Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary Information

Eight coordination compounds assembled from unexplored semi-rigid ether-based unsymmetrical tetracarboxylate and various dipyridyl ligands: structural variation, magnetic and photoluminescence properties

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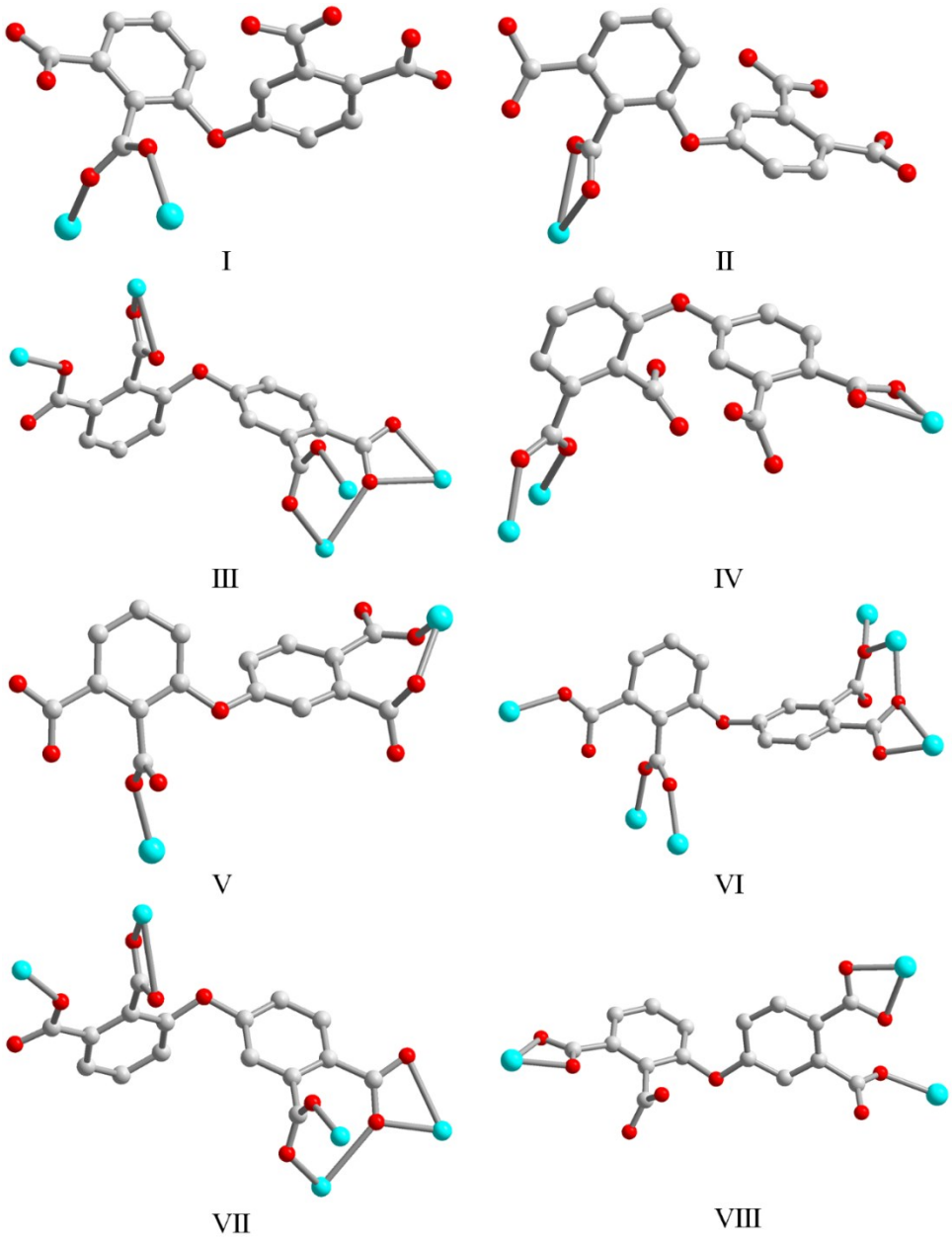


Scheme S1. Coordination modes of 2,3,3',4'-diphenyl ether tetracarboxylate ligands in compounds **1-8**.

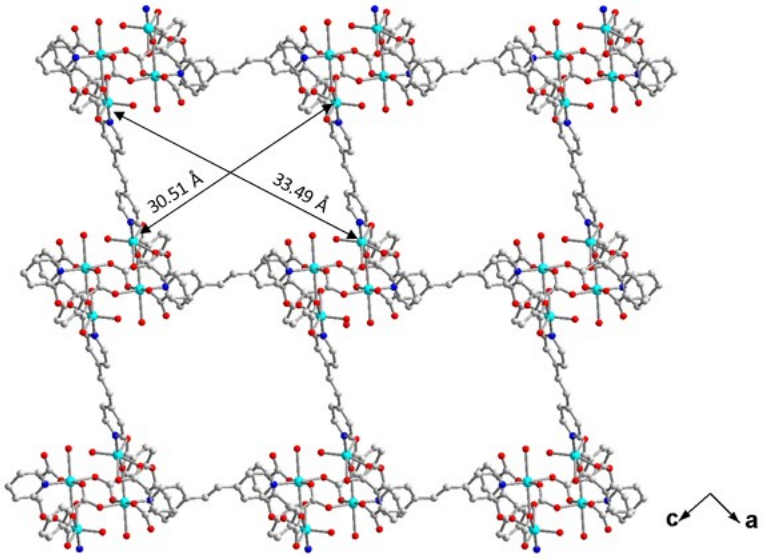


Fig. S1. The 3D framework of **7** viewed along the *b*-axis. The size of the rectangular window is marked.

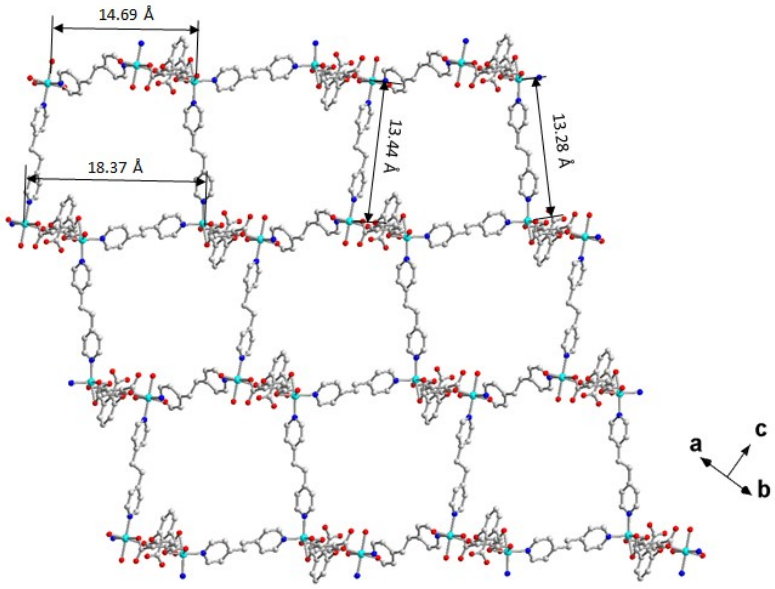


Fig. S2. The 3D framework of **8** viewed from the [60, 76, -57] direction. The size of the trapezoidal window is marked.

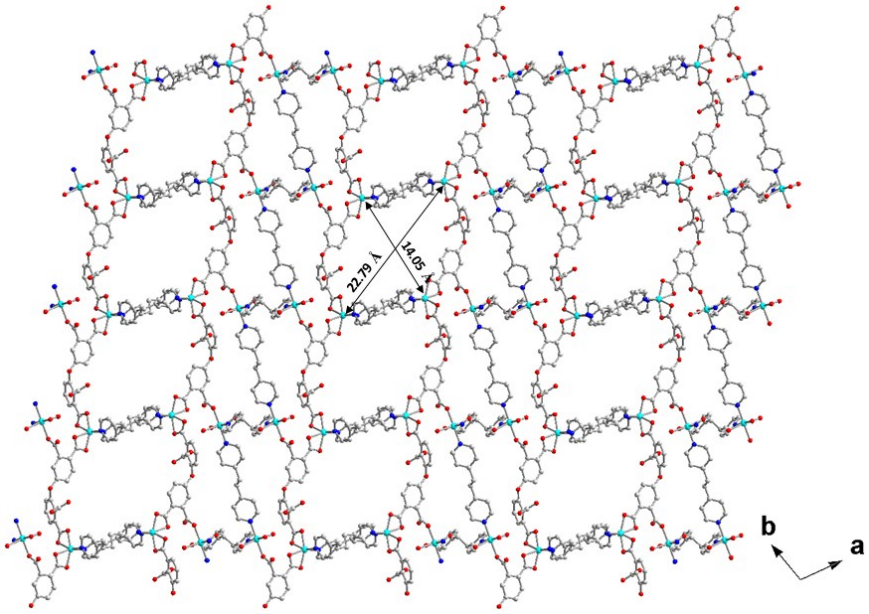
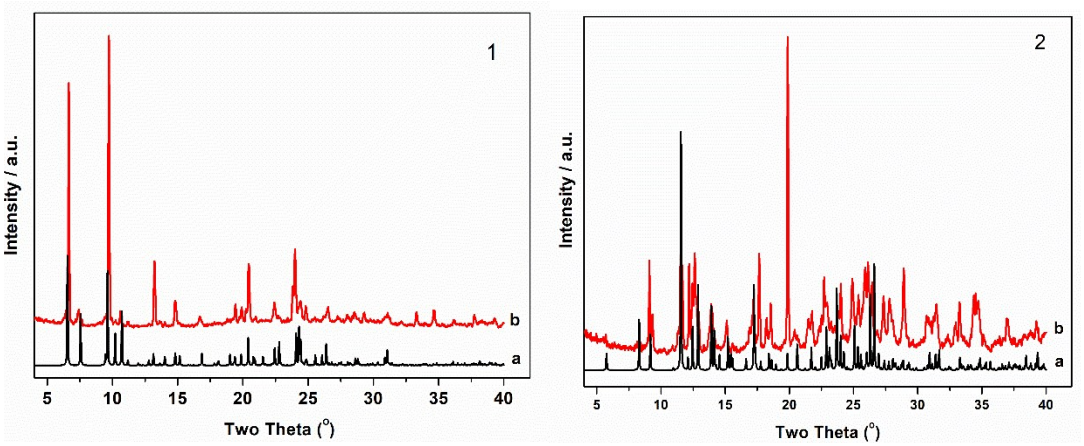
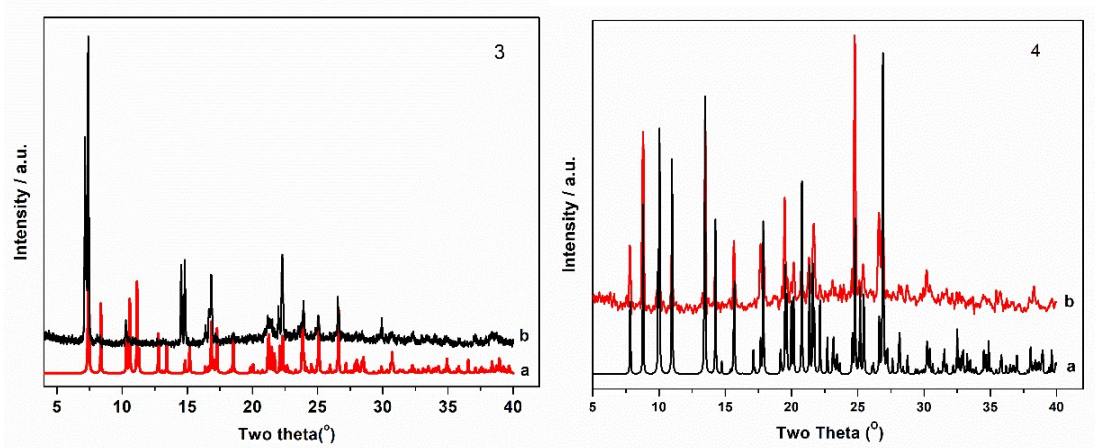
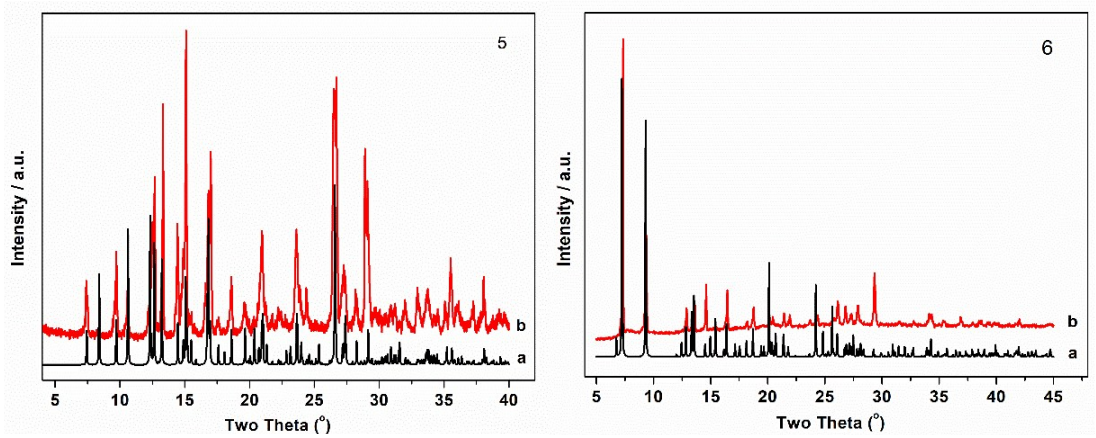


Fig. S3. The 3D framework of **8** viewed from the [0 0 1] direction. The size of the rectangular window is marked.


1
Intensity / a.u.
Two Theta (°)
b
a
2
Intensity / a.u.
Two Theta (°)
b
a


3
Intensity / a.u.
Two theta(°)
b
a
4
Intensity / a.u.
Two Theta (°)
b
a


5
Intensity / a.u.
Two Theta (°)
b
a
6
Intensity / a.u.
Two Theta (°)
b
a

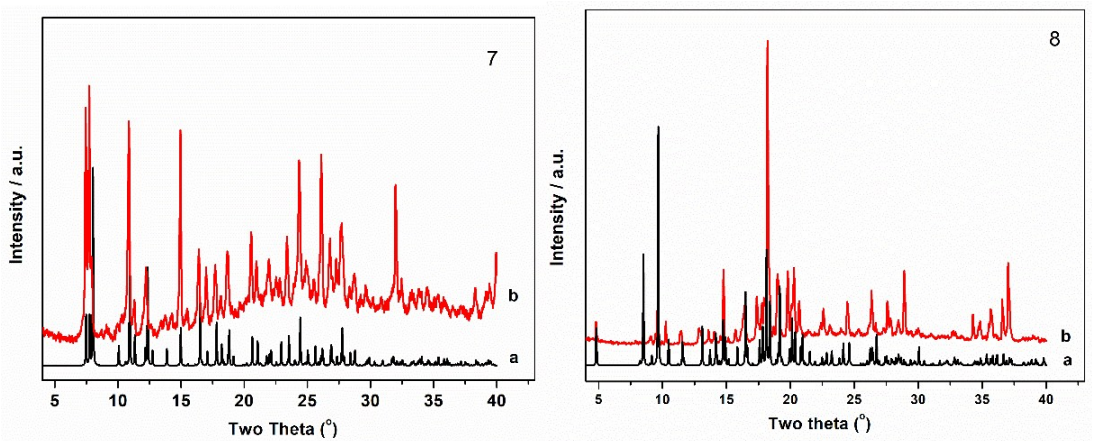


Fig. S4. PXRD patterns of compounds **1-8.** a) Simulated from single crystal structure data. b) Experimental data. The differences between the calculated and observed patterns in intensity may be due to the orientation of the crystals.

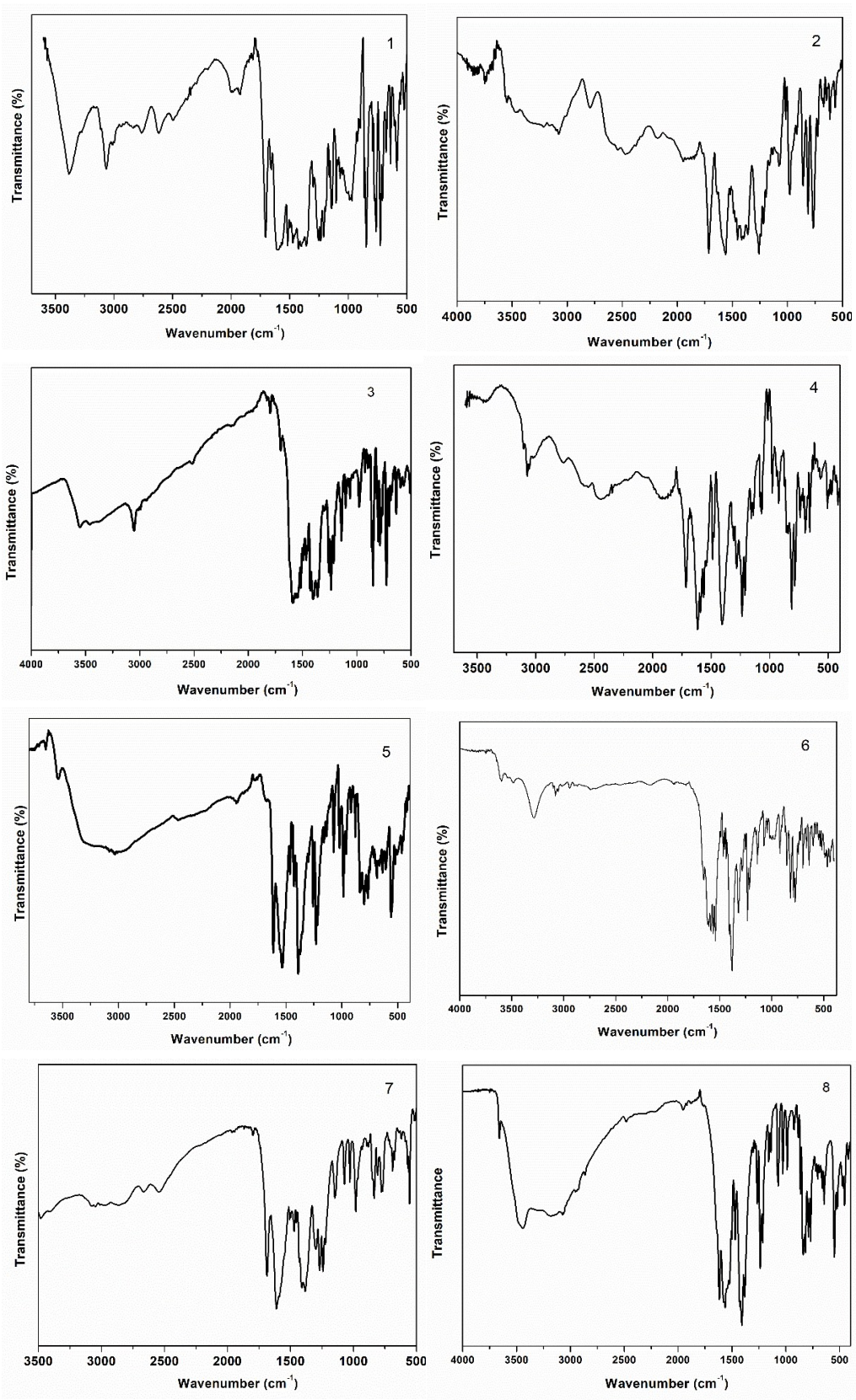


Fig. S5. Infrared spectra of compounds **1-8**.

The presence of ν(C=O) absorption bands about 1700 cm^{-1} in the compounds **1**, **2** and **4** proves the carboxylate groups are partially deprotonation in the structures, whereas the absence of the ν(C=O) absorption bands in compounds **3** and **5-8** in the area of 1700 cm^{-1} indicates full deprotonation of carboxylate groups in compounds **3** and **5-8**. Asymmetric and symmetric ν(C=O) absorptions bands of carboxylate groups are evidenced by strong absorption peaks around 1600 cm^{-1} and 1400 cm^{-1}.

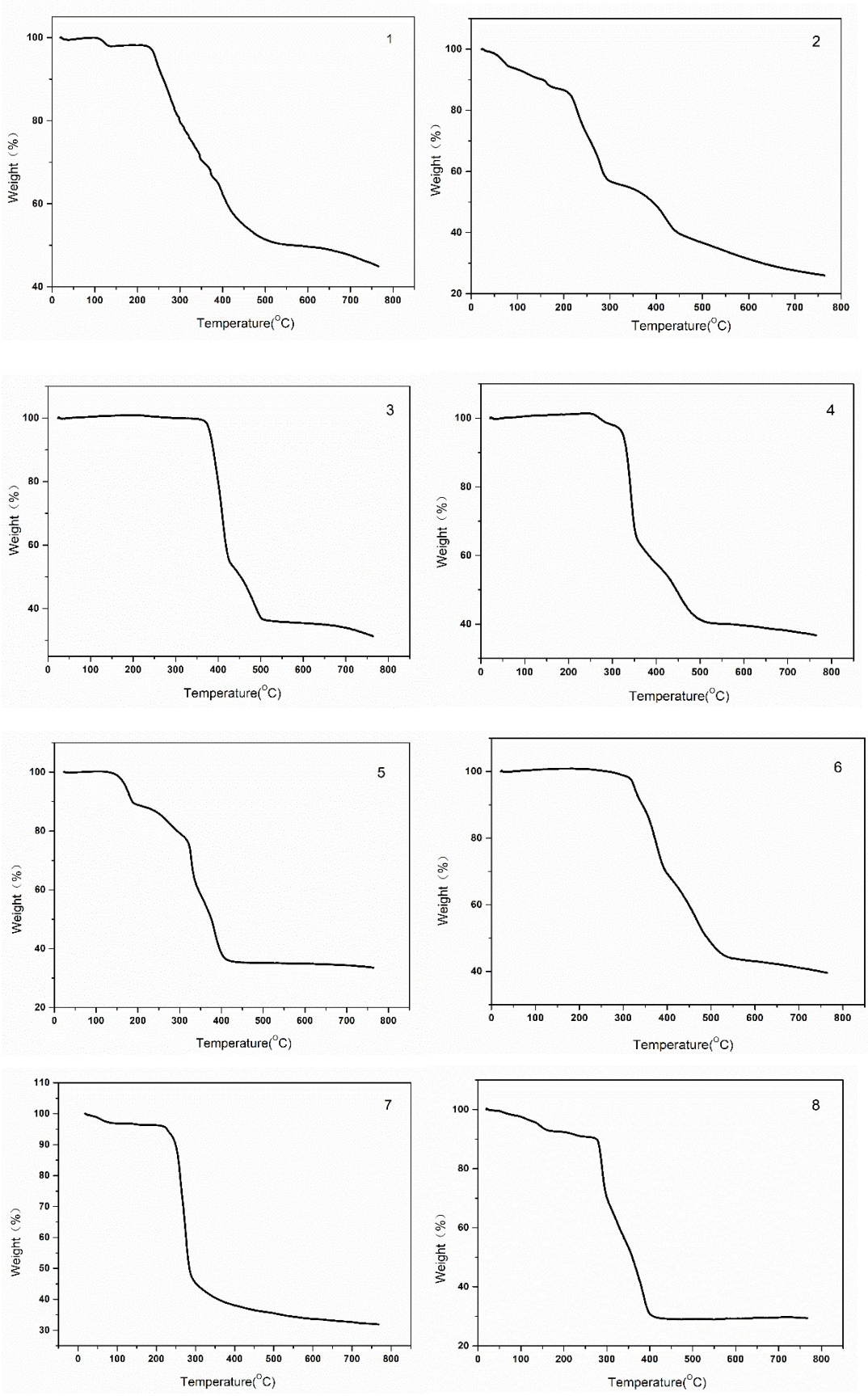


Fig. S6. TGA curves of compounds **1-8**.

For **1**, the weight loss of about 2.10 % from the room temperature to 130 °C corresponds to the departure of one lattice water molecules (calcd 2.26 %), and the remaining framework is thermally stable up to 244 °C, at which the framework begins to collapse. For **2**, the weight loss of about 8.58 % from the room temperature to 127 °C corresponds to the departure of six lattice water molecules (calcd 8.03 %), and then the second stage in the temperature range of 127-159 °C corresponds to the loss of one coordinated water. The framework begins to collapse upon further heating. For **3**, **4** and **6**, the framework is thermally stable up to 362°C, 321°C and 310°C, respectively, at which the frameworks begin to collapse. For **5**, the weight loss of about 10.65 % from the room temperature to 190 °C is the equal of the departure of all lattice and partial coordinated water molecules (calcd of the departure of all water molecules 12.12 %). At temperature above 190 ^{o}C, the remaining framework begins to collapse. For **7**, the weight loss of about 3.20% from the room temperature to 97 °C corresponds to the departure of four lattice water molecules (calcd of 3.79 %), and the remaining framework is thermally stable up to 221 °C. At temperatures above 221 °C, the remaining framework begins to quickly collapse. For **8**, the weight loss of about 10.00 % for the room temperature to 278 °C, but the theoretical loss of three lattice and three coordinated water molecules is 12.3 %. So temperature between 25 °C to 278°C, **8** loses all the lattice and partial coordinated water molecules. At temperature above 278 ^{o}C, the remaining framework begins to collapse.

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Table S1. The comparison of some characteristics for H_4detc ligands in compounds **1-8**.

Complex	The carboxylate groups	The dihedral angle of four carboxylate groups (°)	The dihedral angle between two phenyl rings (°)	coordination modes of $detc^{4-}$ or $Hdetc^{3-}$ anions	coordination modes of carboxylate groups
1	2	68.453	87.288	μ_1-η^1:η^0:η^0:η^0	*syn-skew* bidentate
	3	24.839			
	3′	1.564			
	4′	6.185			
2	2	78.973	77.610	μ_1-η^1:η^0:η^0:η^0	chelating
	3	22.571			
	3′	8.150			
	4′	12.935			
3	2	85.936	84.913	μ_5-η^1:η^1:η^2:η^2	monodentate
	3	6.566			chelating
	3′	83.564			*syn-skew* bidentate
	4′	30.854			chelating-bidentate
4	2	76.480	83.753	μ_3-η^0:η^2:η^0:η^1	
	3	25.779			*syn-skew* bidentate
	3′	57.479			
	4′	27.097			chelating
5	2	87.790	53.974	μ_2-η^1:η^0:η^1:η^1	monodentate
	3	3.593			
	3′	71.132			monodentate
	4′	12.701			monodentate
6	2	85.740	80.401	μ_6-η^1:η^2:η^2:η^2	*syn-syn* bidentate
	3	4.532			monodentate
	3′	76.075			μ_2-η^2:η^0
	4′	23.980			chelating-bidentate
7	2	89.956	81.653	μ_5-η^1:η^1:η^2:η^2	chelating
	3	5.998			monodentate
	3′	81.814			*syn-skew* bidentate
	4′	29.867			chelating-bidentate
8	2	71.559	74.292	μ_3-η^0:η^1:η^1:η^1	
	3	20.591			chelating
	3′	77.575			monodentate
	4′	5.157			chelating

Table S2. Bond lengths [A] and angles [deg] for **1**.

Mn(1)-O(2)#1	2.1264(13)
Mn(1)-O(1)	2.1459(12)
Mn(1)-N(4)	2.2640(16)
Mn(1)-N(2)	2.2700(17)
Mn(1)-N(1)	2.2769(16)
Mn(1)-N(3)	2.2856(15)
O(2)#1-Mn(1)-O(1)	94.42(5)
O(2)#1-Mn(1)-N(4)	97.28(5)
O(1)-Mn(1)-N(4)	89.77(5)
O(2)#1-Mn(1)-N(2)	88.20(5)
O(1)-Mn(1)-N(2)	104.23(6)
N(4)-Mn(1)-N(2)	164.57(6)
O(2)#1-Mn(1)-N(1)	161.10(6)
O(1)-Mn(1)-N(1)	89.24(5)
N(4)-Mn(1)-N(1)	101.27(6)
N(2)-Mn(1)-N(1)	72.94(6)
O(2)#1-Mn(1)-N(3)	91.87(5)
O(1)-Mn(1)-N(3)	162.53(6)
N(4)-Mn(1)-N(3)	73.25(6)
N(2)-Mn(1)-N(3)	92.23(6)
N(1)-Mn(1)-N(3)	90.07(6)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y,-z+1

Table S3. Bond lengths [A] and angles [deg] for **2**.

Cd(1)-O(10)	2.228(2)
Cd(1)-N(1)#1	2.3115(15)
Cd(1)-N(1)	2.3115(15)
Cd(1)-O(1)	2.4141(13)
Cd(1)-O(1)#1	2.4142(13)
Cd(1)-O(2)#1	2.4587(14)
Cd(1)-O(2)	2.4589(14)
O(10)-Cd(1)-N(1)#1	98.76(4)
O(10)-Cd(1)-N(1)	98.76(4)
N(1)#1-Cd(1)-N(1)	162.49(9)
O(10)-Cd(1)-O(1)	133.64(3)
N(1)#1-Cd(1)-O(1)	83.36(5)
N(1)-Cd(1)-O(1)	84.58(5)
O(10)-Cd(1)-O(1)#1	133.64(3)
N(1)#1-Cd(1)-O(1)#1	84.58(5)
N(1)-Cd(1)-O(1)#1	83.36(5)
O(1)-Cd(1)-O(1)#1	92.71(6)
O(10)-Cd(1)-O(2)#1	79.98(3)
N(1)#1-Cd(1)-O(2)#1	86.69(5)
N(1)-Cd(1)-O(2)#1	96.36(5)
O(1)-Cd(1)-O(2)#1	146.00(4)
O(1)#1-Cd(1)-O(2)#1	53.92(4)
O(10)-Cd(1)-O(2)	79.98(3)
N(1)#1-Cd(1)-O(2)	96.36(5)
N(1)-Cd(1)-O(2)	86.68(5)
O(1)-Cd(1)-O(2)	53.92(4)
O(1)#1-Cd(1)-O(2)	146.00(4)
O(2)#1-Cd(1)-O(2)	159.96(6)

Symmetry transformations used to generate equivalent atoms:
#1 -x, y, -z+1/2

Table S4. Bond lengths [A] and angles [deg] for **3**.

Cd(1)-N(3)	2.286(2)
Cd(1)-O(1)	2.306(2)
Cd(1)-N(4)	2.316(2)
Cd(1)-O(9)#1	2.3372(17)
Cd(1)-O(8)#1	2.3628(18)
Cd(1)-O(2)	2.394(2)
Cd(2)-O(3)	2.192(2)
Cd(2)-O(6)#2	2.2582(18)
Cd(2)-O(7)#1	2.3267(18)
Cd(2)-N(2)	2.382(2)
Cd(2)-N(1)	2.390(2)
Cd(2)-O(9)#1	2.5248(19)
N(3)-Cd(1)-O(1)	132.24(8)
N(3)-Cd(1)-N(4)	72.77(8)
O(1)-Cd(1)-N(4)	103.06(8)
N(3)-Cd(1)-O(9)#1	117.15(7)
O(1)-Cd(1)-O(9)#1	99.73(7)
N(4)-Cd(1)-O(9)#1	134.38(7)
N(3)-Cd(1)-O(8)#1	133.97(8)
O(1)-Cd(1)-O(8)#1	91.26(8)
N(4)-Cd(1)-O(8)#1	84.71(7)
O(9)#1-Cd(1)-O(8)#1	55.66(6)
N(3)-Cd(1)-O(2)	84.51(7)
O(1)-Cd(1)-O(2)	55.15(7)
N(4)-Cd(1)-O(2)	118.88(8)
O(9)#1-Cd(1)-O(2)	106.61(7)
O(8)#1-Cd(1)-O(2)	141.06(7)
O(3)-Cd(2)-O(6)#2	98.19(10)
O(3)-Cd(2)-O(7)#1	151.49(9)
O(6)#2-Cd(2)-O(7)#1	96.59(7)
O(3)-Cd(2)-N(2)	123.75(8)
O(6)#2-Cd(2)-N(2)	83.27(7)
O(7)#1-Cd(2)-N(2)	82.10(7)
O(3)-Cd(2)-N(1)	90.55(9)
O(6)#2-Cd(2)-N(1)	152.17(8)
O(7)#1-Cd(2)-N(1)	87.59(7)
N(2)-Cd(2)-N(1)	70.02(8)
O(3)-Cd(2)-O(9)#1	75.24(8)
O(6)#2-Cd(2)-O(9)#1	106.14(7)
O(7)#1-Cd(2)-O(9)#1	77.28(6)
N(2)-Cd(2)-O(9)#1	158.13(6)
N(1)-Cd(2)-O(9)#1	101.63(7)

Symmetry transformations used to generate equivalent atoms:

#1 x+1,y,z #2 -x,-y+2,-z+1 #3 x-1,y,z

Table S5. Bond lengths [A] and angles [deg] for **4**.

Zn(1)-O(2)#1	1.9670(17)
Zn(1)-O(1)	1.9758(16)
Zn(1)-N(1)	2.048(2)
Zn(1)-O(8)#2	2.105(2)
Zn(1)-O(9)#2	2.230(2)
O(2)#1-Zn(1)-O(1)	126.19(8)
O(2)#1-Zn(1)-N(1)	95.70(8)
O(1)-Zn(1)-N(1)	91.73(8)
O(2)#1-Zn(1)-O(8)#2	98.17(8)
O(1)-Zn(1)-O(8)#2	97.81(8)
N(1)-Zn(1)-O(8)#2	153.77(9)
O(2)#1-Zn(1)-O(9)#2	115.35(8)
O(1)-Zn(1)-O(9)#2	117.24(8)
N(1)-Zn(1)-O(9)#2	93.55(8)
O(8)#2-Zn(1)-O(9)#2	60.37(8)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+2,-z+1 #2 x-1,y-1,z #3 x+1,y+1,z

Table S6. Bond lengths [A] and angles [deg] for **5**.

Ni(2)-O(6)	2.045(2)
Ni(2)-O(13)	2.045(3)
Ni(2)-N(4)#1	2.081(3)
Ni(2)-N(3)	2.099(3)
Ni(2)-O(12)	2.105(3)
Ni(2)-O(14)	2.105(3)
Ni(1)-O(1)	2.057(2)
Ni(1)-O(3)	2.068(3)
Ni(1)-O(10)	2.078(2)
Ni(1)-O(11)	2.102(3)
Ni(1)-N(1)	2.105(2)
Ni(1)-N(2)#2	2.112(3)
O(6)-Ni(2)-O(13)	91.57(11)
O(6)-Ni(2)-N(4)#1	88.27(10)
O(13)-Ni(2)-N(4)#1	88.08(11)
O(6)-Ni(2)-N(3)	94.60(10)
O(13)-Ni(2)-N(3)	90.74(12)
N(4)#1-Ni(2)-N(3)	176.93(12)
O(6)-Ni(2)-O(12)	89.98(10)
O(13)-Ni(2)-O(12)	177.39(10)
N(4)#1-Ni(2)-O(12)	89.87(11)
N(3)-Ni(2)-O(12)	91.22(11)
O(6)-Ni(2)-O(14)	177.01(10)
O(13)-Ni(2)-O(14)	90.42(12)
N(4)#1-Ni(2)-O(14)	89.57(11)
N(3)-Ni(2)-O(14)	87.60(11)
O(12)-Ni(2)-O(14)	87.94(11)
O(1)-Ni(1)-O(3)	87.62(10)
O(1)-Ni(1)-O(10)	177.69(9)
O(3)-Ni(1)-O(10)	92.31(12)
O(1)-Ni(1)-O(11)	89.39(11)
O(3)-Ni(1)-O(11)	175.80(11)
O(10)-Ni(1)-O(11)	90.57(12)
O(1)-Ni(1)-N(1)	91.70(9)
O(3)-Ni(1)-N(1)	94.13(12)
O(10)-Ni(1)-N(1)	90.61(9)
O(11)-Ni(1)-N(1)	88.91(12)
O(1)-Ni(1)-N(2)#2	88.81(9)
O(3)-Ni(1)-N(2)#2	89.79(11)
O(10)-Ni(1)-N(2)#2	88.88(10)
O(11)-Ni(1)-N(2)#2	87.20(11)
N(1)-Ni(1)-N(2)#2	176.07(13)

Symmetry transformations used to generate equivalent atoms:

#1 x-1/2,-y+1/2,z-1 #2 x-1,y,z #3 x+1,y,z
#4 x+1/2,-y+1/2,z+1

Table S7. Bond lengths [A] and angles [deg] for **6**.

Co(1)-O(10)	2.041(6)
Co(1)-O(4)#1	2.078(5)
Co(1)-O(1)	2.083(5)
Co(1)-O(9)#2	2.108(5)
Co(1)-O(7)#2	2.143(6)
Co(1)-N(1)	2.172(5)
Co(2)-O(9)#3	1.972(5)
Co(2)-O(3)	1.983(5)
Co(2)-N(2)	2.005(6)
Co(2)-O(6)#4	2.007(5)
O(10)-Co(1)-O(4)#1	85.6(2)
O(10)-Co(1)-O(1)	91.2(2)
O(4)#1-Co(1)-O(1)	93.0(2)
O(10)-Co(1)-O(9)#2	178.5(2)
O(4)#1-Co(1)-O(9)#2	92.9(2)
O(1)-Co(1)-O(9)#2	88.8(2)
O(10)-Co(1)-O(7)#2	94.3(2)
O(4)#1-Co(1)-O(7)#2	178.7(2)
O(1)-Co(1)-O(7)#2	88.3(2)
O(9)#2-Co(1)-O(7)#2	87.1(2)
O(10)-Co(1)-N(1)	88.5(2)
O(4)#1-Co(1)-N(1)	90.1(2)
O(1)-Co(1)-N(1)	176.8(3)
O(9)#2-Co(1)-N(1)	91.5(2)
O(7)#2-Co(1)-N(1)	88.5(2)
O(9)#3-Co(2)-O(3)	101.6(2)
O(9)#3-Co(2)-N(2)	117.6(3)
O(3)-Co(2)-N(2)	107.5(2)
O(9)#3-Co(2)-O(6)#4	99.2(2)
O(3)-Co(2)-O(6)#4	111.4(2)
N(2)-Co(2)-O(6)#4	118.3(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1/2,-y,z+1/2 #2 -x+1/4,y+1/4,z+1/4

#3 x+1/4,-y-1/4,z-1/4 #4 x+1/4,-y-1/4,z+3/4

#5 -x+1/2,-y,z-1/2 #6 x-1/4,-y-1/4,z-3/4

#7 -x+1/4,y-1/4,z-1/4 #8 x-1/4,-y-1/4,z+1/4

#9 x-1/4,-y+1/4,z-1/4 #10 x+1/4,-y+1/4,z+1/4

Table S8. Bond lengths [A] and angles [deg] for **7**.

Cu(1)-O(1)	1.908(2)
Cu(1)-O(7)#1	1.970(2)
Cu(1)-O(6)#2	1.993(2)
Cu(1)-N(1)	1.998(3)
Cu(1)-O(10)	2.424(3)
Cu(2)-O(11)	1.952(3)
Cu(2)-O(3)	1.968(2)
Cu(2)-N(2)	2.000(3)
Cu(2)-O(8)#1	2.001(2)
O(1)-Cu(1)-O(7)#1	173.24(9)
O(1)-Cu(1)-O(6)#2	87.41(10)
O(7)#1-Cu(1)-O(6)#2	87.53(9)
O(1)-Cu(1)-N(1)	90.63(11)
O(7)#1-Cu(1)-N(1)	94.70(11)
O(6)#2-Cu(1)-N(1)	175.76(11)
O(1)-Cu(1)-O(10)	92.77(11)
O(7)#1-Cu(1)-O(10)	91.39(10)
O(6)#2-Cu(1)-O(10)	86.25(11)
N(1)-Cu(1)-O(10)	90.09(12)
O(11)-Cu(2)-O(3)	160.00(11)
O(11)-Cu(2)-N(2)	91.67(11)
O(3)-Cu(2)-N(2)	95.58(11)
O(11)-Cu(2)-O(8)#1	88.11(10)
O(3)-Cu(2)-O(8)#1	90.58(9)
N(2)-Cu(2)-O(8)#1	162.16(10)

Symmetry transformations used to generate equivalent atoms:

#1 x,y-1,z #2 -x,-y+2,-z+1 #3 x,y+1,z

#4 -x+1,-y+1,-z #5 -x-1,-y+2,-z

Table S9. Bond lengths [A] and angles [deg] for **8**.

Ni(1)-O(1)	2.0540(16)
Ni(1)-N(1)	2.070(2)
Ni(1)-O(10)	2.0789(19)
Ni(1)-N(2)	2.088(2)
Ni(1)-O(11)	2.0921(19)
Ni(1)-O(12)	2.105(2)
Ni(2)-N(4)	2.036(2)
Ni(2)-O(8)	2.0438(17)
Ni(2)-N(3)	2.048(2)
Ni(2)-O(4)#1	2.0550(18)
Ni(2)-O(3)#1	2.1368(16)
Ni(2)-O(9)	2.2023(18)
O(1)-Ni(1)-N(1)	178.75(8)
O(1)-Ni(1)-O(10)	92.00(7)
N(1)-Ni(1)-O(10)	87.79(8)
O(1)-Ni(1)-N(2)	88.55(7)
N(1)-Ni(1)-N(2)	91.64(8)
O(10)-Ni(1)-N(2)	178.82(9)
O(1)-Ni(1)-O(11)	83.74(8)
N(1)-Ni(1)-O(11)	95.02(8)
O(10)-Ni(1)-O(11)	88.79(9)
N(2)-Ni(1)-O(11)	90.24(9)
O(1)-Ni(1)-O(12)	88.29(8)
N(1)-Ni(1)-O(12)	92.93(9)
O(10)-Ni(1)-O(12)	88.32(9)
N(2)-Ni(1)-O(12)	92.75(9)
O(11)-Ni(1)-O(12)	171.43(8)
N(4)-Ni(2)-O(8)	94.23(8)
N(4)-Ni(2)-N(3)	95.74(9)
O(8)-Ni(2)-N(3)	96.00(9)
N(4)-Ni(2)-O(4)#1	99.74(8)
O(8)-Ni(2)-O(4)#1	158.70(7)
N(3)-Ni(2)-O(4)#1	98.49(9)
N(4)-Ni(2)-O(3)#1	162.34(9)
O(8)-Ni(2)-O(3)#1	101.67(7)
N(3)-Ni(2)-O(3)#1	90.23(8)
O(4)#1-Ni(2)-O(3)#1	62.88(7)
N(4)-Ni(2)-O(9)	89.81(8)
O(8)-Ni(2)-O(9)	61.77(7)
N(3)-Ni(2)-O(9)	157.49(9)
O(4)#1-Ni(2)-O(9)	102.04(7)
O(3)#1-Ni(2)-O(9)	90.98(7)

Symmetry transformations used to generate equivalent atoms:

#1 x+1, y+1, z #2 x-1, y-1,z #3 -x,-y-2,-z
#4 -x+1, -y-1, -z+1 #5 -x+1, -y+2, -z
#6 -x+1, -y+2, -z+1

Table S10. Hydrogen bond parameters [Å,°] for **1**.

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
O3-H3A	0.864	1.754	171.03	2.610	O10
O10-H10B	0.853	1.904	168.19	2.744	O6 [-x+1, -y, -z+1]
O10-H10C	0.856	1.988	176.87	2.843	O1 [-x+1, -y, -z+1]
C17-H17A	0.930	2.328	151.85	3.178	O4 [-x+1, -y, -z+1]
C27-H27A	0.930	2.376	165.80	3.285	O6 [x+1, y, z]
C18-H18A	0.930	2.658	159.53	3.545	O9 [x-1/2, -y+1/2, z+1/2]
C31-H31A	0.930	2.7727	176.449	3.7014	O4 [1+x, y, 1+z]
C6-H6A	0.930	2.4084	168.762	3.3255	O9[-0.5+x,0.5-y,-0.5+z]
C34-H34A	0.930	2.6949	139.018	3.4513	O8 [1.5-x,-0.5+ y, 1.5-z]
C38-H38A	0.930	2.5544	143.461	3.3477	O8 [1.5-x,-0.5+ y, 1.5-z]
C28-H28A	0.930	2.604	119.56	3.168	O2 [-x+2, -y, -z+1]
C40-H40A	0.930	2.647	120.54	3.221	O1

Table S11. Hydrogen bond parameters [Å,°] for **2**.

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
O4-H4A	0.851	1.777	173.47	2.624	O11
O10-H10B	0.827	1.888	169.87	2.706	O13 [x, y-1, z]
O12-H12A	0.837	1.977	154.57	2.757	O2 [x, y+1, z]
O12-H12B	0.836	1.913	169.76	2.740	O6
O13-H13A	0.832	1.931	162.76	2.737	O12
O13-H13B	0.884	1.831	170.34	2.707	O1
O11-H11A	0.863	2.138	163.15	2.975	O3 [-x, -y+1, -z+1]
O11-H11B	0.821	2.032	172.54	2.848	O13 [-x, -y+2, -z+1]
C16-H16A	0.930	2.594	134.69	3.314	O6 [x, y-1, z]

Table S12. Hydrogen bond parameters [Å,°] for **3**.

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
C29-H29A	0.930	2.613	139.17	3.372	O7[-x, -y+2, -z+1]
C34-H34A	0.930	2.8886	156.523	3.7600	O2 [-x, 1-y, 1-z]
C39-H39A	0.930	2.493	168.73	3.409	O4[x, y-1, z]
C5-H5A	0.930	2.6308	137.318	3.3739	O5 [-x, 0.5+y, 0.5-z]
C16-H16A	0.930	2.7043	153.388	3.5603	O4 [-x, -0.5+y, 0.5-z]
C19-H19A	0.930	2.7006	121.743	3.2865	O8 [-x, 0.5+y, 0.5-z]
C21-H21A	0.930	2.3638	161.284	3.2583	O1 [1-x, -0.5+y, 0.5-z]
C28-H28A	0.930	2.505	123.50	3.116	O6 [-x, -y+2, -z+1]

Table S13. Hydrogen bond parameters [Å,°] for **4**.

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
O7-H7B	0.909	1.657	176.140	2.564	O3 [-x+2, -y+3, -z+1]
C6-H6A	0.930	2.420	150.540	3.262	O9 [x-1, y, z]
C26-H26A	0.930	2.368	144.040	3.168	O4 [x+1, y, z]
C7-H7A	0.930	2.8213	162.344	3.7182	O7 [-1+x, y, z]
C8-H8A	0.930	2.6043	140.050	3.3706	O6 [1-x, 3-y, 1-z]
C25-H25A	0.930	2.5480	122.110	3.142	O3 [-x+2, -y+2, -z]
C16-H16A	0.930	2.9588	155.123	3.8226	O9 [2-x, 3-y, -z]
C19-H19A	0.930	2.7413	133.448	3.4476	O5 [1-x, 2-y, -z]

Table S14. Hydrogen bond parameters [Å,°] for **5**.

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
O11-H11B	0.898	1.938	157.73	2.790	O16 [x-1/2, -y+1/2, z-1]
O12-H12B	0.838	1.770	16798	2.596	O7
O13-H13B	0.836	1.998	161.55	2.804	O16
O12-H12A	0.847	2.012	147.70	2.765	O2 [x, y, z+1]
O13-H13A	0.833	1.790	172.53	2.618	O9 [x-1/2, -y+1/2, z]
O14-H14B	0.824	1.865	168.22	2.677	O8 [x-1/2, -y+1/2, z]
O14-H14C	0.798	2.213	155.62	2.958	O2 [x, y, z+1]
O10-H10A	0.805	2.011	169.13	2.805	O4 [-x+1, -y+1, z-1/2]
O10-H10B	0.774	2.007	168.51	2.770	O9 [-x+2, -y+1, z-1/2]
O11-H11A	0.860	2.012	154.39	2.812	O3 [-x+1, -y+1, z-1/2]

Table S15. Hydrogen bond parameters [Å,°] for **6**.

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
O10-H10B	0.834	1.925	166.29	2.743	O3 [-x+1/2, -y, z-1/2]
C17-H17A	0.930	2.648	110.94	3.105	O10
C24-H24A	0.930	2.285	156.89	3.162	O2

Table S16. Hydrogen bond parameters [Å,°] for **7**.

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
O10-H10B	0.845	2.374	167.58	3.204	O15 [-x+1, -y+1, -z+1]
O10-H10C	0.853	2.004	148.01	2.765	O2
O11-H11A	0.857	1.749	177.95	2.606	O13 [-x, -y+1, -z+1]
O11-H11B	0.839	1.971	157.54	2.765	O7 [-x, -y+2, -z+1]
C16-H16A	0.930	2.569	145.64	3.378	O3 [-x, -y+2, -z]
C17-H17A	0.930	2.657	113.31	3.143	O10
C24-H24A	0.930	2.596	114.69	3.102	O3
C24-H24A	0.930	2.484	163.03	3.384	O5

Table S17. Hydrogen bond parameters [Å,°] for **8**.

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
O11-H11A	0.839	1.913	168.34	2.740	O6 [x-1, y-1, z]
O11-H11B	0.826	2.071	176.45	2.896	O3
O12-H12B	0.830	1.856	172.92	2.682	O7 [x, y-1, z]
C17-H17A	0.930	2.566	146.48	3.381	O7 [x, y-1, z]
C23-H23A	0.930	2.645	116.42	3.171	O12
C24-H24A	0.930	2.585	111.23	3.048	O11
C29-H29A	0.930	2.476	121.40	3.065	O8
O10-H10A	0.845	1.768	157.78	2.570	O2