Coligand-directed synthesis of five Co(II)/Ni(II) coordination polymers with neutral tetradentate ligand: syntheses, crystal structures, and properties

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The PLATON SQUEEZE procedure was used to treat regions of diffuse solvent which could not be sensibly modelled in terms of atomic sites. Their contribution to the diffraction pattern was removed and modified Fo^2 written to a new HKL file. For compound 1, the number of electrons thus located is 1400 per unit cell. This residual electron density was assigned to two molecules of DMF, [1400/16 = 87.5e per one ligand; two molecules of the DMF would give 80e].

For compound 3, the number of electrons thus located is 149 per unit cell. This residual electron density was assigned to two molecules of DMF, [149/2 = 75e per one ligand; four molecules of the water and one and a half CH_3CN would give 73e].

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† Electronic supplementary information (ESI) available: IR, PXRD, Uv-vis, the selected bond lengths and angles. CCDC: 1002453 for **2**, 1002454 for **1**, 1002455 for **5**, 1002456 for **4**, 1002457 for **3**. For ESI and crystallographic data in CIF or other electronic format see DOI: 10.1039/

For compound 4, the number of electrons thus located is 168 per unit cell. This residual electron density was assigned to eight molecules of water, [168/1 = 84e per two ligand; 84/2 = 42e per one ligand; four molecules of the water would give 40e].

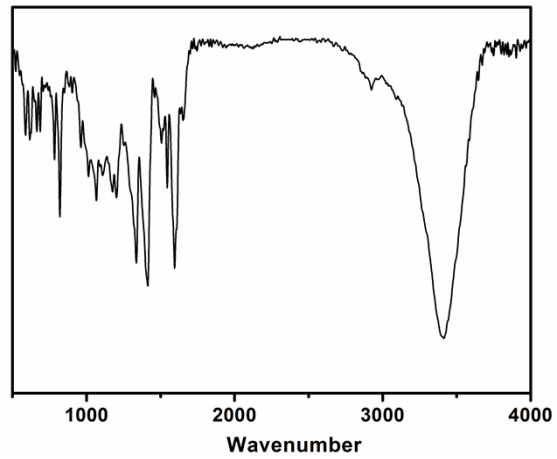

Figure S1. IR of complex **1**

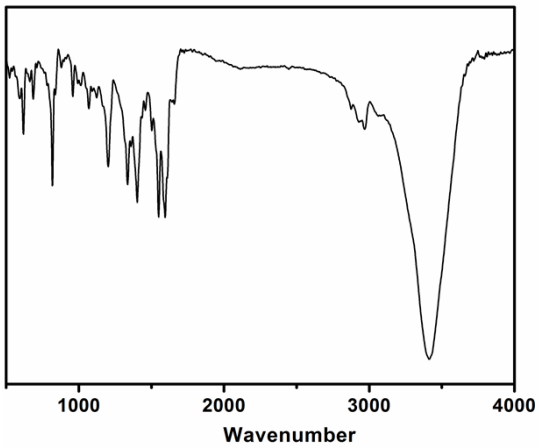

Figure S2. IR of complex **2**

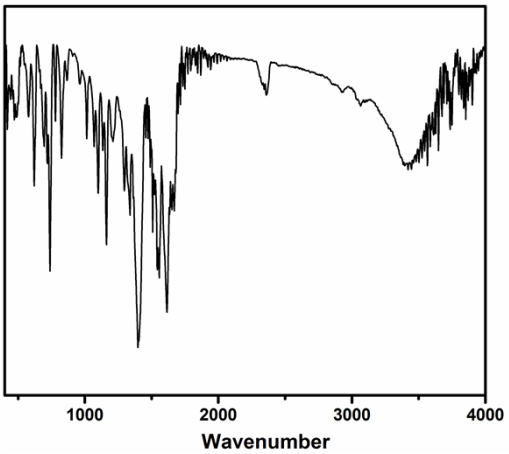

Figure S3. IR of complex **3**

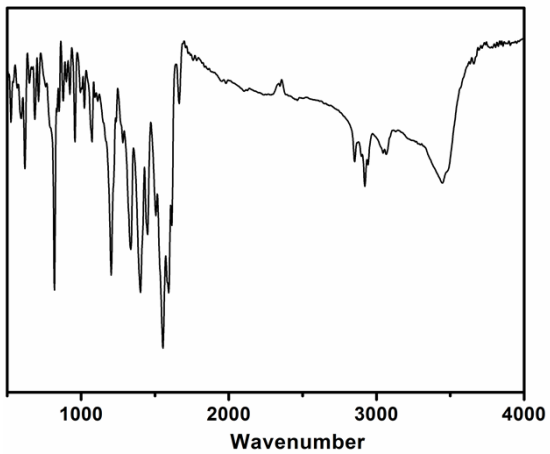

Figure S4. IR of complex **5**

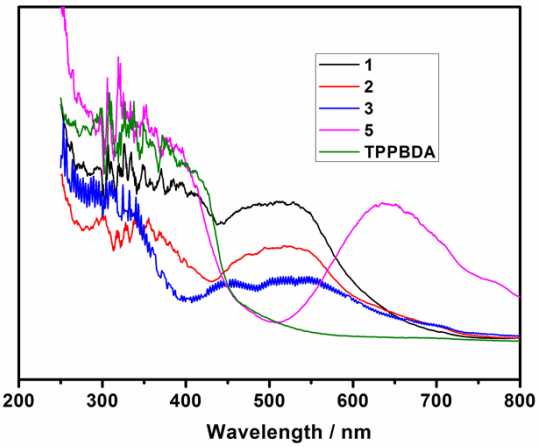

Figure S5. UV-vis absorbance spectra of **1-3** and **5** at room temperature

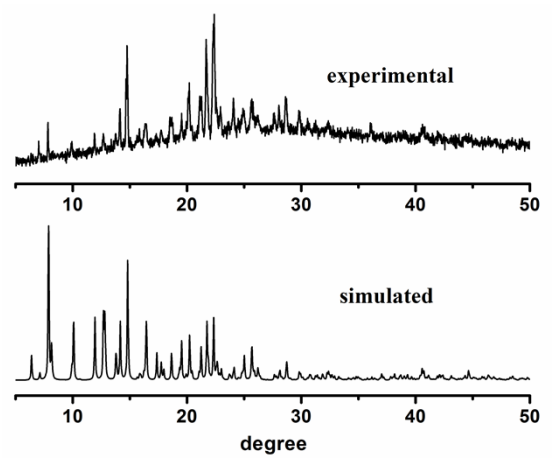

Figure S6. Powder X-ray diffraction patterns of complex **1**

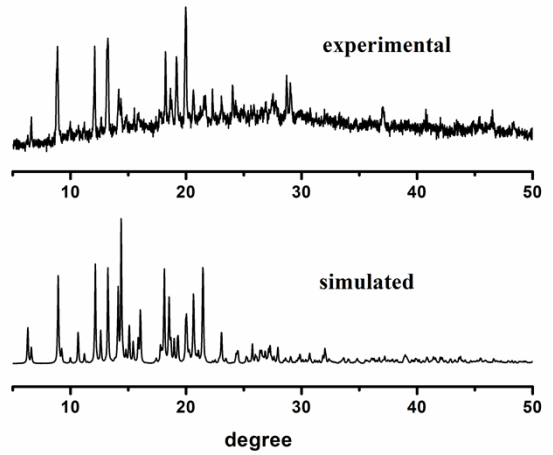

Figure S7. Powder X-ray diffraction patterns of complex **2**

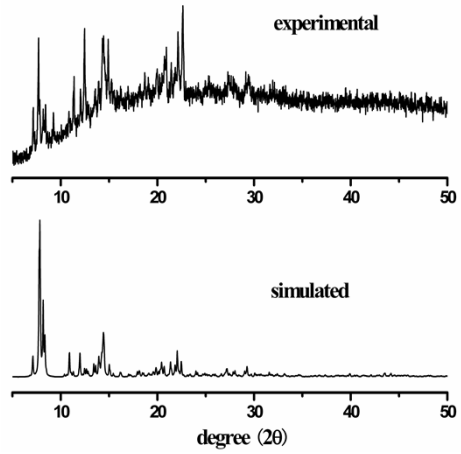

Figure S8. Powder X-ray diffraction patterns of complex **3**

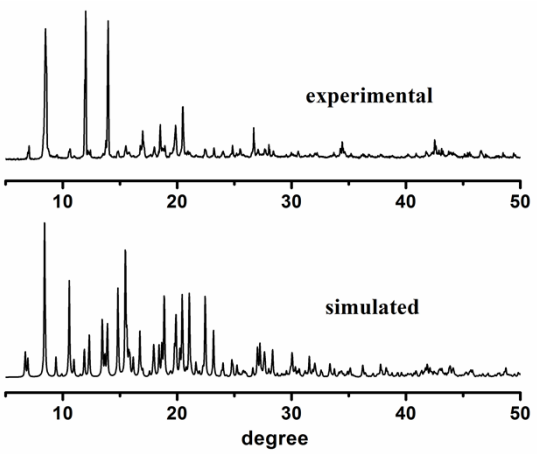

Figure S9. Powder X-ray diffraction patterns of complex **5**

Complex **1**

Co1- N1	2.203(3)	Co1- N3^{a}	2.219(2)
Co1- N4^{b}	2.109(2)	Co1- O2	2.110(2)
Co1- O3	2.162(2)	Co1- O4	2.046(2)
N1 - Co1- N3^{a}	173.25(10)	N1 - Co1- N4^{b}	91.00(9)
N1 - Co1- O2	89.76(9)	N1 - Co1- O3	89.30(9)
N1 - Co1- O4	91.41(10)	N3^{a} - Co1- N4^{b}	88.65(9)
N3^{a} - Co1- O2	83.85(9)	N3^{a} - Co1- O3	89.57(9)
N3^{a} - Co1- O4	95.31(10)	N4^{b} - Co1- O2	105.83(9)
N4^{b} - Co1- O3	167.36(9)	N4^{b} - Co1- O4	97.91(10)
O2- Co1- O3	61.53(8)	O2- Co1- O4	156.21(10)
O3- Co1- O4	94.72(10)		

Complex **2**

Co1- N1	2.179(3)	Co1- N2^{a}	2.117(4)
Co1- O2	2.230(3)	Co1- O3	2.128(3)
Co1- O4^{b}	2.051(3)	Co1- O1W	2.083(3)
N1 - Co1- N2^{a}	85.82(14)	N1 - Co1- O2	87.19(13)
N1 - Co1- O3	88.90(13)	N1 - Co1- O4^{b}	88.25(13)
N1 - Co1- O1W	178.77(13)	N2^{a} - Co1- O2	96.69(13)

N2[a] - Co1- O3	155.82(13)	N2[a] - Co1- O4[b]	95.00(14)
N2[a] - Co1- O1W	93.27(14)	O2 - Co1- O3	59.45(12)
O2 - Co1- O4[b]	167.11(13)	O2 - Co1- O1W	93.75(13)
O3 - Co1- O4[b]	108.43(13)	O3- Co1- O1W	92.26(13)
O4[b] - Co1- O1W	91.01(13)		

Complex **3**

Co1- N1	2.140(3)	Co1- N3[a]	2.172(3)
Co1- O2	2.025(3)	Co1- O8	2.106(2)
Co1- O9	2.337(2)	Co1- O13[b]	2.084(3)
Co2- N2[c]	2.186(3)	Co2- N4[d]	2.122(3)
Co2- O7[e]	2.060(3)	Co2- O15	2.049(2)
Co2- O18[f]	2.011(3)	Co3- O3	2.101(2)
Co3- O6[e]	2.223(2)	Co3- O9	2.199(2)
Co3- O14	2.077(2)	Co3- O19[f]	2.059(3)
Co3- O1w	2.060(3)	N1 - Co1- N3[a]	88.84(12)
N1 - Co1- O2	99.84(11)	N1 - Co1- O8	95.56(10)
N1 - Co1- O9	153.97(10)	N1 - Co1- O13[b]	83.98(11)
N3[a] - Co1- O2	91.11(12)	N3[a] - Co1- O8	91.52(11)
N3[a] - Co1- O9	91.88(10)	N3[a] - Co1- O13[b]	172.11(12)
O2- Co1- O8	164.42(10)	O2- Co1- O9	106.16(9)
O2- Co1- O13[b]	93.33(11)	O8- Co1- O9	58.41(9)
O8- Co1- O13[b]	85.95(11)	O9- Co1- O13[b]	93.14(9)
N2[c]- Co2- N4[d]	95.50(11)	N2[c]- Co2- O7[e]	90.01(11)
N2[c]- Co2- O15	167.65(10)	N2[c]- Co2- O18[f]	88.81(12)
N4[d] - Co2- O7[e]	93.43(11)	N4[d] - Co2- O15	96.82(11)
N4[d] - Co2- O18[f]	92.83(12)	O7[e] - Co2- O15	90.09(11)
O7[e] - Co2- O18[f]	173.71(10)	O15 - Co2- O18[f]	89.74(11)
O3 - Co3- O6[e]	170.59(10)	O3 - Co3- O9	89.93(10)
O3 - Co3- O14	88.76(10)	O3 - Co3- O19[f]	85.13(10)
O3 - Co3- O1w	89.03(11)	O6[e] - Co3- O9	95.52(8)

O6^{e} - Co3- O14	85.11(9)	O6^{e} - Co3- O19^{f}	102.24(9)
O6^{e} - Co3- O1w	83.97(9)	O9 - Co3- O14	174.63(10)
O9 - Co3- O19^{f}	92.52(9)	O9 - Co3- O1w	83.67(10)
O14 - Co3- O19^{f}	92.56(10)	O14 - Co3- O1w	91.10(11)
O19^{f} - Co3- O1w	173.03(9)		

Complex **4**

Ni1- N2	2.099(3)	Ni1- N3^{a}	2.155(3)
Ni1- O2	2.005(2)	Ni1- O8	2.076(2)
Ni1- O9	2.277(2)	Ni1- O13^{b}	2.072(2)
Ni2- N1c	2.154(3)	Ni2- N4d	2.102(3)
Ni2- O7e	2.050(2)	Ni2- O15	2.045(2)
Ni2- O18f	1.993(2)	Ni3- O3	2.073(2)
Ni3- O6e	2.191(2)	Ni3- O9	2.202(2)
Ni3- O14	2.075(3)	Ni3- O19f	2.029(3)
Ni3- O1w	2.034(2)	N2 - Ni1- N3a	88.88(11)
N2 - Ni1- O2	99.80(11)	N2 - Ni1- O8	96.65(11)
N2 - Ni1- O9	153.80(10)	N2 - Ni1- O13b	83.00(10)
N3a - Ni1- O2	90.20(11)	N3a - Ni1- O8	90.77(11)
N3a - Ni1- O9	90.42(9)	N3a - Ni1- O13b	171.70(10)
O2- Ni1- O8	163.53(10)	O2- Ni1- O9	106.39(9)
O2- Ni1- O13^{b}	92.87(10)	O8- Ni1- O9	57.16(9)
O8- Ni1- O13^{b}	88.46(10)	O9- Ni1- O13^{b}	96.10(9)
N1^{c}- Ni2- N4^{d}	94.65(11)	N1^{c}- Ni2- O7^{e}	88.78(10)
N1^{c}- Ni2- O15	167.60(10)	N1^{c}- Ni2- O18^{f}	88.39(10)
N4^{d} - Ni2- O7^{e}	94.33(10)	N4^{d} - Ni2- O15	97.63(11)
N4^{d} - Ni2- O18^{f}	92.36(11)	O7^{e} - Ni2- O15	91.99(10)
O7^{e} - Ni2- O18^{f}	172.93(10)	O15 - Ni2- O18^{f}	89.39(10)
O3 - Ni3- O6^{e}	169.13(10)	O3 - Ni3- O9	88.94(9)
O3 - Ni3- O14	87.17(9)	O3 - Ni3- O19^{f}	84.70(10)
O3 - Ni3- O1w	87.63(10)	O6^{e} - Ni3- O9	98.21(9)

O6^{e} - Ni3- O14	84.90(9)	O6^{e} - Ni3- O19^{f}	103.17(9)
O6^{e} - Ni3- O1w	84.89(9)	O9 - Ni3- O14	173.30(10)
O9 - Ni3- O19^{f}	91.60(9)	O9 - Ni3- O1w	84.85(10)
O14 - Ni3- O19^{f}	93.47(10)	O14 - Ni3- O1w	89.54(11)
O19^{f} - Ni3- O1w	171.61(9)		

Complex **5**

Ni1- N1	2.087(2)	Ni1- N2^{a}	2.0709(19)
Ni1- O2	2.0816(17)	Ni1- O3	2.2535(18)
Ni1- O4^{b}	2.0327(17)	Ni1- O6	2.0586(18)
N1 - Ni1- N2^{a}	88.74(8)	N1 - Ni1- O2	93.45(7)
N1 - Ni1- O3	89.09(7)	N1 - Ni1- O4^{b}	89.19(7)
N1 - Ni1- O6	178.66(8)	N2^{a} - Ni1- O2	93.84(7)
N2^{a} - Ni1- O3	153.87(7)	N2^{a} - Ni1- O4^{b}	93.94(8)
N2^{a} - Ni1- O6	92.51(8)	O2 - Ni1- O3	60.31(7)
O2 - Ni1- O4^{b}	171.84(7)	O2 - Ni1- O6	92.51(8)
O3 - Ni1- O4^{b}	112.07(7)	O3 - Ni1- O6	90.01(7)
O4^{b} - Ni1- O6	90.22(7)		

Symmetry codes: for **1:** a = -0.5 + *x*, 1 - *y*, *z*; b = -0.25 + y, 0.25 + *x*, 0.25 - *z*. for **2:** a = *x*, *y*, 1 + *z*; b = 1 + *x*, *y*, *z*. for **3:** a = - *x*, - *y*, - *z*; b = 3 - *x*, 1 - *y*, - *z*; c = 2 - *x*, 1 - *y*, - *z*; d = 1 + *x*, 1 + *y*, 1 + *z*; e = 1 + *x*, 1 + *y*, *z*; f = 2 - *x*, - *y*, 1 - *z*. for **4:** a = - *x*, 1 - *y*, 1 - *z*; b = 2 - *x*, - *y*, 1 - *z*; c = 1 - *x*, - *y*, 1 - *z*; d = 1 + *x*, -1 + *y*, -1 + *z*; e = 1 + *x*, -1 + *y*, *z*; f = 1 - *x*, 1 - *y*, - *z*. for **5:** a = *x*, *y*, -1 + *z*; b = 1 + *x*, *y*, *z*.