463500
H	-7.02153800	0.99898800	-2.09971900	C	-2.23780300	0.87060400	6.41536600
H	-6.38935000	0.53956700	-3.68156400	H	-2.37049600	1.95408200	6.48474000
H	-6.09279000	2.16902200	-3.05421800	H	-1.54490300	0.56224800	7.20377200
C	-5.03049000	-0.84602600	-1.73028400	H	-3.20007300	0.39408900	6.62268000
H	-4.09824500	-1.22698600	-1.31295700	C	-4.22932900	2.45773100	0.80285600
H	-5.30911100	-1.46499600	-2.59009600	C	-0.28534800	1.08565400	4.90787700
H	-5.81301600	-0.96336500	-0.97487000	H	0.11536400	0.93505400	3.90366000
C	-3.75843200	0.70520300	-3.19840800	H	0.39375100	0.61497500	5.62429000
H	-3.73234400	1.69429400	-3.65826000	H	-0.30846200	2.15671400	5.11374000
H	-3.94490800	-0.03585700	-3.98091000	C	-4.56437800	0.92606200	2.73314800
H	-2.77733900	0.51265000	-2.75876300	H	-4.48443500	-0.02388000	2.18267900
C	-2.85849500	3.60946100	1.77439100	H	-5.62237200	1.19941700	2.78151000
C	-2.26816000	2.59781600	2.76229800	C	-1.56711800	-1.04644800	4.95390100
H	-3.04514900	2.12019000	3.36606300	H	-2.54432900	-1.52722900	5.05714800
H	-1.57785400	3.09017400	3.45496200	H	-0.92019600	-1.44113600	5.74410300
H	-1.72433400	1.81868400	2.22377700	H	-1.15259300	-1.32777600	3.98517800
C	-3.69975800	4.63729700	2.53854800	C	-3.98704400	0.76265700	4.12399800
H	-4.16264800	5.34653700	1.84603500	H	-4.43860400	1.49615800	4.81150900
H	-3.06604200	5.19671000	3.23402000	H	-4.21058700	-0.23675000	4.51417700
H	-4.49243400	4.17006300	3.13022200	C	-5.51981200	3.26271800	0.99239900

C	-1.71712800	4.35191200	1.08537300	H	-6.32903200	2.65494800	1.40652200
H	-1.06482900	3.65404600	0.55849000	H	-5.86934700	3.65302500	0.03129200
H	-1.11812100	4.88061000	1.83169300	H	-5.35109700	4.10612500	1.66693400
H	-2.09465200	5.08323700	0.36867900	C	-2.29971800	4.04025300	3.98356200
C	-3.92454100	5.69769700	-1.74522600	H	-1.68515700	4.14619400	4.89152800
H	-4.80792000	6.24751200	-2.08849600	H	-3.17322900	3.45572900	4.27632400
H	-3.04771500	6.16903900	-2.19985900	C	-3.18494900	3.38458100	0.18400500
H	-3.85105500	5.81809900	-0.66240500	H	-2.25012100	2.85406600	-0.00444800
C	-4.04348300	4.22451100	-2.11737600	H	-2.97014000	4.23288200	0.83571600
H	-4.91134200	3.80282500	-1.60836200	H	-3.56536100	3.77054800	-0.76573100
H	-4.25849800	4.14499700	-3.19565900	C	-2.75856700	5.41917200	3.52990900
C	-1.62423500	3.75658800	-2.37378700	H	-1.92261100	6.05557000	3.22495400
H	-0.93834600	2.95214200	-2.10318000	H	-3.27558900	5.93080000	4.34765800
H	-1.22139900	4.67887600	-1.92441000	H	-3.45179800	5.34700400	2.68853600
C	-1.65633700	3.92315800	-3.88706100	C	-4.49413300	1.29217800	-0.15515800
H	-2.02749000	3.01996800	-4.37692700	H	-3.62627800	0.63074400	-0.22502200
H	-0.64522900	4.11500100	-4.26031300	H	-4.72582400	1.66959000	-1.15508000
H	-2.28314600	4.76256100	-4.20661100	H	-5.35189900	0.69324300	0.16675300
P	0.81408300	-2.16178800	-2.92004600	P	3.13502700	-1.45674700	1.41483800
N	0.53616800	-1.17872900	-1.77708900	N	2.92169600	-2.18930800	2.92628000
N	0.48503600	-1.52660500	-4.46789600	N	4.15333500	-2.52720100	0.55305600
N	0.06246500	-3.70353000	-2.97581600	N	1.81585500	-0.95594100	0.79014700
N	2.37227000	-2.91892800	-3.13492000	N	4.46241700	-0.37175800	1.65893600
C	0.97992200	-4.81681000	-2.94367800	C	1.63581700	-2.19537700	3.59348700
H	1.04747200	-5.31273800	-3.92768900	H	1.63268500	-1.48857600	4.43775800
H	0.67216400	-5.57851700	-2.21639300	H	0.91494400	-1.81520700	2.86881800
C	2.33062800	-4.24529100	-2.55011700	C	1.18915200	-3.56276700	4.09283000
H	2.41744400	-4.22624400	-1.45435300	H	0.20233800	-3.47972300	4.55690000
H	3.13834800	-4.87376100	-2.93890200	H	1.11348800	-4.28258500	3.27528100
C	3.62405700	-2.16280500	-2.95553900	H	1.86548700	-3.97719500	4.84681800
C	4.74904900	-2.88248900	-3.70688200	C	3.81273800	-3.86024000	0.03701700
H	4.98112100	-3.85929500	-3.27254000	C	4.93027100	-4.85390900	0.37229300
H	5.66669300	-2.28673200	-3.66844900	H	5.11425400	-4.88417600	1.44988700
H	4.47808200	-3.03150500	-4.75615600	H	4.64322100	-5.85910600	0.04992000
C	4.00262900	-2.01112500	-1.48073800	H	5.87088200	-4.60740300	-0.12864800
H	3.19773800	-1.50578400	-0.94356700	C	4.29694800	0.99144300	2.19577600
H	4.91299500	-1.41230700	-1.37924500	C	2.51883800	-4.36758100	0.66526300
H	4.19358900	-2.97652000	-1.00168800	H	1.71518700	-3.63649000	0.55810100
C	3.46671300	-0.76600300	-3.54960000	H	2.21083800	-5.29378000	0.17189900
H	3.17720800	-0.80628000	-4.60061900	H	2.65582600	-4.57621000	1.72680100
H	4.41729000	-0.22912300	-3.47650200	C	5.41850000	-0.53622500	0.58233100
H	2.71137500	-0.20303600	-2.99813400	H	5.10004500	-0.03036100	-0.34410100
C	-1.36664400	-3.96037000	-2.77856800	H	6.39934100	-0.13845300	0.85891200
C	-1.65880200	-4.24375500	-1.30165100	C	3.62892000	-3.79147400	-1.48119200
H	-1.10343400	-5.11882000	-0.94729300	H	4.52774400	-3.41267700	-1.97778400
H	-2.72493100	-4.44292200	-1.14382500	H	3.41420000	-4.78152800	-1.89678900
H	-1.36567100	-3.38853000	-0.68823600	H	2.79873500	-3.12453000	-1.71746900
C	-1.79129700	-5.16177300	-3.63091600	C	5.49385900	-2.03159200	0.34734000
H	-1.56125900	-4.98740200	-4.68651200	H	6.21135600	-2.48779500	1.04931900
H	-2.87027200	-5.32039800	-3.53902900	H	5.85205200	-2.24100500	-0.66789700
H	-1.29701300	-6.08753300	-3.32198700	C	5.57331500	1.37958800	2.94996400
C	-2.18721900	-2.75554700	-3.22836000	H	6.44852900	1.41975200	2.29519800
H	-1.89518100	-1.85666600	-2.68297900	H	5.46069100	2.37105200	3.39954200
H	-3.24748500	-2.94517000	-3.04058500	H	5.78009700	0.66185700	3.74778500
H	-2.05119200	-2.56658400	-4.29555100	C	4.04248700	-2.80492600	3.60970000
C	1.66074800	-2.04572900	-6.62765500	H	3.87455100	-3.88933700	3.70337600
H	1.62554600	-1.00556300	-6.96689500	H	4.92314400	-2.69022200	2.97595500
H	1.57985300	-2.68317100	-7.51529600	C	3.13281300	1.03860700	3.18264900
H	2.63767800	-2.22221900	-6.17295900	H	2.18734200	0.80015200	2.69393100
C	0.54178200	-2.36703500	-5.64403100	H	3.27924900	0.33566800	4.00401100
H	-0.42290000	-2.32339600	-6.17432500	H	3.05583900	2.04460800	3.60416600
H	0.64725900	-3.39914500	-5.30659100	C	4.34787100	-2.22821600	4.98530000

C	0.27129300	-0.10813000	-4.66061100	H	3.49739600	-2.31159000	5.66800800
H	1.17409700	0.38064500	-5.06538300	H	5.18570300	-2.76545600	5.44080100
H	0.11027200	0.31610300	-3.66764100	H	4.62279600	-1.17322100	4.91688900
C	-0.90748100	0.22260000	-5.56468400	C	4.03916100	2.00867300	1.07944900
H	-1.83033700	-0.22793600	-5.19271700	H	3.18542000	1.70140200	0.46941200
H	-0.75464000	-0.11664400	-6.59482000	H	3.82737500	2.99292200	1.50614800
H	-1.05165600	1.30609100	-5.60021600	H	4.91288500	2.12071800	0.42843300
P	-0.82453500	-2.26410000	2.84179600	P	-2.24739100	-2.62679900	-1.42011000
N	-0.54203000	-1.24131000	1.73522800	N	-1.45691000	-3.88753700	-2.23396800
N	-0.49243300	-1.68696600	4.41154600	N	-3.59747700	-2.27277500	-2.41140000
N	-0.08004900	-3.81028000	2.84135500	N	-1.28463100	-1.50812600	-0.97550200
N	-2.38622600	-3.02126800	3.02927300	N	-3.27586900	-3.43619000	-0.29230000
C	-1.00266600	-4.91740200	2.76903500	C	-0.01359600	-3.93301800	-2.33619200
H	-1.07244600	-5.44839000	3.73441700	H	0.39941700	-4.71777600	-1.68353900
H	-0.69847200	-5.65362300	2.01452000	H	0.34717000	-2.98078100	-1.94379900
C	-2.35073900	-4.32575300	2.39677600	C	0.51200100	-4.14613900	-3.75029700
H	-2.43753800	-4.26660600	1.30244500	H	1.60600100	-4.14499800	-3.74198100
H	-3.16133500	-4.96415800	2.76271600	H	0.17887900	-3.35468900	-4.42570900
C	-3.63454400	-2.25338900	2.87766900	H	0.19608100	-5.10338900	-4.17635100
C	-4.76262100	-2.99431000	3.60330000	C	-3.58999000	-1.57842800	-3.70192500
H	-4.99935800	-3.95384900	3.13436700	C	-4.53649500	-2.28289100	-4.67962500
H	-5.67750300	-2.39332500	3.58666900	H	-4.25842000	-3.33395200	-4.79788200
H	-4.49201600	-3.18206100	4.64643300	H	-4.48506400	-1.80479000	-5.66260900
C	-4.01293100	-2.04728600	1.40943100	H	-5.57852800	-2.24058300	-4.35046300
H	-3.20594100	-1.52675900	0.89022600	C	-2.82464000	-3.89910000	1.03379600
H	-4.92055800	-1.44103900	1.32990100	C	-2.18869200	-1.58810000	-4.30597400
H	-4.20851600	-2.99402700	0.89624200	H	-1.45291000	-1.20702200	-3.59446500
C	-3.47056100	-0.87948300	3.52128300	H	-2.17099400	-0.96111100	-5.20277700
H	-3.18097000	-0.95869300	4.57006200	H	-1.89628400	-2.59949500	-4.59139100
H	-4.41865200	-0.33593400	3.46785600	C	-4.59925100	-2.84385300	-0.35387200
H	-2.71278000	-0.30060400	2.99000800	H	-4.64941900	-1.87701700	0.17112100
C	1.34786100	-4.06643300	2.63465300	H	-5.34856200	-3.50602900	0.08943300
C	1.63871500	-4.29727400	1.14836000	C	-4.03807500	-0.12710800	-3.50880500
H	1.07925800	-5.15625800	0.76249500	H	-5.04659800	-0.07010400	-3.08892500
H	2.70389800	-4.49557100	0.98324200	H	-4.04686900	0.41404500	-4.46139300
H	1.34963000	-3.41895200	0.56646900	H	-3.35844100	0.37216300	-2.81662600
C	1.76686300	-5.30002200	3.44266900	C	-4.86897500	-2.63932100	-1.83091200
H	1.53762600	-5.16310300	4.50394700	H	-5.26748100	-3.56567300	-2.27665600
H	2.84508300	-5.46024400	3.34490500	H	-5.62220100	-1.85553900	-1.97401200
H	1.26826000	-6.21160500	3.10033400	C	-3.62102100	-5.15459900	1.40698400
C	2.17409100	-2.88265200	3.12787800	H	-4.69355000	-4.95643800	1.48782600
H	1.88636900	-1.96314200	2.61560600	H	-3.28999500	-5.53946700	2.37665100
H	3.23345500	-3.07031900	2.93318900	H	-3.47718500	-5.93762500	0.65813200
H	2.03892100	-2.73199700	4.20125600	C	-2.21506200	-4.97216900	-2.82546100
C	-1.67023800	-2.27865500	6.55140800	H	-2.10750200	-4.95321600	-3.92195900
H	-2.64803100	-2.43406000	6.09091000	H	-3.27093700	-4.78680700	-2.62310000
H	-1.63021000	-1.25164700	6.92812800	C	-1.34571700	-4.27657400	0.99428200
H	-1.59215100	-2.94822400	7.41532700	H	-0.71733500	-3.41513300	0.76451000
C	-0.55289100	-2.56922500	5.55645200	H	-1.15149900	-5.04643300	0.24579900
H	0.41205300	-2.54926200	6.08768200	H	-1.04599500	-4.66642900	1.97062600
H	-0.66315000	-3.58792600	5.18184200	C	-1.85129900	-6.35958100	-2.31456100
C	-0.27212600	-0.27739000	4.65549000	H	-0.80025500	-6.60547300	-2.49206800
H	-1.17256900	0.20050800	5.07810900	H	-2.45425900	-7.11815700	-2.82358600
H	-0.10942600	0.18185600	3.67850600	H	-2.03986200	-6.44500400	-1.24200200
C	0.90842300	0.01498100	5.57040100	C	-3.03988200	-2.82753300	2.10677700
H	0.75433800	-0.36065700	6.58764100	H	-2.57877000	-1.87943100	1.81716700
H	1.05757000	1.09580600	5.64508500	H	-2.60330500	-3.14941300	3.05590900
H	1.82909700	-0.42598800	5.18192300	H	-4.10426100	-2.64576500	2.28750200
P	3.01596700	2.12601400	0.69871000	P	1.25004600	2.47678000	-2.63200900
N	1.72816300	1.31006700	0.54238200	N	0.08263700	2.86447100	-3.75316700
N	2.91414300	3.32730300	1.90617500	N	2.06714700	3.90745300	-2.29829200
N	3.72337800	2.97287900	-0.65167200	N	0.66561900	1.56771400	-1.47209500

N	4.52868300	1.37873000	1.02554800	N	2.60116500	1.77097400	-3.35456600
C	4.81983300	2.17843700	-1.17230700	C	-1.24113100	2.24874400	-3.74916300
H	5.48687000	2.78253300	-1.79548400	H	-1.34542900	1.58314400	-4.61560800
H	4.47214700	1.32472800	-1.77236000	H	-1.29422700	1.61709400	-2.86294000
C	5.55239600	1.67138000	0.05403800	C	-2.37888300	3.25675200	-3.74178600
H	6.14322600	0.78131000	-0.19648900	H	-3.33305500	2.72707300	-3.69706300
H	6.25740400	2.44128600	0.41579100	H	-2.32226000	3.91540300	-2.87326400
C	4.86428000	0.51926300	2.16531100	H	-2.39590100	3.87755300	-4.64251000
C	6.17507200	0.98622800	2.81152100	C	1.56915300	5.03870800	-1.49236000
H	7.02684800	0.89132000	2.13081100	C	1.96495200	6.35023400	-2.17363500
H	6.39329100	0.37882300	3.69571100	H	1.56116300	6.40147000	-3.18863900
H	6.10399700	2.03092500	3.12693300	H	1.57163700	7.19963200	-1.60858600
C	5.02709000	-0.93016700	1.69725300	H	3.05029400	6.47233100	-2.23045800
H	4.09290100	-1.29172400	1.26720600	C	2.70176500	0.41487800	-3.93829100
H	5.30322300	-1.58060900	2.53433700	C	0.04937900	4.97844600	-1.38571000
H	5.80871700	-1.02418300	0.93766100	H	-0.28779100	4.02945300	-0.95918400
C	3.76296200	0.57371900	3.22045500	H	-0.29957300	5.77390600	-0.72294300
H	3.74167900	1.54594100	3.71520300	H	-0.42637500	5.11454400	-2.35784000
H	3.94639100	-0.19554900	3.97599300	C	3.81783700	2.39653600	-2.85611100
H	2.78076700	0.40144900	2.77489900	H	4.13607200	1.94854700	-1.90740300
C	2.87442900	3.65790500	-1.64498000	H	4.62871100	2.27509800	-3.57802900
C	2.27872200	2.68513900	-2.66808100	C	2.16132000	4.97786800	-0.08381000
H	3.05311500	2.22564000	-3.28900200	H	3.25307800	5.03948800	-0.09333900
H	1.59057300	3.20534800	-3.34228700	H	1.79392900	5.81117200	0.52208700
H	1.73127500	1.88989800	-2.15748800	H	1.87704700	4.04273700	0.40055700
C	3.72035600	4.70833000	-2.37238800	C	3.47212000	3.86439200	-2.66600200
H	4.18701100	5.39008300	-1.65523200	H	3.65143800	4.42748300	-3.59355700
H	3.08906700	5.29534000	-3.04701000	H	4.10015300	4.30099700	-1.88509500
H	4.51047800	4.25871800	-2.98089000	C	3.42755200	0.52730000	-5.28396800
C	1.73702600	4.38080700	-0.92913900	H	4.44456700	0.91409000	-5.17756900
H	1.08151800	3.66776300	-0.42715000	H	3.50580100	-0.45997400	-5.74702600
H	1.14030800	4.93879700	-1.65570300	H	2.88252100	1.18345300	-5.96715900
H	2.11845500	5.08417100	-0.18697500	C	0.37258500	3.81971500	-4.81599800
C	3.95091600	5.61351300	1.94689000	H	-0.26661600	4.70510600	-4.69764000
H	3.07636000	6.07218300	2.41853800	H	1.39831900	4.16780800	-4.68315700
H	3.87768400	5.77305600	0.86912400	C	1.31725600	-0.17093100	-4.18803600
H	4.83687300	6.14664200	2.30930200	H	0.75591700	-0.31107000	-3.26230700
C	4.06328500	4.12739100	2.26584000	H	0.72827400	0.45915500	-4.85744100
H	4.92908000	3.72033900	1.74162700	H	1.42565600	-1.15005300	-4.65938600
H	4.27823200	4.00822700	3.34047800	C	0.20569900	3.25337000	-6.21738800
C	1.64199000	3.66145700	2.50633500	H	-0.82344400	2.94739900	-6.42190400
H	0.95240700	2.87040300	2.20714900	H	0.47300100	4.01208100	-6.95829300
H	1.24323500	4.60115700	2.09065500	H	0.85301300	2.38694600	-6.37307800
C	1.67517000	3.77318500	4.02462300	C	3.48353100	-0.50551600	-3.00259700
H	0.66502700	3.95606400	4.40492400	H	3.03173400	-0.54524700	-2.00712100
H	2.30588600	4.59763600	4.37401500	H	3.50103600	-1.51838000	-3.41076300
H	2.04227600	2.85122100	4.48146100	H	4.52424500	-0.18497200	-2.89442700

Table S30. Truncated structure used for MC-PDFT calculations

atom			
P	-2.2382	2.8465	-0.87777
N	-1.49372	4.05639	-1.78695
N	-3.21771	3.65364	0.25701
N	-1.22359	1.76694	-0.39534
N	-3.62159	2.38061	-1.78759
C	-4.76576	2.29298	-0.89845
H	-4.76453	1.36501	-0.30638

H	-5.70323	2.33435	-1.45917
C	-4.63645	3.49176	0.019
H	-5.07029	4.38378	-0.46061
H	-5.1829	3.31957	0.95277
P	2.29938	0.86686	2.7937
N	1.58364	1.78167	4.0165
N	3.27464	-0.28259	3.58485
N	1.26259	0.39815	1.7291
N	3.68689	1.75971	2.31026
C	4.81794	0.85578	2.2036
H	4.79581	0.26675	1.27406
H	5.76308	1.40413	2.2331
C	4.69392	-0.06352	3.40174
H	5.1474	0.40818	4.28834
H	5.22523	-1.00391	3.21929
P	-2.32284	-2.79475	0.88292
N	-1.60927	-4.01861	1.79852
N	-3.3095	-3.58326	-0.25834
N	-1.28191	-1.73574	0.40833
N	-3.70259	-2.29889	1.78256
C	-4.83794	-2.18909	0.88421
H	-4.81353	-1.26211	0.29101
H	-5.78031	-2.21076	1.43757
C	-4.72637	-3.39119	-0.03106
H	-5.18225	-4.27352	0.44617
H	-5.2621	-3.20883	-0.96912
P	2.26243	-0.88101	-2.82242
N	1.52425	-1.78069	-4.0438
N	3.25875	0.24989	-3.61414
N	1.23898	-0.3958	-1.75272
N	3.63374	-1.80478	-2.34726
C	4.78301	-0.92394	-2.24295
H	4.77509	-0.33437	-1.31333
H	5.71719	-1.49072	-2.27542
C	4.67369	-0.00209	-3.44014
H	5.11089	-0.48421	-4.32914
H	5.22754	0.92598	-3.26094
Pr	-0.00501	-0.00008	-0.00215
H	-2.99192	-3.55559	-1.22997
H	-0.59103	-3.9277	1.83411
H	-1.90497	-4.97094	1.56478
H	-3.86539	-2.84111	2.63571

H	1.87619	1.53991	4.96779
H	0.56504	1.81391	3.92411
H	2.94871	-1.25152	3.56901
H	3.8509	2.61061	2.85561
H	-2.90045	3.55606	1.22335
H	-3.46288	1.57974	-2.40442
H	-0.48983	4.13198	-1.60771
H	-1.96307	4.96577	-1.80553
H	2.92442	1.21259	-3.64797
H	3.45197	-2.37492	-1.51568
H	0.66018	-2.24027	-3.7475

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