Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Layered transition metal carboxylates: Synthesis, structural aspects and observation of multi-step magnetic transition through phase diagram

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Table S1. Bond distances (Å) and angles (º) of the compounds **1** and **2**

Compound **1**			
Co1-O1	2.059(2)	O1-Co1-O3	81.52(10)
Co1-O3	2.082(3)	O3-Co1-O7	168.23(11)
Co1-O3	2.058(3)	O3-Co1-O4	100.69(10)
Co1-O4	2.059(3)	O1-Co1-O3	99.09(10)
Co1-O6	2.134(3)	O3-Co1-O3	100.40(6)
Co1-O7	2.121(3)	O4-Co1-O3	80.25(10)
Co2-O2	2.024(2)	O1-Co1-O4	177.76(10)
Co2-O9	2.039(3)	O1-Co1-O7	89.17(11)
Co2-O10	2.236(3)	O4-Co1-O7	88.67(12)
O2-C1	1.261(4)	O1-Co1-O6	89.70(10)
O1-C1	1.257(4)	O3-Co1-O6	88.20(10)
O9-C3	1.270(4)	O4-Co1-O6	90.68(10)
O4-C3	1.252(4)	O2-Co2-O9	90.21(10)
O3-C2	1.409(4)	O2-Co2-O10	88.67(10)
C3-O4	1.252(4)	O9-Co2-O10	82.82(10)
Compound **2**			
Ni1-O1	2.139(3)	O2 -Ni1-O1	85.45(14)
Ni1-O2	2.121(3)	O3-Ni1-O1	88.62(13)
Ni1-O3	2.100(3)	O3-Ni1-O3	98.51(8)
Ni1-O3	2.079(3)	O6-Ni1-O2	90.45(14)
Ni1-O6	2.025(3)	O6-Ni1-O3	97.42(13)
Ni1-O9	2.025(3)	O9-Ni1-O3	81.39(13)
Ni2-O7	2.027(3)	O9-Ni1-O6	177.04(13)
Ni2-O10	2.041(3)	O7-Ni2-O7	179.999(1)
Ni2-O11	2.201(4)	O7-Ni2-O10	88.29(13)
O3-C4	1.420(5)	O7-Ni2-O11	91.69(14)
C5-O6	1.277(5)	O10-Ni2-O10	180.0
C5-O7	1.268(5)	O10-Ni2-O11	96.38(15)
C8-O9	1.270(5)	C4-O3-Ni1	111.2(2)
C8-O10	1.278(5)	Ni1-O3-Ni1	126.74(15)

Table S2. Hydrogen bond dimensions of compound **1**

D-H···A	H···A/ Å	D···A/ Å	D-H···A/^{o}
O(1)-H(1A)…O(11) [1-*x,y-1/2,-z+1/2*]	2.10(2)	2.928(3)	176(3)
O(1)-H(1B)…O(2)[-*x+2,-y,-z+1*]	2.13(2)	2.948(3)	170(3)
O(2)-H(2A)…O(3)[-*x+2,y-1/2,-z+1/2*]	1.86(3)	2.687(3)	174(3)
O(2)-H(2B)…O(100)[*x,y-1,z*]	2.11(2)	2.915(3)	162(2)
O(100)-H(10A)…O(7)[-*x+1,y+1/2,-z+1/2*]	2.04(3)	2.854(3)	176(3)
O(100)-H(10B)…O(6)	2.06(2)	2.857(3)	161(3)
O(11)-H(11A)…O(10)[-*x+1,-y-1,-z*]	1.95(2)	2.773(3)	171(3)
O(11)-H(11B)…O(100)[*x,y-1,z*]	2.40(3)	3.214(3)	166 (3)

Table S3. Hydrogen bond dimensions of Compound **2**

D-H···A	H···A/ Å	D···A/ Å	D-H···A/^{o}
O(1)-H(1A)…O(11) [*x,-y+1/2,z-1/2*]	2.21(2)	3.026(6)	167(4)
O(1)-H(1B)…O(2)[-*x,-y,-z+1*]	2.17(3)	2.987(5)	168(4)
O(2)-H(2A)…O(3)[-*x,y-1/2,-z+3/2*]	1.87(5)	2.684(5)	165(5)
O(2)-H(2B)…O(100)[-*x+1,y-1/2,-z+3/2*]	2.18(3)	2.993(5)	168(4)
O(100)-H(10A)…O(7)	2.13(6)	2.921(6)	160(5)
O(100)-H(10B)…O(6)[-*x+1,y-1/2,-z+3/2*]	2.08(4)	2.909(5)	173(6)
O(11)-H(11A)…O(10)[*x,y+1,z*]	2.01(3)	2.834(5)	176(5)
O(11)-H(11B)…O(100)[*x,-y+1/2,z+1/2*]	2.28(3)	3.098(6)	172 (4)

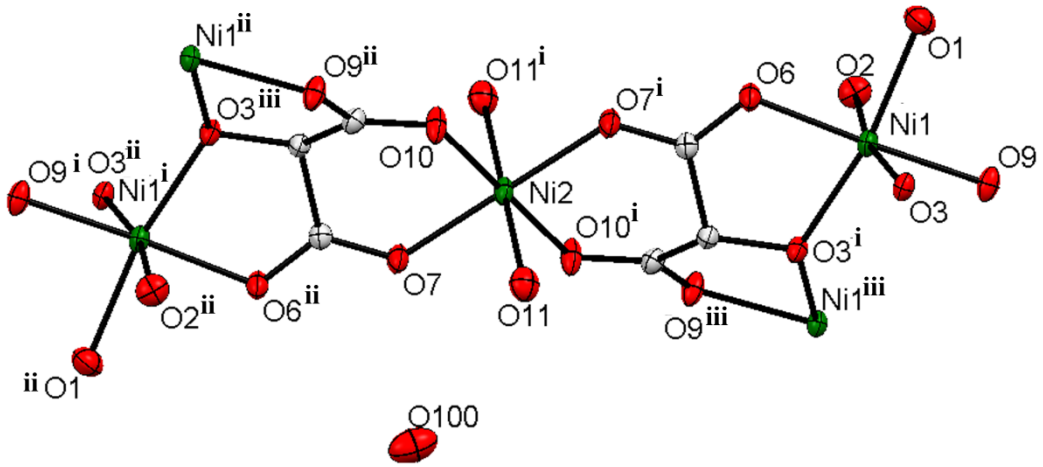

Figure S1. ORTEP diagrams of compounds **2** with 40% ellipsoid probability, [symmetry codes: i= 1-x, -y, 2-z; ii = -x, -1/2+y, 3/2-z, iii = 1+x, ½-y, ½+z].

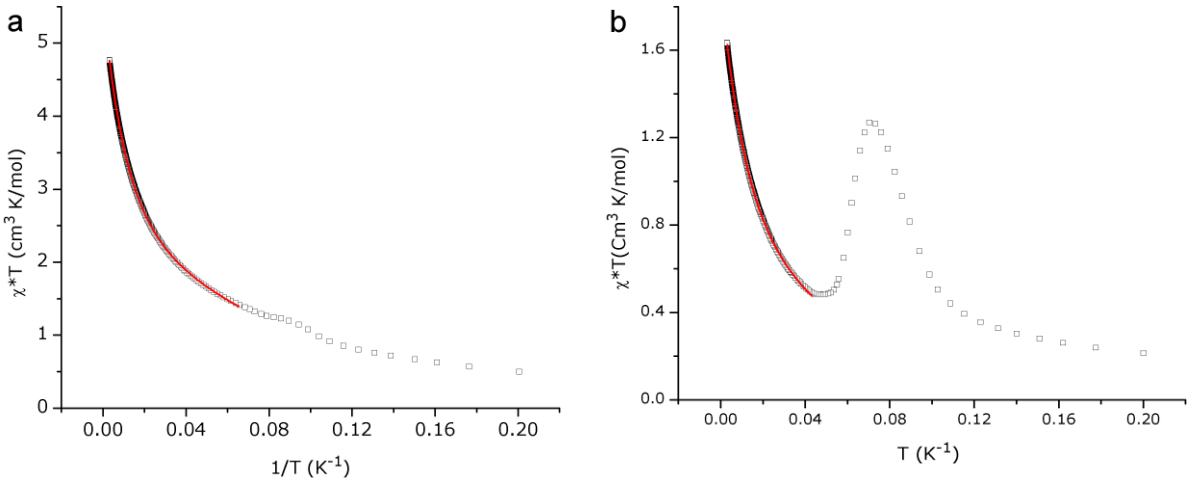

Figure S2. The best fit to the χT experimental data above 15 K using the χT=A exp(E1/kT)+B exp(E2/kT) phenomenological model for **1** (a) and **2** (b). The analysis was performed to the data plotted as χT vs 1/T.

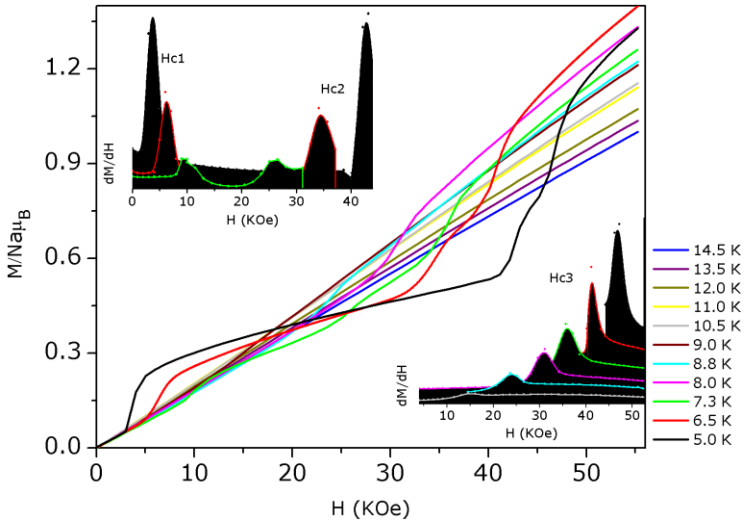

Figure S3. Isothermal magnetization data measured from 5 up to 14.5 K. Only the first quadrant is shown. Insets depict the dM/dH curves evidencing the critical fields.

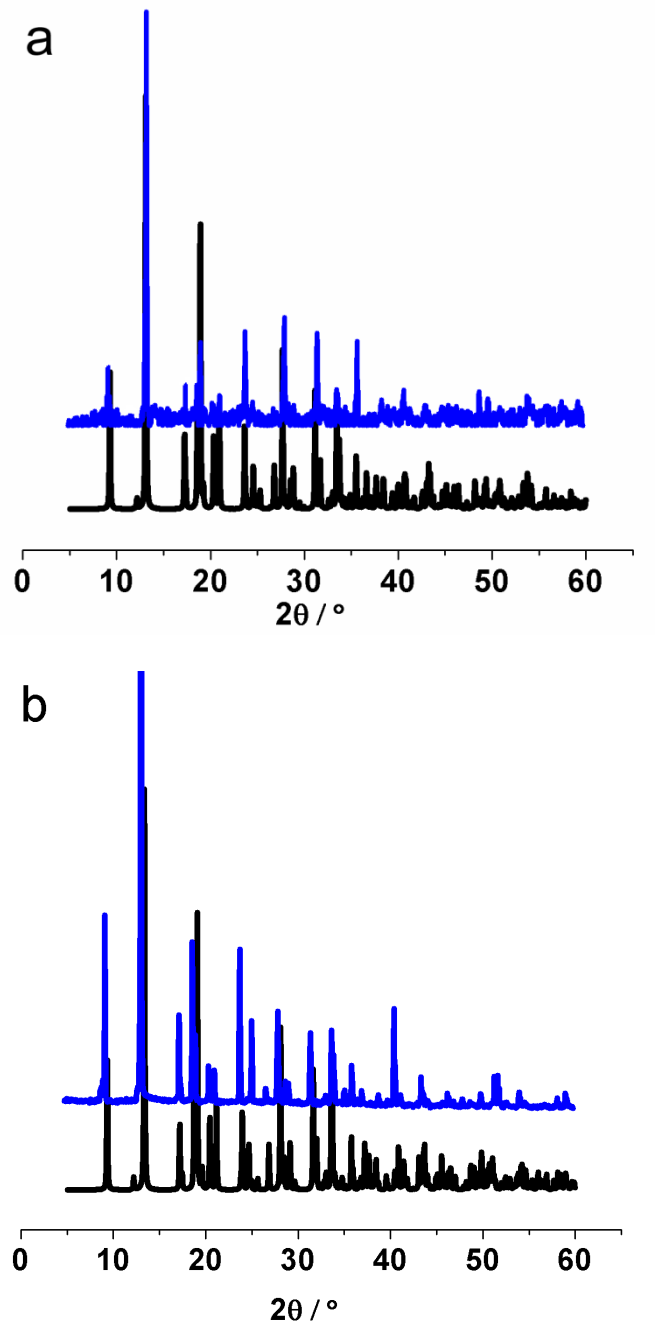

Figure S4. Experimental (blue) and simulated (black) powder X-ray patterns of **1** (a) and **2** (b).