Electronic Supplementary Material (ESI) for CrystEngComm

Synthesis, Crystal Structure and Luminescent Properties of New Lanthanide-Containing Coordination Polymers Involving 4,4'-oxy-bis-benzoate as Ligand.

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SUPPLEMENTARY

Table S1 : Cell parameters for $[Ln_2(oba)_3(H_2O)_5,H_2O]_\infty$ with Ln = La - Pr.

Cell parameters	La	Ce	Pr	Nd
a (Å)	23.622(4)	23.58	23.51	23.51
b (Å)	6.066(1)	6.03	6.01	5.99
c (Å)	29.414(6)	29.33	29.28	29.32
β (°)	102.034(7)	101.96	101.82	101.79

Table S2. Chemical analysis for $[Ln_2(oba)_3(H_2O)_5,H_2O]_\infty$ with Ln = La - Pr.

		Anal. Calculated (found)			
Ln	MW[gmol^{-1}]	Ln [%]	O [%]	C [%]	H [%]
La	1154.53	24.1 (23.3)	29.1 (30.7)	43.7 (42.5)	3.1 (3.3)
Ce	1156.95	24.2 (23.7)	29.0 (31.0)	43.6 (42.0)	3.2 (3.3)
Pr	1158.54	24.3 (23.5)	29.0 (30.9)	43.5 (42.0)	3.2 (3.6)
Nd	1165.20	24.7 (23.8)	28.8 (30.5)	43.3 (42.2)	3.2 (3.5)

Table S3. Chemical analysis for $[Ln_2(oba)_3(H_2O)_6,3H_2O]_\infty$ with Ln = Sm - Ho or Y.

		Anal. Calculated (found)			
Ln	MW[gmol^{-1}]	Ln [%]	O [%]	C [%]	H [%]
Sm	1231.50	24.4 (24.3)	31.2 (31.2)	41.0 (41.1)	3.4 (3.4)
Eu	1234.71	24.6 (24.6)	31.1 (31.0)	40.9 (41.0)	3.4 (3.4)
Gd	1245.30	25.3 (25.5)	30.8 (30.8)	40.5 (40.4)	3.4 (3.3)
Tb	1248.63	25.4 (25.5)	30.8 (30.9)	40.4 (40.4)	3.4 (3.2)
Dy	1255.78	25.9 (26.1)	30.5 (30.3)	40.2 (40.1)	3.4 (3.5)
Ho	1260.64	26.2 (26.0)	30.5 (30.7)	40.0 (40.1)	3.3 (3.2)
Y	1108.59	16.1 (16.0)	34.6 (34.5)	45.5 (45.7)	3.8 (3.8)

Table S4. Chemical analysis for $[Ln_2(oba)_3(H_2O)_{5.5},0.5H_2O]_\infty$ with Ln = Sm - Dy.

		Anal. Calculated (found)			
Ln	MW[gmol^{-1}]	Ln [%]	O [%]	C [%]	H [%]
Sm	1177.50	25.6 (25.5)	28.5 (28.6)	42.8 (42.7)	3.1 (3.2)
Eu	1180.67	25.7 (25.6)	28.5 (28.5)	42.7 (42.6)	3.1 (3.3)
Gd	1191.20	26.4 (26.4)	28.2 (28.1)	42.4 (42.5)	3.0 (3.0)
Tb	1194.59	26.6 (26.5)	28.1 (28.0)	42.3 (42.2)	3.0 (3.3)
Dy	1201.74	27.0 (27.0)	28.0 (28.1)	42.0 (42.1)	3.0 (2.8)

Table S5. Crystallogenesis conditions for family 1.					
Synthesis conditions		La	Ce	Pr	Nd
U-tube	Agar-Agar 0.1%				
	Agar-Agar 0.2%				
	Agar-Agar 0.3%				
	TEOS 7.5%				

Table S6. Crystallogenesis conditions for Family 2.					
Synthesis conditions		Gd	Tb	Er	Ho
U-tube	Agar-Agar 0.1%				
	TEOS 7.5%				

Table S7. Crystallogenesis conditions for Family 3.									
Synthesis conditions		Sm	Eu	Gd	Tb	Dy	Y	Ho	Er
U-tube	Agar-Agar 0.2%								
	TEOS 7.5%								
H-tube									

The darkened cases indicate the single crystals that have been used for solving the crystal structures

Table S8 : Interatomic distances for H-bonds in $[La_2(oba)_3(H_2O)_5,H_2O]_\infty$

Atom1	Atom2	Symmetry code	Distance (Å)
O14	OW1	x, 1+y, z	2.729(4)
O14	OW1	-x, 1-y, 1-z	2.759(1)
OW1	O201	x, y, z	2.822(4)
O201	O15	x, y, z	2.964(4)
O201	O203	x, y, z	3.054(7)
O203	O201	x, y, z	3.054(7)
O203	OW1	-x, 1-y, 1-z	2.725(8)
O14	O203	-x, 1-y, 1-z	2.777(7)
O203	O51	x, y, z	2.770(7)

Table S9 : Interatomic distances for H-bonds in $[Gd_2(oba)_3(H_2O)_6,3H_2O]_\infty$

Atom1	Atom2	Symmetry code	Distance (Å)
O12	OW1	0.5+x, -0.5-y, z	2.886(1)
OW1	OW2	x, y, z	2.567(1)
O15	OW3	0.5+x, -0.5-y, z	2.88(1)