Supplementary Materials: Field Induced SMM and Vis/NIR luminescence on Mononuclear Lanthanide complexes with 9-anthracenecarboxylate and 2,2′:6,2′′-terpyridine

Berta Casanovas, Oriol Porcar, Saskia Speed, Ramon Vicente, Mercè Font-Bardía and M. Salah El Fallah

Table S1. Continuous shape measures (CShM's) using SHAPE software for **2Tb**-**5Yb**.

Polyhedron	Symmetry	2Tb	3Dy	4Er	5Yb
TDD-8	D_{2d}	1.921	1.902	2.342	2.363
BTPR-8	C_{2v}	3.126	3.092	2.426	2.450
JSD-8	T_d	3.155	3.105	3.924	3.931
JBTPR-8	C_{2v}	3.231	3.177	2.516	2.551

Table S2. Hydrogen bonds distances (d; D = donor atom, A = acceptor atom) and angles of 1**Eu**-**5Yb**

	H bond	d(OD···H), Å	d(H···A), Å	d(OD···A), Å	Angle,^{0}	(‘)
1Eu	O1W-H1W…O6	0.94(3)	2.09(4)	2.912(6)	146(5)	-
2Tb	O7-H7A…O6	0.813(12)	1.921(14)	2.6900(15)	157.6(18)	-
	O7-H7B…O1W	0.809(15)	1.886(15)	2.6931(15)	174.6(16)	-
	O1W-H1WA…O2	0.798(19)	2.04(2)	2.8147(16)	165(2)	-
	O1W-H1WB…O1D	0.804(12)	2.083(13)	2.8535(15)	160(2)	-1+x,y,z
3Dy	O7-H7A…O6	0.812(15)	1.909(16)	2.690(2)	161(2)	-
	O7-H7B…O1W	0.801(17)	1.899(18)	2.693(2)	171(2)	-
	O1W-H1WA…O2	0.80(2)	2.03(2)	2.814(3)	167.9(19)	-
	O1W-H1WB…O1D	0.834(6)	2.030(9)	2.855(3)	170(2)	-1+x,y,z
4Er	O7-H7A…O6	0.90(4)	1.80(3)	2.678(3)	164(3)	-
	O7-H7B…O1W	0.896(16)	1.754(14)	2.644(4)	171(3)	-
	O1W-H1WA…O2	0.94(3)	1.89(3)	2.812(4)	168(4)	-
	O1W-H1WB…O1D	0.95(2)	1.86(2)	2.752(6)	156(4)	-
5Yb	O7-H7A…O6	0.90(4)	1.81(5)	2.678(5)	162(4)	-
	O7-H7B…O1W	0.900(16)	1.763(16)	2.660(5)	174(5)	1+x,y,z
	O1W-H1WA…O2	0.90(5)	1.92(5)	2.811(6)	169(6)	-1+x,y,z
	O1W-H1WB…O1D	0.90(3)	1.84(2)	2.721(9)	165(8)	-1+x,y,z

Table S3. Supramolecular π-π stacking interactions for **1Eu**-**5Yb**

Complex	Contact	Symmetry code (‘)	Cg-Cg distance (Å)	Displacement (Å)
1Eu	Cg(1)-Cg(2)'	2-x,1-y,1-z	3.666(2)	1.388
	Cg(4)-Cg(4)'	1-x,1-y,-z	3.632(3)	1.396
2Tb	Cg(1)-Cg(2)'	1-x,-y,-z	3.7575(8)	1.03
	Cg(1)-Cg(7)'	x,y,z	3.5542(8)	1.145
	Cg(3)-Cg(3)'	-x,-y,-z	3.429(4)	0.702
3Dy	Cg(1)-Cg(2)'	1-x,-y,-z	3.7485(14)	1.048
	Cg(1)-Cg(6)'	x,y,z	3.5496(13)	1.136
	Cg(3)-Cg(3)'	-x,-y,-z	3.5642(15)	0.487
4Er	Cg(1)-Cg(3)'	1/2-x,1/2+y,1/2-z	3.739(2)	1.331
	Cg(1)-Cg(6)'	x,y,z	3.551(3)	0.925
5Yb	Cg(1)-Cg(3)'	3/2-z,1/2+y,1/2-z	3.750(3)	1.333
	Cg(1)-Cg(6)'	x,y,z	3.555(4)	0.933

Table S4. Relaxation parameters values for the best fit of χ_M'' and χ_M' *vs* frequency using generalised Debye model for **3Dy**

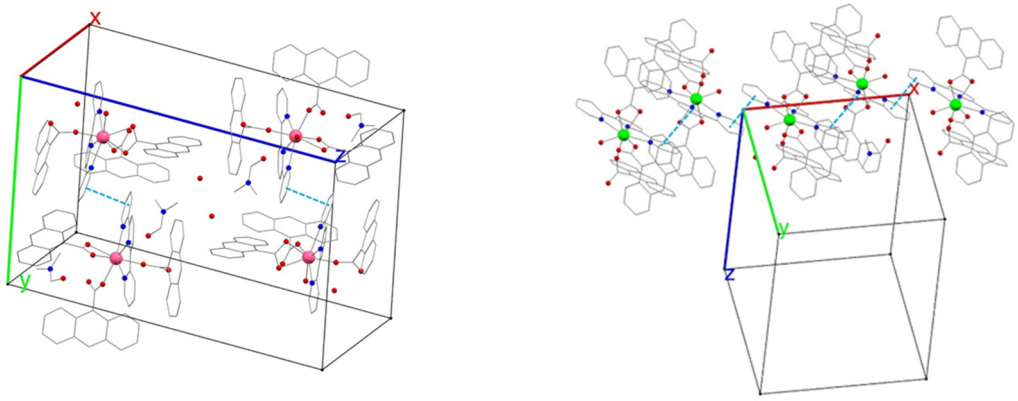
T, K	χ_s, cm³ mol⁻¹	χ_T, cm³ mol⁻¹	τ, s	α
6.2	0.1	2.2	2.0E-04	0.06
6.0	0.1	2.2	2.6E-04	0.06
5.7	0.1	2.3	3.3E-04	0.06
5.5	0.1	2.4	4.3E-04	0.07
5.3	0.1	2.5	5.6E-04	0.07
5.0	0.1	2.7	7.5E-04	0.07
4.7	0.1	2.8	1.0E-03	0.08
4.5	0.1	3.0	1.4E-03	0.08
4.3	0.1	3.1	1.9E-03	0.08
4.1	0.1	3.2	2.5E-03	0.09
4.0	0.1	3.3	2.9E-03	0.09
3.9	0.1	3.4	3.4E-03	0.10
3.8	0.1	3.5	4.1E-03	0.10
3.7	0.1	3.6	4.9E-03	0.11
3.6	0.1	3.7	5.8E-03	0.11
3.5	0.1	3.8	7.0E-03	0.12
3.4	0.1	4.0	8.5E-03	0.13

Table S5. Relaxation parameters values for the best fit of χ_M'' and χ_M' *vs* frequency using generalised Debye model for **4Er**.

T, K	χ_s, cm³ mol⁻¹	χ_T, cm³ mol⁻¹	τ, s	α
2.7	0.31	2.17	1.21E-04	0.05
2.6	0.32	2.24	1.54E-04	0.05
2.5	0.32	2.31	1.92E-04	0.06
2.4	0.32	2.38	2.35E-04	0.07
2.3	0.33	2.47	2.85E-04	0.08
2.2	0.33	2.58	3.53E-04	0.09
2.1	0.33	2.65	3.94E-04	0.09
2.0	0.34	2.78	4.64E-04	0.10
1.9	0.34	2.92	5.40E-04	0.11
1.8	0.35	2.98	5.87E-04	0.10

Table S6. Relaxation parameters values for the best fit of χ_M'' and χ_M' *vs*. frequency using generalised Debye model for compound **5Yb**

T, K	χ_s, cm³ mol⁻¹	χ_T, cm³ mol⁻¹	τ, s	α
3.2	0.03	0.51	1.63E-04	0.12
3.0	0.04	0.55	2.14E-04	0.13
2.8	0.04	0.59	2.79E-04	0.14
2.5	0.04	0.65	3.89E-04	0.16
2.3	0.04	0.72	5.78E-04	0.19
2.0	0.04	0.82	8.74E-04	0.21
1.8	0.04	0.89	1.21E-03	0.24



(**a**) (**b**)

Figure S1. Supramolecular arrangement representation in compounds (**a**) **4Er**; (**b**) **5Yb**. π- π stacking interactions are indicated in blue.

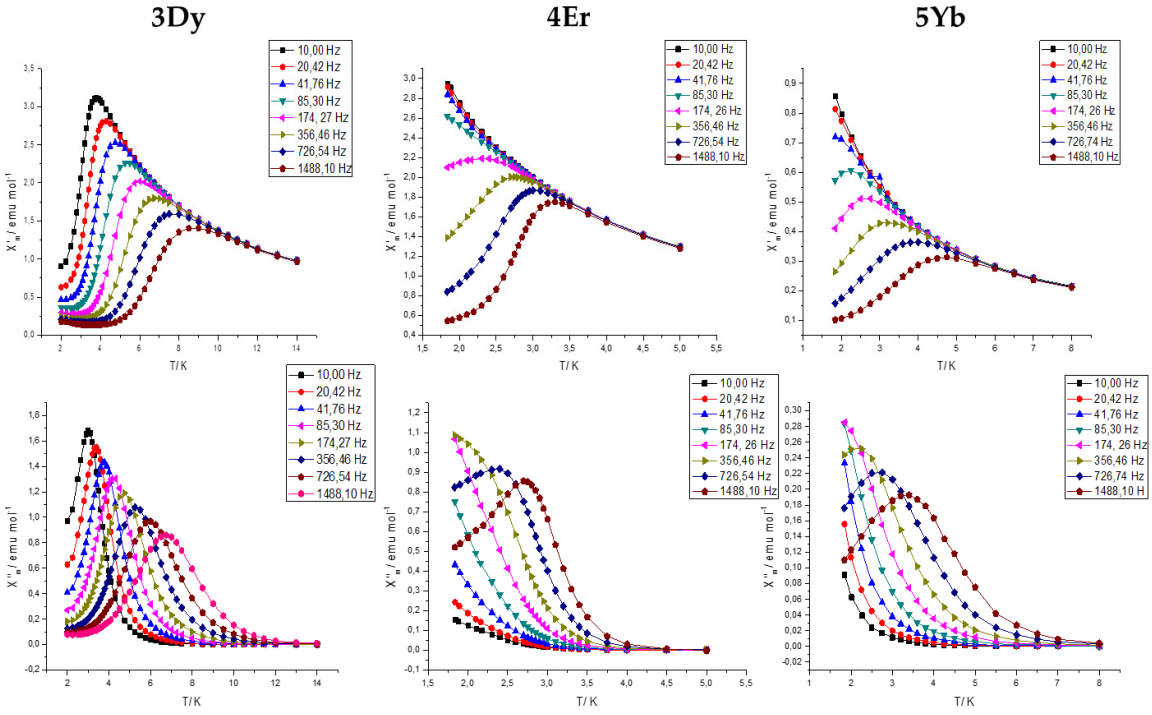


Figure S2. χ_M' and χ_M'' *vs* T plots for compounds **3Dy-5Yb**.

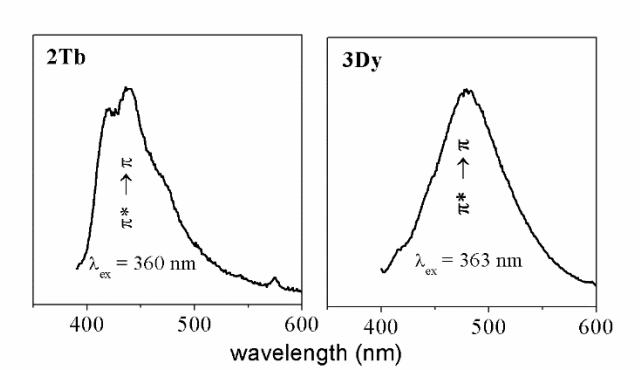


Figure S3. Emission spectra for **2Tb** and **3Dy** at rt.

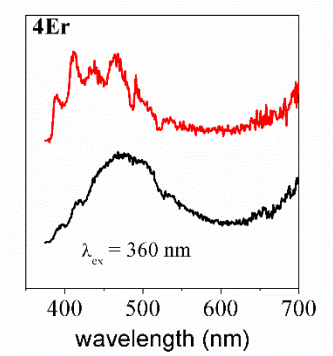


Figure S4. Emission spectra for **4Er** at rt. (back line) and at 77 K (red line).