Supporting Information for:

Auxiliary ligand-directed synthesis of cadmium (II) and zinc (II) complexes from 1-D chains to 3-D architectures with 5-nitroisophthalate

Xinyi Lu, Junwei Ye*, Wei Li, WeitaoGong, Lijian Yang, Yuan Lin and Guiling Ning*

State Key Laboratory of Fine Chemicals and School of Chemical Engineering, Dalian University of Technology, 2 Linggong Road, Dalian 116012, P. R. China.

* *Corresponding author E-mail: junweiye@dlut.edu.cn; ninggl@dlut.edu.cn; Fax: +86-411-84986067.*

CAPTIONS:

Scheme S1. The coordination modes of NIPH ligand.

Fig. S2. Thermogravimetric curve for (a) **1**, (b) **2**, (c) **3,** (d) **4**.

Fig. S3. Thermogravimetric curve for experimental and ion exchanged samples for **4** and **4a.**

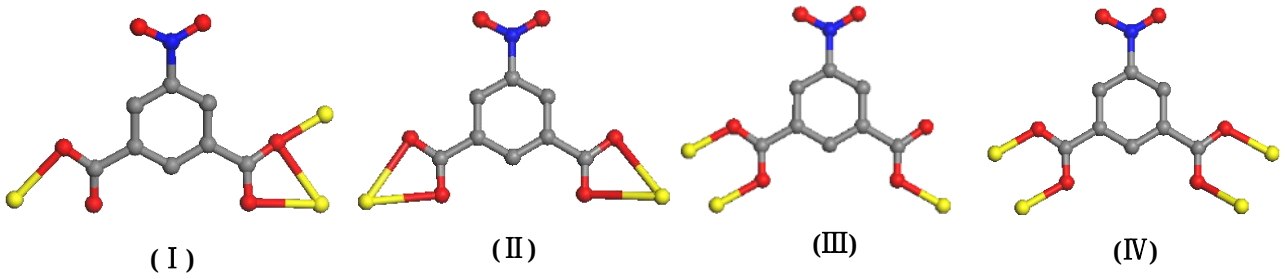
Fig. S4. SEM image (a) and EDS pattern (b) of the K^+ exchange products for **5**. (c) X-ray powder diffraction patterns of **5**: I. ion exchanged samples. II. experimental, III. simulated.

Table S1. Selected bond lengths [Å] for **1** and **2**.

Table S2. Selected bond lengths [Å] for **3-5.**

Table S3. Hydrogen bonds [Å and °] for **1-5.**

Scheme S1



Scheme S1. The coordination modes of NIPH ligand.

Figure S1.

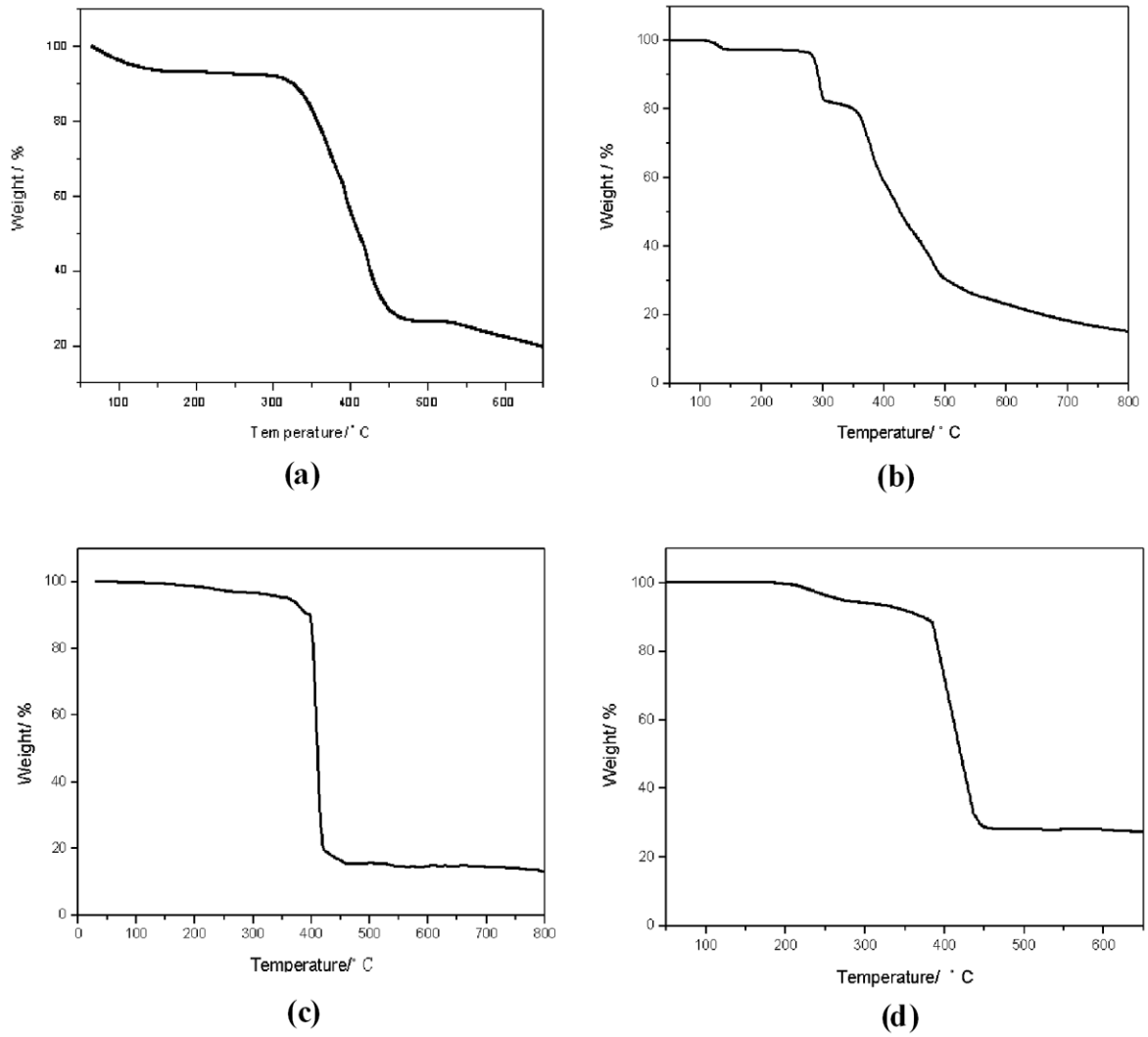


Fig. S2. Thermogravimetric curve for (a) **1**, (b) **2**, (c) **3,** (d) **4**.

Figure S3

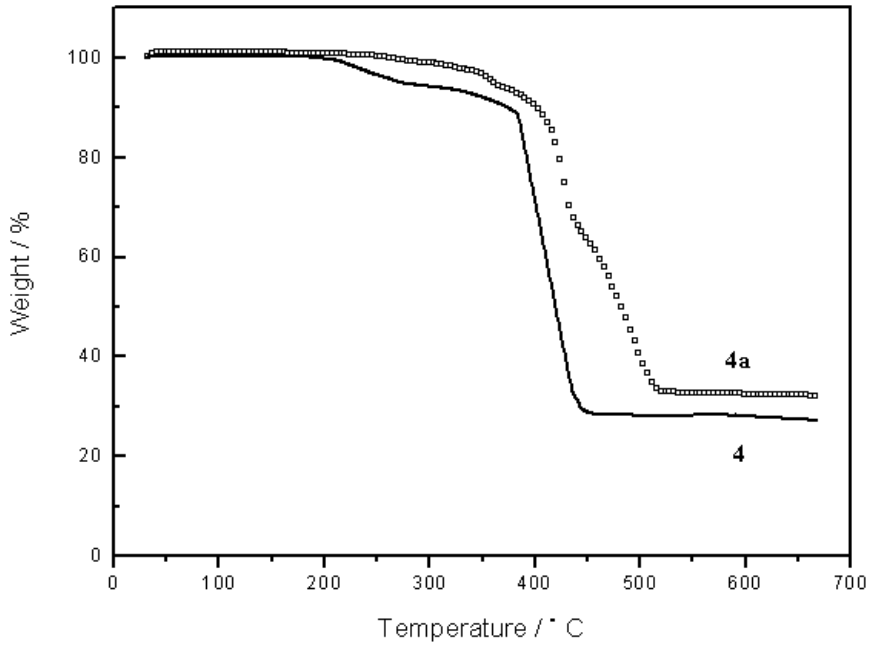


Fig. S3. Thermogravimetric curve for experimental and ion exchanged samples for **4** and **4a.**

Figure S4.

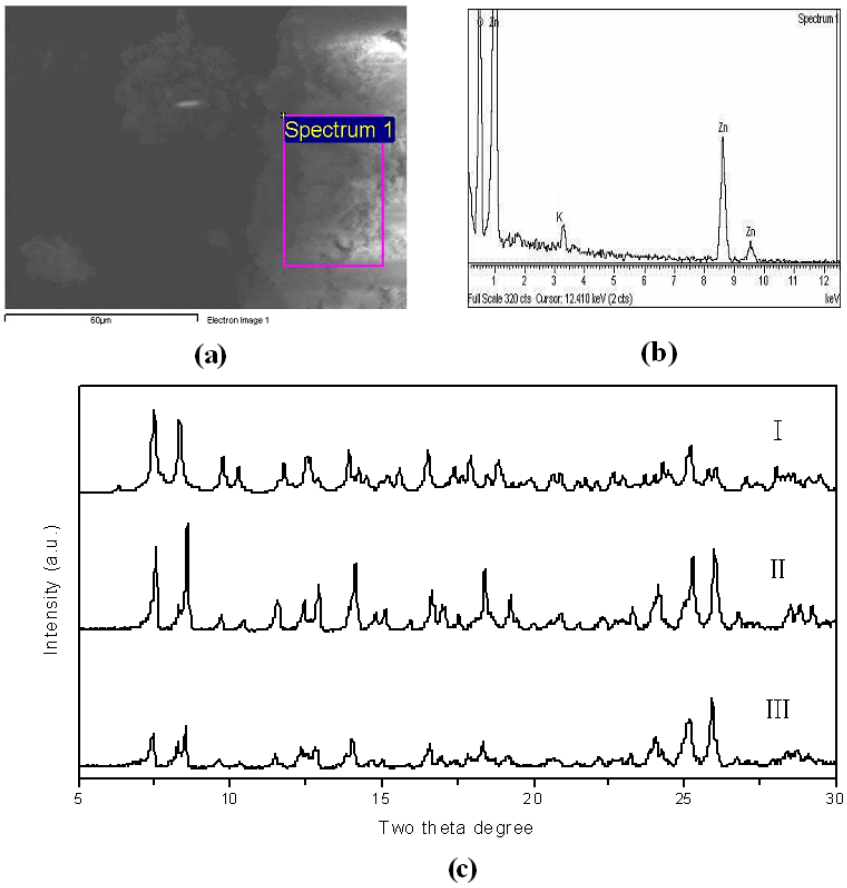


Fig. S4. SEM image (a) and EDS pattern (b) of the K^+ exchange products for **5**. (c) X-ray powder diffraction patterns of **5**: I. ion exchanged samples. II. experimental, III. simulated.

Table S1

Table S1. Selected bond lengths [Å] for **1** and **2**.

1			
Cd-O(4)$^{\#1}$	2.204(2)	Cd-O(2)	2.4701(19)
Cd-N(2)	2.230(2)	Cd-O(1)$^{\#2}$	2.5714(19)
Cd-O(7)	2.275(2)	Cd-O(1)	2.3402(19)
Cd-O(3)$^{\#1}$	2.794(2)	O(4)$^{\#1}$-Cd-O(2)	135.15(8)
O(4)$^{\#1}$-Cd-O(7)	87.22(9)	N(2)-Cd-O(2)	87.67(8)
N(2)-Cd-O(7)	104.93(10)	O(7)-Cd-O(2)	82.53(9)
O(4)$^{\#1}$-Cd-O(1)	90.70(7)	O(1)-Cd-O(2)	54.03(6)
N(2)-Cd-O(1)	120.64(8)	O(4)$^{\#1}$-Cd-O(1)$^{\#2}$	79.14(7)
O(7)-Cd-O(1)	111.38(9)	N(2)-Cd-O(1)$^{\#2}$	81.59(7)
O(2)-Cd-O(1)$^{\#2}$	111.45(7)	O(7)-Cd-O(1)$^{\#2}$	165.07(8)
O(1)-Cd-O(1)$^{\#2}$	75.13(7)	O(4)$^{\#1}$-Cd-N(2)	137.05(8)
Symmetry codes: #1 x,y,z-1, #2 -x+1,-y+2,-z			
2			
Cd-O(4)$^{\#1}$	2.2543(19)	Cd-O(1)	2.462(2)
Cd-N(2)	2.308(3)	Cd-O(3)$^{\#1}$	2.7105(19)
Cd-O(2)	2.408(2)	Cd-N(4)	2.285(2)
Cd-O(7)	2.420(3)	N(2)-Cd-O(1)	92.10(8)
O(4)$^{\#1}$-Cd-N(4)	138.88(7)	O(7)-Cd-O(1)	89.00(8)
O(4)$^{\#1}$-Cd-N(2)	92.97(9)	O(3)$^{\#1}$-Cd-C(7)	155.52(8)
N(4)-Cd-N(2)	91.15(9)	O(2)-Cd-O(1)	53.18(7)
O(4)$^{\#1}$-Cd-O(2)	130.90(7)	O(7)-Cd-O(1)	89.00(8)
N(4)-Cd-O(2)	87.90(8)	O(4)$^{\#1}$-Cd-O(3)$^{\#1}$	51.59(6)
N(2)-Cd-O(2)	101.62(9)	N(4)-Cd-O(3)$^{\#1}$	87.53(7)
O(4)$^{\#1}$-Cd-O(7)	86.69(9)	N(2)-Cd-O(3)$^{\#1}$	90.19(8)
N(4)-Cd-O(7)	88.35(9)	O(2)-Cd-O(3)$^{\#1}$	167.42(9)
N(2)-Cd-O(7)	178.78(8)	O(7)-Cd-O(3)$^{\#1}$	88.68(8)
O(2)-Cd-O(7)	79.48(10)	O(1)-Cd-O(3)$^{\#1}$	131.54(6)
O(4)$^{\#1}$-Cd-O(1)	79.96(7)	O(2)-Cd-O(1)	53.18(7)
N(4)-Cd-O(1)	140.76(7)		
Symmetry codes: #1 x,y+1,z			

Table S2

Table S2. Selected bond lengths [Å] for **3-5.**

3			
Zn(1)-O(13)	1.9411(19)	Zn(2)-O(13)	2.092(2)
Zn(1)-O(9)$^{\#1}$	1.945(2)	Zn(2)-O(13)$^{\#2}$	2.096(2)
Zn(1)-O(2)	1.985(2)	Zn(2)-O(14)	2.266(3)
Zn(1)-O(7)$^{\#2}$	2.001(2)	Zn(2)-O(8)	2.082(2)
Zn(2)-O(4)$^{\#3}$	1.989(2)	Zn(2)-O(1)$^{\#2}$	2.087(2)
O(13)-Zn(1)-O(9)$^{\#1}$	108.23(9)	O(4)$^{\#3}$-Zn(2)-O(14)	80.10(10)
O(13)-Zn(1)-O(2)	116.71(10)	O(8)-Zn(2)-O(14)	89.73(11)
O(9)$^{\#1}$-Zn(1)-O(2)	111.53(10)	O(1)$^{\#2}$-Zn(2)-O(14)	78.63(10)
O(13)-Zn(1)-O(7)$^{\#2}$	106.71(9)	O(13)-Zn(2)-O(14)	95.96(11)
O(9)$^{\#1}$-Zn(1)-O(7)$^{\#2}$	115.59(10)	O(13)$^{\#2}$-Zn(2)-O(14)	172.36(9)
O(2)-Zn(1)-O(7)$^{\#2}$	97.97(10)	O(8)-Zn(2)-O(13)	172.17(8)
O(4)$^{\#3}$-Zn(2)-O(8)	95.76(10)	O(1)$^{\#2}$-Zn(2)-O(13)	86.66(9)
O(4)#3-Zn(2)-O(1)$^{\#2}$	158.12(9)	O(4)$^{\#3}$-Zn(2)-O(13)$^{\#2}$	106.90(9)
O(8)-Zn(2)-O(1)$^{\#2}$	89.19(10)	O(8)-Zn(2)-O(13)$^{\#2}$	92.56(8)
O(4)$^{\#3}$-Zn(2)-O(13)	90.54(9)	O(1)$^{\#2}$-Zn(2)-O(13)$^{\#2}$	94.10(9)
O(13)-Zn(2)-O(13)$^{\#2}$	81.13(8)		
Symmetry codes: #1 -x-2,-y,-z, #2 -x-1,-y,-z, #3 -x-1,-y+1,-z			
4			
Zn(1)-O(14)	1.9342(18)	Zn(3)-O(8)$^{\#2}$	2.1469(16)
Zn(1)-O(25)	1.9369(17)	Zn(3)-O(25)$^{\#1}$	2.1551(18)
Zn(1)-O(7)	1.9411(17)	Zn(4)-O(28)$^{\#4}$	2.1117(17)
Zn(1)-O(1)	1.9616(19)	Zn(4)-O(19)	2.1260(17)
Zn(2)-O(26)	1.901(2)	Zn(4)-O(10)$^{\#5}$	2.1875(16)
Zn(2)-O(21)$^{\#1}$	1.9417(17)	Zn(4)-O(27)	2.054(2)
Zn(2)-O(13)	1.9587(18)	Zn(4)-O(28)$^{\#3}$	2.0754(17)
Zn(2)-O(20)	1.9707(17)	Zn(4)-O(16)$^{\#3}$	2.1008(18)
Zn(3)-O(26)$^{\#1}$	1.985(2)	Zn(5)-O(3)$^{\#6}$	1.9140(18)
Zn(3)-O(25)$^{\#2}$	2.0651(17)	Zn(5)-O(28)	1.9456(17)
Zn(3)-O(2)$^{\#2}$	2.0880(19)	Zn(5)-O(9)$^{\#7}$	1.9501(17)
Zn(3)-O(22)	2.1433(17)	Zn(5)-O(15)	1.9634(18)
O(14)-Zn(1)-O(25)	115.58(8)	O(25)$^{\#2}$-Zn(3)-O(25)$^{\#1}$	81.26(7)
O(14)-Zn(1)-O(7)	109.48(9)	O(2)$^{\#2}$-Zn(3)-O(25)$^{\#1}$	174.67(7)
O(25)-Zn(1)-O(7)	114.29(8)	O(22)-Zn(3)-O(25)$^{\#1}$	95.84(8)
O(14)-Zn(1)-O(1)	103.25(8)	O(8)$^{\#2}$-Zn(3)-O(25)$^{\#1}$	88.15(7)

O(25)-Zn(1)-O(1)	107.41(8)	O(27)-Zn(4)-O(28)$^{\#3}$	168.90(8)
O(7)-Zn(1)-O(1)	105.73(8)	O(27)-Zn(4)-O(16)$^{\#3}$	90.71(9)
O(26)-Zn(2)-O(21)$^{\#1}$	115.97(9)	O(28)$^{\#3}$-Zn(4)-O(16)$^{\#3}$	98.76(7)
O(26)-Zn(2)-O(13)	113.24(10)	O(27)-Zn(4)-O(28)$^{\#4}$	89.62(8)
O(21)$^{\#1}$-Zn(2)-O(13)	111.91(8)	O(28)$^{\#3}$-Zn(4)-O(28)$^{\#4}$	80.30(7)
O(26)-Zn(2)-O(20)	98.73(9)	O(16)$^{\#3}$-Zn(4)-O(28)$^{\#4}$	173.30(7)
O(21)$^{\#1}$-Zn(2)-O(20)	111.57(8)	O(27)-Zn(4)-O(19)	100.09(8)
O(13)-Zn(2)-O(20)	103.99(7)	O(28)$^{\#3}$-Zn(4)-O(19)	86.44(7)
O(26)$^{\#1}$-Zn(3)-O(25)$^{\#2}$	170.04(9)	O(16)$^{\#3}$-Zn(4)-O(19)	85.79(7)
O(26)$^{\#1}$-Zn(3)-O(2)$^{\#2}$	95.05(9)	O(28)$^{\#4}$-Zn(4)-O(19)	100.74(7)
O(25)$^{\#2}$-Zn(3)-O(2)$^{\#2}$	94.00(7)	O(27)-Zn(4)-O(10)$^{\#5}$	84.36(8)
O(26)$^{\#1}$-Zn(3)-O(22)	96.82(9)	O(28)$^{\#3}$-Zn(4)-O(10)$^{\#5}$	90.10(7)
O(25)$^{\#2}$-Zn(3)-O(22)	87.88(7)	O(16)$^{\#3}$-Zn(4)-O(10)$^{\#5}$	88.42(7)
O(2)$^{\#2}$-Zn(3)-O(22)	86.38(8)	O(28)$^{\#4}$-Zn(4)-O(10)$^{\#5}$	84.96(7)
O(26)$^{\#2}$-Zn(3)-O(8)$^{\#3}$	85.58(9)	O(19)-Zn(4)-O(10)$^{\#5}$	172.72(7)
O(25)$^{\#3}$-Zn(3)-O(8)$^{\#3}$	90.37(7)	O(3)$^{\#6}$-Zn(5)-O(28)	106.31(8)
O(2)$^{\#3}$-Zn(3)-O(8)$^{\#3}$	89.44(8)	O(3)$^{\#6}$-Zn(5)-O(9)$^{\#7}$	115.01(9)
O(22)-Zn(3)-O(8)$^{\#3}$	175.35(7)	O(28)-Zn(5)-O(9)$^{\#7}$	106.66(8)
O(26)$^{\#2}$-Zn(3)-O(25)$^{\#2}$	89.51(9)	O(3)$^{\#6}$-Zn(5)-O(15)	111.51(9)
O(9)$^{\#7}$-Zn(5)-O(15)	109.08(8)	O(28)-Zn(5)-O(15)	107.91(8)
Symmetry codes:#1 -x+1,-y,-z, #2 x-1,y,z, #3 -x+1,-y+1,-z, #4 x,y,z-1, #5 x,y+1,z-1, #6 -x+2,-y,-z+1, #7 -x+1,-y,-z+1,			
5			
Zn(1)-O(26)$^{\#1}$	1.985(3)	Zn(3)-O(20)$^{\#6}$	1.944(3)
Zn(1)-O(27)$^{\#2}$	2.064(3)	Zn(3)-O(13)	1.959(3)
Zn(1)-O(14)$^{\#2}$	2.090(3)	Zn(4)-O(28)	2.057(3)
Zn(1)-O(27)$^{\#3}$	2.145(3)	Zn(4)-O(25)	2.069(3)
Zn(1)-O(1)	2.151(3)	Zn(4)-O(4)	2.113(3)
Zn(1)-O(19)$^{\#4}$	2.153(3)	Zn(4)-O(10)	2.117(3)
Zn(2)-O(26)	1.897(3)	Zn(4)-O(28)$^{\#7}$	2.123(3)
Zn(2)-O(2)$^{\#1}$	1.946(3)	Zn(4)-O(22)	2.155(3)
Zn(2)-O(7)$^{\#5}$	1.954(3)	Zn(5)-O(15)$^{\#8}$	1.924(3)
Zn(2)-O(3)	1.976(3)	Zn(5)-O(21)	1.949(3)
Zn(3)-O(8)	1.930(3)	Zn(5)-O(28)	1.952(3)
Zn(3)-O(27)	1.942(3)	Zn(5)-O(9)	1.969(3)
O(26)$^{\#1}$-Zn(1)-O(27)$^{\#2}$	170.18(13)	O(8)-Zn(3)-O(13)	101.82(16)
O(26)$^{\#1}$-Zn(1)-O(14)$^{\#2}$	95.07(14)	O(27)-Zn(3)-O(13)	106.81(14)
O(27)$^{\#2}$-Zn(1)-O(14)$^{\#2}$	94.09(13)	O(20)$^{\#6}$-Zn(3)-O(13)	105.92(16)
O(26)$^{\#1}$-Zn(1)-O(27)$^{\#3}$	89.93(12)	O(28)-Zn(4)-O(25)	169.64(12)
O(27)$^{\#2}$-Zn(1)-O(27)$^{\#3}$	80.86(12)	O(28)-Zn(4)-O(4)	86.28(12)
O(14)$^{\#2}$-Zn(1)-O(27)$^{\#3}$	174.91(13)	O(25)-Zn(4)-O(4)	97.69(13)
O(26)$^{\#1}$-Zn(1)-O(1)	96.71(14)	O(28)-Zn(4)-O(10)	99.58(12)
O(27)$^{\#2}$-Zn(1)-O(1)	87.32(13)	O(25)-Zn(4)-O(10)	90.23(13)
O(14)$^{\#2}$-Zn(1)-O(1)	86.61(15)	O(4)-Zn(4)-O(10)	86.51(13)

O(27)$^{\#3}$-Zn(1)-O(1)	93.79(13)	O(28)-Zn(4)-O(28)$^{\#7}$	80.36(12)
O(26)$^{\#1}$-Zn(1)-O(19)$^{\#4}$	85.67(13)	O(25)-Zn(4)-O(28)$^{\#7}$	89.57(12)
O(27)$^{\#2}$-Zn(1)-O(19)$^{\#4}$	90.90(13)	O(4)-Zn(4)-O(28)$^{\#7}$	98.49(12)
O(14)$^{\#2}$-Zn(1)-O(19)$^{\#4}$	89.53(14)	O(10)-Zn(4)-O(28)$^{\#7}$	174.97(13)
O(27)$^{\#3}$-Zn(1)-O(19)$^{\#4}$	89.87(12)	O(28)-Zn(4)-O(22)	91.41(12)
O(1)-Zn(1)-O(19)$^{\#4}$	175.62(13)	O(25)-Zn(4)-O(22)	85.44(13)
O(26)-Zn(2)-O(2)$^{\#1}$	115.66(14)	O(4)-Zn(4)-O(22)	174.47(13)
O(26)-Zn(2)-O(7)$^{\#5}$	117.76(15)	O(10)-Zn(4)-O(22)	88.93(13)
O(2)$^{\#1}$-Zn(2)-O(7)$^{\#5}$	108.93(15)	O(28)$^{\#7}$-Zn(4)-O(22)	86.05(12)
O(26)-Zn(2)-O(3)	99.20(14)	O(15)$^{\#8}$-Zn(5)-O(21)	113.92(16)
O(2)$^{\#1}$-Zn(2)-O(3)	106.75(15)	O(15)$^{\#8}$-Zn(5)-O(28)	105.89(15)
O(7)$^{\#5}$-Zn(2)-O(3)	107.18(14)	O(21)-Zn(5)-O(28)	106.61(13)
O(8)-Zn(3)-O(27)	114.59(15)	O(15)$^{\#8}$-Zn(5)-O(9)	114.29(15)
O(8)-Zn(3)-O(20)$^{\#6}$	111.60(17)	O(21)-Zn(5)-O(9)	109.13(15)
O(27)-Zn(3)-O(20)$^{\#6}$	114.73(13)	O(28)-Zn(5)-O(9)	106.38(13)

Symmetry codes: #1 -x+1, -y-1, -z+2, #2 -x, -y, -z+2, #3 x, y-1, z, #4 x-1, y-1, z+1, #5 -x+1, -y, -z+2, #6 -x+1, -y+1, -z+1, #7 -x+1, -y, -z+1, #8 -x, -y+1,-z+1

Table S3

Table S3. Hydrogen bonds [Å and °] for **1-5.**

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
1				
N(3)-H(3A)...O(7)	0.86	2.45	3.230(4)	151.9
N(3)-H(3A)...O(3)$^{\#1}$	0.86	2.58	3.169(3)	126.1
N(3)-H(3B)...O(5)$^{\#2}$	0.86	2.14	2.988(3)	167.9
O(7)-H(7A)...O(2)$^{\#3}$	0.66(5)	2.07(5)	2.714(3)	164(5)
O(8)-H(8A)...O(3)$^{\#4}$	0.77(5)	2.06(5)	2.804(4)	162(4)
O(7)-H(7B)...O(8)$^{\#5}$	0.71(5)	2.03(5)	2.723(4)	165(5)
O(8)-H(8B)...O(6)$^{\#6}$	0.73(5)	2.47(5)	3.165(4)	161(5)
Symmetry codes: #1 x,y,z-1, #2 x+1,y-1,z-1, #3 -x+2,-y+2,-z, #4 -x+1,-y+1,-z+1, #5 x+1,y+1,z-1, #6 -x,-y+2,-z+1				
2				
N(5)-H(5B)...O(5)$^{\#1}$	0.86	2.67	3.079(3)	110.7
N(5)-H(5A)...O(6)$^{\#1}$	0.77	2.53	3.147(4)	138.8
N(3)-H(3B)...O(1)$^{\#2}$	0.79	2.35	3.060(4)	149.9
N(3)-H(3A)...O(1)$^{\#3}$	0.85	2.57	3.306(4)	145.0
N(3)-H(3A)...O(4)$^{\#4}$	0.85	2.53	3.142(3)	129.6
O(7)-H(7B)...O(3)$^{\#5}$	0.59	2.21	2.756(3)	157.1
Symmetry codes: #1 x+1,y,z+1, #2 -x+1,-y+1,-z, #3 x+1,y,z, #4 x+1,y+1,z, #5 -x,-y,-z+1				
3				
N(4)-H(4A)...O(10)$^{\#2}$	0.86	2.08	2.811(4)	142.0
N(4)-H(4B)...O(3)$^{\#1}$	0.86	1.92	2.769(4)	169.8
C(18)-H(18A)...O(10)$^{\#2}$	0.93	1.97	2.778(4)	144.8
C(18)-H(18A)...O(7)$^{\#3}$	0.93	2.63	3.209(4)	120.9
C(20)-H(20A)...O(6)$^{\#4}$	0.93	2.63	3.310(6)	130.6
Symmetry codes: #1 -x-1,-y,-z, #2 -x-2,-y-1,-z+1 #3 -x-1,-y-1,-z+1, #4 -x,-y,-z+1				
4				
O(28)-H(28A)...O(6)	0.69(3)	2.34(3)	2.986(3)	155(3)
O(27)-H(27A)...O(26)	0.75(5)	2.04(5)	2.786(3)	170(5)
O(25)-H(25)...O(17)$^{\#1}$	0.67(3)	2.31(4)	2.916(3)	152(4)
O(27)-H(27B)...O(5)$^{\#2}$	0.76(5)	2.19(5)	2.924(3)	162(5)
N(6)-H(6B)...O(24)$^{\#4}$	0.86	2.52	3.147(5)	130.8
N(5)-H(5A)...O(4)$^{\#3}$	0.86	1.93	2.692(4)	146.8
Symmetry codes: #1 -x+1,-y+1,-z, #2 x,y,z-1, #3 -x+2,-y,-z+1, #4 -x,-y+1,-z				
5				
O(25)-H(25A)...O(17)$^{\#2}$	0.69	2.32	2.911(5)	145.0

O(25)-H(25A)...O(22)	0.69	2.51	2.867(5)	115.1
O(25)-H(25B)...O(26)	0.71	2.08	2.781(5)	169.0
O(27)-H(27A)...O(11)[#1]	0.65	2.29	2.923(5)	166.1
O(28)-H(28)...O(18)	0.68	2.34	2.980(5)	158.0
N(5)-H(5A)...O(16)[#3]	0.86	1.93	2.700(8)	148.6
N(6)-H(6A)...O(3)[#2]	0.86	2.55	3.353(8)	155.4
N(6)-H(6B)...O(29)	0.86	2.00	2.835(10)	164.6
O(29)-H(29A)...N(6)	0.82	2.71	2.835(10)	90.3

Symmetry codes: #1 -x+1, -y, -z+2, #2 -x+1, -y, -z+1, #3 x+1,y,z