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Supporting information for

New Functionalized MIL-53(In) Solids: Syntheses, Characterization, Sorption, and Structural Flexibility

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Table S1 The selected bond lengths (Å) and bond angles (º) of MIL-53(In)_$(OH)_2$_lp_DMF.

MIL-53(In)_$(OH)_2$_lp_DMF			
In(1)-O(8)#1	2.052(4)	In(1)-O(8)	2.071(4)
In(1)-O(4)#2	2.145(3)	In(1)-O(4)#3	2.145(3)
In(1)-O(3)	2.177(3)	In(1)-O(3)#4	2.178(3)
In(2)-O(7)	2.0657(19)	In(2)-O(7)#5	2.0658(19)
In(2)-O(1)#6	2.147(3)	In(2)-O(1)	2.148(3)
In(2)-O(2)#7	2.181(3)	In(2)-O(2)#8	2.181(3)
O(2)-In(2)#5	2.181(3)	O(4)-In(1)#1	2.145(3)
O(7)-In(2)#7	2.0657(19)	O(8)-In(1)#2	2.052(4)
O(8)#1-In(1)-O(8)	173.28(11)	O(8)#1-In(1)-O(4)#2	91.27(12)
O(8)-In(1)-O(4)#2	93.20(12)	O(8)#1-In(1)-O(4)#3	91.27(12)
O(8)-In(1)-O(4)#3	93.20(12)	O(4)#2-In(1)-O(4)#3	96.6(2)
O(8)#1-In(1)-O(3)	89.54(12)	O(8)-In(1)-O(3)	85.75(12)
O(4)#2-In(1)-O(3)	177.02(16)	O(4)#3-In(1)-O(3)	86.25(15)
O(8)#1-In(1)-O(3)#4	89.54(12)	O(8)-In(1)-O(3)#4	85.75(12)
O(4)#2-In(1)-O(3)#4	86.25(15)	O(4)#3-In(1)-O(3)#4	177.02(16)
O(3)-In(1)-O(3)#4	90.9(2)	O(7)-In(2)-O(7)#5	174.14(2)
O(7)-In(2)-O(1)#6	93.30(11)	O(7)#5-In(2)-O(1)#6	90.94(11)
O(7)-In(2)-O(1)	90.94(11)	O(7)#5-In(2)-O(1)	93.30(11)
O(1)#6-In(2)-O(1)	87.4(2)	O(7)-In(2)-O(2)#7	89.90(11)
O(7)#5-In(2)-O(2)#7	85.75(11)	O(1)#6-In(2)-O(2)#7	94.36(14)
O(1)-In(2)-O(2)#7	178.02(14)	O(7)-In(2)-O(2)#8	85.75(11)
O(7)#5-In(2)-O(2)#8	89.90(11)	O(1)#6-In(2)-O(2)#8	178.02(14)
O(1)-In(2)-O(2)#8	94.36(14)	O(2)#7-In(2)-O(2)#8	83.9(2)

Symmetry transformations used to generate equivalent atoms: #1 -x,-y+1/2,z-1/2; #2 -x,-y+1/2,z+1/2; #3 x,-y+1/2,z+1/2 ; #4 -x,y,z; #5 -x+1/2,-y+1,z-1/2; #6 x,-y+1,-z+2; #7 -x+1/2,-y+1,z+1/2; #8 -x+1/2,y,-z+3/2.

Table S2 The selected bond lengths (Å) and bond angles (º) of MIL-53(In)_Br_lp_DMF.

MIL-53(In)_Br_lp_DMF			
In(1)-O(2)	2.0778(15)	In(1)-O(2)#1	2.0779(15)
In(1)-O(1)#1	2.1615(18)	In(1)-O(1)#2	2.1614(18)
In(1)-O(1)#1	2.167(7)	In(1)-O(1)#3	2.1615(18)
O(2)-In(1)#4	2.0778(15)		
O(2)-In(1)-O(2)#1	180.0	O(2)-In(1)-O(1)	90.85(7)
O(2)#1-In(1)-O(1)	89.15(7)	O(2)-In(1)-O(1)#2	90.85(7)
O(2)#1-In(1)-O(1)#2	89.15(7)	O(1)-In(1)-O(1)#2	91.77(10)
O(2)-In(1)-O(1)#1	89.15(7)	O(2)#1-In(1)-O(1)#1	90.85(7)
O(1)-In(1)-O(1)#1	180.0	O(1)#2-In(1)-O(1)#1	88.23(10)
O(2)-In(1)-O(1)#3	89.15(7)	O(2)#1-In(1)-O(1)#3	90.85(7)
O(1)-In(1)-O(1)#3	88.23(10)	O(1)#2-In(1)-O(1)#3	180.0
O(1)#1-In(1)-O(1)#3	91.77(10)		

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y,-z+1; #2 -x+1,y,z; #3 x,-y,-z+1; #4 -x+1,-y+1/2,z.

Table S3 The selected bond lengths (Å)and bond angles (º) of MIL-53(In)_NO_2_lp_DMF.

MIL-53(In)_NO_2_lp_DMF			
In(1)-O(2)	2.082(3)	In(1)-O(2)#1	2.082(3)
In(1)-O(1)#2	2.164(3)	In(1)-O(1)#3	2.164(3)
In(1)-O(1)#1	2.164(3)	In(1)-O(1)	2.164(3)
O(2)-In(1)#4	2.082(3)		
O(2)-In(1)-O(2)#1	180.0	O(2)-In(1)-O(1)#2	89.73(15)
O(2)#1-In(1)-O(1)#2	90.27(15)	O(2)-In(1)-O(1)#3	90.27(15)
O(2)#1-In(1)-O(1)#3	89.73(15)	O(1)#2-In(1)-O(1)#3	179.999(1)
O(2)-In(1)-O(1)#1	89.73(15)	O(2)#1-In(1)-O(1)#1	90.27(15)
O(1)#2-In(1)-O(1)#1	92.8(3)	O(1)#3-In(1)-O(1)#1	87.2(3)
O(2)-In(1)-O(1)	90.27(15)	O(2)#1-In(1)-O(1)	89.73(15)
O(1)#2-In(1)-O(1)	87.2(3)	O(1)#3-In(1)-O(1)	92.8(3)
O(1)#1-In(1)-O(1)	179.999(1)		

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y,-z+1; #2 x,-y,-z+1; #3 -x+1,y,z; #4 -x+1,-y+1/2,z.

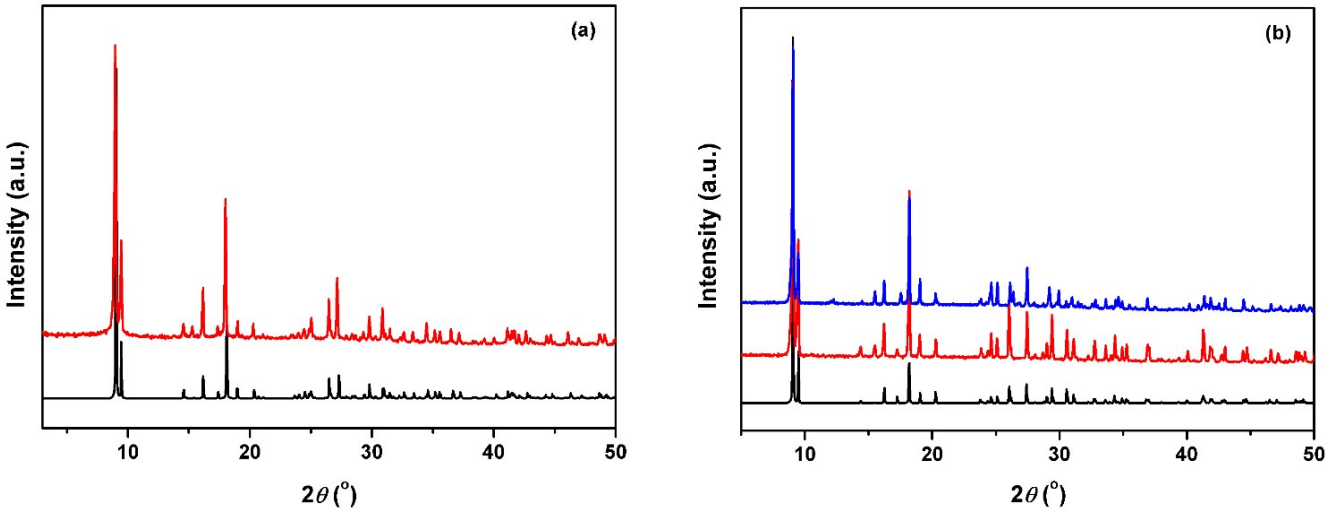

Fig. S1 PXRD patterns of (a) a simulated one calculated from single-crystal structure of MIL-53(In)_$(OH)_2$_lp_DMF (bulk crystal) (black); MIL-53(In)_$(OH)_2$_lp_DMF (microcrystalline) (red); (b) a simulated one calculated from single-crystal structure of MIL-53(In)_NO_2_lp_DMF (bulk crystal) (black); MIL-53(In)_NO_2_lp_DMF (microcrystalline) (red); MIL-53(In)_Br_lp_DMF (microcrystalline) (blue).

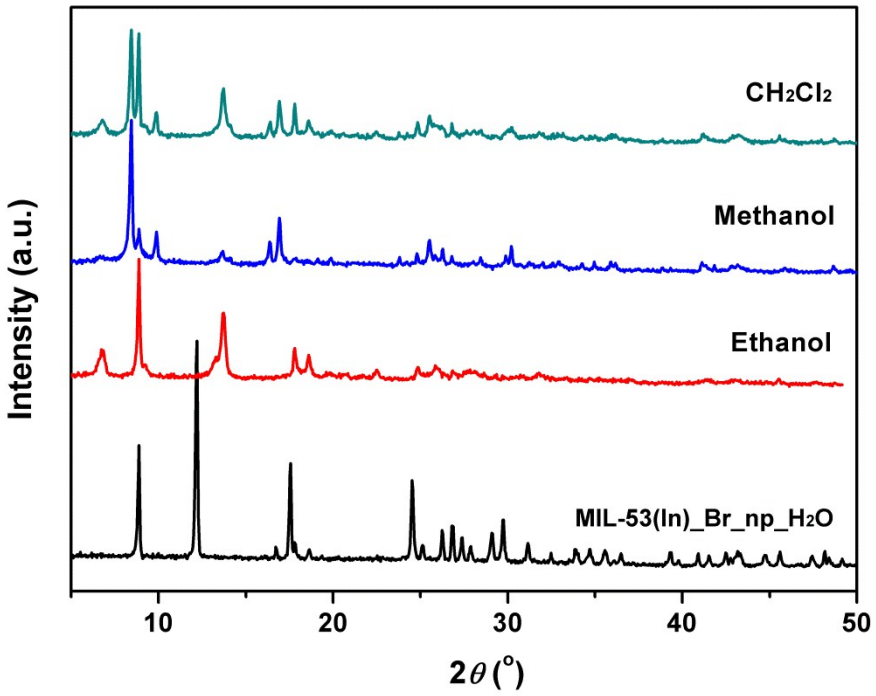

Fig. S2 PXRD patterns of MIL-53(In)_Br_np_H_2O (black), MIL-53(In)_$(OH)_2$_lp_DMF soaked in ethanol (red), methanol (blue) and CH_2Cl_2 (green).

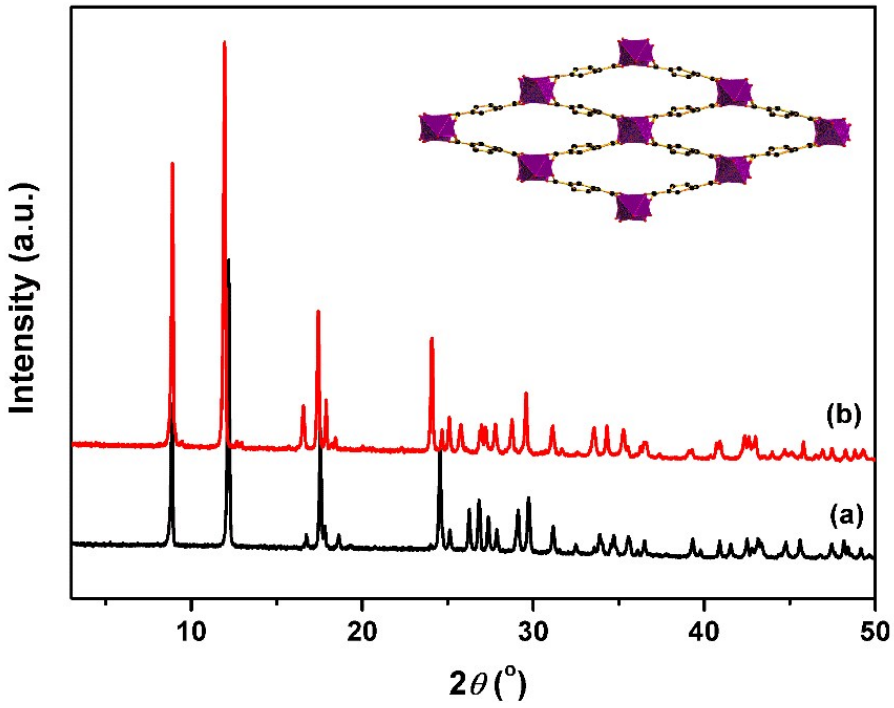

Fig. S3 PXRD patterns of (a) MIL-53(In)_Br_np_H_2O (black) and (b) MIL-53(In)_NO_2_np_H_2O (red).

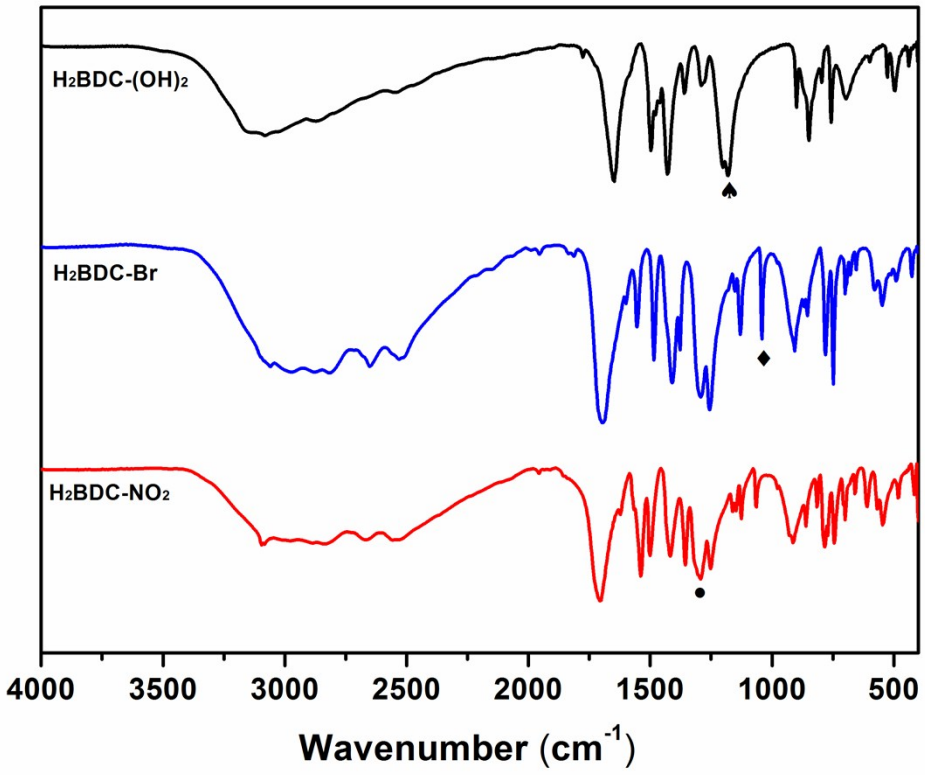

Fig. S4 IR spectra of the organic sources: (a) $H_2BDC\text{-}(OH)_2$; (b) $H_2BDC\text{-}Br$; (c) $H_2BDC\text{-}NO_2$ (♠, $\nu_{(C-O)}$; ♦, $\nu_{(C-Br)}$; ●, $\nu_{s(C-N)}$).