Electronic Supporting Information (ESI)

Homochiral lanthanoid(III) mesoxalate metal-organic frameworks: synthesis, crystal growth, chirality, magnetic and luminescent properties

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Content:

Table S1. Elemental analyses

		C (%)	H (%)
La	Calculated	13.71	2.28
	Experimental	13.73	2.29
Ce	Calculated	13.67	2.28
	Experimental	13.61	2.31
Pr	Calculated	13.66	2.28
	Experimental	13.63	2.20
Nd	Calculated	13.53	2.26
	Experimental	13.58	2.30
Sm	Calculated	13.33	2.22
	Experimental	13.39	2.29
Eu	Calculated	13.27	2.21
	Experimental	13.21	2.18
Gd	Calculated	13.1	2.19
	Experimental	13.15	2.24
Tb	Calculated	13.04	2.18
	Experimental	13.07	2.19
Dy	Calculated	12.94	2.16
	Experimental	12.99	2.23
Er	Calculated	12.79	2.13
	Experimental	12.72	2.18
Yb	Calculated	12.62	2.10
	Experimental	12.67	2.05

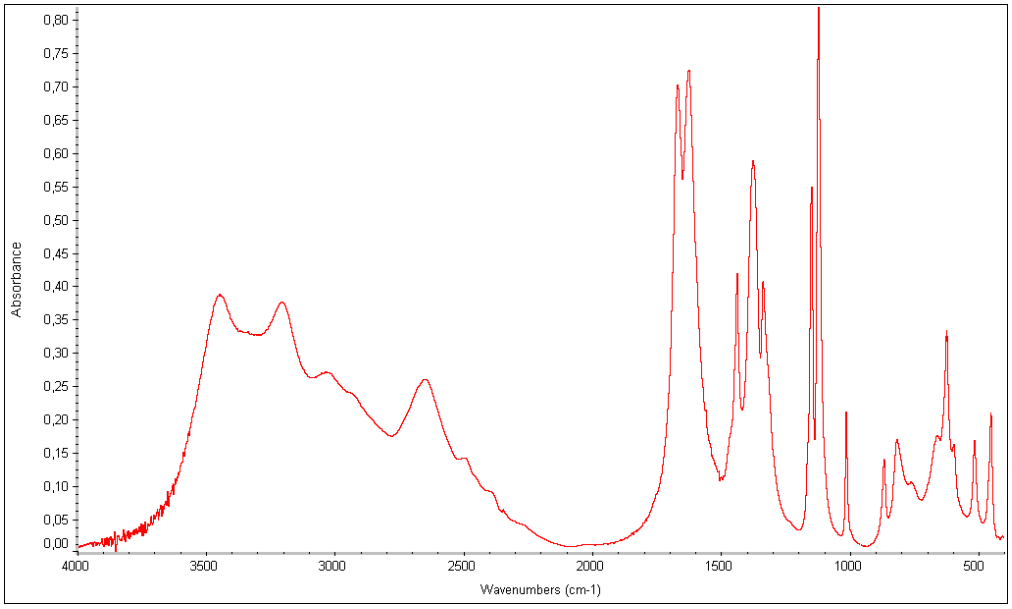
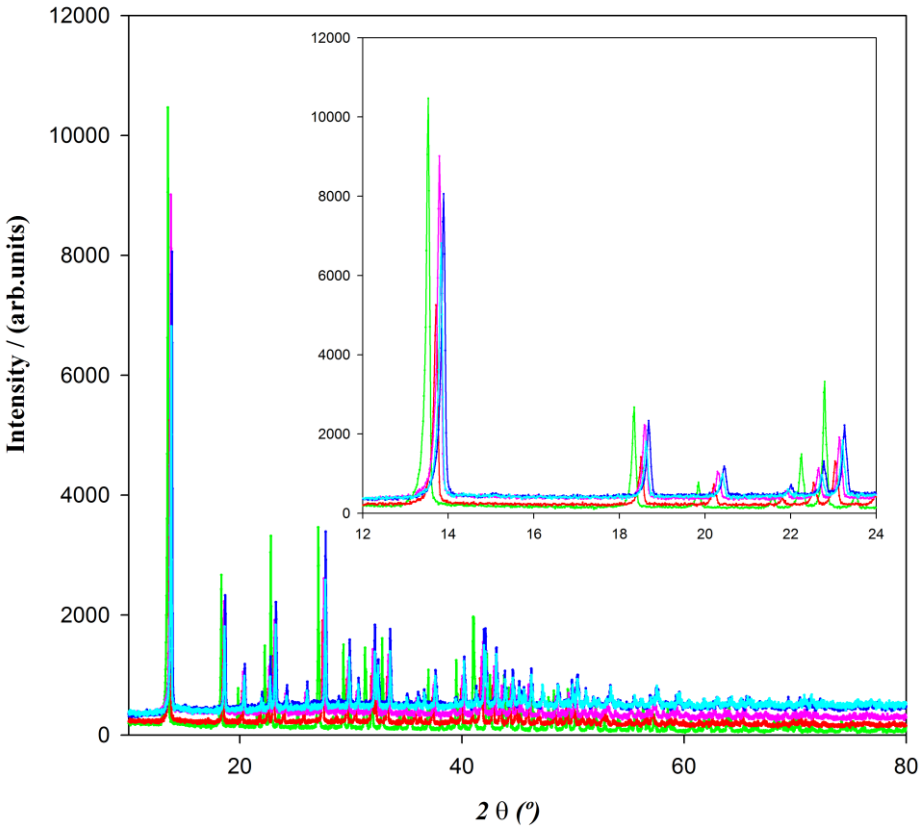


Fig S1: IR spectra for Nd (**4**) compound. The other compounds are IR isostructural, not shown for clarity.



FigS2a (insert) X-ray powder diffraction patterns of compounds **1-11**. All of them show the same pattern.
Fig S2b X-Ray diffraction pattern for compounds (**4**) (**5**) (**6**) (**8**) (**9**), green, red, pink, cyan and blue, respectively. It can be deduced that all of them are isostructural.

Additional crystallographic information:

In the first dataset, the crystal structure (which was that of compound **1** in the Δ configuration) could not be solved directly in the final space group *R*32 (no. 155) but could be solved in the triclinic space group *P*1. After obtaining a basic structure model, this solution was transformed to *R*32.

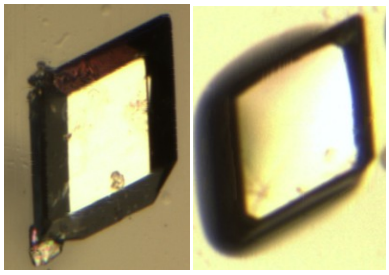


Fig. S3 Crystals of La(mesox) (1) with different configurations; left Λ -, right Δ -metal-centered chirality. The potential crystal enantiomorphism cannot be recognized.

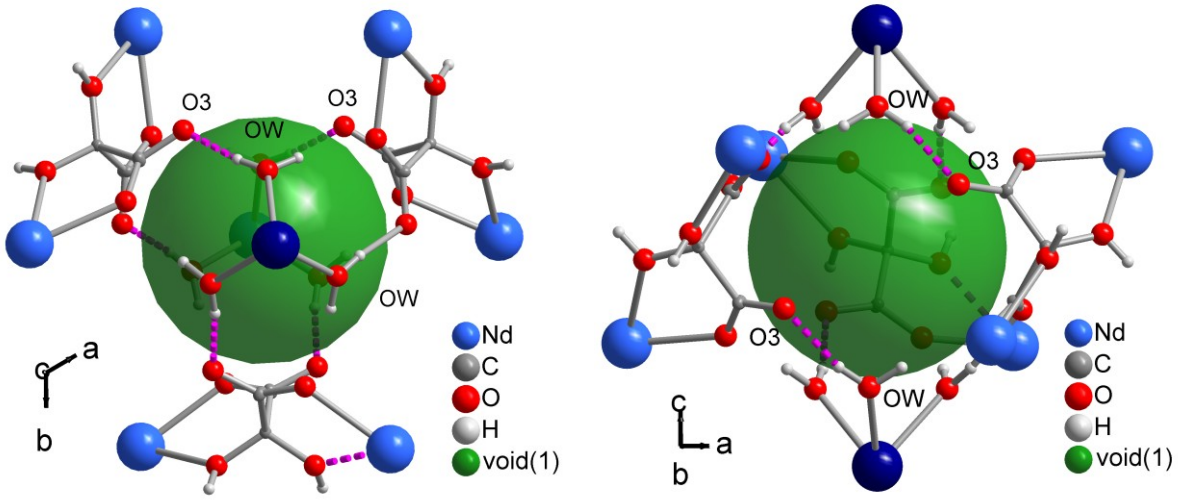


Fig. S4 Two views of void(1) in the structure of compound **4**. Void(1) is depicted with a space-filling radius of 2.9 Å. Inter-layer hydrogen bonds are shown as dashed pink lines; intra-layer hydrogen bonds (*cf*. Fig. 5 in paper) are omitted for clarity. Different blue colours of the Nd atoms indicate different layers. In Fig. 8 electron density maps are shown of the same views.

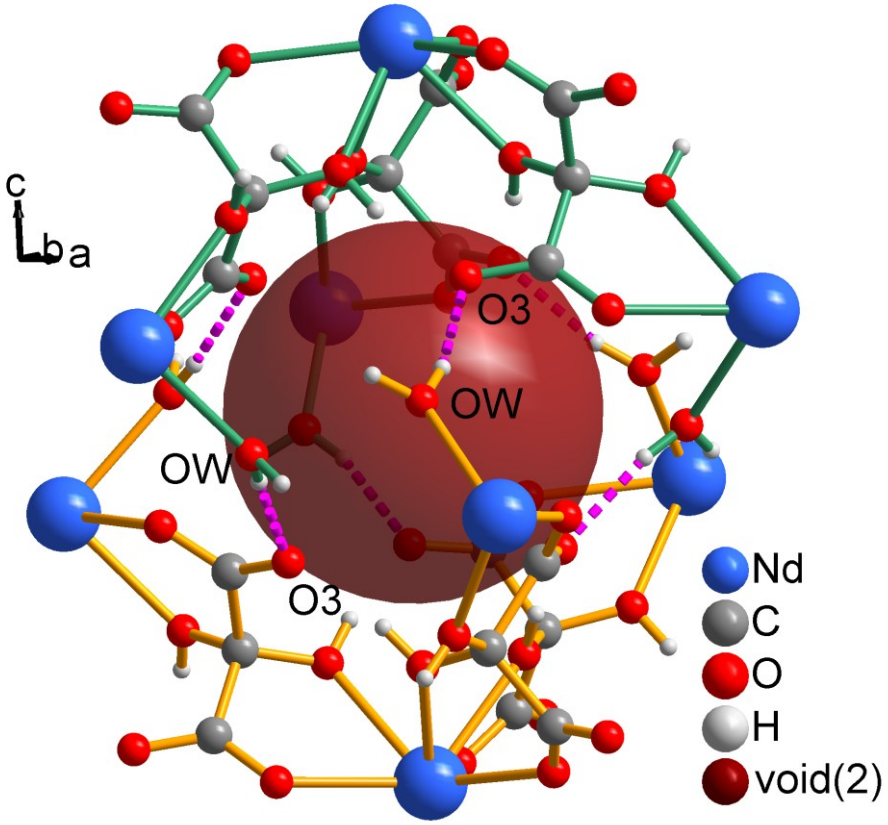


Fig. S5 Void(2) from adjacent layer interdigitation with surrounding inter-layer hydrogen bonds as dashed pink lines; intra-layer hydrogen bonds (*cf*. Fig. 6 in paper) are omitted for clarity.

Table S2 Potential solvent area volumes calculated by PLATON[1] in compound **1-11**.[a]

Compound	Pore volume as potential solvent area volume [Å^3]	Unit cell volume [Å^3]	Pore volume/unit cell volume [%]	Packing index [% filled space]
1	234.4	1752.50(13)	13.4	70.2
2	235.4	1733.6(5)	13.6	70.1
3	242.3	1758.39(13)	13.8	69.2
4	222.1	1708.30(5)	13.0	70.1
7	215.9	1669.3(2)	12.9	71.0
10	193.7	1627.53(7)	11.9	71.7
11	194.9	1612.93(4)	12.1	72.7

[a] The packing index (percent filled space) was obtained with "calc void".

Table S3 Centroid distances void(1)-void(2) and from void centers to closest oxygen atoms (see Fig. S4 and S5 for atom labels).

Com-pound	Distance from void(1) to void(2) [Å]	Distance from center of void(1) to OW [Å]	Distance from center of void(1) to O3 [Å]	Distance from center of void(2) to OW [Å]	Distance from center of void(2) to O3 [Å]
1	6.6540	3.5510(14)	3.5462(10)	4.2005(11)	3.2494(11)
2	6.6302	3.5557(26)	3.5480(16)	4.1743(23)	3.2248(17)
3	6.6614	3.5983(16)	3.5693(15)	4.1899(18)	3.2306(18)
4	6.6006	3.5660(14)	3.5446(14)	4.1633(18)	3.1891(14)
7	6.5518	3.5759(24)	3.5484(26)	4.1283(23)	3.1302(23)
10	6.4994	3.5697(21)	3.5440(16)	4.1087(19)	3.0734(22)
11	6.4801	3.5731(17)	3.5362(18)	4.0947(14)	3.0584(20)

[1] A.L. Spek, *J. Appl. Cryst.*, 2003, **36**, 7-13. *PLATON* – A Multipurpose Crystallographic Tool, Utrecht University, Utrecht, The Netherlands, A.L. Spek (2008); Windows implementation: L.J. Farrugia, University of Glasgow, Scotland, Version 40608 (2008).