

ELECTRONIC SUPPORTING INFORMATION

A 1-D coordination polymer based on a Mn₄₀ octagonal super-structure

Maria Manoli,^a Ross Inglis,^b Manolis J. Manos,^a Giannis S Papaefstathiou,^c Euan K. Brechin^{*b},
and Anastasios J. Tasiopoulos^{*a}

^aDepartment of Chemistry, University of Cyprus, 1678 Nicosia, Cyprus; Fax: (+357) 22895451; Tel: (+357) 22892765; E-mail: atasio@ucy.ac.cy

^bEaStCHEM School of Chemistry, The University of Edinburgh, West Mains Road, Edinburgh, EH9 3JJ, UK. Fax: +44 (0) 131-650-6453; Tel: +44(0) 131-650-7545; E-mail: ebrechin@staffmail.ed.ac.uk

^cLaboratory of Inorganic Chemistry, Department of Chemistry, National and Kapodistrian University of Athens, Panepistimiopolis 157 71 Zografou, Greece.

Experimental Procedure

{(Et₄N)[Mn₂₁(μ₃-O)₆(μ₃-OH)₂(sao)₁₂Br₃(O₂CMe)₁₂(H₂O)₁₀(CH₃CN)]Br₂}_n (**1**)_n: 1,3-butanediol (H₂bd) (0.502 ml, 0.505g, 5.60 mmol), saoH₂ (0.096 g, 0.70 mmol) and Et₄NBr (0.147 g, 0.70 mmol) were added to a solution of MnBr₂·4H₂O (0.200 g, 0.70 mmol) and Mn(O₂CMe)₂·4H₂O (0.171 g, 0.70 mmol) in 12 ml MeCN. The resulting green-brown solution was stirred for 1 hour, filtered off and layered with Et₂O. X-ray quality crystals of **1**·10MeCN·H₂O were formed after three weeks in ~30% yield. Vacuum – dried microcrystalline solid was analyzed as **1**·MeCN. Calcd. (found): C 32.71 (32.89), H 3.29 (3.35), N 4.77 (4.82).

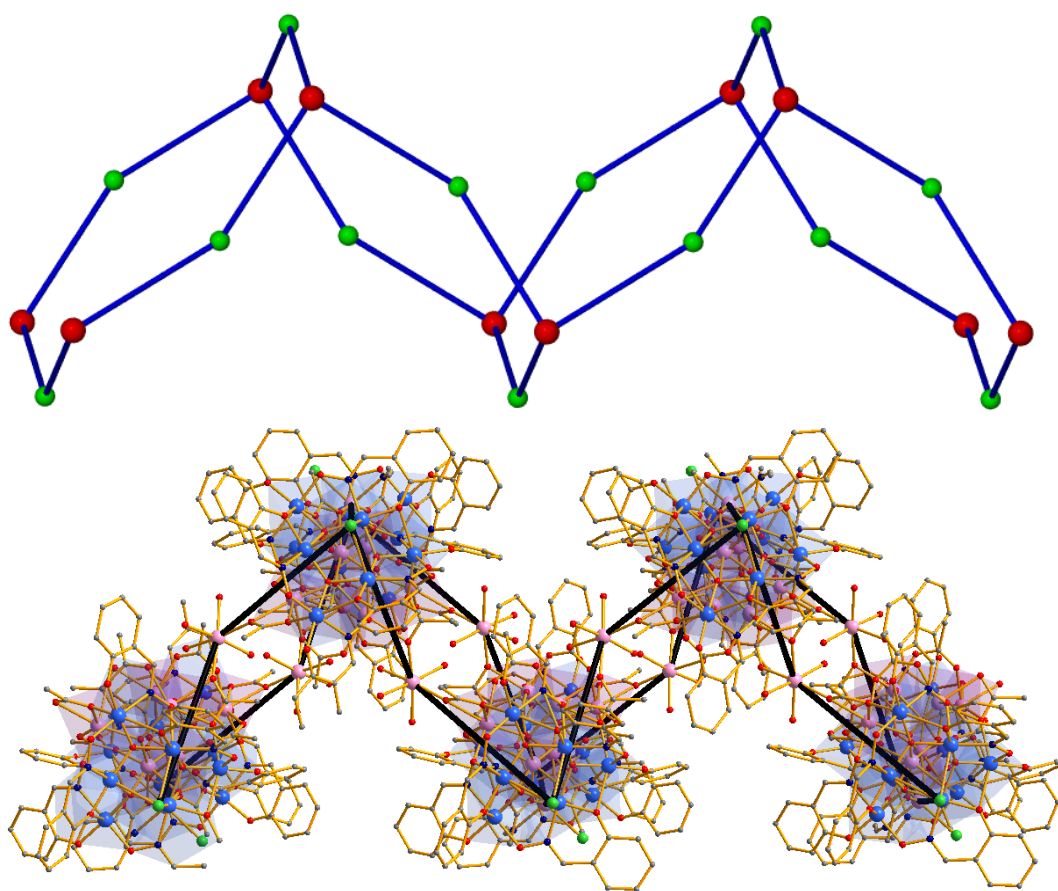


Fig. S1. A simplified (top) and ball and stick (bottom) representations of a part of the zig-zag chain of $(\mathbf{1})_n$ from a viewpoint that emphasizes the connection of the Mn_{40} octagons to form the ribbon-shaped 1-D chain. The black solid line and metal ion polyhedra are included to emphasize the Mn_{40} superstructure; Colour scheme: Mn^{III} : blue; Mn^{II} : pink; O: red; Br: green; N: dark blue; C: gray. Hydrogen atoms have been omitted for clarity

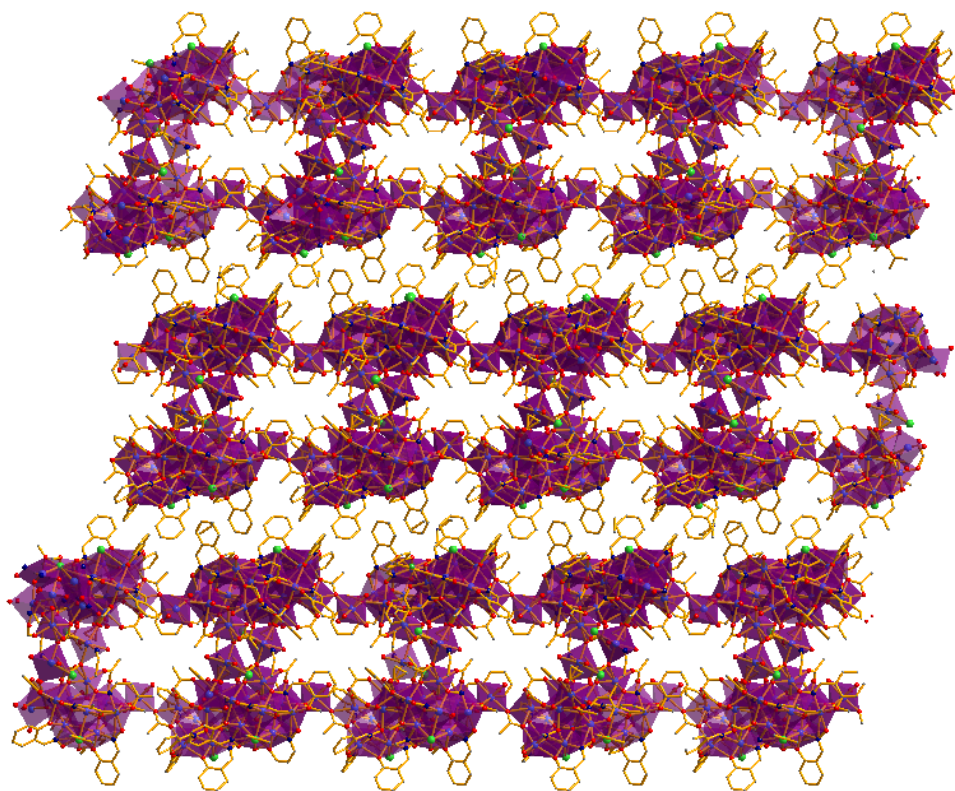


Fig. S2. Representation along the *b* axis of the packing of $(\mathbf{1})_n$. The metal ion polyhedra are included to emphasize the 1-D chains of $(\mathbf{1})_n$ consisting of Mn_{40} octagons that run parallel in the crystal. Colour scheme: As in Fig. S1. Hydrogen atoms have been omitted for clarity.

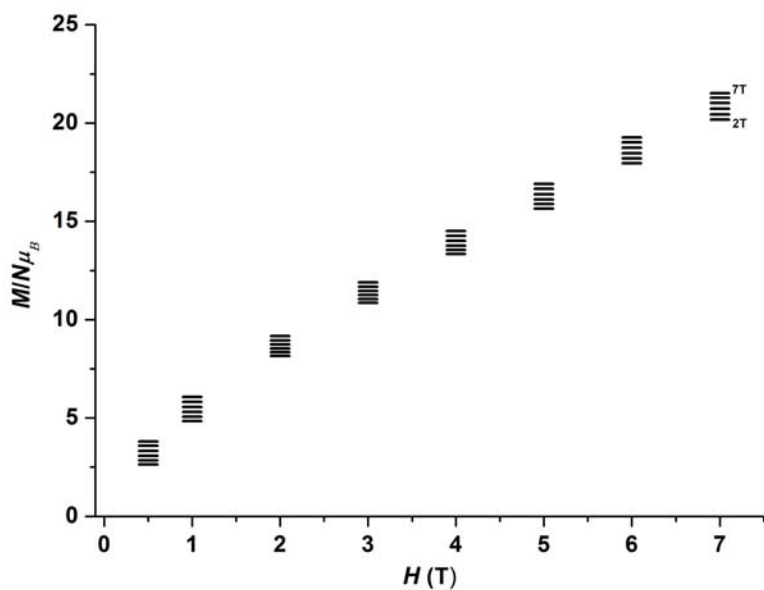


Fig. S3. Plot of magnetisation ($M/N\mu_B$) versus field for **1**·MeCN.

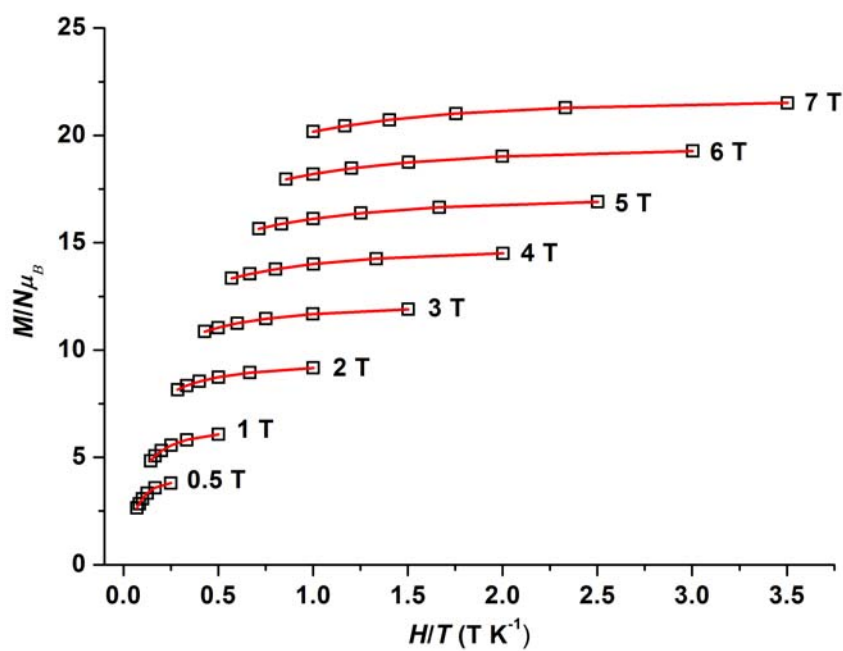


Fig. S4. Plot of $M/N\mu_B$ versus H/T for **1**·MeCN. The solid red lines are a guide to the eye only.

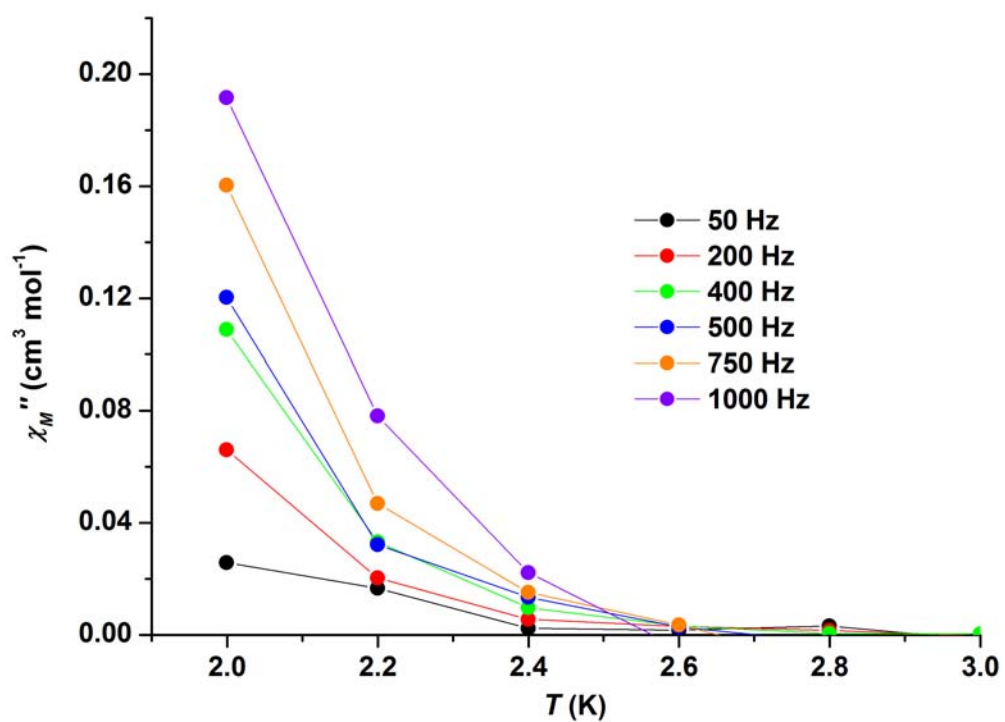


Fig. S5. Plot of the out-of-phase (χ_M'') ac susceptibility versus T , in the indicated frequency range for **1-MeCN**. The data was collected in a 3.5G ac field and zero-applied dc field. The presence of frequency-dependent signals is indicative of slow relaxation of the magnetisation.