

High structural diversity controlled by temperature and induction agent†

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Table S1. Selective Bond Lengths (Å) and Angles (deg) for Compounds **1** – **5**.^a

1			
Zn(1)–O(7)#1	1.986(5)	Zn(1)–O(2)	2.035(5)
Zn(1)–N(6)#2	2.057(5)	Zn(1)–O(17)	2.069(5)
Zn(1)–O(18)	2.182(5)	Zn(2)–O(6)	1.979(4)
Zn(2)–O(4)	1.998(5)	Zn(2)–N(2)#3	2.031(6)
Zn(2)–O(20)	2.160(5)	Zn(2)–O(19)	2.162(5)
Zn(3)–O(9)	1.982(5)	Zn(3)–O(16)#1	2.031(4)
Zn(3)–O(22)	2.059(5)	Zn(3)–N(8)#4	2.071(5)
Zn(3)–O(21)	2.110(5)	Zn(4)–O(12)	1.998(4)
Zn(4)–O(14)	2.010(5)	Zn(4)–N(12)#4	2.035(5)
Zn(4)–O(23)	2.141(5)	Zn(4)–O(24)	2.156(5)
O(7)#1–Zn(1)–O(2)	118.84(19)	O(7)#1–Zn(1)–N(6)#2	96.4(2)
O(2)–Zn(1)–N(6)#2	144.3(2)	O(7)#1–Zn(1)–O(17)	93.0(2)
O(2)–Zn(1)–O(17)	90.0(2)	N(6)#2–Zn(1)–O(17)	93.9(2)
O(7)#1–Zn(1)–O(18)	92.9(2)	O(2)–Zn(1)–O(18)	87.1(2)
N(6)#2–Zn(1)–O(18)	85.5(2)	O(17)–Zn(1)–O(18)	174.1(2)
O(6)–Zn(2)–O(4)	94.3(2)	O(6)–Zn(2)–N(2)#3	120.9(2)
O(4)–Zn(2)–N(2)#3	144.5(2)	O(6)–Zn(2)–O(20)	90.7(2)

O(4)–Zn(2)–O(20)	86.5(2)	N(2)#3–Zn(2)–O(20)	88.5(2)
O(6)–Zn(2)–O(19)	97.2(2)	O(4)–Zn(2)–O(19)	91.0(2)
N(2)#3–Zn(2)–O(19)	89.1(2)	O(20)–Zn(2)–O(19)	171.9(2)
O(9)–Zn(3)–O(16)#1	118.4(2)	O(9)–Zn(3)–O(22)	93.2(2)
O(16)#1–Zn(3)–O(22)	87.3(2)	O(9)–Zn(3)–N(8)#4	100.7(2)
O(16)#1–Zn(3)–N(8)#4	140.8(2)	O(22)–Zn(3)–N(8)#4	92.2(2)
O(9)–Zn(3)–O(21)	95.0(2)	O(16)#1–Zn(3)–O(21)	88.9(2)
O(22)–Zn(3)–O(21)	171.8(2)	N(8)#4–Zn(3)–O(21)	86.1(2)
O(12)–Zn(4)–O(14)	92.6(2)	O(12)–Zn(4)–N(12)#4	120.7(2)
O(14)–Zn(4)–N(12)#4	146.4(2)	O(12)–Zn(4)–O(23)	91.1(2)
O(14)–Zn(4)–O(23)	85.2(2)	N(12)#4–Zn(4)–O(23)	89.4(2)
O(12)–Zn(4)–O(24)	96.8(2)	O(14)–Zn(4)–O(24)	91.0(2)
N(12)#4–Zn(4)–O(24)	89.5(2)	O(23)–Zn(4)–O(24)	171.4(2)

2

Zn(1)–O(3)#1	1.9968(18)	Zn(1)–O(1)	2.048(2)
Zn(1)–N(3)#2	2.134(2)	Zn(1)–N(2)#3	2.143(2)
Zn(1)–O(5)	2.2252(18)	Zn(1)–O(5)#4	2.2890(18)
O(3)#1–Zn(1)–O(1)	171.17(8)	O(3)#1–Zn(1)–N(3)#2	98.60(8)
O(1)–Zn(1)–N(3)#2	90.08(8)	O(3)#1–Zn(1)–N(2)#3	91.12(8)
O(1)–Zn(1)–N(2)#3	88.72(8)	N(3)#2–Zn(1)–N(2)#3	101.68(9)
O(3)#1–Zn(1)–O(5)	87.75(8)	O(1)–Zn(1)–O(5)	89.80(7)
N(3)#2–Zn(1)–O(5)	95.38(7)	N(2)#3–Zn(1)–O(5)	162.88(8)
O(3)#1–Zn(1)–O(5)#4	84.37(7)	O(1)–Zn(1)–O(5)#4	86.80(7)
N(3)#2–Zn(1)–O(5)#4	169.46(7)	N(2)#3–Zn(1)–O(5)#4	88.32(7)
O(5)–Zn(1)–O(5)#4	74.57(8)		

3

Zn(1)–O(2)	1.965(2)	Zn(1)–O(3)#1	1.903(2)
Zn(1)–O(5)	1.970(2)	Zn(1)–N(3)#2	2.058(3)
O(3)#1–Zn(1)–O(2)	123.72(12)	O(3)#1–Zn(1)–O(5)	124.72(10)
O(2)–Zn(1)–O(5)	103.40(11)	O(3)#1–Zn(1)–N(3)#2	104.70(11)
O(2)–Zn(1)–N(3)#2	92.17(10)	O(5)–Zn(1)–N(3)#2	100.22(11)

4

Zn(1)–O(2)	1.925(4)	Zn(1)–O(3)#1	1.974(3)
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Zn(1)–N(2)#2	2.024(4)	Zn(1)–O(1)#3	2.163(4)
Zn(1)–O(5)	2.332(4)	O(2)–Zn(1)–O(3)#1	142.03(16)
O(2)–Zn(1)–N(2)#2	116.96(17)	O(3)#1–Zn(1)–N(2)#2	99.69(16)
O(2)–Zn(1)–O(1)#3	94.36(16)	O(3)#1–Zn(1)–O(1)#3	93.53(15)
N(2)#2–Zn(1)–O(1)#3	92.52(15)	O(2)–Zn(1)–O(5)	89.91(15)
O(3)#1–Zn(1)–O(5)	81.39(15)	N(2)#2–Zn(1)–O(5)	88.00(15)
O(1)#3–Zn(1)–O(5)	174.91(14)		

5

Zn(1)–O(34)	1.931(11)	Zn(1)–O(9)	1.962(12)
Zn(1)–O(17)#1	2.007(12)	Zn(1)–N(8)#2	2.029(14)
Zn(2)–O(19)#3	1.964(12)	Zn(2)–O(37)	2.000(10)
Zn(2)–N(15)	2.038(14)	Zn(2)–O(27)#4	2.119(12)
Zn(2)–O(28)#4	2.345(14)	Zn(3)–O(3)	1.947(11)
Zn(3)–O(33)	1.922(11)	Zn(3)–N(3)#3	2.032(13)
Zn(3)–O(11)	1.996(11)	Zn(4)–N(24)#2	2.015(14)
Zn(4)–O(24)	2.011(13)	Zn(5)–O(15)#3	1.979(12)
Zn(5)–O(34)#5	1.943(11)	Zn(5)–N(12)	2.067(14)
Zn(5)–O(7)#6	2.040(13)	Zn(6)–N(20)	2.031(14)
Zn(6)–O(38)	1.995(10)	Zn(6)–O(25)#2	1.954(11)
Zn(6)–O(1)#5	2.050(12)	Zn(7)–O(5)	1.961(12)
Zn(7)–O(33)	1.942(11)	Zn(7)–N(5)#2	2.037(14)
Zn(7)–O(29)#7	2.031(12)	Zn(8)–O(14)	2.014(13)
Zn(8)–O(37)	2.006(10)	Zn(8)–N(17)	2.035(13)
Zn(8)–O(21)#2	2.019(11)	Zn(9)–O(36)	2.039(11)
Zn(9)–O(22)#2	2.001(11)	Zn(9)–O(35)	2.150(12)
Zn(9)–O(12)	2.096(11)	Zn(9)–O(13)	2.210(14)
Zn(9)–O(37)	2.161(11)	Zn(10)–O(39)	2.041(11)
Zn(10)–O(32)	2.006(10)	Zn(10)–O(18)#7	2.146(13)
Zn(10)–O(40)	2.132(14)	Zn(10)–O(38)	2.178(11)
Zn(10)–O(23)	2.148(13)		
O(34)–Zn(1)–O(9)	117.0(5)	O(34)–Zn(1)–O(17)#1	109.1(5)
O(9)–Zn(1)–O(17)#1	103.0(5)	O(34)–Zn(1)–N(8)#2	110.7(6)
O(9)–Zn(1)–N(8)#2	100.1(6)	O(17)#1–Zn(1)–N(8)#2	116.8(6)

O(19)#3–Zn(2)–O(37)	112.6(5)	O(19)#3–Zn(2)–N(15)	100.8(6)
O(37)–Zn(2)–N(15)	107.5(5)	O(19)#3–Zn(2)–O(27)#4	99.3(5)
O(37)–Zn(2)–O(27)#4	99.4(5)	N(15)–Zn(2)–O(27)#4	136.7(5)
O(19)#3–Zn(2)–O(28)#4	141.6(5)	O(37)–Zn(2)–O(28)#4	102.0(5)
N(15)–Zn(2)–O(28)#4	83.5(5)	O(27)#4–Zn(2)–O(28)#4	57.7(5)
O(33)–Zn(3)–O(3)	116.0(5)	O(33)–Zn(3)–O(11)	108.5(5)
O(3)–Zn(3)–O(11)	104.6(5)	O(33)–Zn(3)–N(3)#3	112.9(5)
O(3)–Zn(3)–N(3)#3	99.8(5)	O(11)–Zn(3)–N(3)#3	114.8(5)
O(31)–Zn(4)–O(38)	106.6(5)	O(31)–Zn(4)–O(24)	122.7(6)
O(38)–Zn(4)–O(24)	105.9(5)	O(31)–Zn(4)–N(24)#2	101.9(5)
O(38)–Zn(4)–N(24)#2	129.1(6)	O(24)–Zn(4)–N(24)#2	92.2(5)
O(34)#5–Zn(5)–O(15)#3	111.9(5)	O(34)#5–Zn(5)–O(7)#6	102.0(5)
O(15)#3–Zn(5)–O(7)#6	100.2(5)	O(34)#5–Zn(5)–N(12)	119.8(5)
O(15)#3–Zn(5)–N(12)	99.3(5)	O(7)#6–Zn(5)–N(12)	122.0(5)
O(25)#2–Zn(6)–O(38)	113.3(5)	O(25)#2–Zn(6)–N(20)	99.7(5)
O(38)–Zn(6)–N(20)	107.3(5)	O(25)#2–Zn(6)–O(1)#5	104.5(5)
O(38)–Zn(6)–O(1)#5	102.4(5)	N(20)–Zn(6)–O(1)#5	129.9(5)
O(33)–Zn(7)–O(5)	118.2(5)	O(33)–Zn(7)–O(29)#7	101.7(5)
O(5)–Zn(7)–O(29)#7	102.9(5)	O(33)–Zn(7)–N(5)#2	113.0(6)
O(5)–Zn(7)–N(5)#2	98.6(5)	O(29)#7–Zn(7)–N(5)#2	123.2(5)
O(37)–Zn(8)–O(14)	103.8(5)	O(37)–Zn(8)–O(21)#2	101.6(4)
O(14)–Zn(8)–O(21)#2	126.5(6)	O(37)–Zn(8)–N(17)	138.5(6)
O(14)–Zn(8)–N(17)	90.5(6)	O(21)#2–Zn(8)–N(17)	100.4(5)
O(22)#2–Zn(9)–O(36)	173.0(5)	O(22)#2–Zn(9)–O(12)	91.6(5)
O(36)–Zn(9)–O(12)	93.1(5)	O(22)#2–Zn(9)–O(35)	86.6(5)
O(36)–Zn(9)–O(35)	88.6(5)	O(12)–Zn(9)–O(35)	85.8(5)
O(22)#2–Zn(9)–O(37)	87.8(4)	O(36)–Zn(9)–O(37)	88.8(4)
O(12)–Zn(9)–O(37)	167.4(4)	O(35)–Zn(9)–O(37)	106.7(4)
O(22)#2–Zn(9)–O(13)	99.1(5)	O(36)–Zn(9)–O(13)	86.4(5)
O(12)–Zn(9)–O(13)	85.9(5)	O(35)–Zn(9)–O(13)	170.0(6)
O(37)–Zn(9)–O(13)	81.8(5)	O(32)–Zn(10)–O(39)	170.8(5)
O(32)–Zn(10)–O(40)	88.8(5)	O(39)–Zn(10)–O(40)	88.0(5)
O(32)–Zn(10)–O(18)#7	92.9(4)	O(39)–Zn(10)–O(18)#7	95.3(5)

O(40)–Zn(10)–O(18)#7	83.5(5)	O(32)–Zn(10)–O(23)	98.1(5)
O(39)–Zn(10)–O(23)	86.9(5)	O(40)–Zn(10)–O(23)	166.2(6)
O(18)#7–Zn(10)–O(23)	84.3(5)	O(32)–Zn(10)–O(38)	85.4(4)
O(39)–Zn(10)–O(38)	87.5(5)	O(40)–Zn(10)–O(38)	108.9(5)
O(18)#7–Zn(10)–O(38)	167.5(4)	O(23)–Zn(10)–O(38)	83.7(4)

^a Symmetry transformations used to generate equivalent atoms: #1 $x + 1, y, z - 1$; #2 $x, y, z - 1$; #3 $x - 1, y, z$; #4 $x + 1, y, z$ for **1**; #1 $x + 1/2, y - 1/2, z$; #2 $x, -y + 2, z - 1/2$; #3 $-x + 2, y, -z + 3/2$; #4 $-x + 2, -y + 1, -z + 1$ for **2**; #1 $-x + 1, y - 1/2, -z + 5/2$; #2 $-x + 1, y - 1/2, -z + 3/2$ for **3**; #1 $x - 1/2, -y + 3/2, z + 1/2$; #2 $x - 1, -y + 1, z - 1/2$; #3 $x, -y + 1, z + 1/2$ for **4**; #1 $-x - 1, -y + 1, -z + 2$; #2 $x - 1, y, z$; #3 $x + 1, y, z$; #4 $x - 1, y, z - 1$; #5 $-x, -y + 2, -z + 2$; #6 $-x + 1, -y + 2, -z + 1$; #7 $-x + 1, -y + 1, -z + 2$ for **5**.

Table S2. Hydrogen bonding data for compounds **1** and **3**.^a

D–H...A	d(D...A) (Å)	∠D–H...A (°)
1		
O(17)–H(17A)...O(8)#1	2.686(8)	168
O(18)–H(18B)...O(16)#2	2.644(8)	134
O(19)–H(19B)...O(5)#3	2.732(8)	167
O(20)–H(20A)...O(14)	3.140(7)	146
O(20)–H(20B)...O(12)	2.963(8)	138
O(21)–H(21A)...O(8)#2	2.952(8)	146
O(22)–H(22A)...O(10)#4	2.751(8)	159
O(23)–H(23A)...O(6)	2.924(8)	176
O(23)–H(23B)...O(26)#5	2.696(9)	144
O(24)–H(24A)...N(9)#6	3.090(9)	167
O(24)–H(24B)...O(11)#7	2.696(7)	156
3		
O(5)–H(5A)...N(2)#1	2.805(4)	178
O(5)–H(5B)...O(4)#2	2.648(3)	178

^a Symmetry transformations used to generate equivalent atoms: #1 $-x + 1, -y + 1, -z + 2$; #2 $x + 1, y, z - 1$; #3 $-x, -y + 1, -z + 2$; #4 $-x + 1, -y + 2, -z + 1$; #5 $x, y, z + 1$; #6 $-x, -y + 2, -z + 2$; #7 $-x + 1, -y + 2, -z + 2$ for **1**; #1 $x + 1, y, z + 1$; #2 $-x + 1, -y + 2, -z + 2$ for **3**.

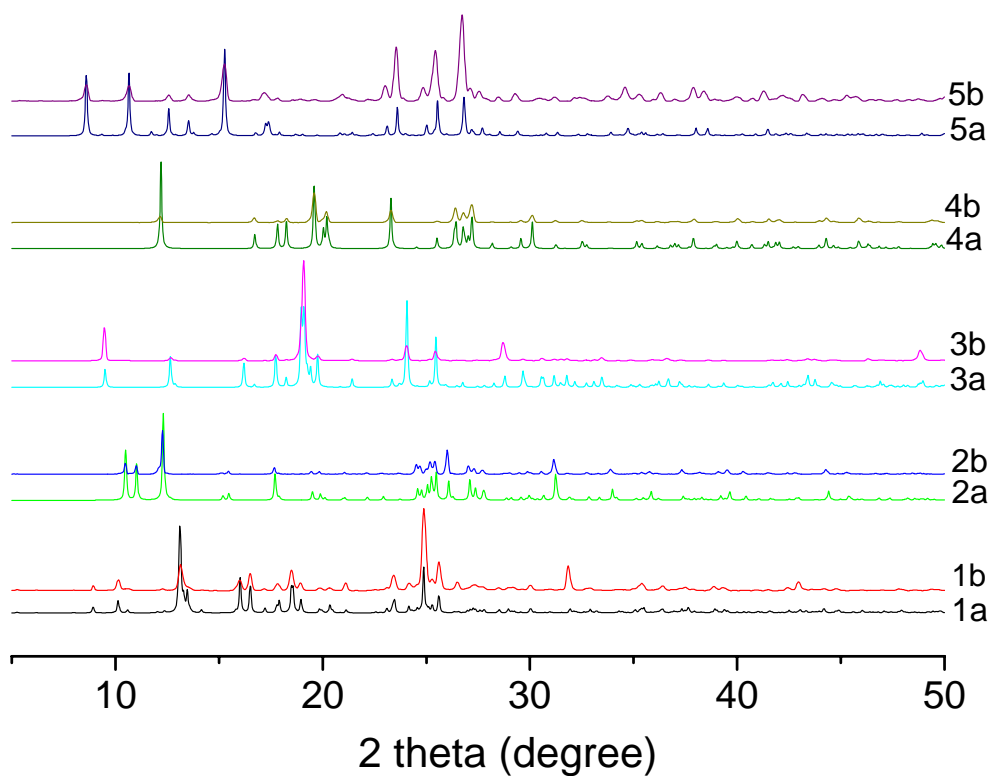


Fig. S1. The PXRD patterns of **1 - 5**: a – simulated; b – as-synthesized.

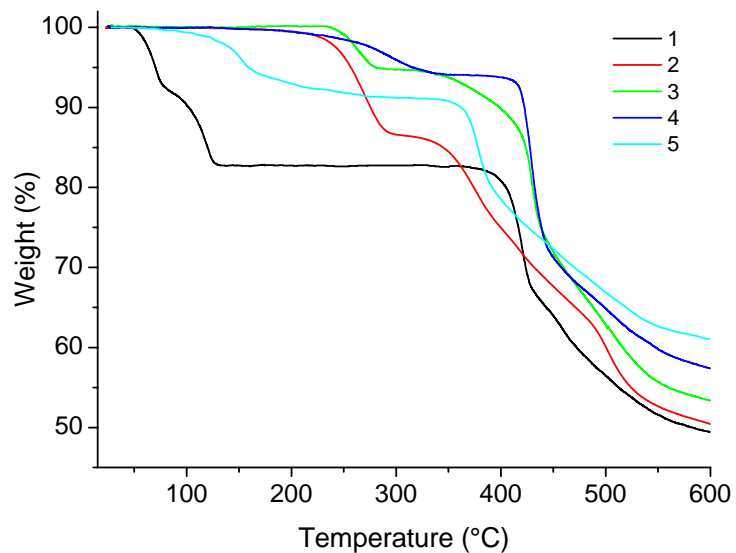


Fig. S2. The TGA curves of **1 - 5**.

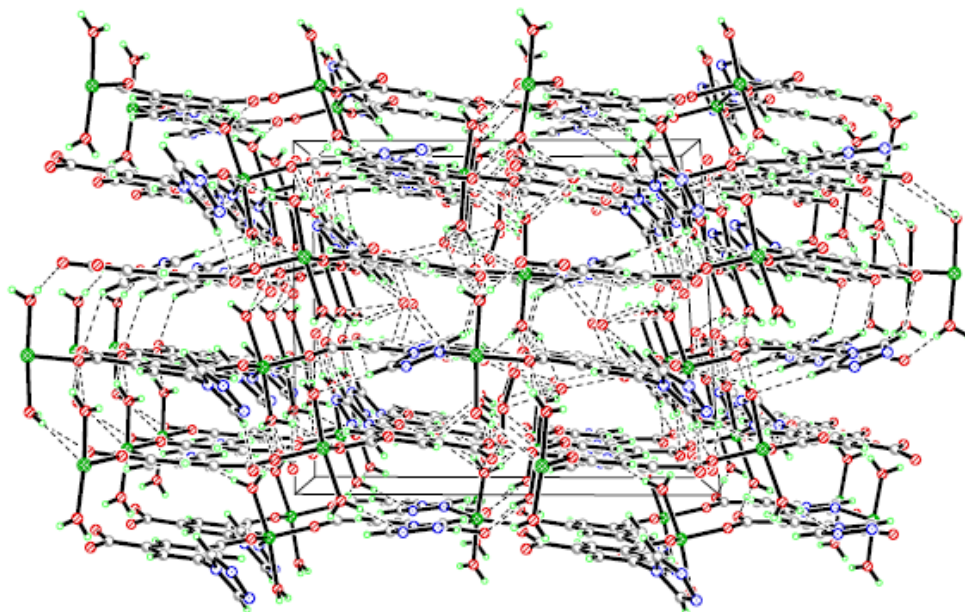
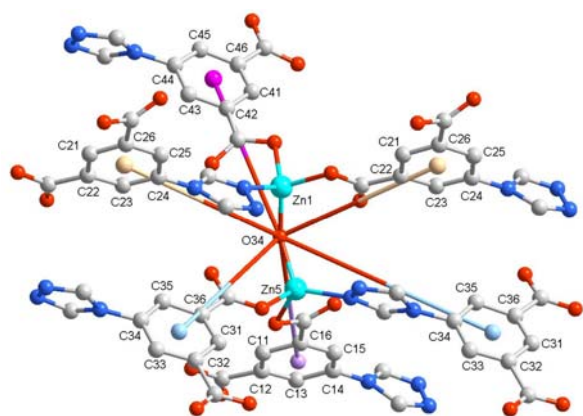
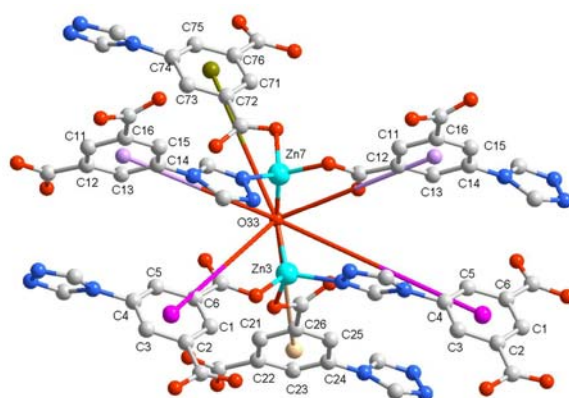


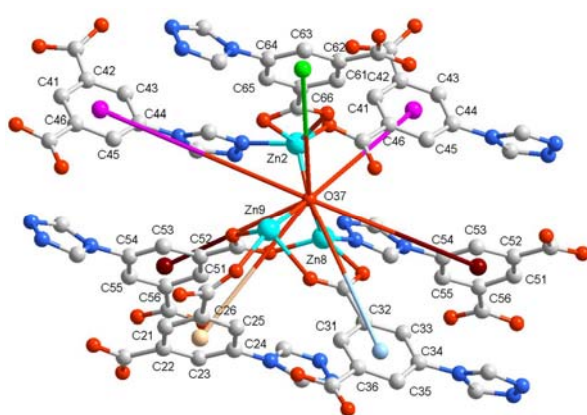
Fig. S3. 3D structure of **1** with hydrogen bonds indicated by dashed lines.



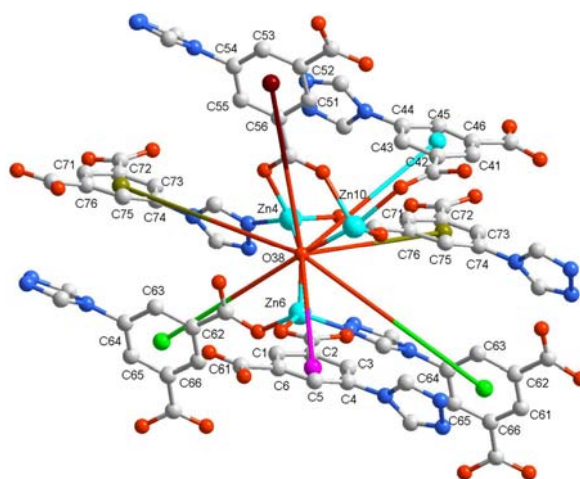
(i)



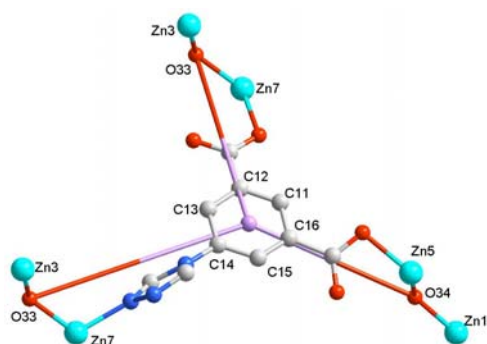
(ii)



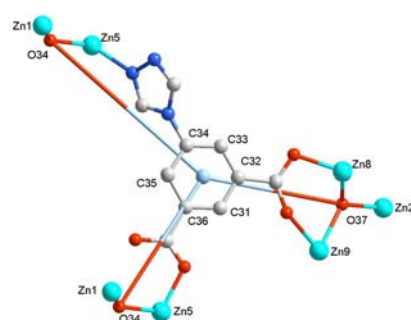
(iii)



(iv)



(v)



(vi)

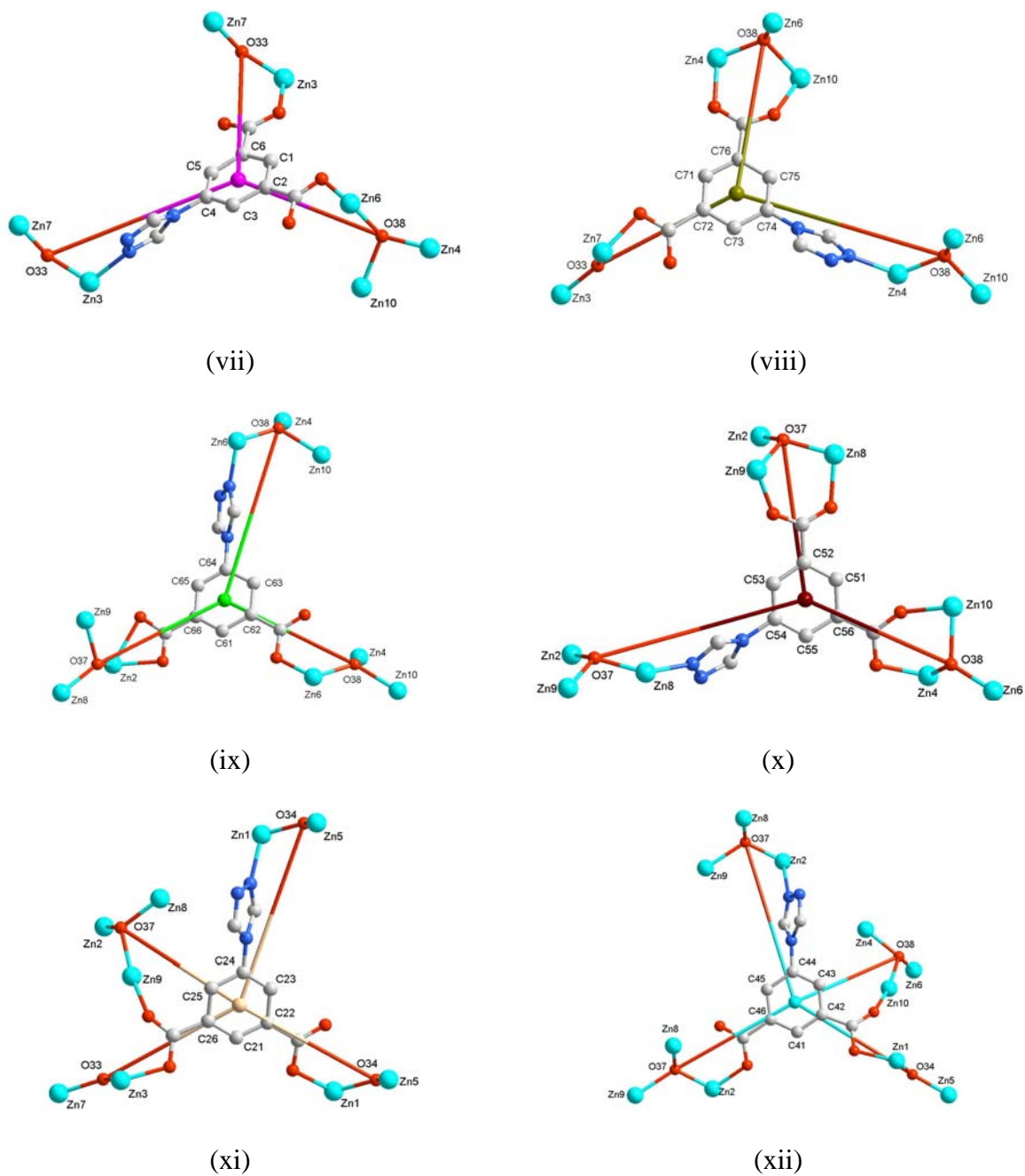


Fig. S4. The twelve types of nodes in **5**: (i) and (ii): 6-connected nodes of Zn1–Zn5 and Zn3–Zn7 units; (iii) and (iv): 7-connected nodes of Zn2–Zn8–Zn9 and Zn4–Zn6–Zn10 units; (v - x): 3-connected nodes of L^{2-} ligands; (xi) and (xii): 4-connected nodes of L^{2-} ligands.