Structural Characterization and Solvent Vapor Sorption of Two Solvent-Dependent Zn(II) Supramolecular Architectures Based on a Flexible Tripodal Thioether-based Pyridyl Ligand and a Dicarboxylate-based Ligand

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5.516%.

Figure S5 (a) N_2 ad-/desorption isotherms of dehydrated species **1** at 77 K. (b) N_2 ad-/desorption isotherms of dehydrated species **2** at 77 K.

Table S1. Selected bond lengths (Å) and angle (°) around Zn(II) ion for **1**[a]

Zn(1)─O(1)	2.082(3)	Zn(2)─N(3)	2.038(4)
Zn(1)─O(1)#1	2.082(3)	Zn(2)─N(2)#2	2.048(4)
Zn(1)─N(1)	2.142(3)	Zn(2)─Cl(2)	2.2149(14)
Zn(1)─N(1) #1	2.142(3)	Zn(2)─Cl(1)	2.2211(14)
Zn(1)─O(4)	2.159(3)		
Zn(1)─O(4)#1	2.159(3)		
O(1)-Zn(1)-O(1)#1	180.0	O(1)#1-Zn(1)-O(4)#1	87.87(12)
O(1)-Zn(1)-N(1)#1	89.22(13)	N(1)#1-Zn(1)-O(4)#1	87.39(13)
O(1)#1-Zn(1)-N(1)#1	90.78(13)	N(1)-Zn(1)-O(4)#1	92.61(13)
O(1)-Zn(1)-N(1)	90.78(13)	O(4)-Zn(1)-O(4)#1	180.0
O(1)#1-Zn(1)-N(1)	89.22(13)	N(3)-Zn(2)-N(2)#2	100.00(18)
N(1)#1-Zn(1)-N(1)	180.0	N(3)-Zn(2)-Cl(2)	107.13(13)
O(1)-Zn(1)-O(4)	87.87(12)	N(2)#2-Zn(2)-Cl(2)	109.32(14)
O(1)#1-Zn(1)-O(4)	92.13(12)	N(3)-Zn(2)-Cl(1)	108.37(13)
N(1)#1-Zn(1)-O(4)	92.61(13)	N(2)#2-Zn(2)-Cl(1)	104.10(14)
N(1)-Zn(1)-O(4)	87.39(13)	Cl(2)-Zn(2)-Cl(1)	125.11(6)
O(1)-Zn(1)-O(4)#1	92.13(12)		

Symmetry transformations used to generate equivalent atoms:
#1 -x+2, -y, -z #2 -x-1,-y,-z+1 #3 –x+2, -y-1, -z

Table S2. The parameters of O–H···O and O–H···Cl hydrogen bonds for **1**[a]

D–H (Å)	D···A(Å)	H···A(Å)	∠ D–H···Acceptor(°)
O(3)–H(3)	O(3)···O(2)	H(3)···O(2)	∠ O(3)–H(3)···O(2)
0.840	2.543	1.811	144.6
O(4)–H(4)	O(4)···$O(2)_i$	H(4)···$O(2)_i$	∠ O(4)–H(4)···$O(2)_i$
0.883	2.633	1.800	144.6
O(5)–H(5)	O(5)···O(6)	H(5)···O(6)	∠ O(5)–H(5)···O(6)
0.840	2.792	2.181	129.6
O(7)–H(7)	O(7)···O(5)	H(7)···O(5)	∠ O(7)–H(7)···O(5)
0.840	2.677	2.204	115.6
O(6)–H(6)	O(6)···Cl(2)	H(6)···Cl(2)	∠ O(6)–H(6)···Cl(2)
0.840	3.207	2.417	157.0

[a]Symmetry operations used to generate equivalent atoms: (i) -x+5/2, y+1/2, -z+1/2;

Table S3. Selected bond lengths (Å) and angle (°) around Zn(II) ion for **2**[a]

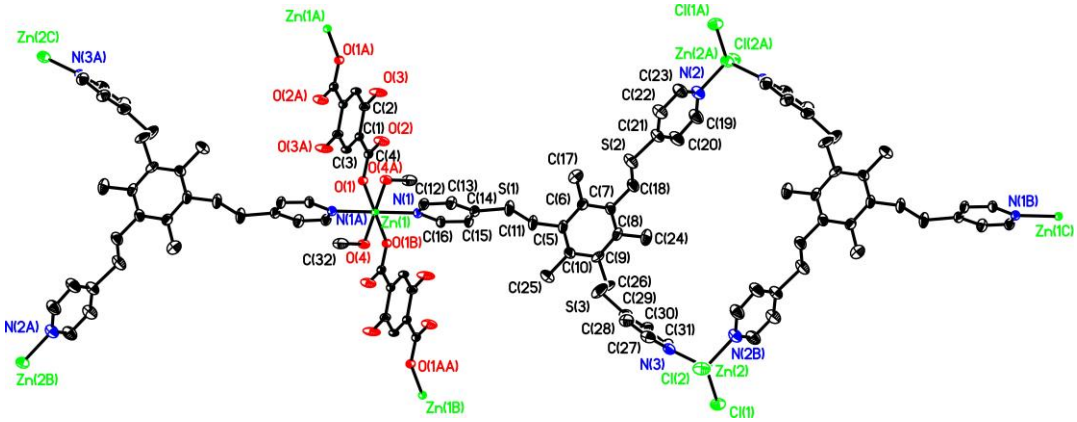
Zn(1)-O(4)	2.104(4)	Zn(1)-N(3)#1	2.155(12)
Zn(1)-O(1)	2.116(3)	Zn(1)-N(2)#2	2.179(5)
Zn(1)-O(7)	2.131(4)	Zn(1)-N(1)	2.151(5)
O(4)-Zn(1)-O(1)	87.07(15)	O(7)-Zn(1)-N(3)#1	82.80(3)
O(4)-Zn(1)-O(7)	91.94(15)	N(1)-Zn(1)-N(3)#1	98.20(3)
O(1)-Zn(1)-O(7)	91.61(15)	O(4)-Zn(1)-N(2)#2	172.38(17)
O(4)-Zn(1)-N(1)	85.86(16)	O(1)-Zn(1)-N(2)#2	87.42(16)
O(1)-Zn(1)-N(1)	87.26(16)	O(7)-Zn(1)-N(2)#2	93.46(18)
O(7)-Zn(1)-N(1)	177.57(16)	N(1)-Zn(1)-N(2)#2	88.64(19)
O(4)-Zn(1)-N(3)#1	90.60(3)	N(3)#1-Zn(1)-N(2)#2	95.40(3)
O(1)-Zn(1)-N(3)#1	173.90(3)		

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

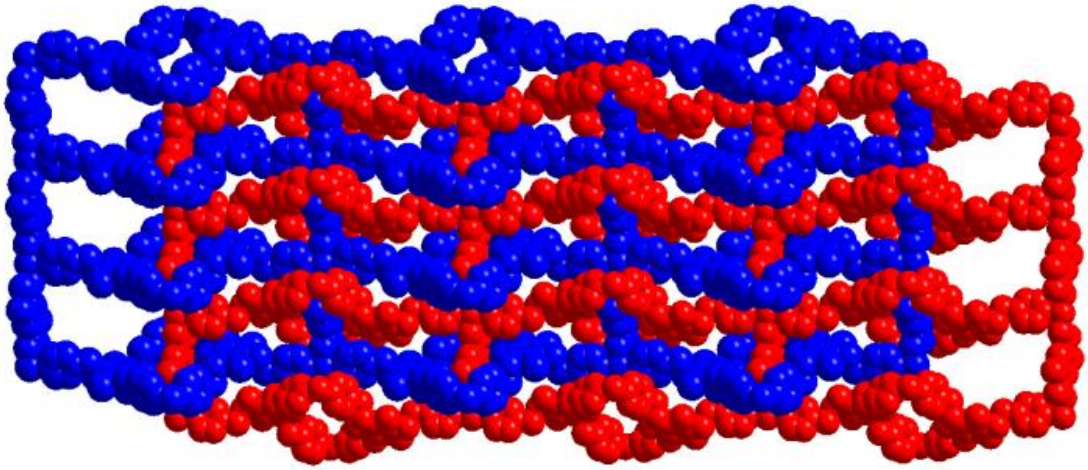
Table S4. The parameters of O–H···O hydrogen bonds for **2**[a]

D–H (Å)	D···A(Å)	H···A(Å)	∠ D–H···Acceptor(°)
O(1S)–H(1S)	O(1S)···O(3S)$_{i}$	H(1S)···O(3S)$_{i}$	∠ O(1S)–H(1S)···O(3S)$_{i}$
0.840	2.879	2.243	132.5
O(2S)–H(2S)	O(2S)···O(6)$_{ii}$	H(2S)···O(6)$_{ii}$	∠ O(2S)–H(2S)···O(6)$_{ii}$
0.840	2.680	1.840	163.0
O(3)–H(3)	O(3)···O(2)	H(3)···O(2)	∠ O(3)–H(3)···O(2)
0.839	2.541	1.791	148.0
O(3S)–H(3S)	O(3S)···O(3)$_{iii}$	H(3S)···O(3)$_{iii}$	∠ O(3S)–H(3S)···O(3)$_{iii}$
0.840	2.789	2.056	145.5
O(6)–H(6)	O(6)···O(2S)$_{iv}$	H(6)···O(2S)$_{iv}$	∠ O(6)–H(6)···O(2S)$_{iv}$
0.839	2.655	1.921	145.4
O(7)–H(7A)	O(7)···O(2)	H(7A)···O(2)	∠ O(7)–H(7A)···O(2)
0.815	2.709	1.899	172.5
O(7)–H(7B)	O(7)···O(5)	H(7B)···O(5)	∠ O(7)–H(7B)···O(2)
0.824	2.702	2.010	141.3

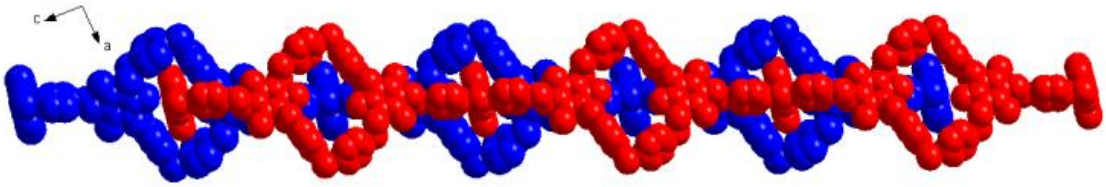
[a]Symmetry operations used to generate equivalent atoms:
(i) -x+1, y+3/2, -z+3/2; (ii) x, y, z–1; (iii) –x+2, y+3/2, -z+5/2; (iv) x, y, z+1.



(a)

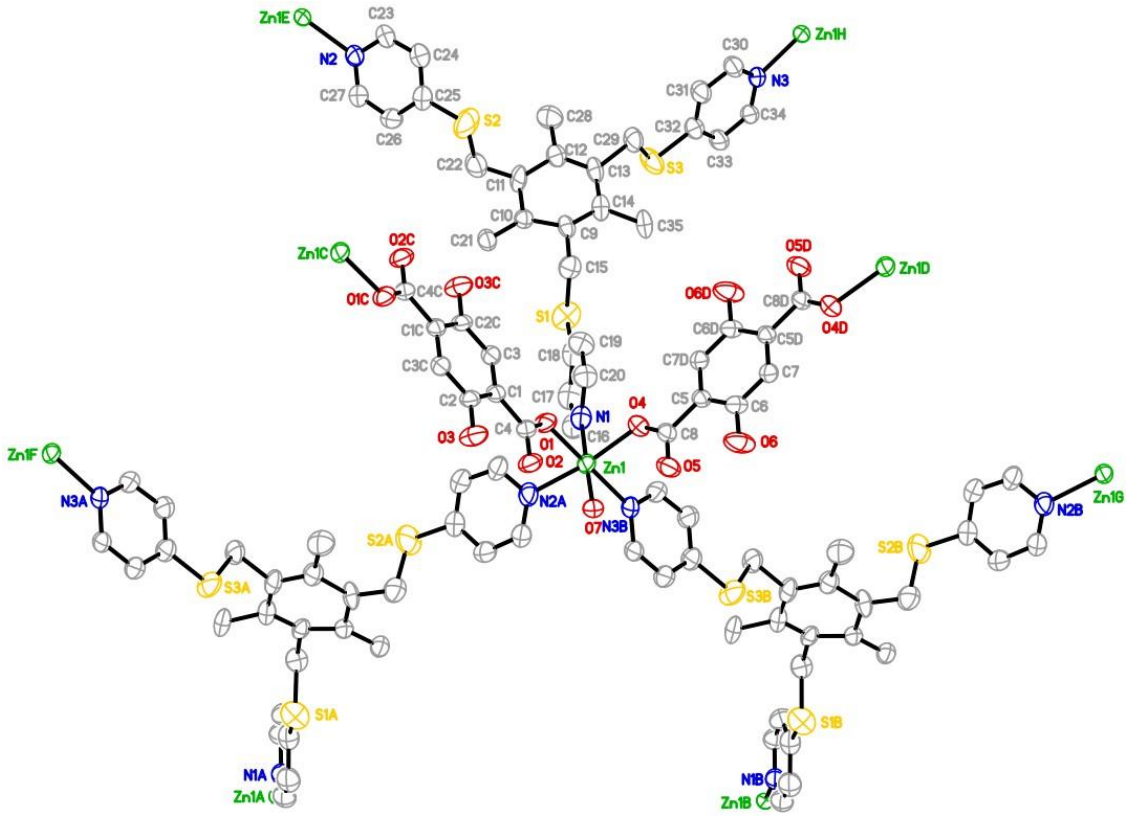


(b)

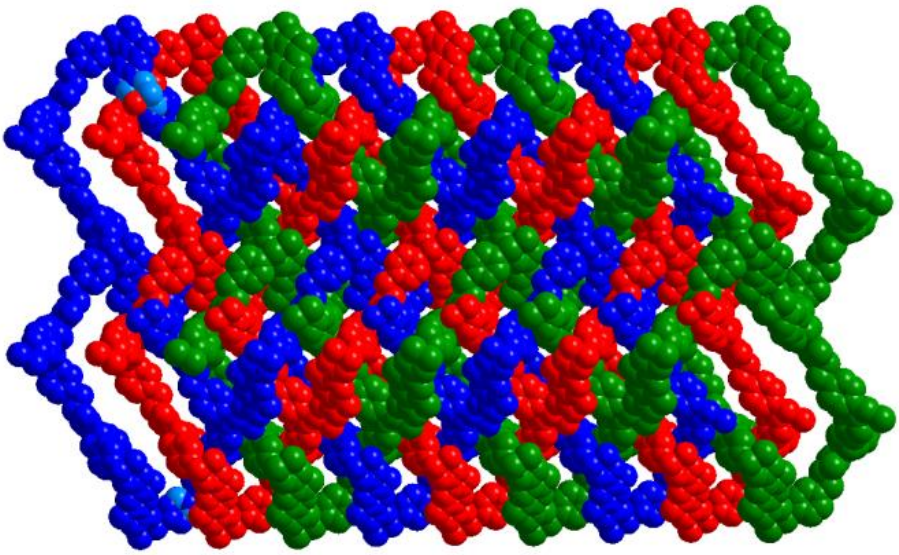


(c)

Figure S1. (a) Coordination environments about Zn(II) ion in $[Zn_3(L^1)_2(L^2)(Cl)_4(CH_3OH)_2]\cdot 6CH_3OH$ (**1**) with atom labelling scheme (ORTEP drawing, 50 % thermal ellipsoids). Hydrogen atoms and guest CH_3OH molecules are omitted for clarity. (b) The 2D doubly-interpenetrating network with space-filling mode; (c) The 2D doubly-interpenetrating network with space-filling mode viewing along the *b* axis.

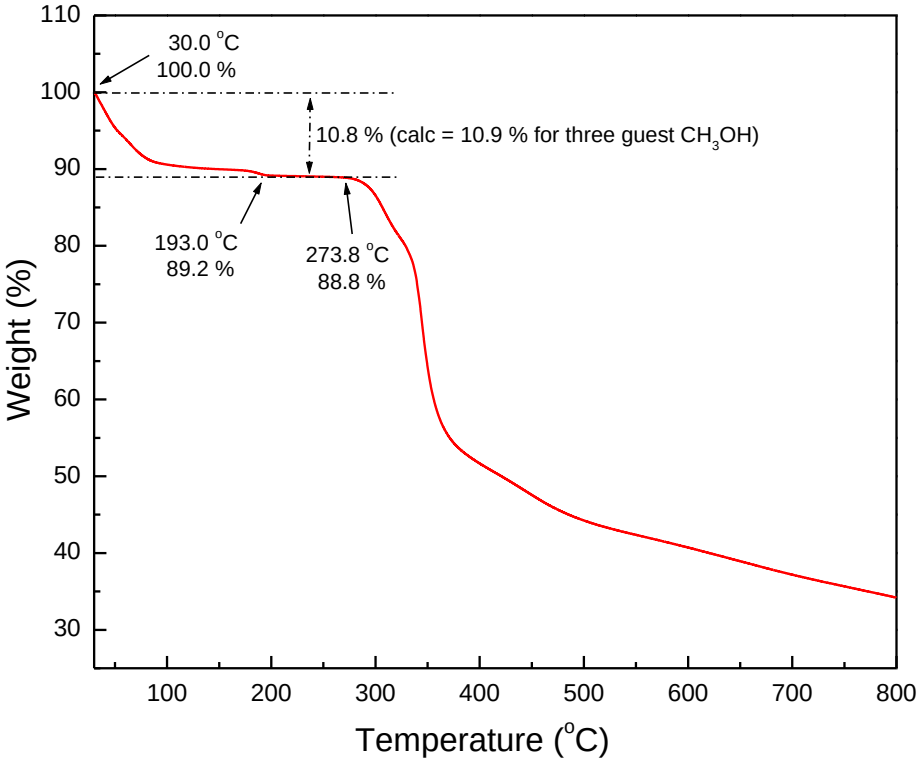


(a)

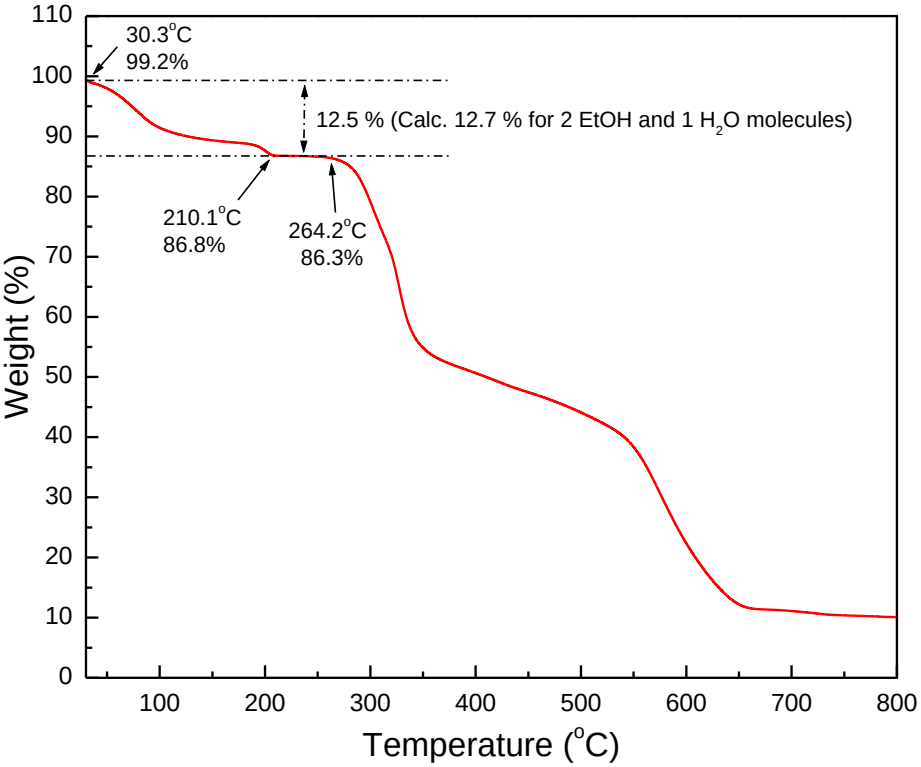


(b)

Figure S2. (a) Coordination environments about Zn(II) ion in $[Zn(L^1)(L^2)(H_2O)]\cdot 2C_2H_5OH$ (**2**) with atom labelling scheme (ORTEP drawing, 30 % thermal ellipsoids). Hydrogen atoms and guest C_2H_5OH molecules are omitted for clarity. (b) The triply-interpenetrating 3D supramolecular architecture with space-filling mode.

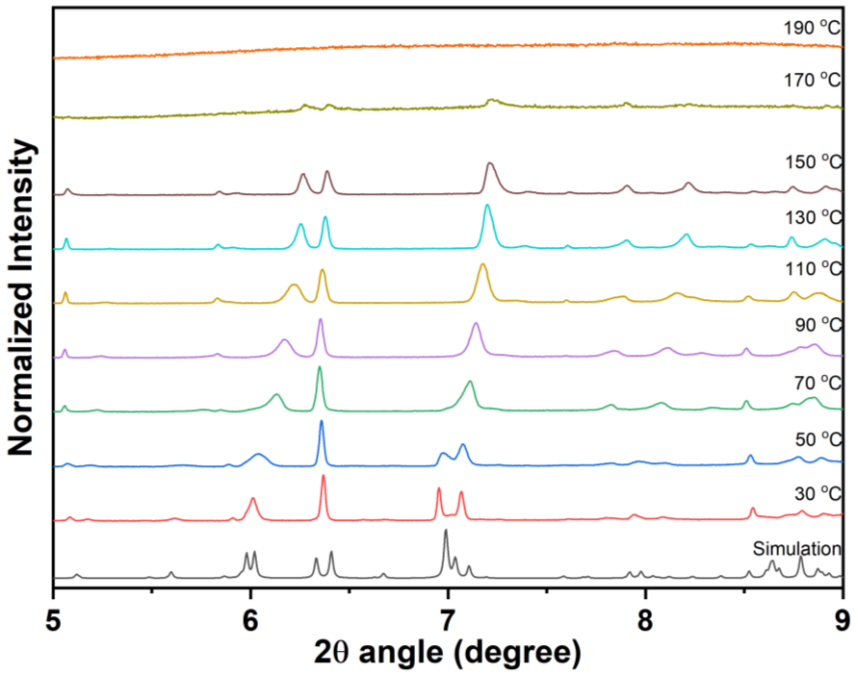


(a)

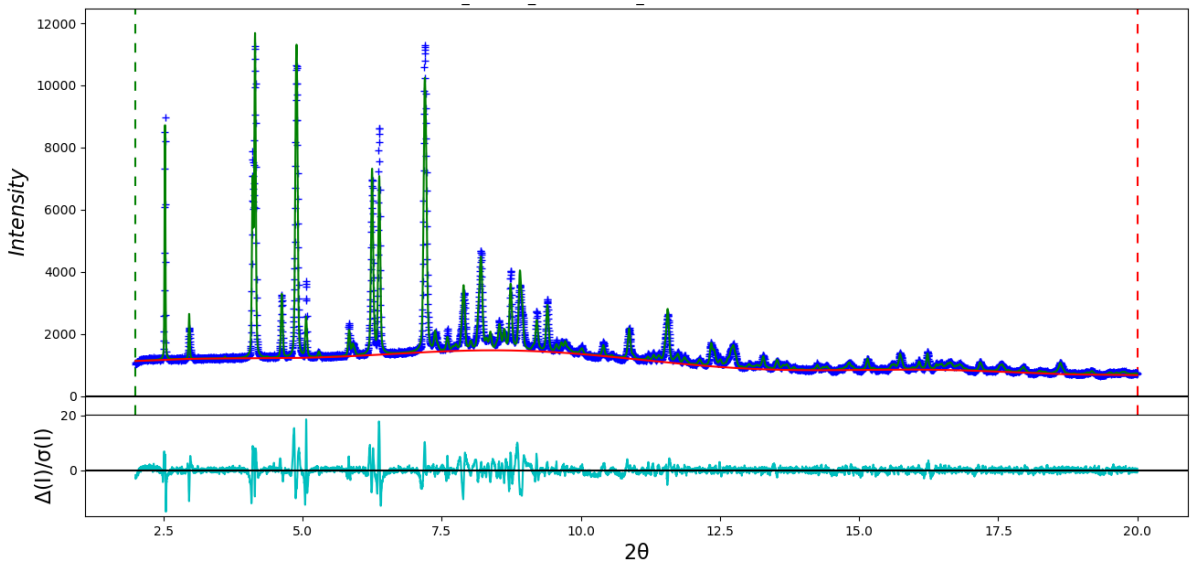


(b)

Figure S3. Thermogravimetric (TG) measurement of (a) **1** and (b) **2**.

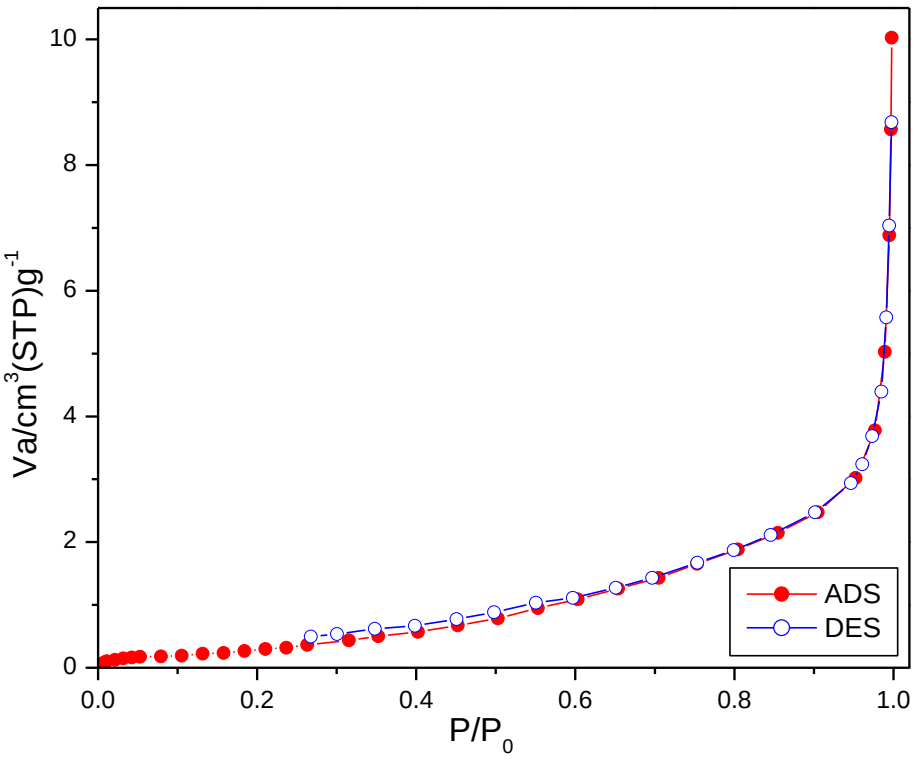


(a)

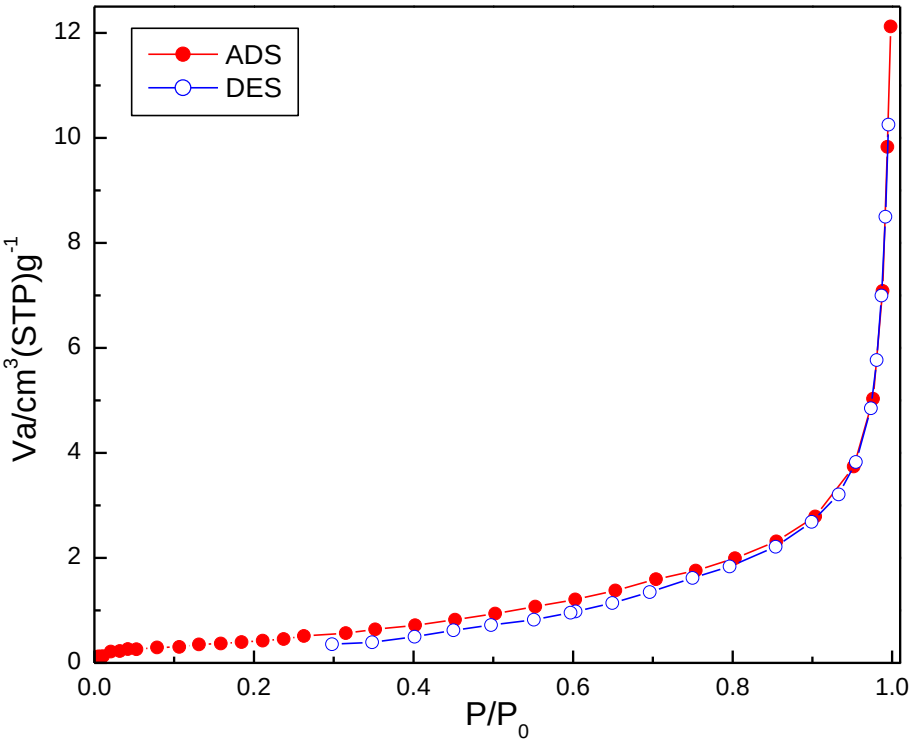


(b)

Figure S4. (a) Enlarge in-situ XRD powder diffraction patterns of **1**, (b) The Le Bail refinement of 130 °C de-hydrated form of sample **2** and agreement factor R_{wp} is 5.516%.



(a)



(b)

Figure S5. N_2 ad-/desorption isotherms of (a) dehydrated species **1** and (b) dehydrated species **2** at 77 K.