Electronic Supplementary Information for

Syntheses, structures and magnetic properties of cobalt(II) and nickel(II) complexes based on 5-methylisophthalate and different pyridyl-containing ligands

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Table S1. Selected bond lengths (Å) and angles (°) for 1

Co(1)–O(2)#1	2.007(3)	O(1)–Co(1)–N(1)	94.81(12)
Co(1)–O(1)	2.033(3)	O(3)#2–Co(1)–N(1)	89.72(12)
Co(1)–O(3)#2	2.120(3)	O(2)#1–Co(1)–N(2)#3	89.19(13)
Co(1)–N(1)	2.176(3)	O(1)–Co(1)–N(2)#3	86.91(12)
Co(1)–N(2)#3	2.184(3)	O(3)#2–Co(1)–N(2)#3	88.01(12)
Co(1)–O(4)#2	2.262(3)	N(1)–Co(1)–N(2)#3	177.57(14)
O(2)#1–Co(1)–O(1)	105.50(11)	O(2)#1–Co(1)–O(4)#2	158.43(11)
O(2)#1–Co(1)–O(3)#2	98.56(12)	O(1)–Co(1)–O(4)#2	95.73(11)
O(1)–Co(1)–O(3)#2	155.32(11)	O(3)#2–Co(1)–O(4)#2	59.96(11)
O(2)#1–Co(1)–N(1)	91.99(13)	N(1)–Co(1)–O(4)#2	89.98(12)□

Symmetry equivalent atoms: #1 –*x*, –*y*+1, –*z*+1; #2 *x*, *y*+1, *z*; #3 *x*–1, *y*, *z*+1

Table S2. Selected bond lengths (Å) and angles (°) for 2

Co(1)–O(4)#1	2.0373(14)	O(3)#2–Co(1)–N(1)	91.10(7)
Co(1)–O(3)#2	2.0400(15)	O(2)–Co(1)–N(1)	90.97(7)
Co(1)–O(2)	2.1374(15)	O(4)#1–Co(1)–N(2)#3	87.04(7)
Co(1)–N(1)	2.1571(19)	O(3)#2–Co(1)–N(2)#3	87.19(7)
Co(1)–N(2)#3	2.175(2)	O(2)–Co(1)–N(2)#3	93.82(7)
Co(1)–O(1)	2.2247(15)	N(1)–Co(1)–N(2)#3	174.89(6)

O(4)#1–Co(1)–O(3)#2	115.54(6)	O(4)#1–Co(1)–O(1)	95.02(6)
O(4)#1–Co(1)–O(2)	154.98(6)	O(3)#2–Co(1)–O(1)	149.02(6)
O(3)#2–Co(1)–O(2)	89.47(6)	O(2)–Co(1)–O(1)	60.00(6)
O(4)#1–Co(1)–N(1)	89.37(7)	N(1)–Co(1)–O(1)	94.34(7)

Symmetry equivalent atoms: #1 *x*, *y*+1, *z*; #2 –*x*+1, –*y*+1, –*z*+2; #3 –*x*+1, –*y*+2, –*z*+2

Table S3. Selected bond lengths (Å) and angles (º) for 3

Ni(1)–O(4)#1	2.0307(12)	O(3)#2–Ni(1)–N(1)	91.99(6)
Ni(1)–O(3)#2	2.0414(13)	O(2)–Ni(1)–N(1)	90.24(6)
Ni(1)–O(2)	2.1083(12)	O(4)#1–Ni(1)–N(2)#3	87.14(6)
Ni(1)–N(1)	2.1157(15)	O(3)#2–Ni(1)–N(2)#3	88.35(6)
Ni(1)–N(2)#3	2.1197(15)	O(2)–Ni(1)–N(2)#3	87.82(5)
Ni(1)–O(1)	2.1865(13)	N(1)–Ni(1)–N(2)#3	178.06(6)
O(4)#1–Ni(1)–O(3)#2	100.86(5)	O(4)#1–Ni(1)–O(1)	97.96(5)
O(4)#1–Ni(1)–O(2)	159.21(5)	O(3)#2–Ni(1)–O(1)	160.68(5)
O(3)#2–Ni(1)–O(2)	99.15(5)	O(2)–Ni(1)–O(1)	61.72(5)
O(4)#1–Ni(1)–N(1)	94.67(6)	N(1)–Ni(1)–O(1)	90.84(6)

Symmetry equivalent atoms:#1 *x*, *y*–1 , *z*; #2 –*x*+1, –*y*+2, –*z*+1; #3 *x*–1, *y*, *z*+1

Table S4. Selected bond lengths (Å) and angles (º) for 4

Ni(1)–O(4)#1	2.0095(12)	O(2)–Ni(1)–N(1)	91.20(5)
Ni(1)–O(2)	2.0760(11)	N(2)#2–Ni(1)–N(1)	96.84(5)
Ni(1)–N(2)#2	2.0817(14)	O(4)#1–Ni(1)–O(5)	86.03(6)
Ni(1)–N(1)	2.0908(14)	O(2)–Ni(1)–O(5)	90.91(5)
Ni(1)–O(5)	2.1134(13)	N(2)#2–Ni(1)–O(5)	91.91(5)
Ni(1)–O(1)	2.1949(12)	N(1)–Ni(1)–O(5)	170.89(5)
O(4)#1–Ni(1)–O(2)	161.93(5)	O(4)#1–Ni(1)–O(1)	99.92(5)
O(4)#1–Ni(1)–N(2)#2	105.20(5)	O(2)–Ni(1)–O(1)	62.08(4)
O(2)–Ni(1)–N(2)#2	92.69(5)	N(2)#2–Ni(1)–O(1)	154.64(5)
O(4)#1–Ni(1)–N(1)	89.24(6)	N(1)–Ni(1)–O(1)	86.83(5)

Symmetry equivalent atoms: #1 *x*–1, *y*, *z*; #2 *x*, *y*–1, *z*+1

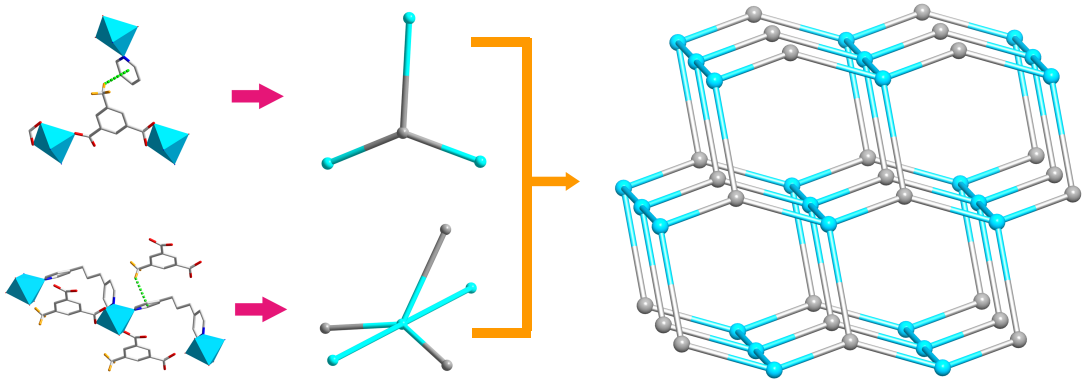

Fig. S1 Schematic view of the 3D (3,5)-connected framework with the $(6^3)(6^9.8)$ topology in **4**.

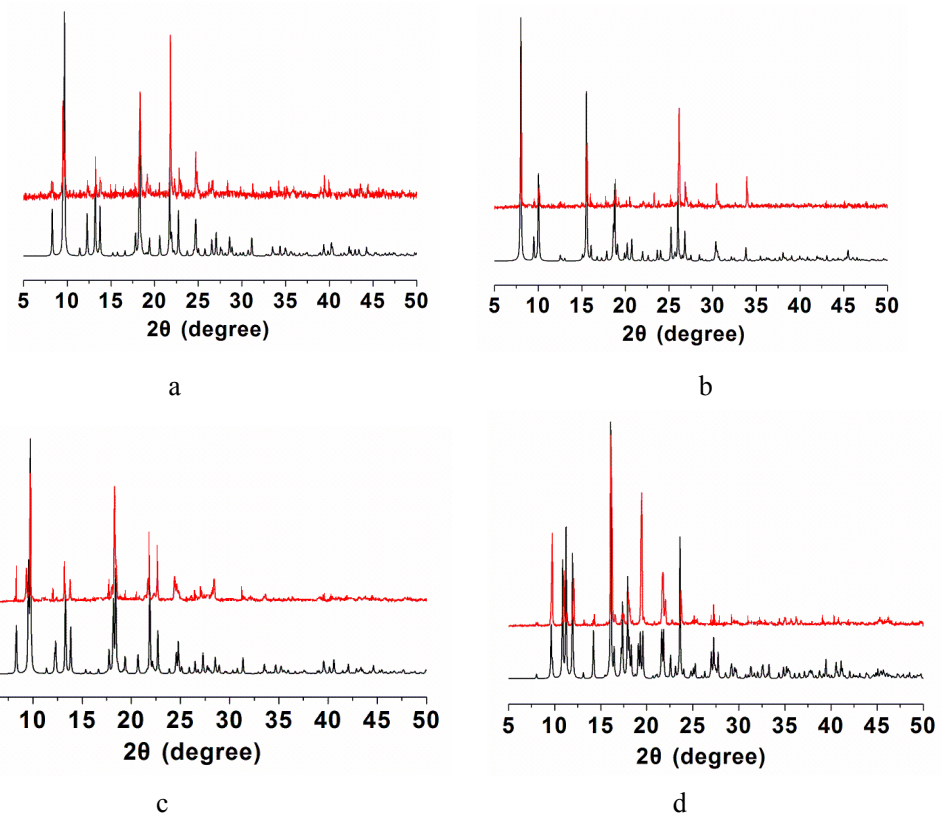

Fig. S2 XPRD pattern of the single crystal of complexes **1** (a), **2** (b) **3** (c) and **4** (d). Observed XPRD patterns (black); as-synthesized (red).