Syntheses, characterization, and magnetic properties of novel divalent Co/Ni coordination polymers based on a V-shaped pyridine ligand and dicarboxylate acids

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Table S1. Selected bond distances and angles for 1.

Co(1)-O(6)	2.0163(14)	Co(1)-O(4)	2.0589(15)
Co(1)-O(1)	2.1400(14)	Co(1)-N(2)	2.1442(17)
Co(1)-O(2)	2.1475(14)	Co(1)-N(1)	2.1648(17)
Co(2)-O(8)	2.0648(14)	Co(2)-O(8)#1	2.0648(14)
Co(2)-O(3)	2.1384(14)	Co(2)-O(3)#1	2.1384(14)
Co(2)-N(3)	2.1386(17)	Co(2)-N(3)#1	2.1387(17)
O(6)-Co(1)-O(4)	175.93(6)	O(6)-Co(1)-O(1)	91.27(6)
O(4)-Co(1)-O(1)	87.81(6)	O(6)-Co(1)-N(2)	91.67(7)
O(4)-Co(1)-N(2)	92.34(7)	O(1)-Co(1)-N(2)	93.18(6)
O(6)-Co(1)-O(2)	91.20(6)	O(4)-Co(1)-O(2)	89.58(6)
O(1)-Co(1)-O(2)	176.75(5)	N(2)-Co(1)-O(2)	88.86(6)
O(6)-Co(1)-N(1)	91.94(7)	O(4)-Co(1)-N(1)	84.09(7)

O(1)-Co(1)-N(1)	89.44(6)	N(2)-Co(1)-N(1)	175.49(7)
O(2)-Co(1)-N(1)	88.36(6)	O(8)-Co(2)-O(8)#1	180.0
O(8)-Co(2)-O(3)	89.53(6)	O(8)#1-Co(2)-O(3)	90.47(6)
O(8)-Co(2)-O(3)#1	90.47(6)	O(8)#1-Co(2)-O(3)#1	89.53(6)
O(3)-Co(2)-O(3)#1	180.000(19)	O(8)-Co(2)-N(3)	86.84(7)
O(8)#1-Co(2)-N(3)	93.16(7)	O(3)-Co(2)-N(3)	87.48(6)
O(3)#1-Co(2)-N(3)	92.52(6)	O(8)-Co(2)-N(3)#1	93.16(7)
O(8)#1-Co(2)-N(3)#1	86.84(7)	O(3)-Co(2)-N(3)#1	92.52(6)
O(3)#1-Co(2)-N(3)#1	87.48(6)	N(3)-Co(2)-N(3)#1	180.00(10)

Symmetry codes: #1 = − *x*+2,− *y*+2, − *z*.

Table S2. Selected bond distances and angles for 2.

Ni(1)-O(4)	2.009(2)	Ni(1)-O(8)	2.044(2)
Ni(1)-N(3)#1	2.086(3)	Ni(1)-O(6)	2.089(3)
Ni(1)-N(2)	2.103(3)	Ni(1)-O(7)	2.105(3)
Ni(2)-O(1)	2.057(2)	Ni(2)-O(1)#2	2.057(2)
Ni(2)-N(1)#2	2.082(3)	Ni(2)-N(1)	2.082(3)
Ni(2)-O(3)#2	2.089(3)	Ni(2)-O(3)	2.089(3)
O(4)-Ni(1)-O(8)	176.06(12)	O(4)-Ni(1)-N(3)#1	91.67(14)
O(8)-Ni(1)-N(3)#1	92.24(14)	O(4)-Ni(1)-O(6)	92.27(10)
O(8)-Ni(1)-O(6)	87.11(11)	N(3)#1-Ni(1)-O(6)	92.87(12)
O(4)-Ni(1)-N(2)	91.46(12)	O(8)-Ni(1)-N(2)	84.65(12)
N(3)#1-Ni(1)-N(2)	175.93(14)	O(6)-Ni(1)-N(2)	89.61(11)
O(4)-Ni(1)-O(7)	89.54(10)	O(8)-Ni(1)-O(7)	90.97(10)
N(3)#1-Ni(1)-O(7)	88.81(12)	O(6)-Ni(1)-O(7)	177.49(10)
N(2)-Ni(1)-O(7)	88.60(12)	O(1)-Ni(2)-O(1)#2	180.00(16)
O(1)-Ni(2)-N(1)#2	93.35(13)	O(1)#2-Ni(2)-N(1)#2	86.65(13)

O(1)-Ni(2)-N(1)	86.65(13)	O(1)#2-Ni(2)-N(1)	93.35(13)
N(1)#2-Ni(2)-N(1)	180.00(18)	O(1)-Ni(2)-O(3)#2	91.22(10)
O(1)#2-Ni(2)-O(3)#2	88.78(10)	N(1)#2-Ni(2)-O(3)#2	87.31(12)
N(1)-Ni(2)-O(3)#2	92.69(12)	O(1)-Ni(2)-O(3)	88.78(10)
O(1)#2-Ni(2)-O(3)	91.22(10)	N(1)#2-Ni(2)-O(3)	92.69(12)
N(1)-Ni(2)-O(3)	87.31(12)	O(3)#2-Ni(2)-O(3)	180.0

Symmetry codes: #1 = *x*, − *y* −1/2, *z*+1/2; #2 = − *x*+1,− *y*+1, − *z*.

Table S3. Selected bond distances and angles for 3.

Co(1)-O(1)	1.991(3)	Co(1)-O(2)#1	2.002(3)
Co(1)-N(3)	2.143(3)	Co(1)-N(1)#3	2.155(4)
Co(1)-O(3)	2.175(4)	Co(1)-O(4)	2.273(4)
O(1)-Co(1)-O(2)#1	122.53(14)	O(1)-Co(1)-N(3)	91.14(13)
O(2)#1-Co(1)-N(3)	86.19(13)	O(1)-Co(1)-N(1)#3	94.06(13)
O(2)#1-Co(1)-N(1)#3	89.80(14)	N(3)-Co(1)-N(1)#3	174.61(14)
O(1)-Co(1)-O(3)	145.70(14)	O(2)#1-Co(1)-O(3)	91.73(13)
N(3)-Co(1)-O(3)	89.37(14)	N(1)#3-Co(1)-O(3)	87.16(14)
O(1)-Co(1)-O(4)	88.70(13)	O(2)#1-Co(1)-O(4)	147.63(13)
N(3)-Co(1)-O(4)	84.80(14)	N(1)#3-Co(1)-O(4)	96.75(15)
O(3)-Co(1)-O(4)	57.19(13)		

Symmetry codes: #1 = − *x*+1, − *y*+2, − *z*+1; #3 = *x*−1,− *y*+2, *z*−1/2.

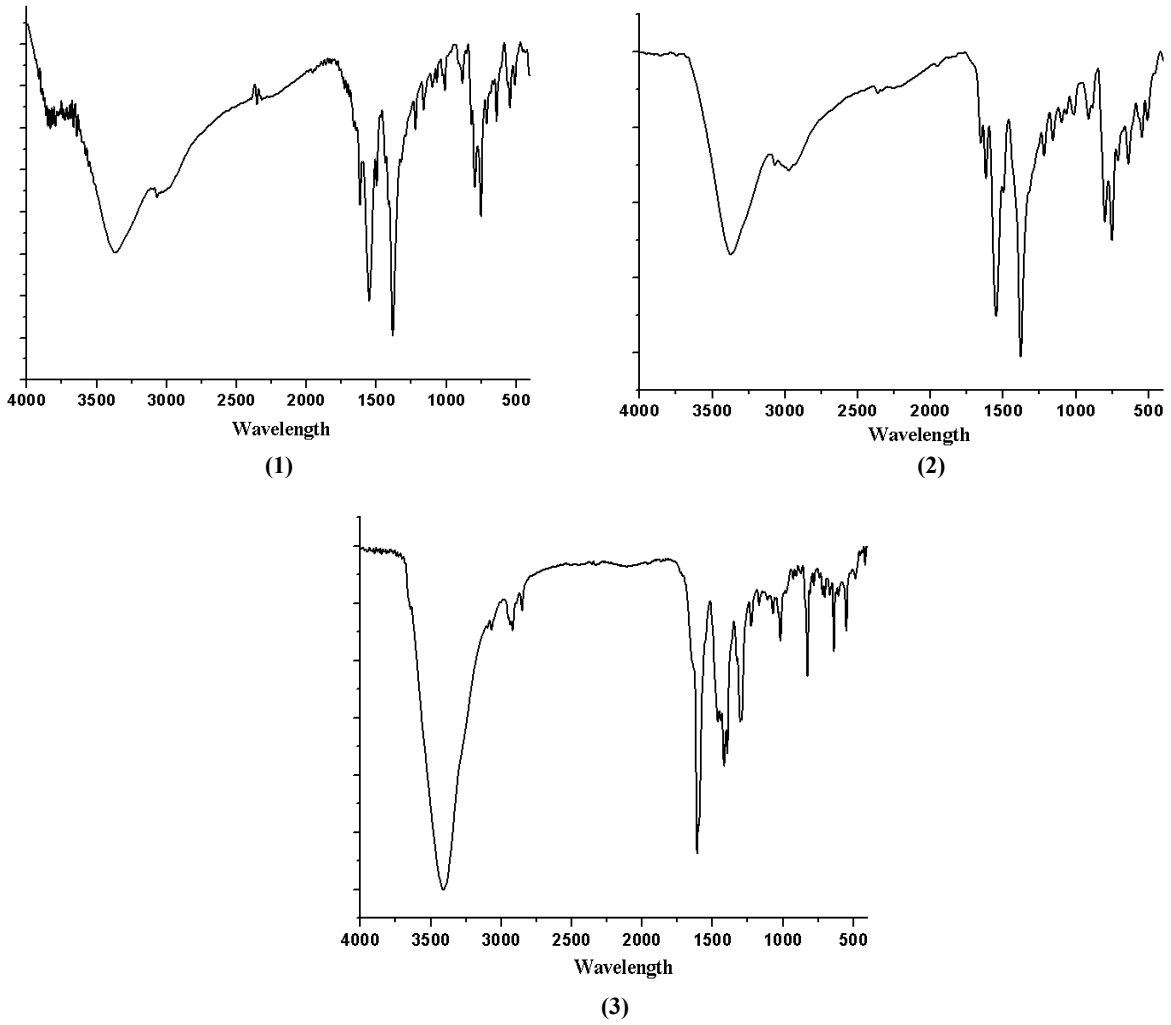

Fig. S1 IR spectra of compounds **1-3.**

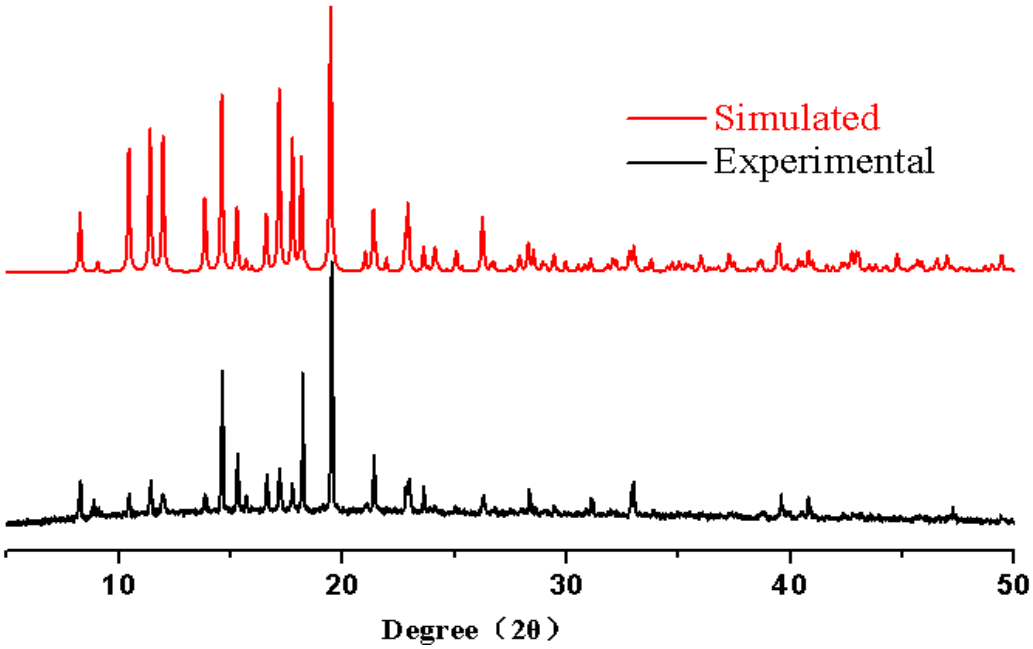

Fig. S2 Powder X-ray diffraction patterns of compound **1**.

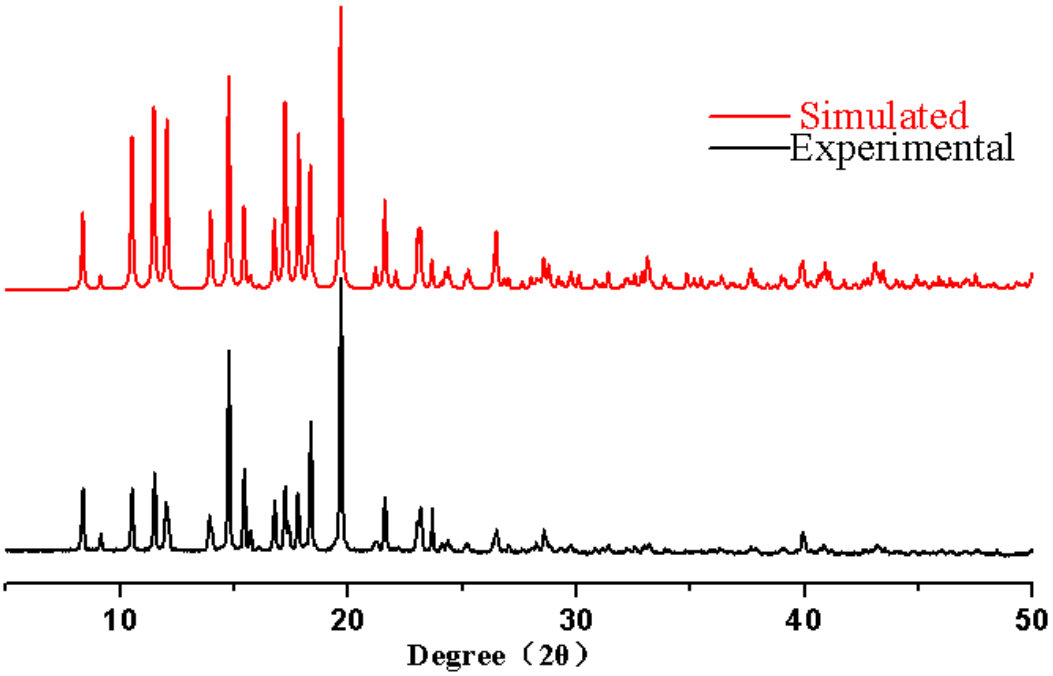

Fig. S3 Powder X-ray diffraction patterns of compound **2**.

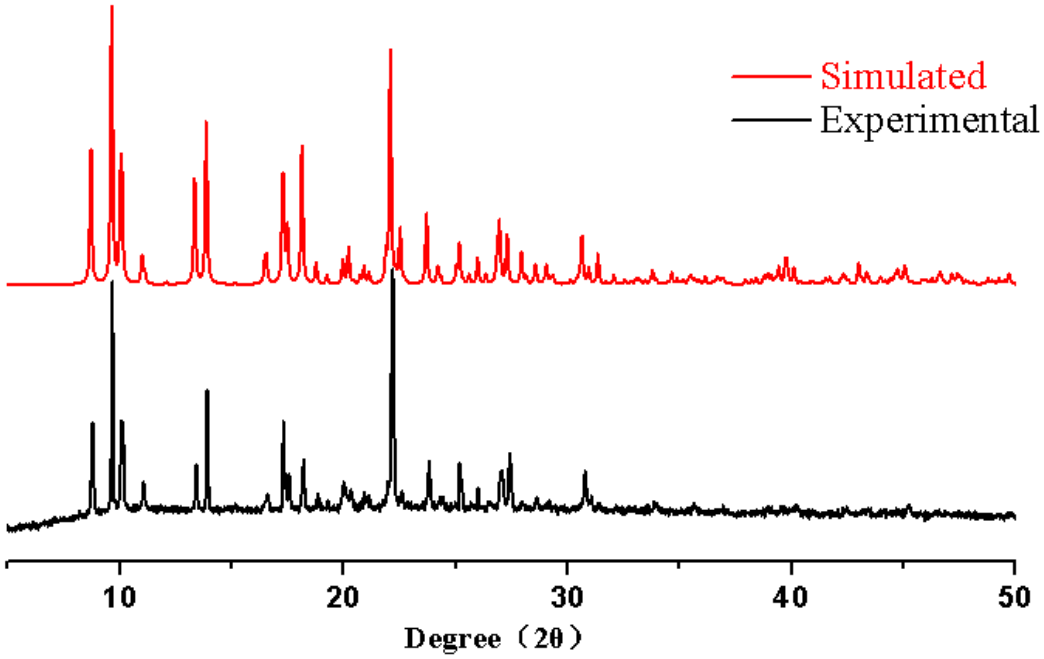

Fig. S4 Powder X-ray diffraction patterns of compound **3**.

Fig. S5 Coordination environment of the Ni(II) cation in **2**. The hydrogen atoms are omitted for clarity. Symmetry codes: #1 = *x*, − 1/2− *y*, 1/2+ *z*.

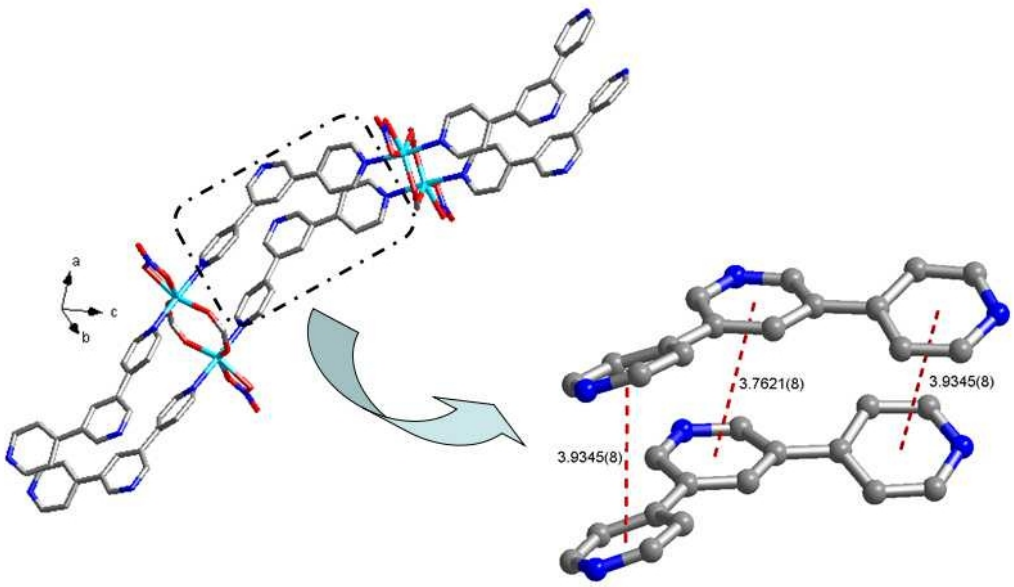

Fig. S6 The weak π···π stacking interactions (centroid-to-centroid distance of 3.7621(8) and 3.9345(8) Å) among adjacent pyridine cycles of BPYPY ligands in compound **3**.