Electronic Supporting Information

Luminescence thermometry based on one-dimensional benzoato-bridged coordination polymers containing lanthanide ions

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Table S1. Crystallographic data, details of data collection and structure refinement parameters for **1** and **3**.

Compounds	**1**	**3**
Formula	$C_{58}H_{70}O_{22}Tb_2$	$C_{27}H_{31}O_{11}Nd$
Molecular weight	1436.98	675.76
Temperature (K)	293(2)	293(2)
Crystal system	*triclinic*	*monoclinic*
Space group	*P*-1	$P2_1/c$
a (Å)	9.8516(2)	10.0703(3)
b (Å)	12.2547(3)	9.7655(3)
c (Å)	13.9649(3)	28.8888(9)
α (deg)	107.133(2)	90
β (deg)	98.272(5)	91.964(3)
γ (deg)	102.315(2)	90
V (Å^3)	1497.64(6)	2839.30(15)
Z	1	4
D_{calc} (g cm^{-3})	1.593	1.581
F (000)	724.0	1364.0
Wavelength (Å)	0.71073	0.71073
Final R_1[a], wR_2[b] $[I > 2\sigma(I)]$	0.0367, 0.0781	0.0619, 0.2022
R_1[a], wR_2[b] (all data)	0.0415, 0.0810	0.0672, 0.2045
Goodness-of-fit on F^2	1.035	1.647
Largest peak in final difference (e Å^{-3})	1.07, -1.09	2.33, -1.86

[a]$R_1 = \sum||F_o|-|F_c||/\sum|F_o|$. [b]$wR_2 = [\sum w(F_o^2 - F_c^2)^2/\sum w(F_o^2)^2]^{1/2}$; $w = 1/[\sigma^2(F_0^2)+(aP)^2+bP]$ where $P = [\max(F_0^2, 0) + 2F_c^2]/3$.

Table S2. Continuous Shape Measures for the coordination polyhedron around the Ln^{III} ion

Geometry	**Tb^{III} (1)**	**Nd^{III} (3)**
OP-8	28.788	30.550
HPY-8	22.332	23.505
HBPY-8	12.277	16.124
CU-8	89.642	10.370
SAPR-8	2.172	1.288
TDD-8	2.246	1.508
JGBF-8	11.706	14.491
JETBPY-8	26.951	28.572
JBTPR-8	1.985	1.084
BTPR-8	**1.801**	**0.909**
JSD-8	2.720	3.302
TT-8	10.240	10.726
ETBPY-8	24.264	25.028

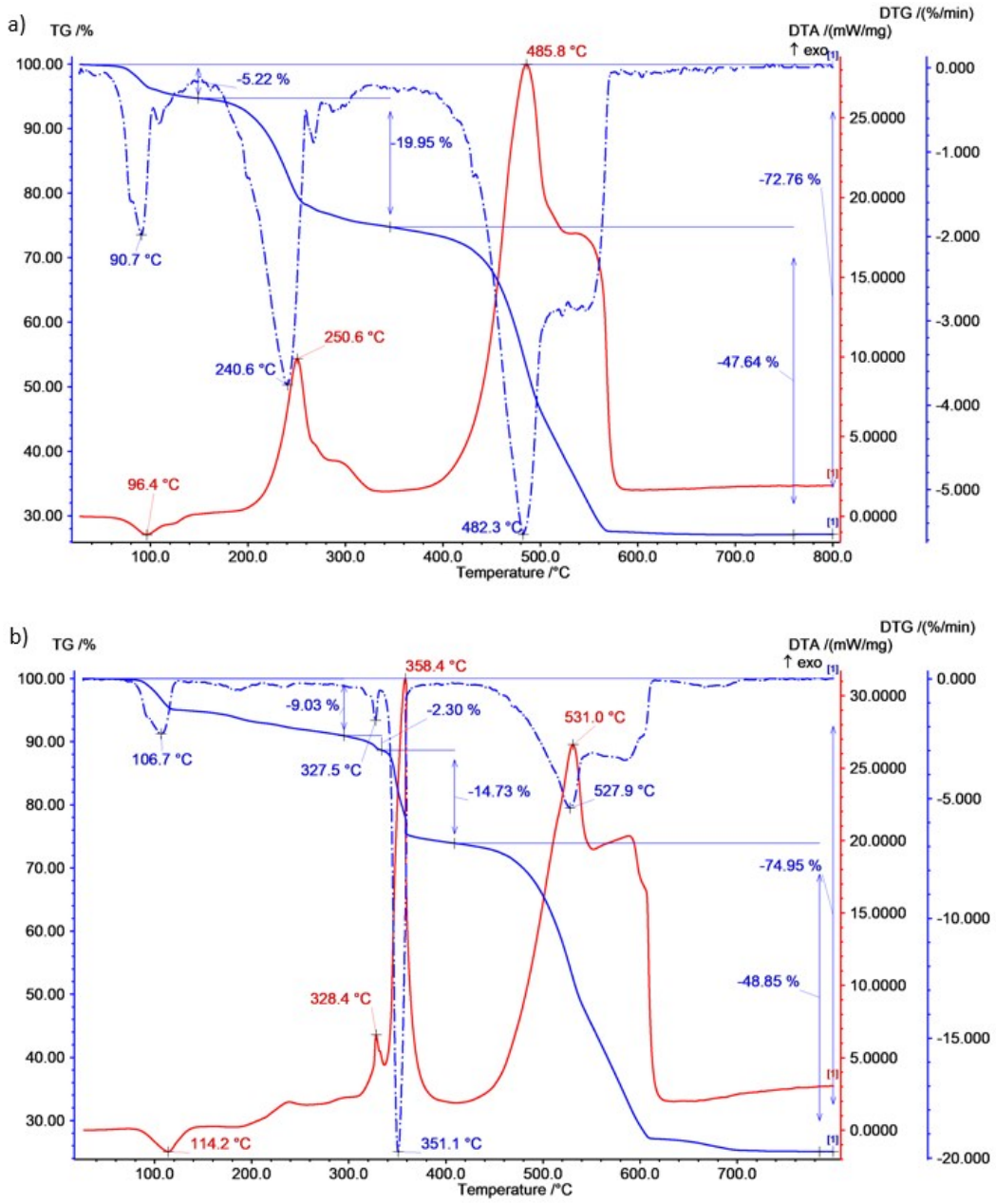

Figure S1. Thermogravimetry, Differential thermogravimetry and Differential Thermal Analysis plots of compounds **1** (a) and **3** (b).

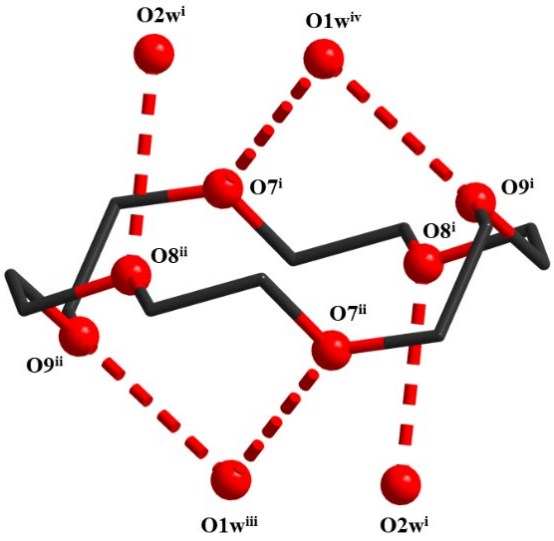

Figure S2. Hydrogen bonds formed via 18C6 molecules in compound **3**

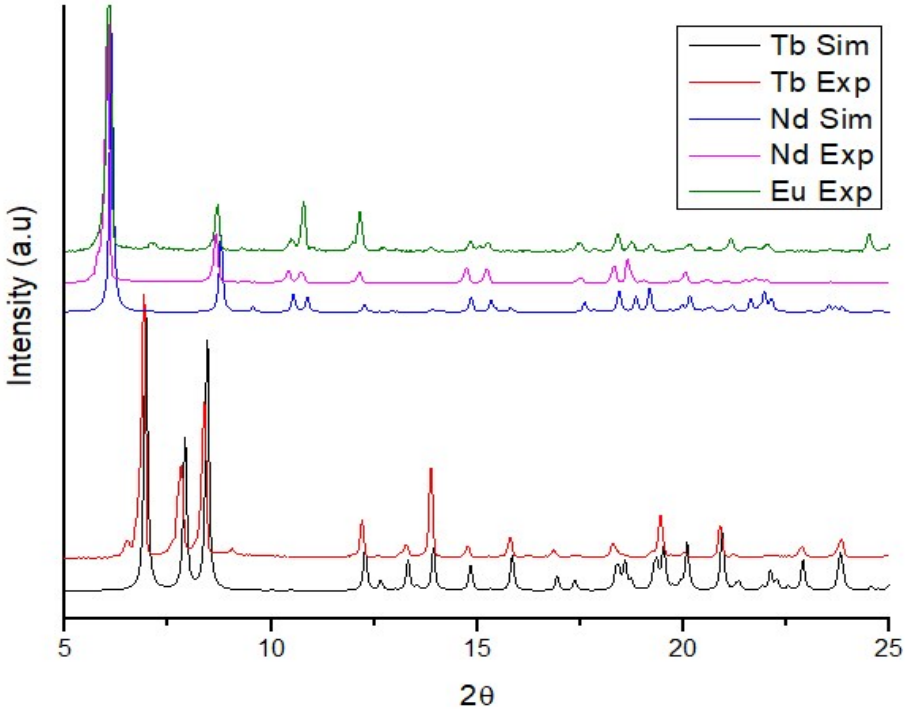

Figure S3. Simulated PXRD patterns for compounds **1** (black) and **3** (blue), experimental PXRD patterns for compounds **1** (red), **2** (green) and **3** (violet)

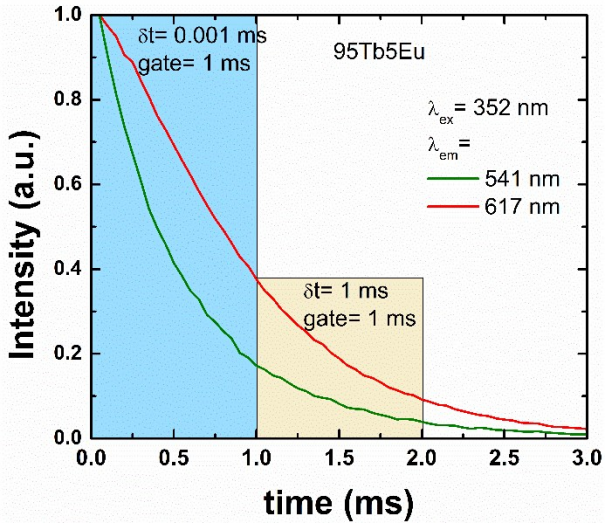

Figure S4. Selection of time delay and gate width used in PL thermometry measurements.

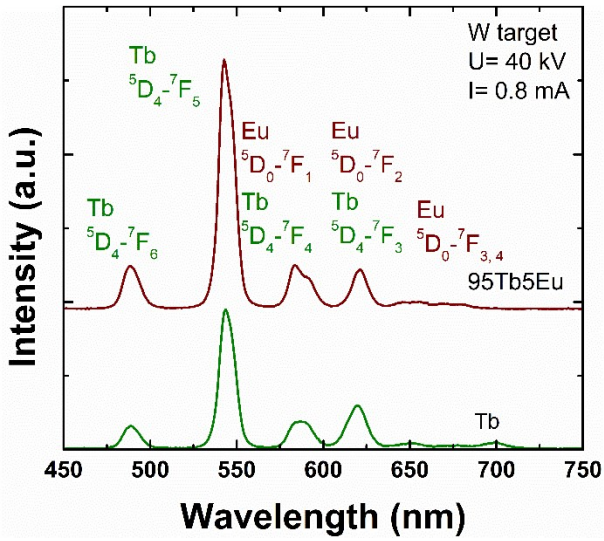

Figure S5. XEOL spectra of **1** (Tb) and **4** (95Tb5Eu) measured upon X-ray irradiation with a W target at U= 40 kV and I= 0.8 mA.