

Supplementary Information

A gadolinium(III) complex based on pyridoxine molecule with single-ion magnet and magnetic resonance imaging properties

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Table S1. Selected bond lengths (Å) for compound **1**.

Compound	1
Gd(1)-O(1)	2.255(1)
Gd(1)-O(2)	2.433(1)
Gd(1)-O(4)	2.308(1)
Gd(1)-O(5)	2.444(1)
Gd(1)-O(1w)	2.423(1)
Gd(1)-O(2w)	2.410(1)
Gd(1)-O(3w)	2.414(1)
Gd(1)-O(4w)	2.449(1)
O(1)-C(2)	1.303(2)
O(2)-C(7)	1.441(2)
O(3)-C(8)	1.432(2)
O(4)-C(10)	1.313(2)
O(5)-C(15)	1.436(2)
O(6)-C(16)	1.424(2)
C(1)-N(1)	1.343(2)
C(5)-N(1)	1.352(2)
C(9)-N(2)	1.343(2)
C(13)-N(2)	1.349(2)
C(1)-C(2)	1.415(2)
C(1)-C(6)	1.485(2)
C(2)-C(3)	1.415(2)
C(3)-C(4)	1.400(2)
C(3)-C(7)	1.502(2)
C(4)-C(5)	1.381(2)
C(4)-C(8)	1.506(2)
C(9)-C(10)	1.415(2)

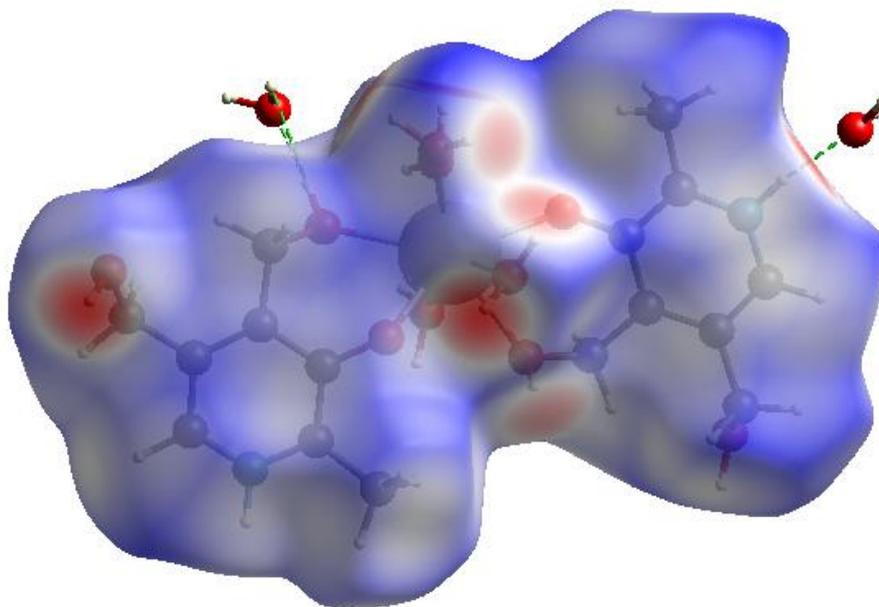


Figure S1. Hirshfeld surface mapped with d_{norm} function, showing the shorter intermolecular H \cdots O contacts (dashed lines) between alcohol and N-H groups and non-coordinated water molecules for **1**.

Table S2. Parameters of the three main sequences to obtain the maps of T2, T2* and T1, respectively. Subindex p of METSEp, MEGREp and MAPp refers to the sequences used in the Philips Achieva (3T) equipment for compound **1**.

	METSEp	MEGREp	MAPp
Scanner	Philips Achieva	Philips Achieva	Philips Achieva
FA [°]	90	10	2,5,10,15,25,45
TR [ms]	5000	100	14
TE ₁ [ms]	10	0.9	4.6
nTE [a.u.]	32	32	1
ΔTE [ms]	10	0.7	NA
Voxel Size [mm]	1.8	1.8	1.8
Slice Thickness [mm]	5	5	5
FOV [mm]	230x230	230x230	288x288
N Slices [a.u.]	1	15	15
Duration [s]	315	75	5 x 64

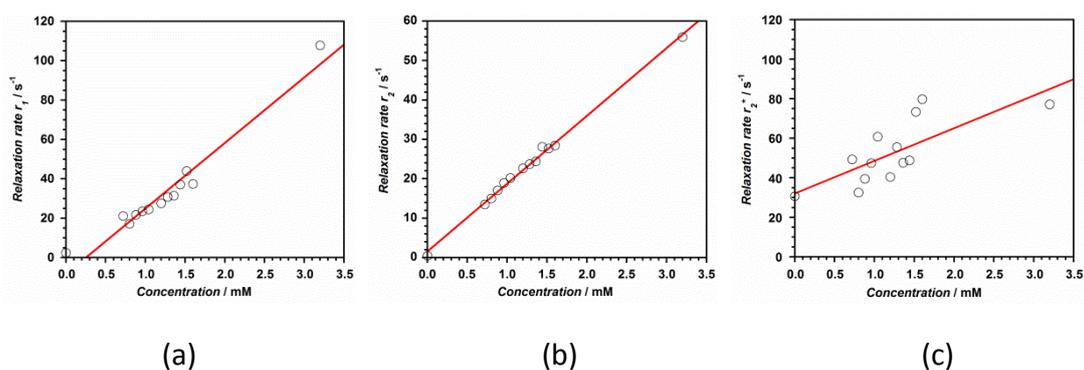


Figure S2. Relaxation rate vs. contrast concentration plot obtained for the relaxivities r_1 (a), r_2 (b) and r_2^* (c) of compound **1**. The red line represents the best linear fit of the experimental data.

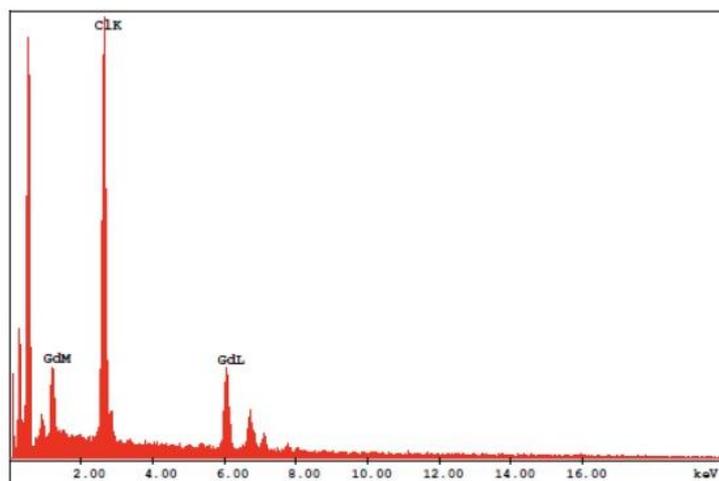


Figure S3. SEM-EDAX spectrum for compound **1**.

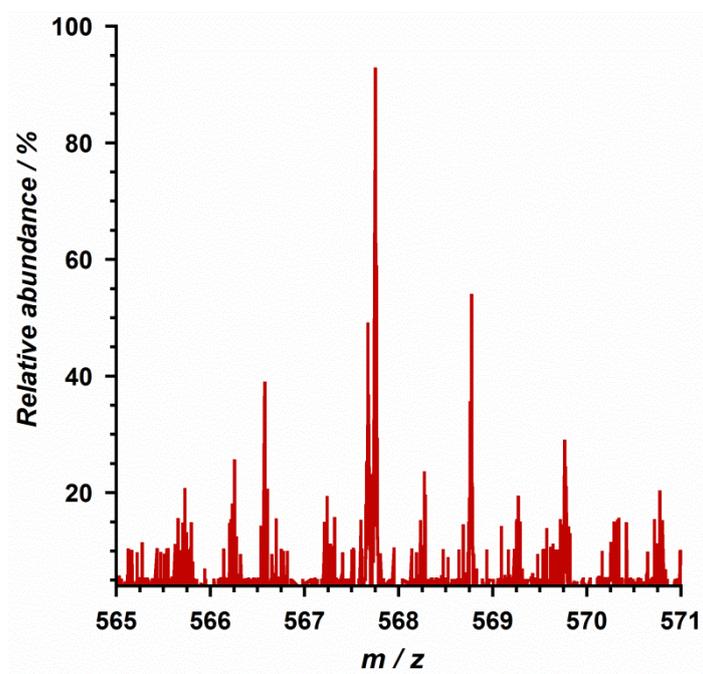


Figure S4. Electrospray ionization mass spectrum (ESI-MS) for compound **1** showing the isotopic distribution for the $[\text{Gd}(\text{pyr})_2(\text{H}_2\text{O})_4]^{3+}$ cation.

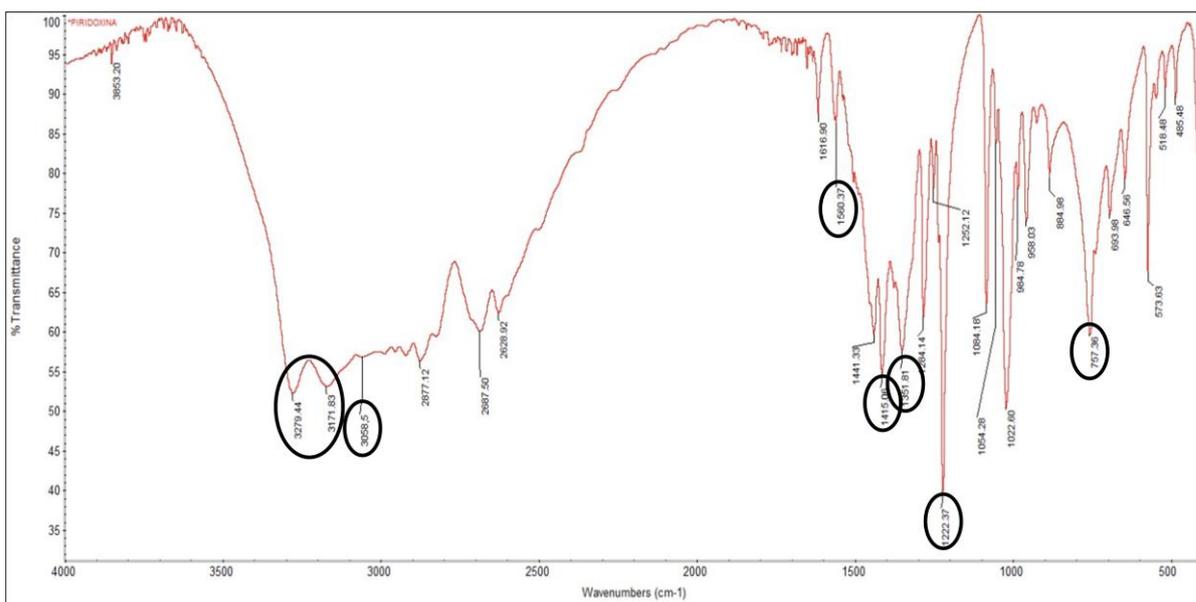


Figure S5. FT-IR spectrum for compound 1.