Magnetic properties of isostructural $M(H_2O)_4[Au(CN)_4]_2$-based coordination polymers (M = Mn, Co, Ni, Cu, Zn) by SQUID and μSR studies

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Electronic Supplementary Information

Table S1. Lengths of hydrogen bonds (Å) for $M(H_2O)_4[Au(CN)_4]_2 \cdot 4H_2O$ (M = Mn, Co, Ni, Zn) coordination polymers

Selected Atoms	Hydrogen Bond Lengths for $M(H_2O)_4[Au(CN)_4]_2 \cdot 4H_2O$ (Å)			
	Mn	Co	Ni	Zn
O(1) – H(11) ··· O(3)″	2.762(6)	2.752(8)	2.735(14)	2.751(10)
O(1) – H(12) ··· N(22)	2.763(6)	2.754(8)	2.749(14)	2.764(10)
O(2) – H(21) ··· N(21)$^{\$}$	2.890(6)	2.880(8)	2.901(14)	2.881(10)
O(2) – H(22) ··· O(4)$^{€}$	2.769(6)	2.756(8)	2.762(14)	2.767(10)
O(3) – H(31) ··· O(4)$^{£}$	2.793(6)	2.779(8)	2.765(14)	2.777(10)
O(3) – H(32) ··· N(12)	2.927(6)	2.903(8)	2.913(14)	2.925(10)
O(4) – H(41) ··· O(1)	2.922(6)	2.929(8)	2.933(14)	2.915(10)
O(4) – H(42) ··· O(3)	2.888(6)	2.891(8)	2.911(14)	2.892(10)

Symmetry transformations: ″ ≡ 2-x, 1-y, 2-z; $^{\$}$ ≡ x, y, 1+z; $^{€}$ ≡ 1-x, -y, 2-z; 1-x, $^{£}$ ≡ 1-y, 2-z

Table S2. Selected bond lengths (Å) for $Cu(H_2O)_4[Au(CN)_4]_2 \cdot 4H_2O$

Selected Atoms	Bond Length	Selected Atoms	Bond Length
Au(1) – C(11)	1.997(3)	Au(1) – C(13)	1.994(3)
Au(1) – C(12)	1.998(3)	Au(1) – C(14)	1.989(3)
C(11) – N(11)	1.145(3)	C(13) – N(13)	1.146(3)
C(12) – N(12)	1.142(4)	C(14) – N(14)	1.142(4)
Au(2) – C(21)	1.994(4)	Au(2) – C(22)	1.988(3)
C(21) – N(21)	1.143(5)	C(22) – N(22)	1.139(4)
Au(3) – C(31)	1.995(3)	Au(3) – C(32)	1.987(3)
C(31) – N(31)	1.148(4)	C(32) – N(32)	1.144(4)
Cu(1) – O(11)	1.995(2)	Cu(1) – O(12)	1.986(2)
Cu(1) – N(11)	2.312(2)	Cu(2) – O(21)	2.280(2)
Cu(2) – O(22)	1.985(2)	Cu(2) – N(13)	2.010(2)

Selected Atoms	Bond Length	Selected Atoms	Bond Length
Au(1) – N(21)	3.159(3)	Au(1) – N(31)	3.158(3)
Au(2) – N(14)´	3.278(3)	Au(3) – N(12)†	3.156(3)
O(1) – H(11) ··· O(3)	2.848(5)	O(1) – H(12) ··· N(14)˝	2.879(5)
O(2) – H(21) ··· O(1)‡	2.899(5)	O(2) – H(22) ··· O(1)	2.745(5)
O(3) – H(31) ··· O(21)˝	2.800(5)	O(3) – H(32) ··· O(4)	2.757(5)
O(4) – H(41) ··· N(12)§	2.882(5)	O(4) – H(42) ··· O(2)	2.820(5)
O(11) – H(111) ··· O(1)	2.696(5)	O(11) –H(112) ··· N(32)$^{¥}$	2.726(5)
O(12) – H(121) ··· O(2)	2.711(5)	O(12) –H(122) ··· N(21)§	2.857(5)
O(21) – H(211) ··· O(4)$^{\$}$	2.748(5)	O(21) –H(212) ··· N(22)$^{\$}$	2.785(5)
O(22) – H(221) ··· O(3)$^{\$}$	2.714(5)	O(12) –H(122) ··· N(31)‡	2.872(5)

Symmetry transformations: * ≡ -x, 1-y, -z; † ≡ 1+x, y, z; ‡ ≡ -1+x, y, z; ´ ≡ -1+x, -1+y, z; ˝ ≡ -x, 2-y, 1-z; § ≡ -1-x, 1-y, 1-z; $^{¥}$ ≡ -x, 1-y, 1-z; $^{\$}$ ≡ -1-x, 2-y, 1-z; $^{£}$ ≡ -1-x, 1-y, -z

Table S3. Selected angles (deg) for $Cu(H_2O)_4[Au(CN)_4]_2 \cdot 4H_2O$

Selected Atoms	Angle	Selected Atoms	Angle
C(11) – Au(1) – C(12)	90.10(12)	C(12) – Au(1) – C(13)	89.63(12)
C(11) – Au(1) – C(13)	178.93(12)	C(12) – Au(1) – C(14)	179.35(11)
C(11) – Au(1) – C(14)	89.63(12)	C(13) – Au(1) – C(14)	90.94(12)
Au(1) – C(11) – N(11)	179.4(3)	Au(1) – C(13) – N(13)	178.9(3)
Au(1) – C(12) – N(12)	179.9(3)	Au(1) – C(14) – N(14)	179.3(3)
C(11) – N(11) – Cu(1)	169.9(3)	C(13) – N(13) – Cu(2)	175.6(3)
C(12) – N(12) – Au(3)‡	132.4(3)	C(14) – N(14) – Au(2)†	129.0(3)
C(11) – Au(1) – N(21)	74.51(11)	C(13) – Au(1) – N(21)	104.44(11)
C(12) – Au(1) – N(21)	87.98(11)	C(14) – Au(1) – N(21)	92.17(11)
C(11) – Au(1) – N(31)	105.32(11)	C(13) – Au(1) – N(31)	75.71(11)
C(12) – Au(1) – N(31)	88.14(11)	C(14) – Au(1) – N(31)	91.70(11)
N(21) – Au(1) – N(31)	176.12(8)		

Selected Atoms	Angle	Selected Atoms	Angle
C(21) – Au(2) – C(22)	88.38(14)	C(22) – Au(2) – C(21)$^{\$}$	91.62(14)
C(21) – Au(2) – C(21)$^{\$}$	180	C(22) – Au(2) – C(22)$^{\$}$	180
C(21) – Au(2) – C(22)$^{\$}$	91.62(14)	C(21)$^{\$}$ – Au(2) – C(22)$^{\$}$	88.38(14)
Au(2) – C(21) – N(21)	178.2(3)	Au(2) – C(22) – N(22)	177.9(3)
C(21) – N(21) – Au(1)	98.5(2)	N(14)‡ – Au(2) – N(14)$^{\prime\prime}$	180
C(21) – Au(2) – N(14)‡	75.61(12)	C(21)$^{\$}$ – Au(2) – N(14)‡	104.39(12)
C(22) – Au(2) – N(14)‡	107.38(12)	C(22)$^{\$}$ – Au(2) – N(14)‡	72.62(12)
C(31) – Au(3) – C(32)	91.54(13)	C(32) – Au(3) – C(31)*	88.46(13)
C(31) – Au(3) – C(31)*	180	C(32) – Au(3) – C(32)*	180
C(31) – Au(3) – C(32)*	88.46(13)	C(31)* – Au(3) – C(32)*	91.54(13)
Au(3) – C(31) – N(31)	178.4(3)	Au(3) – C(32) – N(32)	178.0(3)
C(31) – N(31) – Au(1)	101.9(2)	N(12)† – Au(3) – N(12)$^{\pounds}$	180
C(31) – Au(3) – N(12)†	77.40(12)	C(31)* – Au(3) – N(12)†	102.60(12)
C(32) – Au(3) – N(12)†	75.11(12)	C(32)* – Au(3) – N(12)†	104.89(12)

Symmetry transformations: * ≡ -x, 1-y, -z; † ≡ 1+x, y, z; ‡ ≡ -1+x, y, z; $^{\prime}$ ≡ -1+x, -1+y, z; $^{\prime\prime}$ ≡ -x, 2-y, 1-z; § ≡ -1-x, 1-y, 1-z; $^{¥}$ ≡ -x, 1-y, 1-z; $^{\$}$ ≡ -1-x, 2-y, 1-z; $^{\pounds}$ ≡ -1-x, 1-y, -z

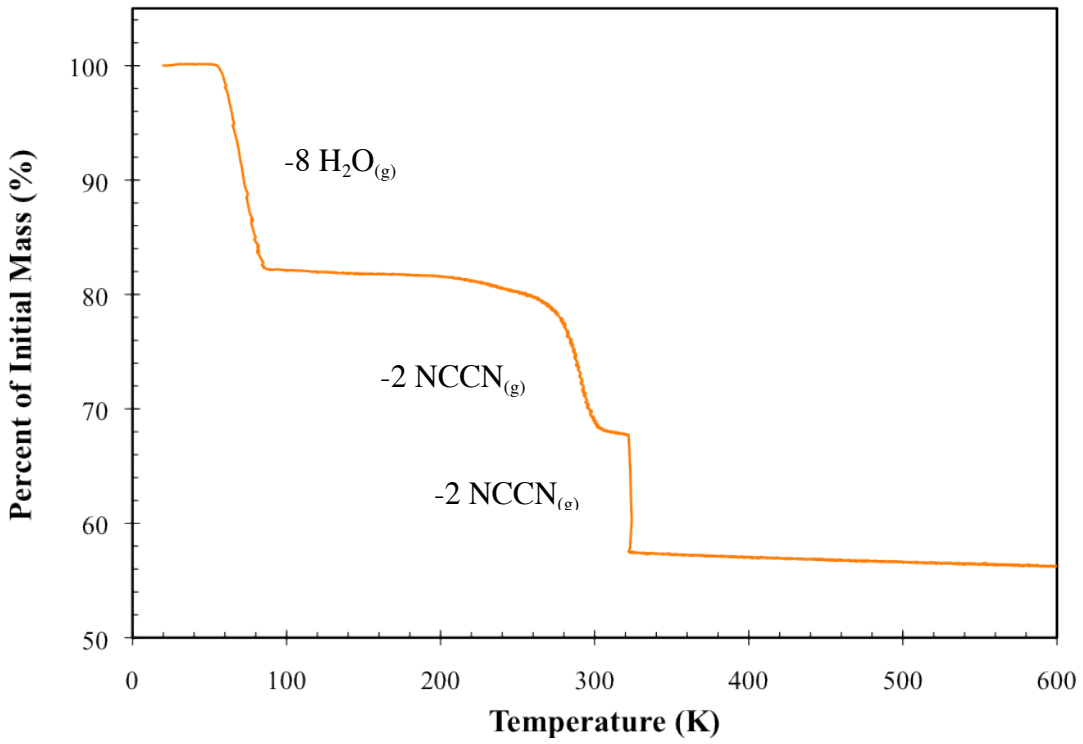

Figure S1. The thermal decomposition profile (TGA) for $Co(H_2O)_4[Au(CN)_4]_2 \cdot 4H_2O$, showing loss of eight water molecules and the subsequent, stepwise loss of four equivalents of cyanogen gas.

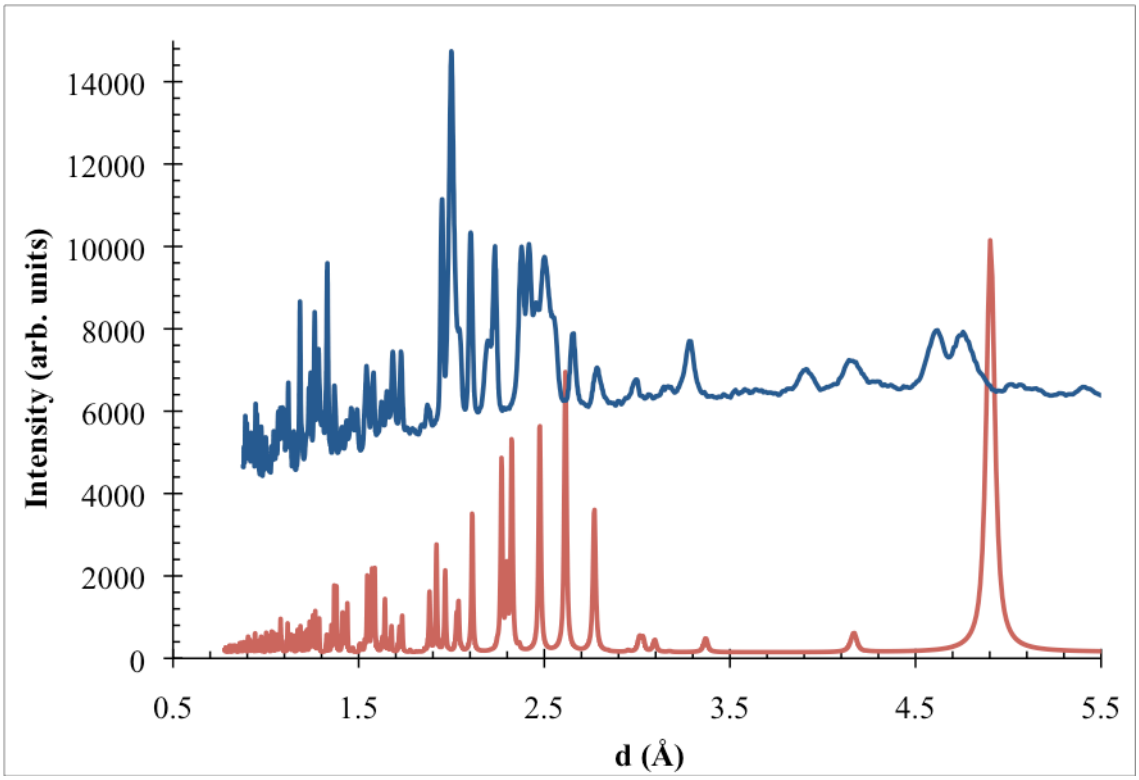

Figure S2 Comparison of the powder X-ray diffraction pattern (generated from the single-crystal data) for $Cu(H_2O)_4[Au(CN)_4]_2 \cdot 4H_2O$ (bottom) and experimentally collected (top) for partially-dehydrated $Cu(H_2O)_4[Au(CN)_4]_2$, indicating the lack of isostructurality.