Electronic Supplementary Material (ESI) for CrystEngComm.

Electronic Supplementary Information

Two isomeric Zn(II)-based metal-organic frameworks constructed from a bifunctional triazolate-carboxylate tecton exhibiting distinct gas sorption behaviors

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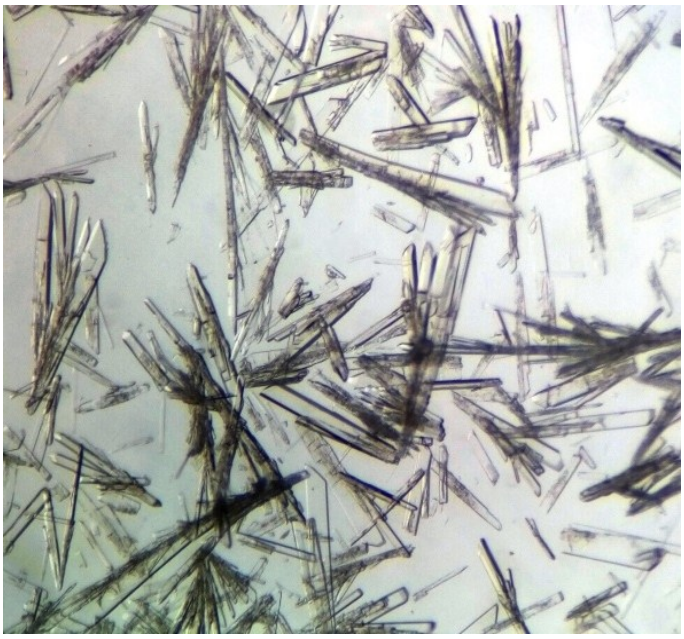
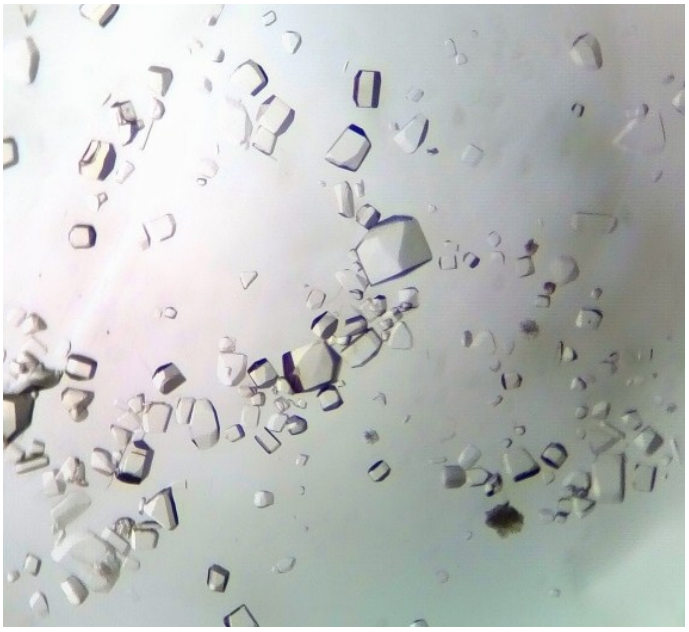


(a)



(b)

Fig. S1 Optical microscopic photographs of **1**(a) and **2**(b).

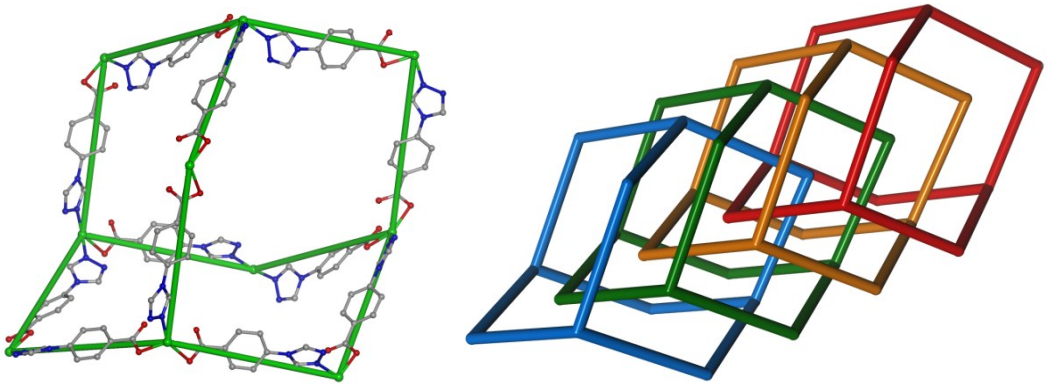


Fig. S2 A single diamond net (left) and topological representation of the 4-fold interpenetrated diamond net (right) in **1** and **2**.

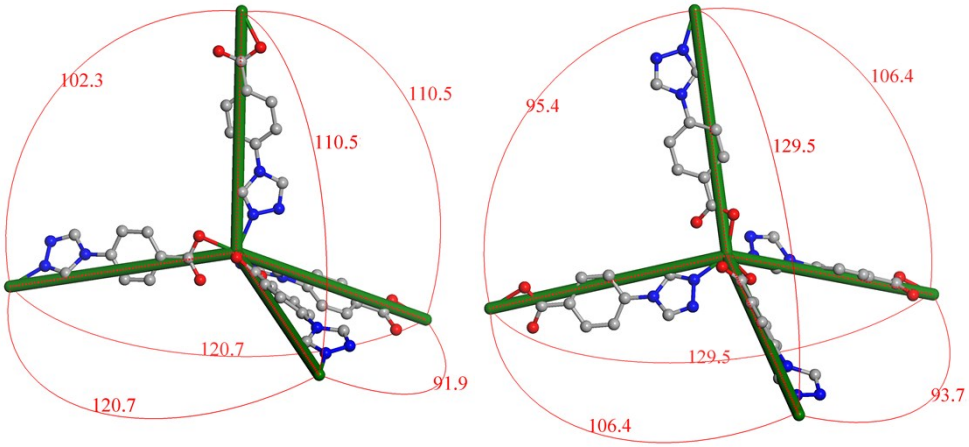
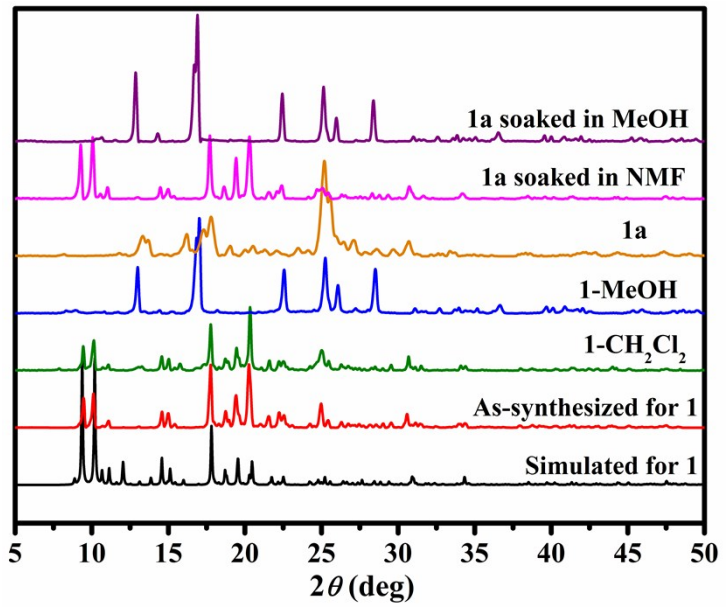
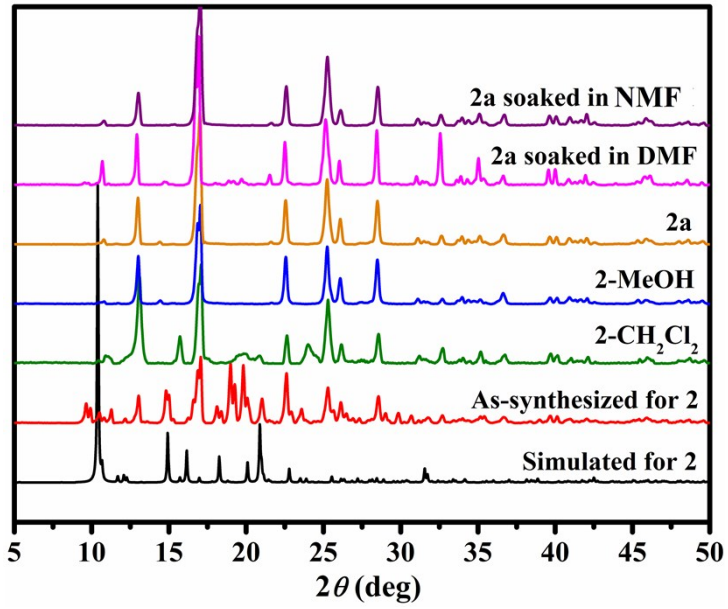


Fig. S3 The Zn···Zn···Zn angels for **1**(left) and **2**(right).



(a)



(b)

Fig. S4 PXRD patterns of **1**(a) and **2(b)**.

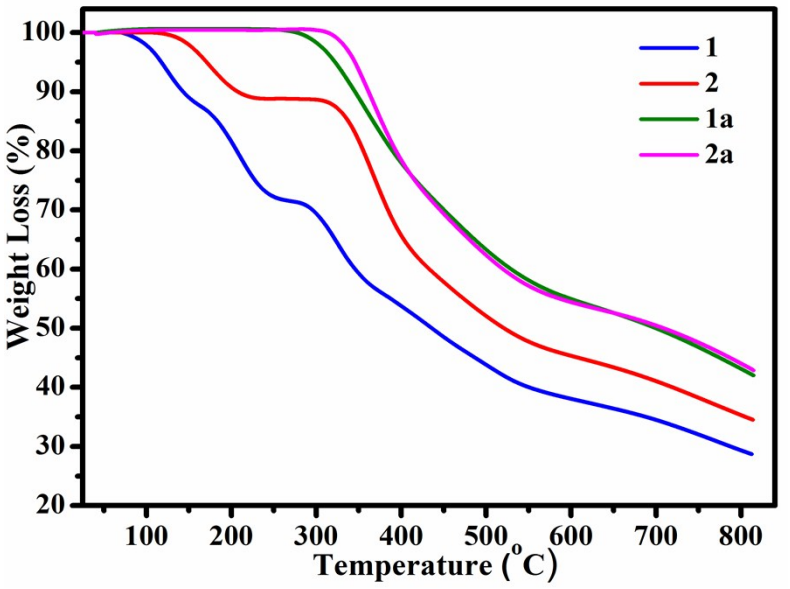


Fig. S5 TGA curves for **1**, **1a**, **2**, and **2a**.

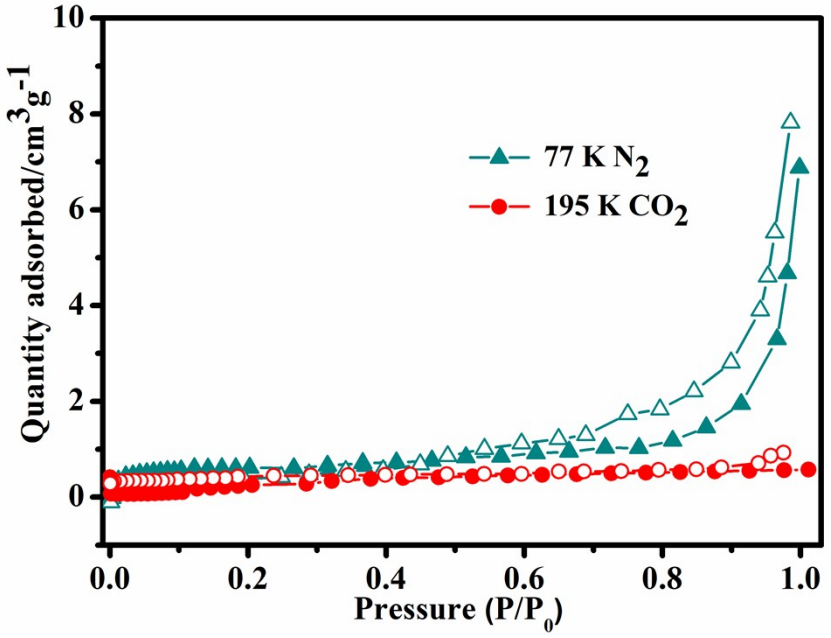


Fig. S6 Sorption isotherms of **2a**: CO_2 at195 K and N_2 at 77 K.

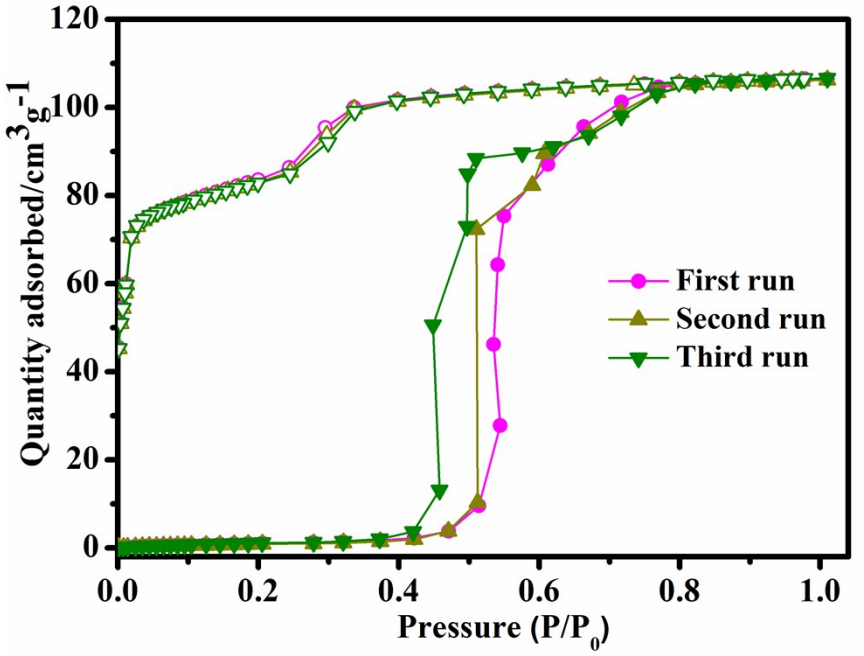


Fig. S7 Three-runs sorption isotherms of **1a** for CO_2 at 195 K.

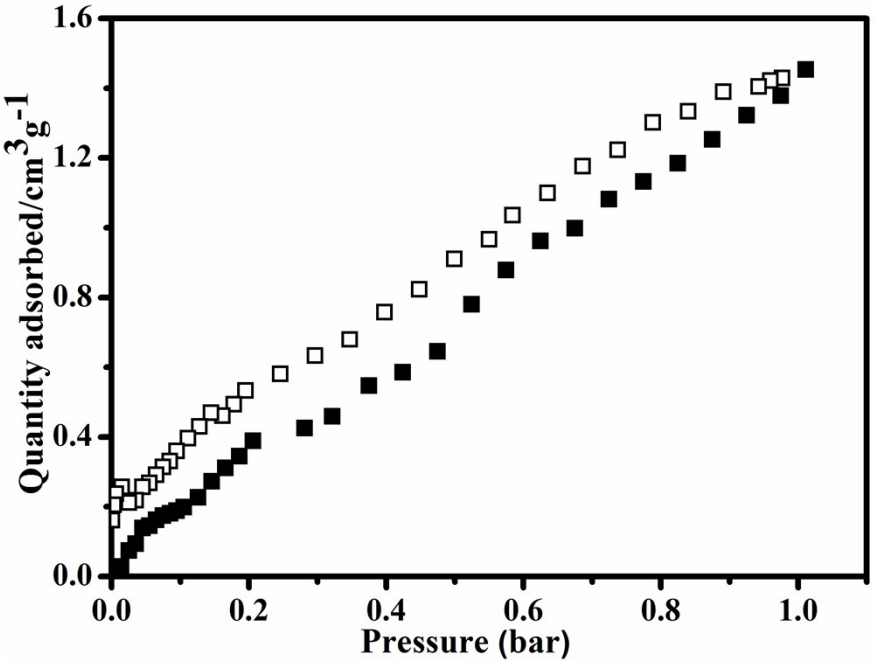


Fig. S8 Sorption isotherm of **1a** for CO_2 at 273 K.

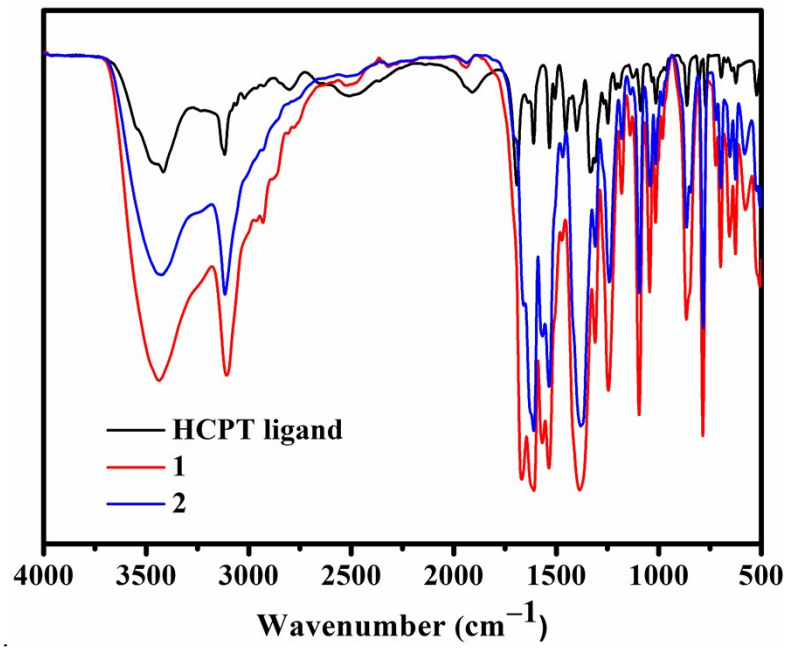


Fig. S9 IR spectra for HCPT ligand (black), **1**(red), and **2**(blue).

Computational details.

The potential surface of the torsion between the triazol ring and phenyl ring of HCPT were calculated by the conformers calculation in Material Studio 8.0 with a step-width of 2 degree. MM calculations for the framework energy of the structures were performed with the smart algorithm based on the universal forcefield (UFF) in the Forcite module. The charge-Eq method was used to calcuate the charges of the framework.

############################
TOPOS analysis results for **1**
############################

Topology for Zn1

Atom Zn1 links by bridge ligands and has
Common vertex with R(A-A)

Zn 1 0.7423 -0.5110 -0.0327 (0-1 0) 12.058A 1
Zn 1 -0.2577 -0.5110 -0.0327 (-1-1 0) 12.058A 1
Zn 1 0.2423 0.4890 -0.4673 (0 0-1) 12.102A 1
Zn 1 0.2423 0.4890 0.5327 (0 0 0) 12.102A 1

Structural group analysis

Structural group No 1

Structure consists of 3D framework with Zn
There are 4 interpenetrating nets
TIV: Translating interpenetration vectors

[0,1,0] (15.88A)

NISE: Non-translating interpenetration symmetry elements

1: -1

PIC: [0,2,0][1,0,0][0,0,1] (PICVR=2)

Zt=2; Zn=2

Class IIIa Z=4[2*2]

Coordination sequences

Zn1: 1 2 3 4 5 6 7 8 9 10
Num 4 12 24 42 64 92 124 162 204 252
Cum 5 17 41 83 147 239 363 525 729 981

TD10=981

Vertex symbols for selected sublattice

Zn1 Point symbol:{6^6}
Extended point symbol:[6(2).6(2).6(2).6(2).6(2).6(2)]

Point symbol for net: {6^6}
4-c net; uninodal net

Topological type: dia Diamond; 4/6/c1; sqc6 (topos&RCSR.ttd) {6^6} - VS [6(2).6(2).6(2).6(2).6(2).6(2)] (16813 types in 3 databases)

##
TOPOS analysis results for **2**
##

Topology for Zn1

Atom Zn1 links by bridge ligands and has

Common vertex with					R(A-A)	
Zn 1	0.2498	0.7467	0.8170	(-1 1 0)	12.146A	1
Zn 1	1.2498	0.7467	-0.1830	(0 1-1)	12.146A	1
Zn 1	0.2498	-0.2533	-0.1830	(-1 0-1)	12.295A	1
Zn 1	1.2498	-0.2533	0.8170	(0 0 0)	12.295A	1

Topology for Zn2

Atom Zn2 links by bridge ligands and has

Common vertex with					R(A-A)	
Zn 2	-0.2538	0.7470	0.3595	(-1 1-1)	12.153A	1
Zn 2	0.7462	0.7470	1.3595	(0 1 0)	12.153A	1
Zn 2	-0.2538	-0.2530	1.3595	(-1 0 0)	12.288A	1
Zn 2	0.7462	-0.2530	0.3595	(0 0-1)	12.288A	1

Structural group analysis

Structural group No 1

Structure consists of 3D framework with Zn
There are 2 interpenetrating nets
FIV: Full interpenetration vectors

[1,0,0] (10.44A)

PIC: [2,0,0][1,0,1][1,1,0] (PICVR=2)

Zt=2; Zn=1

Class Ia Z=2

Coordination sequences

Zn1: 1 2 3 4 5 6 7 8 9 10
Num 4 12 24 42 64 92 124 162 204 252
Cum 5 17 41 83 147 239 363 525 729 981

TD10=981

Vertex symbols for selected sublattice

Zn1 Point symbol:{6^6}
Extended point symbol:[6(2).6(2).6(2).6(2).6(2).6(2)]

Point symbol for net: {6^6}
4-c net; uninodal net

Topological type: dia Diamond; 4/6/c1; sqc6 (topos&RCSR.ttd) {6^6} - VS [6(2).6(2).6(2).6(2).6(2).6(2)] (16813 types in 3 databases)

Structural group No 2

Structure consists of 3D framework with Zn
There are 2 interpenetrating nets
FIV: Full interpenetration vectors

[1,0,0] (10.44A)

PIC: [2,0,0][1,0,1][1,1,0] (PICVR=2)

Zt=2; Zn=1

Class Ia Z=2

Coordination sequences

Zn2: 1 2 3 4 5 6 7 8 9 10
Num 4 12 24 42 64 92 124 162 204 252
Cum 5 17 41 83 147 239 363 525 729 981

TD10=981

Vertex symbols for selected sublattice

Zn2 Point symbol:{6^6}

Extended point symbol:[6(2).6(2).6(2).6(2).6(2).6(2)]

Point symbol for net: {6^6}

4-c net; uninodal net

Topological type: dia Diamond; 4/6/c1; sqc6 (topos&RCSR.ttd) {6^6} - VS [6(2).6(2).6(2).6(2).6(2).6(2)] (16813 types in 3 databases)

Totally **4(2+2)** interpenetrating nets

Table S1 Bond Lengths for **1.**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Zn1	O3	1.981(2)	N6	C18	1.350(4)
Zn1	N3	2.056(2)	O2	C1	1.230(5)
Zn1	N4	2.066(3)	N2	C9	1.302(4)
Zn1	O1	2.043(3)	C13	C14	1.383(5)
Zn1	O2	2.327(3)	C13	C12	1.383(5)
Zn1	$C10^{1}$	2.586(3)	C14	C15	1.384(4)
O3	$C10^{1}$	1.254(4)	C10	$Zn1^{2}$	2.586(3)
N1	C8	1.348(4)	C10	$O3^{2}$	1.254(4)
N1	C9	1.371(4)	C10	C11	1.504(4)
N1	C5	1.426(4)	C12	C11	1.387(4)
N3	N2	1.381(4)	C2	C3	1.381(5)
N3	C8	1.307(4)	C2	$C1^{3}$	1.509(5)
O4	C10	1.230(4)	C2	C7	1.376(6)
N4	C17	1.309(4)	C3	C4	1.401(5)
N4	N5	1.365(4)	C5	C6	1.396(5)
C17	N6	1.339(4)	C5	C4	1.376(4)
O1	C1	1.259(5)	N5	C18	1.304(5)
C16	C11	1.397(4)	C6	C7	1.390(5)
C16	C15	1.380(4)	C1	$C2^{4}$	1.509(5)
N6	C14	1.436(4)			

Table S2 Bond Angles for **1**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O3	Zn1	N3	103.94(10)	C12	C13	C14	118.5(3)
O3	Zn1	N4	93.08(10)	N3	C8	N1	109.5(3)
O3	Zn1	O1	149.95(12)	C13	C14	N6	119.1(3)
O3	Zn1	O2	103.87(10)	C13	C14	C15	121.7(3)
O3	Zn1	$C10^{1}$	28.10(10)	C15	C14	N6	119.2(3)
N3	Zn1	N4	98.13(10)	$O3^{2}$	C10	$Zn1^{2}$	48.07(15)
N3	Zn1	O2	150.63(10)	$O3^{2}$	C10	C11	116.8(3)
N3	Zn1	$C10^{1}$	96.61(10)	O4	C10	$Zn1^{2}$	74.52(18)
N4	Zn1	O2	89.61(11)	O4	C10	$O3^{2}$	122.5(3)
N4	Zn1	$C10^{1}$	121.14(10)	O4	C10	C11	120.6(3)
O1	Zn1	N3	91.53(11)	C11	C10	$Zn1^{2}$	164.6(2)
O1	Zn1	N4	110.29(11)	C13	C12	C11	120.9(3)
O1	Zn1	O2	59.33(11)	C3	C2	$C1^{3}$	120.9(3)

O1	Zn1	C10[1]	125.89(11)	C7	C2	C3	120.5(3)
O2	Zn1	C10[1]	103.52(10)	C7	C2	C1[3]	118.6(3)
C10[1]	O3	Zn1	103.8(2)	C16	C11	C10	119.6(3)
C8	N1	C9	105.3(2)	C12	C11	C16	119.5(3)
C8	N1	C5	127.5(3)	C12	C11	C10	120.9(3)
C9	N1	C5	127.2(3)	N2	C9	N1	110.4(3)
N2	N3	Zn1	121.91(18)	C2	C3	C4	120.1(3)
C8	N3	Zn1	129.4(2)	C16	C15	C14	119.3(3)
C8	N3	N2	108.5(2)	C6	C5	N1	118.3(3)
C17	N4	Zn1	123.4(2)	C4	C5	N1	119.8(3)
C17	N4	N5	108.2(3)	C4	C5	C6	121.9(3)
N5	N4	Zn1	128.1(2)	C18	N5	N4	105.6(3)
N4	C17	N6	110.1(3)	C7	C6	C5	118.2(3)
C1	O1	Zn1	94.9(2)	C5	C4	C3	118.6(3)
C15	C16	C11	120.0(3)	O1	C1	C2[4]	117.1(4)
C17	N6	C14	126.0(3)	O2	C1	O1	122.0(3)
C17	N6	C18	104.5(3)	O2	C1	C2[4]	120.9(4)
C18	N6	C14	129.6(3)	C2	C7	C6	120.7(3)
C1	O2	Zn1	82.7(2)	N5	C18	N6	111.6(3)
C9	N2	N3	106.3(2)				

[1]-1/2+X,-1/2-Y,-Z; [2]1/2+X,-1/2-Y,-Z; [3]+X,1/2-Y,-1/2+Z; [4]+X,1/2-Y,1/2+Z

Table S3 Bond Lengths for **2**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Zn1	O4	2.097(8)	N4	C18	1.386(14)
Zn1	N2	2.015(8)	C29	C28	1.486(15)
Zn1	O1	1.980(6)	C29	C34	1.383(15)
Zn1	O3	2.284(10)	C29	C30	1.436(16)
Zn1	N5	2.021(8)	C15	C14	1.397(15)
Zn2	O8	2.133(8)	C15	C16	1.415(15)
Zn2	O5	1.978(6)	C23	C22	1.409(14)
Zn2	N8	2.093(9)	C23	C24[2]	1.343(17)
Zn2	O7	2.358(9)	C28	Zn2[3]	2.536(11)
Zn2	N11	2.073(9)	C28	O8[3]	1.284(14)
O8	C28[1]	1.284(14)	C28	O7[3]	1.221(15)
O5	C19	1.247(12)	C19	C20	1.525(13)
N8	C27	1.312(12)	C14	C13	1.364(13)
N8	N9	1.355(13)	C20	C21	1.408(15)
O4	C10	1.243(14)	C20	C25	1.386(14)

N2	C9	1.289(12)	C2	C3	1.411(16)
N2	N3	1.422(14)	C2	C1[4]	1.519(14)
C32	N10	1.408(12)	C2	C7	1.423(15)
C32	C31	1.472(14)	C31	C30	1.316(15)
C32	C33	1.354(15)	C36	N12	1.306(15)
O1	C1	1.254(12)	C16	C11	1.384(15)
O7	C28[1]	1.221(15)	N6	C18	1.265(14)
O3	C10	1.267(14)	C11	C10[5]	1.415(16)
C35	N11	1.252(12)	C11	C12	1.428(14)
C35	N10	1.327(13)	C21	C22[6]	1.381(16)
O6	C19	1.222(12)	C34	C33	1.413(14)
N1	C9	1.294(13)	C4	C3	1.302(17)
N1	C5	1.443(15)	C4	C5	1.409(16)
N1	C8	1.441(16)	C10	C11[7]	1.415(16)
N5	C17	1.312(12)	C22	C21[2]	1.381(16)
N5	N6	1.407(11)	C5	C6	1.389(17)
N7	C27	1.345(12)	C8	N3	1.300(19)
N7	C23	1.415(12)	C6	C7	1.340(18)
N7	C26	1.412(13)	N9	C26	1.352(15)
N11	N12	1.380(13)	C12	C13	1.383(13)
C17	N4	1.353(12)	C25	C24	1.375(14)
N10	C36	1.320(13)	C1	C2[8]	1.519(14)
O2	C1	1.251(12)	C24	C23[6]	1.343(17)
N4	C14	1.445(12)			

Table S4 Bond Angles for **2**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O4	Zn1	O3	58.2(3)	C14	C15	C16	118.9(9)
N2	Zn1	O4	96.0(4)	C22	C23	N7	118.1(9)
N2	Zn1	O3	103.5(4)	C24[2]	C23	N7	120.7(9)
N2	Zn1	N5	115.2(4)	C24[2]	C23	C22	120.8(9)
O1	Zn1	O4	109.3(3)	O8[3]	C28	Zn2[3]	57.2(5)
O1	Zn1	N2	94.3(3)	O8[3]	C28	C29	116.9(11)
O1	Zn1	O3	159.0(3)	O7[3]	C28	Zn2[3]	67.6(7)
O1	Zn1	N5	100.3(3)	O7[3]	C28	O8[3]	124.7(11)
N5	Zn1	O4	134.9(3)	O7[3]	C28	C29	118.4(10)
N5	Zn1	O3	82.4(3)	C29	C28	Zn2[3]	172.7(9)
O8	Zn2	O7	59.0(3)	O5	C19	C20	117.0(8)
O5	Zn2	O8	107.7(3)	O6	C19	O5	122.4(9)
O5	Zn2	N8	95.6(3)	O6	C19	C20	120.5(9)

O5	Zn2	O7	160.4(3)	C15	C14	N4	118.0(8)
O5	Zn2	N11	102.0(3)	C13	C14	N4	120.2(9)
N8	Zn2	O8	100.9(4)	C13	C14	C15	121.6(9)
N8	Zn2	O7	100.9(3)	C21	C20	C19	121.8(9)
N11	Zn2	O8	135.4(3)	C25	C20	C19	119.0(8)
N11	Zn2	N8	108.5(4)	C25	C20	C21	118.9(9)
N11	Zn2	O7	82.7(3)	C3	C2	C1[4]	125.1(10)
C28[1]	O8	Zn2	92.4(7)	C3	C2	C7	116.5(10)
C19	O5	Zn2	110.8(6)	C7	C2	C1[4]	118.2(9)
C27	N8	Zn2	125.7(7)	C30	C31	C32	120.4(10)
C27	N8	N9	111.0(8)	N12	C36	N10	111.7(10)
N9	N8	Zn2	122.7(6)	C11	C16	C15	120.3(10)
C10	O4	Zn1	97.2(7)	C18	N6	N5	107.3(8)
C9	N2	Zn1	132.1(7)	N2	C9	N1	114.4(9)
C9	N2	N3	106.6(8)	C16	C11	C10[5]	120.4(10)
N3	N2	Zn1	120.3(7)	C16	C11	C12	118.4(10)
N10	C32	C31	121.8(9)	C10[5]	C11	C12	121.2(10)
C33	C32	N10	120.8(9)	C22[6]	C21	C20	120.3(10)
C33	C32	C31	117.4(10)	C29	C34	C33	120.1(10)
C1	O1	Zn1	111.4(6)	C36	N12	N11	103.3(9)
C28[1]	O7	Zn2	83.8(7)	C31	C30	C29	122.2(10)
C10	O3	Zn1	87.8(8)	C3	C4	C5	119.5(11)
N11	C35	N10	110.8(8)	N6	C18	N4	110.9(10)
C9	N1	C5	130.0(10)	O4	C10	O3	116.7(10)
C9	N1	C8	103.0(9)	O4	C10	C11[7]	123.4(11)
C8	N1	C5	126.0(11)	O3	C10	C11[7]	119.9(11)
C17	N5	Zn1	130.2(6)	C4	C3	C2	123.0(10)
C17	N5	N6	106.8(7)	C32	C33	C34	122.1(10)
N6	N5	Zn1	123.0(6)	C21[2]	C22	C23	118.3(10)
C27	N7	C23	130.6(8)	C4	C5	N1	121.9(11)
C27	N7	C26	106.1(8)	C6	C5	N1	117.9(11)
C26	N7	C23	123.3(8)	C6	C5	C4	119.7(12)
C35	N11	Zn2	130.2(7)	N3	C8	N1	109.3(12)
C35	N11	N12	109.1(8)	C7	C6	C5	120.3(12)
N12	N11	Zn2	120.6(6)	C26	N9	N8	106.2(8)
N8	C27	N7	108.9(8)	C13	C12	C11	121.1(9)
N5	C17	N4	110.1(8)	N9	C26	N7	107.8(9)
C35	N10	C32	129.4(8)	C24	C25	C20	119.4(10)
C36	N10	C32	126.1(9)	C8	N3	N2	105.4(9)
C36	N10	C35	104.5(8)	O1	C1	C2[8]	117.4(9)
C17	N4	C14	127.4(8)	O2	C1	O1	126.3(9)

C17	N4	C18	104.4(8)	O2	C1	C2[8]	116.2(9)
C18	N4	C14	127.6(9)	C14	C13	C12	119.4(9)
C34	C29	C28	119.1(10)	C23[6]	C24	C25	121.3(10)
C34	C29	C30	117.7(9)	C6	C7	C2	120.7(11)
C30	C29	C28	122.9(10)				

[1]1/2+X,1-Y,1/2+Z; [2]1/2+X,-Y,-1/2+Z; [3]-1/2+X,1-Y,-1/2+Z; [4]-1/2+X,-Y,-1/2+Z; [5]1/2+X,1-Y,-1/2+Z; [6]-1/2+X,-Y,1/2+Z; [7]-1/2+X,1-Y,1/2+Z; [8]1/2+X,-Y,1/2+Z