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Versatile functionalities in MOFs assembled from the same building units: Interplay of structural flexibility, rigidity and regularity

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Table S1: Selected Bond lengths (Å) and angles (º) for **1**

Cu1 - O1	1.9682(19)	Cu1 - O2	1.9617(19)
Cu1 - O3	1.9728(19)	Cu1 - O4	1.958(2)
Cu1 - O5	2.126(2)		
O1 - Cu1 - O2	169.16(9)	O1 - Cu1 - O3	89.37(9)
O1 - Cu1 - O4	91.30(9)	O1 - Cu1 - O5	94.01(8)
O2 - Cu1 - O3	88.93(9)	O2 - Cu1 - O4	88.29(9
O2 - Cu1 - O5	96.83(8)	O3 - Cu1 - O4	168.64(9)
O3 - Cu1 - O5	98.04(8)	O4 - Cu1 - O5	93.23(8)

Table S2: Selected Bond lengths (Å) and angles (º) for **2**

Cu1 - O1	1.973(5)	Cu1 - O5	2.136(5
Cu1 - O2_a	1.950(5)	Cu1 - O4_b	1.951(5)
Cu1 - O3_d	1.957(5)		
O1 - Cu1 - O5	93.5(2)	O1 - Cu1 - O2_a	88.8(2)
O1 - Cu1 -O4_b	170.0(2)	O1 - Cu1 - O3_d	88.5(2)
O2_a - Cu1 - O5	95.4(2)	O4_b - Cu1 - O5	96.5(2)
O3_d - Cu1 - O5	96.8(2)	O2_a - Cu1 - O4_b	88.9(2)
O2_a - Cu1 -O3_d	167.6(2)	O3_d - Cu1 - O4_b	91.6(2)

Symmetry codes : a = -x, y, 3/2 – z ; b = -1/2 + x, -1/2 + y, 3/2 – z ; d =1/2 - x,-1/2 + y, z

Table S3: Selected Bond lengths (Å) and angles (º) for **3**

Cu1-O1	1.939(6)	Cu1-O1W	2.100(14)
Cu1-O1_a	1.939(6)	Cu1-O1_b	1.939(6)
Cu1-O1_c	1.939(6)		
O1-Cu1-O1W	95.75(17)	O1-Cu1-O1_a	89.43(3)
O1-Cu1-O1_b	168.5(3)	O1-Cu1-O1_c	89.43(3)
O1_a-Cu1-O1W	95.75(17)	O1_b-Cu1-O1W	95.75(17)
O1_c-Cu1-O1W	95.75(17)	O1_a-Cu1-O1_b	89.43(3)
O1_a-Cu1-O1_c	168.5(3)	O1_b-Cu1-O1_c	89.43(3)

a = 1-y, x, z; b = 1-x,1-y, z; c = y, 1-x, z

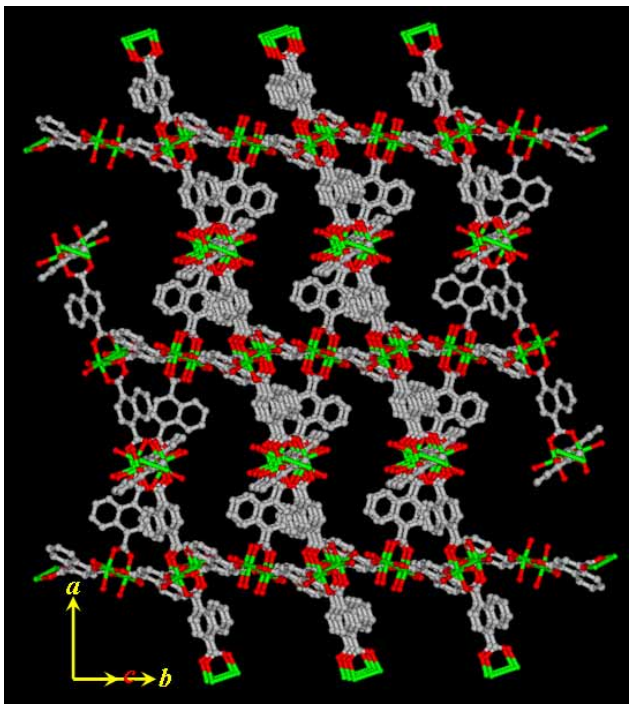

Fig. S1 View of a single 3D net in **1**. Color specification: Cu, green; O, red; C, grey. Guest water molecules are not shown for clarity.

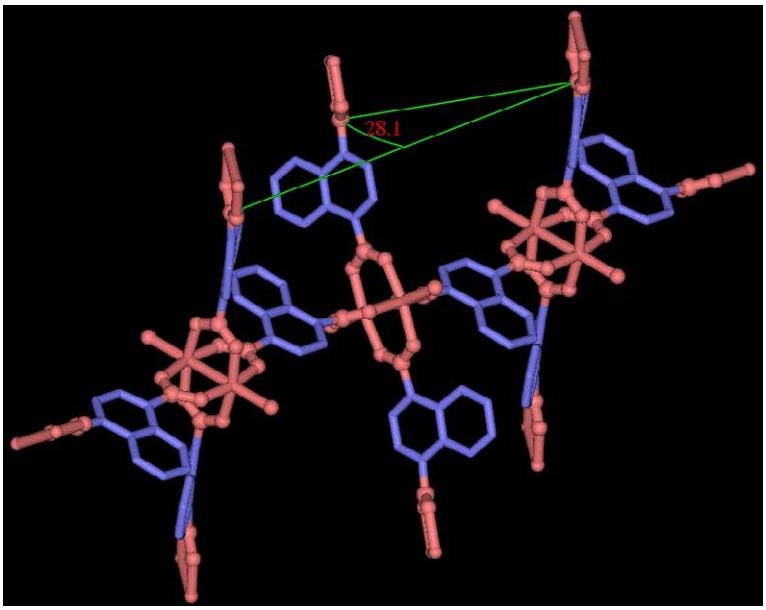

Fig. S2 Perspective view of the paddle-wheels showing the bending of neighbouring paddle-wheels by 28.1 º which dictates the formation of 3D structure.

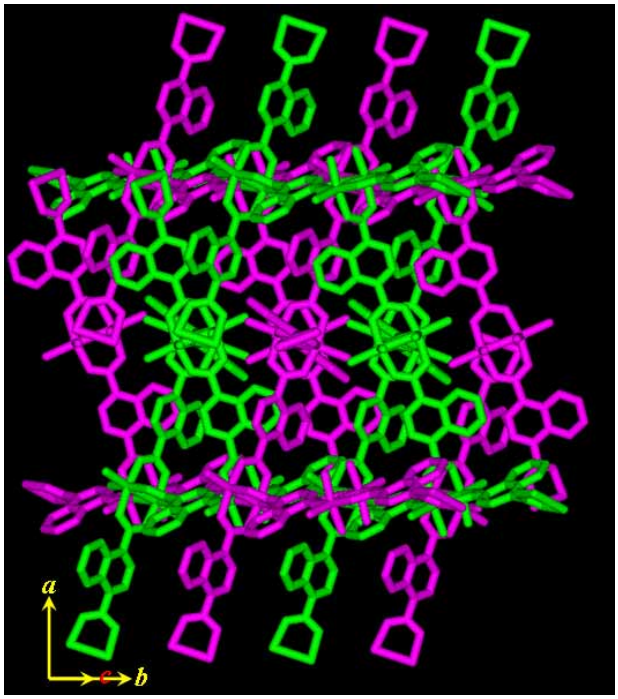

Fig. S3 Unusual two-fold interpenetrated 3D network found in compound **1**. The two-folds are designated with green and pink color. Guest water molecules are not shown for clarity.

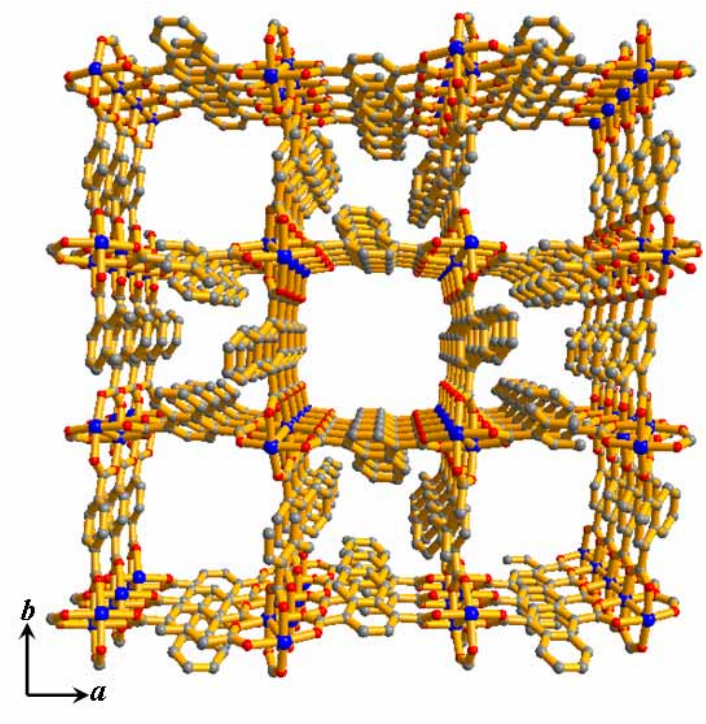

Fig. S4 Perspective view of the 3D coordination framework **1** showing two different channels along *c*-direction (pendent benzene rings align in one channels forming hydrophobic nature).

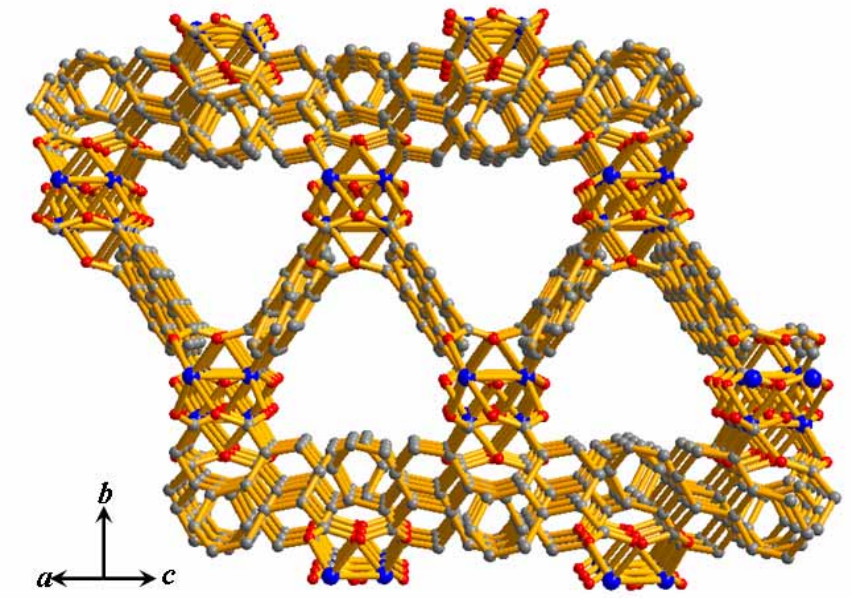

Fig. S5 Three dimensional view of **2** showing the presence of triangular channels.

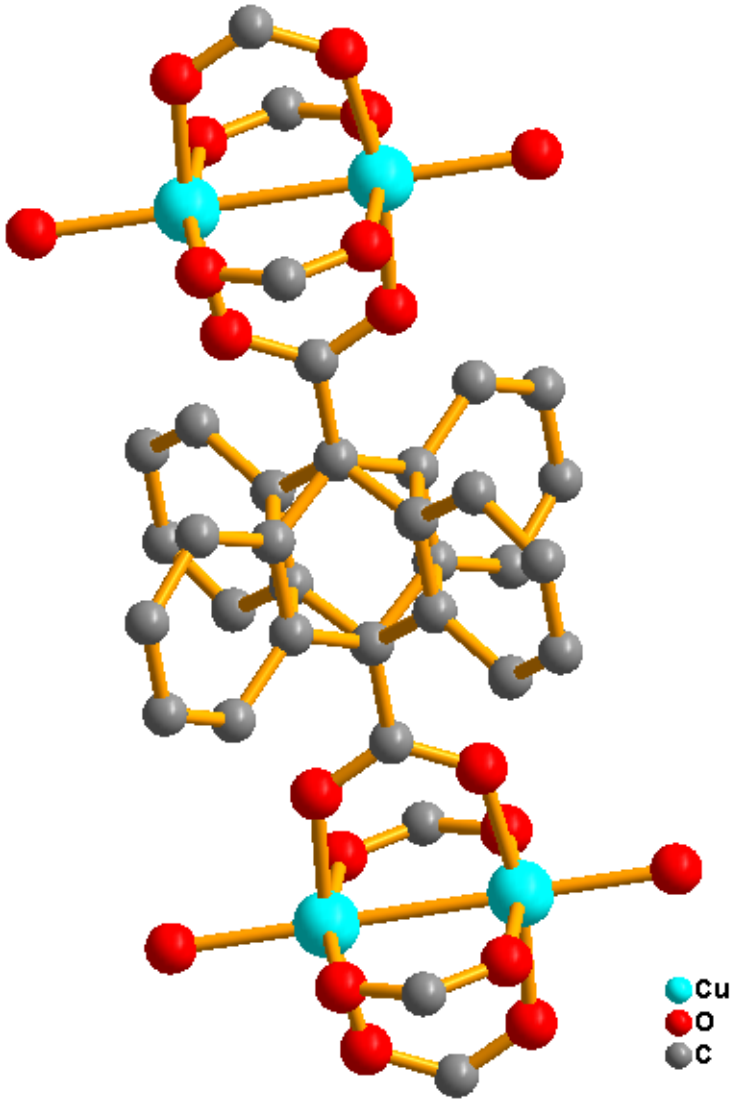

Fig. S6 Figure shows the presence of 4-fold disorder in the naphthalene ring of 1,4-ndc ligand in compound **3**.

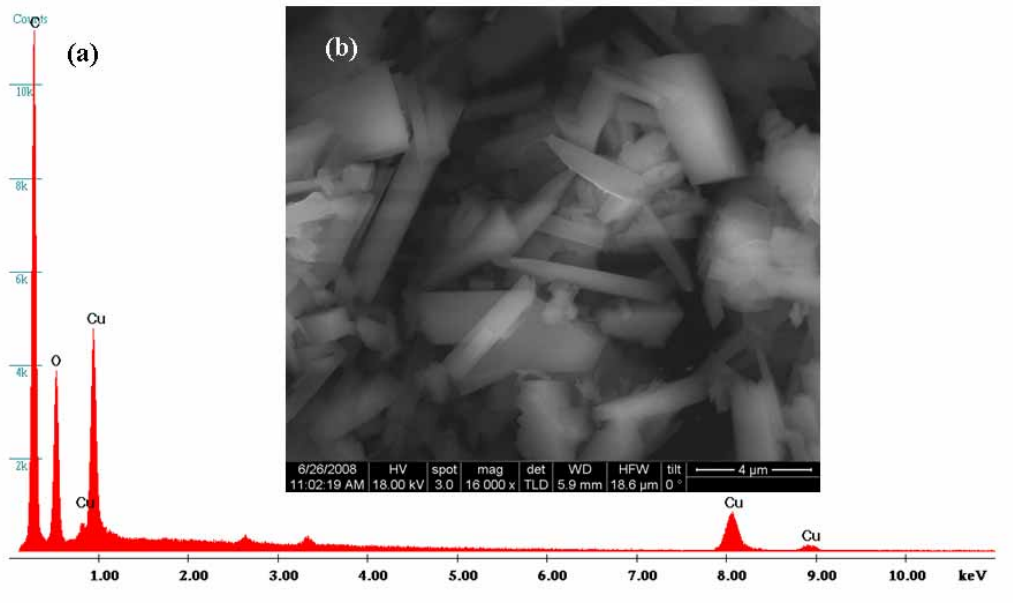

Fig. S7 EDX analysis and FESEM images (inset) for compound **4** showing micron size crystals.

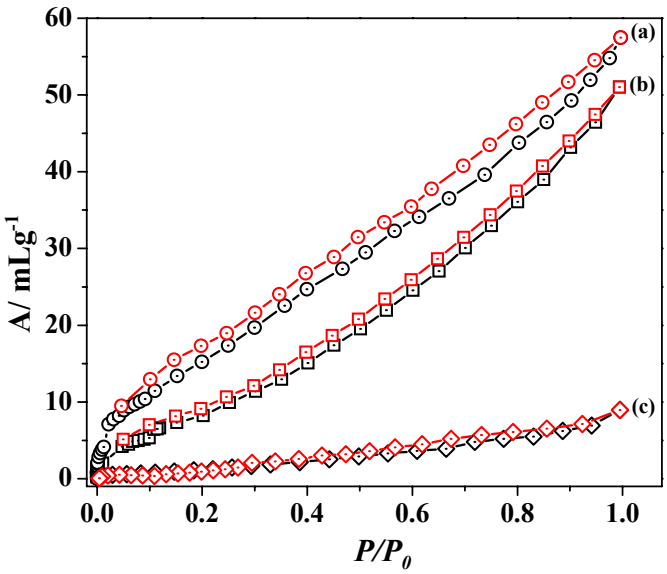

Fig. S8 N_2 adsorption isotherm for **1′** (b), **2′**(a) and **4′**(c) measured at 77 K (P_0 is the saturated vapour pressure of N_2).

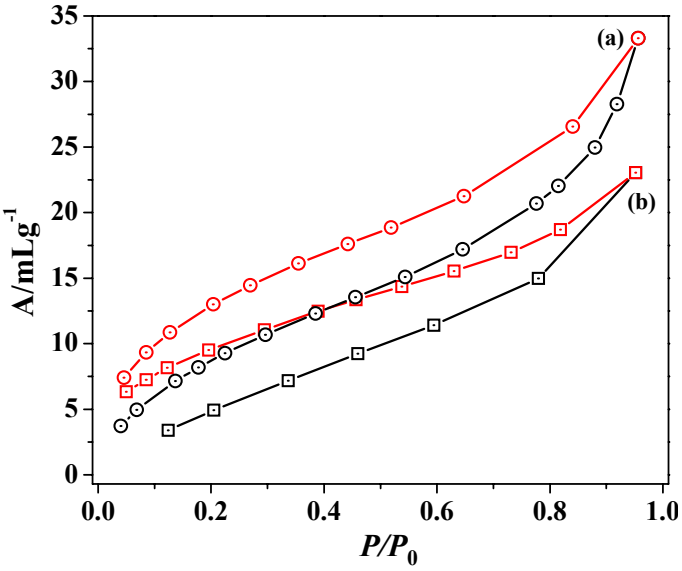

Fig. S9 Vapor sorption isotherms for **3′;** (a) MeOH at 293 K; and (b) H_2O at 298 K (P_0 is the saturated vapour pressure of the solvents at respective temperature).

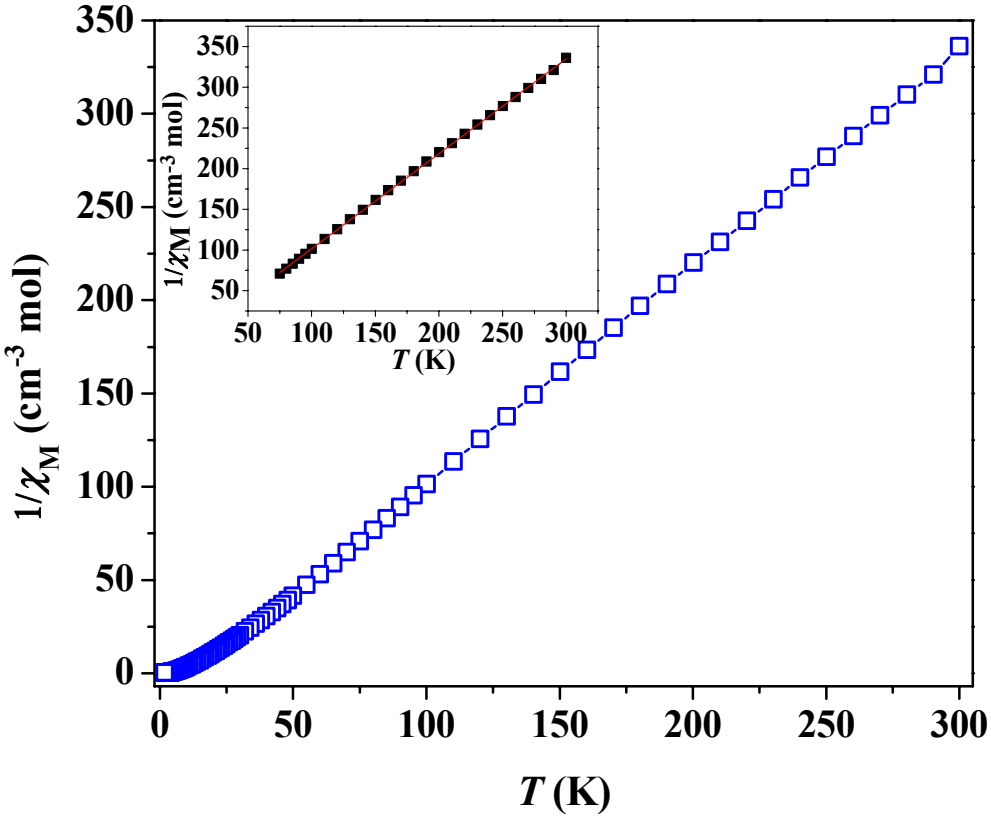

Fig. S10 Plot of temperature dependency of χ_M^{-1} for **4**. Inset shows the Curie-Weiss fitting in the temperature range 75 – 300 K.