

Supplementary information for

“Morpholine-Derived Hydrophilic 1,10-phenanthroline-2,9-dicarboxamide for Americium–Lanthanide Separation in Phosphine Oxide Extraction Systems”

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1. NMR, IR and HRMS spectra of L

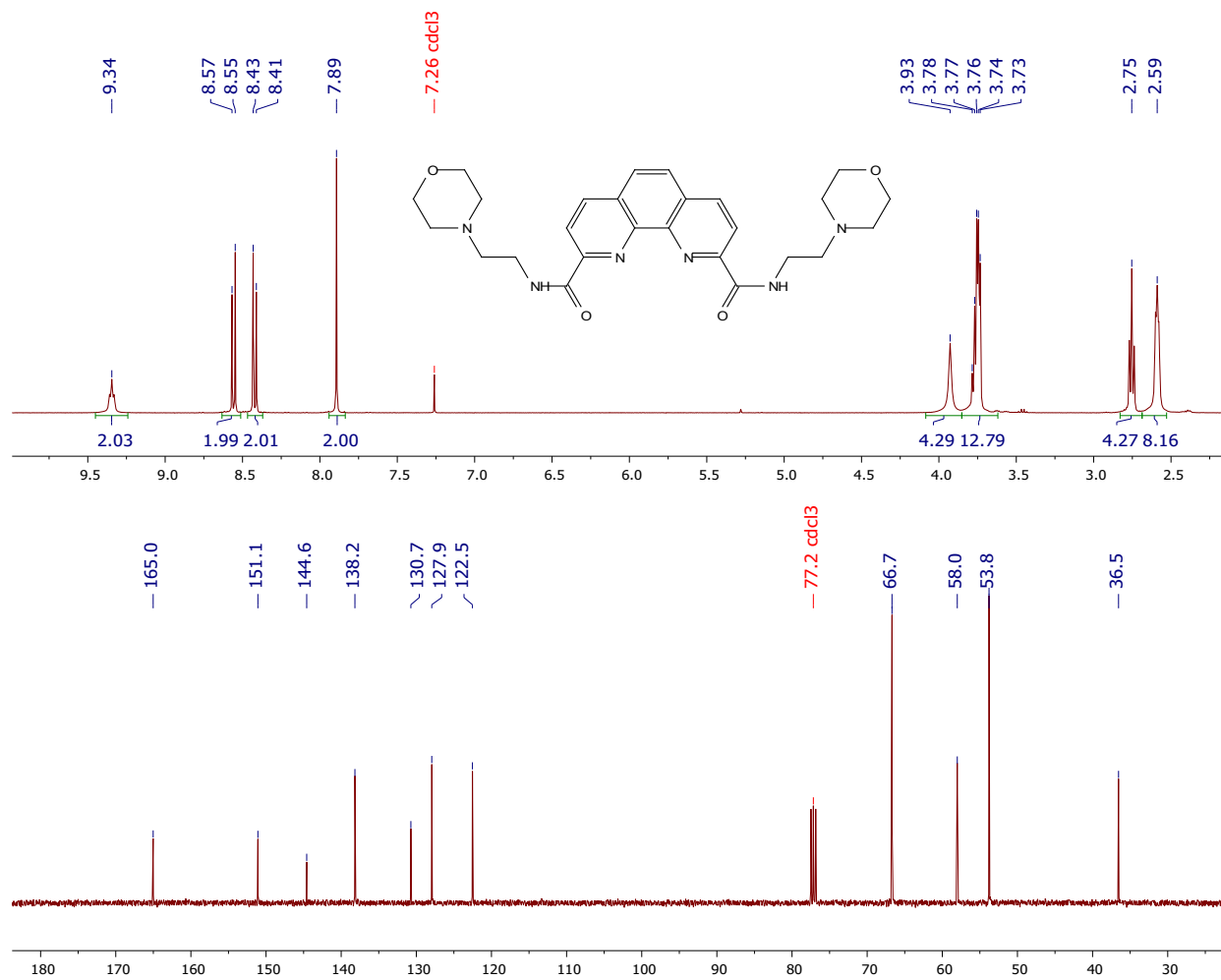


Figure S1. ¹H and ¹³C NMR spectra (CDCl₃, 25 °C).

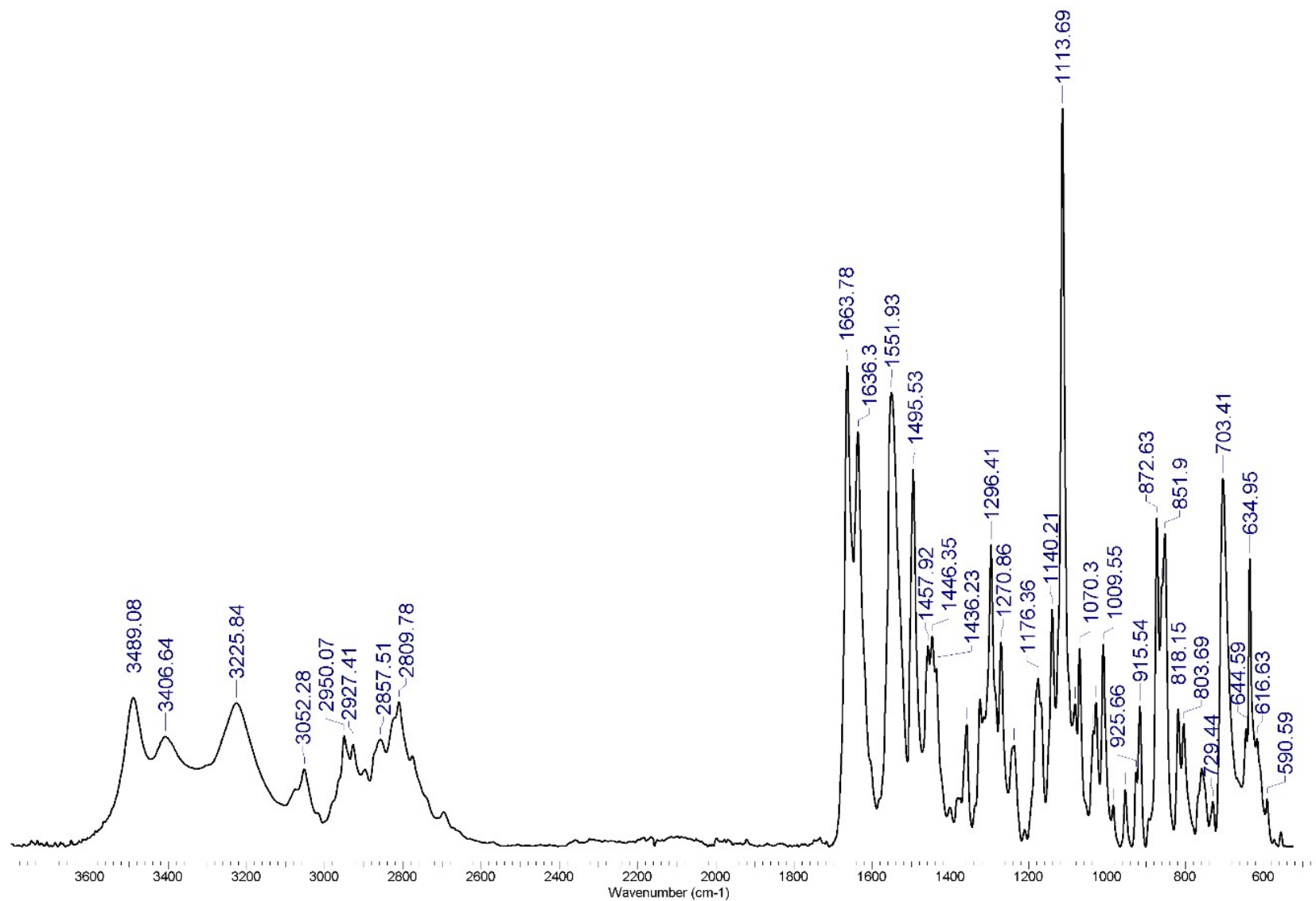


Figure S2. Solid-state IR spectrum of **L**.

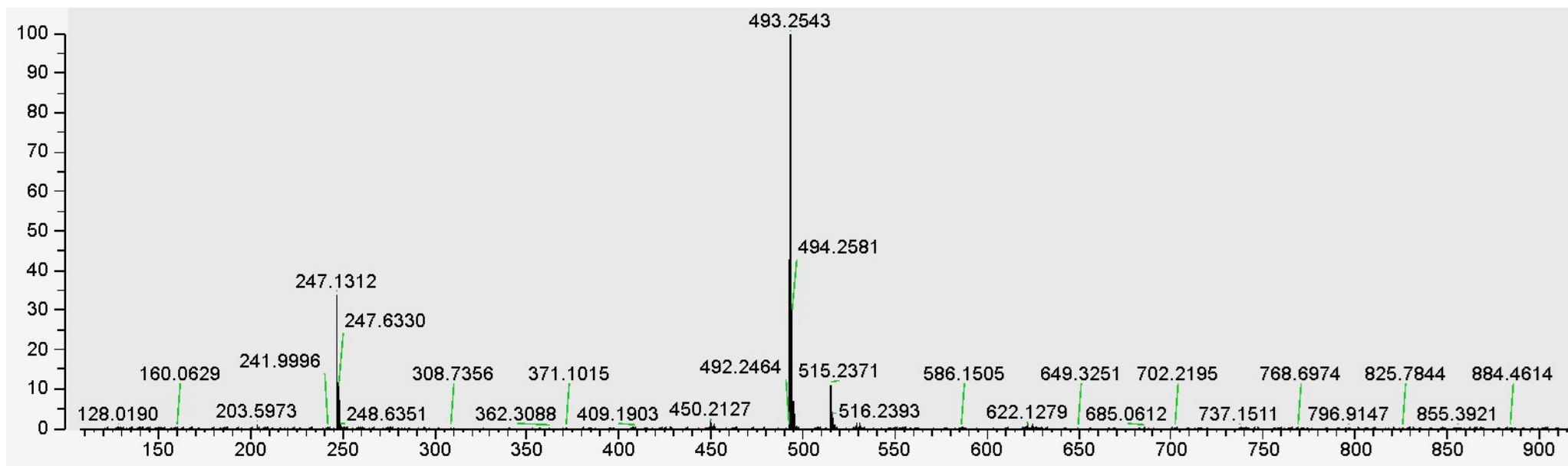


Figure S3. HRMS spectrum of **L**.

2. Potentiometric titration data

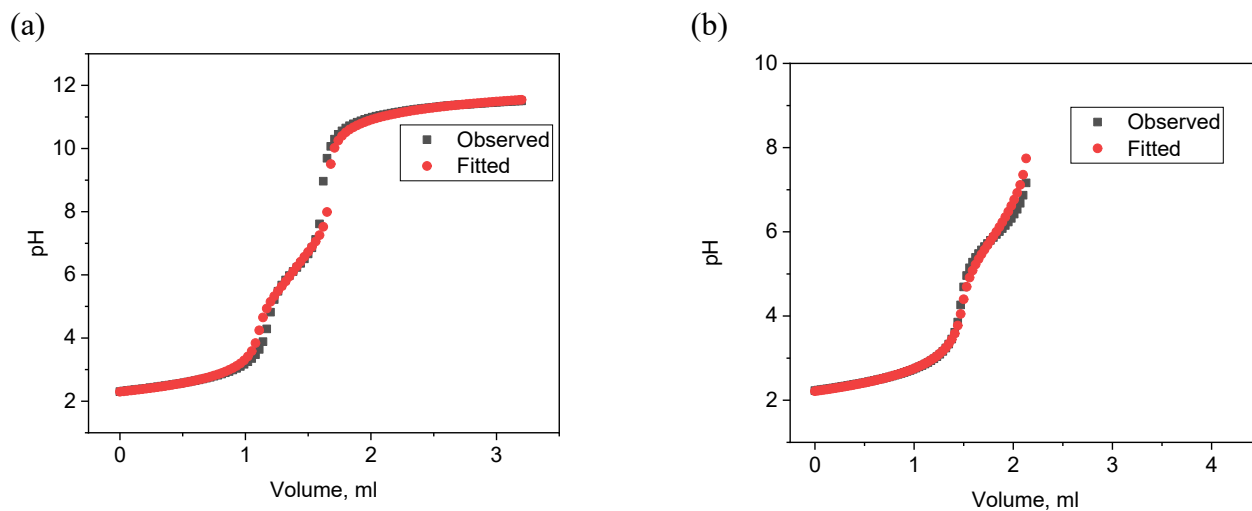


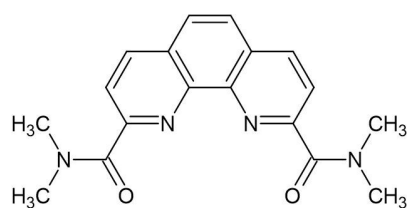
Figure S4. (a) Potentiometric titration curves observed (black points) and fitted (red points) for aqueous solution of ligand **L** ($[L]_{\text{total}} = 1.0 \text{ mM}$) as a function of pH. (b) Potentiometric titration curves observed (black points) and fitted (red points) for aqueous solution of ligand **L** ($[L]_{\text{total}} = 2.0 \text{ mM}$) in the presence of Eu(III) ($[Eu]_{\text{total}} = 1.0 \text{ mM}$) as a function of pH.

3. X-ray crystallography

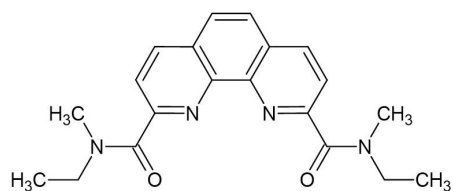
Table S1. Crystal data and structure refinement parameters.

Identification code	LaL	EuL	ErL
Empirical formula	C ₂₆ H ₃₅ LaN ₁₀ O ₁₇	C ₂₆ H ₃₇ EuN ₁₀ O ₁₈	C ₂₆ H ₄₄ ErN ₁₁ O ₂₄
Formula weight	898.55	929.61	1061.98
Temperature/K	100	100	100
Crystal system	triclinic	triclinic	monoclinic
Space group	P-1	P-1	C2/c
a/Å	9.1879(3)	9.2372(6)	29.3427(15)
b/Å	9.3337(3)	9.2714(5)	7.2948(4)
c/Å	21.2534(8)	21.8651(12)	36.3733(17)
α /°	88.7220(10)	98.190(2)	90
β /°	79.5490(10)	92.689(2)	91.742(2)
γ /°	69.9790(10)	110.491(2)	90
Volume/Å ³	1682.51(10)	1726.71(18)	7782.1(7)
Z	2	2	8
ρ_{calc} /g/cm ³	1.774	1.788	1.813
μ /mm ⁻¹	1.363	1.912	2.264
F(000)	908.0	940.0	4296.0
Crystal size/mm ³	0.13 × 0.1 × 0.01	0.17 × 0.05 × 0.03	0.39 × 0.18 × 0.01
Radiation	MoK α (λ = 0.71073)	MoK α (λ = 0.71073)	MoK α (λ = 0.71073)
2 Θ range for data collection/°	3.902 to 52.9	3.784 to 53.996	4.482 to 51.124
Reflections collected	22739	25475	30311
Independent reflections	6919 [R _{int} = 0.0397, R _{sigma} = 0.0465]	7524 [R _{int} = 0.0523, R _{sigma} = 0.0552]	7262 [R _{int} = 0.0558, R _{sigma} = 0.0502]
Data/restraints/parameters	6919/0/499	7524/106/529	7262/2/569
Goodness-of-fit on F ²	1.060	1.156	1.073
Final R indexes [I > 2 σ (I)]	R ₁ = 0.0362, wR ₂ = 0.0735	R ₁ = 0.0591, wR ₂ = 0.1349	R ₁ = 0.0437, wR ₂ = 0.0775
Final R indexes [all data]	R ₁ = 0.0426, wR ₂ = 0.0758	R ₁ = 0.0628, wR ₂ = 0.1389	R ₁ = 0.0536, wR ₂ = 0.0807
Largest diff. peak/hole / e Å ⁻³	0.94/-1.07	4.10/-3.71	1.49/-1.47
CCDC	2481118	2481119	2481120

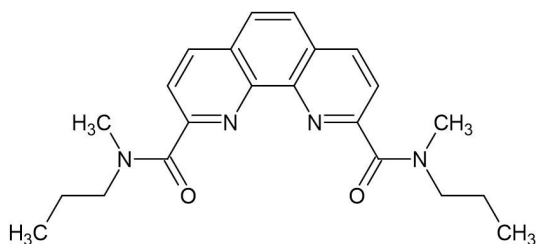
4. Structural formulas of some ligands discussed in the work



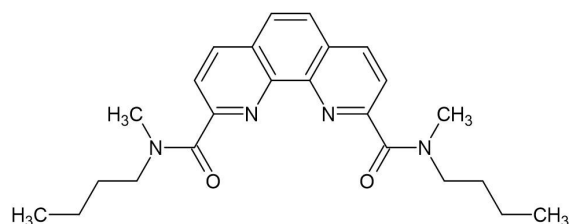
DAPhen-1



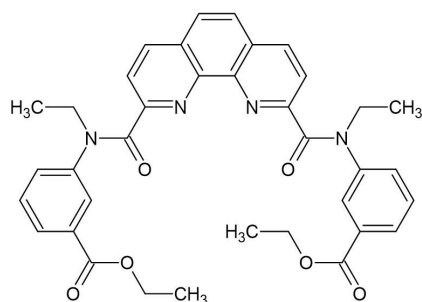
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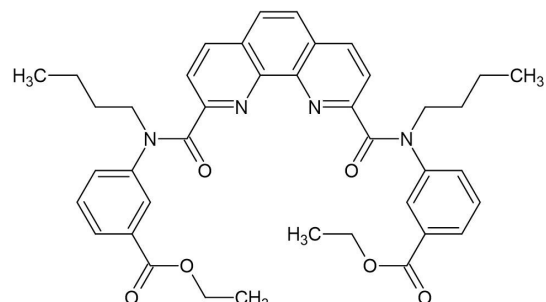
DAPhen-3



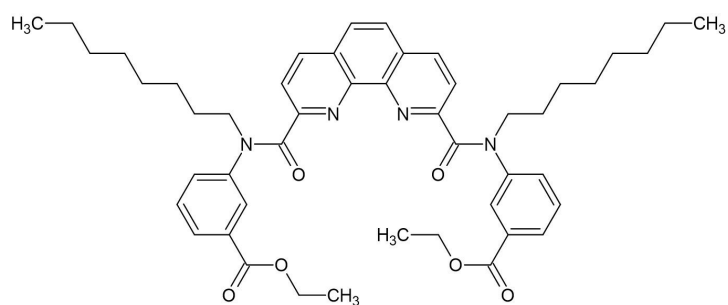
DAPhen-4



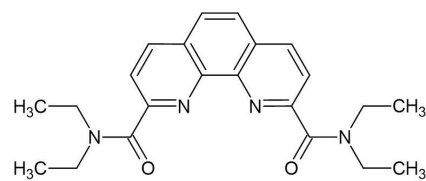
Et-EB-DAPhen



But-EB-DAPhen



Oct-EB-DAPhen



Et-Et-DAPhen

Figure S5. Structural formulas of selected ligands discussed in the work.

5. Solvent extraction with TODGA

