Electronic Supplementary Material (ESI) for CrystEngComm

Supporting Information

Structural Isomerism of an Anionic Nanoporous In-MOF with Interpenetrated Diamond-Like Topology

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Table S1. Selected bond angles around In(1) and In(2) atoms for In-MOF **1**.

Atoms			Angle (°)
C(114)#2	IN(1)	C(114)#3	98.46(1)
C(114)#3	IN(1)	C(11)#1	97.96(1)
C(11)#1	IN(1)	C(11)	98.81(1)
C(11)	IN(1)	C(114)#2	97.96(1)
C(21)#6	IN(2)	C(21)	100.95(1)
C(21)	IN(2)	C(214)#4	96.89(1)
C(214)#4	IN(2)	C(214)#5	93.12(1)
C(214)#5	IN(2)	C(21)#6	96.89(1)

#1 -x+1/4,y,-z+1/4 #2 x+1/4,y+1/4,-z #3 -x,y+1/4,z+1/4

#4 x+1/4,-y+1,z+1/4 #5 -x+3/2,y-1/4,z+1/4 #6 -x+7/4,-y+3/4,z

#7 x-1/4,y-1/4,-z #8 x-1/4,-y+1,z-1/4

Figure S1. Diagrams of the solvent-free In-MOF **1** along the *b*-axis (a) and *c*-axis (b). Counter-ions, $H_2N(CH_3)_2^+$, are represented in a CPK model without hydrogen atoms. Nitrogen atoms of $H_2N(CH_3)_2^+$ are shown in blue spheres.

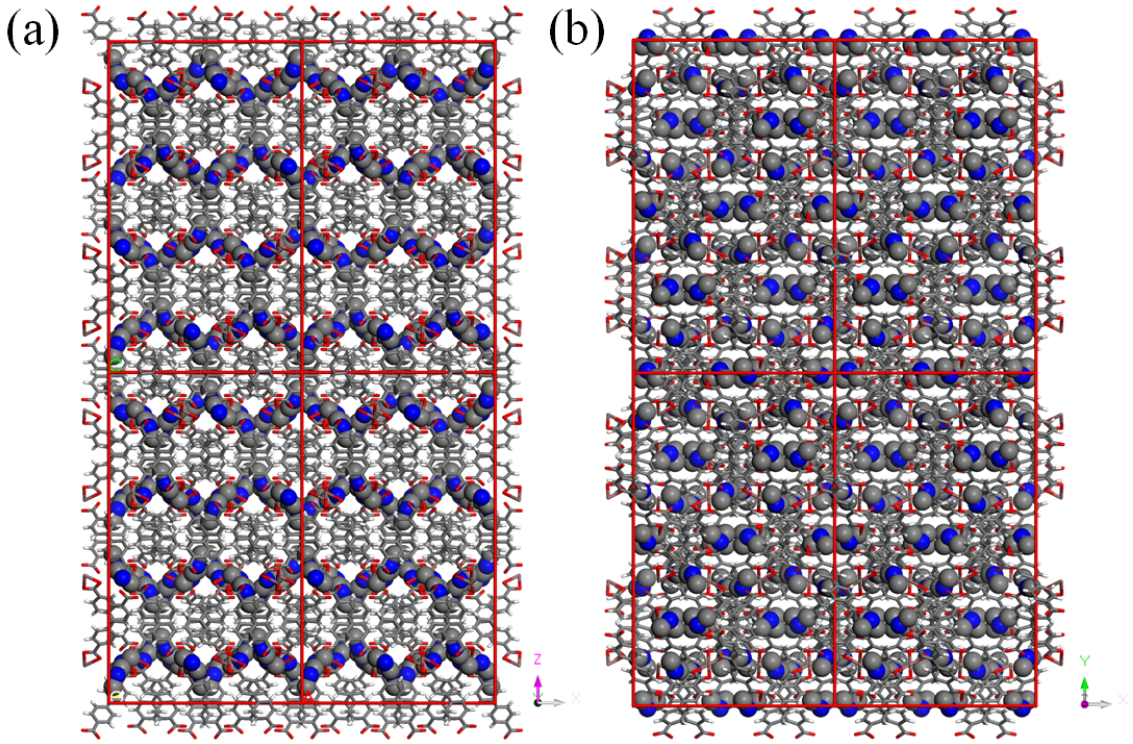


Figure S2. TGA profile for the as-preapred In-MOF **1**.

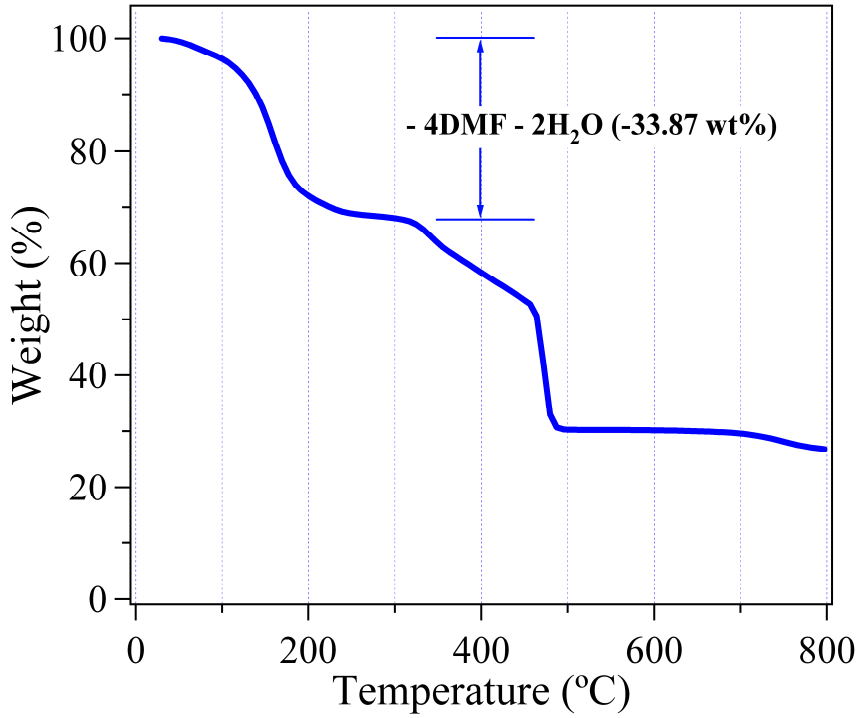


Figure S3. The Connolly surface of solvent-free In-MOF **1** obtained with 1.0 Å probe radius (Materials Studio 4.3, Accelrys) along the *a*-axis (a) and its 45°-rotated view along the *b*-axis (b).

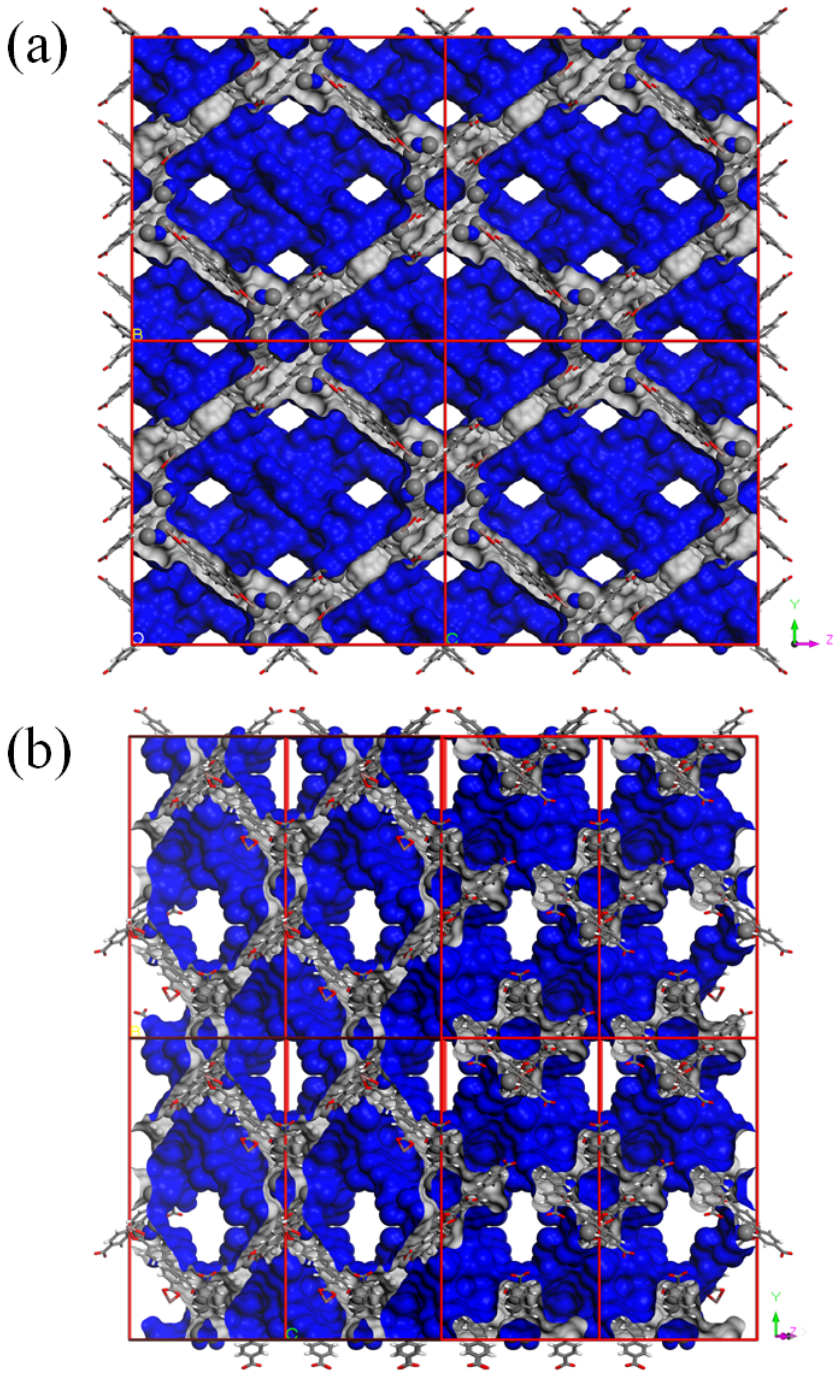
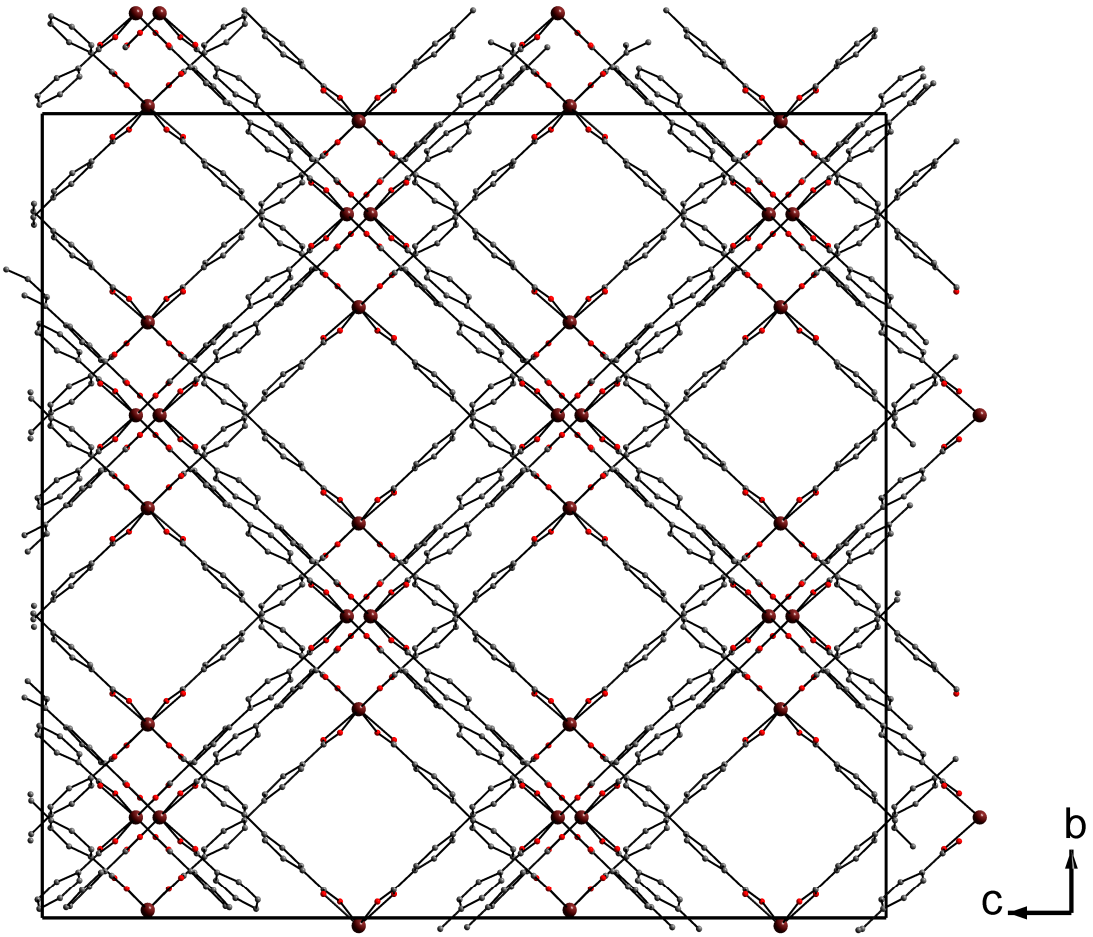
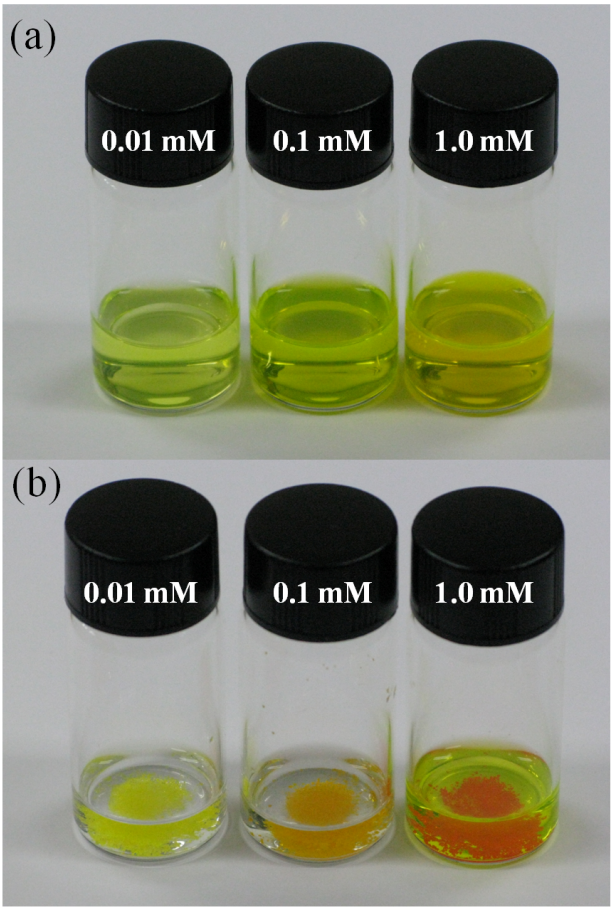


Figure S4. The framework structure of the AO-encapsulated In-MOF **1** along the *a*-axis. Hydrogen atoms are omitted for clarity. The unit cell dimensions of as-prepared **1** and AO-encapsulated **1** are also compared in the table.



Unit cell dimensions	As-prepared In-MOF **1**	AO-encapsulated In-MOF **1**
a	23.760(5) Å	23.088(3) Å
b	39.331(8) Å	39.262(5) Å
c	40.610(9) Å	41.133(5) Å
α	90.00°	90.00°
β	90.00°	90.00°
γ	90.00°	90.00°
Volume	37951(14) $Å^3$	37286(8) $Å^3$

Figure S5. Concentration dependence on the acridine orange hydrochloride (AO) encapsulation by the as-prepared In-MOF **1**. (a) Digital image of the initial ethanolic solutions of various AO concentrations. (b) Image taken after 7 d of immersion of 20 mg of the as-prepared In-MOF **1**. (c) Time course of AO encapsulation by In-MOF **1** for 1.0 mM AO solution.



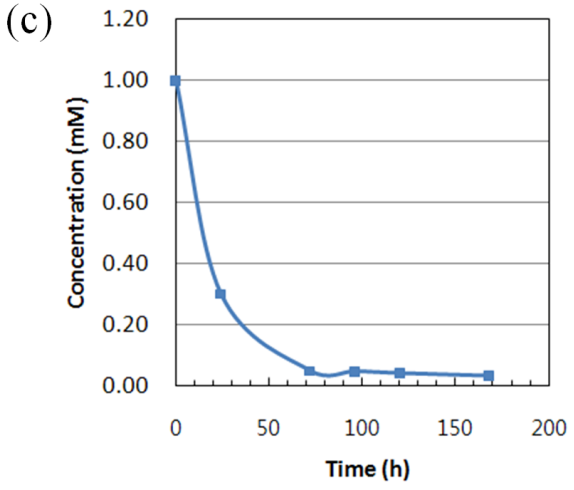


Figure S6. TGA profile for the as-preapred In-MOF **2**.