Electronic Supplementary Material for CrystEngComm

Supplementary information

Design of bimetallic magnetic chains based on oxalate complexes: towards single chain magnets

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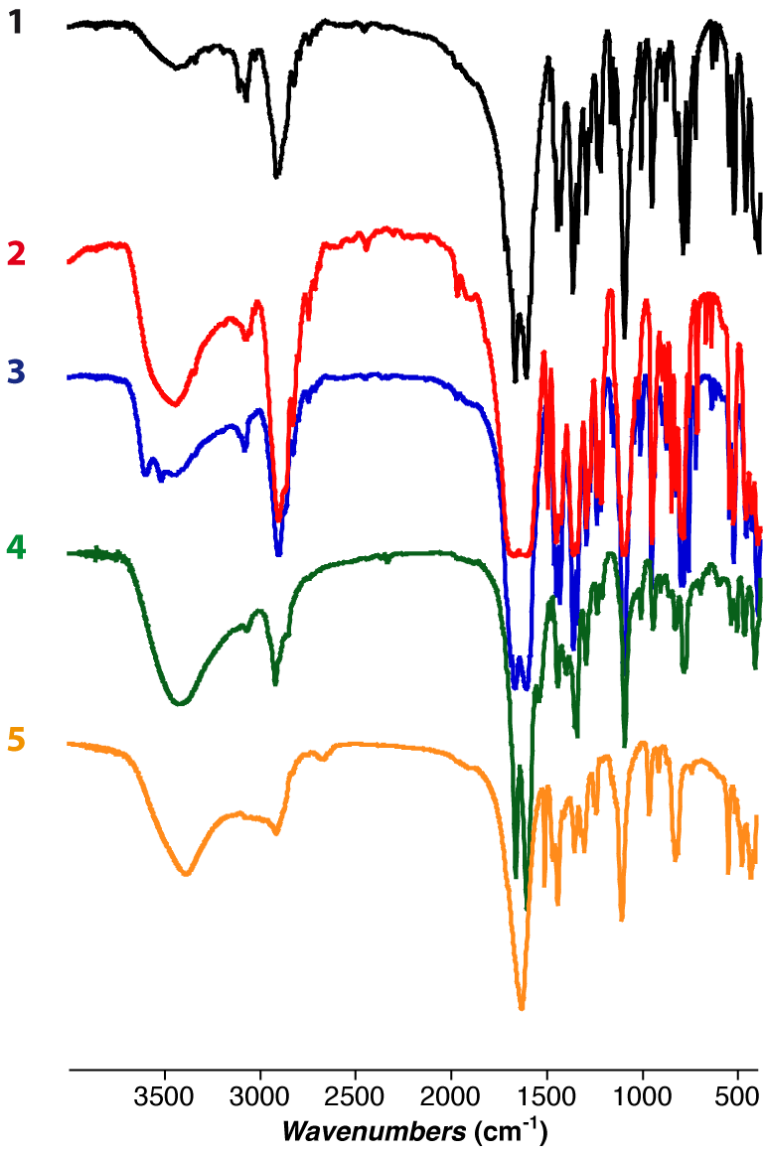
SI 1. FT-IR spectroscopy.

Infrared spectra were recorded in a FT-IR Nicolet 5700 spectrometer in the 4000-400 cm^{-1} range using powdered samples diluted in KBr pellets:



Most characteristic vibration modes for compounds **1-5** were assigned as follows:[1] **1**) υ[C-H]: 2918, 2905, 2826, 1457, 1441 cm^{-1}; υ[C=O]: 1728, 1698, 1676, 1617 cm^{-1}; υ[C-O]: 1304, 1285, 1248, 1233 cm^{-1}; υ[C-O]: 1107 cm-$^{-1}$; υ[C-C]: 964, 907 cm^{-1}; υ[O-C=O]: 839, 803 cm^{-1};

[1] Socrates, G. *Infrared characteristic group frequencies: tables and charts;* 2nd Ed. John Wiley & Sons. West Sussex, UK, **1994**.

υ[M-O]: 565, 477, 420, 409 cm^{-1}. (**2**) υ[C-H]: 2903, 2831, 1460, 1444 cm^{-1}; υ[C=O]: 1697, 1677, 1616 cm^{-1}; υ[C-O]: 1373, 1353, 1304, 1286 cm^{-1}; υ[C-O]: 1109 cm^{-1}; υ[C-C]: 966, 910 cm^{-1}; υ[O-C=O]: 815, 802 cm^{-1}; υ[M-O]: 563, 539, 475, 444, 413 cm^{-1}. (**3**) υ[C-H]: 2906, 2831, 2803, 1462, 1439 cm^{-1}; υ[C=O]: 1674, 1612 cm^{-1}; υ[C-O]: 1371, 1353, 1306, 1286 cm^{-1}; υ[C-O]: 1110 cm^{-1}; υ[C-C]: 965, 911 cm^{-1}; υ[O-C=O]: 839, 815, 802 cm^{-1}; υ[M-O]: 551, 476, 445, 413 cm^{-1}. (**4**) υ[C-H]: 2921, 1454, 1409 cm^{-1}; υ[C=O]: 1673, 1613 cm^{-1}; υ[C-O]: 1364, 1354, 1305, 1249 cm^{-1}; υ[C-O]: 1106 cm^{-1}; υ[C-C]: 959, 910 cm^{-1}; υ[O-C=O]: 844 cm^{-1}; υ[M-O]: 553, 533, 484, 427 cm^{-1}. (**5**) υ[C-H]: 2913, 1464, 1438 cm^{-1}; υ[C=O]: 1627 cm^{-1}; υ[C-O]: 1352, 1300, 1236 cm^{-1}; υ[C-O]: 1103 cm^{-1}; υ[C-C]: 960, 911 cm^{-1}; υ[O-C=O]: 824, 810 cm^{-1}; υ[M-O]: 546, 511, 475, 428 cm^{-1}.

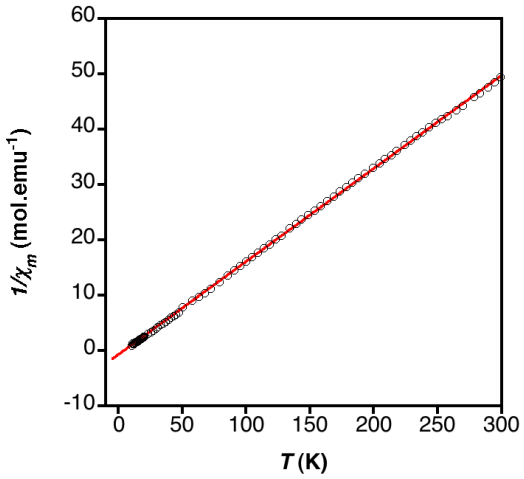
SI 2. Metallic composition.

Metallic composition of hand collected grounded crystals of **1**, **3**, **4** and **5** together with polycrystalline powder of **4** were estimated by electron probe microanalysis (EPMA). The analysis was performed in a Philips SEM XL30 equipped with an EDAX microprobe. The obtained results are summarized in Table 1.

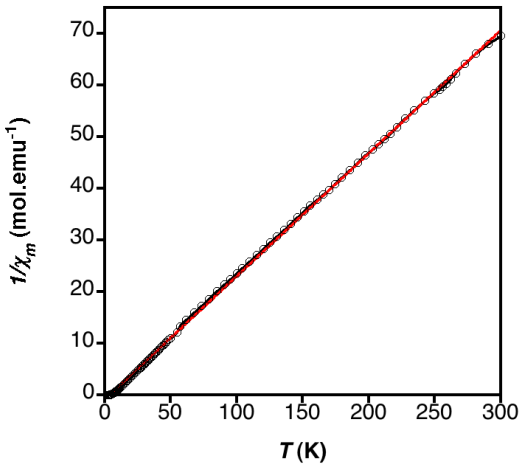
Table 1. Metallic composition of compounds **1**-**5** expressed as atomic percentage.

Sample	$\%M^{II}$		$\%M^{III}$		%K	
	Theor.	Exp.	Theor.	Exp.	Theor.	Exp.
1	33.3	33.8	33.3	33.2	33.3	33.0
2	33.3	34.3	33.3	32.6	33.3	33.1
3	33.3	33.5	33.3	33.0	33.3	33.5
4	33.3	33.4	33.3	34.1	33.3	32.5
5	40.0	41.5	40.0	39.3	20.0	19.2

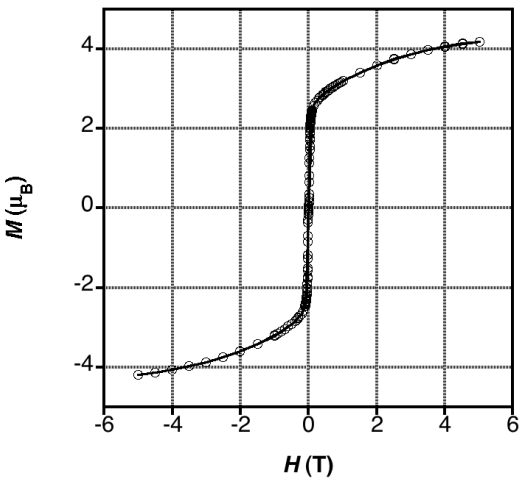
SI 3. Best fitting of the susceptibility data of **1** to the Curie-Weiss law in the 50-300 K interval (red line represents the best fitting; R = 99.9%).

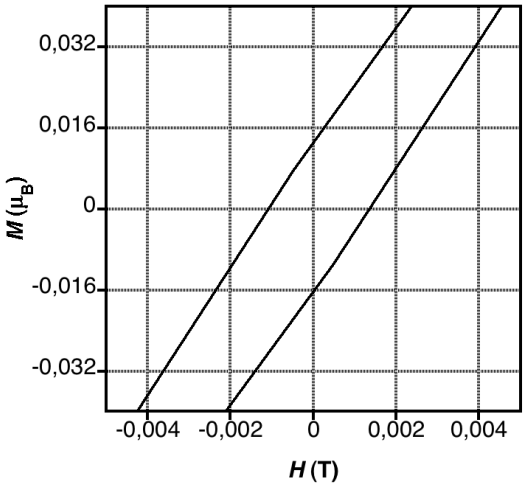


SI 4. Best fitting of the susceptibility data of **2** to the Curie-Weiss law in the 50-300 K interval (red line represents the best fitting; R = 99.9%).

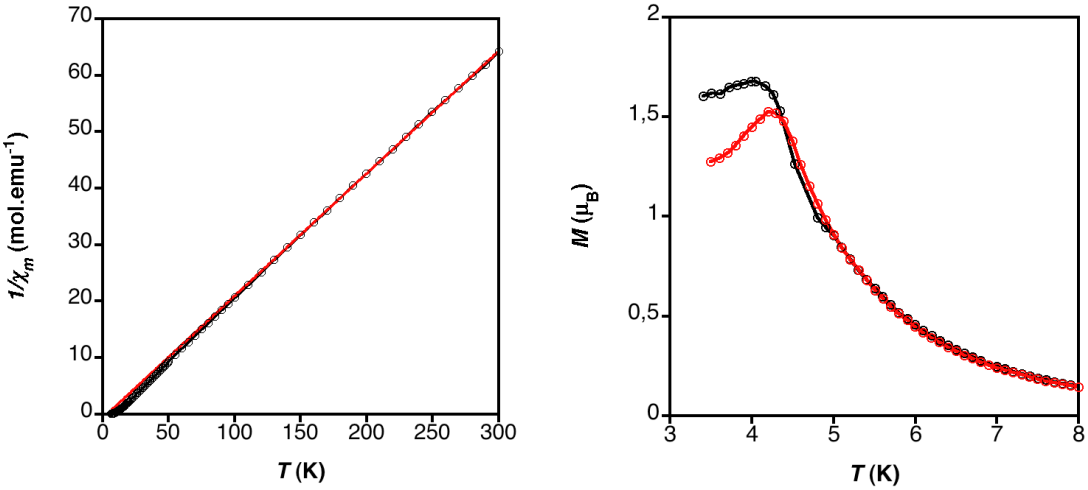


SI 5. Hysteresis loops of **2** at 2 K (*left*). Magnification at low fields (*right*). Solid lines are only a guide to the eye.

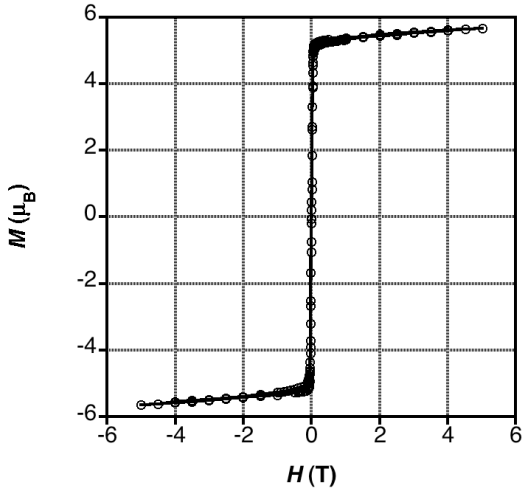




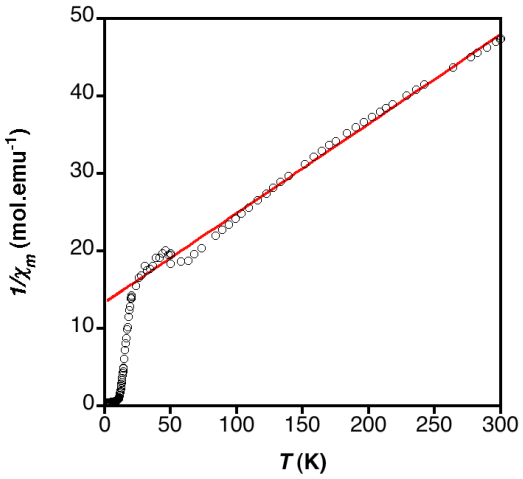
SI 6. *Left*: Best fitting (red line; R = 99.9%) of the susceptibility data of **3** to a Curie-Weiss law in the 150-300 K interval. *Right*: Field-cooled (black symbols) and zero field-cooled (red symbols) magnetizations under an external applied field of 50 G. Solid lines are only a guide to the eye.

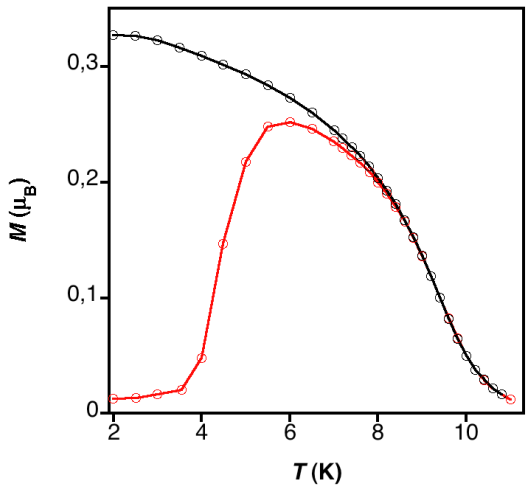


SI 7. Hysteresis loops of **3** at 2 K.

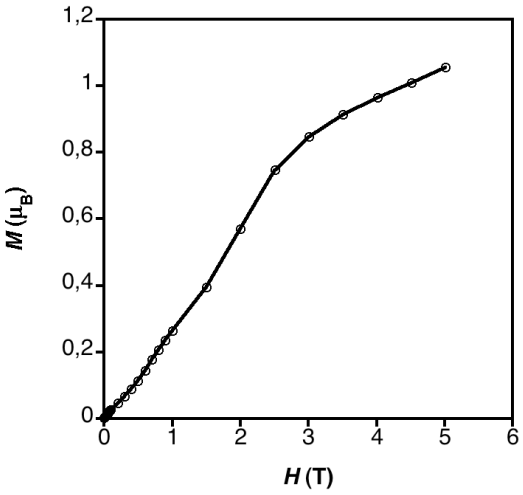


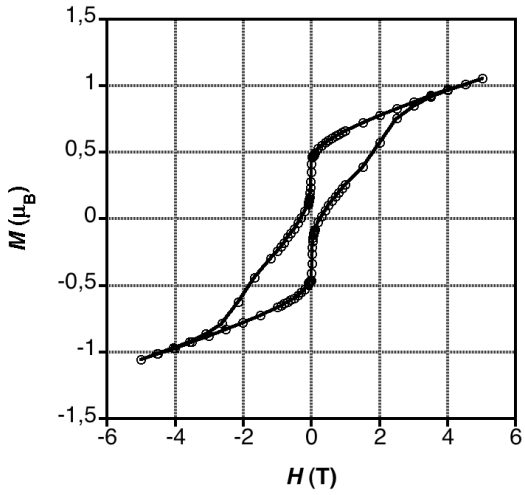
SI 8. *Left*: Best fitting (red line; R = 99.7%) of the susceptibility data of **4** to a Curie-Weiss law in the 150-300 K interval. *Right*: Field-cooled (black symbols) and zero field-cooled (red symbols) magnetizations under an external applied field of 50 G. Solid lines are only a guide to the eye.



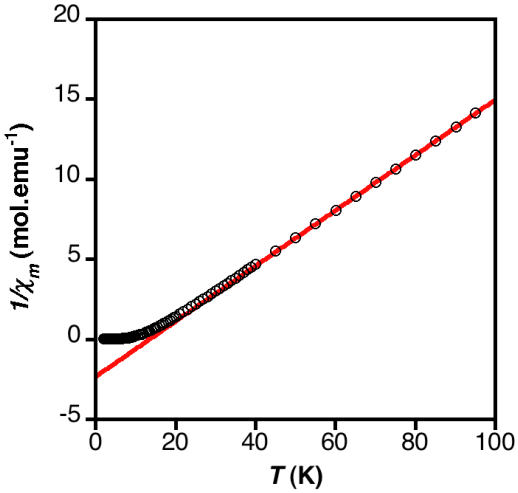


SI 9. Field dependence of the magnetization (*left*) and hysteresis loop of **4** at 2K (*right*).

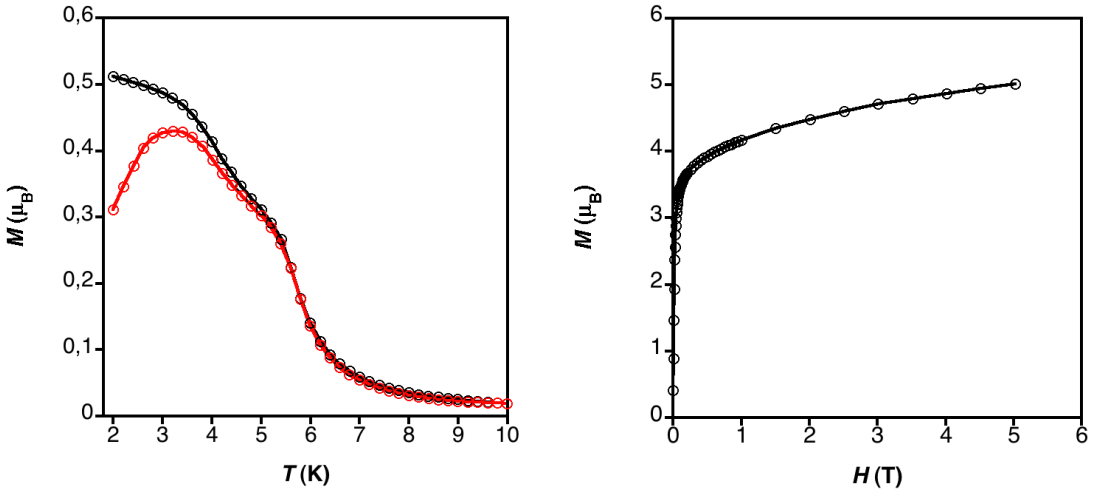




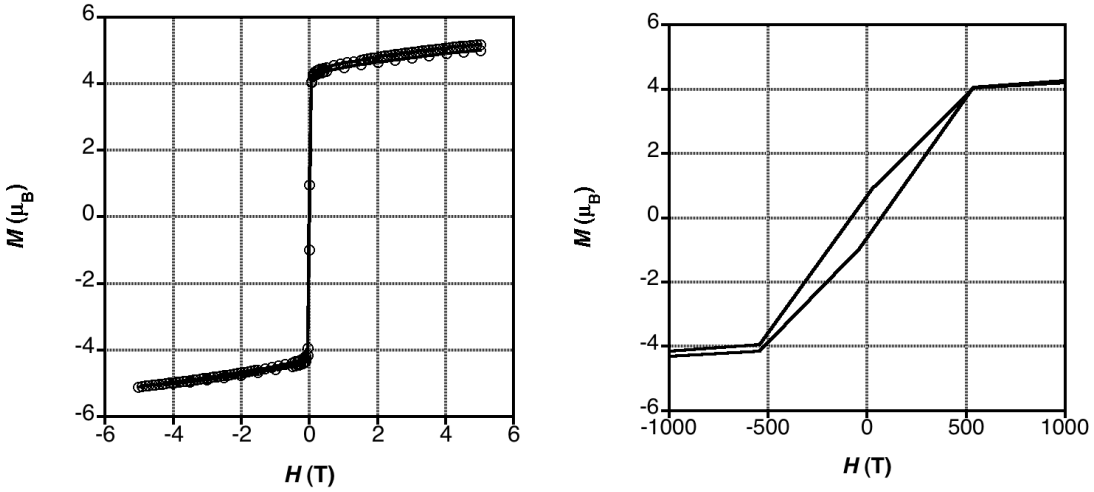
SI 10. Best fitting (red line; R = 99.5%) of the susceptibility data of **4** to a Curie-Weiss law in the 150-300 K interval.



SI 11. Field-cooled (black symbols) and zero field-cooled (red symbols) magnetizations of **5** under an external applied field of 25 G (*left*). Field dependence of the isothermal magnetization at 2 K (right). Solid lines are only a guide to the eye.



SI 12. Hysteresis loops at 2 K (*left*) and its magnification at low fields (*right*) for 5. Solid lines are only a guide to the eye.



SI 13. Plot of Ln(χ_M´T) vs. 1/T for 5. Solid line represents the best fitting to a linear regime. AC data were measured at 1 Hz frequency, 3.95 G oscillating field and zero external field.