Electronic Supplementary Material (ESI) for CrystEngComm

Structures and Magnetic Properties of Mn and Co Inorganic-Organic Frameworks with Mixed Linear Dicarboxylate Ligands

Electronic Supplementary Information

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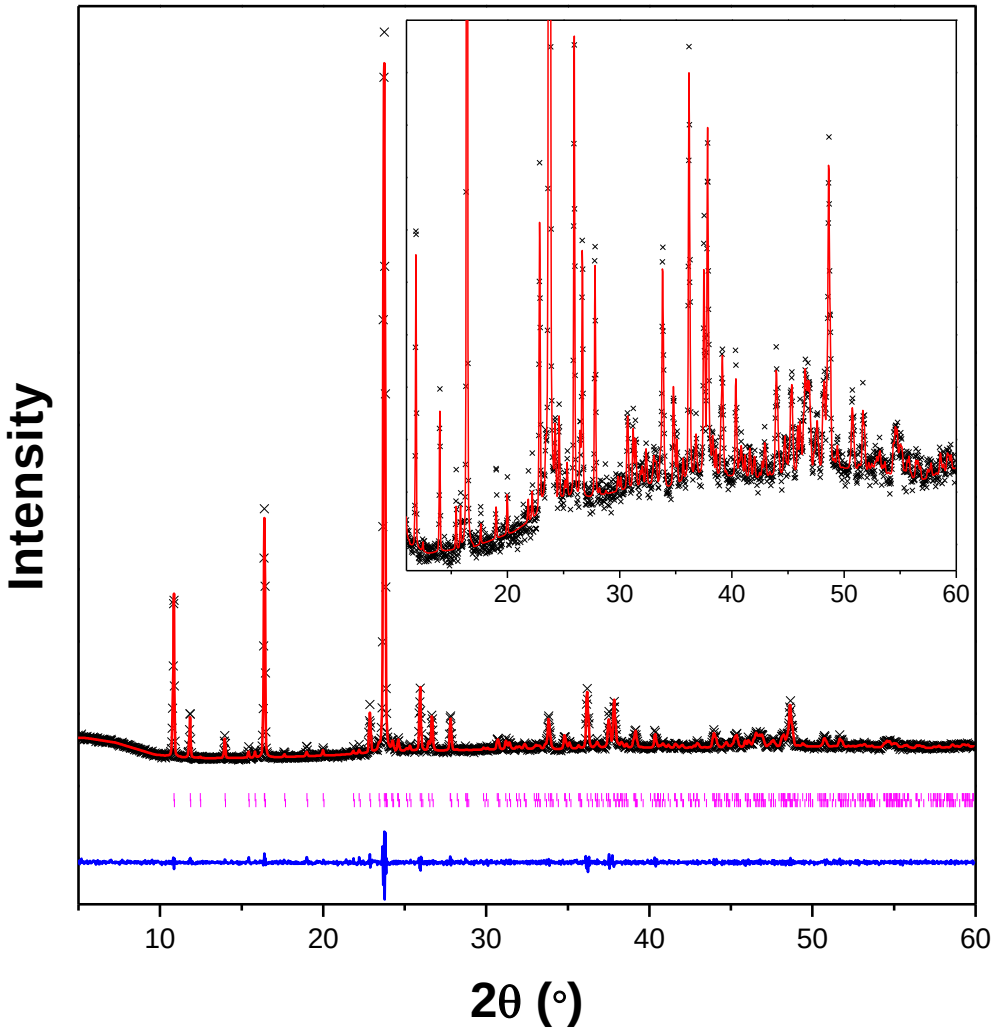

Fig. S1 Le Bail fit to the X-ray diffraction pattern of a sample of **1**, indicating its purity. The crosses, and upper and lower continuous lines are the experimental, calculated and difference profiles, respectively. The inset shows the weaker peaks in the higher angle data in more detail. The vertical markers indicate the allowed Bragg reflections, with the upper and lower symbols indicating $K_{\alpha 1}$ and $K_{\alpha 2}$ reflections, respectively. The final R_p, R_{wp} and χ^2 values are 2.6 %, 3.4 % and 1.7 and the cell parameters were determined to be a = 7.6184(5) Å, b = 7.9371(4) Å, c = 8.2133(5) Å, α = 85.051(5)°, β = 81.151(3)° and γ = 69.585(5)°.

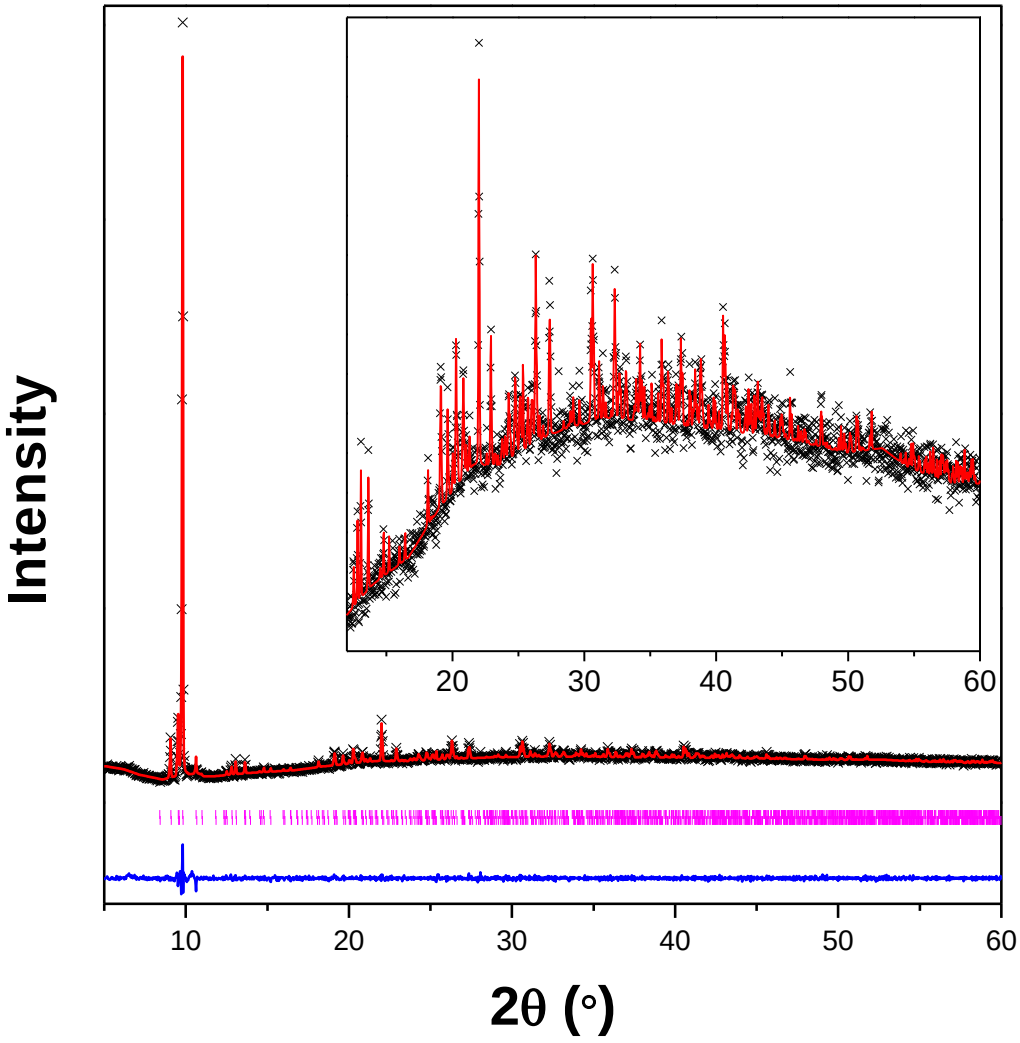

Fig. S2 Le Bail fit to the X-ray diffraction pattern of a sample of **2**, indicating its purity. The crosses, and upper and lower continuous lines are the experimental, calculated and difference profiles, respectively. The inset shows the weaker peaks in the higher angle data in more detail. The vertical markers indicate the allowed Bragg reflections, with the upper and lower symbols indicating $K_{\alpha 1}$ and $K_{\alpha 2}$ reflections, respectively. The final R_p, R_{wp} and χ^2 values are 2.4 %, 3.3 % and 1.2 and the cell parameters were determined to be a = 9.1898(5) Å, b = 10.7227(7) Å, c = 19.6178(11) Å, α = 89.320(5)°, β = 87.515(5)° and γ = 80.515(6)°. The increase in background at higher angles is caused by Co fluorescence.

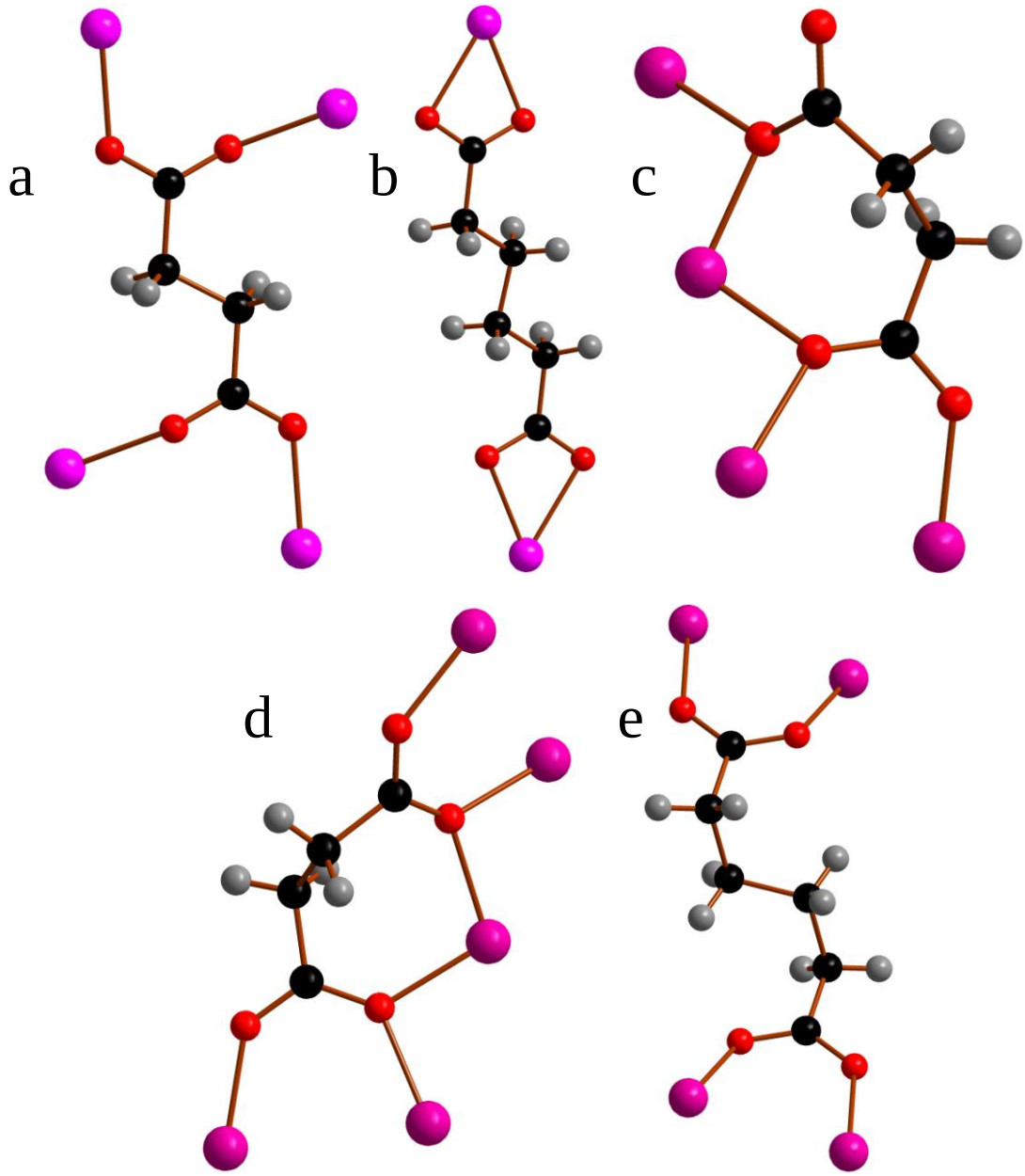

Fig. S3 The coordination modes of the ligands in compounds **1** (a) and b) and **2** (c), d) and e)). Compound **1** has succinate and adipate ligands with (1111) coordination while compound **2** has succinate ligands with (0212) and (1212) connectivity and adipate ligands with (1111) coordination. All colours are the same as those used in the main article.

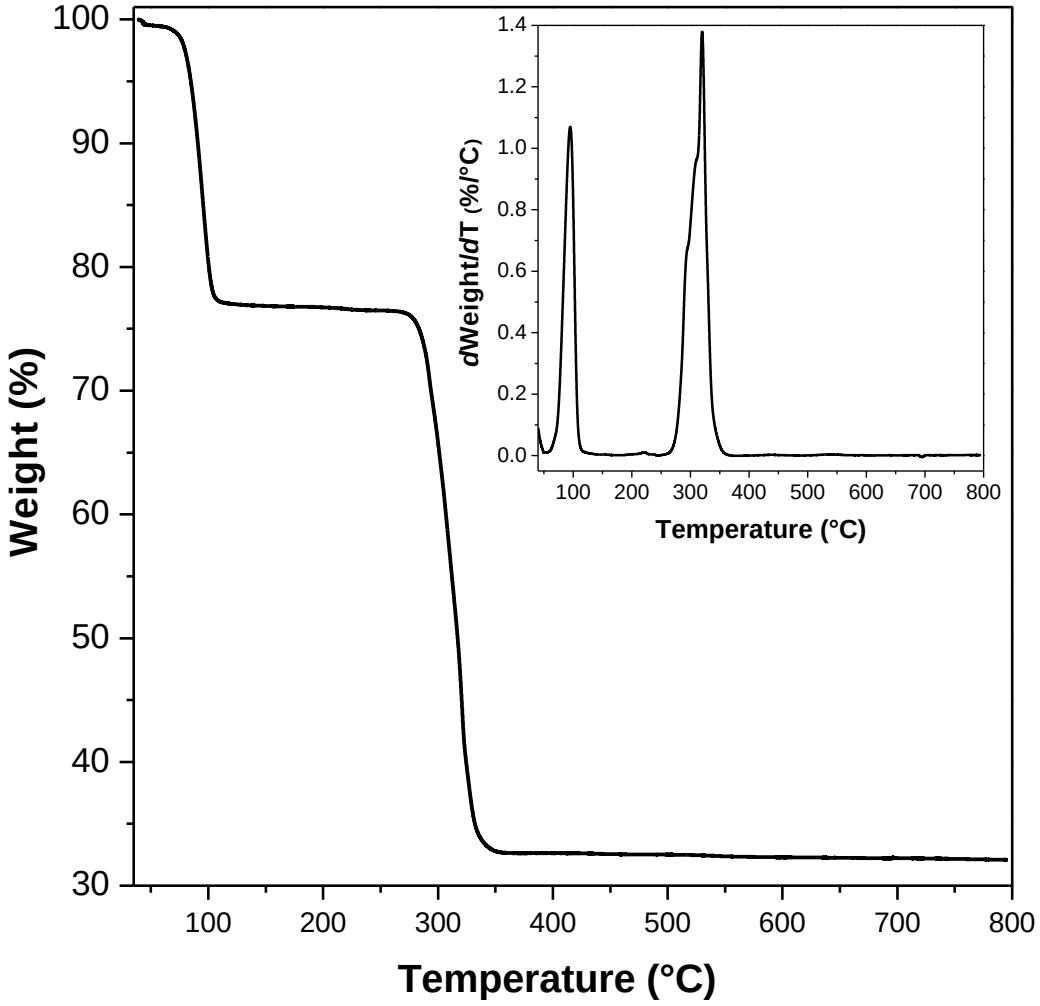

Fig. S4 Weight, expressed as a percentage of intial weight, versus temperature for compound **1** determined using TGA. The inset shows the rate of change in weight with temperature.

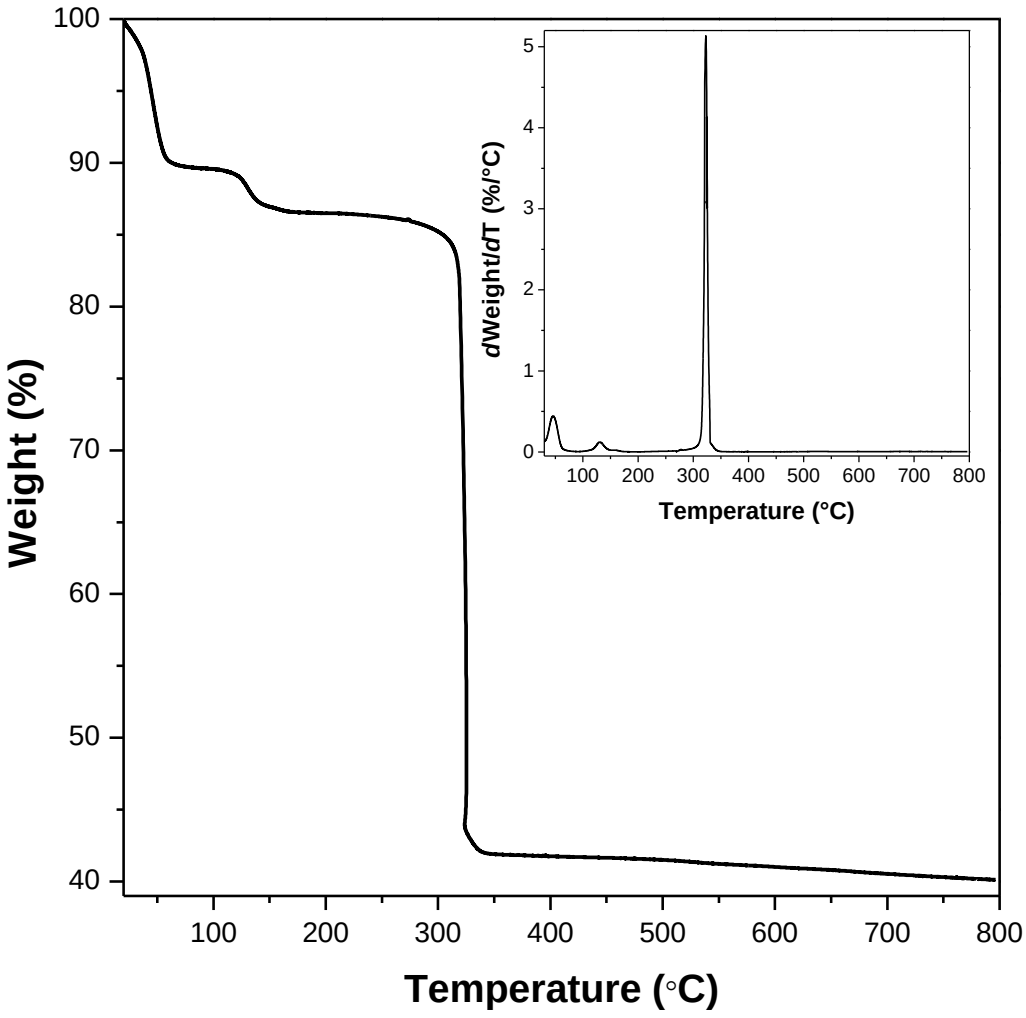

Fig. S5 Weight, expressed as a percentage of intial weight, versus temperature for compound **2** determined using TGA. The inset shows the rate of change in weight with temperature.

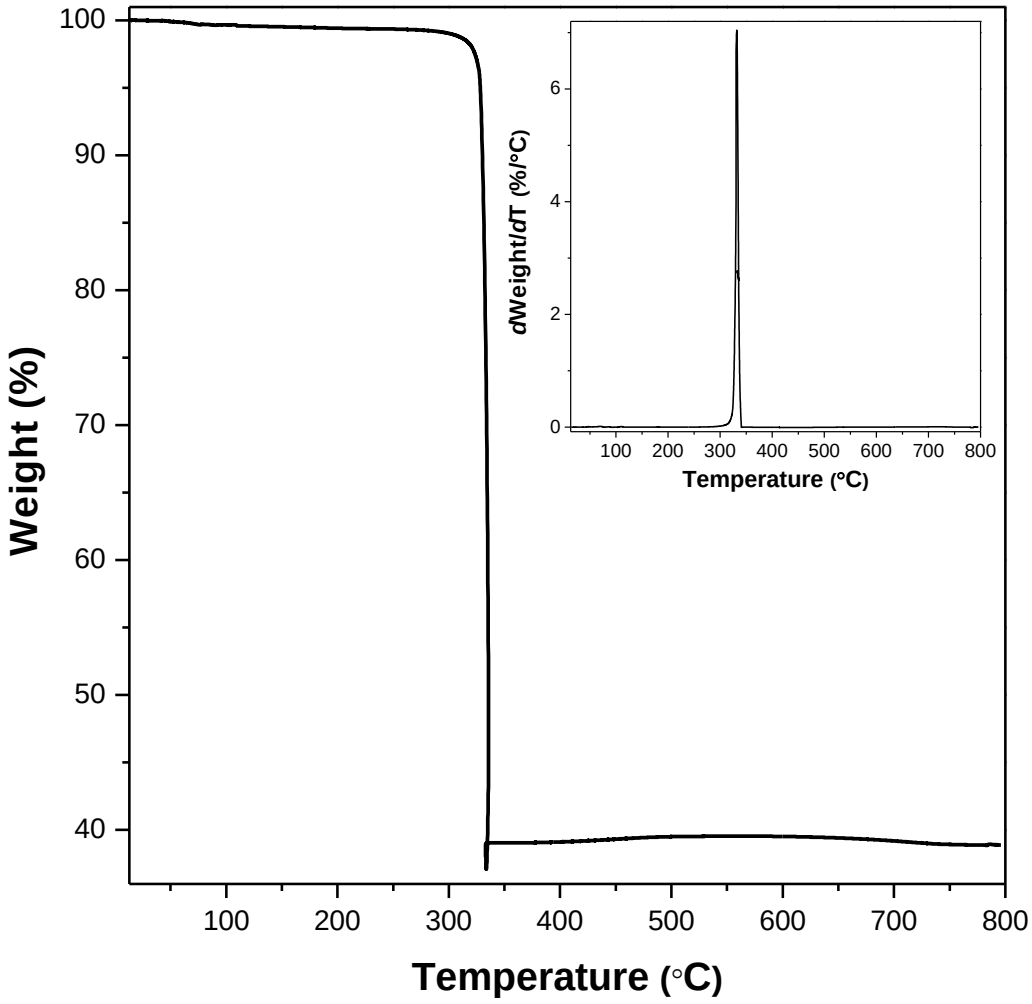

Fig. S6 Weight, expressed as a percentage of intial weight, versus temperature for compound **3** determined using TGA. The inset shows the rate of change in weight with temperature.

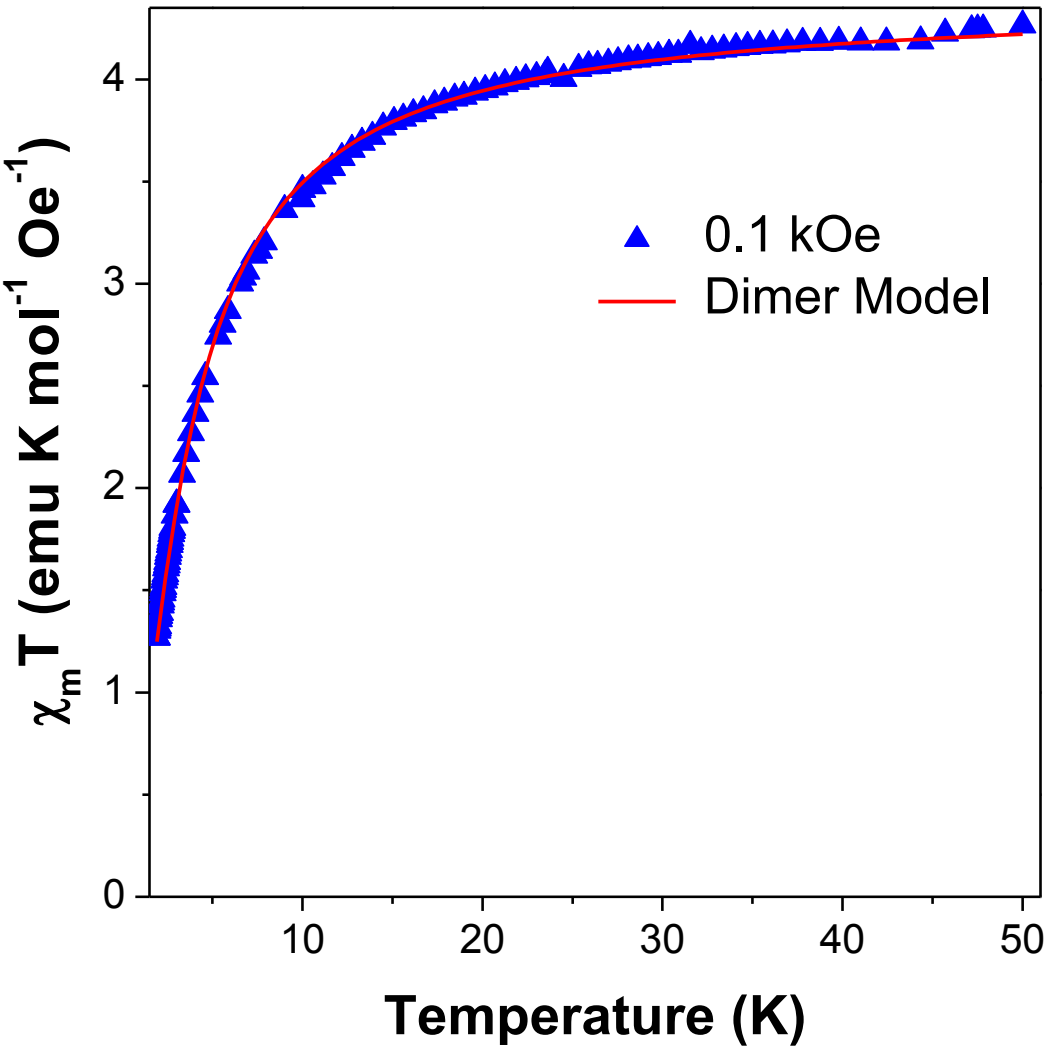

Fig. S7 Fit of the Heisenburg dimer model to the 0.1 kOe field-cooled susceptability measurement of compound **1.**

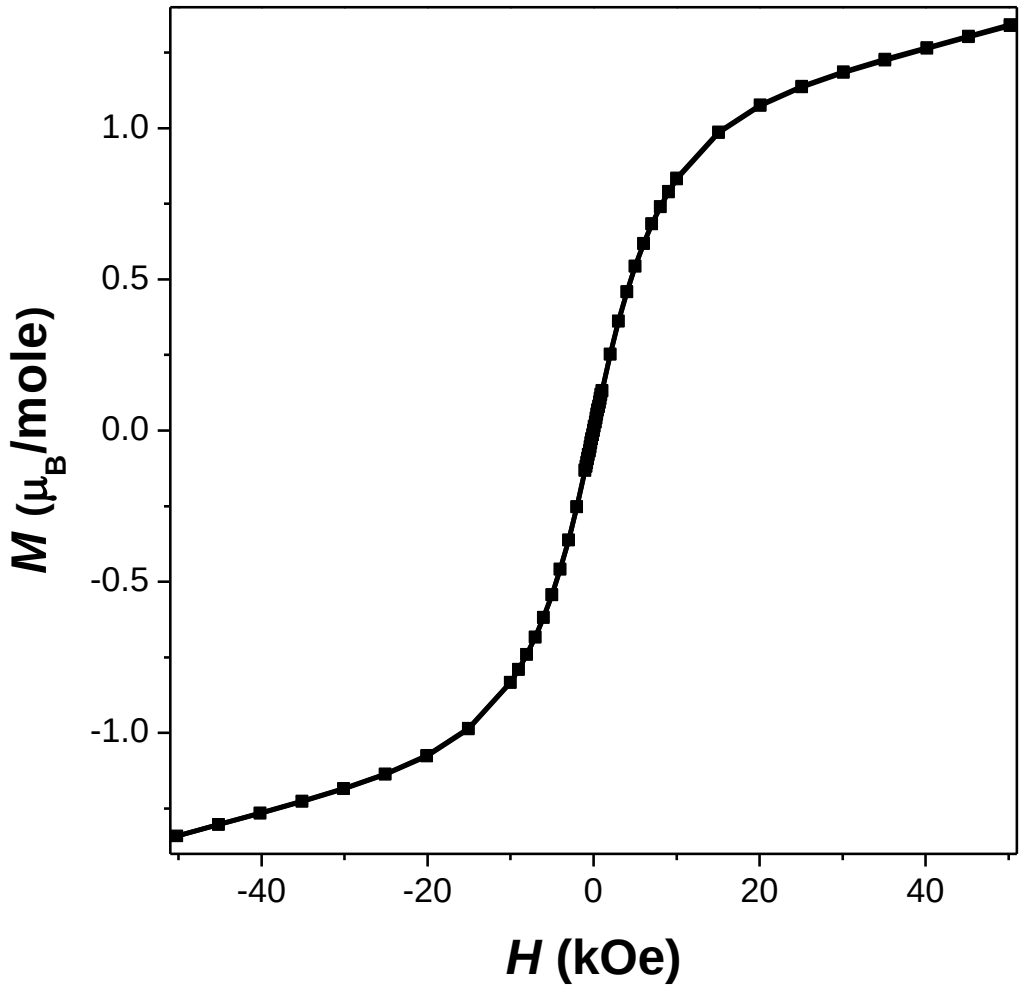

Fig. S8 Isothermal magnetisation of compound **2** measured at 1.9 K.

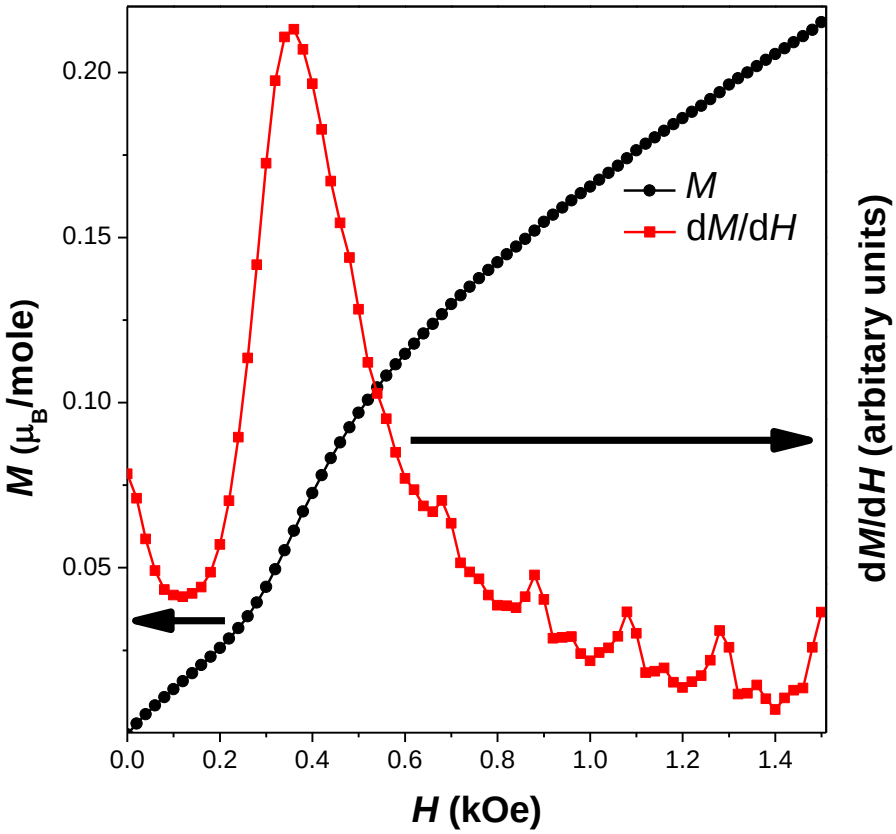

Fig. S9 Isothermal magnetisation and derivative of magnetisation of compound **2**, at lower fields, measured at 1.9 K.

Table S1 Selected co-ordination bond distances (Å) in compounds **1**, **2** and **3**.

1		Co1-O7W	2.146(3)	Co4-O2H	2.029(2)	Co7-O23	2 × 2.085(2)
Mn1-O2	2.111(1)	Co2-O14	2.055(3)	Co4-O52	2.095(3)	Co7-O34	2 × 2.091(3)
Mn1-O1W	2.119(1)	Co2-O1H	2.072(3)	Co4-O32	2.123(3)	Co8-O11	2 × 2.067(2)
Mn1-O1	2.155(1)	Co2-O3	2.079(3)	Co4-O24	2.131(2)	Co8-O4	2 × 2.083(3)
Mn1-O2W	2.200(1)	Co2-O9W	2.102(3)	Co4-O34	2.132(3)	Co8-O2	2 × 2.113(3)
Mn1-O11	2.276(1)	Co2-O2H	2.115(3)	Co4-O21	2.141(3)	**3**	
Mn1-O12	2.311(1)	Co2-O8W	2.156(3)	Co5-O42	2 × 2.008(2)	Co1-O3	1.955(6)
2		Co3-O1H	2.008(3)	Co5-O13	2 × 2.118(2)	Co1-O2	1.958(6)
Co1-O33	2.064(3)	Co3-O41	2.098(3)	Co5-O12	2 × 2.160(2)	Co1-O1	1.969(6)
Co1-O2H	2.071(3)	Co3-O12	2.103(2)	Co6-O51	2 × 2.003(3)	Co1-O4	1.974(6)
Co1-O22	2.098(2)	Co3-O13	2.112(2)	Co6-O24	2 × 2.149(2)		
Co1-O1H	2.121(3)	Co3-O4	2.148(3)	Co6-O21	2 × 2.152(2)		
Co1-O6W	2.145(3)	Co3-O2	2.159(3)	Co7-O32	2 × 2.075(3)		