Electronic Supplementary Material (ESI) for Journal of Materials Chemistry

Supporting Information

Homochiral Porous Metal-Organic Frameworks Containing Only Achiral Building Blocks for Enantioselective Separation

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Materials and Instrumentation. All reagents were purchased commercially and used without further purification. All Powder X-ray diffraction (PXRD) analyses were recorded on a Rigaku Dmax2500 diffractometer with Cu Kα radiation (λ = 1.54056 Å) with a step size of 0.05°. Thermal stability studies were carried out on a NETSCHZ STA-449C thermoanalyzer with a heating rate of 10 °C/min under an N_2 atmosphere. The adsorption experiments were performed on Micromeritics ASAP 2020 surface area and pore size analyzer.

Measurements of solid CD spectra: The mixture of three single crystals of **1**⊃DMPU and 200 mg dry KCl powder was well grounded and then pressed into a disk for the CD measurement with a MOS-450 spectropolarimeter.

Table S1 A Summary of Crystal Data and Refinement Results

Compound reference	1_DMPU	1_ethanol	1_acetonitrile	1_cyclohexane	1P_styreneoxide	1P_2-butanol	1M_(S)-1-phenylethanol	1P_(R)-1-phenylethanol
Chemical formula	$C_{36}H_{42}Co_2N_8O_{11}$	$C_{24}H_{18}Co_2N_4O_9$	$C_{28}H_{24}Co_2N_6O_9$	$C_{30}H_{30}Co_2N_4O_9$	$C_{32}H_{18}Co_2N_4O_{10}$	$C_{26}H_{23}Co_2N_4O_{9\cdot50}$	$C_{32}H_{28}Co_2N_4O_{10}$	$C_{32}H_{28}Co_2N_4O_{10}$
Formula Mass	880.64	624.28	706.39	708.44	736.36	661.34	746.44	746.44
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic
a/ Å	11.4398(2)	11.3503(3)	11.249(4)	11.3749(4)	11.379(3)	11.2690(17)	11.4777(2)	11.4659(3)
b/ Å	13.2955(2)	13.1581(3)	13.238(4)	13.3596(5)	13.386(4)	13.382(2)	13.3164(3)	13.2732(3)
c/ Å	26.2483(4)	26.2130(6)	26.050(9)	25.9691(11)	25.904(8)	25.592(4)	26.0307(4)	26.1201(12)
α/°	90.00	90.00	90.00	90.00	90.00	90.00	90.00	90.00
β/°	90.00	90.00	90.00	90.00	90.00	90.00	90.00	90.00
γ/°	90.00	90.00	90.00	90.00	90.00	90.00	90.00	90.00
Unit cell volume/^{3}	3992.31(11)	3914.87(16)	3879(2)	3946.4(3)	3945(2)	3859.4(10)	3978.57(13)	3975.2(2)
Temperature/K	298(2)	173(2)	173(2)	173(2)	173(2)	173(2)	173(2)	173(2)
Space group	*P2(1)2(1)2(1)*	*P2(1)2(1)2(1)*	*P2(1)2(1)2(1)*	*P2(1)2(1)2(1)*	*P2(1)2(1)2(1)*	*P2(1)2(1)2(1)*	*P2(1)2(1)2(1)*	*P2(1)2(1)2(1)*
No. of formula units per unit cell, *Z*	4	4	4	4	4	4	4	4
No. of reflections measured	9865	10317	33922	10082	29672	30673	10910	10381
No. of independent reflections	6664	6592	8859	6476	8886	8749	6599	6431
R_{int}	0.0243	0.0238	0.1093	0.0277	0.0438	0.0318	0.0244	0.0300
Final R_1 values ($I > 2\sigma(I)$)	0.0289	0.0479	0.0856	0.0460	0.0671	0.0326	0.0479	0.0567
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.0679	0.1572	0.2186	0.1375	0.1995	0.1043	0.1665	0.1789
Final R_1 values (all data)	0.0369	0.0567	0.0954	0.0509	0.0743	0.0338	0.0532	0.0737
Final $wR(F^2)$ values (all data)	0.0691	0.1624	0.2343	0.1433	0.2176	0.1052	0.1725	0.1964
Goodness of fit on F^2	1.003	1.173	1.174	1.144	1.056	1.112	1.178	1.156
Flack parameter	0.003(12)	-0.03(3)	0.11(3)	0.01(2)	0.00(2)	-0.002(11)	-0.01(2)	0.02(3)

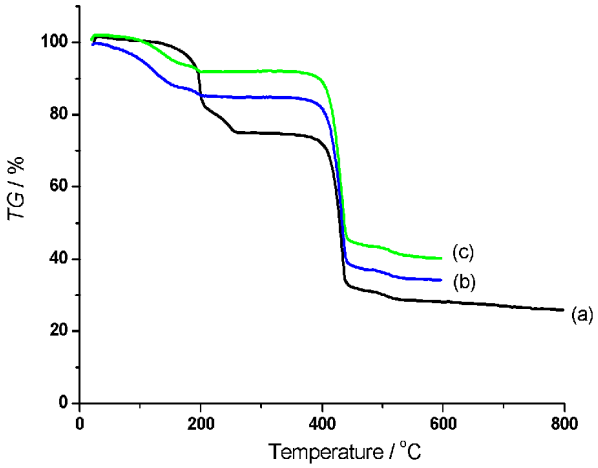

Figure S1. TGA curves of compounds **1**⊃DMPU (a), **1**⊃ethanol (b), **1**⊃acetonitrile (c).

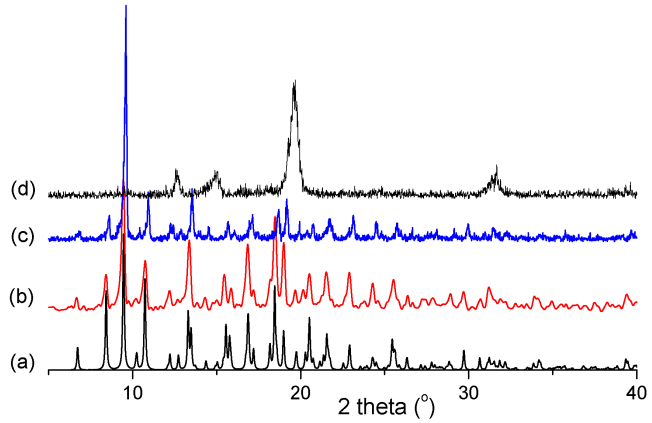

Figure S2. The Powder XRD patterns of 1: (a) stimulated from 1⊃DMPU; (b) the as-synthesized sample of 1⊃DMPU; (c) the as-synthesized sample of 1⊃ ethanol; (d) the sample of **1** after heating at 300 °C for ten minutes. The powder X-ray diffraction pattern of the desolvated form shows that the broadened peaks keep the positions, indicating the maintenance of the framework structure. It also reveals that the crystalline sample tends to be amorphous after the departure of the guest molecules.

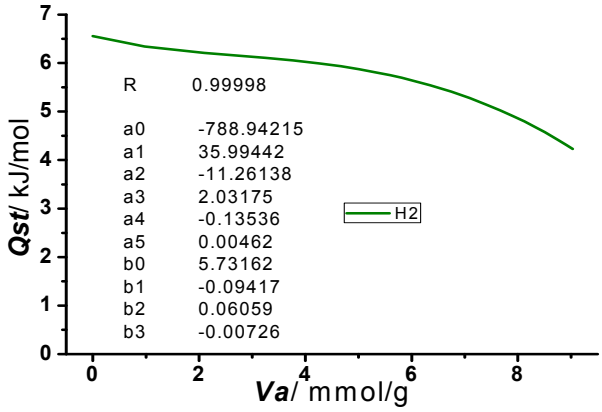

Figure S3. The Isosteric heat of H_2 adsorption for **1** estimated by the virial equation.