

Supplementary Electronic Information

Synthesis and structural characterization of lanthanide (III) nitrate complexes of a tetraaminodiphenol macrocycle in the solid state and in solution †

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† Electronic supplementary information (ESI) available: COSY spectrum of **1** (**Fig. S1**), ¹H NMR spectrum of **1** at different temperatures (**Fig. S2**), plots of $\Delta_{ij} / \langle S_z \rangle_j$ vs $C_j / \langle S_z \rangle_j$ according to equation (4) for the lanthanide complexes (**Fig. S3**), absorption spectrum of [Nd(LH₂)(NO₃)₃] (**4**) (**Fig. S4**) and absorption spectral data for some of the lanthanide complexes (**Table S1**).

See <http://www.rsc.org/suppdata>

Electronic supplementary information (ESI)

Fig. S1 $\{^1\text{H} - ^1\text{H}\}$ COSY spectrum of $[\text{La}(\text{LH}_2)(\text{NO}_3)_3]$ (**1**) in $(\text{CD}_3)_2\text{SO}$.

Fig. S2 ^1H NMR spectra of $[\text{La}(\text{LH}_2)(\text{NO}_3)_3]$ (**1**) in $(\text{CD}_3)_2\text{SO}$ at different temperatures.

Fig. S3 Plots of $\Delta_{ij} / \langle S_z \rangle_j$ vs. $C_j / \langle S_z \rangle_j$ according to equation (4) for the proton **e** in $\text{Ln}(\text{LH}_2)(\text{NO}_3)_3$ compounds.

Fig. S4 The absorption spectrum of $[\text{Nd}(\text{LH}_2)(\text{NO}_3)_3]$ (**4**) in *N,N*-dimethylformamide.

Table S1 Absorption spectral data for some of the lanthanide (III) complexes.

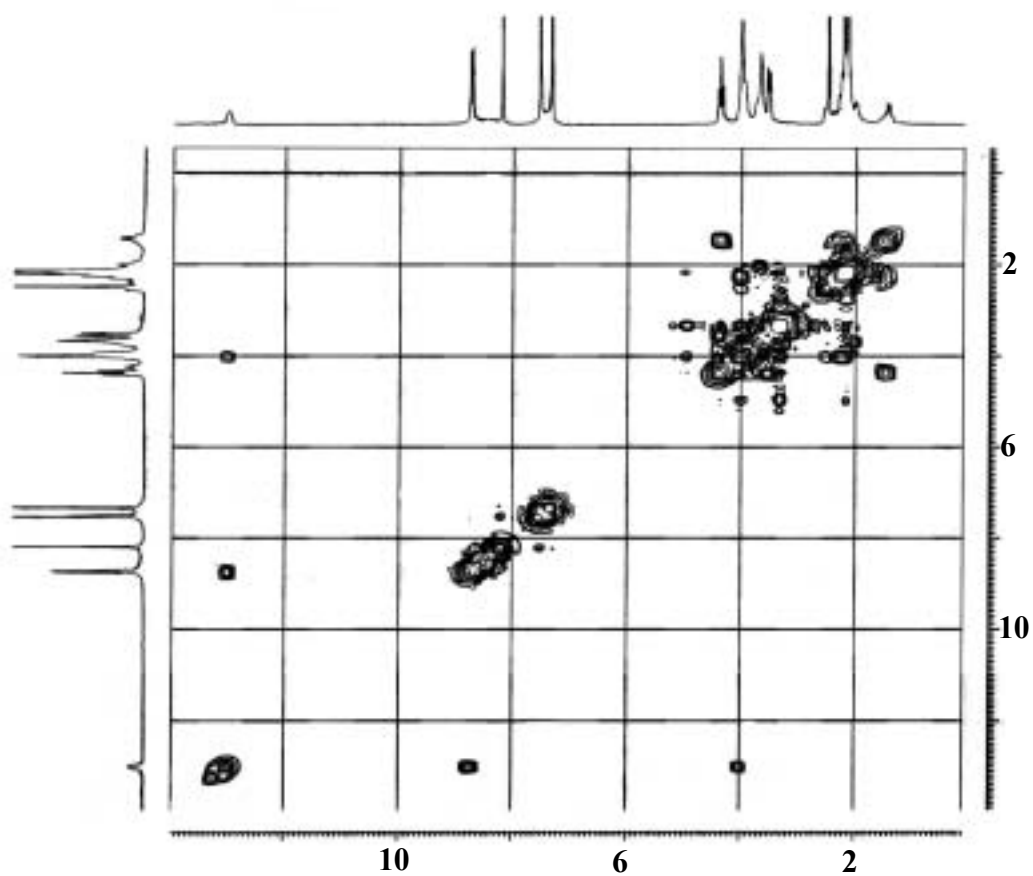


Fig. S1 $\{^1\text{H} - ^1\text{H}\}$ COSY spectrum of $[\text{La}(\text{LH}_2)(\text{NO}_3)_3]$ (**1**) in $(\text{CD}_3)_2\text{SO}$.

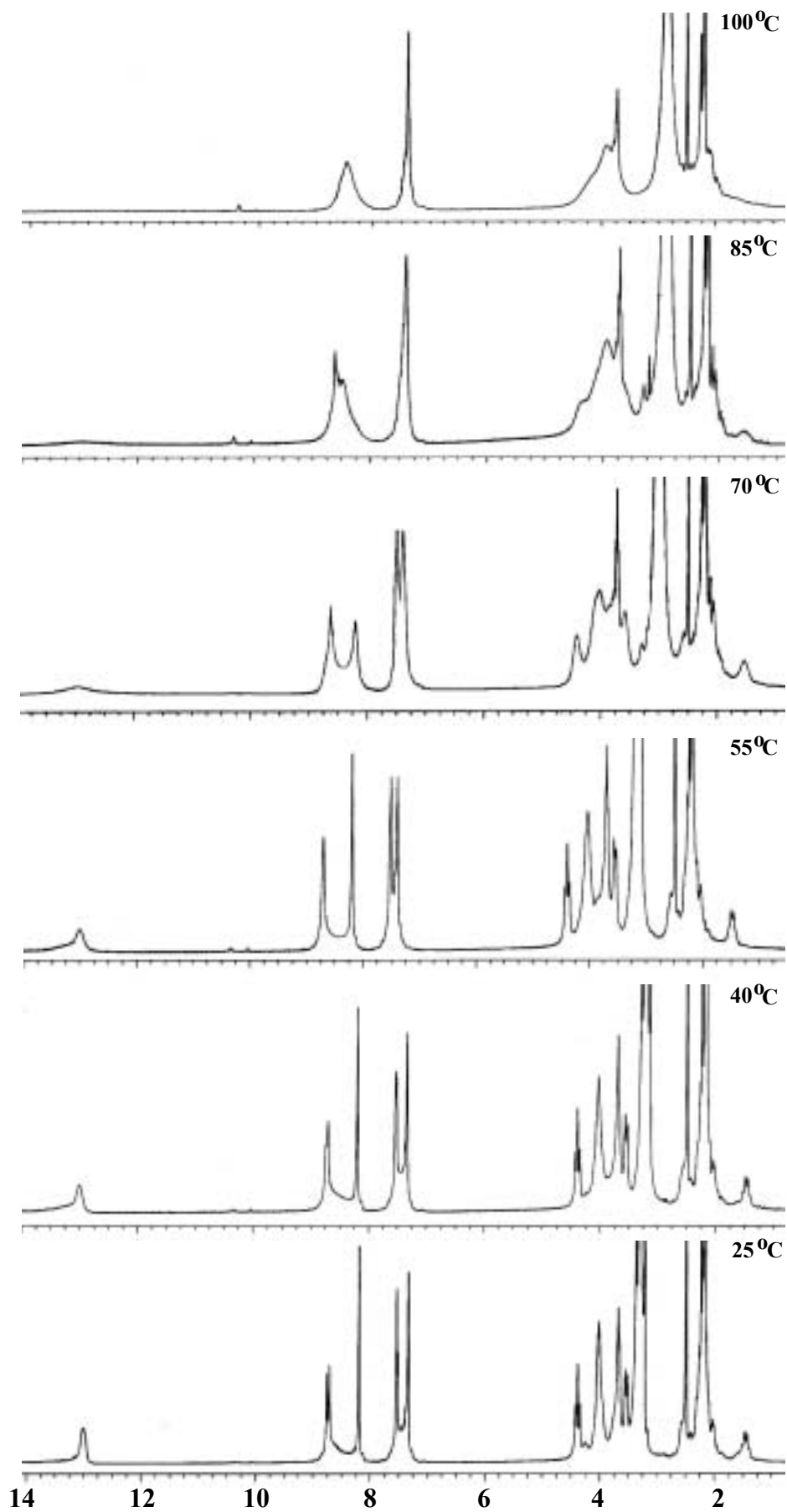


Fig. S2 ^1H NMR spectra of $[\text{La}(\text{LH}_2)(\text{NO}_3)_3]$ (**1**) in $(\text{CD}_3)_2\text{SO}$ at different temperatures.

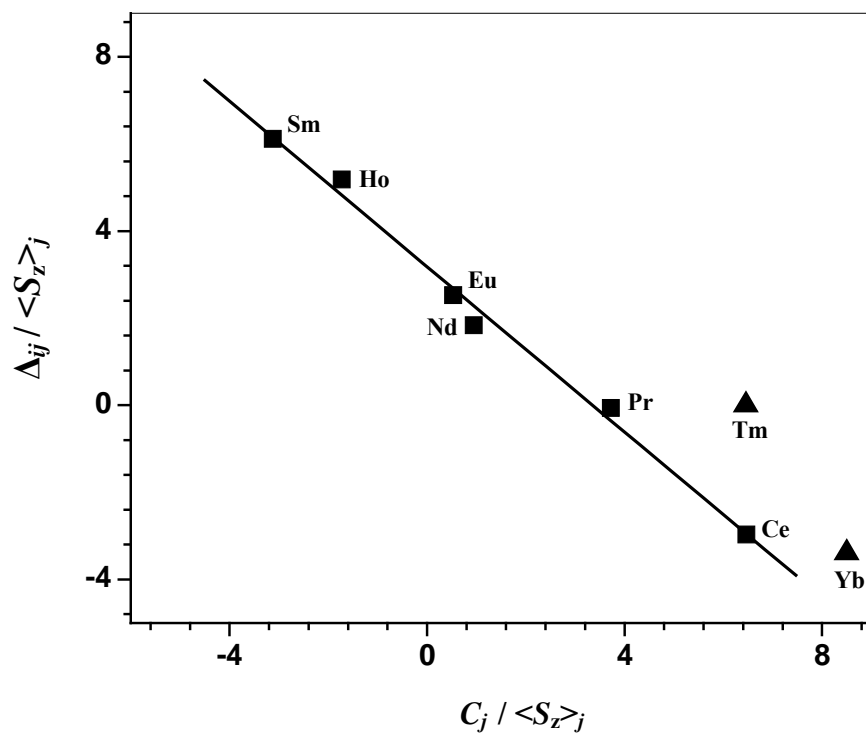


Fig. S3 Plots of $\Delta_{ij} / \langle S_z \rangle_j$ vs. $C_j / \langle S_z \rangle_j$ according to equation (4) for the proton e in $\text{Ln}(\text{LH}_2)(\text{NO}_3)_3$ compounds.

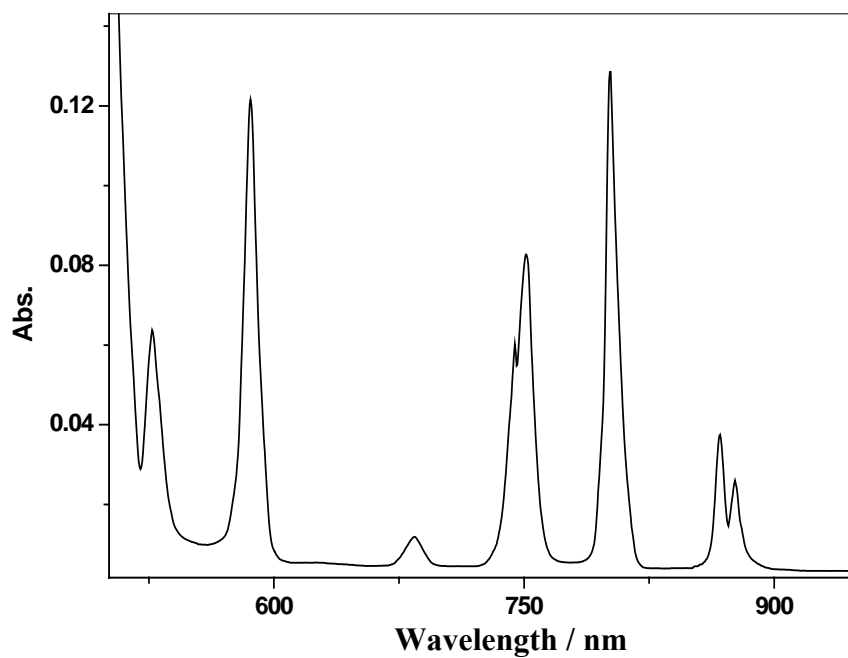


Fig. S4 The absorption spectrum of $[\text{Nd}(\text{LH}_2)(\text{NO}_3)_3]$ (**4**) in N,N -dimethylformamide

Table S1 Absorption spectral data for some of the lanthanide (III) complexes ^a

[Ln(LH ₂)(NO ₃) ₃]		
Ln ³⁺	λ_{\max} / nm (ϵ / dm ³ mol ⁻¹ cm ⁻¹)	Transition
Pr 3	585 (3.5)	³ H ₄ → ¹ D ₂ ^b
	1000 (1.5)	→ ¹ G ₄
Nd 4	530 (6.3)	⁴ I _{9/2} → ⁴ G _{7/2} , ⁴ G _{9/2} ^b
	585 (12.2)	→ ⁴ G _{5/2} , ² G _{7/2} ^b
	685 (1.3)	→ ⁴ F _{9/2}
	738 (7.5)	→ ⁴ F _{7/2}
	802 (12.9)	→ ⁴ F _{5/2}
	867 (3.8)	→ ⁴ F _{3/2}
Ho 10	550 (9.8)	⁵ I ₈ → ⁵ G ₂
	645 (5.4)	→ ⁵ G ₃
Er 11	520 (13.5)	⁴ I _{15/2} → ² H _{11/2} , ⁴ G _{11/2} ^b
	630 (3)	→ ⁴ F _{9/2}
	980 (1)	→ ⁴ I _{11/2}
Tm 12	688 (7.0)	
	790 (5.4)	³ H ₆ → ³ H ₄

^a In *N,N*-dimethylformamide. ^b Hypersensitive transition.