Supplementary Information

Synthesis, Structures, and Water Adsorption of Two Coordination Polymers Constructed by M(II) (M = Ni (1) and Zn (2)) with 1,3-bis(4-pyridyl)propane (bpp) and 1,2,4,5-benzenetetracarboxylate (BT^{4-}) Ligands

Supporting Information

Table S1. Bond lengths (Å) and angles (°) around Ni(II) ion in **1**.

Ni(1)–O(5)	2.039(3)	Ni(1)–N(3)	2.063(4)
Ni(1)–N(1)	2.069(4)	Ni(1)–O(11)	2.089(3)
Ni(1)–O(9)	2.095(3)	Ni(1)–O(10)	2.099(4)
Ni(2)–O(1)	2.051(3)	Ni(2)–N(2)	2.060(4)
Ni(2)–N(4)	2.083(4)	Ni(2)–O(13)	2.088(3)
Ni(2)–O(14)	2.091(3)	Ni(2)–O(12)	2.103(3)
O(5)–Ni(1)–N(3)	170.95(1)	O(5)–Ni(1)–O(1)	90.66 (2)
N(3)–Ni(1)–N(1)	96.38(2)	O(5)–Ni(1)–O(11)	82.19(1)
N(3)–Ni(1)–O(11)	91.80(2)	N(1)–Ni(1)–O(11)	92.48(1)
O(5)–Ni(1)–O(9)	84.23(1)	N(3)–Ni(1)–O(9)	89.05(1)
N(1)–Ni(1)–O(9)	173.90(2)	O(11)–Ni(1)–O(9)	90.13(1)
O(5)–Ni(1)–O(10)	91.71(1)	N(3)–Ni(1)–O(10)	94.38(2)
N(1)–Ni(1)–O(10)	86.54(2)	O(11)–Ni(1)–O(10)	173.81(2)
O(9)–Ni(1)–O(10)	90.27(1)	O(1)–Ni(2)–N(2)	171.96(1)
O(1)–Ni(2)–N(4)	90.89(2)	N(2)–Ni(2)–N(4)	93.15(2)
O(1)–Ni(2)–O(13)	80.99(1)	N(2)–Ni(2)–O(13)	91.77(2)
N(4)–Ni(2)–O(13)	94.20(1)	O(1)–Ni(2)–O(14)	86.31(1)
N(2)–Ni(2)–O(14)	90.17(1)	N(4)–Ni(2)–O(14)	174.84(2)
O(13)–Ni(2)–O(14)	89.64(1)	O(1)–Ni(2)–O(12)	91.48(1)
N(2)–Ni(2)–O(12)	95.59(1)	N(4)–Ni(2)–O(12)	88.14(1)
O(13)–Ni(2)–O(12)	172.14(1)	O(14)–Ni(2)–O(12)	87.60(1)

Table S2. Related parameters of O–H···O hydrogen bonds in **1**. [1]

D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	∠ D–H···A (°)
O(9)–H(9A)···O(4)$_{i}$	0.83	1.87	2.675(1)	163
O(9)–H(9B)···O(7)	0.83	2.07	2.871(1)	163
O(10)–H(10A)···O(6)	0.83	1.94	2.752(1)	164
O(10)–H(10B)···O(2)$_{ii}$	0.83	1.94	2.726(1)	157
O(11)–H(11A)···O(3)$_{i}$	0.83	1.91	2.668(1)	153
O(11)–H(11B)···O(8)	0.82	2.41	3.094(1)	141
O(12)–H(12A)···O(2)	0.83	1.94	2.689(1)	150
O(12)–H(12B)···O(6)$_{iii}$	0.83	1.91	2.713(1)	163
O(13)–H(13A)···O(7)$_{iv}$	0.83	1.85	2.689(1)	178
O(13)–H(13B)···O(4)	0.84	2.38	3.170(1)	157
O(14)–H(14A)···O(8)$_{iv}$	0.83	1.89	2.705(1)	169
O(14)–H(14B)···O(3)	0.83	1.98	2.799(1)	172
O(15)–H(15A)···O(12)$_{v}$	0.91	2.09	2.869(1)	143
O(15)–H(15B)···O(7)$_{vi}$	0.94	1.87	2.719(1)	150
O(16)–H(16)···O(15)	0.84	2.00	2.610(1)	129
O(17)–H(17C)···O(3)$_{ii}$	0.96	2.22	2.862(1)	123
O(18)–H(18)···O(16)	0.84	2.23	2.813(1)	127

[1] Symmetry transformations used to generate equivalent atoms: i = x,–y–1, z+1/2; ii = x–1,–y–1, z+1/2; iii = x,–y, z+1/2; iv = x–1,–y, z+1/2; v = x–1/2, y+3/2, z–1; vi = x–1/2,–y+1/2, z–1/2

Table S3. Bond lengths (Å) and angles (°) around Zn(II) ion in **2**.[1]

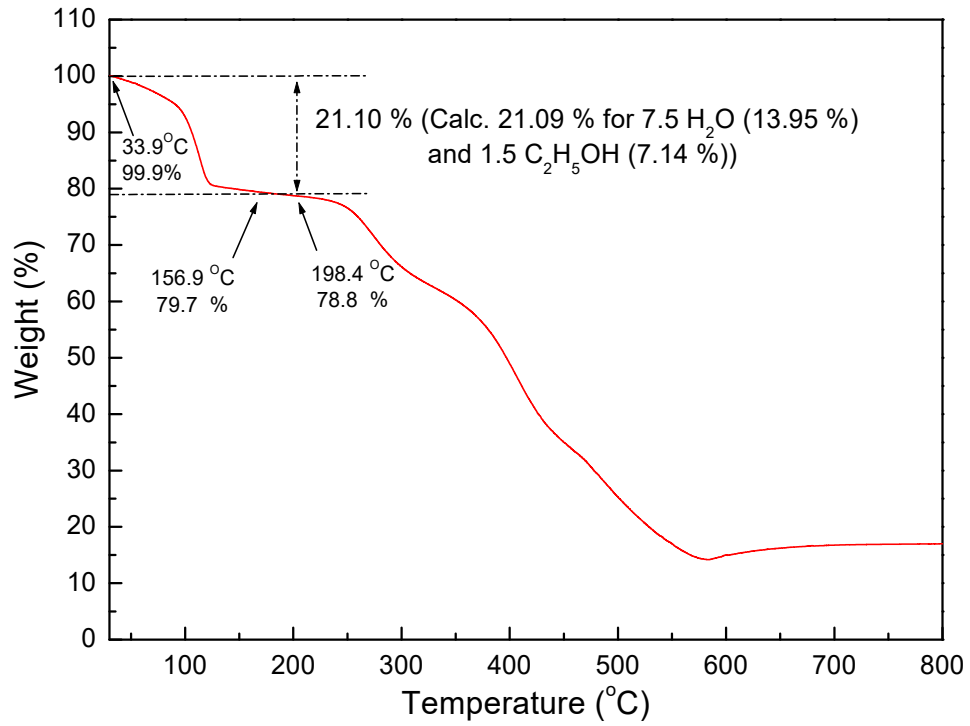
Zn(1)–O(1)	1.997(9)	Zn(1)–N(1)	2.024(1)
Zn(1)–N(2)	2.025(1)	Zn(1)–O(3)$_i$	2.030(9)
O(1)–Zn(1)–N(1)	110.05(4)	O(1)–Zn(1)–N(2)	108.05(4)
N(1)–Zn(1)–N(2)	110.25(4)	O(1)–Zn(1)–O(3)$_i$	102.29(4)
N(1)–Zn(1)–O(3)$_i$	117.72(4)	N(2)–Zn(1)–O(3)$_i$	107.90(4)

[1] Symmetry transformations used to generate equivalent atoms: i x,-y+1/2,z-1/2.

Table S4. Related parameters of O–H···O hydrogen bonds in **2**. [1]

D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	∠ D–H···A (°)
O(5)–H(5A)···O(8)	0.83	1.95	2.766(1)	167
O(5)–H(5B)···O(1)$_i$	0.79	2.08	2.867(1)	171
O(6)–H(6A)···O(7)	0.81	1.93	2.725(1)	171
O(6)–H(6B)···O(4)$_{ii}$	0.83	2.07	2.854(1)	159
O(7)–H(7A)···O(9)$_{ii}$	0.88	1.95	2.818(1)	170
O(7)–H(7B)···O(5)$_{iii}$	0.82	1.99	2.804(1)	174
O(8)–H(8A)···O(9)	0.84	1.90	2.735(1)	178
O(8)–H(8B)···O(3)$_{iv}$	0.82	2.10	2.884(1)	160
O(9)–H(9A)···O(2)	0.81	1.96	2.771(1)	175
O(9)–H(9B)···O(6)	0.81	1.95	2.757(1)	176

[1] Symmetry transformations used to generate equivalent atoms: i = –x–1,–y–1,–z; ii = –x, y+1/2,–z+3/2; iii = –x,–y,–z; iv = –x–1, y+1/2,–z+3/2



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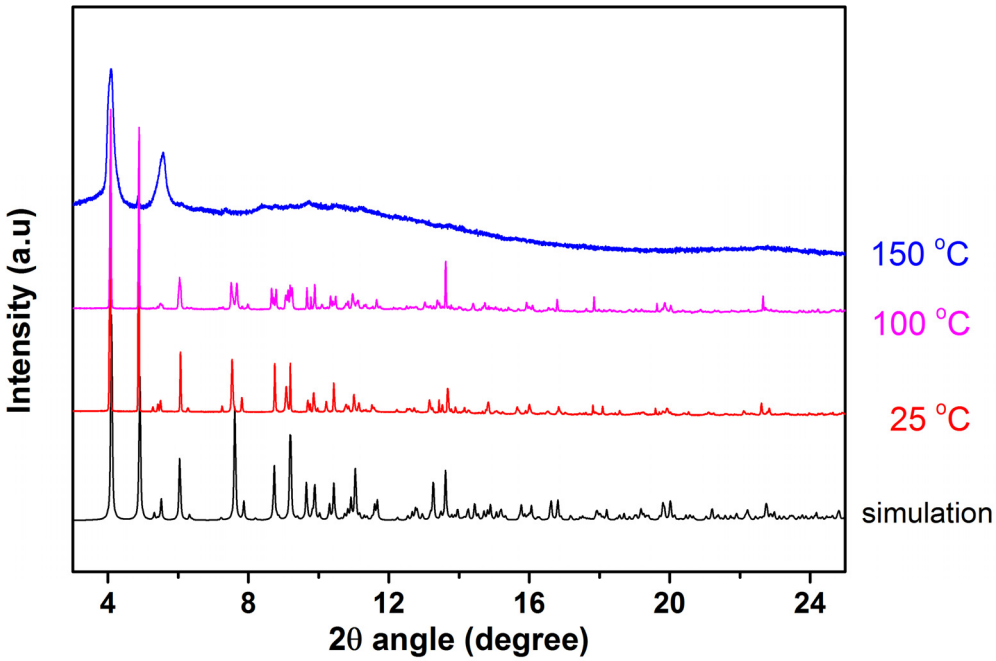
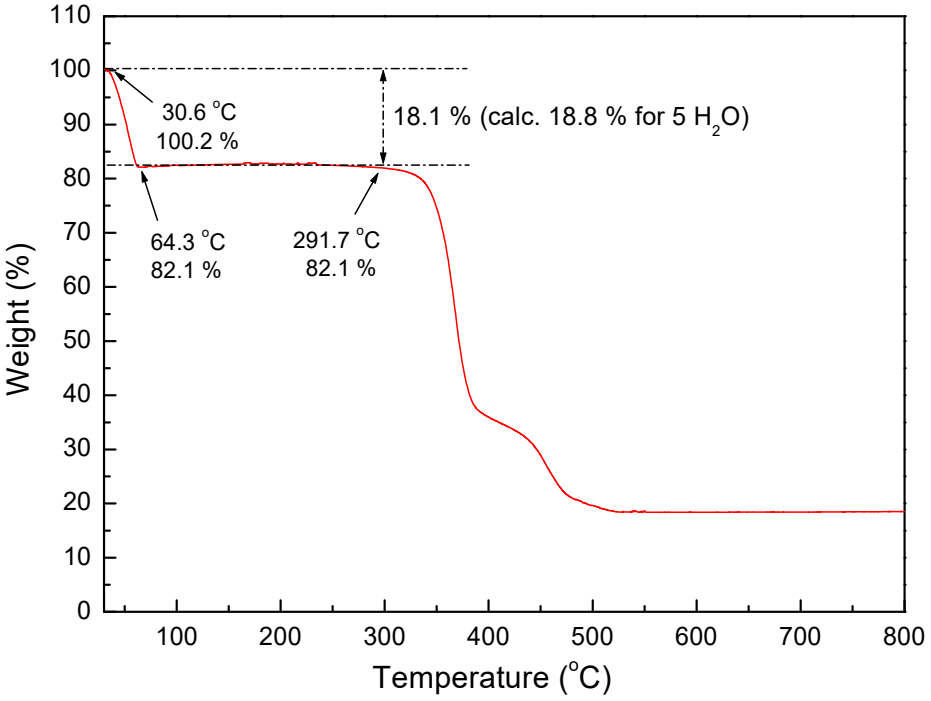
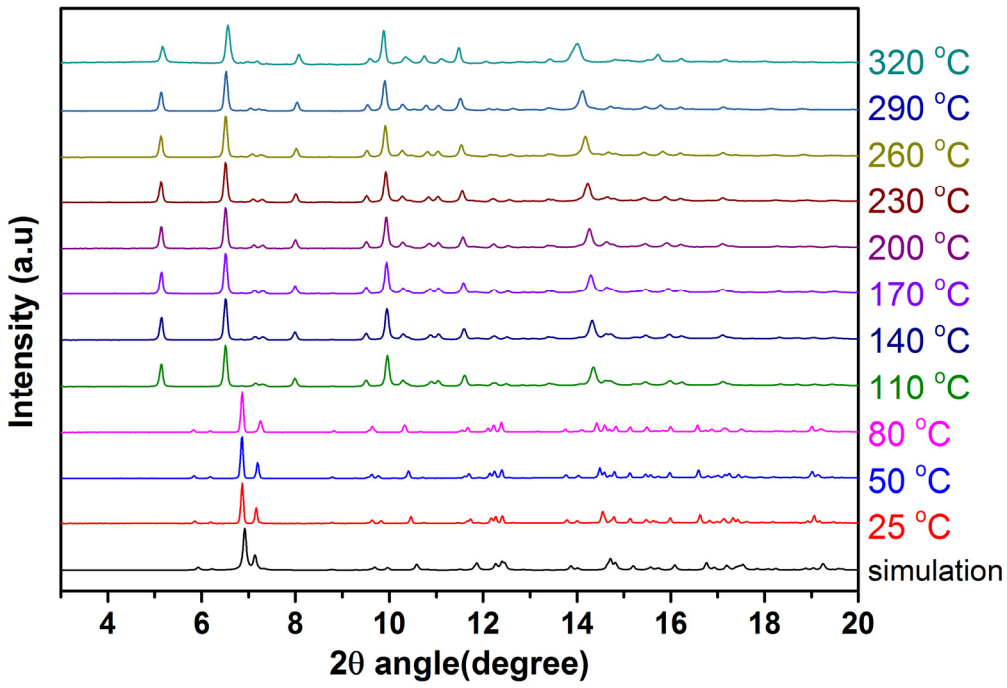


(b)

Figure S1 (a) Thermogravimetric (TG) measurement of **1**. (b) Powder X-ray diffraction patterns at RT and selected temperatures and its simulation from single-crystal diffraction data of **1**.



(a)



(b)

Figure S2 (a) Thermogravimetric (TG) measurement of **2**. (b) Powder X-ray diffraction patterns at RT and selected temperatures and its simulation from single-crystal diffraction data of **2**.