Electronic supplementary information (ESI)

Zinc(II) coordination polymers with substituted benzenedicarboxylate and tripodal imidazole ligands: syntheses, structures and properties

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Table S1 Hydrogen bonding data for complexes **2-4**.

Complex **2**				
D–H ··A	d(*D*–H) (Å)	d(H ··A) (Å)	d(*D* ··A) (Å)	∠*D*–H ··A (°)
O7W–H7WB ··O2W#1	0.97	2.02	2.935(6)	156
O1W–H1WA ··O1#2	0.82	1.92	2.700(5)	160
O1W–H1WB ··O5#3	0.89	1.72	2.593(5)	165
C1–H1 ··O6W#4	0.93	2.40	3.310(6)	166
C9–H9 ··O6W#4	0.93	2.34	3.235(6)	161
O2W–H2WA ··O4W#4	0.82	2.05	2.788(5)	150
O2W–H2WB ··O3W#5	0.96	1.90	2.849(5)	174
O6W–H6WB ··O5#6	0.97	1.93	2.867(6)	163
O3W–H3WA ··O7W#7	0.90	1.98	2.808(6)	151
O4W–H4WA ··O7W#8	0.95	1.85	2.752(6)	158
O4W–H4WB ··O3#9	0.95	1.87	2.813(5)	173
O5W–H5WA ··O8#10	0.89	1.88	2.759(6)	171
C12–H12 ··O7#11	0.93	2.34	2.961(6)	124

Symmetry codes: #1 1-x, -y, 1-z; #2 2-x, 1-y, 1-z; #3 2-x, -y, 1-z; #4 x, -1+y, z; #5 1-x, -y, -z; #6 x, 1+y, z; #7 1-x, 1-y, 1-z; #8 x, y, -1+z; #9 1-x, 1-y, -z; #10 -1+x, 1+y, z; #11 -1+x, y, z.

Complex **3**

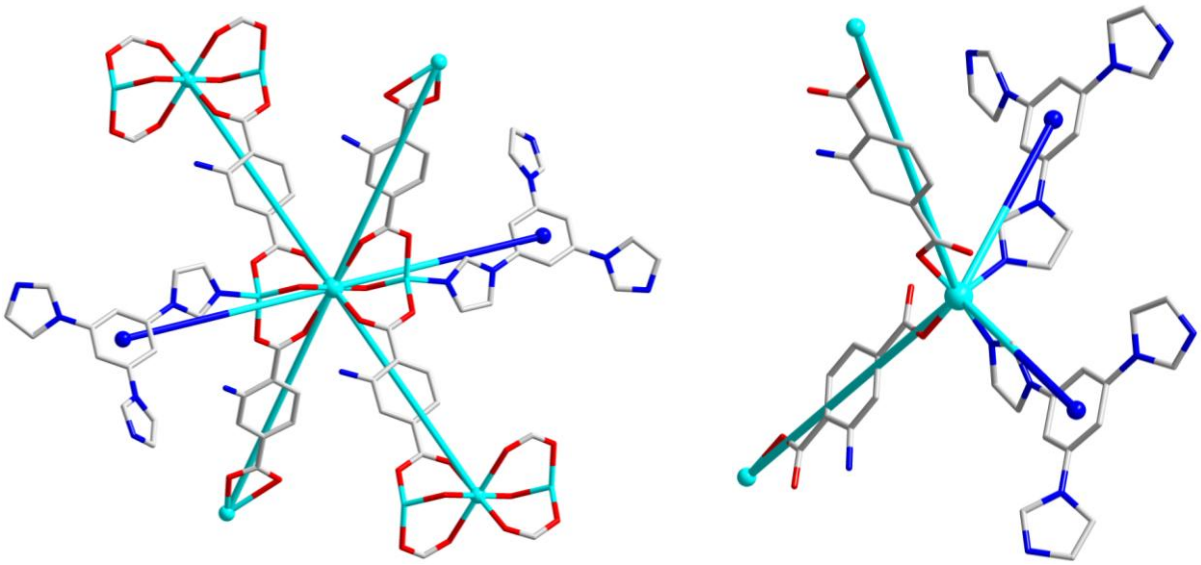
D–H ··A	d(*D*–H) (Å)	d(H ··A) (Å)	d(*D* ··A) (Å)	∠*D*–H ··A (°)
O(4)–H(4A) ··N(5)#1	1.05	1.52	2.573(4)	178
C(3)–H(3) ··O(7)#2	0.93	2.50	3.351 (4)	151
C(9)–H(9) ··O(7)#2	0.93	2.53	3.341 (4)	146
C(12)–H(12) ··O(2)#2	0.93	2.36	3.261 (4)	164
C(13)–H(13) ··O(3)#2	0.93	2.58	3.178(4)	123

Symmetry codes: #1 1+x, 1/2-y, -1/2+z; #2 x, 1/2-y, 1/2+z.

Complex **4**

D–H ··A	d(*D*–H) (Å)	d(H ··A) (Å)	d(*D* ··A) (Å)	∠*D*–H ··A (°)
C(12)–H(12) ··O(7)#1	0.93	2.41	3.312(4)	163
C(3)–H(3) ··N(5)#2	0.93	2.40	3.306(3)	166
C(5)–H(5) ··O(5)#3	0.93	2.55	3.481(3)	178
C(9)–H(9) ··O(5)#4	0.93	2.58	3.492(4)	168
C(1)–H(1) ··O(7)#5	0.93	2.60	3.524(4)	173

Symmetry codes: #1 1-x, 1-y, 1-z; #2 3/2-x, -1/2+y, 3/2-z; #3 2-x, 1-y, 1-z; #4 3/2-x, 1/2+y, 3/2-z; #5 1/2-x, 1/2+y, 3/2-z.



(a) (b)

Fig. S1 (a) The 6-connected node of $Zn_3(OCO)_4(\mu_2\text{-}OH)_2$ in **1**. (b) The 4-connected node of Zn1 building unit in **1**.

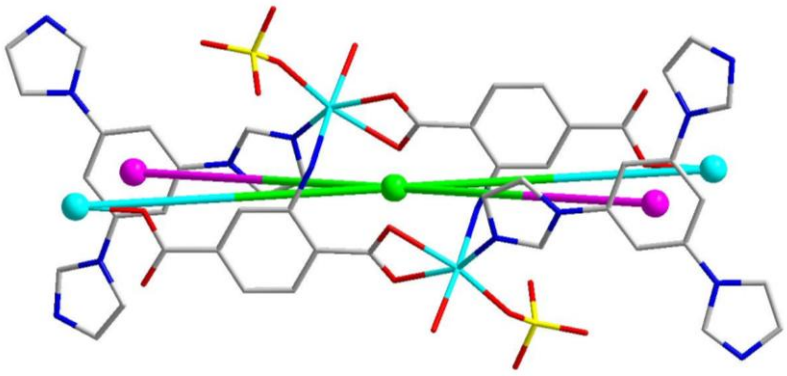
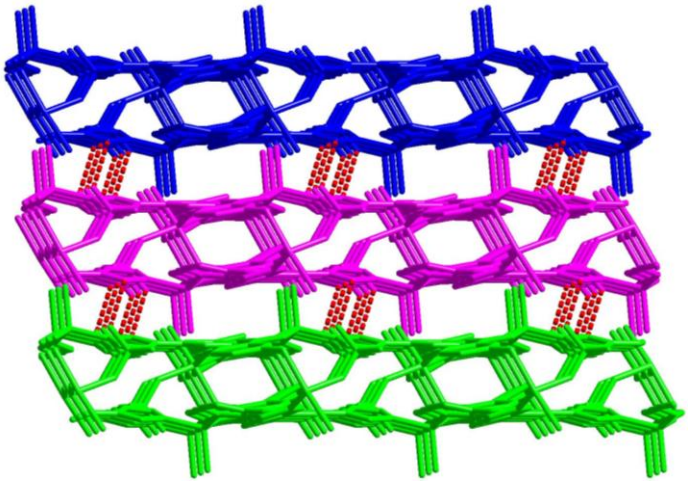
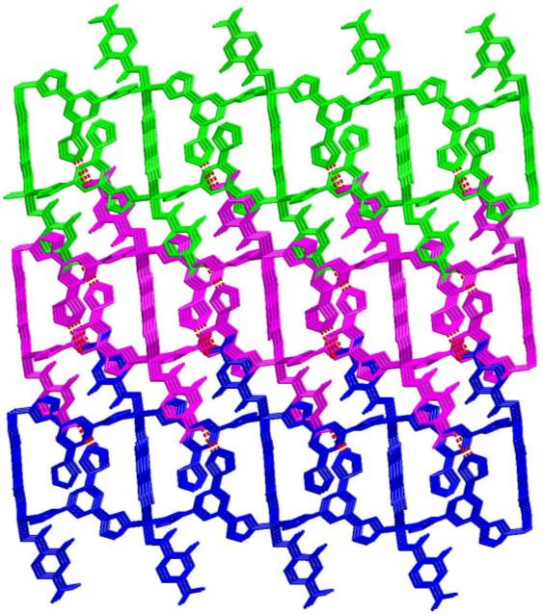
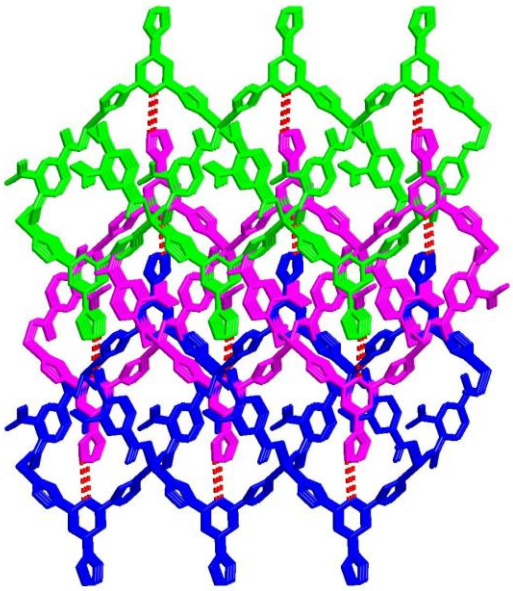


Fig. S2 The 4-connected node of $Zn_2(BDC\text{-}NH_2)_2$ building unit in **2**.



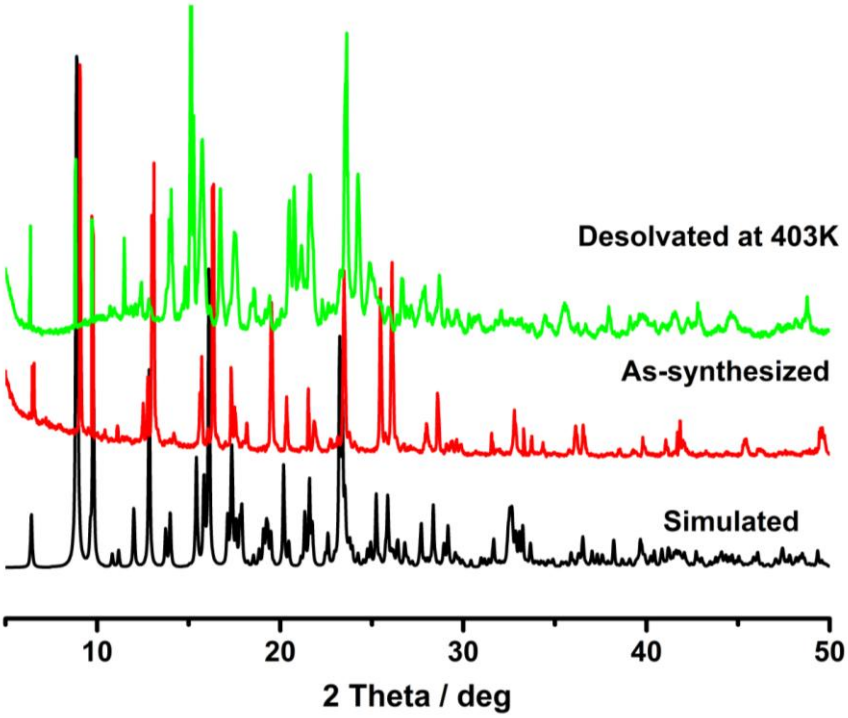
(a)



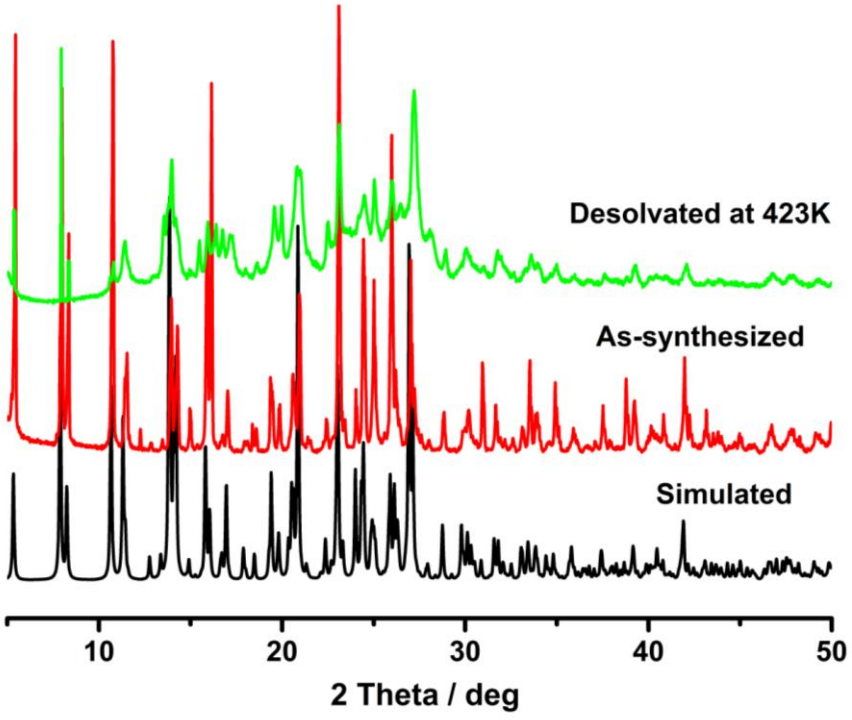


(b) (c)

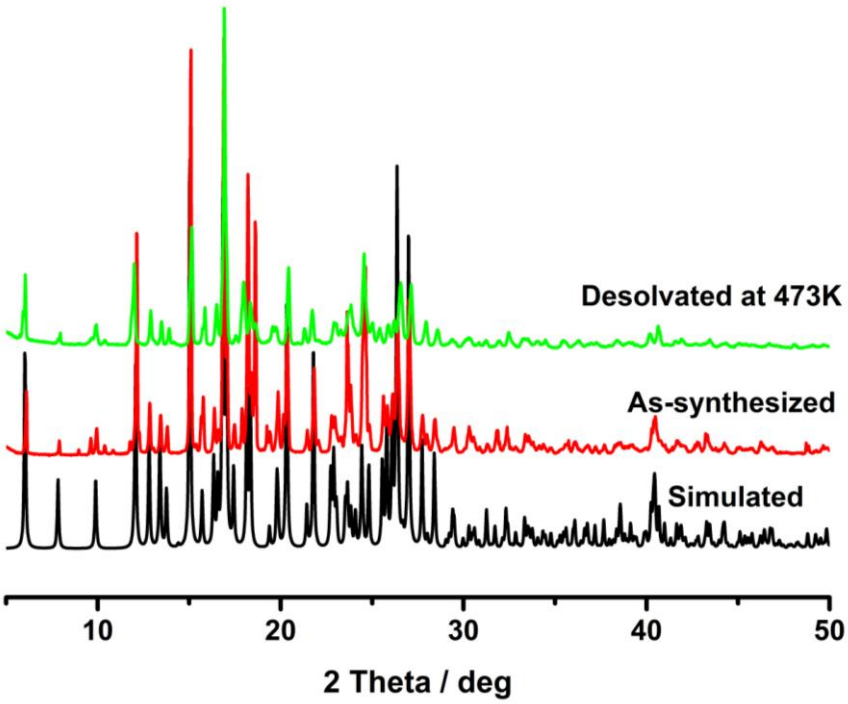
Fig. S3 The 2D layers are further held by C12-H12 ··O7, O4-H4A ··N5 and C3-H3 ··N5 hydrogen bonds respectively to obtain 3D supramolecular structures of **2** (a), **3** (b) and **4** (c): different colors indicate the different layers. The hydrogen bonds are indicated by the red dashed lines.


Desolvated at 403K
As-synthesized
Simulated
10
20
30
40
50
2 Theta / deg

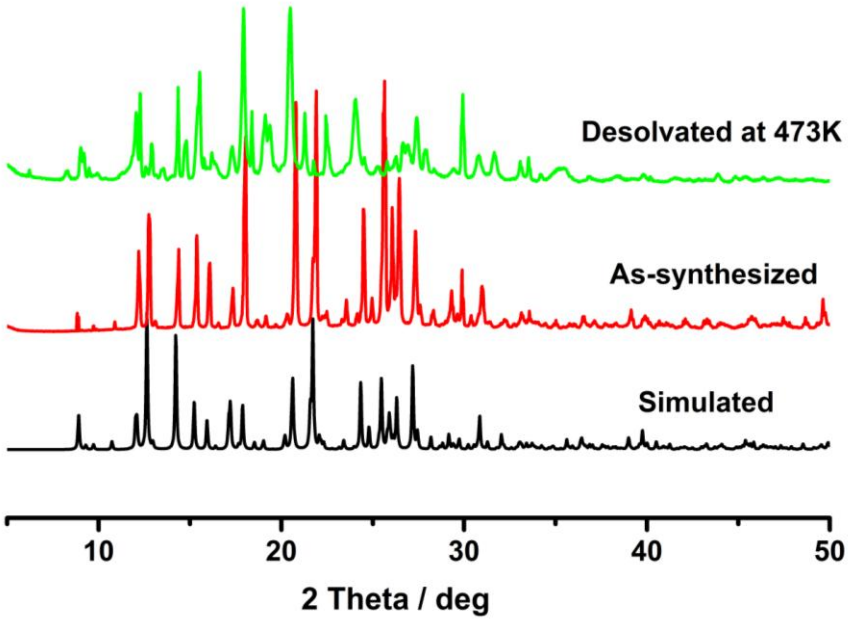
(a)


Desolvated at 423K
As-synthesized
Simulated
10
20
30
40
50
2 Theta / deg

(b)

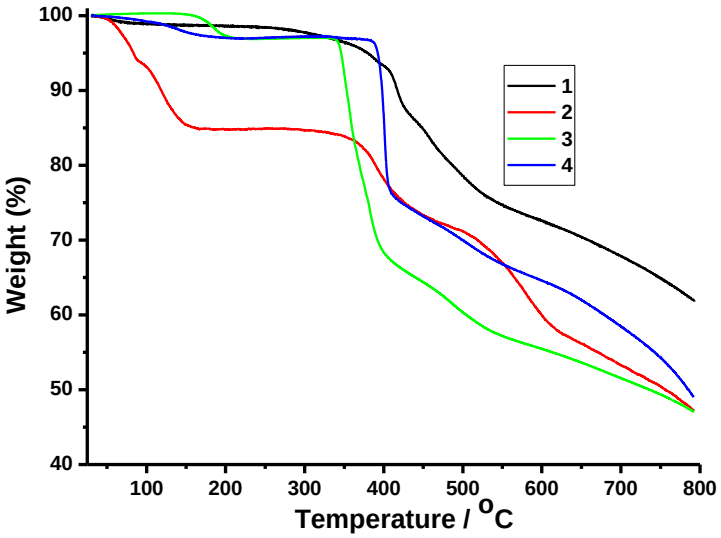


(c)

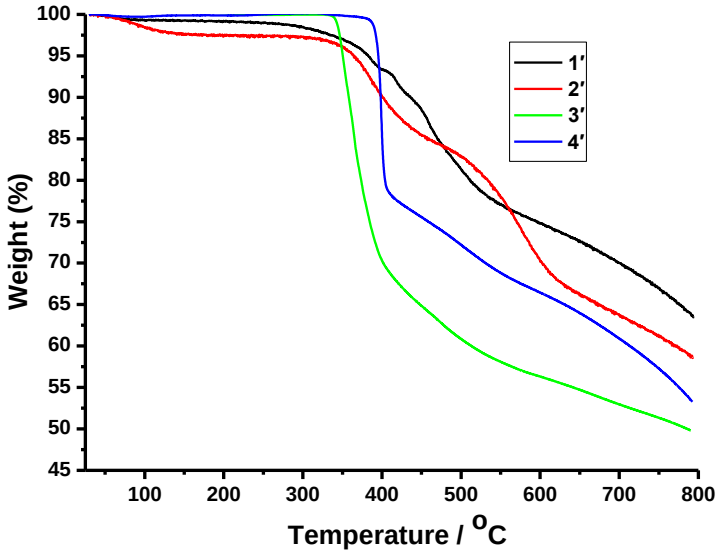


(d)

Fig. S4 The PXRD patterns of **1** (a)-**4** (d).



(a)



(b)

Fig. S5 The TGA curves of complexes **1**-**4** (a) and desolvated samples **1′**-**4′** (b).