Slow magnetic relaxation and luminescence properties in tetra - diketonate lanthanide(III) complexes.

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SUPPLEMENTARY INFORMATION

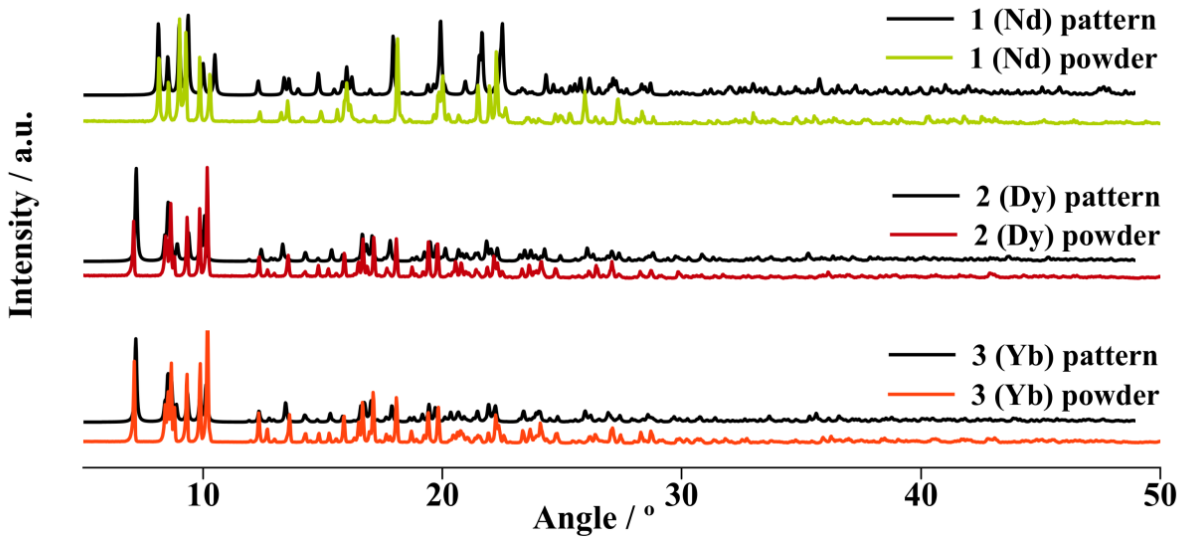

Figure S1. Powder X-Ray Diffraction (PDRX) of all the polycrystalline samples. The PDRX spectra of the polycrystalline samples were compared with the simulated PDRX spectra from the structures obtained by monocrystal X-Ray Diffraction.

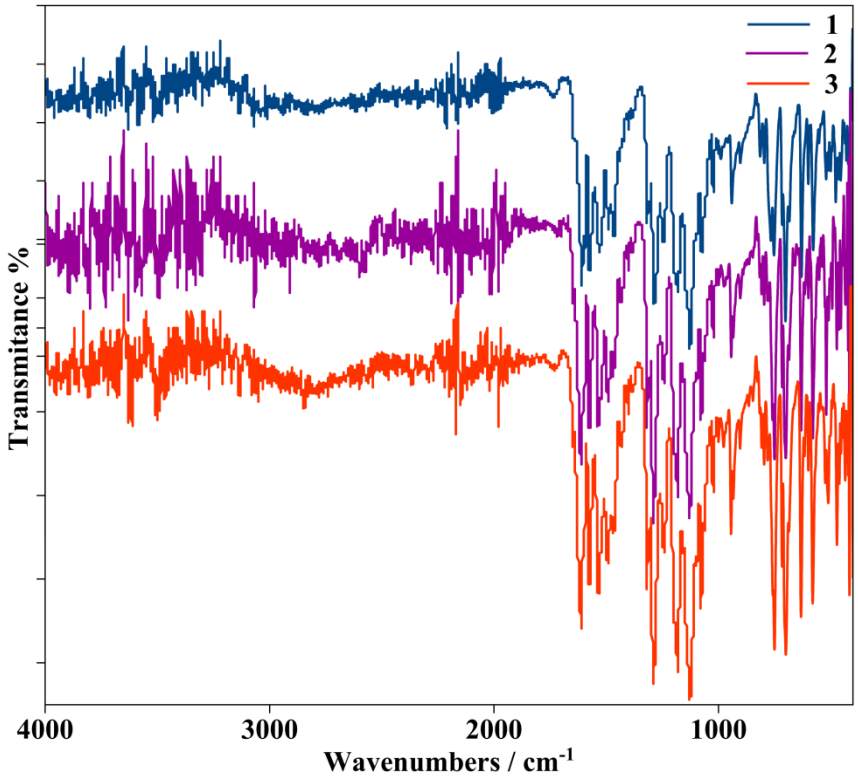

Figure S2. Infra-Red Spectra of compounds 1-3.

Table S1. Continuous shape measures (CShM's) using SHAPE software for.compounds 1-3.

		1(Nd)
CU-8	Oh	0.026
TT-8	T_d	0.978
HBPY-8	D_{6h}	7.924
TDD-8	D_{2d}	7.934

		2(Dy)	3(Yb)
TDD-8	D_{2d}	0.360	0.422
SAPR-8	D_{4d}	1.666	1.373
BTPR-8	C_{2v}	2.273	2.040
JBTPR-8	C_{2v}	2.849	2.558

Table S2. Relaxation parameters values for the best fit of χ_M'' and χ_M' in front of frequency using the one component generalised Debye model for compound **1**.

T (K)	χ_S (cm^{3}Kmol^{-1})	χ_T (cm^{3}Kmol^{-1})	(s)	
1.83962	0.0455	0.31734	0.002	0.06556
1.88732	0.04206	0.30921	0.00152	0.07221
1.99563	0.04023	0.2931	0.00103	0.06035
2.09453	0.03677	0.27889	6.94346E-4	0.05252
2.19774	0.0362	0.27019	5.46854E-4	0.04596
2.3044	0.03318	0.25631	3.64038E-4	0.03809
2.40117	0.03119	0.24564	2.57573E-4	0.03385
2.50108	0.02977	0.23572	1.86695E-4	0.02777
2.59803	0.028	0.22687	1.36275E-4	0.02536
2.69581	0.02549	0.21874	9.79094E-5	0.02664
2.79577	0.02352	0.21116	7.18483E-5	0.03203

Table S3. Relaxation parameters values for the best fit of χ_M'' and χ_M' in front of frequency using the one component generalised Debye model for compound **2.**

T (K)	χ_S (cm^{3}Kmol^{-1})	χ_T (cm^{3}Kmol^{-1})	(s)	
1.79711	0.33409	6.51147	0.02539	0.20192
1.89644	0.32045	6.18647	0.02107	0.19353
2.00023	0.31244	5.86218	0.0166	0.17471
2.09788	0.30113	5.5674	0.01268	0.1581
2.3033	0.28247	5.12006	0.0073	0.12635
2.49529	0.26234	4.76426	0.00379	0.10196
2.69827	0.24811	4.45505	0.0019	0.08707
2.90236	0.23298	4.18945	9.14465E-4	0.08134
3.09913	0.22158	3.95721	4.32091E-4	0.08158
3.30013	0.17581	3.74919	2.00062E-4	0.08957
3.49969	0.08911	3.56102	9.34182E-5	0.09614
3.70212	2.95341E-18	3.38881	4.49466E-5	0.09836

Table S4. Relaxation parameters values for the best fit of χ_M'' and χ_M' in front of frequency using the one component generalised Debye model (Eq S1) for compound **3.**

T (K)	χ_S (cm^{3}Kmol^{-1})	χ_T (cm^{3}Kmol^{-1})	τ (s)	α
1.88843	0.05903	0.48819	0.00431	0.15698
1.99543	0.0559	0.48361	0.00382	0.1592
2.09444	0.05491	0.45621	0.00274	0.12562
2.19757	0.05247	0.43312	0.00193	0.0999
2.30387	0.05098	0.41924	0.00154	0.0849
2.40208	0.04806	0.39716	0.00103	0.06436
2.50073	0.04631	0.38062	7.37139E-4	0.04941
2.59353	0.04426	0.3656	5.31522E-4	0.04161
2.69378	0.04333	0.35153	3.89679E-4	0.0298
2.79486	0.04053	0.33902	2.88188E-4	0.02637
2.89796	0.03978	0.32734	2.16683E-4	0.02048
2.99848	0.03938	0.3166	1.64892E-4	0.01455
3.09816	0.0398	0.30641	1.27739E-4	0.01174
3.19864	0.04065	0.29721	1.0025E-4	0.00895
3.30053	0.04398	0.28806	8.02924E-5	6.91582E-5
3.39966	0.04593	0.27992	6.349E-5	9.47705E-5

$$\chi_{AC}(\omega) = \chi_S + \frac{\chi_T - \chi_S}{1+(i\omega\tau)^{(1-\alpha)}} \qquad \text{Eq S1}$$

Generalized Debye model that describes a system with a distribution of the magnetization relaxation time. Where χ_S and χ_T are the adiabatic and thermal susceptibilities, τ is the relaxation of the magnetization time and ω is the angular frequency of the ac field (ω= 1/2πf). χ_T is the susceptibility in the limit of the lowest field frequencies where the thermal equilibrium of the system is observed. χ_S (lower than the χ_T) is observed when the oscillations of the ac field are fast compared to the time constant, τ, and the magnetic system remains isolated from its environment. The α parameter quantifies the width of the τ distribution and it ranges from 0 to 1. The wider the distribution, α acquires a larger value.