Electronic Supplementary Information for Dalton Transactions

Electronic Supplementary Information

Novel Manganese(II) and cobalt(II) 3D polymers with mixed cyanate and carboxylate bridges: crystal structure and magnetic properties

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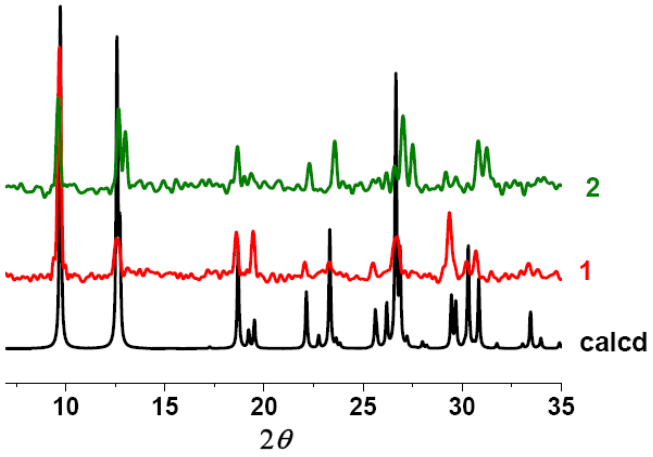

Fig. S1 The XRD patterns calculated from the single crystal data of **1** and observed for **1** and **2**. The similarity of the patterns suggests that the two compounds are isomorphous, although **2** shows some obvious peak shifts with respect to **1**. To confirm the isomorphism, we performed unit cell refinement on **2** using the CELREF program (J. Laugier and B. Bochu, LMGP-Suite, http://www.inpg.fr/LMGP). Using the unit cell dimensions of **1** as initial parameters in the same orthorhombic space group, the final refinement yielded a = 7.551(4) Å, b = 7.317(4) Å, c =18.373(9) Å, and V = 1015.1(9) Å^3, with good agreement between the observed and calculated peak positions (Table S1). Obviously, the peak shifts for **2** with respect to **1** is due to the changes in cell dimensions. For instance, the (101) and (011) peaks of **1** are very close and given a broad envelope peak around 2θ = 12.58°, while corresponding peaks of **2** appear as separate peaks at 12.66° and 13.01°.

Table S1. Relevant data of the unit cell refinement

H	K	L	$2\theta_{obsd}$/°	$2\theta_{Calcd}$ /°	difference/°
0	0	2	9.6177	9.6275	-0.0098
1	0	1	12.6621	12.6742	-0.0121
0	1	1	13.0147	13.0239	-0.0092
1	0	3	18.6639	18.6544	0.0095
0	0	4	19.3551	19.3238	0.0313
1	1	3	22.2956	22.2920	0.0036
2	0	0	23.5729	23.5634	0.0095
2	0	1	23.9886	24.0630	-0.0744
0	2	0	24.3037	24.3298	-0.0261
2	0	2	25.4863	25.5068	-0.0205
1	1	4	25.8050	25.7609	0.0441
0	2	2	26.1842	26.2199	-0.0357
2	1	0	26.5770	26.5665	0.0105
2	1	1	27.0221	27.0141	0.0080
1	2	1	27.5079	27.5233	-0.0154
0	0	6	29.1742	29.1623	0.0119
1	1	5	29.6885	29.6659	0.0226
2	1	3	30.2852	30.3759	-0.0907
1	2	3	30.8094	30.8341	-0.0247
0	2	4	31.2460	31.2565	-0.0105
1	0	6	31.5680	31.5266	0.0414
1	1	6	33.8276	33.8812	-0.0536
2	2	0	34.1304	34.1258	0.0046
2	2	1	34.5572	34.4838	0.0734
2	2	2	35.5019	35.5386	-0.0367
1	0	7	36.1734	36.2326	-0.0592
1	2	5	36.6340	36.6479	-0.0139
0	3	1	37.1948	37.1881	0.0067
3	1	1	38.1786	38.1248	0.0538
3	0	3	38.6738	38.6751	-0.0013
0	0	8	39.2472	39.2263	0.0209
2	2	4	39.5781	39.5138	0.0643
0	3	3	39.8035	39.7818	0.0217

Mean square deviation: $(\Sigma (2\theta_{obsd}-2\theta_{calcd})^2)^{1/2}/N_{ref} = 0.0367$

(N_{ref} is the number of the peaks used in the refinement)