Two new Cu(II) and La(III) 2D coordination polymers, synthesis and *in situ* structural analysis by X-ray diffraction

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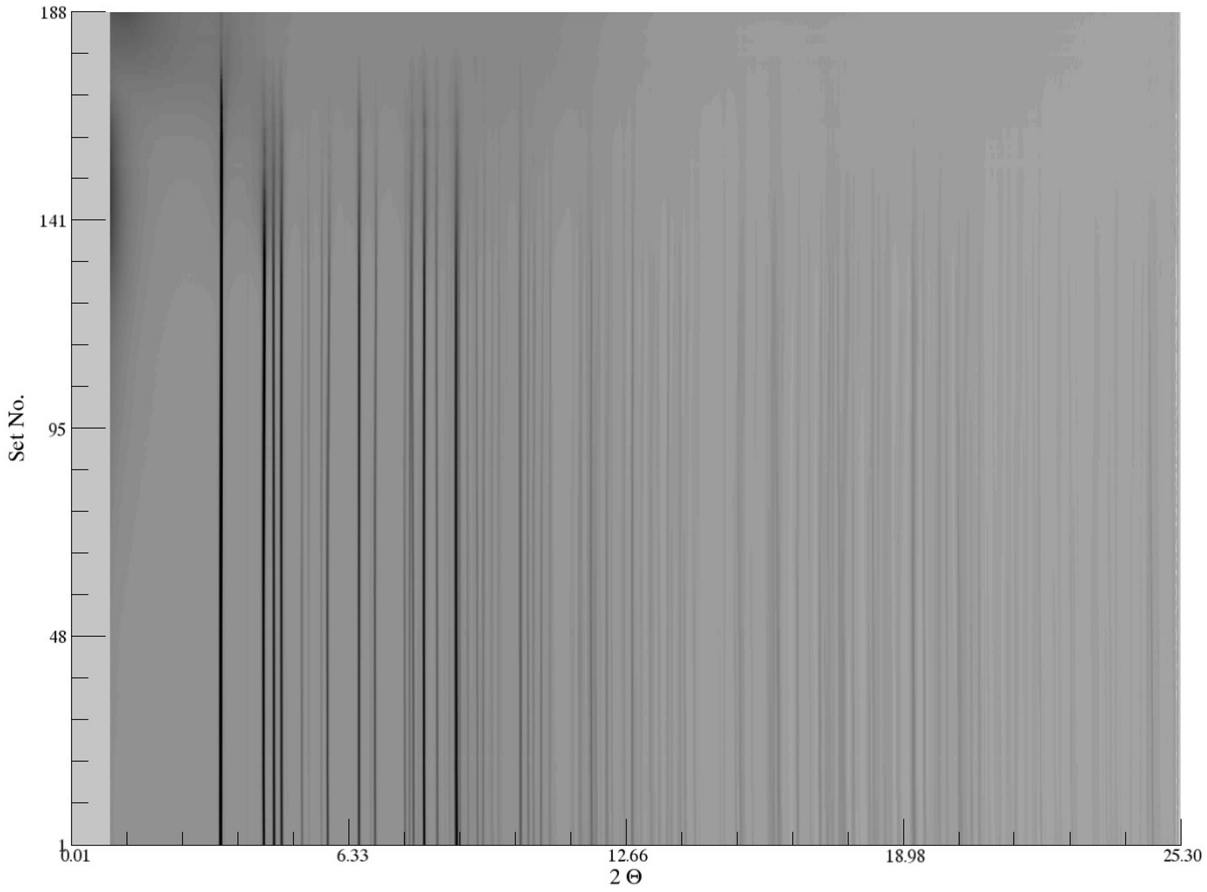

Figure S 1. The VT measurement of CPO-71-Cu, y-axis = scan number (increasing temperature), x-axis = reflection angle in degrees 2Θ (λ = 0.69396 Å).

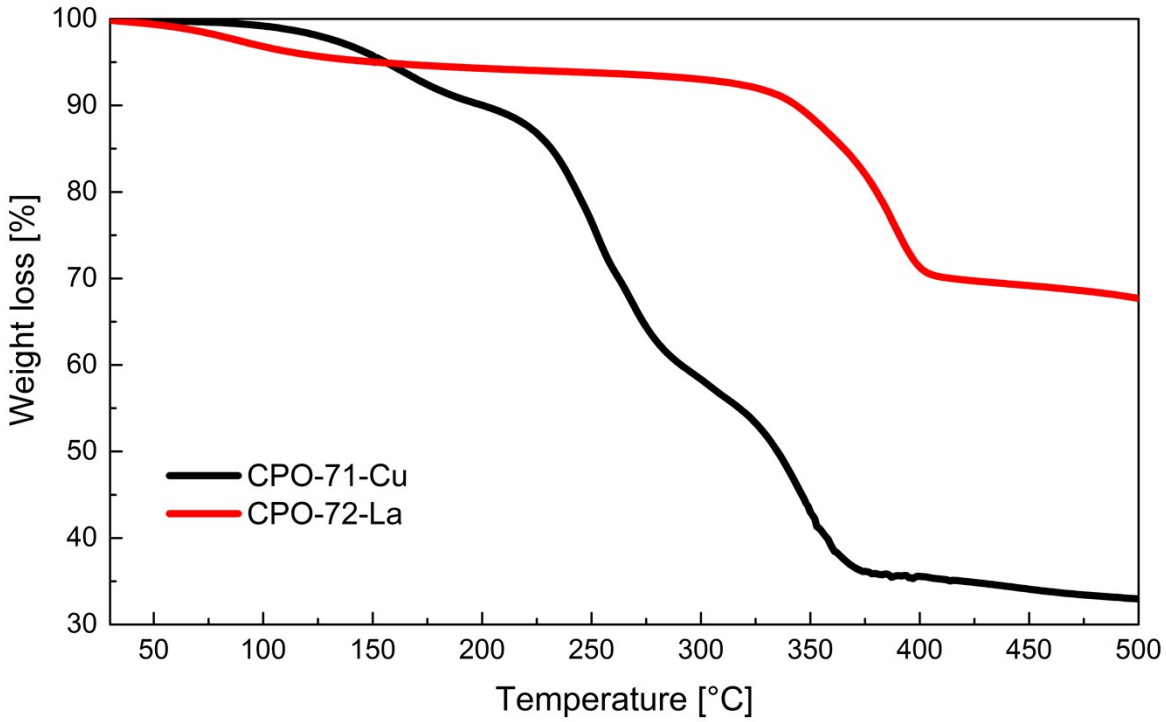

Figure S 2. Thermogravimetric analysis of CPO-71-Cu and CPO-72-La. The samples were heated in alumina crucibles at 2K/min in N_2.

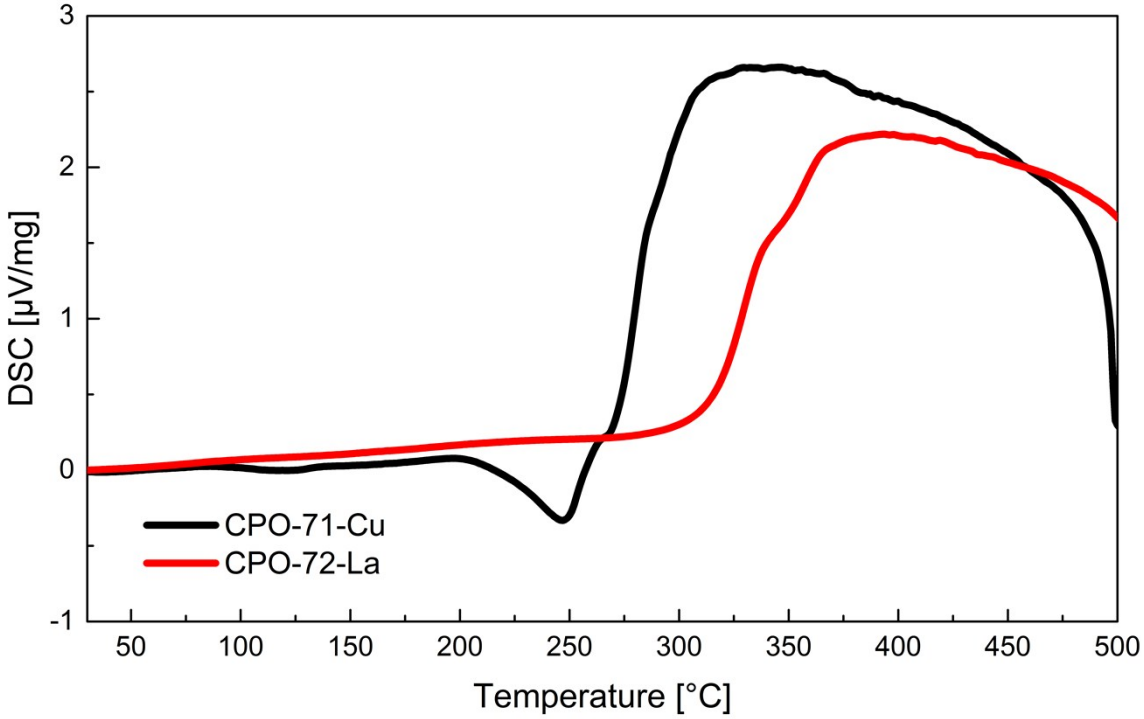

Figure S 3. Differential scanning calorimetric analysis of CPO-71-Cu and CPO-72-La. The samples were heated in platinum crucibles at 5K/min in N_2.

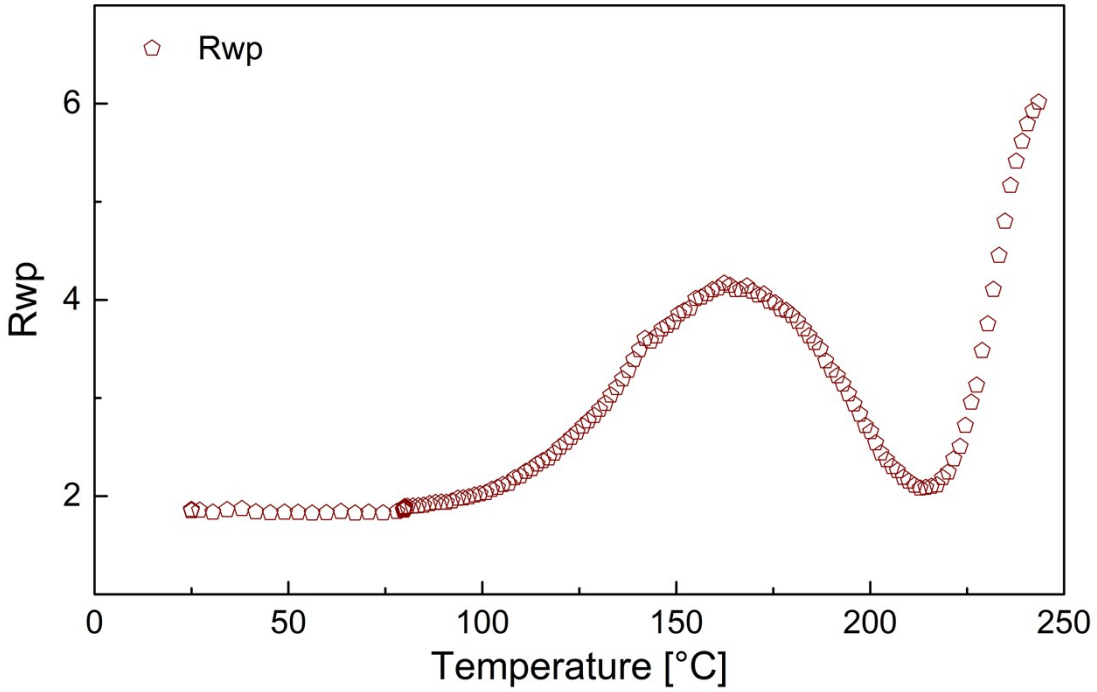

Figure S 4. Rwp from the parametric refinement of CPO-71-Cu plotted against temperature.

Table S 1. Unit cell parameters of CPO-71-Cu extracted from the variable temperature S-XRD experiment. Calculated standard deviations in parentheses.

Temp. (°C)	a-axis (Å)	b-axis (Å)	c-axis (Å)	beta-angle (°)	volume (Å^3)
20	18.2076 (2)	10.4482(2)	23.4284 (3)	96.1861 (10)	4430.97 (9)
70	18.2577 (4)	10.4644 (3)	23.4579 (5)	96.1696 (19)	4455.79 (17)
80	18.2422 (4)	10.4552 (3)	23.4343 (5)	96.1640 (19)	4444.16 (17)
90	18.2661 (4)	10.4655 (3)	23.4540 (5)	96.1541 (19)	4457.72 (17)
100	18.2610 (4)	10.4611 (3)	23.4393 (5)	96.1404 (19)	4451.94 (17)
110	18.2185 (4)	10.4374 (3)	23.3735 (5)	96.1180 (20)	4419.24 (18)
120	18.2674 (4)	10.4599 (3)	23.4285 (5)	96.1020 (20)	4451.25 (18)
130	18.3916 (4)	10.5287 (3)	23.5785 (6)	96.0850 (20)	4520.00 (20)
140	18.2803 (4)	10.4647 (3)	23.4271 (5)	96.0641 (19)	4456.48 (18)
150	18.2912 (4)	10.4728 (3)	23.4336 (5)	96.0430 (20)	4464.00 (18)
160	18.2843 (4)	10.4679 (3)	23.4188 (6)	96.0260 (20)	4457.56 (19)
170	18.3218 (4)	10.4928 (3)	23.4589 (6)	96.0030 (20)	4485.20 (20)
180	18.3501 (4)	10.5073 (4)	23.4922 (7)	95.9870 (30)	4504.80 (30)
220	18.1863 (4)	10.4897 (4)	23.3243 (8)	96.3820 (30)	4422.00 (30)
230	18.2094 (4)	10.4994 (3)	23.3512 (5)	96.4050 (20)	4436.59 (18)
240	18.2251 (4)	10.5054 (3)	23.3680 (5)	96.4230 (20)	4446.01 (18)
250	18.1754 (5)	10.4733 (3)	23.2993 (5)	96.4450 (20)	4406.90 (20)

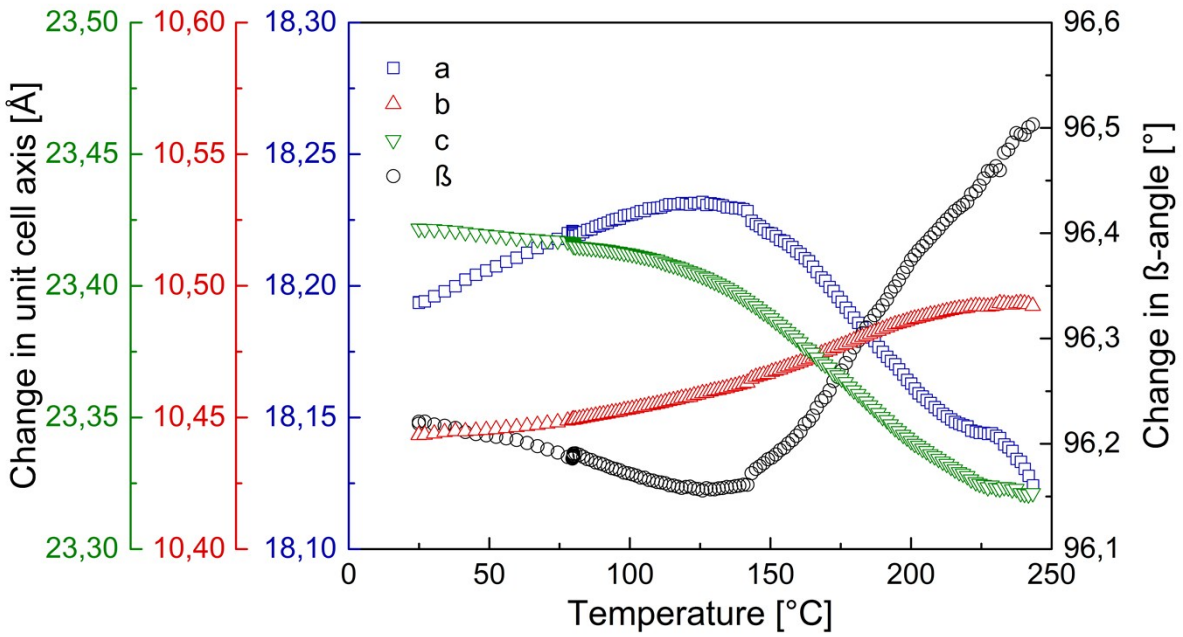

Figure S 5. Unit cell parameters of CPO-71-Cu extracted from the parametric refinement of the variable temperature P-XRD experiment.

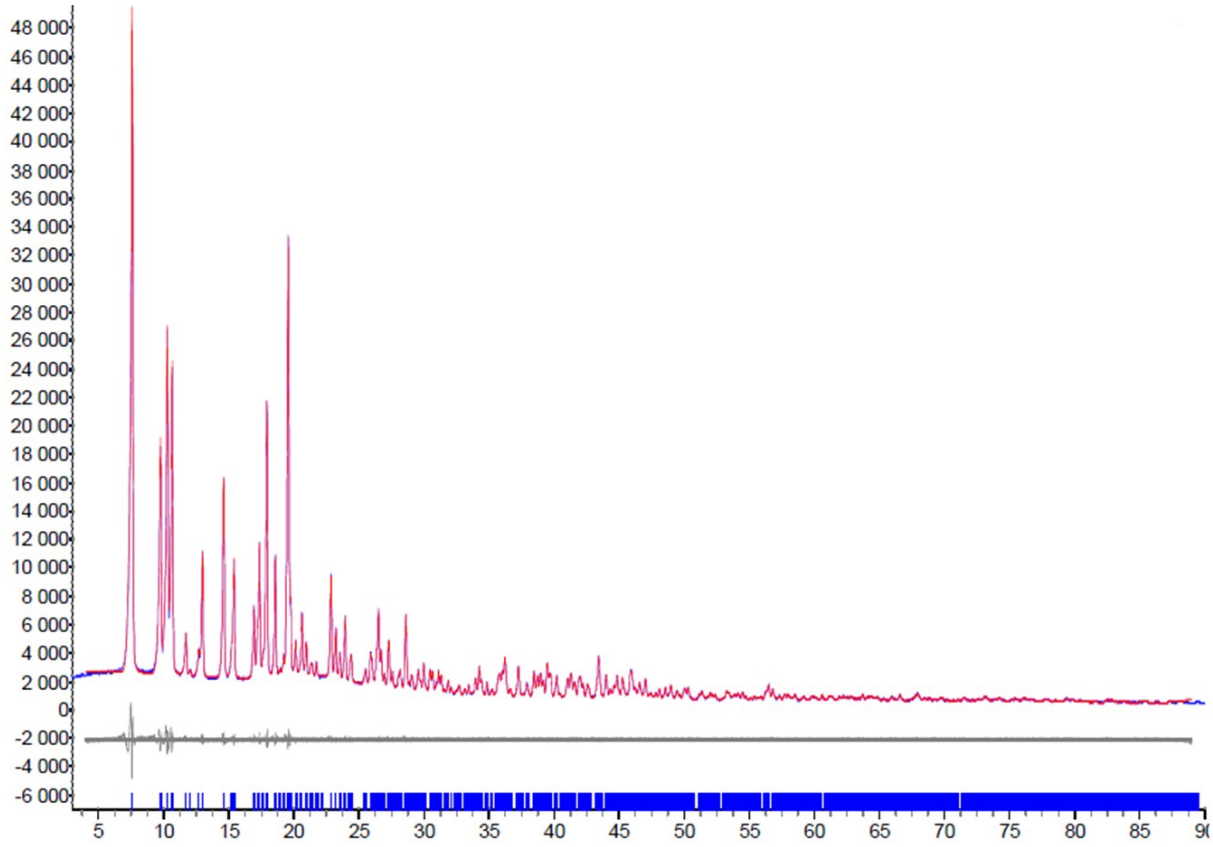

Figure S 6. P-XRD and Pawley fit for CPO-71-Cu. P-XRD in blue, simulated pattern in red and difference in grey. $\lambda = 1.5406$ Å

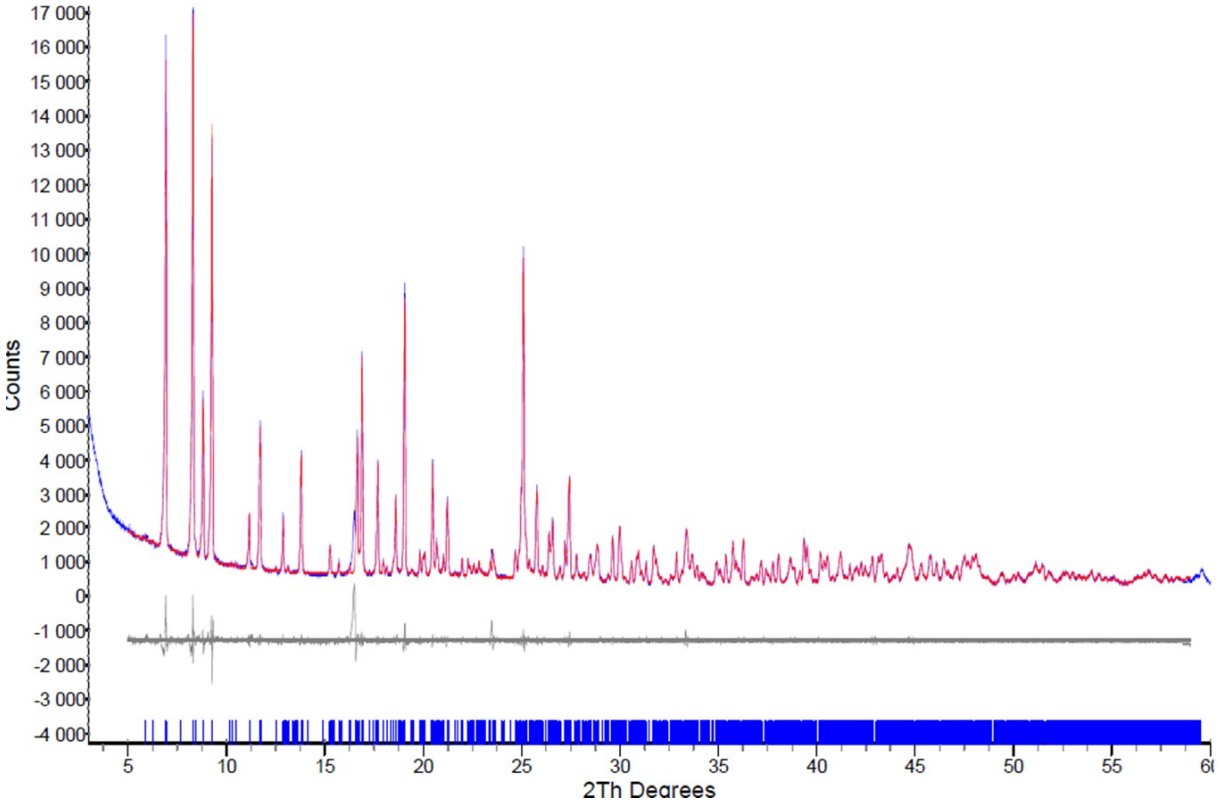

Figure S 7. P-XRD and Pawley fit for CPO-72-La. P-XRD in blue, simulated pattern in red and difference in grey. $\lambda = 1.5406$ Å

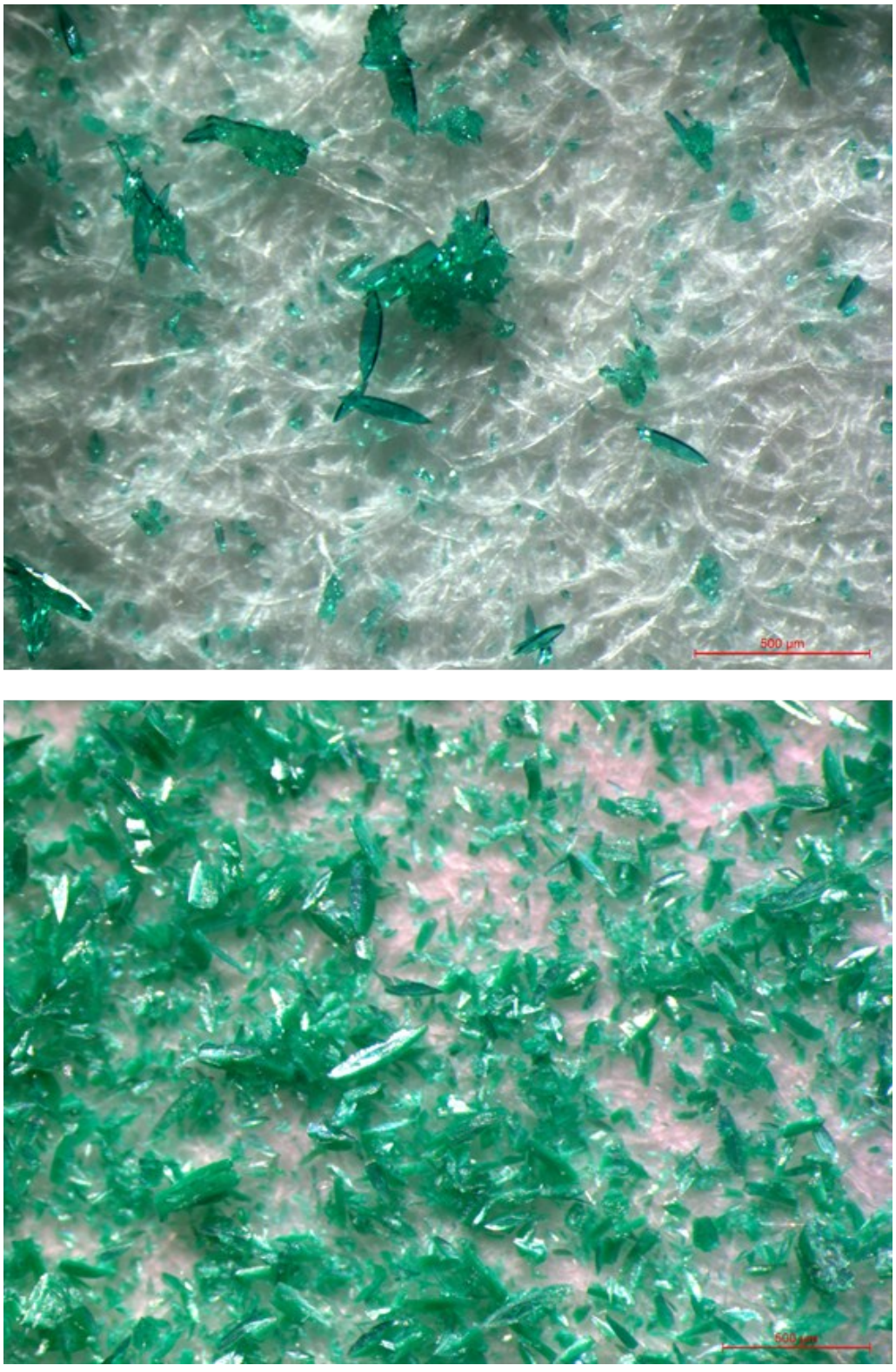

Figure S 8. Microscope images of CPO-71-Cu before (top) and after (bottom) solvent exchange with methanol for 48 hours. The red scale bar is set to 500 µm in both images.

Table S 2. La—O bond lengths (Å) in CPO-72-La. Calculated standard deviations in parentheses.

CPO-72-La	
La1—O3C[i]	2.504 (2)
La1—O4C[i]	2.677 (2)
La1—O1	2.466 (2)
La1—O4	2.567 (2)
La1—O5	2.581 (2)
La1—O7	2.772 (2)
La1—O8	2.597 (2)
La1—O13	2.427 (2)
La1—O17	2.520 (2)
La2—O1C[ii]	2.481 (2)
La2—O2C[i]	2.641 (2)
La2—O1	2.868 (2)
La2—O2	2.563 (2)
La2—O7	2.464 (2)
La2—O10	2.592 (2)
La2—O11	2.558 (2)
La2—O14	2.501 (2)
La2—O16	2.419 (2)
(i) H_2O; (ii) DMF	

Table S 3. Hydrogen bond geometry in CPO-72-La between selected oxygen atoms in the framework, the coordinated solvent, and the interlayer solvent (Å, °). Calculated standard deviations in parentheses.

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O2^{iii}	0.87	2.02	2.880 (3)	168
O1W—H1WB···O2W^{v}	0.87	1.94	2.765 (4)	158
O2W—H2WA···O11	0.87	1.99	2.848 (3)	169
O2W—H2WB···O4W	0.87	2.03	2.886 (4)	168
O3W—H3WA···O5	0.87	2.05	2.887 (3)	160
O3W—H3WB···O1W	0.87	2.00	2.851 (4)	164
O4W—H4WA···O8^{i}	0.86 (2)	2.09 (2)	2.875 (3)	153 (4)
O4W—H4WB···O3W^{vi}	0.84 (2)	1.93 (2)	2.737 (4)	160 (4)
O2C—H2CD···O15^{iii}	0.90	2.18	3.066 (3)	170
O2C—H2CE···O1W^{vii}	0.90	2.01	2.746 (3)	139
O3C—H3CD···O4C^{viii}	0.86 (2)	1.99 (2)	2.827 (3)	167 (3)
O3C—H3CE···O1S	0.85 (2)	1.84 (2)	2.687 (3)	177 (3)
O4C—H4CA···O4W^{viii}	0.92	1.84	2.686 (3)	153
O4C—H4CB···O18^{i}	0.92	2.09	3.007 (3)	173

(i) x−1, y, z; (iii) x+1, y, z; (v) x+1, y, z+1; (vi) x−1, y, z−1; (vii) −x+2, −y, −z+1; (viii) −x, −y+1, −z