Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Chemical transformation of a luminescent two-dimensional Eu(III) coordination polymer under aqueous phase

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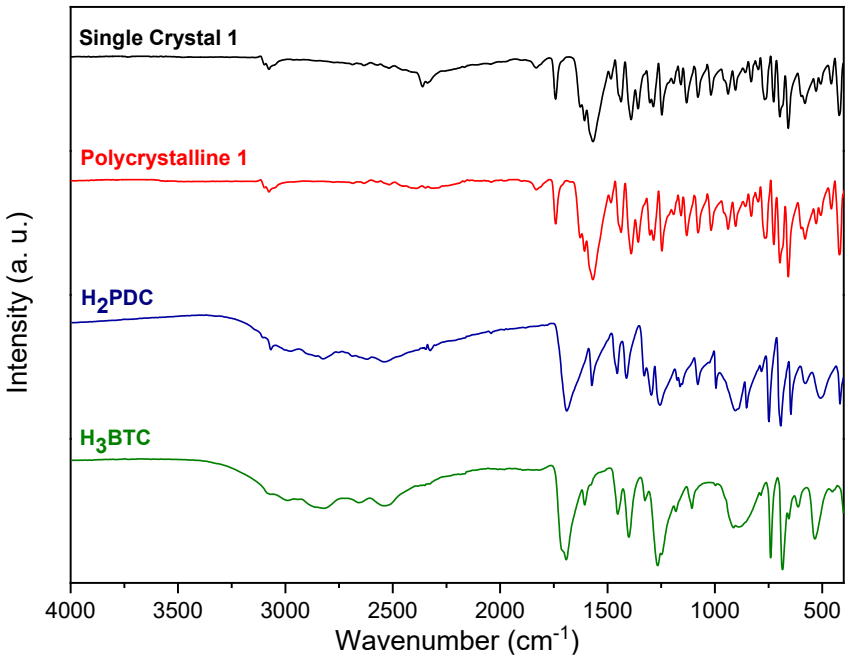


Fig. S1. FTIR spectra of compound {[Eu(HPDC)(PDC)]}$_n$ (**1**) (single crystal and polycrystalline forms) and ligands.

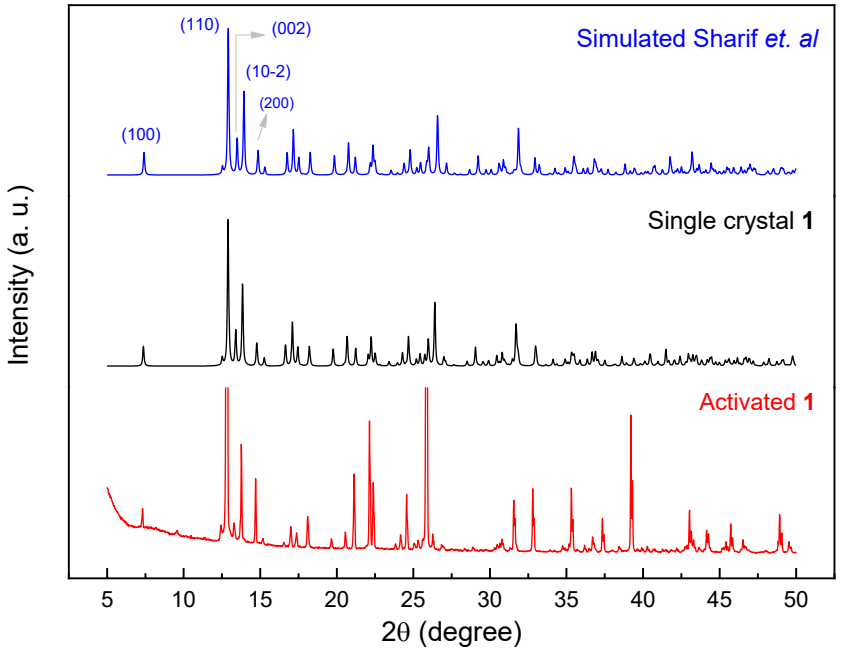


Fig. S2. PXRD patterns of **1** activated polycrystalline sample (red line), simulated from single crystal X-ray diffraction results (black line) and simulated PXRD pattern of the known phase [Eu(PDC)(HPDC)]$_n$ (CCDC 872843) (blue line).[1]

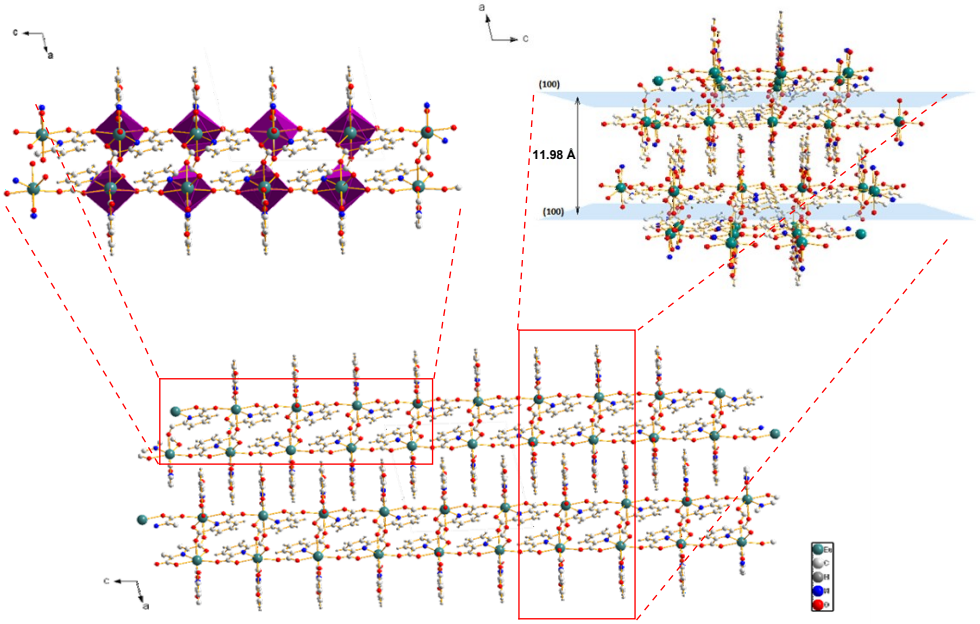


Fig. S3. Polymeric extension and 3D supramolecular framework packing of $\{[Eu(HPDC)(PDC)]\}_n$ (**1**) and the magnified representation of schematic polyhedral of 2D MOF and the interplanar distance between the sheets.

Table S1. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for **1**.

Atom	x	y	z	U_{iso}*/U_{eq}
C101	-0.0936 (5)	0.2971 (7)	0.1079 (5)	0.0305 (13)
H101	-0.153827	0.227017	0.096007	0.037*
Eu1	0.30185 (2)	0.23362 (3)	0.18215 (2)	0.01148 (10)
O2	0.2687 (4)	0.2747 (4)	0.0029 (3)	0.0234 (8)
O1	0.3885 (3)	0.0036 (4)	0.2768 (3)	0.0192 (7)
O2W	0.2803 (3)	0.2900 (5)	0.3461 (3)	0.0216 (8)
O3	0.2833 (3)	0.5137 (4)	0.1725 (3)	0.0208 (8)
O1W	0.4863 (3)	0.3092 (4)	0.2135 (2)	0.0181 (7)
C007	0.4339 (4)	-0.2493 (6)	0.0733 (4)	0.0159 (10)
H007	0.466461	-0.339889	0.107204	0.019*
N2	0.1037 (3)	0.3338 (5)	0.1441 (3)	0.0167 (9)
C009	0.4114 (4)	-0.1148 (6)	0.1258 (4)	0.0148 (9)

C010	0.4396 (4)	-0.1003 (6)	0.2389 (3)	0.0140 (9)
C011	0.3411 (4)	0.0233 (6)	-0.0218 (4)	0.0145 (9)
N1	0.3637 (3)	0.0151 (5)	0.0794 (3)	0.0132 (8)
O4	0.1439 (3)	0.0298 (5)	0.1525 (3)	0.0239 (8)
C014	0.2930 (4)	0.1813 (6)	-0.0615 (4)	0.0166 (10)
C015	0.3627 (4)	-0.1039 (6)	-0.0800 (4)	0.0204 (11)
H015	0.348410	-0.096301	-0.150269	0.024*
O5	-0.0370 (3)	-0.0342 (5)	0.1102 (4)	0.0392 (11)
C017	0.0143 (4)	0.2404 (6)	0.1266 (4)	0.0182 (11)
C018	0.4061 (5)	-0.2434 (6)	-0.0313 (4)	0.0194 (11)
H018	0.416441	-0.332964	-0.068997	0.023*
C019	0.0347 (5)	0.0643 (6)	0.1277 (4)	0.0239 (11)
C020	0.0869 (5)	0.4927 (6)	0.1427 (4)	0.0208 (11)
C022	0.1936 (5)	0.5900 (6)	0.1623 (4)	0.0222 (11)
O6	0.1868 (4)	0.7366 (5)	0.1680 (5)	0.0467 (14)
C027	-0.0189 (5)	0.5590 (7)	0.1246 (5)	0.0277 (12)
H027	-0.025 (6)	0.662 (9)	0.129 (5)	0.033*
C028	-0.1102 (5)	0.4605 (7)	0.1072 (5)	0.0321 (14)
H028	-0.181968	0.502827	0.095224	0.039*
H4	0.160 (7)	-0.060 (11)	0.153 (6)	0.06 (3)*

Table S2. Atomic displacement parameters (Å^2) for **1**.

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C101	0.018 (3)	0.023 (3)	0.049 (4)	0.002 (2)	0.006 (3)	0.006 (3)
Eu1	0.01411 (15)	0.00993 (15)	0.01026 (15)	0.00035 (8)	0.00232 (10)	-0.00050 (8)
O2	0.039 (2)	0.0160 (18)	0.0154 (18)	0.0101 (16)	0.0071 (17)	0.0027 (14)
O1	0.0269 (19)	0.0146 (17)	0.0160 (17)	0.0054 (15)	0.0042 (14)	0.0014 (14)
O2W	0.032 (2)	0.0219 (19)	0.0112 (17)	0.0002 (16)	0.0062 (15)	-0.0041 (15)
O3	0.0258 (19)	0.0102 (17)	0.0269 (19)	0.0002 (15)	0.0068 (15)	-0.0002 (14)
O1W	0.0183 (17)	0.0208 (18)	0.0148 (16)	-0.0078 (15)	0.0029 (14)	-0.0036 (14)
C007	0.009 (2)	0.014 (2)	0.024 (3)	0.0014 (17)	0.003 (2)	0.0001 (19)
N2	0.021 (2)	0.009 (2)	0.020 (2)	0.0031 (17)	0.0060 (17)	0.0004 (16)
C009	0.014 (2)	0.012 (2)	0.019 (2)	0.0022 (18)	0.0050 (18)	0.0013 (19)
C010	0.017 (2)	0.011 (2)	0.014 (2)	-0.0034 (19)	0.0044 (19)	0.0022 (18)
C011	0.013 (2)	0.014 (2)	0.015 (2)	0.0020 (18)	0.0007 (18)	-0.0022 (19)
N1	0.0146 (19)	0.0117 (19)	0.0131 (19)	0.0026 (15)	0.0026 (15)	-0.0006 (15)

O4	0.0203 (19)	0.0093 (18)	0.042 (2)	0.0018 (15)	0.0059 (17)	-0.0013 (16)
C014	0.021 (2)	0.015 (2)	0.015 (2)	-0.005 (2)	0.006 (2)	-0.0002 (19)
C015	0.024 (3)	0.022 (3)	0.016 (2)	0.000 (2)	0.006 (2)	-0.002 (2)
O5	0.024 (2)	0.016 (2)	0.074 (3)	-0.0069 (17)	0.004 (2)	0.001 (2)
C017	0.018 (3)	0.016 (3)	0.022 (3)	0.0032 (19)	0.005 (2)	0.0027 (19)
C018	0.026 (3)	0.016 (2)	0.019 (3)	0.003 (2)	0.012 (2)	-0.0041 (19)
C019	0.025 (3)	0.014 (3)	0.031 (3)	-0.001 (2)	0.003 (2)	0.003 (2)
C020	0.030 (3)	0.010 (2)	0.022 (3)	0.006 (2)	0.004 (2)	0.003 (2)
C022	0.034 (3)	0.007 (2)	0.026 (3)	0.005 (2)	0.005 (2)	0.002 (2)
O6	0.039 (3)	0.013 (2)	0.087 (4)	0.0016 (18)	0.011 (3)	-0.003 (2)
C027	0.034 (3)	0.015 (3)	0.034 (3)	0.007 (2)	0.007 (2)	0.002 (2)
C028	0.020 (3)	0.025 (3)	0.049 (4)	0.012 (2)	0.003 (3)	0.007 (3)

Table S3. Geometric parameters (Å, °) for **1**.

C101—H101	0.9300	N2—C017	1.326 (7)
C101—C017	1.376 (8)	N2—C020	1.345 (7)
C101—C028	1.381 (8)	C009—C010	1.500 (7)
Eu1—O2	2.395 (4)	C009—N1	1.327 (6)
Eu1—O1	2.426 (3)	C011—N1	1.338 (6)
Eu1—O2W	2.336 (3)	C011—C014	1.498 (7)
Eu1—O3	2.354 (4)	C011—C015	1.382 (7)
Eu1—O1W	2.299 (3)	O4—C019	1.340 (7)
Eu1—N2	2.517 (4)	O4—H4	0.78 (9)
Eu1—C010	3.269 (5)	C015—H015	0.9300
Eu1—N1	2.509 (4)	C015—C018	1.388 (7)
Eu1—O4	2.547 (4)	O5—C019	1.192 (7)
Eu1—C022	3.250 (5)	C017—C019	1.493 (7)
O2—C014	1.251 (6)	C018—H018	0.9300
O1—C010	1.245 (6)	C020—C022	1.515 (8)
O2W—C014^{i}	1.248 (6)	C020—C027	1.384 (8)
O3—C022	1.253 (6)	C022—O6	1.232 (7)
O1W—C010^{ii}	1.249 (6)	C027—H027	0.86 (7)
C007—H007	0.9300	C027—C028	1.369 (9)
C007—C009	1.388 (7)	C028—H028	0.9300
C017—C101—H101	120.8	C018—C007—H007	121.3
C017—C101—C028	118.5 (6)	C018—C007—C009	117.5 (5)

C028—C101—H101	120.8	C017—N2—Eu1	124.5 (3)
O2—Eu1—O1	127.43 (12)	C017—N2—C020	117.4 (5)
O2—Eu1—N2	78.38 (13)	C020—N2—Eu1	118.0 (3)
O2—Eu1—C010	109.09 (12)	C007—C009—C010	124.0 (4)
O2—Eu1—N1	63.23 (12)	N1—C009—C007	122.5 (5)
O2—Eu1—O4	88.77 (14)	N1—C009—C010	113.4 (4)
O2—Eu1—C022	78.89 (13)	O1—C010—Eu1	38.7 (2)
O1—Eu1—N2	131.78 (13)	O1—C010—O1W^{iii}	125.9 (4)
O1—Eu1—C010	18.70 (11)	O1—C010—C009	116.8 (4)
O1—Eu1—N1	64.19 (12)	O1W^{iii}—C010—Eu1	157.0 (3)
O1—Eu1—O4	77.57 (12)	O1W^{iii}—C010—C009	117.4 (4)
O1—Eu1—C022	153.59 (12)	C009—C010—Eu1	80.5 (3)
O2W—Eu1—O2	154.45 (13)	N1—C011—C014	112.9 (4)
O2W—Eu1—O1	77.60 (12)	N1—C011—C015	121.3 (4)
O2W—Eu1—O3	79.75 (13)	C015—C011—C014	125.7 (4)
O2W—Eu1—N2	79.98 (13)	C009—N1—Eu1	119.3 (3)
O2W—Eu1—C010	96.18 (12)	C009—N1—C011	119.9 (4)
O2W—Eu1—N1	141.42 (13)	C011—N1—Eu1	120.6 (3)
O2W—Eu1—O4	92.71 (13)	Eu1—O4—H4	117 (6)
O2W—Eu1—C022	76.46 (13)	C019—O4—Eu1	125.5 (3)
O3—Eu1—O2	78.94 (12)	C019—O4—H4	117 (6)
O3—Eu1—O1	147.60 (12)	O2—C014—C011	115.8 (4)
O3—Eu1—N2	65.15 (13)	O2W^{iv}—C014—O2	125.4 (5)
O3—Eu1—C010	154.41 (12)	O2W^{iv}—C014—C011	118.8 (4)
O3—Eu1—N1	136.98 (12)	C011—C015—H015	120.8
O3—Eu1—O4	126.56 (12)	C011—C015—C018	118.5 (5)
O3—Eu1—C022	18.22 (13)	C018—C015—H015	120.8
O1W—Eu1—O2	95.37 (13)	C101—C017—C019	119.6 (5)
O1W—Eu1—O1	79.55 (13)	N2—C017—C101	123.8 (5)
O1W—Eu1—O2W	94.41 (13)	N2—C017—C019	116.6 (5)
O1W—Eu1—O3	79.42 (13)	C007—C018—C015	120.1 (5)
O1W—Eu1—N2	144.57 (14)	C007—C018—H018	120.0
O1W—Eu1—C010	75.70 (12)	C015—C018—H018	120.0
O1W—Eu1—N1	84.26 (13)	O4—C019—C017	111.8 (5)
O1W—Eu1—O4	153.94 (13)	O5—C019—O4	123.8 (5)
O1W—Eu1—C022	97.55 (14)	O5—C019—C017	124.4 (5)
N2—Eu1—C010	139.47 (13)	N2—C020—C022	113.9 (5)
N2—Eu1—O4	61.44 (13)	N2—C020—C027	122.2 (5)
N2—Eu1—C022	47.05 (14)	C027—C020—C022	123.9 (5)

N1—Eu1—N2	121.48 (13)	O3—C022—Eu1	36.0 (2)
N1—Eu1—C010	46.03 (12)	O3—C022—C020	116.8 (4)
N1—Eu1—O4	74.67 (13)	C020—C022—Eu1	81.0 (3)
N1—Eu1—C022	142.04 (13)	O6—C022—Eu1	159.9 (5)
O4—Eu1—C010	78.63 (12)	O6—C022—O3	124.7 (6)
O4—Eu1—C022	108.49 (13)	O6—C022—C020	118.5 (5)
C022—Eu1—C010	169.77 (13)	C020—C027—H027	119 (5)
C014—O2—Eu1	126.9 (3)	C028—C027—C020	119.4 (5)
C010—O1—Eu1	122.6 (3)	C028—C027—H027	122 (5)
C014^{i}—O2W—Eu1	166.6 (4)	C101—C028—H028	120.7
C022—O3—Eu1	125.8 (3)	C027—C028—C101	118.7 (5)
C010^{ii}—O1W—Eu1	147.1 (3)	C027—C028—H028	120.7
C009—C007—H007	121.3		
C101—C017—C019—O4	-176.6 (5)	C011—C015—C018—C007	-4.4 (8)
C101—C017—C019—O5	2.5 (9)	N1—C009—C010—Eu1	6.6 (4)
Eu1—O2—C014—O2W^{iv}	-175.8 (4)	N1—C009—C010—O1	20.5 (6)
Eu1—O2—C014—C011	4.3 (6)	N1—C009—C010—O1W^{iii}	-157.9 (4)
Eu1—O1—C010—O1W^{iii}	156.1 (4)	N1—C011—C014—O2	-8.0 (6)
Eu1—O1—C010—C009	-22.3 (6)	N1—C011—C014—O2W^{iv}	172.0 (4)
Eu1—O3—C022—C020	-7.2 (7)	N1—C011—C015—C018	1.6 (8)
Eu1—O3—C022—O6	172.0 (5)	C014—C011—N1—Eu1	8.3 (5)
Eu1—N2—C017—C101	178.6 (4)	C014—C011—N1—C009	-176.9 (4)
Eu1—N2—C017—C019	-1.4 (7)	C014—C011—C015—C018	-179.1 (5)
Eu1—N2—C020—C022	1.6 (6)	C015—C011—N1—Eu1	-172.3 (4)
Eu1—N2—C020—C027	-178.6 (4)	C015—C011—N1—C009	2.5 (7)
Eu1—O4—C019—O5	176.7 (5)	C015—C011—C014—O2	172.6 (5)
Eu1—O4—C019—C017	-4.3 (7)	C015—C011—C014—O2W^{iv}	-7.3 (8)
C007—C009—C010—Eu1	-174.2 (5)	C017—C101—C028—C027	0.3 (10)
C007—C009—C010—O1	-160.3 (5)	C017—N2—C020—C022	-179.4 (5)
C007—C009—C010—O1W^{iii}	21.2 (7)	C017—N2—C020—C027	0.4 (8)
C007—C009—N1—Eu1	171.0 (4)	C018—C007—C009—C010	-178.1 (5)
C007—C009—N1—C011	-3.8 (7)	C018—C007—C009—N1	1.0 (7)
N2—C017—C019—O4	3.5 (7)	C020—N2—C017—C101	-0.3 (8)
N2—C017—C019—O5	-177.5 (6)	C020—N2—C017—C019	179.6 (5)
N2—C020—C022—Eu1	-1.1 (4)	C020—C027—C028—C101	-0.3 (10)
N2—C020—C022—O3	3.2 (7)	C022—C020—C027—C028	179.6 (6)
N2—C020—C022—O6	-176.1 (6)	C027—C020—C022—Eu1	179.1 (5)
N2—C020—C027—C028	-0.1 (9)	C027—C020—C022—O3	-176.6 (5)
C0	3.2 (8)	C027—C020—C022—O6	4.2 (9)

09—C007—C018—C015			
C010—C009—N1—Eu1	-9.8 (5)	C028—C101—C017—N2	0.0 (10)
C010—C009—N1—C011	175.3 (4)	C028—C101—C017—C019	-180.0 (6)

Symmetry codes: (i) *x*, -*y*+1/2, *z*+1/2; (ii) -*x*+1, *y*+1/2, -*z*+1/2; (iii) -*x*+1, *y*-1/2, -*z*+1/2; (iv) *x*, -*y*+1/2, *z*-1/2.

Table S4. Hydrogen-bond interactions (Å) for **1.**

D—H···A	D—H	H···A	D—O···H	D—O	O···H
C028—H028···O2	0.9300	2.394	C019—O5···H027	1.192	2.550
C111—H111···O2	0.9300	2.480			

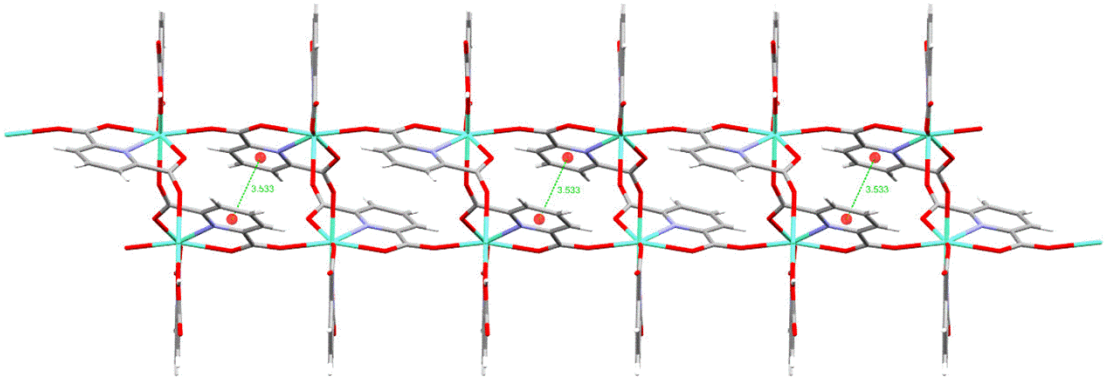


Fig. S4. π–π stacking interactions in the structure of the solid **1**.

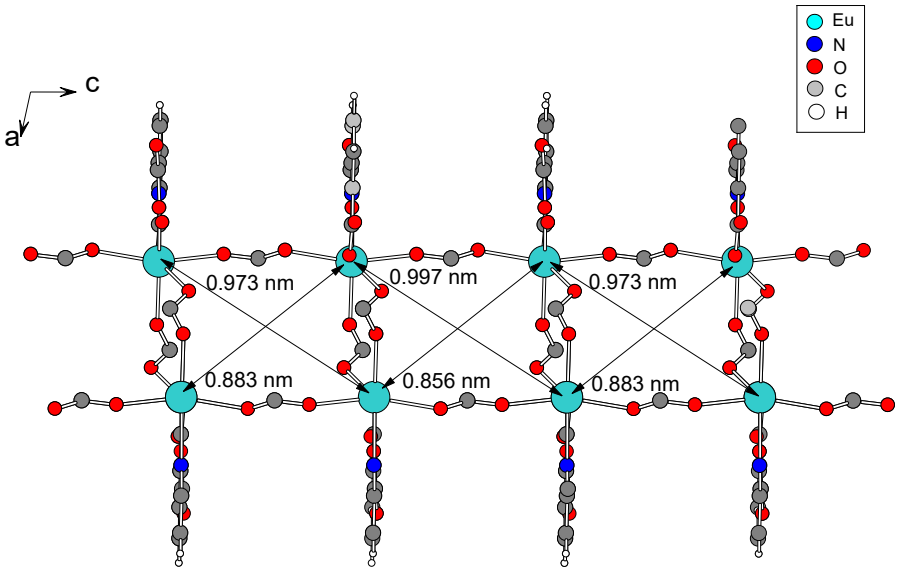


Fig. S5. Nanosized cavities along the polymeric extension in the bc plane of the solid **1**. All atoms present in the center of the cavity have been omitted for clarity.

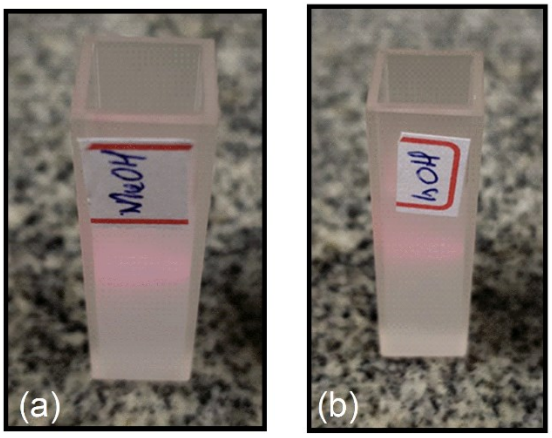


Fig. S6. Images of the suspension of nanosheets of **1** in methanol (a) and isopropanol (b) showing characteristic Tyndall scattering of laser light.

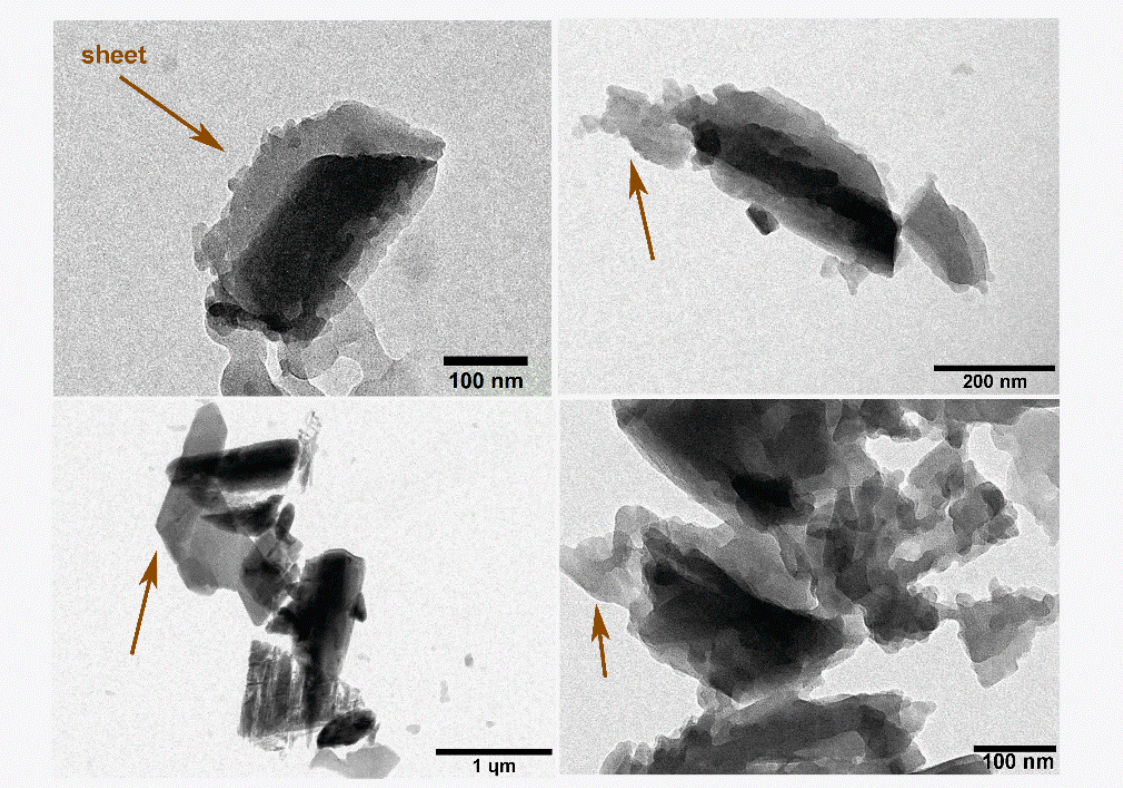


Fig. S7. TEM images of {[Eu(HPDC)(PDC)]}$_n$ (**1**) dispersed in isopropanol.

Table S5. Elemental analysis data of compounds.

Compounds	Found/Calc. (%)		
	C	H	N
{[Eu(HPDC)(PDC)]}$_n$ (**1**)	34.88 (34.80)	1.47 (1.46)	5.62 (5.80)
{[Eu(HPDC)(PDC)(H$_2$O)$_2$] · 4H$_2$O}$_n$ (**2**)	28.53 (28.39)	3.02 (3.40)	4.71 (4.73)

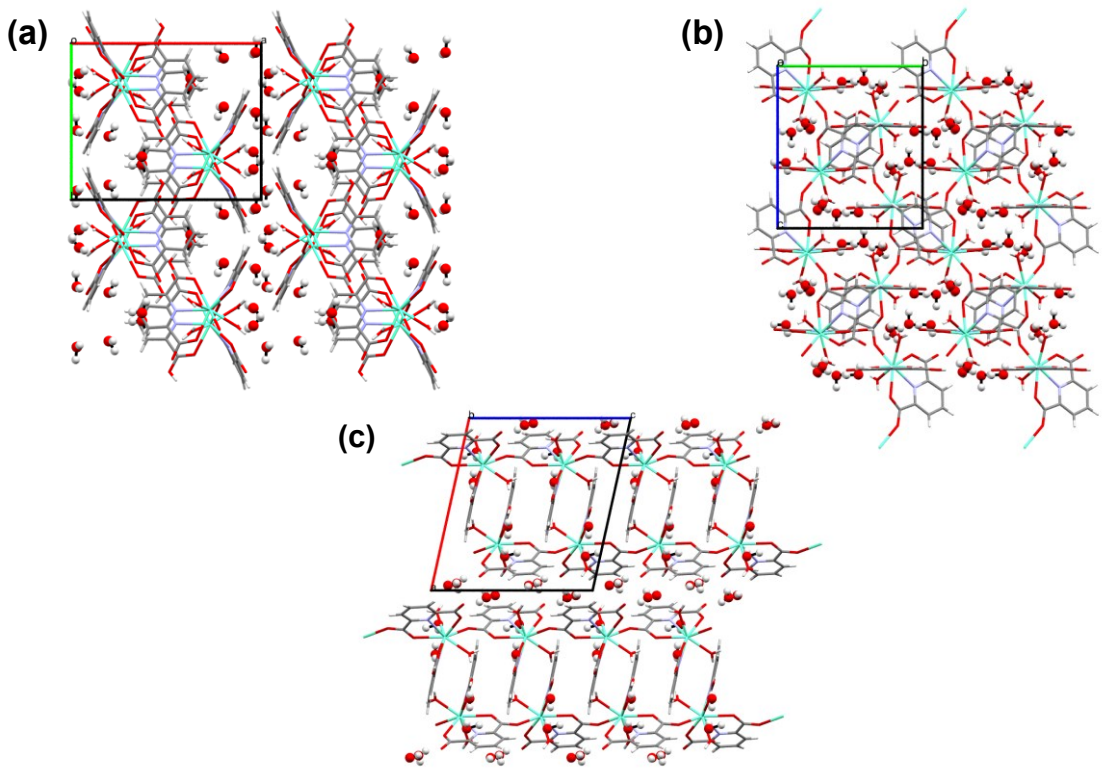
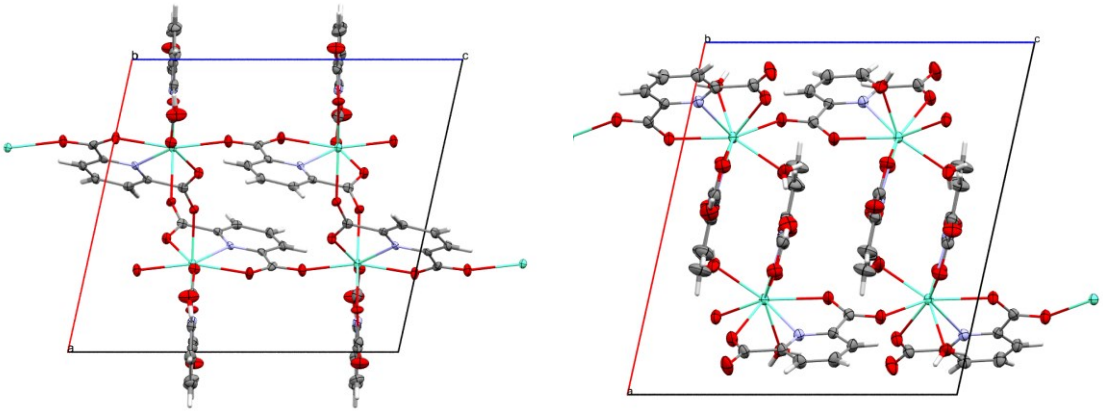


Fig. S8. Unit cell content of {[Eu(HPDC)(PDC)(H_2O)$_2$]·4H_2O}$_n$ (**2**), projected on: (a) *c* axis, (b) *a* axis and (c) *b* axis. The *a* axis are depicted in red, *b* axis in green and the *c* axis in blue. Crystallographic data were obtained from the Cambridge Crystallographic Data Center under number CCDC 740891.[2]



(1) **(2)**

Fig. S9. Display of the contents of the unit cell packing of compound **1** (this work) and the compound **2** reported in the literature[2]. The hydrate water molecules in **2** have been omitted for clarity. Eu atoms are depicted in sky blue, O in red, C in grey, N in violet and H in white. The *a* axis is represented in red and the *c* axis in blue.

Table S6. Experimental intensity parameters radiative (A_{rad}), non-radiative (A_{nrad}) transitions, lifetime values (**τ**), quantum efficiency (ϕ) and the number of water molecules (n_w) in **2**.

Sample	**τ** (ms)	r^2	A (ms^{-1})	n_w	ϕ (%)
2	τ_1 = 0.4118	0.987	A_{rad} = 0.2131 A_{nrad} = 0.2215	2.11	8.78

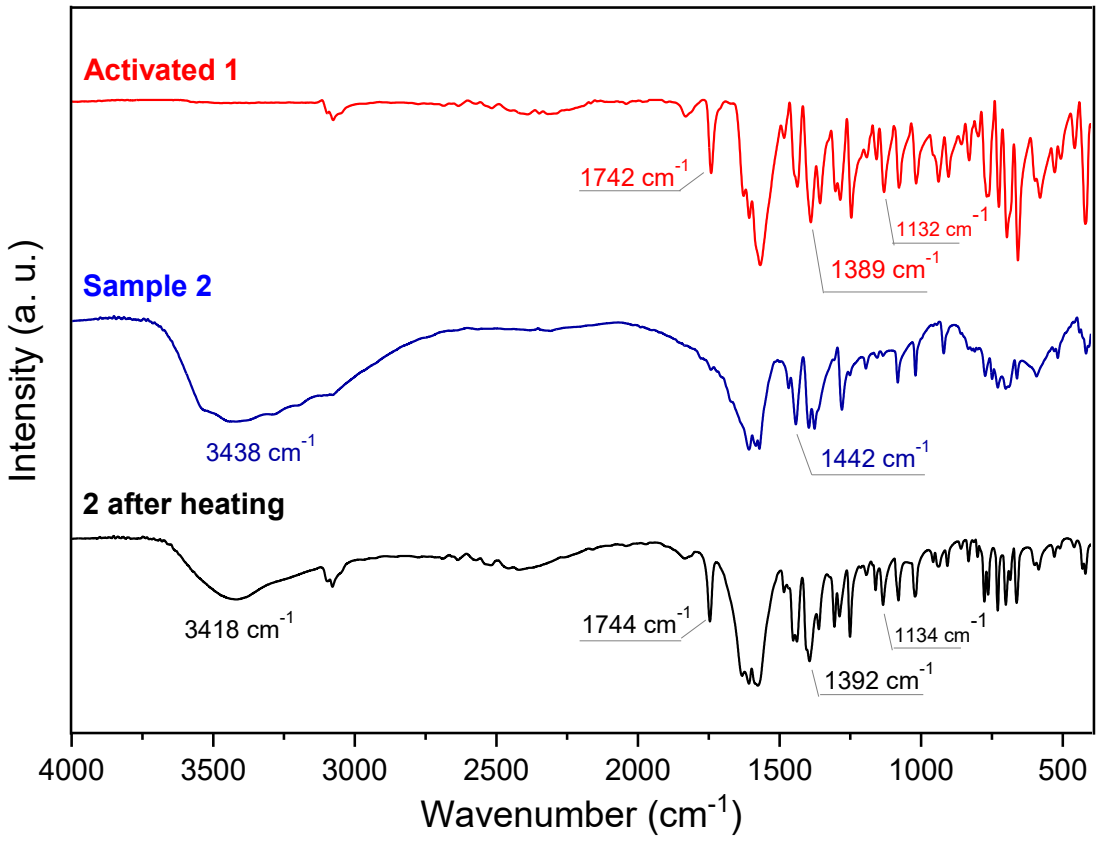


Fig. S10. FTIR spectra of compounds activated **1**, **2** and **2** after heating.

Table S7. Observed bond frequencies and assignments for compound **1** and **2** (as-synthesized and after heating).

Samples	FTIR (cm^{-1})			
	υ(OH)	υ(C=O)	υ_s(COO)	υ(C-O-M)
Activated **1**	-	1742	1389	1132
Sample **2**	3438	-	1442	-
2 after heating	3418	1744	1392	1134

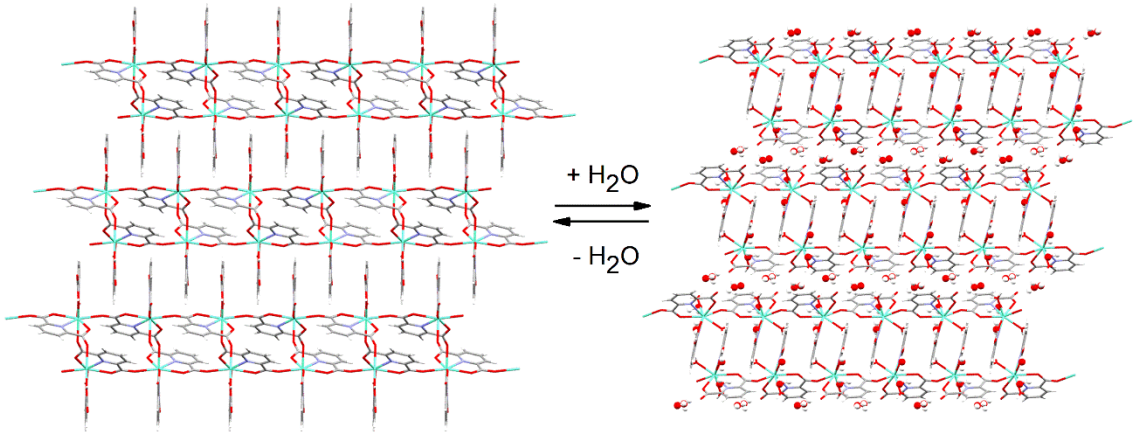


Fig. S11. Proposed scheme for the reversible behavior of the solid **1** in water.

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