Electronic Supplementary Material (ESI) for CrystEngComm.

A series of six-member lanthanide-rings based on 2,2-bis(hydroxymethyl)-2,2',2''-nitrilotriethanol : synthesis, crystal structures and magnetic properties

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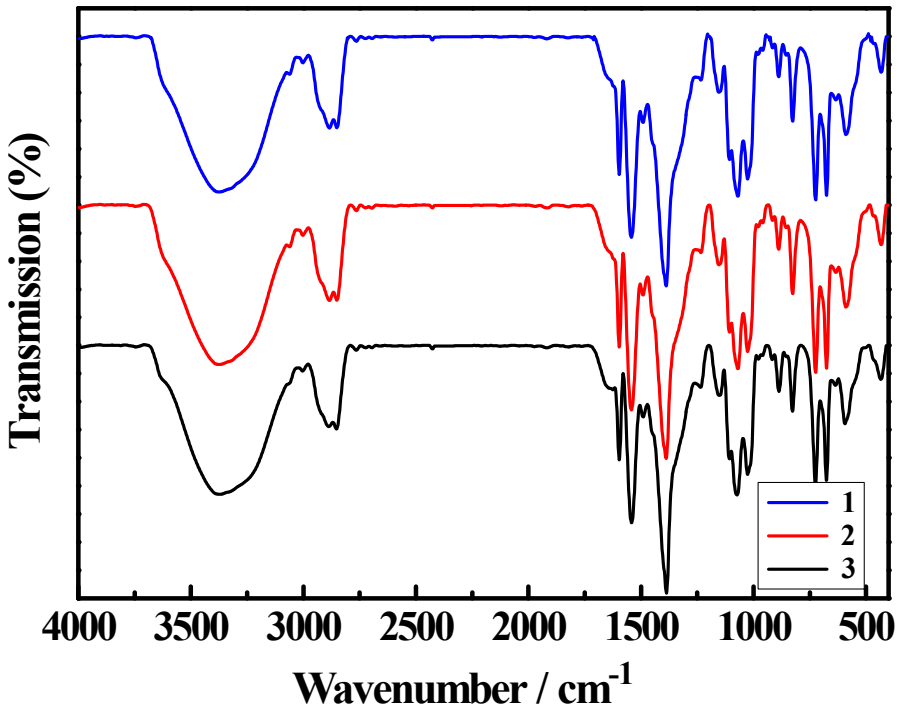

Fig. S1. FT-IR spectra of **1** (red), **2** (blue) and **3** (black).

Table S1. Crystal data and structure refinement for **1**, **2** and **3**.

	1	2	3
Empirical formula	$C_{97}H_{144}Gd_6N_6O_{44}$	$C_{97}H_{144}Tb_6N_6O_{44}$	$C_{90}H_{136}Dy_6N_6O_{44}$
Formula weight	3041.69	3051.74	2981.05
Temperature/K	293(2)	293(2)	173(2)
Crystal system	trigonal	trigonal	monoclinic
Space group	*R*-3	*R*-3	*C*2/*c*
a/Å	26.842(4)	26.742(4)	32.664(7)
b/Å	26.842(4)	26.742(4)	11.254(2)

c/Å	78.271(16)	78.391(16)	30.378(6)
α/°	90	90	90
β/°	90	90	111.76(3)
γ/°	120	120	90
Volume/Å^3	48838(17)	48548(17)	10371(4)
Z	18	18	4
D_{calc} (g/cm^3)	1.976	1.879	1.886
M (mm^{-1})	3.700	3.967	4.358
F(000)	27636.0	25920.0	5784.0
R_{int}	0.0283	0.0341	0.0370
parameters	1332	1331	670
Goodness-of-fit on F^2	1.009	1.051	1.076
Final R indexes [$I>2\sigma(I)$]	R_1 = 0.0283, wR_2 = 0.0764	R_1 = 0.0341, wR_2 = 0.0877	R_1 = 0.0559, wR_2 = 0.1662
Final R indexes [all data]	R_1 = 0.0299, wR_2 = 0.0775	R_1 = 0.0414, wR_2 = 0.0911	R_1 = 0.0610, wR_2 = 0.1722
$\Delta\rho_{max}/\Delta\rho_{min}$/e Å^{-3}	2.81/-1.23	3.18/-1.30	3.93/-1.60

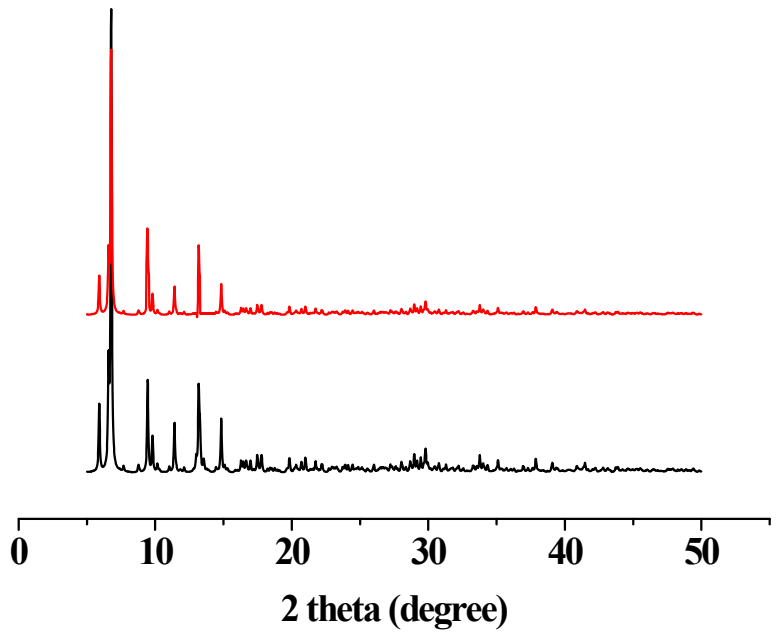

Fig. S2. The simulated X-ray powder diffraction patterns (black) and the experimental one (red) of compound **1**.

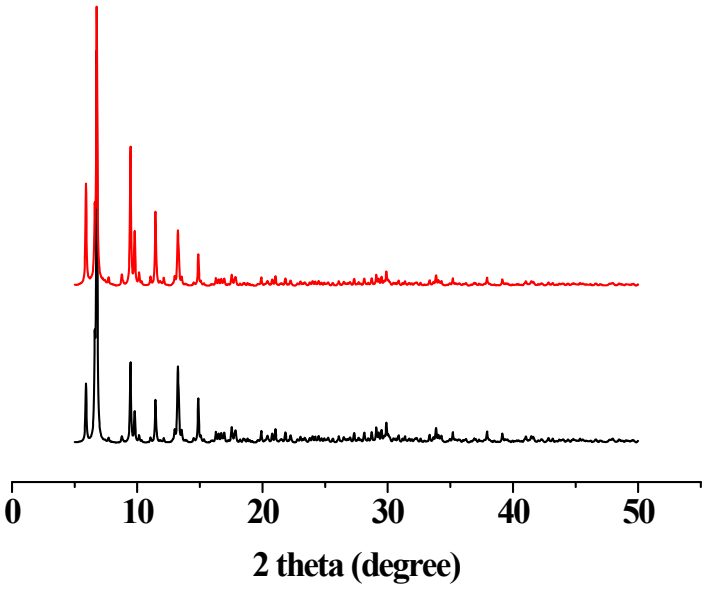

Fig. S3. The simulated X-ray powder diffraction patterns (black) and the experimental one (red) of compound **2**.

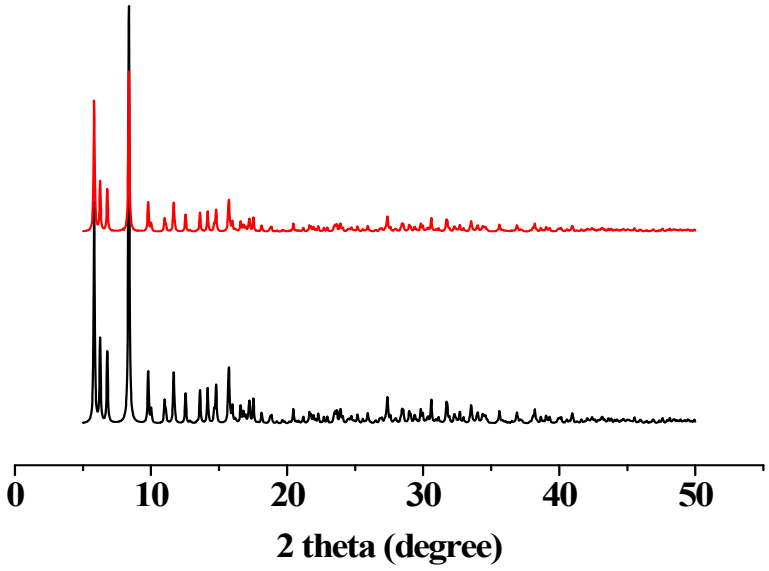

Fig. S4. The simulated X-ray powder diffraction patterns (black) and the experimental one (red) of compound **3**.

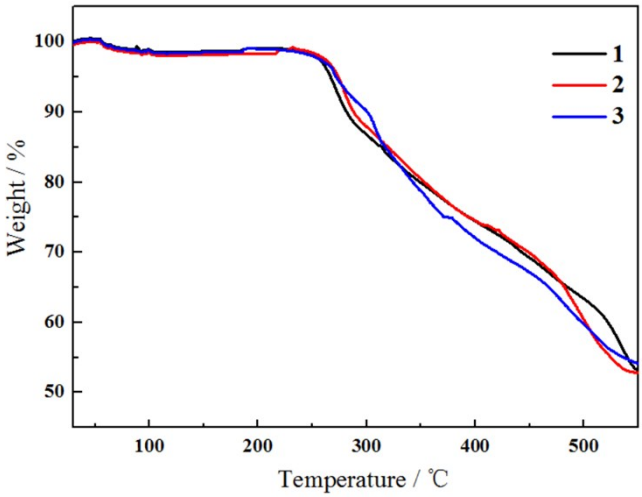

Figure S5. TGA curves of 1-3