Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

1D chains, 2D network and 3D interdigitated framework of isorotic acid with 4,4′-bipyridyl: Syntheses, structures, and sorption properties

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Table S1: Selected bond distances (Å) and angles (°) for $\{Cu(H_2iso)_2]\cdot 2H_2O\}_n$ (**1**).

Cu1-O1	1.939(5)	Cu1-O2	1.904(5)
Cu1-O3_a	2.705(5)	Cu1-O1_c	1.939(5)
Cu1-O2_c	1.904(5)	Cu1-O3_d	2.705(5)
O1-Cu1-O2	93.62(16)	O1-Cu1-O3_a	85.78(15)
O1-Cu1-O1_c	180.00	O1-Cu1-O2_c	86.38(16)
O1-Cu1-O3_d	94.22(15)	O2-Cu1-O3_a	95.19(19)
O1_c-Cu1-O2	86.38(16)	O2-Cu1-O2_c	180.00
O2-Cu1-O3_d	84.81(19)	O1_c-Cu1-O3_a	94.22(15)
O2_c-Cu1-O3_a	84.81(19)	O3_a-Cu1-O3_d	180.00
O1_c-Cu1-O2_c	93.62(16)	O1_c-Cu1-O3_d	85.78(15)
O2_c-Cu1-O3_d	95.19(19)		

Symmetry code: a = -1+x, y, z; c = 2-x, -y, 2-z; d = 3-x, -y, 2-z.

Table S2: Hydrogen bonds (Å,°) for $\{Cu(Hiso)_2]\cdot 2H_2O\}_n$ (**1**).

D-H···A	D-H	H···A	D···A	<D-H···A
O4-H2···N1^{i}	0.8200	2.1100	2.879(7)	156.00
C3-H1···O3	0.9300	2.4200	2.758(7)	101.00
C3-H1···OW^{ii}	0.9300	2.0800	2.960(9)	158.00

Symmetry code: i = 2-x, 1-y, 2-z; ii = 7/2-x, 1/2+y, 5/2-z

Table S3: Selected bond distances (Å) and angles (°) for $\{Mn(Hiso)(H_2O)_3\}_n$ (**2**).

Mn1-O1	2.207(2)	Mn1-O2	2.204(2)
Mn1-O3	2.198(2)	Mn1-N1	2.248(2)
O1-Mn1-O2	87.60(8)	O1-Mn1-O3	170.51(9)
O1-Mn1-N1	96.85(8)	O2-Mn1-O3	88.36(8)
O2-Mn1-N1	91.06(7)	O3-Mn1-N1	91.81(8)

Table S4 : Hydrogen bonds (Å°) for $\{Mn(Hiso)(H_2O)_3\}_n$ (**2**).

D-H···A	D-H	H···A	D···A	<D-H···A
O1-- H1···O4^{i}	0.72(4)	2.23(4)	2.936(3)	172(4)
O1-- H2···O2^{ii}	0.95(4)	1.90(4)	2.845(3)	177(4)
O2-- H3···O6^{iii}	0.85(4)	1.82(4)	2.655(3)	168(4)
O2-- H4···O6^{iv}	0.84(4)	1.86(4)	2.699(3)	174(4)
O3-- H5···O7^{v}	0.80(3)	1.97(4)	2.764(3)	171(3)
O3-- H6···O4	0.74(5)	1.99(5)	2.687(3)	158(5)
C3-- H7···O6	0.96(4)	2.43(3)	2.770(3)	100(2)

Symmetry Code: i = 3/2-x,-1/2+y,1/2-z; ii = 1+x,y,z; iii = 2-x,-y,-z; iv = -1+x,y,z; v = -3/2+x,1/2-y,1/2+z

Table S5 : Selected bond distances (Å) and angles (°) for $\{Mn(Hiso)(H_2O)_2\}_n$ (**3**).

Mn1-O1	2.176(3)	Mn1-O2	2.117(4)
Mn1-O3	2.130(3)	Mn1-O5	2.139(3)
O1-Mn1-O2	94.32(12)	O1-Mn1-O3	92.80(12)
O1-Mn1-O5	89.92(10)	O2-Mn1-O3	86.68(12)
O2-Mn1-O5	167.87(13)	O3-Mn1-O5	81.77(11)
Mn1_a-O6-Mn1_c	100.19(11)		

Symmetry code: a = 1/2+x,1/2-y,1-z; c = 5/2-x,1/2+y,z.

Table S6: Hydrogen bonds (Å,°) for $\{Mn(Hiso)(H_2O)_2\}_n$ (**3**).

D-H···A	D-H	H···A	D···A	<D-H···A
O1-H1···O4^{i}	0.90(4)	1.86(4)	2.738(4)	166(4)
O1-H2···O5^{ii}	0.67(4)	2.03(4)	2.700(4)	178(3)
O2-H3···O4^{iii}	1.03(10)	1.68(9)	2.683(4)	163(7)
O2-H4···O1^{iv}	0.60(4)	2.32(4)	2.884(5)	158(6)
C5-H5···O4	0.87(3)	2.45(3)	2.763(5)	102(2)

Symmetry code: i = 2-x,1/2+y,3/2-z; ii = 2-x,1-y,1-z; iii = 2-x,-1/2+y,3/2-z; iv = 2-x,-1/2+y,3/2-z.

Table S7: Selected bond distances (Å) and angles (°) for {[Ni(Hiso)(4,4′-bipy)]·0.5(4,4′-bipy)}$_n$ (**5**).

Ni1-O1	2.0221(16)	Ni2-O3	2.0606(16)
Ni1-O2	2.0122(15)	Ni2-O4	2.0865(17)
Ni1-N3	2.154(2)	Ni2 -N5	2.122(2)
Ni1-O1_b	2.0221(16)	Ni2 -O3_d	2.0606(16)
Ni1-O2_b	2.0122(15)	Ni2 -O4_d	2.0865(17)
O1-Ni1-O2	90.30(7)	O3 -Ni2 -O4	95.01(6)
O1-Ni1-N3	86.37(5)	O3-Ni2-N5	88.49(5)
O1-Ni1-O1_b	172.75(7)	O3-Ni2-O3_d	176.98(7)
O1-Ni1-O2_b	89.80(7)	O3-Ni2-O4_d	85.15(6)
O2 -Ni1-N3	90.77(4)	O4-Ni2 -N5	93.12(5)
O1_b-Ni1-O2	89.80(7)	O3_d-Ni2 -O4	85.15(6)
O2-Ni1-O2_b	178.46(6)	O4-Ni2-O4_d	173.77(7)
O1_b-Ni1-N3	86.37(5)	O3_d-Ni2-N5	88.49(5)
O2_b-Ni1-N3	90.77(4)	O4_d -Ni2-N5	93.12(5)
O1_b-Ni1-O2_b	90.30(7)	O3_d -Ni2 -O4_d	95.01(6)

Symmetry code: b = 1/2-x, y, 3/2-z; e = 3/2-x, y, 3/2-z; d = 3/2-x,y,3/2-z

Table S8: Hydrogen bonds (Å,°) for {[Ni(Hiso)(4,4′-bipy)]·0.5(4,4′-bipy)}$_n$ (**5**).

D-H···A	D-H	H···A	D···H	<D-H···A
C5-H5···O3	0.9300	2.41	2.764(3)	103.00
C5-H5···N2^{i}	0.9300	2.48	3.307(4)	149.00
C11-H11···O2^{ii}	0.9300	2.56	2.9604(4)	112.00
C12-H12···O3^{iii}	0.9300	2.47	3.0313(3)	147.00
C22-H22···O1^{iv}	0.9300	2.47	3.383(4)	155.00

Symmetry code: i = 1-x, 1-y, z; ii = x, 1+y, z; iii = 3/2-x,y,3/2-z; iv = 1/2+x,1-y,1/2+z

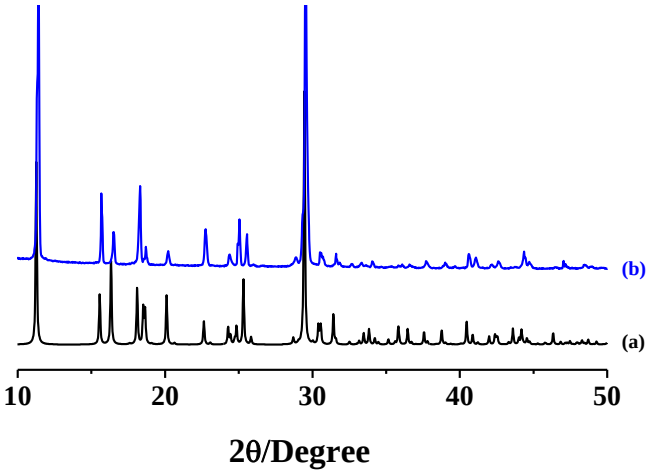

Fig. S1: PXRD patterns of compound **1** (a) simulated (b) as-synthesized.

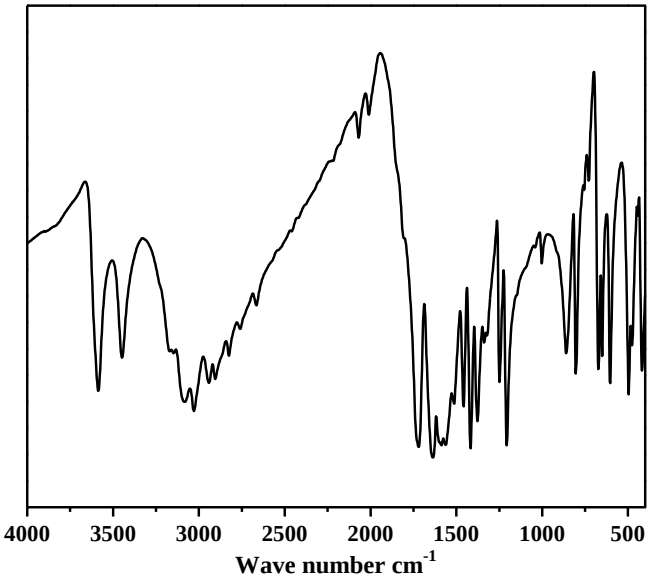

Fig. S2: FT-IR spectrum of compound **1**.

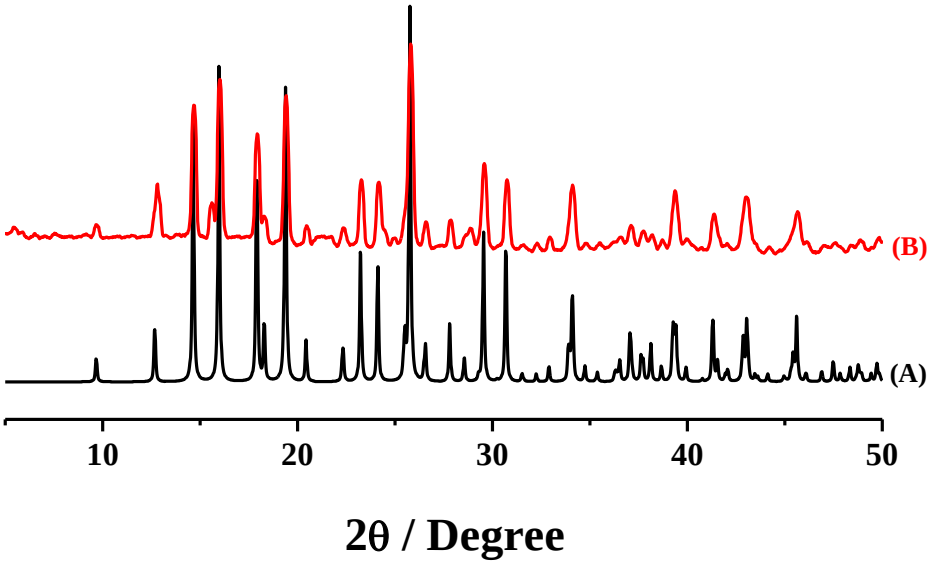

Fig. S3: PXRD patterns of compound **2** (A) simulated (B) as-synthesized.

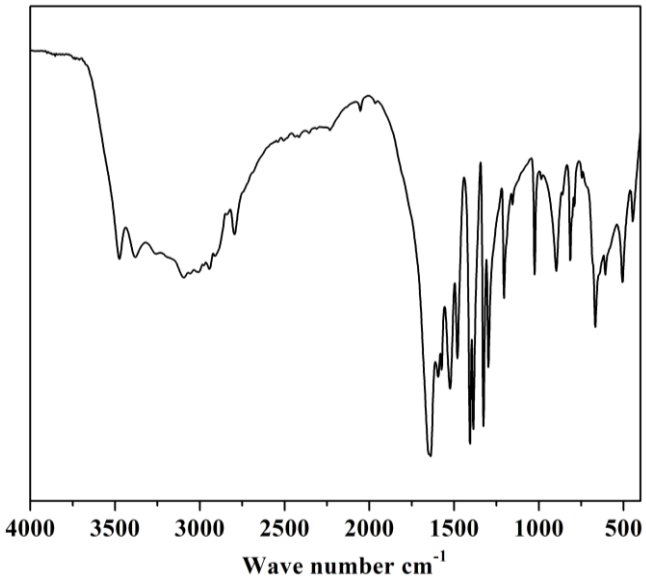

Fig. S4: FT-IR spectrum of compound **2**.

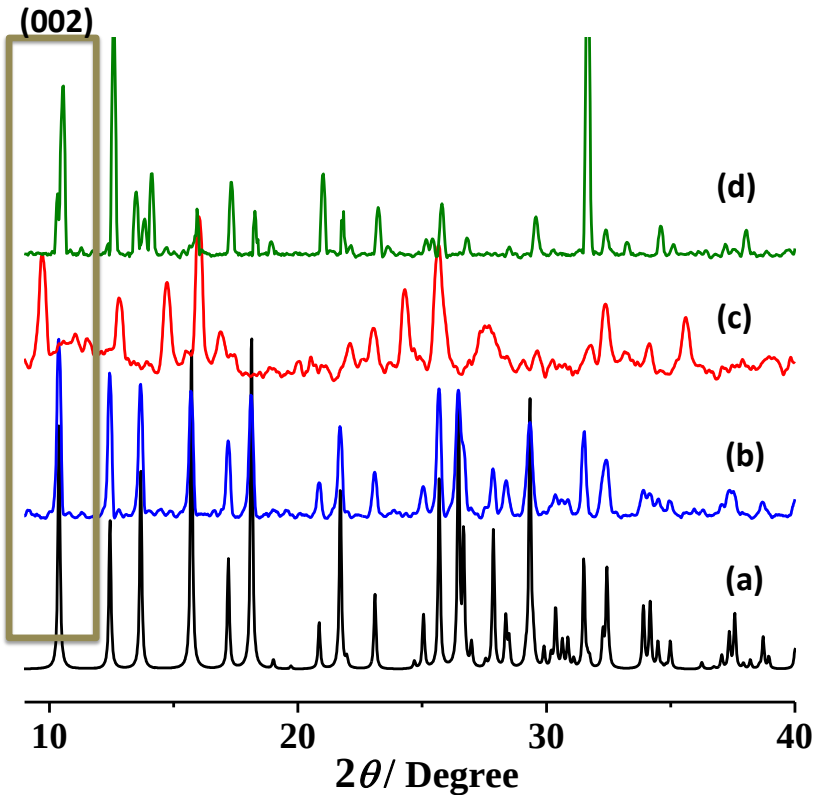

Fig. S5: PXRD patterns of compound **3** in different state; (a) simulated from X-ray single crystal data, (b) as-synthesized; (c) dehydrated at 250 °C and (d) rehydrated by exposing the water vapor for 72 h.

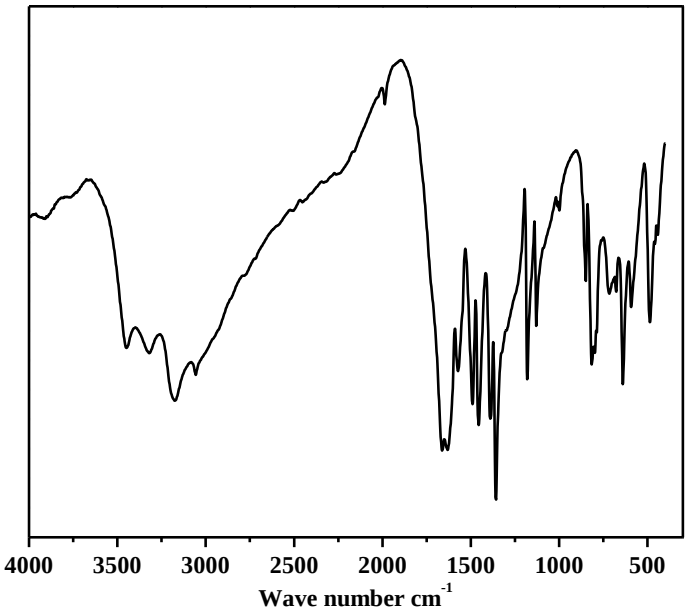

Fig. S6: FT-IR spectrum of compound **3**.

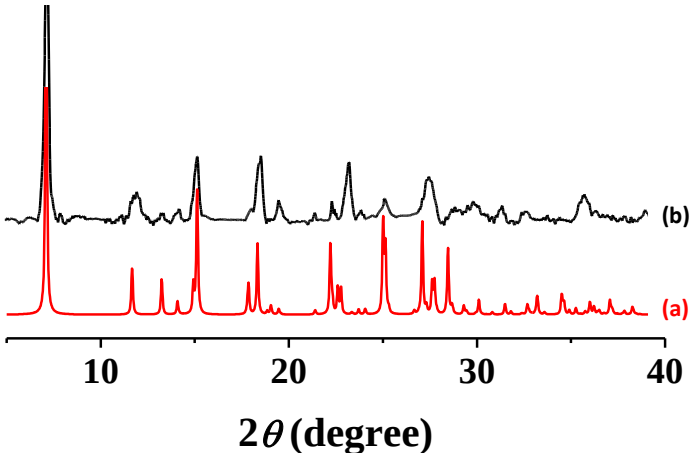

Fig. S7: PXRD patterns of compound **4** (a) simulated (b) as-synthesized.

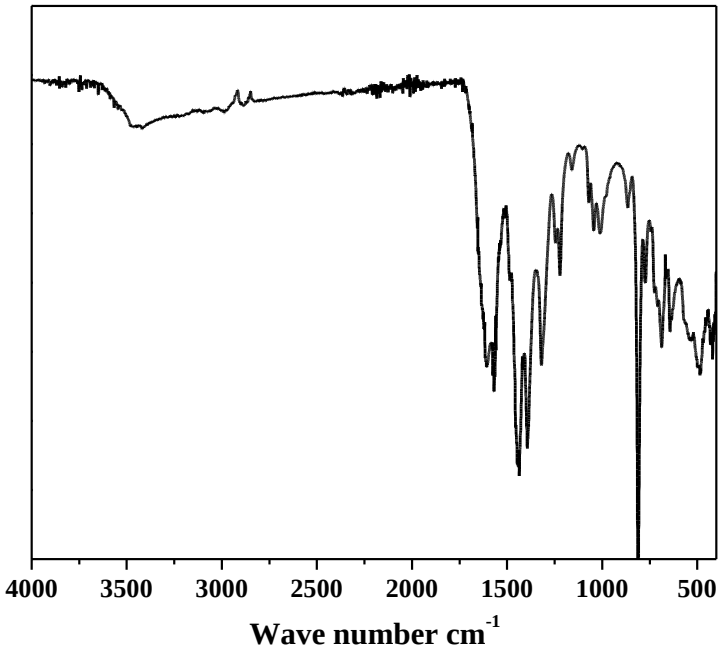

Fig. S8: FT-IR spectrum of compound **4**.

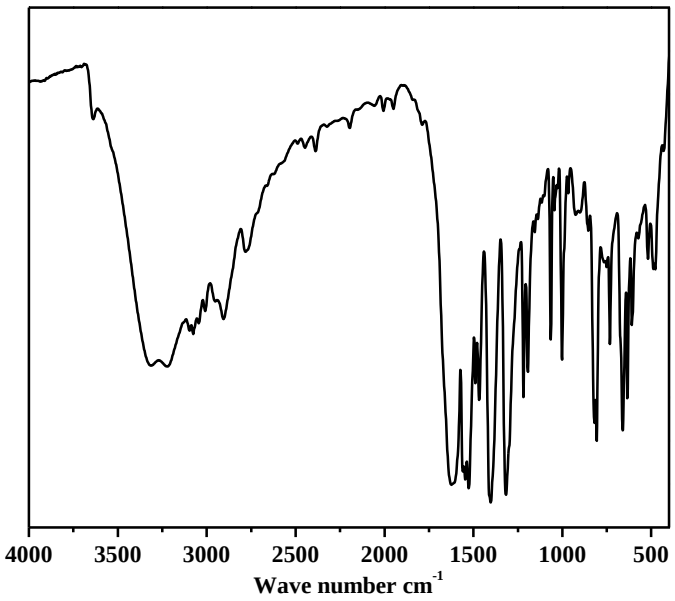

Fig. S9: FT-IR spectrum of compound **5**.

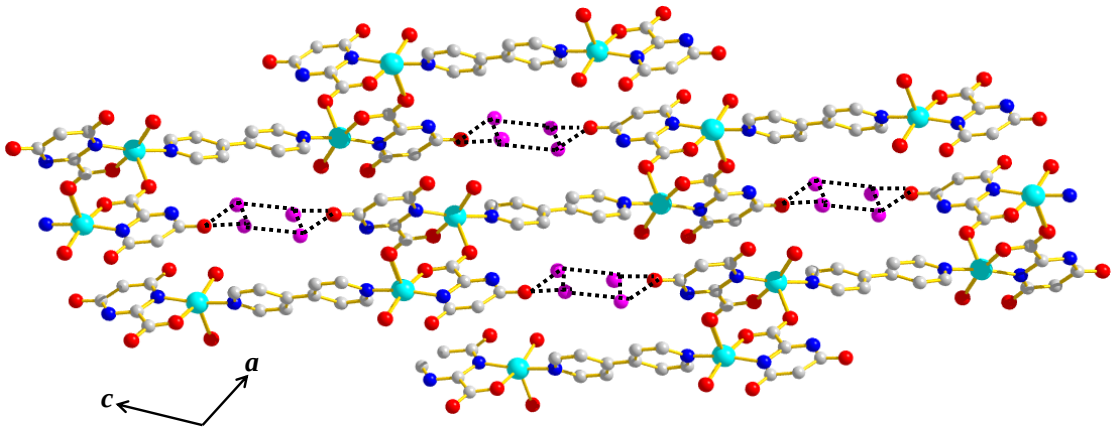

Fig. S10: Hydrogen bonding between the guest water molecules and the pendent oxygen of Hiso linker in compound **4**. Cyan: Cu, grey: C, blue: N, red: O.

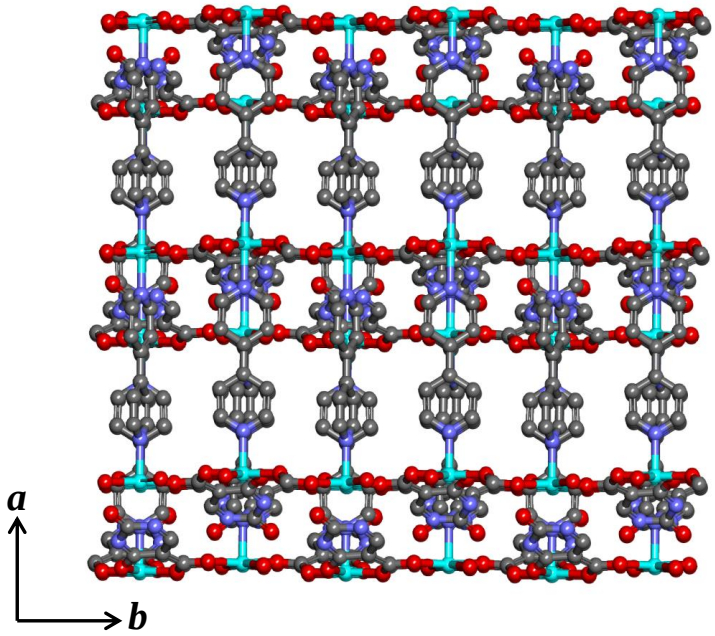

Fig. S11: View of the 2D rectangular grid of compound **5** along *c*-axis. Cyan: Ni, grey: C, blue: N, red: O.

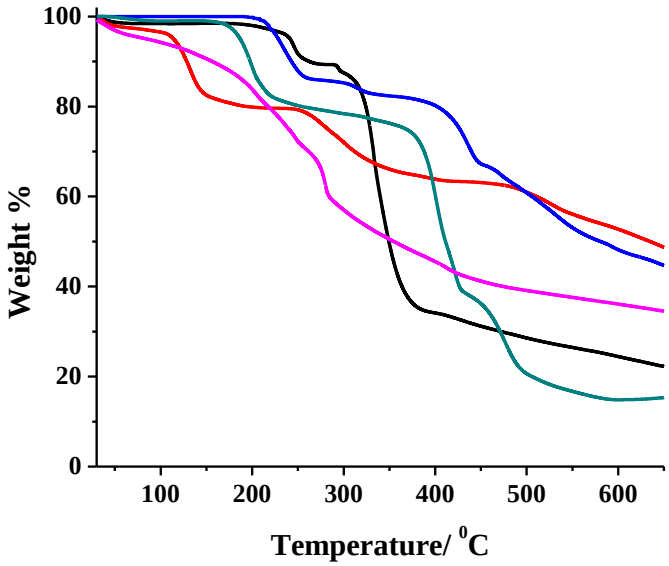

Fig. S12: TGA plot. Black: **1,** red: **2** , blue: **3**, pink: **4** and green: **5** over the temperature range from 25–600 °C at a heating rate of 3 °C/min under the N_2 atmosphere.

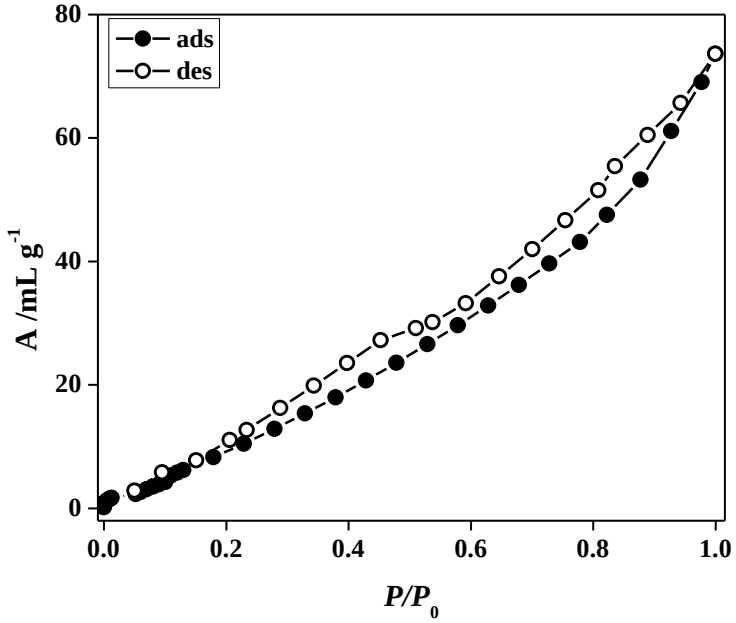

Fig. S13: N_2 Adsorption and desorption isotherms for **3′** at 77K.

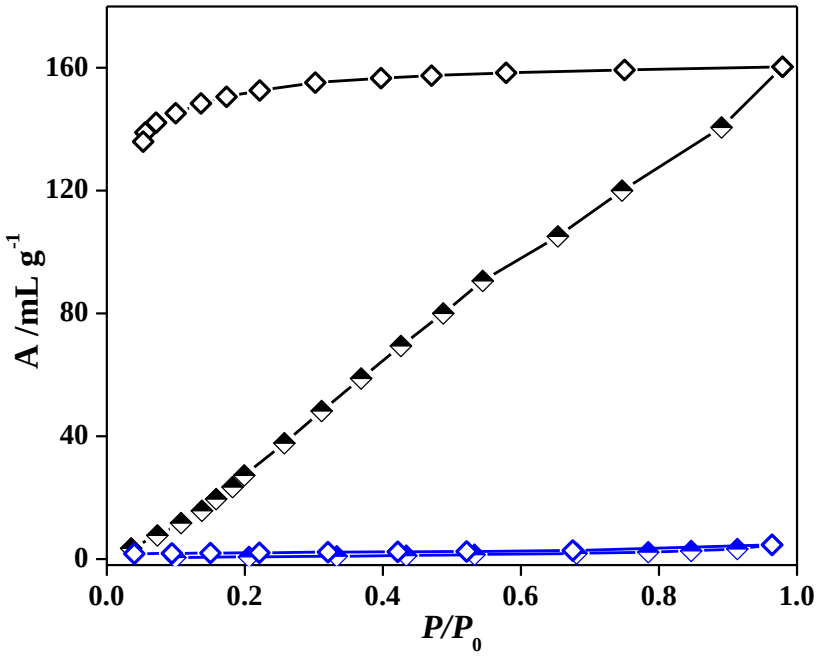

Fig. S14: Vapor sorption isotherm for **3′.** Black curve represents for water (298 K) and blue color curve represents for MeOH (293 K).

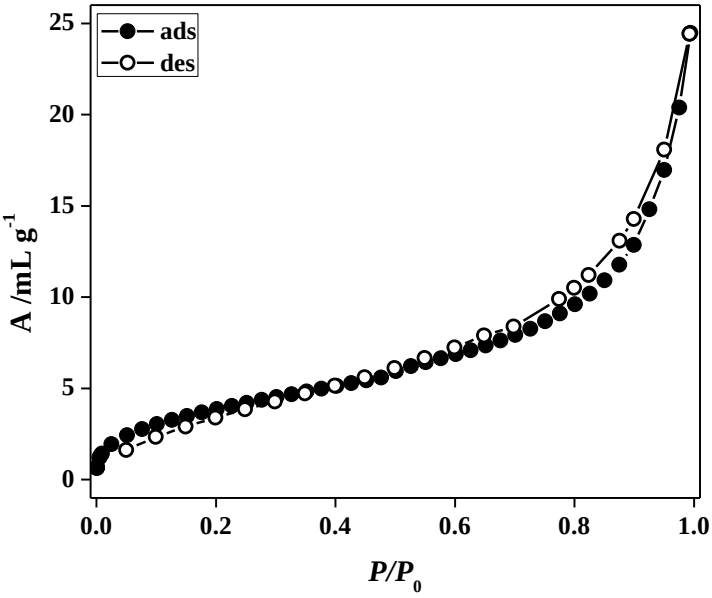

Fig. S15: N_2 Adsorption and desorption isotherms for **5′**.

Indexing result of the powder pattern of compound 5′

Cell parameters : a = 10.81057 (9) Å, b = 10.81057 (4) Å, c = 15.02864 (6) Å , V = 1756.73(6)Å^3

H	K	L	SST-OBS	SST-CALC	DELTA	2TH-OBS	2TH-CALC	D-OBS	FREE PARAM.
			.004648			7.818		11.2989	28
0	0	2	.010512	.010508	.000004	11.770	11.768	7.5130	50
2	0	1	.022983	.022936	.000047	17.440	17.421	5.0811	57
2	1	1	.028085	.028013	.000072	19.295	19.270	4.5965	76
1	0	4	.047129	.047111	.000018	25.077	25.072	3.5482	82
3	0	2	.056097	.056203	.000106	27.401	27.428	3.2523	100
4	0	0	.081259	.081235	.000024	33.125	33.120	2.7022	0

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LOUER, D. & LOUER, M. (1972). J. APPL. CRYST. 5, 271-275.
BOULTIF, A. & LOUER, D. (1991). J. APPL. CRYST. 24, 987-993.