Electronic Supplementary Information

For

Guest-triggered assembly of zinc(II) supramolecular isomers with accompanying dimensional change and reversible single-crystal-to-single-crystal transformation

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List of Tables and Figures

Table S1 Crystallographic data and structure refinement for **1**, **2**, **2a**, **3** and **4**

	1	**2**	**2a**	**3**	**4**
Formula	$C_{44}H_{40}N_8O_8Zn_2$	$C_{60}H_{88}N_{12}O_{18}Zn_2$	$C_{22}H_{20}N_4O_4Zn$	$C_{37}H_{35}N_4O_4Zn$	$C_{60}H_{81}N_9O_{13}Zn_2$
Formula weight	939.58	1396.16	469.79	665.06	1267.08
Temperature (K)	173(2)	173(2)	173(2)	173(2)	173(2)
Crystal system	Monoclinic	Monoclinic	Orthorhombic	Monoclinic	Monoclinic
Space group	*C*2/*c*	$P2_1/c$	*Pbca*	$P2_1$/c	$P2_1/n$
Z	8	4	8	4	2
a (Å)	12.0935(6)	19.5006(5)	18.6866(13)	9.987(4)	10.3361(4)
b (Å)	34.0051(17)	20.5981(6)	15.8553(12)	22.605(12)	20.4349(7)
c (Å)	31.9458(16)	18.7188(5)	22.302(2)	17.815(6)	16.2418(5)
α (°)	90	90	90	90	90
β (°)	93.564(3)	116.0640(10)	90	121.513(17)	91.807(2)
γ (°)	90	90	90	90	90
V (Å^3)	13112.0(11)	6754.2(3)	6607.6(9)	3429(3)	3428.8(2)
D_{calc} (g/cm^3)	0.952	1.373	0.944	1.288	1.227
μ (mm^{-1})	0.773	0.787	0.767	0.760	0.762
$2\theta_{max}$ (°)	52.00	52.00	52.00	52.00	52.00
reflections collected	80312	108241	57668	24532	47173
independent reflections	12888 [R(int) = 0.0798]	13269 [R(int) = 0.0928]	6101 [R(int) = 0.1110]	6730 [R(int) = 0.0949]	6741 [R(int) = 0.0916]
goodness-of-fit on F2	0.889	1.108	1.024	1.021	1.095
R1, wR2 [I > 2σ(I)]	R1 = 0.0535, wR2 = 0.1332	R1 = 0.0701, wR2 = 0.1779	R1 = 0.1201, wR2 = 0.3174	R1 = 0.0677, wR2 = 0.13.88	R1 = 0.0782, wR2 = 0.2376
R1, wR2 (all data)	R1 = 0.1069, wR2 = 0.1446	R1 = 0.1227, wR2 = 0.2044	R1 = 0.2215, wR2 = 0.3491	R1 = 0.1547, wR2 = 0.1801	R1 = 0.1281, wR2 = 0.2753

Table S2 Selected bond lengths (Å) and bond angles (°) for **1**[a]

Zn1-O5	1.938(2)	Zn1-O1	1.956(2)
Zn1-N1	1.994(3)	Zn1-N5	2.042(3)
Zn2-O3A	1.944(3)	Zn2-O8	1.990(2)
Zn2-N7	2.001(3)	Zn2-N4B	2.035(3)
O5-Zn1-O1	105.53(1)	O5-Zn1-N1	126.30(1)
O1-Zn1-N1	111.62(1)	O5-Zn1-N5	105.55(1)
O1-Zn1-N5	98.69(1)	N1-Zn1-N5	105.57(1)
O3A-Zn2-O8	114.55(1)	O3A-Zn2-N7	123.72(1)
O8-Zn2-N7	104.39(1)	O3A-Zn2-N4B	108.83(1)
O8-Zn2-N4B	97.51(1)	N7-Zn2-N4B	104.31(1)

[a]Symmetry operations: (A) x-1/2,y-1/2,z; (B) x-1,-y+1,z+1/2.

Table S3 Selected bond lengths (Å) and bond angles (°) for **2**[a]

Zn1-O1	1.954(4)	Zn1-N1	2.041(4)
Zn1-O3A	1.955(3)	Zn1-N8B	2.012(4)
Zn2-O5	1.967(3)	Zn2-N4	2.025(4)
Zn2-O7C	1.967(4)	Zn2-N5	2.023(4)
O1-Zn1-O3A	108.9(2)	O1-Zn1-N8B	121.3(2)
O3A-Zn1-N8B	107.0(2)	O1-Zn1-N1	113.0(2)
O3A-Zn1-N1	98.8(2)	N8B-Zn1-N1	105.4(2)
O7C-Zn2-O5	110.3(2)	O7C-Zn2-N5	113.4(2)
O5-Zn2-N5	99.4(2)	O7C-Zn2-N4	122.2(2)
O5-Zn2-N4	108.4(2)	N5-Zn2-N4	100.5(2)

[a]Symmetry operations: (A) x,-y+3/2,z+1/2; (B) x,y+1,z; (C) x,-y+1/2,z+1/2.

Table S4 Selected bond lengths (Å) and bond angles (°) for **3**[a]

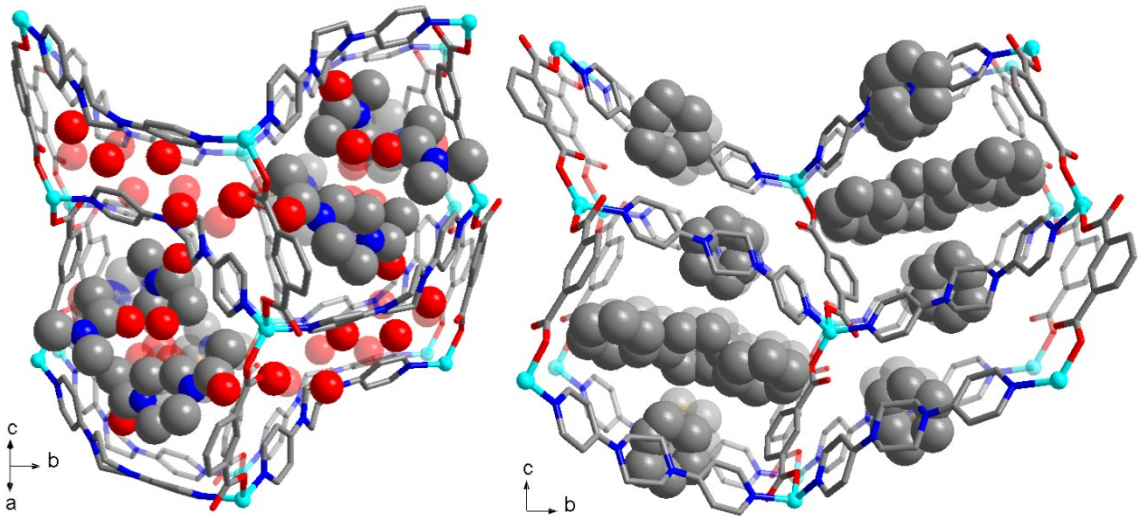
Zn1-O1	1.941(3)	Zn1-N1	2.033(5)
Zn1-O3A	1.960(3)	Zn1-N4 B	2.038(4)
O1-Zn1-O3A	110.1(2)	O1-Zn1-N1	128.1(2)
O3A-Zn1-N1	105.0(2)	O1-Zn1-N4B	108.3(2)
O3A-Zn1-N4B	100.9(2)	N1-Zn1-N4B	100.9(2)

[a]Symmetry operations: (A) x - 1, -y + 3/2, z - 1/2; (B) –x + 1, y – 1/2, -z + 1/2.

Table S5 Selected bond lengths (Å) and bond angles (°) for **4**[a]

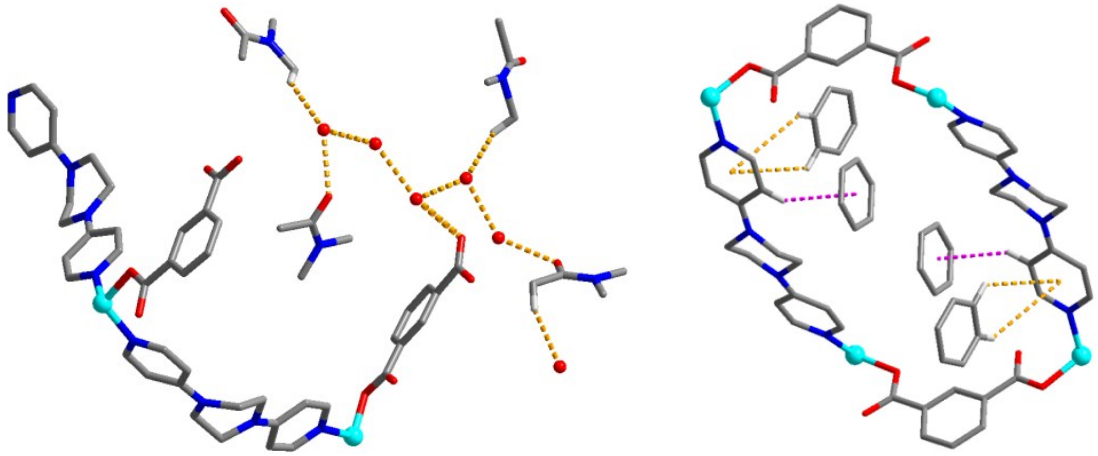
Zn1-O1	1.957(1)	Zn1-N1	2.024(2)
Zn1-O3A	1.928(1)	Zn1-N4B	2.031(2)
O1-Zn1-O3A	113.8(6)	O1-Zn1-N1	107.0(6)
O3A-Zn1-N1	118.9(6)	O1-Zn1-N4B	97.6(6)
O3A-Zn1-N4B	113.7(6)	N1-Zn1-N4B	103.3(7)

[a]Symmetry operations: (A) x - 1/2, -y + 1/2, z - 1/2; (B) –x + 1/2, y + 1/2, -z + 1/2.



(a) (b)

Fig. S1 Packing structures of (a) **2** and (b) **3**.



(a) (b)

Fig. S2 The interactions between the solvent molecules and the 2D networks. (a) The H-bonded DMA and water molecules in **2** and (b) the benzene molecules showing the edge-to-face π-π stacking interactions (yellow dashed lines: 3.62 and 3.63 Å; pink dashed lines: 3.01Å) in **3**.

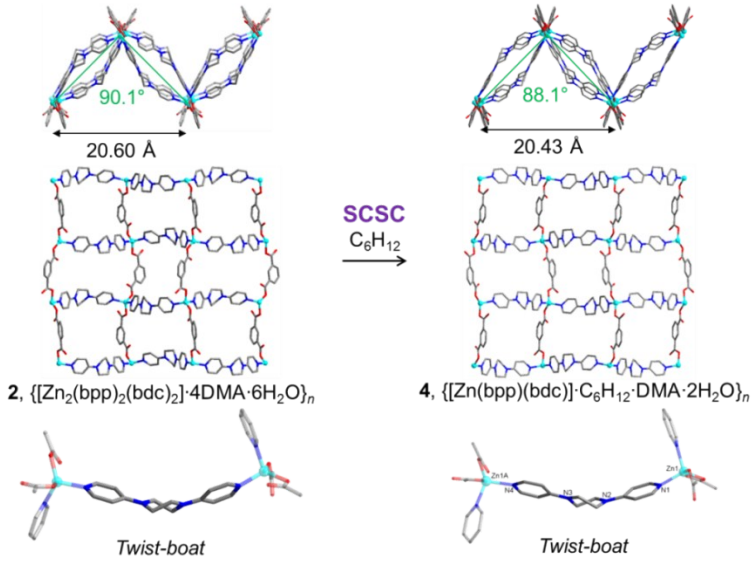


Fig. S3 Irreversible conversion of (a) **2** to (b) **4** via the SCSC transformation after immersion in cyclohexane.

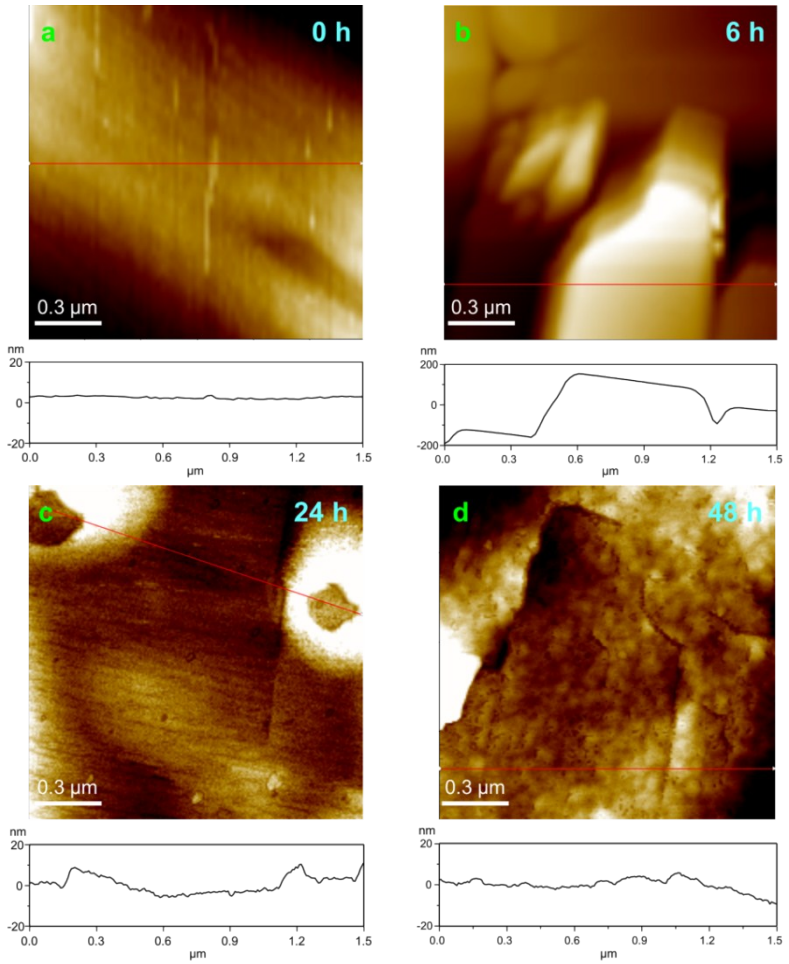


Fig. S4 AFM images (top) and profiles (bottom) of the surface of a crystal of **2** after immersing in benzene: (a) before solvent exchange, (b) 6 h, (c) 24 h and (d) 48 h. Image size is 1.5 × 1.5 µm in all cases.

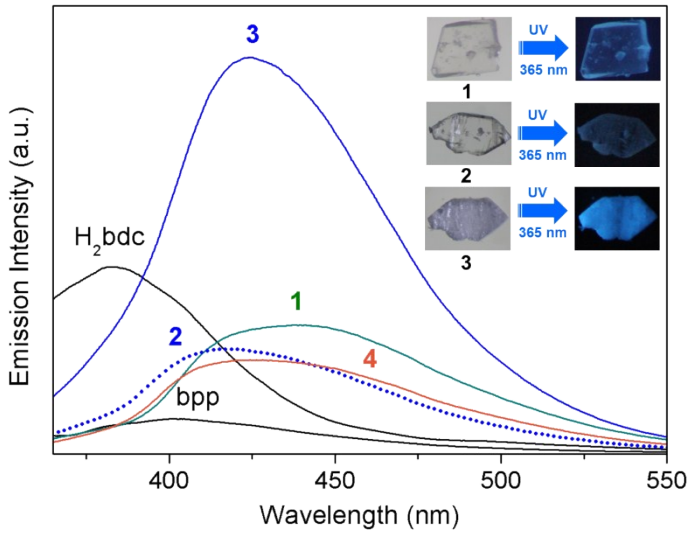


Fig. S5 Solid-state photoluminescence spectra of bpp, H_2bdc, **1**, **2**, **3** and **4** at room temperature (excitation at 290 nm).

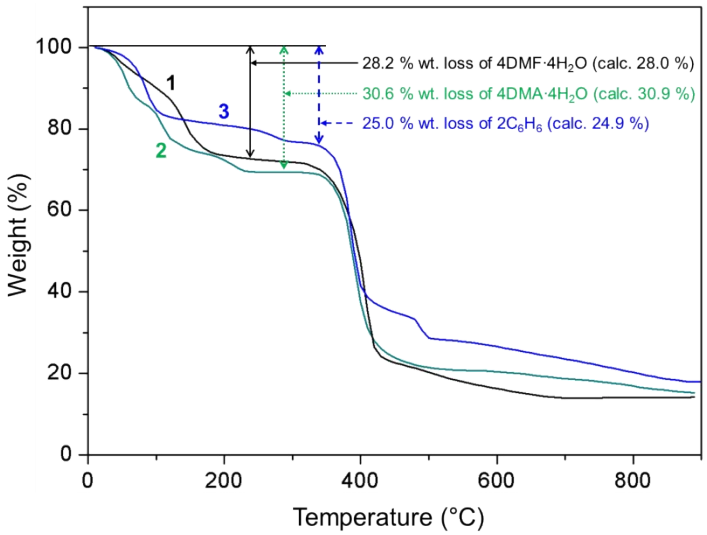


Fig. S6 TGA curves for **1**, **2** and **3**.