Electronic Supplementary Information for

A pair of 3D homochiral metal-organic frameworks: spontaneous resolution, single-crystal-to-single-crystal transformation and selective adsorption properties

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Table S1 Selected bond distances (Å) and angles (deg) for **1a**, **1b** and **1a'**

1a

Eu(1)-O(4i)	2.302(4)	Eu(1)-O(1)	2.320(5)	Eu(1)-O(12ii)	2.321(4)
Eu(1)-O(8iii)	2.328(4)	Eu(1)-O(6iv)	2.334(5)	Eu(1)-O(10v)	2.343(4)
Eu(1)-O(1W)	2.457(4)	O(4)-Eu(1)-O(1v)	134.1(2)	O(4v)-Eu(1)-O(12ii)	86.99(18)
O(1)-Eu(1)-O(12ii)	87.92(17)	O(4i)-Eu(1)-O(8iii)	92.78(19)	O(1)-Eu(1)-O(8iii)	90.59(17)
O(12ii)- Eu(1)-O(8iii)	177.68(17)	O(4i)Eu(1)-O(6i)	149.1(2)	O(1)-Eu(1)-O(6i)	76.4(2)
O(12ii)- Eu(1)-O(6i)	89.8(2)	O(8iii)-Eu(1)-O(6i)	91.61(15)	O(1)-Eu(1)-O(10v)	151.0(2)
O(4)-Eu(1)-O(1Wi)	67.9(2)	O(6i)-Eu(1)-O(10v)	74.7(2)	O(8iii)-Eu(1)-O(10v)	87.62(16)
O(12ii)-Eu(1)-O(10v)	94.54(16)	O(1)-Eu(1)-O(1W)	66.52(18)	O(6)-Eu(1)-O(1Wi)	142.9(2)
O(8)-Eu(1)-O(1Wiii)	87.91(15)	O(10)-Eu(1)-O(1Wv)	142.22(19)	O(12)-Eu(1)-O(1Wii)	89.86(15)

1b

Eu(1)-O(4i)	2.304(6)	Eu(1)-O(1ii)	2.316(7)	Eu(1)-O(12ii)	2.318(5)
Eu(1)-O(6iii)	2.331(8)	Eu(1)-O(8iv)	2.331(7)	Eu(1)-O(10v)	2.346(7)
Eu(1)-O(1W)	2.454(7)	O(4)-Eu(1)-O(1i)	133.0(4)	O(4i)-Eu(1)-O(12ii)	86.8(2)
O(1)-Eu(1)-O(12ii)	88.3(2)	O(4i)-Eu(1)-O(6iii)	150.3(4)	O(1)-Eu(1)-O(6iii)	76.2(3)
O(12)ii-Eu(1)-O(6)iii	89.6(3)	O(4iv)-Eu(1)-O(8i)	92.8(3)	O(1)-Eu(1)-O(8iv)	89.9(3)
O(12ii)-Eu(1)-O(8i)v	177.0(3)	O(6iii)-Eu(1)-O(8iv)	92.2(2)	O(4i)-Eu(1)-O(10v)	74.6(4)
O(1)-Eu(1)-O(10v)	152.4(3)	O(12ii)-Eu(1)-O(10v)	94.8(2)	O(6iii)-Eu(1)-O(10v)	76.4(3)
O(8iv)-Eu(1)-O(10v)	87.9(2)	O(4)-Eu(1)-O(1Wi)	67.0(3)	O(1)-Eu(1)-O(1W)	66.3(3)
O(6)-Eu(1)-O(1Wiii)	142.5(3)	O(8)-Eu(1)-O(1Wiv)	87.4(2)	O(10)-Eu(1)-O(1Wv)	141.0(3)

1a'

Eu(1)-O(1i)	2.298(11)	Eu(1)-O(1)	2.298(11)	Eu(1)-O(1ii)	2.298(11)
Eu(1)-O(1iii)	2.298(11)	Eu(1)-O(1iv)	2.298(11)	Eu(1)-O(1v)	2.298(11)
O(1i)-Eu(1)-O(1)	167.6(8)	O(1i)-Eu(1)-O(1ii)	84.8(6)	O(1)-Eu(1)-O(1ii)	87.4(4)
O(1i)-Eu(1)-O(1iii)	87.4(4)	O(1)-Eu(1)-O(1iii)	84.8(6)	O(1ii)-Eu(1)-O(1iii)	101.8(7)
O(1i)-Eu(1)-O(1iv)	101.8(7)	O(1)-Eu(1)-O(1iv)	87.4(4)	O(1ii)-Eu(1)-O(1iv)	87.4(4)
O(1iii)-Eu(1)-O(1iv)	167.6(8)	O(1i)-Eu(1)-O(1v)	87.4(4)	O(1)-Eu(1)-O(1v)	101.8(7)
O(1ii)-Eu(1)-O(1v)	167.6(8)	O(1iii)-Eu(1)-O(1v)	87.4(4)	O(1iv)-Eu(1)-O(1v)	84.8(6)

Symmetry transformations used to generate equivalent atoms: **1a:** (i) -x+1, y+1/2,-z; (ii) x, y, z-1; (iii) 1-x, y+1/2, 1-z; (iv) x+1, y, z; (v) x+1, y, z-1; (vi) 1-x, y-1/2, -z; (vii) x-1, y, z; (viii) 1-x, y-1/2, 1-z; (ix) x-1, y, z+1; (x) x, y, z+1; **1b**: (i) 1-x, y-1/2, 2-z; (ii) x, y, z+1; (iii) x-1, y, z; (iv) 1-x, y-1/2, 1-z; (v) x-1, y, z+1; (vi) 1-x, y+1/2, 2-z; (vii) x+1, y, z; (viii) 1-x, y+1/2, 1-z; (ix) x+1, y, z-1; (x) x, y, z-1; **1a'**: (i) -y, -x, -z; (ii) -y, x-y, z; (iii) -x+y, y, -z; (iv) -x+y, -x, z; (v) x, x-y, -z; (vi) -x+y, -x+1, z; (vii) -y+1, x-y+1, z; (viii) x, x-y+1, -z+1; (ix) -x+y, y, -z+1; (x) -y, -x, -z+1.

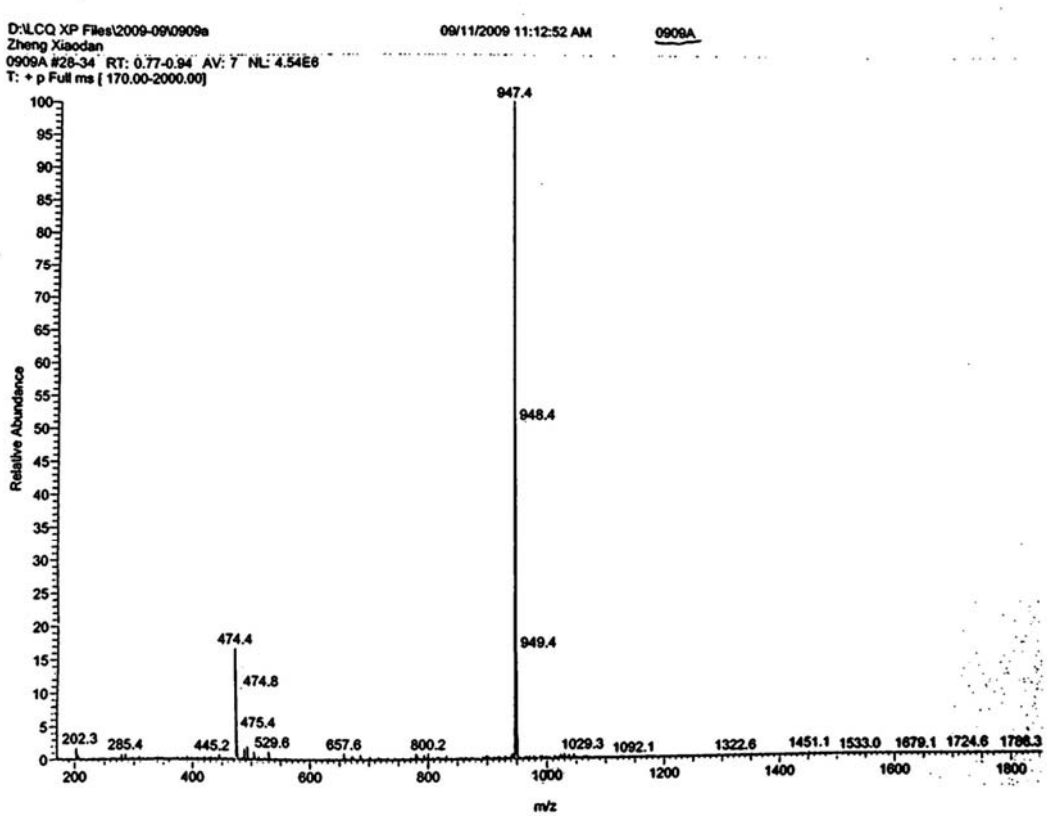


Fig. S1 ESI mass spectra of the ligand **L**.

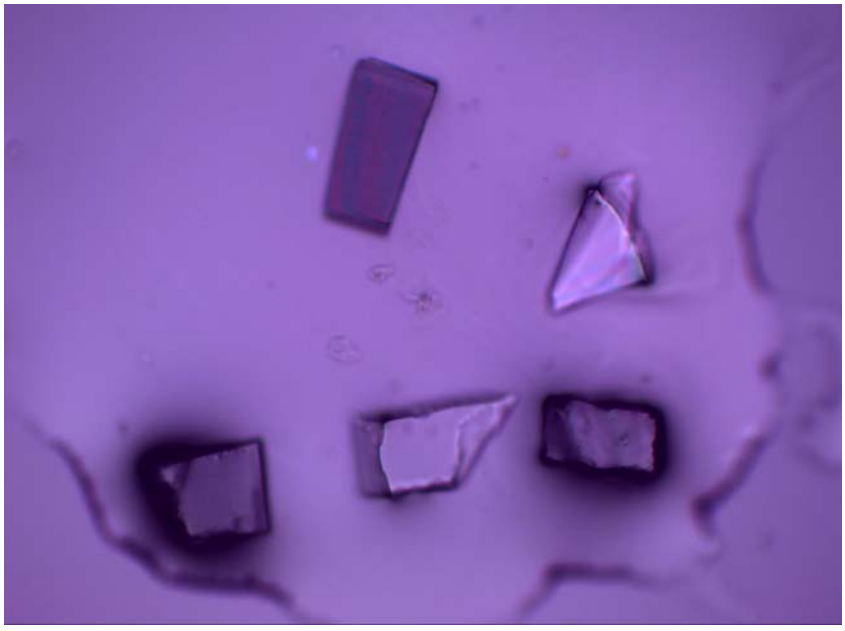


Fig. S2 View of the enantiomers of **1a** (light) and **1b** (dark) in the presence of polarized light by using a polarized light microscope.

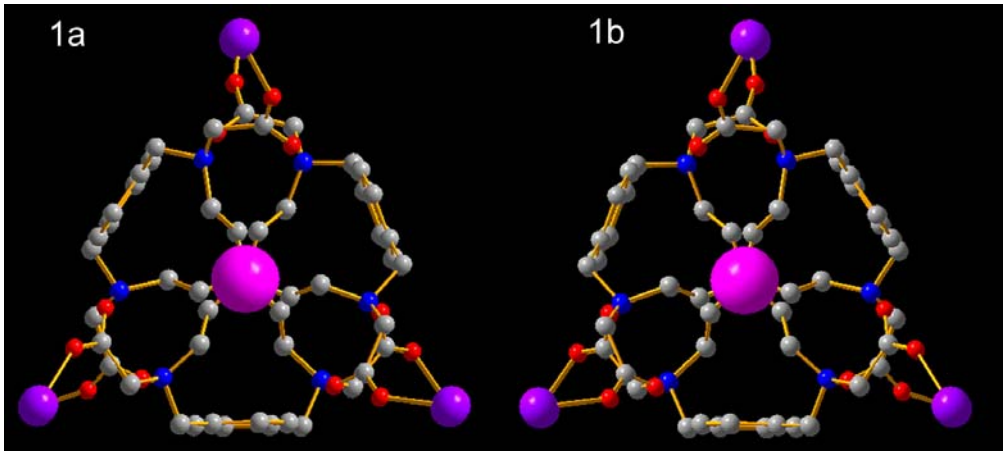


Fig. S3 C_3 symmetric conformation of the ligand in **1a** (left) and **1b** (right) viewed down the *c* axis (the middle pink spheres represent the C_3 axis).

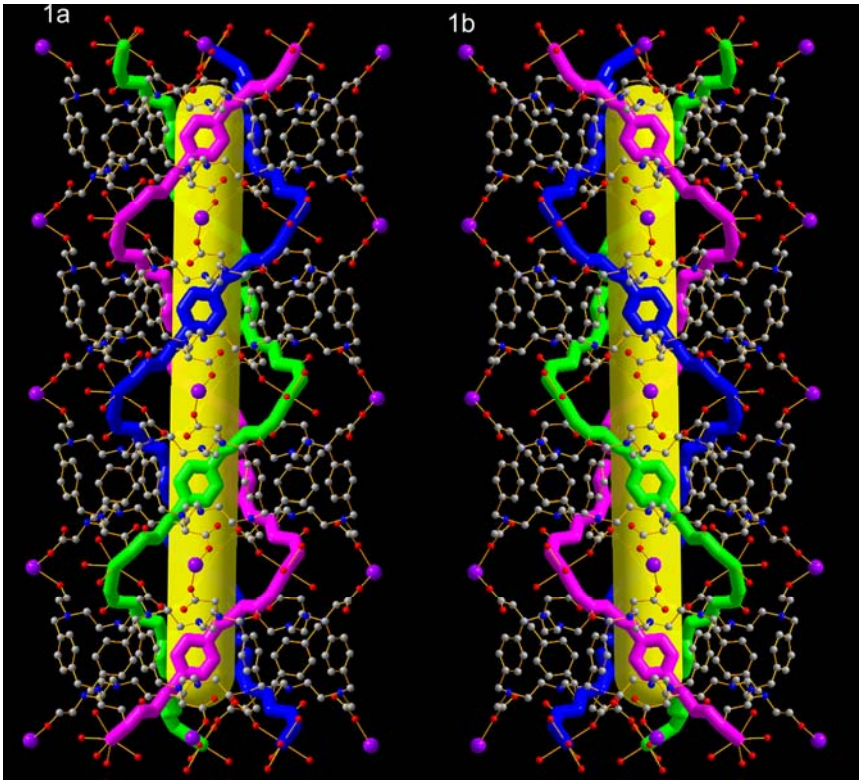
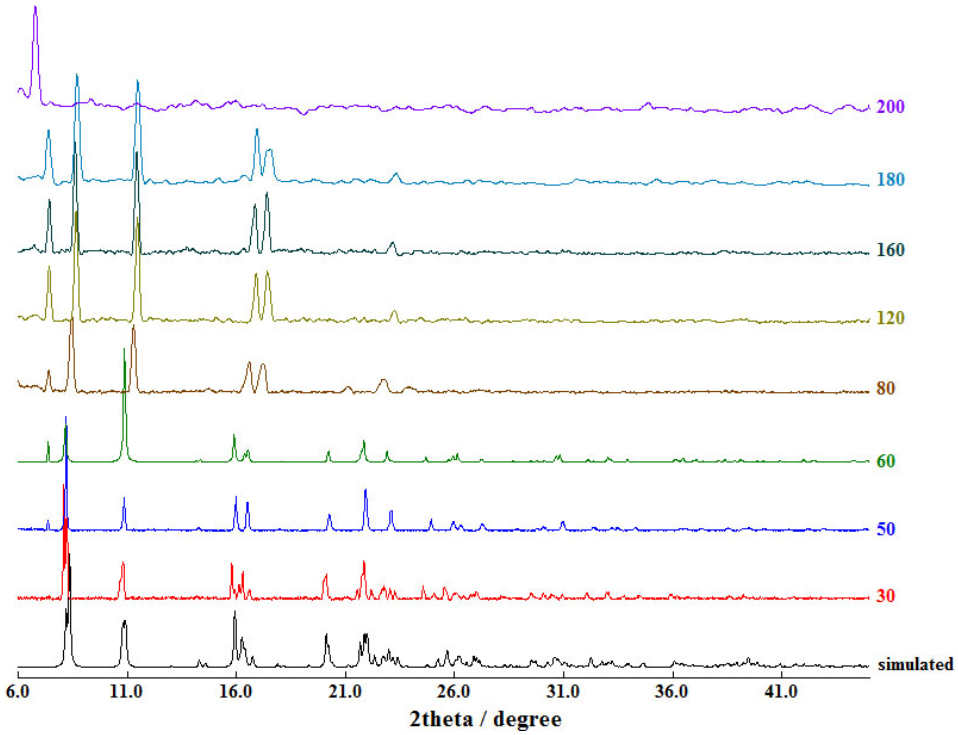


Fig. S4 Right-handed triple-stranded helical channel in **1a** (left) and left-handed triple-stranded helical channel in **1b** (right) along the *c* axis (yellow pillars represent the helical channels, water molecules and H atoms are omitted for clarity).

a)



b)

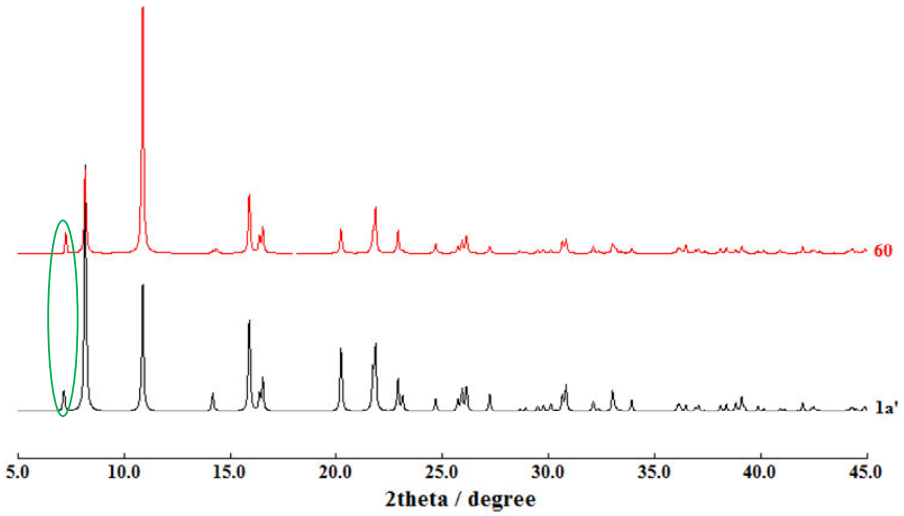


Fig. S5 a) The XRPD patterns of **1** at different temperatures, and b) the XRD patterns of **1a'** as simulated and **1** at 60°C (the simulated patterns are generated from the single-crystal diffraction data).

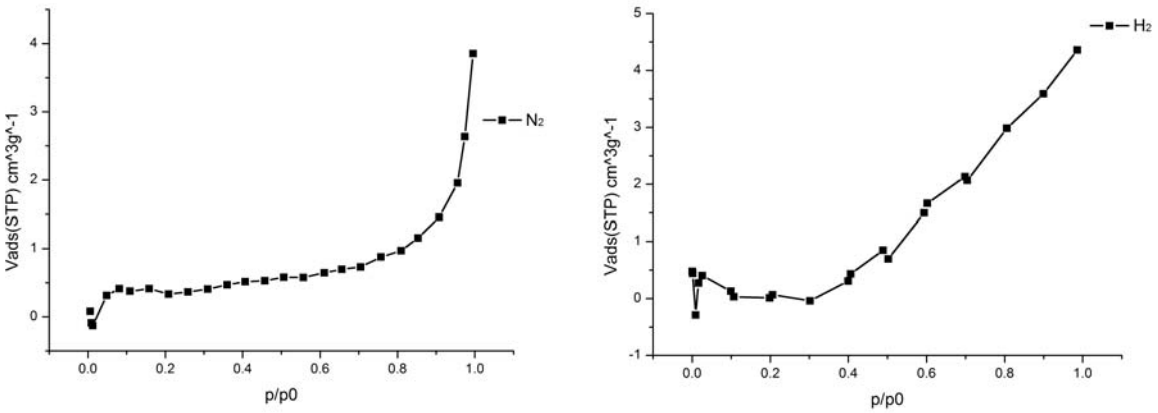


Fig. S6 The gas sorption isotherms of nitrogen (left) and hydrogen (right) for dehydrated **1**, implying that only surface adsorption occurred.

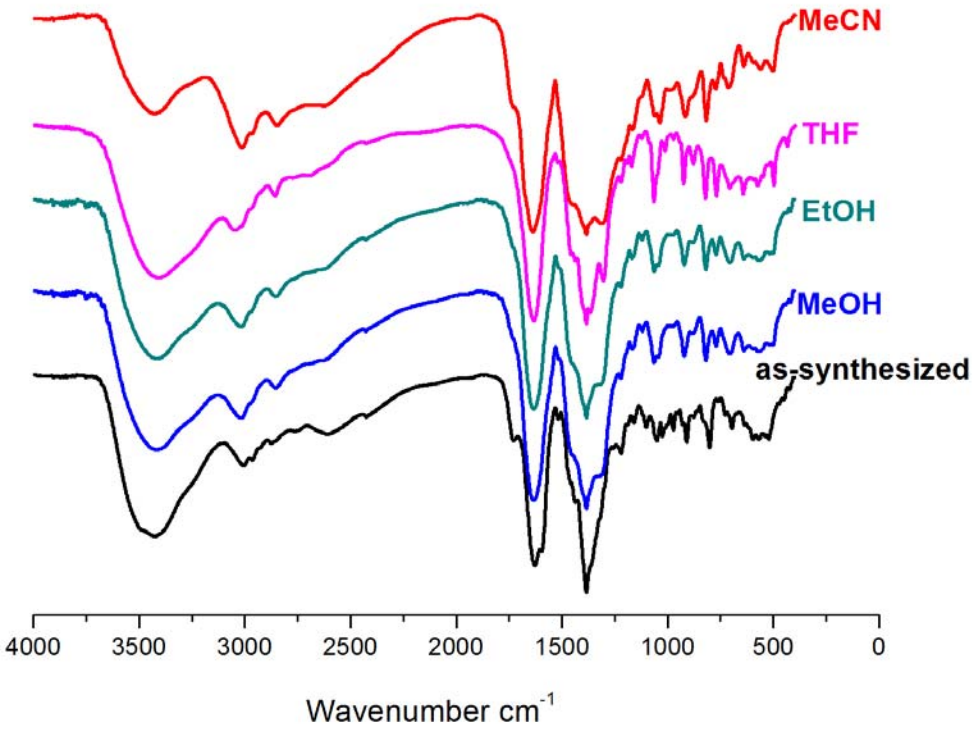


Fig. S7 The IR spectra for the synthesized crystals, and the samples after the dehydrated crystals were immersed in different solvents for 1 day, indicating only water molecules were adsorbed by dehydrated **1**.

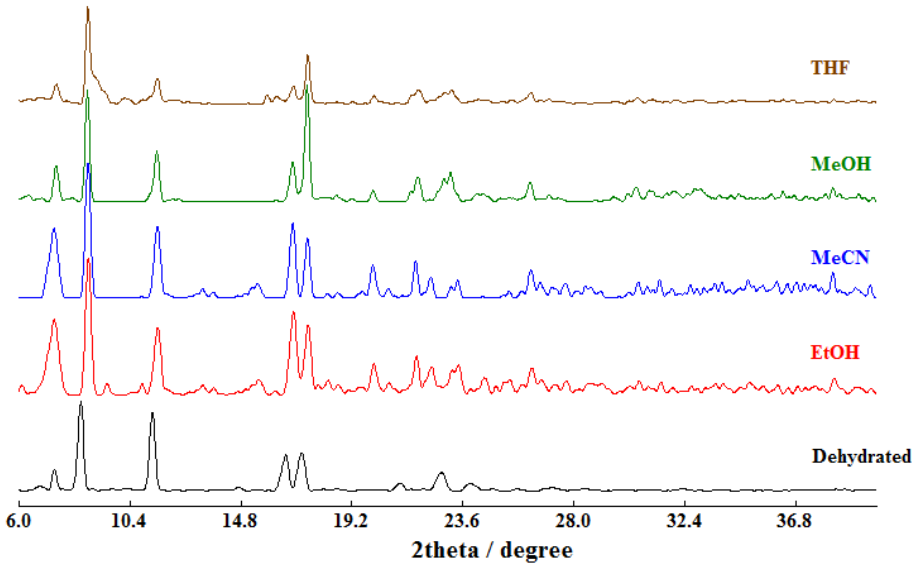


Fig. S8 The XRPD patterns of dehydrated **1** after immersed in different dry solvents for 24 h.