Four 3D coordination polymers based on layers with single syn-
anti carboxylate bridges: synthesis, structures, and magnetic
properties

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Table S1 Selected bond lengths (Å) and angles (°) for CPs 2-4

|                  | 2 (M = Co) | 3 (M = Ni) | 4 (M = CoNi) |
|------------------|------------|------------|--------------|
| M1-O1            | 2.149(2)   | 2.111(3)   | 2.119(3)     |
| M1-O4A           | 2.023(2)   | 2.004(3)   | 2.010(3)     |
| M1-O5B           | 2.087(2)   | 2.061(3)   | 2.070(3)     |
| M1-O7            | 2.117(3)   | 2.071(3)   | 2.096(4)     |
| M1-O6C           | 2.174(2)   | 2.108(3)   | 2.130(3)     |
| M1-N1B           | 2.117(3)   | 2.056(3)   | 2.077(3)     |
| M2-O2            | 2.107(2)   | 2.010(3)   | 2.021(3)     |
| M2-O8            | 2.013(3)   | 2.072(6)   | 2.083(6)     |
| M2-O9            | 2.158(3)   | 2.055(4)   | 2.074(5)     |
| O4A-M1-O5B       | 168.70(10) | 172.19(12) | 171.89(12)   |
| O4A-M1-O7        | 91.62(10)  | 94.02(13)  | 93.91(13)    |
| O5B-M1-O7        | 98.37(10)  | 93.58(13)  | 94.00(13)    |
| O4A-M1-N1B       | 92.65(10)  | 92.31(13)  | 92.67(12)    |
| O5B-M1-N1B       | 78.16(10)  | 80.48(12)  | 79.86(12)    |
| O7-M1-N1B        | 171.32(11) | 168.86(14) | 167.86(14)   |
| O4A-M1-O1        | 92.49(10)  | 92.21(12)  | 92.20(12)    |
| O5B-M1-O1        | 83.44(10)  | 86.25(13)  | 86.21(13)    |
| O7-M1-O1         | 83.67(11)  | 88.22(14)  | 88.74(14)    |
| N1B-M1-O1        | 103.67(10) | 100.69(13) | 101.21(13)   |
| O4A-M1-O6C       | 98.39(10)  | 92.48(12)  | 92.87(12)    |
| O5B-M1-O6C       | 86.87(10)  | 89.63(13)  | 89.32(13)    |
| O7-M1-O6C        | 90.28(11)  | 87.50(14)  | 86.86(14)    |
| Bond                  | A   | B   | C   |
|-----------------------|-----|-----|-----|
| N1B-M1-O6C            | 81.63(10) | 83.08(13) | 82.62(13) |
| O1-M1-O6C             | 167.70(9)  | 173.86(12) | 173.50(12) |
| O8D-M2-O8             | 180.00(2)   | 180.000(2)  | 180.000(2)  |
| O8D-M2-O2             | 93.02(12)   | 89.0(2)     | 89.14(19)   |
| O8-M2-O2              | 86.98(12)   | 91.0(2)     | 90.86(19)   |
| O2-M2-O2D             | 180.00(13)  | 180.0(2)    | 180.00(19)  |
| O8-M2-O9D             | 91.10(18)   | 89.3(3)     | 89.7(2)     |
| O8-M2-O9              | 88.90(18)   | 90.7(3)     | 90.3(2)     |
| O2-M2-O9D             | 83.63(11)   | 93.28(16)   | 93.49(17)   |
| O2-M2-O9              | 96.37(11)   | 86.72(16)   | 86.51(17)   |
| O9-M2-O9D             | 180.0       | 180.000(1)  | 180.000(2)  |

Symmetry codes: A x, -y+1/2, z-1/2; B -x+3, -y+1, -z+1; C -x+3, y+1/2, -z+1/2; D -x+4, -y+1, -z+1.
Fig. S1 Powder X-ray diffraction profiles (black) of CPs 1-4 together with a simulation from the single crystal data (red).

Fig. S2 TGA curves of CPs 1-4.
**Fig. S3** The 3D structures with hydrogen bonding interactions in CP 2.

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

| D   | A[Transformation] | d(D-H) | d(H···A) | d(D···A) | <(DHA) |
|-----|-------------------|--------|----------|----------|--------|
| O7  | O10[ x-1, y, z+1 ]| 0.817  | 2.072    | 2.862    | 162.63 |
| O8  | O7[ -x, -y+1, -z+1 ]| 0.847  | 2.035    | 2.852    | 162.01 |
| O8  | O11[ x-1, -y+3/2, z-1/2 ]| 0.849  | 1.849    | 2.683    | 167.18 |
| O9  | O10[ x-1, y, z ]| 0.880  | 1.760    | 2.635    | 172.33 |
| O9  | O11[ -x+1, -y+1, -z+1 ]| 0.869  | 2.027    | 2.894    | 174.84 |
| O10 | O1[ x+1, y, z ]| 0.924  | 1.819    | 2.734    | 170.03 |
| O10 | O5[ -x+2, y-1/2, -z+1/2 ]| 0.849  | 2.145    | 2.824    | 136.71 |
| O11 | O3[ x+1, y, z ]| 0.833  | 1.982    | 2.739    | 150.55 |
| O11 | O9[ -x+1, y+1/2, -z+1/2 ]| 0.845  | 2.013    | 2.846    | 168.64 |

*a D, donor; A, acceptor.
Fig. S4 The ZFC and FC curves of CP 4.

Fig. S5 $\chi_M'$ and $\chi_M''$ plots for CP 4 at frequencies of 10, 100, and 100 Hz with $H_{dc} = 0$ and $H_{ac} = 3.0$ Oe.