Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supplementary Information

Theoretical evaluation of Lanthanide Binding Tags as biomolecular handles for the organization of Single Ion Magnets and spin qubits

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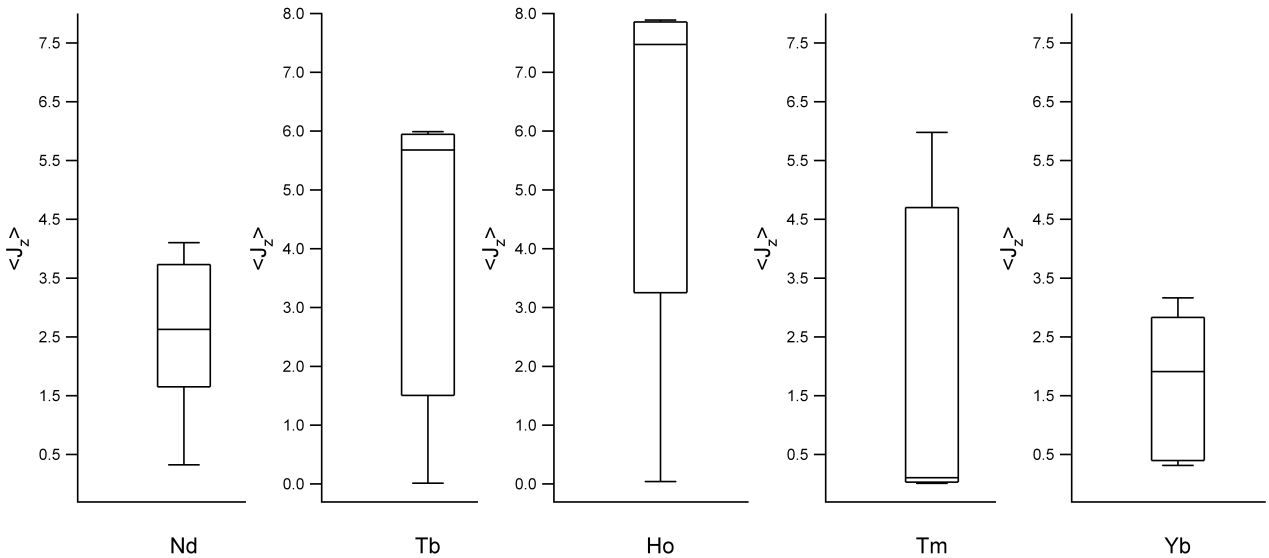

Fig S1: Box plots with the full distribution of expectation values $\langle J_z \rangle$ for diverse LBT structures substituted, from left to right, by Nd, Tb, Ho, Tm and Yb.

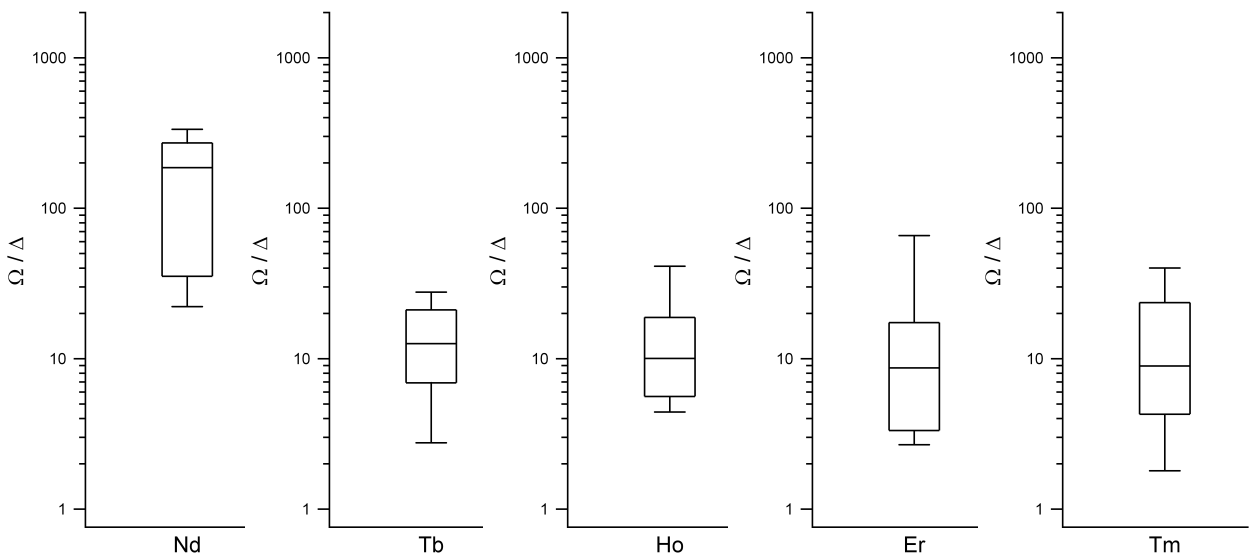

Fig S2: Box plots with the full distribution of Ω/Δ ratios for diverse LBT structures substituted, from left to right, by Nd, Tb, Ho, Er and Tm.

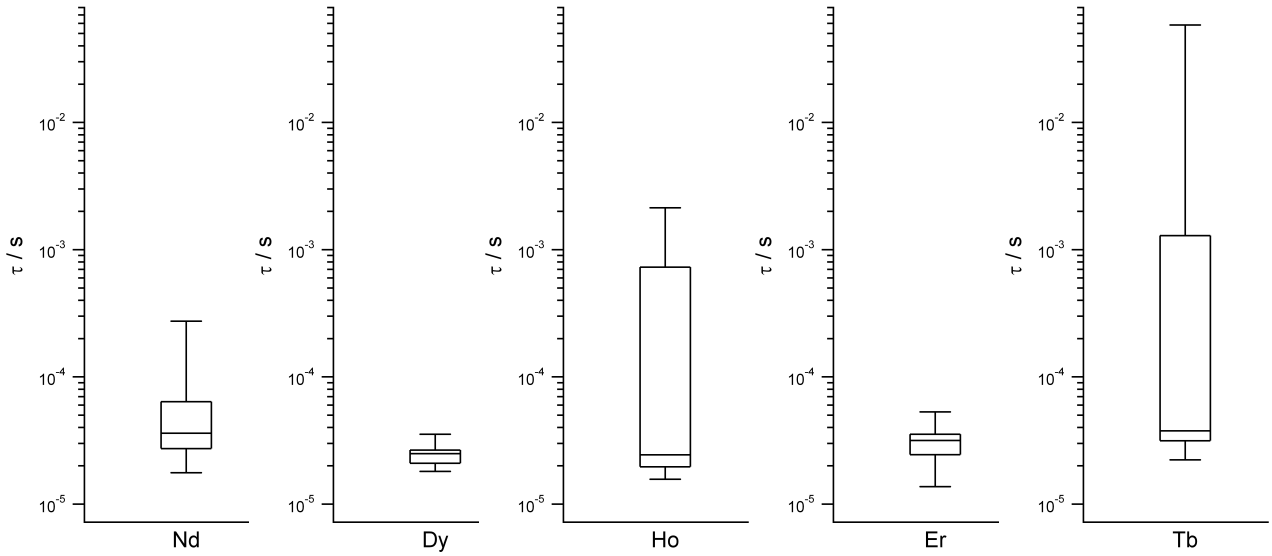

Fig S3: Box plots with the full distribution of estimates decoherence times t for diverse LBT structures substituted, from left to right, by Nd, Dy, Ho, Er and Tb.

Table S1: Ionic radii employed for the lanthanide series and the corresponding contraction/expansion for their coordination spheres. Starting from crystal structures of the Tb^{+3}/Gd^{+3} derivatives.

	Nd	**Gd**	**Tb**	**Dy**	**Ho**	**Er**	**Tm**	**Yb**
r_i	1.249	1.193	1.180	1.167	1.155	1.144	1.134	1.125
Tb Correction	0.069	0.013	0.000	-0.013	-0.025	-0.036	-0.046	-0.055
Gd Correction	0.056	0.000	-0.013	-0.026	-0.038	-0.049	-0.059	-0.068

Table S2: SIMPRE parameters calculated from chemical parameters: electronegativity of the metal (E_M), radial displacement (D_r) and effective charge (Z_i). In all cases number of ligands (N_L) is 8, valence of the metal (V_M) is 3, and electronegativity of the oxygen ligand (E_L) is 3.44.

	Nd	**Tb**	**Dy**	**Ho**	**Er**	**Tm**	**Yb**
E_M	1.14	1.10	1.22	1.23	1.24	1.25	1.10
D_r	1.02	1.04	0.98	0.98	0.98	0.97	1.04
Z_i	0.092	0.091	0.095	0.096	0.096	0.096	0.091

