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Supporting information for article:

Seven new metal–organic frameworks assembled from semi-rigid polycarboxylate and auxiliary N-donor ligands: syntheses, structures and properties

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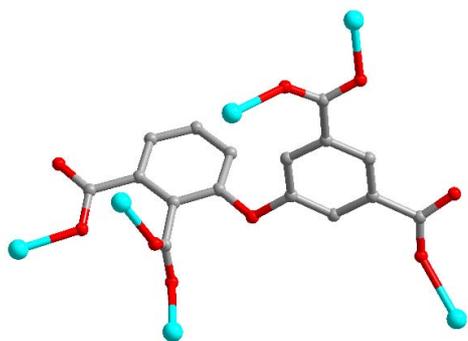
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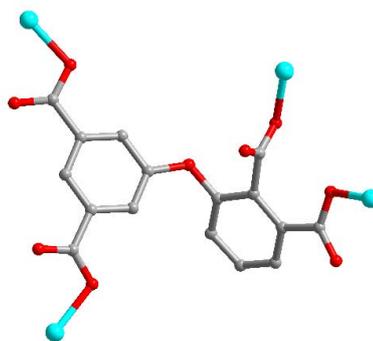
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Table S1. Selected Bond Lengths (Å) and Angles (°) for compounds **1-7**.

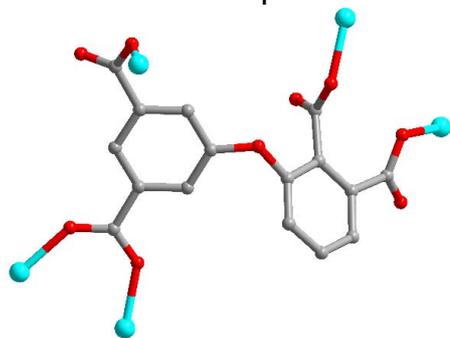
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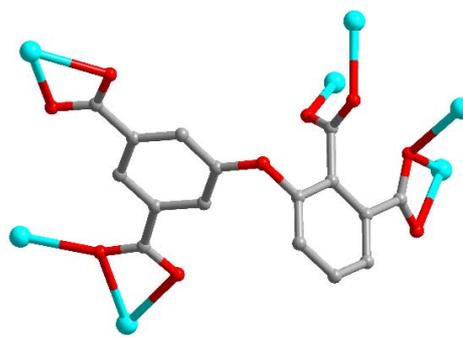
I



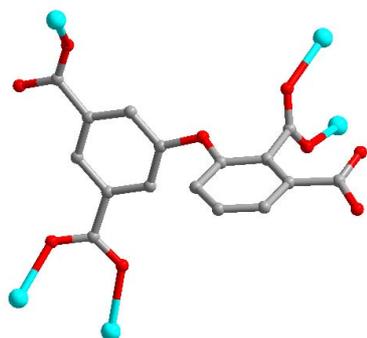
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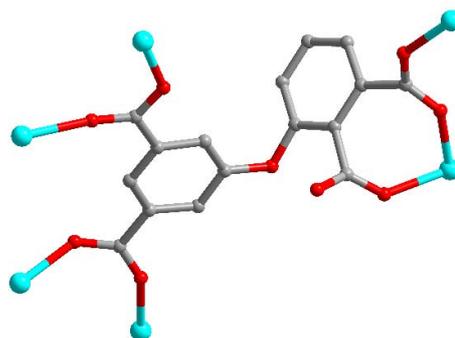
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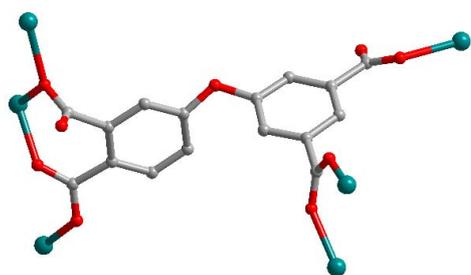
IV



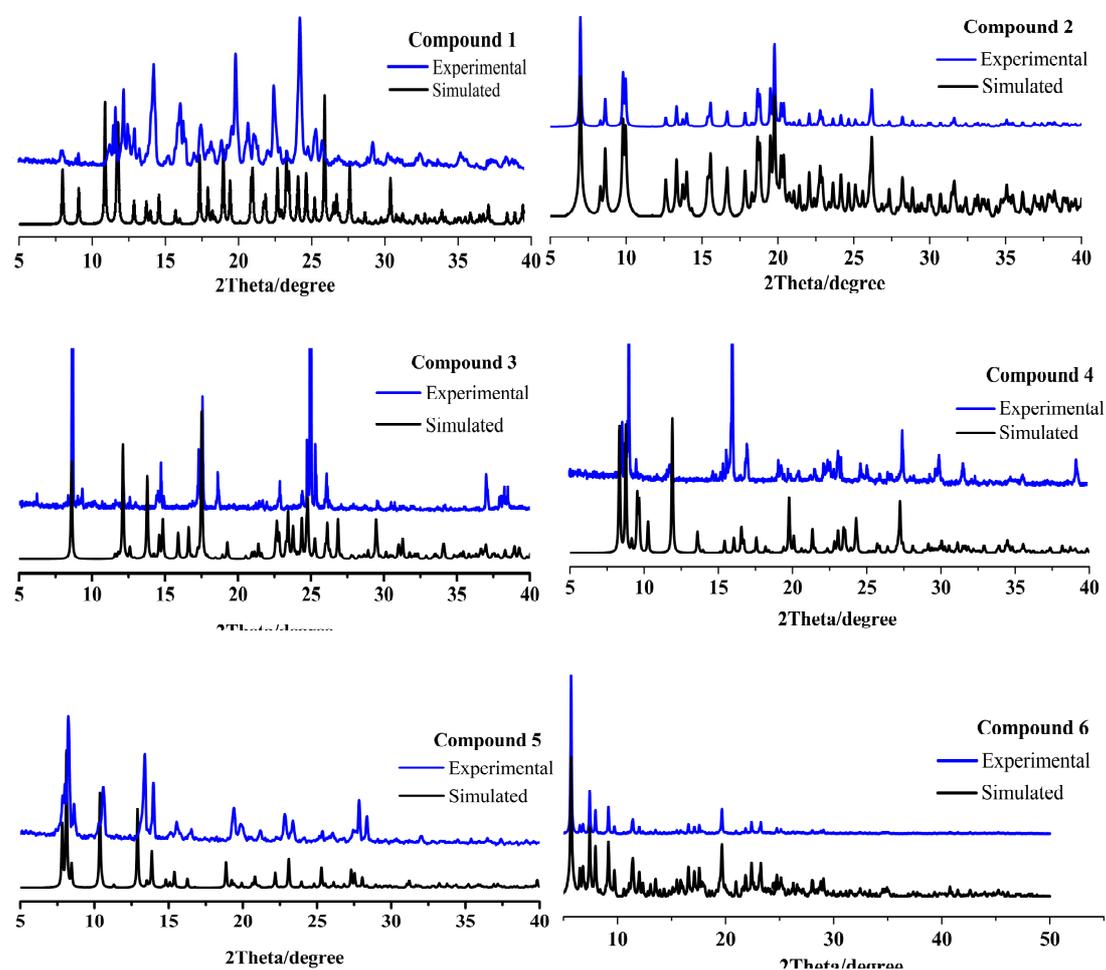
V



VI



VII

Scheme S1. Coordination modes of H₄L ligands in compounds 1-7.

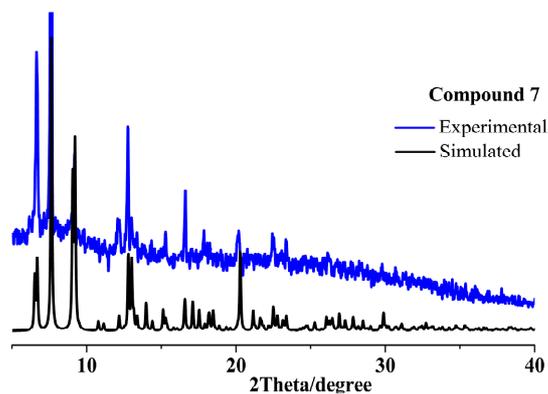


Fig. S1. PXRD patterns of compounds 1-7. (black) Simulated from single crystal structure data. (blue) Experimental data. The differences between the calculated and observed patterns in intensity may be due to the orientation of the crystals.

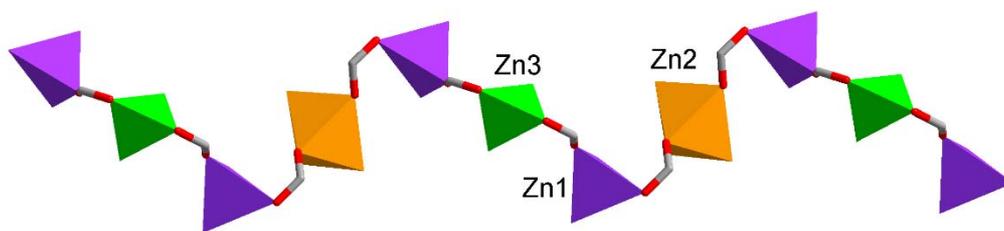


Fig. S2. 1D chain formed by Zn1, Zn2, Zn3 and bridged carboxyl group in compound 1.

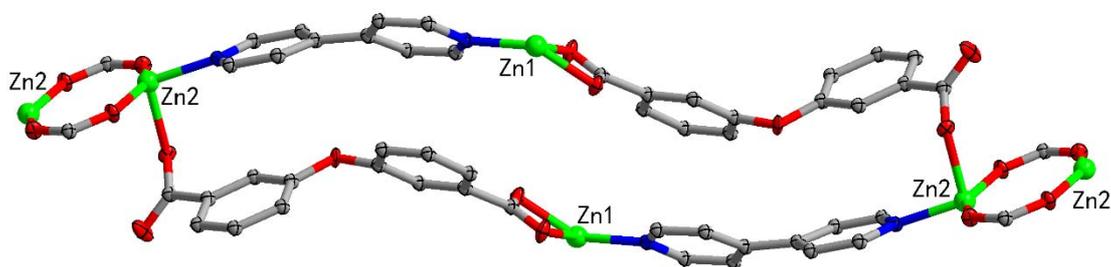


Fig. S3. The linkage between L_1^{4-} ligand and 4,4'-bipy in Zn (II) ion forms an elongated ring structure in compound 3.

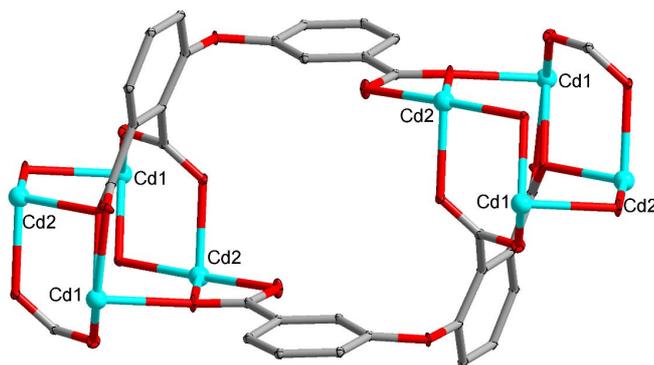


Fig. S4. The ligand of compound **4** forms a cyclic structure with a Cd (II) ion and a tetranuclear metal unit.

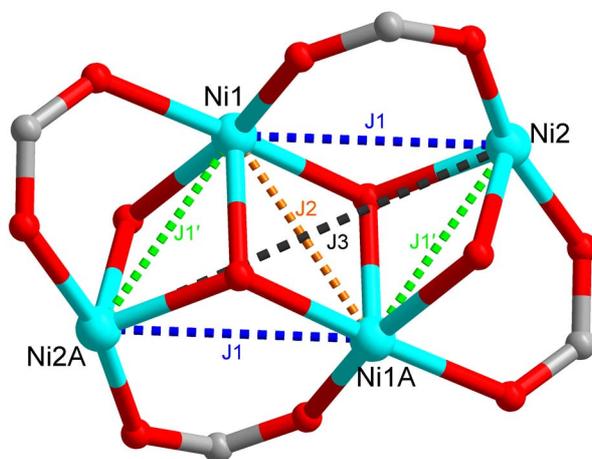


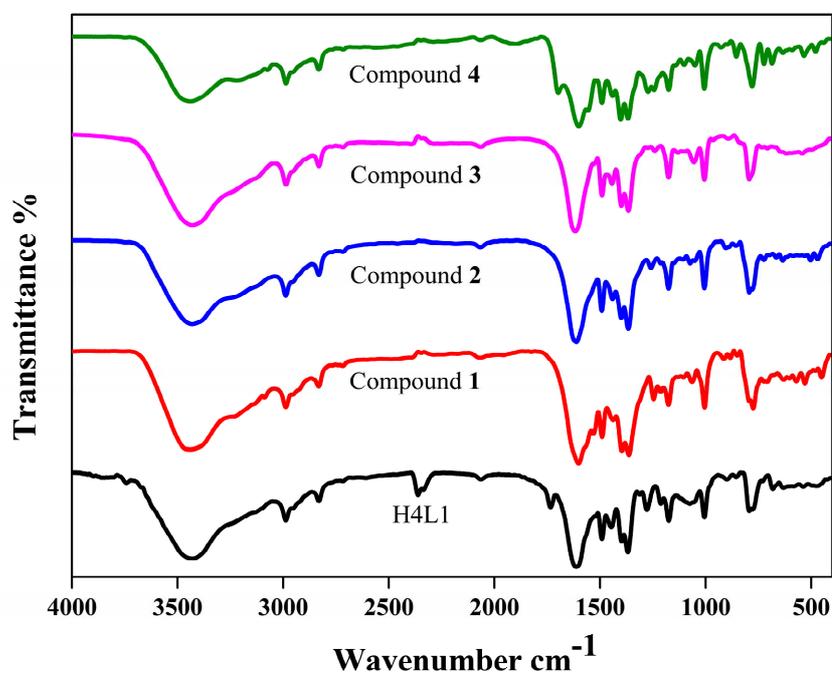
Fig. S5. The chair-shaped $[\text{Ni}_4(\mu_3\text{-OH})_2(\mu_2\text{-H}_2\text{O})_2(\text{COO})_4]^{2+}$ SBU in **5**. Considering the distance of Ni (II) ions in the tetranuclear nickel cluster of **5**, $[\text{Ni1}\cdots\text{Ni2}=3.5349(8)\text{ \AA}$, $\text{Ni2}\cdots\text{Ni1A}=3.0812(9)\text{ \AA}$, $\text{Ni1}\cdots\text{Ni1A}=3.1904(9)\text{ \AA}$, $\text{Ni2}\cdots\text{Ni2A}=5.8137(9)\text{ \AA}]$, we defined the $J1'\approx J1$. The tetranuclear nickel cluster can be considered as a parallelogram-shaped model, which provides three different magnetic exchange pathways: $J1$, $J2$ and $J3$.

The expression of the magnetic susceptibility of **5**:

$$\chi_{\text{Ni}_4}=(Ng^2\beta^2/3kT)[A/B]+TIP$$

$$A = [180 \exp((20J_1 + 6J_2 + 6J_3)/kT) + 84 \exp((12J_1 + 6J_2 + 6J_3)/kT) + 30 \exp((6J_1 + 6J_2 + 6J_3)/kT) + 6 \exp((2J_1 + 6J_2 + 6J_3)/kT) + 84 \exp((12J_1 + 6J_2 + 2J_3)/kT) + 30 \exp((6J_1 + 6J_2 + 2J_3)/kT) + 6 \exp((2J_1 + 6J_2 + 2J_3)/kT) + 30 \exp((6J_1 + 6J_2)/kT) + 84 \exp((12J_1 + 2J_2 + 6J_3)/kT) + 30 \exp((6J_1 + 2J_2 + 6J_3)/kT) + 6 \exp((2J_1 + 2J_2 + 6J_3)/kT) + 30 \exp((6J_1 + 2J_2 + 2J_3)/kT) + 6 \exp((2J_1 + 2J_2 + 2J_3)/kT) + 6 \exp((2J_1 + 2J_2)/kT)]$$

$$B = [9 \exp((20J_1 + 6J_2 + 6J_3)/kT) + 7 \exp((12J_1 + 6J_2 + 6J_3)/kT) + 5 \exp((6J_1 + 6J_2 + 6J_3)/kT) + 3 \exp((2J_1 + 6J_2 + 6J_3)/kT) + \exp((6J_2 + 6J_3)/kT) + 7 \exp((2J_1 + 6J_2 + 2J_3)/kT) + 5 \exp((6J_1 + 6J_2 + 2J_3)/kT) + 3 \exp((2J_1 + 6J_2 + 2J_3)/kT) + 5 \exp((6J_1 + 6J_2)/kT) + 7 \exp((12J_1 + 2J_2 + 6J_3)/kT) + 5 \exp((6J_1 + 2J_2 + 6J_3)/kT) + 3 \exp((2J_1 + 2J_2 + 6J_3)/kT) + 5 \exp((6J_1 + 2J_2 + 2J_3)/kT) + 3 \exp((2J_1 + 2J_2 + 2J_3)/kT) + \exp((2J_2 + 2J_3)/kT) + 3 \exp((2J_1 + 2J_2)/kT) + 1]$$



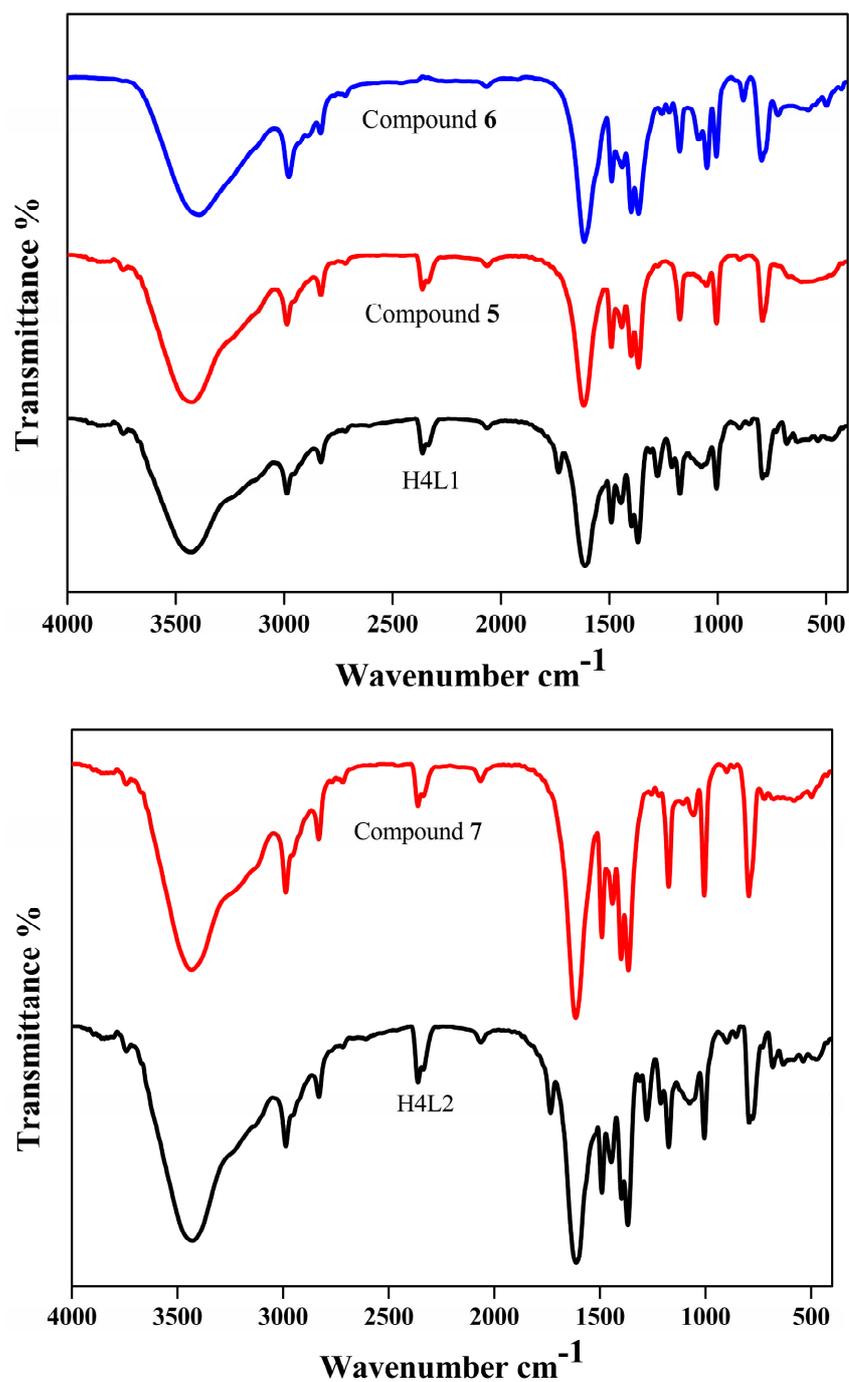


Fig. S6. Infrared spectra of compounds 1-7.

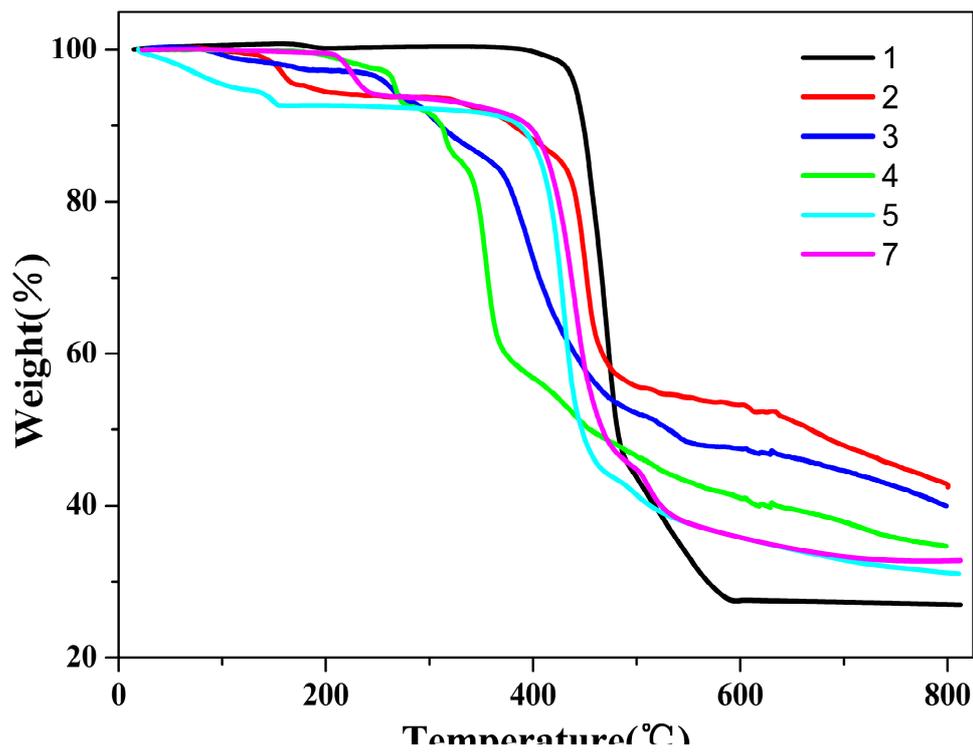


Fig. S7. The TG curves of compounds 1-7.

Table S1. Selected Bond Lengths (Å) and Angles (°) for Compounds 1-7.

Compound 1					
Zn1-O7	1.9288(15)	Zn2-O6#2	2.0857(15)	Zn2-O8#2	2.1227(15)
Zn1-O1#1	1.9451(15)	Zn2-O12#2	2.0978(15)	Zn3-O10	1.9530(16)
Zn1-O4	1.9507(15)	Zn2-O12	2.0978(15)	Zn3-O3	1.9602(15)
Zn1-O11	2.0019(15)	Zn2-O8	2.1227(15)	Zn3-O3#4	1.9603(15)
Zn2-O6	2.0857(15)				
O7-Zn1-O1#1	108.86(6)	O6-Zn2-O12#2	174.71(6)	O12-Zn2-O8	85.41(6)
O7-Zn1-O4	111.90(7)	O6-Zn2-O12	90.41(6)	O12#2-Zn2-O8	89.34(6)
O1#1-Zn1-O4	109.86(7)	O12-Zn2-O12#2	84.31(9)	O8#2-Zn2-O8	172.93(8)
O7-Zn1-O11	120.21(6)	O6-Zn2-O8#2	94.24(6)	O10#4-Zn3-O10	105.16(11)

O1#1-Zn1-O11	106.36(6)	O6-Zn2-O8	90.54(6)	O10-Zn3-O3#4	119.71(7)
O4-Zn1-O11	99.04(6)	O12-Zn2-O8#2	89.35(6)	O10-Zn3-O3	110.35(7)
O6-Zn2-O6#2	94.87(8)	O12-Zn2-O8	85.41(6)	O10#4-Zn3-O3#4	110.35(7)
O6#2-Zn2-O12#2	90.41(6)	O6#2-Zn2-O8#2	90.54(6)	O10#4-Zn3-O3	119.71(7)
O6#2-Zn2-O12	174.71(6)	O6#2-Zn2-O8	94.24(6)	O3#4-Zn3-O3	92.11(9)

Symmetry codes for #1 0.5-x, 0.5-y, 2-z; #2 1-x, y, 1.5-z; #3 0.5+x, 0.5-y, 0.5+z; #4 1-x, y, 2.5-z.

Compound 2

N1-Zn1	1.982(4)	O6-Zn1	1.944(4)	O9-Zn2	1.978(4)
O8-Zn1	2.006(4)	O5-Zn2	1.939(4)	O11-Zn2	2.011(4)
O1-Zn1	1.974(4)	N3-Zn2	1.997(5)		
O6-Zn1-O1	113.55(16)	O1-Zn1-O8	99.47(16)	O9-Zn2-N3	112.11(18)
O6-Zn1-N1	121.23(18)	N1-Zn1-O8	100.68(17)	O5-Zn2-O11	110.99(18)
O1-Zn1-N1	107.28(17)	O5-Zn2-O9	99.01(16)	O9-Zn2-O11	114.37(17)
O6-Zn1-O8	111.78(17)	O5-Zn2-N3	119.1(2)	N3-Zn2-O11	101.94(18)

Symmetry codes for #1 1-x, 1-y, -z; #2 -1+x, y, z; #3 2-x, -1-y, 1 -z; #4 2-x, -y, -z.

Compound 3

Zn1-O3#1	1.951(2)	Zn1-N1	2.043(2)	Zn2-N2#2	2.055(2)
Zn1-O11	1.986(2)	Zn2-O8#3	1.966(2)	Zn2-O10	2.115(2)
Zn1-O2	1.988(2)	Zn2-O7#4	1.973(2)	Zn2-O5	2.126(2)
O3#1-Zn1-O11	92.95(10)	O8#3-Zn2-O7#4	142.94(9)	N2#2-Zn2-O10	90.93(9)
O3#1-Zn1-O2	104.25(10)	O8#3-Zn2-N2#2	107.52(10)	O8#3-Zn2-O5	84.41(9)
O11-Zn1-O2	110.81(10)	O7#4-Zn2-N2#2	109.52(10)	O7#4-Zn2-O5	88.45(9)
O3#1-Zn1-N1	112.76(10)	O8#3-Zn2-O10	88.46(9)	N2#2-Zn2-O5	99.45(9)
O11-Zn1-N1	97.63(10)	O7#4-Zn2-O10	92.07(9)	O10-Zn2-O5	168.79(8)
O2-Zn1-N1	131.59(10)				

Symmetry codes for #1 2-x, -y, -z; #2 1-x, -y, -z; #3 1+x, -1+y, z; #4 2-x, -y, 1-z.

Compound 4

Cd1–O1#1	2.2791(18)	Cd1–O8#2	2.3721(17)	Cd2–O4#1	2.4240(19)
Cd1–O2	2.3066(18)	Cd1–O9#2	2.3628(19)	Cd2–O8#4	2.736(3)
Cd1–O4	2.3220(18)	Cd2–O7	2.2721(18)	Cd2–N1	2.342(2)
Cd1–O6#3	2.1927(19)	Cd2–O3#1	2.3310(19)	Cd2–N2	2.342(2)
O1#1–Cd1–O2	57.44(6)	O1#1–Cd1–O9#2	100.34(7)	O2–Cd1–O9#2	93.19(7)
O1#1–Cd1–O4	153.03(7)	O2–Cd1–O6#3	124.73(7)	O4–Cd1–O6#3	77.92(7)
O1#1–Cd1–O6#3	104.12(7)	O2–Cd1–O4	98.83(6)	O4–Cd1–O8#2	83.26(6)
O1#1–Cd1–O8#2	123.59(6)	O2–Cd1–O8#2	148.84(7)	O4–Cd1–O9#2	93.06(7)
O6#3–Cd1–O8#2	86.24(7)	O7–Cd2–N1	84.53(7)	O4#1–Cd2–O8#4	123.03(6)
O6#3–Cd1–O9#2	141.78(7)	O7–Cd2–N2	155.64(8)	O4#1–Cd2–N1	145.89(7)
O8#2–Cd1–O9#2	55.67(6)	O3#1–Cd2–O4#1	54.84(6)	O4#1–Cd2–N2	101.28(7)
O7–Cd2–O3#1	93.00(7)	O3#1–Cd2–O8#4	176.92(7)	O8#4–Cd2–N1	90.71(7)
O7–Cd2–O4#1	101.64(7)	O3#1–Cd2–N1	91.63(7)	O8#4–Cd2–N2	89.17(7)
O7–Cd2–O8#4	85.24(6)	O3#1–Cd2–N2	93.45(8)	N1–Cd2–N2	71.83(8)

Symmetry codes for #1 -x, -y, -z; #2 1-x, 1-y, 1-z; #3 -1+x, y, z; #4 2-x, 1-y, 1-z.

Compound 5

Ni1–O9	2.013(3)	Ni1–O4#1	2.110(2)	Ni2–O11#2	2.026(2)
Ni1–O11	2.066(2)	Ni1–O10	2.109(2)	Ni2–N2#3	2.094(3)
Ni1–O11#2	2.082(2)	Ni2–O8	1.987(2)	Ni2–O10#2	2.159(2)
Ni1–N1	2.094(3)	Ni2–O3#5	1.995(3)	Ni2–O1#4	2.280(3)
O9–Ni1–O11#2	98.26(10)	O9–Ni1–O10	162.84(10)	O11#2–Ni2–N2#3	99.14(10)
O9–Ni1–O11#2	93.73(10)	O11#2–Ni1–O10	96.64(9)	O8–Ni2–O10#2	84.49(9)
O11–Ni1–O11#2	79.46(9)	O11#2–Ni1–O10	80.65(9)	O3#5–Ni2–O10#2	93.80(9)
O9–Ni1–N1	95.20(11)	N1–Ni1–O10	93.05(10)	O11#2–Ni2–O10#2	80.74(8)
O11#2–Ni1–N1	90.82(9)	O4#1–Ni1–O10	82.36(9)	N2#3–Ni2–O10#2	175.74(10)
O11#2–Ni1–N1	167.66(11)	O8–Ni2–O3#5	164.87(11)	O8–Ni2–O1#4	83.06(10)
O9–Ni1–O4#1	82.38(10)	O8–Ni2–O11#2	102.63(10)	O3#5–Ni2–O1#4	81.81(11)

O11#2–Ni1–O4#1	177.36(8)	O3#5–Ni2–O11#2	91.89(11)	O11#2–Ni2–O1#4	162.63(9)
O11#2–Ni1–O4#1	97.95(9)	O8–Ni2–N2#3	91.40(11)	N2#3–Ni2–O1#4	97.09(10)
N1–Ni1–O4#1	91.67(10)	O3#5–Ni2–N2#3	90.46(11)	O10#2–Ni2–O1#4	83.53(9)

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

Compound 6

Co1–O14	1.935(6)	Co2–O4	2.100(6)	Co3–O10	2.128(5)
Co1–O9	1.981(5)	Co2–N3	2.151(6)	Co3–N8	2.167(6)
Co1–O16	2.011(5)	Co2–N4	2.167(6)	Co4–O2	1.961(5)
Co1–N6	2.125(7)	Co3–O15	2.051(6)	Co4–O3	1.974(5)
Co1–N5	2.186(6)	Co3–O11	2.080(6)	Co4–O5	1.980(5)
Co2–O1	2.022(5)	Co3–N7	2.121(6)	Co4–N2	2.142(6)
Co2–O6	2.049(6)	Co3–O13	2.118(5)	Co4–N1	2.174(7)
Co2–O17	2.081(5)				
O14–Co1–O9	125.1(2)	O6–Co2–N3	97.9(2)	O13–Co3–O10	92.2(2)
O14–Co1–O16	111.5(2)	O17–Co2–N3	89.9(2)	O15–Co3–N8	90.9(2)
O9–Co1–O16	123.0(2)	O4–Co2–N3	88.7(2)	O11–Co3–N8	101.8(2)
O14–Co1–N6	91.4(3)	O1–Co2–N4	90.4(2)	N7–Co3–N8	172.5(3)
O9–Co1–N6	90.0(2)	O6–Co2–N4	87.0(2)	O13–Co3–N8	89.6(2)
O16–Co1–N6	94.8(3)	O17–Co2–N4	90.1(2)	O10–Co3–N8	87.2(2)
O14–Co1–N5	90.0(3)	O4–Co2–N4	86.5(2)	O2–Co4–O3	124.0(2)
O9–Co1–N5	90.9(2)	N3–Co2–N4	175.2(3)	O2–Co4–O5	112.1(2)
O16–Co1–N5	82.7(2)	O15–Co3–O11	81.3(2)	O3–Co4–O5	123.8(2)
N6–Co1–N5	177.5(3)	O15–Co3–N7	90.2(2)	O2–Co4–N2	94.6(2)
O1–Co2–O6	83.1(2)	O11–Co3–N7	85.7(2)	O3–Co4–N2	91.3(2)
O1–Co2–O17	170.5(2)	O15–Co3–O13	168.0(2)	O5–Co4–N2	87.1(2)
O6–Co2–O17	87.5(2)	O11–Co3–O13	86.8(2)	O2–Co4–N1	86.1(2)
O1–Co2–O4	92.7(2)	N7–Co3–O13	90.8(2)	O3–Co4–N1	88.1(2)
O6–Co2–O4	172.2(2)	O15–Co3–O10	99.8(2)	O5–Co4–N1	92.9(2)

O17–Co2–O4	96.8(2)	O11–Co3–O10	170.9(2)	N2–Co4–N1	179.3(3)
O1–Co2–N3	90.3(2)	N7–Co3–O10	85.3(2)		

Symmetry codes for #1 -x, -0.5+y, 1.5-z; #2 x, -1+y, z; #3 x, 0.5-y, -0.5+z; #4 1-x, 1-y, 2-z; #5 1-x, -0.5+y, 1.5-z; ; #6 x, 1.5-y, 0.5+z; #7 -x, 0.5+y, 1.5-z.

Compound 7

Co1–O1	2.061(3)	Co1–O8	2.157(3)	Co2–O9	2.132(3)
Co1–O6#2	2.089(2)	Co1–N3	2.172(3)	Co2–N1	2.147(3)
Co1–O7#3	2.117(3)	Co2–O2	2.051(3)	Co2–N4	2.174(3)
Co1–N2	2.145(3)	Co2–O3#1	2.072(2)	Co2–O8	2.247(2)
O1–Co1–O6#2	174.12(10)	O1–Co1–N3	89.09(11)	O9–Co2–N1	91.91(11)
O1–Co1–O7#3	88.42(11)	O6#2–Co1–N3	96.77(10)	O2–Co2–N4	92.15(11)
O6#2–Co1–O7#3	90.37(10)	O7#3–Co1–N3	97.31(11)	O3#1–Co2–N4	84.92(10)
O1–Co1–N2	88.48(12)	N2–Co1–N3	176.13(11)	O9–Co2–N4	86.20(11)
O6#2–Co1–N2	85.69(11)	O8–Co1–N3	91.45(10)	N1–Co2–N4	91.22(11)
O7#3–Co1–N2	85.64(11)	O2–Co2–O3#1	84.10(10)	O2–Co2–O8	93.94(10)
O1–Co1–O8	94.87(10)	O2–Co2–O9	174.30(10)	O3#1–Co2–O8	84.32(9)
O6#2–Co1–O8	85.47(10)	O3#1–Co2–O9	90.31(10)	O9–Co2–O8	86.63(10)
O7#3–Co1–O8	170.70(9)	O2–Co2–N1	93.58(12)	N1–Co2–O8	99.81(10)
N2–Co1–O8	85.76(11)	O3#1–Co2–N1	175.41(11)	N4–Co2–O8	167.02(11)

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

Table S2. Hydrogen bond parameters [\AA , $^\circ$] for compounds 1-7.

Compound 1

D–H \cdots A	D–H	H \cdots A	D \cdots A	D–H \cdots A
O(1)–H(10B) \cdots O(2) #4	0.82	1.92	2.7206	165
O(10)–H(10C) \cdots O(9) #2	0.92	1.87	2.7774	168

O(11)–H(11A)···O(9) #5	0.82	1.74	2.5529	174
O(11)–H(11B)···O(2)	0.87	2.40	2.9969	126
O(11)–H(11B)···O(8) #6	0.87	2.59	3.3209	142
O(12)–H(12B)···O(11) #3	0.82	2.06	2.8476	160
O(12)–H(12C)···O(2) #7	0.94	1.86	2.7876	167
C(10)–H(10A)···O(10) #2	0.93	2.42	3.3201	162
C(12)–H(12A)···O(6) #1	0.93	2.35	3.2118	154

Symmetry code: #1 -x, y, 0.5-z; #2 -0.5-x, 0.5-y, -z; #3 0.5-x, 0.5-y, -z; #4 -0.5+x, 0.5-y, -0.5+z; #5 1+x, y, z; #6 -x, 1-y, -z; #7 0.5-x, -0.5+y, 0.5-z.

Compound 2

D–H···A	D–H	H···A	D···A	D–H···A
O(8)–H(8A)···O(10) #4	0.85	1.80	2.5843	154
O(8)–H(8C)···O(7) #1	0.85	1.92	2.7131	155
O(11)–H(11A)···O(2) #2	0.85	1.83	2.6293	156
O(11)–H(11C)···O(1) #3	0.85	2.56	2.9353	108
O(11)–H(11C)···O(6) #3	0.85	2.17	2.9057	145
C(18)–H(18)···O(5)	0.93	2.43	3.2774	152
C(22)–H(22)···O(2) #2	0.93	2.34	3.0713	135
C(25)–H(25)···O(8) #3	0.93	2.56	3.4808	172

Symmetry code: #1 1+x, y, z; #2 1-x, -y, -z; #3 x, -1+y, z; #4 1+x, 1+y, z.

Compound 3

D–H···A	D–H	H···A	D···A	D–H···A
O(1W)–H(1WA)···O(4) #7	0.89	1.93	2.7998	165
O(1W)–H(1WB)···O(2) #4	0.93	2.07	2.9392	155
O(1W)–H(1WB)···O(3) #4	0.93	2.59	3.1307	118
O(10)–H(10A)···O(6) #6	0.87	1.86	2.7241	170
O(10)–H(10B)···O(5) #5	0.77	2.43	3.0930	145
O(10)–H(10B)···O(6) #5	0.77	2.14	2.8199	146

O(11)–H(11A)···O(1) #3	0.88	1.84	2.7047	165
O(11)–H(11B)···O(1W) #2	0.88	1.90	2.7082	151
O(11)–H(11B)···O(1W) #3	0.88	2.50	2.9394	112
C(1)–H(1)···O(10) #3	0.93	2.52	3.2849	140
C(2)–H(2)···O(5) #1	0.93	2.852	3.4173	163
C(9)–H(9)···O(1)	0.93	2.40	3.0756	130

Symmetry code: #1 2-x, -y, -z; #2 1+x, y, z; #3 1-x, 1-y, -z; #4 1-x, -y, -z; #5 -1+x, 1+y, z; #6 2-x, 1-y, 1-z; #7 -1+x, y, -z.

Compound 4

D–H···A	D–H	H···A	D···A	D–H···A
C(3)–H(3)···O(1)	0.93	2.45	2.7635	100
C(5)–H(5)···O(3)	0.93	2.42	2.7437	100
C(7)–H(7)···O(2) #2	0.93	2.50	3.4268	177
C(17)–H(17)···O(7) #3	0.93	2.55	3.1485	122
C(19)–H(19)···O(3) #4	0.93	2.54	3.3279	142
C(24)–H(24)···O(2) #5	0.93	2.56	3.2919	136
C(26)–H(26)···O(6) #1	0.93	2.58	3.2222	126

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

Compound 5

D–H···A	D–H	H···A	D···A	D–H···A
O(2)–H(2)···O(7) #2	0.90	1.64	2.5188	164
O(3)–H(3)···N(2) #2	0.93	2.34	2.9039	119
O(10)–H(10A)···O(6) #4	0.85	1.84	2.6579	161
O(10)–H(10B)···O(7) #1	0.77	1.96	2.7097	165
C(20)–H(20)···O(1) #5	0.93	2.59	3.4743	160
C(24)–H(24)···O(3) #3	0.93	2.50	3.0259	116
C(25)–H(25)···O(8) #5	0.93	2.38	2.9660	120

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

Compound 6

D-H...A	D-H	H...A	D...A	D-H...A
C(3)-H(3)...O(14) #4	0.93	2.40	2.7202	100
C(30)-H(30)...O(3) #6	0.93	2.48	3.0094	117
C(46)-H(46)...O(3) #7	0.93	2.53	3.0576	116
C(74)-H(74)...O(9)	0.93	2.59	3.1326	118
C(83)-H(83)...N(13) #8	0.93	2.50	3.3150	146
C(84)-H(84)...O(10) #2	0.93	2.55	3.0607	115
C(91)-H(91)...O(15) #5	0.93	2.58	3.0477	111
C(99)-H(99)...O(7) #3	0.93	2.35	3.0610	134
C(106)-H(106)...O(7) #3	0.93	2.59	3.5068	167
C(119)-H(119)...O(7) #1	0.93	2.30	3.1206	146

Symmetry code: #1 x, y, 1+z; #2 -x, -0.5+y, 0.5-z; #3 x, 0.5-y, 0.5+z; #4 x, 1.5-y, -0.5+z; #5 x, 1.5-y, 0.5+z; #6 -x, 1-y, -z; #7 1-x, 0.5+y, 0.5-z; #8 -x, -y, 1-z.

Compound 7

D-H...A	D-H	H...A	D...A	D-H...A
O(9)-H(9A)...O(10) #2	0.94	1.82	2.7171	159
O(9)-H(9B)...O(4) #4	0.76	1.91	2.6519	164
C(16)-H(16)...O(2) #1	0.93	2.56	3.1425	121
C(19)-H(19)...O(4) #2	0.93	2.53	3.2654	136
C(34)-H(34)...O(3) #4	0.93	2.34	3.1966	152
C(38)-H(38)...O(6) #3	0.93	2.41	3.2570	152
C(40)-H(40)...O(10) #5	0.93	2.50	3.3399	150
C(43)-H(43)...O(3) #4	0.93	2.57	2.9017	102

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

