Electronic Supplementary Material (ESI) for CrystEngComm.

Hydrogen bonded-extended lanthanide coordination polymers decorated with 2,3-thiophenedicarboxylate and oxalate: synthesis, structures, and properties

Table S1 Crystal data and structure refinements for **1–5**

Compounds	**1**	**2**	**3**	**4**	**5**
Formula	$C_{14}H_{14}O_{17}S_2Nd_2$	$C_{14}H_{14}O_{17}S_2Eu_2$	$C_{14}H_{14}O_{17}S_2Gd_2$	$C_{14}H_{14}O_{17}S_2Tb_2$	$C_{14}H_{14}O_{17}S_2Ho_2$
Formula weight	806.85	822.29	832.87	836.21	848.23
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
space group	C2/c	C2/c	C2/c	C2/c	C2/c
a/Å	19.965(3)	19.746(6)	19.671(4)	19.621(3)	19.489(5)
b/Å	6.1120(10)	6.0662(19)	6.0556(13)	6.0421(9)	6.0107(16)
c/Å	19.828(3)	19.785(6)	19.793(4)	19.795(3)	19.762(5
α/°	90.00	90.00	90.00	90.00	90.00
β/°	111.194(2)	111.051(3)	111.098(2)	111.0900(10)	111.257(2)
γ/°	90.00	90.00	90.00	90.00	90.00
V/Å^3	2255.9(6)	2211.7(12)	2199.7(8)	2189.5(6)	2157.5(10)
Z	4	4	4	4	4
D_c (g cm^{-3})	2.376	2.469	2.515	2.537	2.611
μ/mm^{-1}	4.821	5.893	6.253	6.684	7.562
F(000)	1544	1568	1576	1584	1600
Reflections collected/unique	7958/2101	7791/2060	7618/2042	7571/2033	6495/2008
Data/restraints/parameters	2101/0/160	2060/0/160	2042/0/160	2033/0/160	2008/0/160
GOF(F^2)	1.029	1.268	1.095	1.155	1.166
R_1[a]/wR_2[b] [$I > 2\sigma(I)$]	0.0189/0.0509	0.0225/ 0.0559	0.0206/0.0528	0.0224/0.0580	0.0215/0.0531
R_1[a]/wR_2[b] (all data)	0.0191/0.0511	0.0227/0.0560	0.0210/0.0530	0.0225/0.0580	0.0221/0.0533

[a] $R_1 = \sum \left| |F_o| - |F_c| \right| / \sum |F_o|$. [b] $wR_2 = \{\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]\}^{1/2}$

Table S2 Selected bond lengths (Å) for **1–5**[a]

	1	**2**	**3**	**4**	**5**
Ln(1)-O(8)	2.443(2)	2.398(3)	2.390(3)	2.373(3)	2.350(3)
Ln(1)-O(7)	2.462(3)	2.418(3)	2.400(3)	2.388(4)	2.356(3)
Ln(1)-O(1)#1	2.469(2)	2.426(3)	2.416(3)	2.400(3)	2.377(3)
Ln(1)-O(5)	2.480(2)	2.440(3)	2.431(3)	2.419(3)	2.402(3)
Ln(1)-O(6)#2	2.494(2)	2.458(3)	2.448(3)	2.439(3)	2.414(3)
Ln(1)-O(4)	2.508(2)	2.474(3)	2.465(3)	2.454(3)	2.430(3)
Ln(1)-O(3)	2.528(2)	2.482(3)	2.476(3)	2.455(3)	2.433(3)
Ln(1)-O(2)#3	2.537(2)	2.484(3)	2.478(3)	2.457(3)	2.424(3)
Ln(1)-O(1)#3	2.631(2)	2.618(3)	2.605(3)	2.616(3)	2.605(3)

[a] Symmetry codes:#1 x, y+1, z #2 -x, -y+2, -z+1 #3 -x+1/2,-y+3/2,-z+1

Table S3 Hydrogen bond lengths (Å) and bond angles (º) in **1**[a]

Compound **1**				
D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(9)-H(5W)...O(4)#4	0.85	1.97	2.759(3)	154.7
O(8)-H(4W)...O(3)#5	0.85	1.92	2.760(3)	169.6
O(8)-H(3W)...O(2)#5	0.85	2.38	2.918(4)	121.4
O(8)-H(3W)...O(6)#6	0.85	2.29	3.074(4)	154.1
O(7)-H(2W)...O(5)	0.85	2.54	3.003(4)	115.7
O(7)-H(1W)...O(9)#7	0.85	2.32	2.744(3)	111.3

[a] Symmetry codes: #4 -x+1,y-1,-z+1/2 #5-x+1/2,-y+5/2,-z+1 #6 -x,-y+3,-z+1 #7 x-1,y+1,z

Scheme 1. Coordination modes of tdc and oxalate ligands.

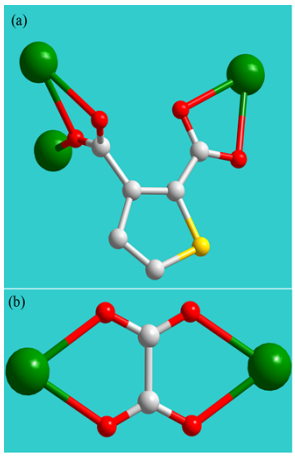

Fig. S1 View of the 3D supramolecular structure of **1**. The intra- and intermolecule hydrogen bonds are shown in yellow and blue colours, respectively. C–H···π stacking interactions are shown in pink colour.

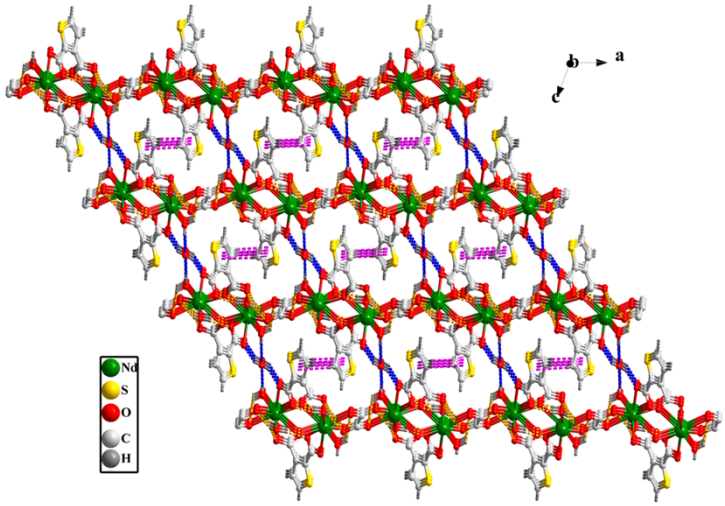

Fig. S2 PXRD patterns of as-synthesized **1-5** and simulated **1.**

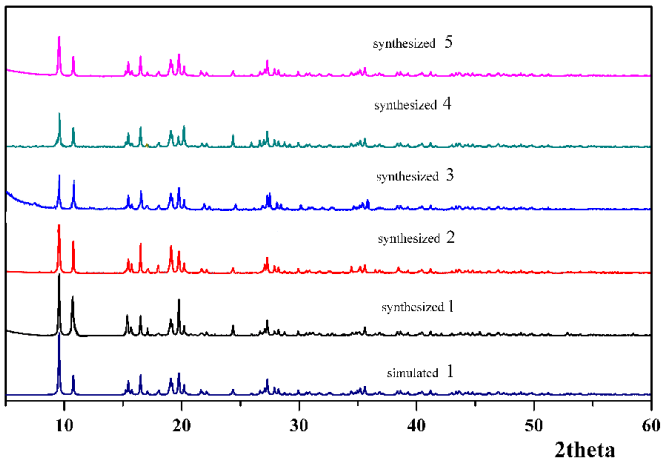

Fig. S3 TG curve of **1-5**.

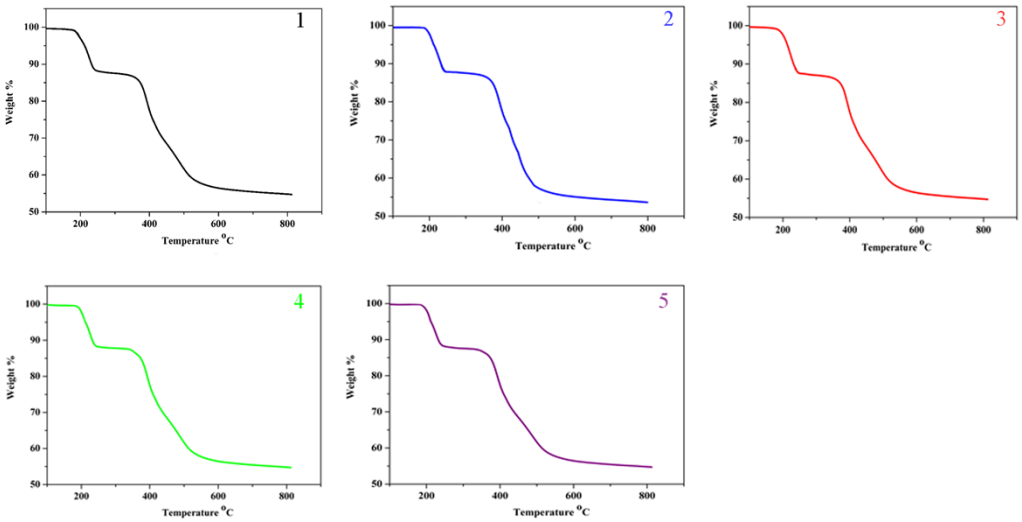

Fig. S4 PXRD patterns of fresh dehydrated **1**, recovered **1** after run 4(activated) and synthesized **1.**

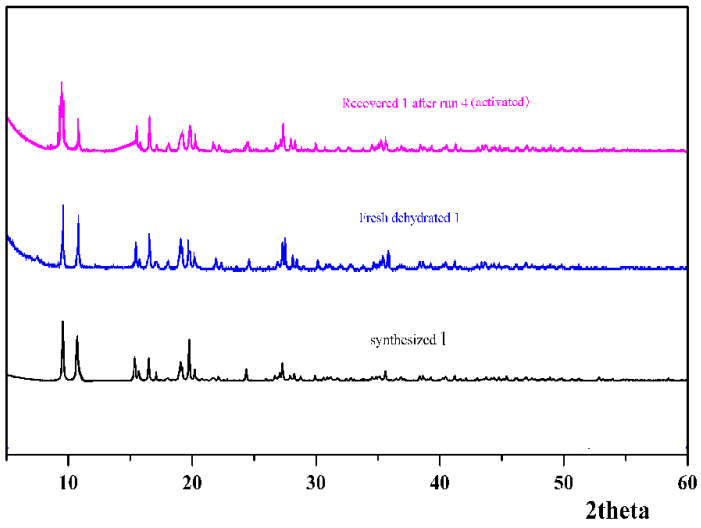

Fig. S5 ^{1}HNMR of (Dimethoxymethyl)benzene

^{1}H NMR (400 MHz, $CHCl_3$): δ 7.41-7.35 (m, 5H), 5.43 (s, 1H), 3.32 (s, 6H).