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SUPPORTING INFORMATION FOR

A High-Pressure Crystallographic and Magnetic Study of $Na_5[Mn(L\text{-}tart)_2]\cdot 12H_2O$ (L-tart = L-tartrate)

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Crystal System	Monoclinic										
Space Group	$C2$										
λ/Å	0.4859										
Pressure/GPa	0.34	0.60	0.85	1.09	1.32	1.57	1.80	2.29	2.65	3.05	3.49
a/Å	20.1905(14)	20.1241(14)	20.0669(14)	20.0069(12)	19.9615(16)	19.9008(13)	19.8482(14)	19.7638(18)	19.6986(13)	19.6368(15)	19.5753(19)
b/Å	6.830(2)	6.800(2)	6.771(2)	6.7361(19)	6.715(3)	6.689(2)	6.664(2)	6.621(3)	6.5700(18)	6.512(2)	6.476(3)
c/Å	9.5946(7)	9.5772(7)	9.5645(7)	9.5511(6)	9.5408(8)	9.5275(7)	9.5173(7)	9.5007(9)	9.4982(6)	9.5039(7)	9.5153(10)
β/°	112.981(4)	113.069(4)	113.161(4)	113.257(4)	113.331(4)	113.453(3)	113.535(4)	113.677(5)	113.778(4)	113.862(4)	114.033(6)
V/Å^3	1218.0(4)	1205.8(4)	1194.9(4)	1182.6(4)	1174.3(5)	1163.6(4)	1154.1(4)	1138.6(5)	1124.9(3)	1111.5(4)	1101.7(5)
Z	2										
D_{calc}/g cm^{-3}	1.849	1.868	1.885	1.905	1.918	1.936	1.952	1.978	2.002	2.027	2.044
Reflections	4189	4356	4120	4041	3903	3716	3968	3915	3814	3036	3086
Unique Reflections	1044	1130	1029	1052	1026	951	982	965	969	701	921
R_{int}	0.046	0.051	0.046	0.051	0.058	0.044	0.047	0.044	0.045	0.038	0.059
R	0.041	0.043	0.036	0.046	0.043	0.035	0.033	0.033	0.036	0.034	0.049
R_w	0.064	0.104	0.061	0.072	0.071	0.060	0.061	0.058	0.063	0.060	0.078
S	0.99	1.02	0.99	0.99	1.00	0.99	1.00	1.00	1.00	1.00	1.00
Flack Parameter	0.06(6)	0.06(10)	0.06(6)	0.04(7)	0.13(6)	0.01(5)	0.08(6)	0.04(5)	−0.01(6)	−0.07(8)	0.06(10)
ρ_{max}, ρ_{min}/eÅ^{-3}	0.55,−0.58	0.58,−0.63	0.43,−0.52	0.30,−0.38	0.41,−0.50	0.37,−0.51	1.09,−1.31	0.56,−0.68	1.22,−1.16	0.45,−0.41	1.43,−1.32

Table S1. Selected crystallographic data for compound **1**.

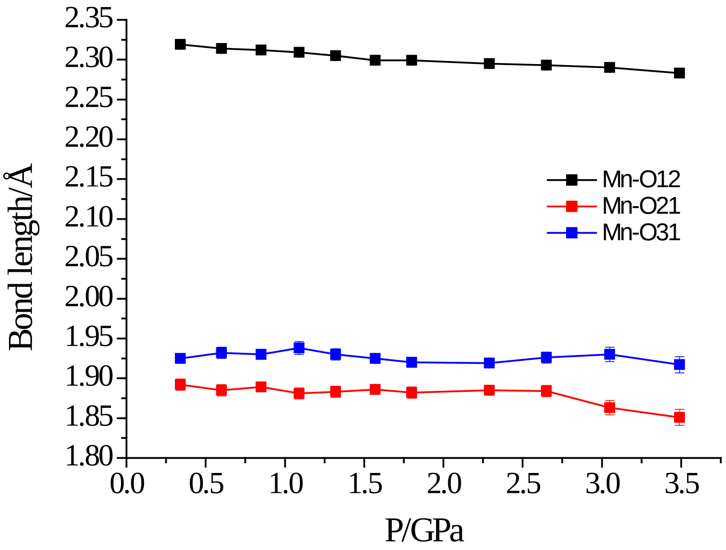

Figure S1. Variation with pressure of the average Mn-O bond lengths in the first coordination sphere of compound **1**.

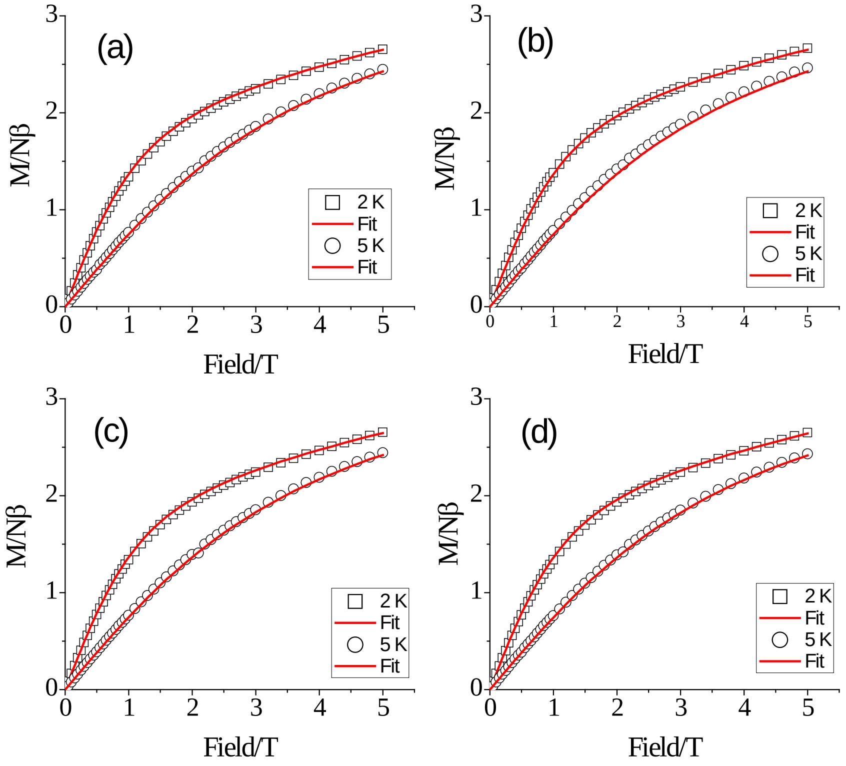

Figure S2. Magnetisation of **1** as a function of applied field at (a) ambient pressure inside the cell, (b) 0.5 GPa, (c) 1.0 GPa, and (d) 1.6 GPa. Solid lines correspond to fits of the data, performed with the program Phi.[1] Both the parameters *D* and *g* were allowed to vary as part of the fitting routine. A rhombic contribution, *E*, was not included to avoid over-parameterisation of the fit, and also because *E* had been previously found by EPR to be extremely small (0.032 cm^{-1}). The resulting parameters are given in Table S2. While the parameter *D* matches that found previously for **1** at ambient pressure,[2] the value of *g* is slightly lower. In this way, the *g* value accounts for the imperfect background correction for the high pressure SQUID cell.

P/GPa	*g*	D/cm^{-1}
0	1.81	−3.23
0.5	1.81	−3.23
1.0	1.81	−3.23
1.6	1.81	−3.23

Table S2. Values of *g* and *D* derived from the simultaneous fits of the *M* v *H* data at 2 and 5 K for **1**

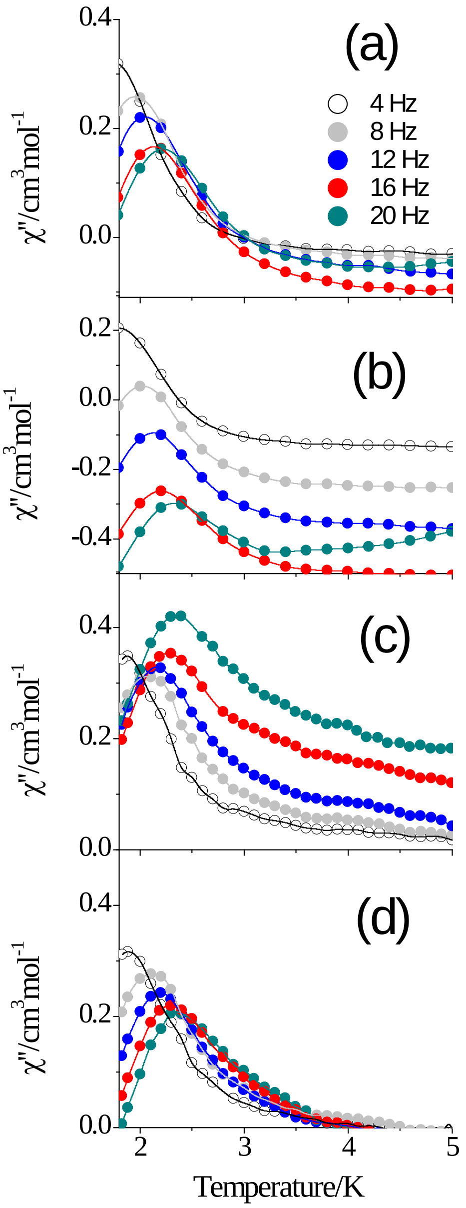

Fig S3. Out-of-phase susceptibility χ'' of **1** as a function of temperature at H_{DC} = 2500 Oe, scanned at various frequencies of alternating current (see key), at (a) ambient pressure; (b) 0.5 GPa; (c) 1.0 GPa; and (d) 1.6 GPa. Solid lines are guides to the eye. The limited frequency range is due to a broadening of the peak observed as well as an increasing non-linear background in the pressure cell above 30 Hz, rendering it impossible to determine the maxima in χ''. For this reason, we chose to scan the temperature at different frequencies, rather than scan frequencies at different temperatures, as in ref [2]. The negative values of χ'' registered in some of the measurements are caused by an imperfect background correction of the cell. This arises because the exact mass of the pressure transmitting medium is not known. The dc field of 2500 Oe was chosen because it was shown in in ref [2] to yield the highest signal in χ''.

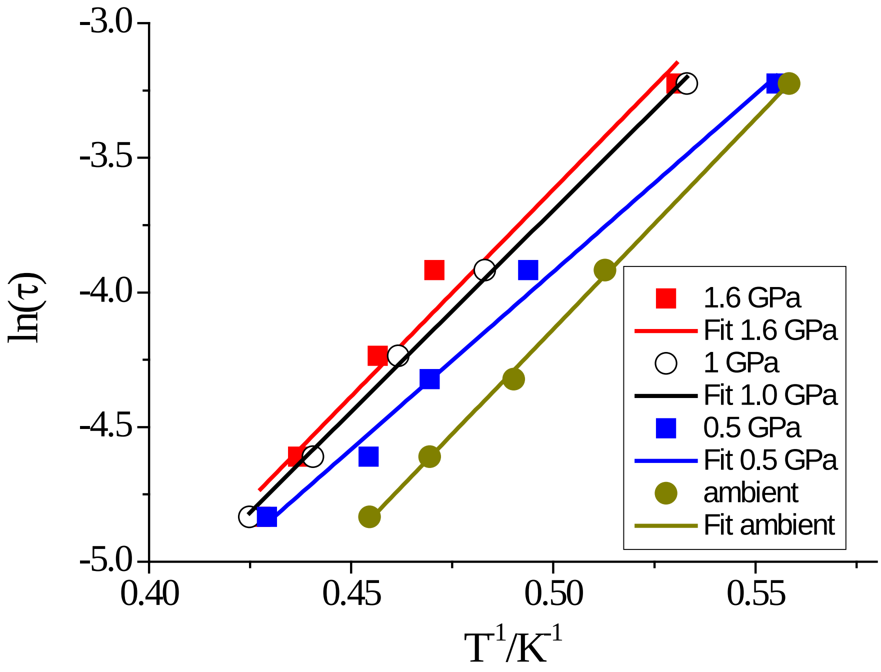

Figure S4. Arrhenius plots derived from the ac susceptibility data presented in Fig. S3. The lines correspond to straight line fits of the data, yielding the barriers to relaxation of the magnetisation U_{eff}, given in Table S3.

P/GPa	$U_{\mathrm{eff}}/\mathrm{cm}^{-1}$
1.6	10.7(10)
1.0	10.4(3)
0.5	9.2(5)
0	10.8(2)

Table S3. Values of U_{eff} derived for **1** at the pressures measured.

References

[1] N. F. Chilton, R. P. Anderson, L. D. Turner, A. Soncini and K. S. Murray, *J. Comput. Chem.*, 2013, **34**, 1164-1175.

[2] G. A. Craig, J. J. Marbey, S. Hill, O. Roubeau, S. Parsons and M. Murrie, *Inorg. Chem.*, 2015, **54**, 13-15.