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Supplementary Material

Coordination assemblies of Co^{II}/Ni^{II}/Zn^{II}/Cu^{II} with 3,3',4,4'-Biphenyltetracarboxylic acid and three positional isomeric ligands

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Table S1. Crystal data and structure refinement for **1**–**8**.

Complex	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**
Empirical formula	$C_{20}H_{18}N_5CoO_7$	$C_{20}H_{18}N_5NiO_7$	$C_{40}H_{30}N_{10}Zn_2O_{11}$	$C_{20}H_{14}N_5CoO_5$	$C_{32}H_{25}N_{10}NiO_6$	$C_{20}H_{16}CuN_5O_6$	$C_{20}H_{22}CoN_5O_9$	$C_{20}H_{22}N_5NiO_9$
Formula weight	499.32	499.09	957.51	463.29	704.31	485.92	535.36	535.12
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	triclinic	monoclinic	triclinic	triclinic
Space group	$P2_1/n$	$P2_1/n$	$C2/c$	$C2/c$	P-1	$P2_1/n$	P-1	P-1
a (Å)	8.2637(5)	8.2622 (3)	25.0845(8)	25.144(6)	10.7917(10)	7.0471(8)	10.3859(7)	10.3239(13)
b (Å)	12.2275(9)	12.1100 (6)	10.3487(2)	10.0502(3)	12.0386(12)	12.4408(10)	10.5288(6)	10.4640(15)
c (Å)	19.7018(19)	19.6599 (9)	16.3895(7)	15.907(3)	12.7146(11)	22.398(2)	12.4029(6)	12.3735(16)
α (°)	90.00	90.00	90.00	90.00	70.344(9)	90.00	70.674(5)	109.379(12)
β (°)	95.421(8)	95.452 (4)	114.587(5)	114.67(3)	82.435(7)	95.547(11)	89.513(5)	89.865(11)
γ (°)	90.00	90.00	90.00	90.00	72.872(8)	90.00	63.781(6)	116.093(14)
Volume ($Å^3$)	1981.8(3)	1958.19 (15)	3868.8(2)	3652.8(14)	1485.6(2)	1954.5(3)	1132.88(11)	1116.1(3)
Z	4	4	4	8	2	4	2	2
Calculated density(Mg/m^3)	1.673	1.696	1.642	1.685	1.574	1.651	1.569	1.592
Goodness-of-fit on F^2	1.054	1.169	1.018	1.042	1.025	1.073	1.046	1.020
Independent reflections	4051	4003	3939	3734	6062	3989	4632	4566
$R_1[I>2\sigma(I)]$	0.0511	0.1164	0.0480	0.0342	0.0467	0.0786	0.0442	0.0536
wR_2 (all data)	0.1085	0.3090	0.1007	0.0836	0.1607	0.1789	0.1078	0.1185

Table S2. Selected bond lengths (Å) and angles (º) for **1**–**8**.

1 (Symmetry codes: A: −*x*+3/2, *y*+1/2, −*z*+1/2; B: *x*−1/2, −*y*+3/2, *z*−1/2.)

Co1—O1	2.120 (2)	Co1—O3	2.040 (2)	Co1—N1	2.164 (3)
Co1—O2	2.116 (3)	Co1—O5A	2.143 (2)	Co1—N5B	2.153 (3)
O1—Co1—O5A	91.70 (9)	O2—Co1—N1	89.51 (10)	O3—Co1—N1	94.44 (10)
O1—Co1—N1	83.22 (10)	O2—Co1—N5B	88.63 (10)	O3—Co1—N5B	93.97 (10)
O1—Co1—N5B	88.32 (11)	O3—Co1—O1	177.29(10)	O5A—Co1—N1	88.69 (10)
O2—Co1—O1	89.16 (10)	O3—Co1—O2	89.45 (10)	O5A—Co1—N5B	93.32 (10)
O2—Co1—O5A	177.90 (9)	O3—Co1—O5A	89.61 (9)	N5B—Co1—N1	171.36(10)

2 (Symmetry codes: A: −*x*+5/2, *y*−1/2, −*z*+3/2; B: *x*−1/2, −*y*+3/2, *z*−1/2.)

Ni1—O1	2.051 (7)	Ni1—O5	2.072 (8)	Ni1—N1	2.109 (9)
Ni1—O4A	2.098 (7)	Ni1—O6	2.073 (8)	Ni1—N5B	2.109 (9)
O1—Ni1—O4A	88.2 (3)	O4A—Ni1—N1	89.7 (3)	O5—Ni1—N5B	89.8 (3)
O1—Ni1—O5	89.3 (3)	O4A—Ni1—N5B	91.8 (3)	O6—Ni1—O4A	93.2 (3)
O1—Ni1—O6	177.1 (3)	O5—Ni1—O4A	177.1 (3)	O6—Ni1—N1	83.7 (3)
O1—Ni1—N1	93.8 (3)	O5—Ni1—O6	89.2 (3)	O6—Ni1—N5B	89.3 (3)
O1—Ni1—N5B	93.3 (3)	O5—Ni1—N1	89.0 (3)	N1—Ni1—N5B	172.8 (4)

3 (Symmetry codes: A: −*x*+1/2, *y*+1/2, −*z*+1/2; B: −*x*, *y*, −*z*+1/2.)

Zn1—O1	2.134 (3)	Zn1—O4A	1.981 (2)	Zn1—N5B	2.079 (3)
Zn1—O2	2.157 (3)	Zn1—N1	2.101 (3)		
O1—Zn1—O2	59.21 (10)	O4A—Zn1—N5B	106.87(10)	N5B—Zn1—O2	151.05(10)
O4A—Zn1—O1	150.23(13)	N1—Zn1—O1	103.73(13)	N5B—Zn1—N1	95.71 (11)
O4A—Zn1—O2	97.58 (9)	N1—Zn1—O2	96.53 (12)		
O4A—Zn1—N1	96.85 (10)	N5B—Zn1—O1	92.39 (10)		

4 (Symmetry codes: A: −*x*+1/2, *y*+1/2, −*z*+1/2; B: *x*−1/2, −*y*+3/2, *z*−1/2.)

Co1—O4A	2.0259(14)	Co1—O3	2.1227(16)	Co1—N1B	2.2354(19)
Co1—O1	2.0831(18)	Co1—O2	2.1407(15)	Co1—N5	2.2430(19)
O4A—Co1—O1	93.20 (6)	O4A—Co1—N1B	91.18 (6)	O3—Co1—N5	86.65 (7)
O4A—Co1—O3	108.13 (6)	O1—Co1—N1B	89.73 (7)	O2—Co1—N5	91.97 (7)
O1—Co1—O3	158.39 (6)	O3—Co1—N1B	93.20 (7)	N1B—Co1—N5	179.59 (7)
O4A—Co1—O2	170.02 (6)	O2—Co1—N1B	88.30 (7)	O4A—Co1—C13	138.99 (7)
O1—Co1—O2	96.76 (6)	O4A—Co1—N5	88.50 (7)		
O3—Co1—O2	61.97 (6)	O1—Co1—N5	90.55 (7)		

5 (Symmetry codes: Symmetry codes: A: −*x*+1, −*y*+2, −*z*; B : −*x*+2, −*y*+1, −z.)

Ni1—O1	2.0603(18)	Ni1—N1	2.111 (2)	Ni2—O6	2.042 (2)
Ni1—O5	2.060 (2)	Ni2—O3	2.0900(19)	Ni2—N6	2.105 (3)
O1—Ni1—N1A	85.46 (8)	O5—Ni1—N1A	89.17 (9)	O6B—Ni2—O3B	88.47 (8)
O1A—Ni1—N1A	94.54 (8)	O5A—Ni1—N1A	90.83 (9)	O6—Ni2—O3	88.47 (8)
O1—Ni1—N1	94.54 (8)	O5—Ni1—N1	90.83 (9)	O6B—Ni2—O3	91.53 (8)
O1A—Ni1—N1	85.46 (8)	O5A—Ni1—N1	89.17 (9)	O6—Ni2—O3B	91.53 (8)
O5—Ni1—O1	89.24 (8)	O3B—Ni2—N6B	90.14 (9)	O6—Ni2—N6B	88.90 (13)
O5A—Ni1—O1A	89.24 (8)	O3—Ni2—N6B	89.86 (9)	O6B—Ni2—N6B	91.10 (13)
O5A—Ni1—O1	90.76 (8)	O3B—Ni2—N6	89.86 (9)	O6B—Ni2—N6	88.90 (13)
O5—Ni1—O1A	90.76 (8)	O3—Ni2—N6	90.14 (9)	O6—Ni2—N6	91.10 (13)

6 (Symmetry codes: A: −*x*+1/2, *y*+1/2, −*z*+1/2; B: *x*−1/2, −*y*+1/2, *z*−1/2;.)

Cu1—O2A	2.047 (18)	Cu1—O5	2.324 (8)	Cu1—N5B	2.042 (5)
Cu1—O3	2.000 (4)	Cu1—N1	2.026 (5)		
O2A—Cu1—O5	107.3 (7)	O3—Cu1—N5B	91.73 (18)	N5B—Cu1—O2A	92.8 (5)
O3—Cu1—O2A	154.5 (6)	N1—Cu1—O2A	88.8 (5)	N5B—Cu1—O5	88.2 (3)
O3—Cu1—O5	97.9 (3)	N1—Cu1—O5	85.9 (3)		
O3—Cu1—N1	89.26 (18)	N1—Cu1—N5B	174.1 (2)		

7 (Symmetry codes: A: −*x*+2, −*y*+1, −*z*+2; B: *x*+1, *y*−1, *z*+1; C: −*x*+1, −*y*+2, −*z*+1; D: −*x*+2, −*y*+2, −*z*+2;)

Co1—O2	2.0714(18)	Co1—N5C	2.176 (2)	Co2—O5	2.133(2)
Co1—O3	2.046 (2)	Co2—O1	2.0841(18)	Co2—N1	2.183(2)
Co1—N5B	2.176 (2)				
O2A—Co1—N5C	88.86 (8)	O3A—Co1—N5B	87.06 (8)	O1D—Co2—N1	90.32 (8)
O2—Co1—N5C	91.14 (8)	O3—Co1—N5B	92.94 (8)	O1—Co2—N1	89.68 (8)
O2A—Co1—N5B	91.14 (8)	O3—Co1—N5C	87.06 (8)	O1D—Co2—N1D	89.68 (8)
O2—Co1—N5B	88.86 (8)	N5B—Co1—N5C	180.000(1)	O1—Co2—N1D	90.32 (8)
O3A—Co1—O2A	90.61 (8)	O1—Co2—O5D	92.34 (8)	O5—Co2—N1	92.73 (9)
O3—Co1—O2	90.61 (8)	O1D—Co2—O5D	87.66 (8)	O5D—Co2—N1	87.27 (9)
O3—Co1—O2A	89.39 (8)	O1D—Co2—O5	92.34 (8)	O5—Co2—N1D	87.27 (9)
O3A—Co1—O2	89.39 (8)	O1—Co2—O5	87.66 (8)	O5D—Co2—N1D	92.73 (9)
O3A—Co1—N5C	92.94 (8)				

8 (Symmetry codes: A: −*x*, −*y*, −*z*+1; B: *x*−1, *y*−1, *z*−1; C: −*x*+1, −*y*+1, −*z*+2; D: −*x*, −*y*+1, −*z*+1.)

Ni1—O1	2.045 (2)	Ni1—N5C	2.120 (3)	Ni2—O5	2.099 (3)
Ni1—O3	2.024 (2)	Ni2—O2	2.061 (2)	Ni2—N1	2.133 (3)
Ni1—N5B	2.120 (3)				
O1A—Ni1—N5C	89.23(10)	O3—Ni1—N5B	93.28(10)	O2D—Ni2—N1	90.05(10)
O1—Ni1—N5C	90.77(10)	O3A—Ni1—N5B	86.72(10)	O2—Ni2—N1	89.95(10)
O1A—Ni1—N5B	90.77(10)	O3A—Ni1—N5C	93.28(10)	O2D—Ni2—N1D	89.95(10)
O1—Ni1—N5B	89.23(10)	N5B—Ni1—N5C	180.0	O2—Ni2—N1D	90.05(10)
O3—Ni1—O1A	88.47(10)	O2—Ni2—O5D	92.58 (10)	O5—Ni2—N1	92.34(11)
O3A—Ni1—O1	88.47 (10)	O2D—Ni2—O5D	87.42 (10)	O5D—Ni2—N1	87.66 (11)
O3A—Ni1—O1A	91.53 (10)	O2D—Ni2—O5	92.58 (10)	O5—Ni2—N1D	87.66 (11)
O3—Ni1—O1	91.53 (10)	O2—Ni2—O5	87.42 (10)	O5D—Ni2—N1D	92.34 (11)
O3—Ni1—N5C	86.72(10)				

Table S3. Selected Hydrogen-bond Geometry (Å) for complex **2, 3, 5**

D—H···*A*	*D*—*H*	*H*···*A*	*D*···*A*	*D*—H···*A*
		2		
N3—H3···O7^{vi}	0.86	2.29	2.939 (14)	133
N4—H4···O2^{i}	0.86	1.84	2.693 (11)	173
O5—H5A···O3^{vii}	0.85	1.82	2.673 (11)	172
O6—H6A···O3^{i}	0.85	2.12	2.695 (11)	125
O6—H6B···O2^{vii}	0.84	2.30	2.979 (12)	138
O7—H7A···O5	0.85	2.36	2.738 (13)	108

O7—H7B···N3^{viii}	0.84	2.52	2.939 (14)	112
Symmetry codes: (i) −*x*+5/2, *y*−1/2, −*z*+3/2; (vi) *x*, *y*−1, *z*; (vii) *x*−1, *y*, *z*; (viii) *x*, *y*+1, *z*.				
		3		
N3—H3···O3^{iv}	0.86	1.95	2.813 (5)	177
O5—H5A···N2	0.85	2.23	3.074 (5)	179
O6—H6A···O6^{v}	0.85	2.47	3.031 (9)	124
Symmetry codes: (iv) *x*+1/2, *y*+3/2, *z*; (v) −*x*+1/2, −*y*−1/2, −*z*.				
		5		
N4—H4···O2^{iv}	0.86	1.85	2.712 (3)	175
O5—H5B···N10^{iii}	0.85	2.02	2.773 (4)	147
O6—H6A···N5^{iii}	0.83	1.89	2.701 (4)	168
O6—H6B···O4^{ii}	0.86	1.93	2.630 (4)	139
N8—H8···O2^{v}	0.86	2.55	3.017 (4)	115
Symmetry codes: (ii) −x+2, −y+1, −z; (iii) −x+1, −y+1, −z+1; (iv) −x+1, −y+2, −z+1; (v) −x+2, −y+1, −z+1.				

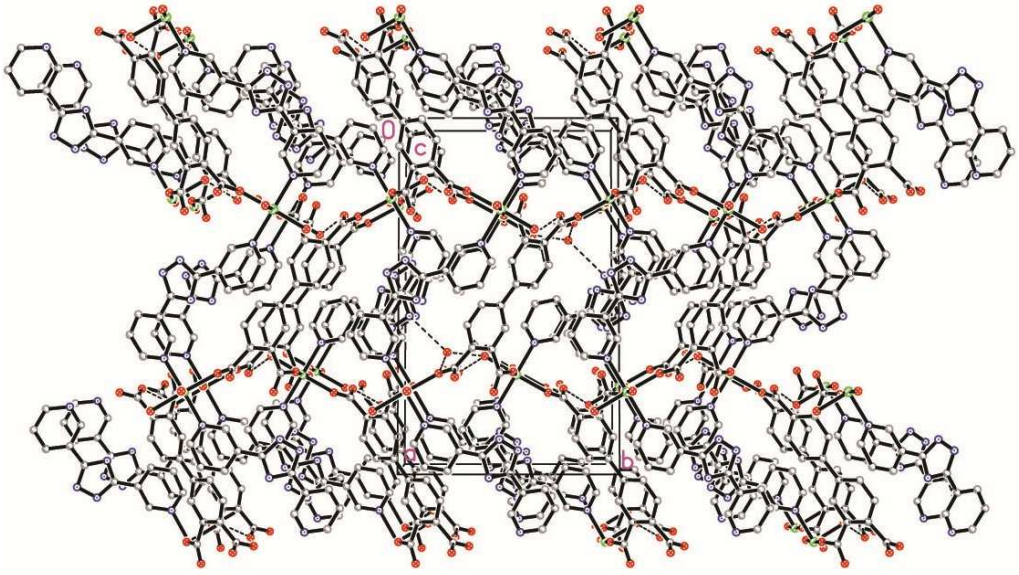

Fig S 1. Show the 3-D packing drawing of **2**.

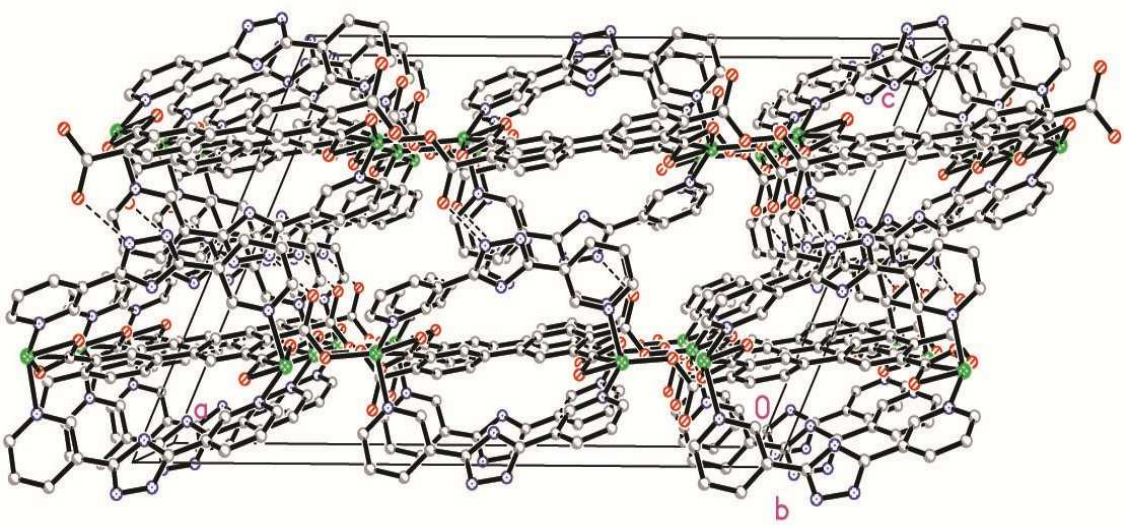

Fig S 2. Show the 3-D packing drawing of **3**

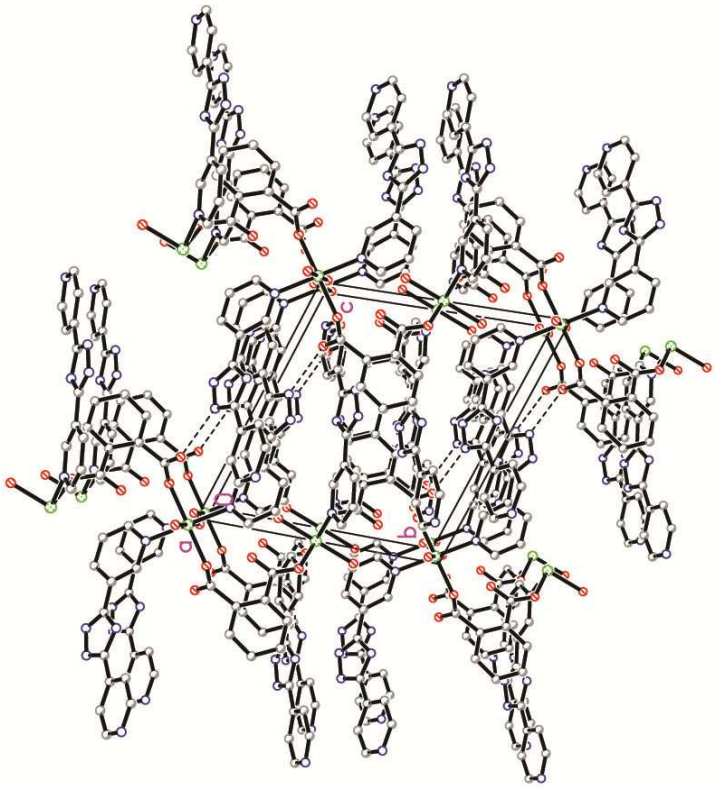

Fig **S 3**. Show the 3-D packing drawing of **5**.