

Electronic Supplementary Information

of

Unraveling the Complexation Mechanism of Actinide(III) and Lanthanide(III) by a New Tetradentate Phenanthroline-Derived Phosphonate Ligand

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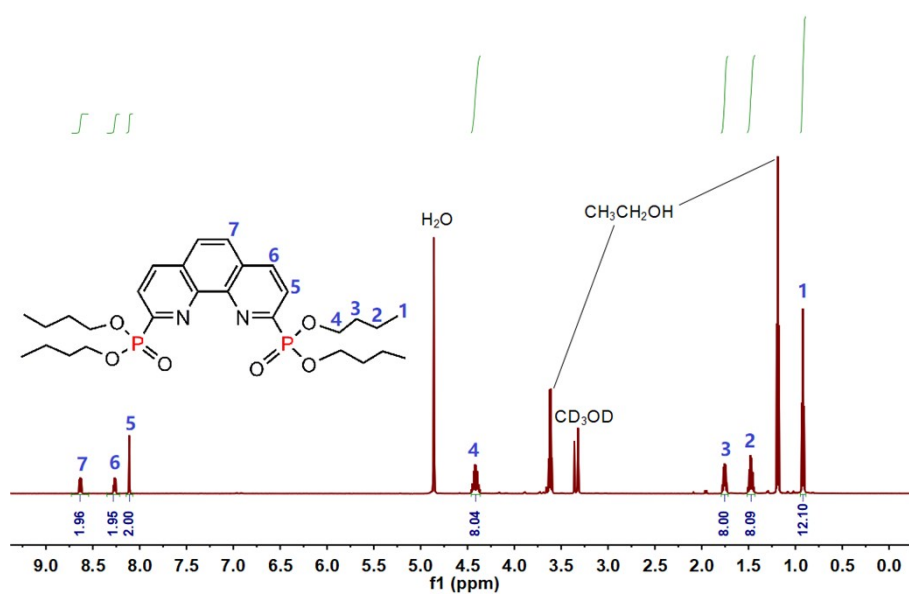


Fig. S1 The ^1H NMR spectrum of ligand C4-POPhen in CD_3OD .

^1H NMR (600 MHz, CD_3OD): δ =0.92 ppm (t, 12H, $-\text{CH}_3$), 1.47 ppm (m, 8H, $-\text{CH}_2-$), 1.76 ppm (m, 8H, $-\text{CH}_2-$), 4.41 ppm (m, 8H, $-\text{CH}_2-$), 8.11 ppm (s, 2H, $-\text{Ar-H}$), 8.26 ppm (dd, 2H, $-\text{Ar-H}$), 8.63 ppm (dd, 2H, $-\text{Ar-H}$).

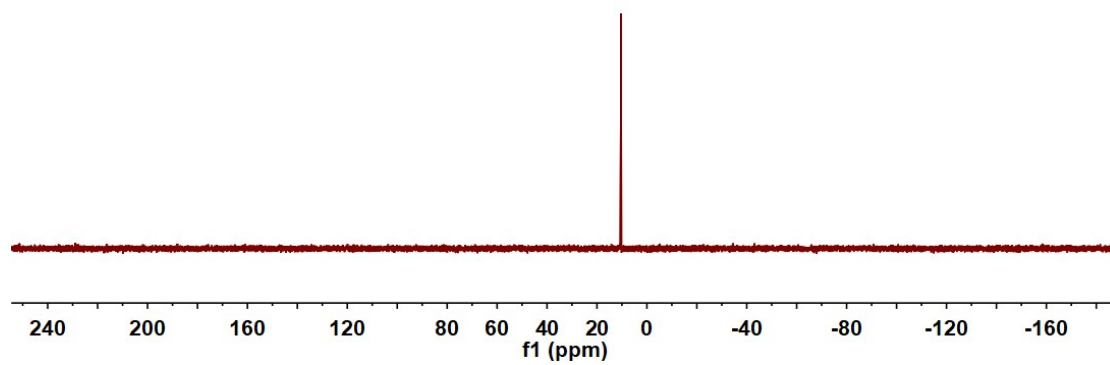


Fig. S2 The ^{31}P NMR spectrum of ligand C4-POPhen (600 MHz, CD_3OD).

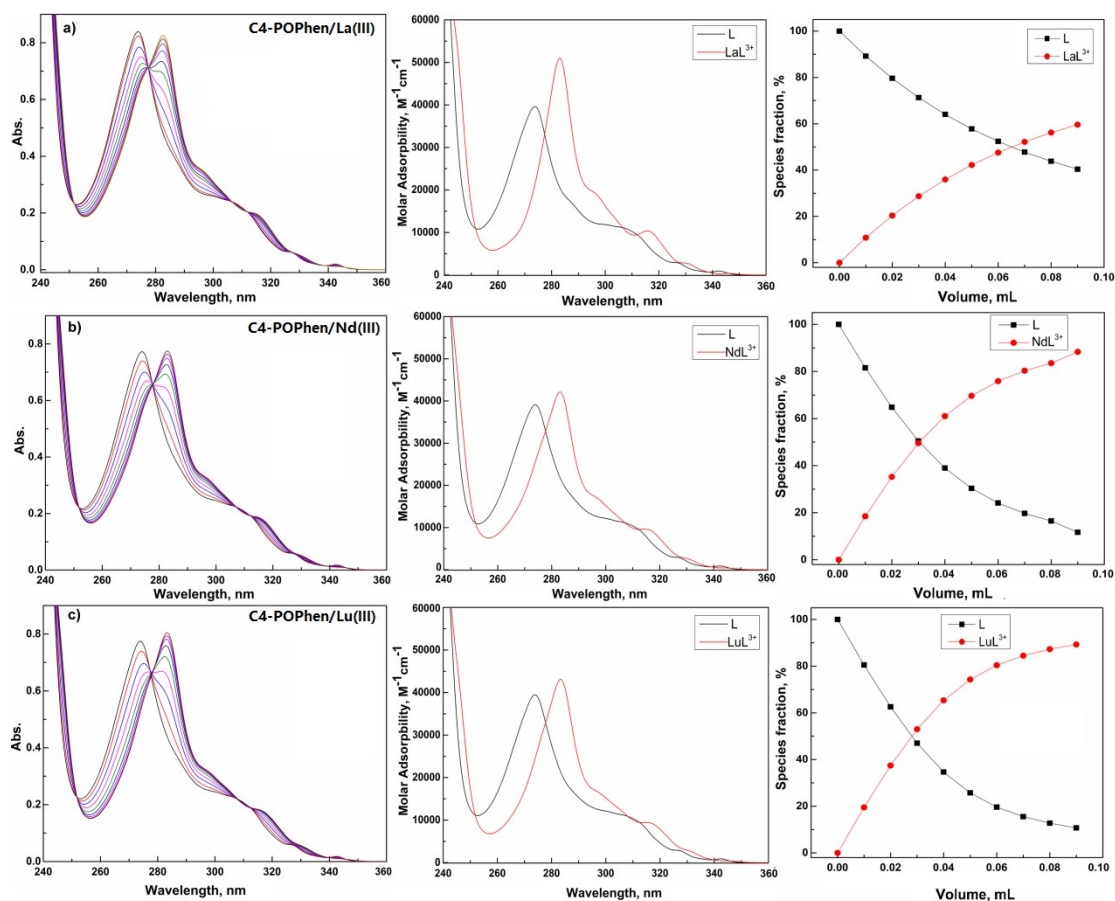


Fig. S3 Spectra of C4-POPhen titrated with three representative Lanthanides(III) in methanol solution ($T=298\text{K}$, $I=0.01\text{ M Et}_4\text{NNO}_3$, $V_0=2.20\text{ mL}$). Left: the normalized absorption spectra of C4-Phen-PO titrated with a) $\text{La}(\text{NO}_3)_3$, b) $\text{Nd}(\text{NO}_3)_3$, and c) $\text{Lu}(\text{NO}_3)_3$; Middle: the fitted molar absorptivities of ligand and its Ln(III) complexes; Right: the fraction curves of species formed during titration. a) $C_L/C_{\text{La(III)}}=0.022\text{ mM}/1.0\text{ mM}$, 0.09 mL of titrant was added; b) $C_L/C_{\text{Nd(III)}}=0.02\text{ mM}/1.0\text{ mM}$, 0.08 mL of titrant was added; c) $C_L/C_{\text{Lu(III)}}=0.02\text{ mM}/1.0\text{ mM}$, 0.08 mL of titrant was added.

**The coordinates of the optimized structures of Am(III) and Eu(III) complexes
calculated by DFT methods.**

EuL(NO₃)₃ Complex

Symbolic Z-Matrix:

C	2.8042	3.89594	-0.67997
C	3.45705	2.71602	-0.39438
C	2.684	1.56765	-0.12169
N	1.35424	1.56576	-0.14035
C	0.70066	2.72626	-0.37972
C	1.39283	3.93529	-0.66397
C	-0.74947	2.74072	-0.31979
C	-1.44044	3.95893	-0.56614
C	-0.70372	5.15154	-0.87007
C	0.65653	5.14023	-0.91598
N	-1.40275	1.5955	-0.02001
C	-2.72983	1.61177	0.03112
C	-3.50569	2.76547	-0.20228
C	-2.85087	3.94152	-0.49863
P	-3.46825	-0.0112	0.39887
P	3.4694	-0.00885	0.386
O	2.4363	-1.09054	0.48326
O	-2.39709	-1.04033	0.60879
O	-4.51976	-0.36939	-0.74705
O	-4.38518	0.33094	1.66013
O	4.25055	0.33034	1.73555
O	4.70104	-0.24126	-0.59192
C	-4.23109	-1.31369	-1.84485
C	-3.86341	-0.56851	-3.11269
C	-5.04929	-0.74242	2.40048
C	-5.69743	-0.12515	3.62246
C	3.62233	0.08246	3.04222
C	4.58669	0.56723	4.10349
C	4.56906	-0.98735	-1.8577
C	4.71949	-2.47778	-1.6219
H	3.3618	4.80079	-0.90517
H	4.53955	2.65544	-0.3793
H	-1.25623	6.06712	-1.05972
H	1.21002	6.04709	-1.1415
H	-4.58719	2.71597	-0.14612
H	-3.40627	4.85661	-0.68391
H	-3.43501	-1.99178	-1.53065
H	-5.16218	-1.87388	-1.95692

H	-4.63578	0.15935	-3.37968
H	-2.89834	-0.0637	-3.016
H	-4.29638	-1.48732	2.67337
H	-5.7883	-1.20516	1.73877
H	-6.43478	0.62947	3.33475
H	-4.94636	0.34347	4.26374
H	3.4299	-0.98943	3.12549
H	2.66559	0.6088	3.08625
H	4.77392	1.64035	4.00448
H	5.54161	0.03872	4.03598
H	5.37725	-0.58738	-2.47356
H	3.60842	-0.75116	-2.32119
H	3.89137	-2.86218	-1.02193
H	5.66509	-2.70177	-1.11954
N	-0.33458	-3.53261	-1.23499
O	0.54401	-3.281	-0.33327
O	-1.07511	-2.53079	-1.56633
O	-0.46174	-4.62841	-1.73997
N	0.2681	-0.88776	2.92515
O	0.3112	0.20447	2.23871
O	-0.00612	-1.94372	2.26491
O	0.49708	-0.89803	4.12327
N	0.48259	-0.11163	-2.89684
O	1.34132	-0.78547	-2.22577
O	-0.56102	0.2562	-2.24419
O	0.65047	0.17991	-4.06716
C	4.70481	-3.20358	-2.98006
H	4.79027	-4.25835	-2.82173
H	3.78676	-2.99231	-3.48745
C	5.88842	-2.71538	-3.83581
H	6.15555	-3.47434	-4.54117
H	5.60715	-1.82537	-4.35894
H	6.72493	-2.50724	-3.20192
C	3.97866	0.30536	5.49394
H	3.14993	0.96383	5.65058
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C	5.04524	0.55612	6.57612
H	4.60862	0.42566	7.54423
H	5.85	-0.13792	6.45133
H	5.41817	1.55485	6.4847
C	-6.41352	-1.22146	4.43296
H	-7.17394	-1.67175	3.82972
H	-5.70493	-1.9667	4.72865
C	-7.05499	-0.59712	5.68608

H	-7.74183	0.16855	5.39132
H	-7.57747	-1.35342	6.23374
H	-6.29135	-0.17271	6.30385
C	-3.73882	-1.58467	-4.26312
H	-4.70701	-1.97143	-4.50379
H	-3.09876	-2.38754	-3.96209
C	-3.14197	-0.88866	-5.50044
H	-2.09009	-0.75185	-5.35999
H	-3.31041	-1.49431	-6.36629
H	-3.61073	0.06378	-5.63471
Eu	0.00497	-0.89269	-0.01889

AmL(NO₃)₃ Complex

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O	2.4363	-1.09054	0.48326
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H	3.3618	4.80079	-0.90517
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H	-3.43501	-1.99178	-1.53065
H	-5.16218	-1.87388	-1.95692
H	-4.63578	0.15935	-3.37968
H	-2.89834	-0.0637	-3.016
H	-4.29638	-1.48732	2.67337
H	-5.7883	-1.20516	1.73877
H	-6.43478	0.62947	3.33475
H	-4.94636	0.34347	4.26374
H	3.4299	-0.98943	3.12549
H	2.66559	0.6088	3.08625
H	4.77392	1.64035	4.00448
H	5.54161	0.03872	4.03598
H	5.37725	-0.58738	-2.47356
H	3.60842	-0.75116	-2.32119
H	3.89137	-2.86218	-1.02193
H	5.66509	-2.70177	-1.11954
Am	0.00497	-0.89269	-0.01889
N	-0.33458	-3.53261	-1.23499
O	0.54401	-3.281	-0.33327
O	-1.07511	-2.53079	-1.56633
O	-0.46174	-4.62841	-1.73997
N	0.2681	-0.88776	2.92515
O	0.3112	0.20447	2.23871
O	-0.00612	-1.94372	2.26491
O	0.49708	-0.89803	4.12327
N	0.48259	-0.11163	-2.89684
O	1.34132	-0.78547	-2.22577
O	-0.56102	0.2562	-2.24419
O	0.65047	0.17991	-4.06716
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H	4.79027	-4.25835	-2.82173
H	3.78676	-2.99231	-3.48745
C	5.88842	-2.71538	-3.83581
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H	3.64385	-0.70928	5.55147
C	5.04524	0.55612	6.57612
H	4.60862	0.42566	7.54423
H	5.85	-0.13792	6.45133
H	5.41817	1.55485	6.4847
C	-6.41352	-1.22146	4.43296
H	-7.17394	-1.67175	3.82972
H	-5.70493	-1.9667	4.72865
C	-7.05499	-0.59712	5.68608
H	-7.74183	0.16855	5.39132
H	-7.57747	-1.35342	6.23374
H	-6.29135	-0.17271	6.30385
C	-3.73882	-1.58467	-4.26312
H	-4.70701	-1.97143	-4.50379
H	-3.09876	-2.38754	-3.96209
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H	-3.31041	-1.49431	-6.36629
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EuL₂³⁺ Complex

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AmL₂³⁺ Complex

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