

ESI for 'Pressure-induced Jahn-Teller switching in a Mn₁₂ single-molecule magnet'
Pascal Parois *et al.*

Geometry around Mn8. Bold = significantly elongated.					
Crystal	0	2	1&2	1	2
Data-set	SP8038	MNJTRT	MN0311	MNJT04	MNJT12
Conditions	150 K/0 GPa	RT/0 GPa	RT/1.5 GPa	RT/2.5 GPa	RT/0GPa
Distance/Å					
Mn8-O108	1.893(3)	1.930(4)	1.98(2)	1.88(3)	1.932(4)
Mn8-O13	1.963(3)	2.002(5)	2.02(3)	1.89(3)	1.994(4)
Mn8-O208	2.049(2)	1.966(4)	1.94(2)	1.90(3)	1.956(4)
Mn8-O25	2.145(3)	2.025(4)	2.04(3)	2.03(3)	2.022(5)
Mn8-O14	1.961(2)	2.012(5)	2.082(15)	2.105(17)	2.015(5)
Mn8-O26	1.956(3)	2.010(5)	2.034(17)	2.19(2)	2.005(5)

Table S1. Mn-O bond lengths at Mn8 as a function of pressure.

Experimental details

In each case the crystal system is triclinic and the space group P-1. The value of $Z = 2$.

Structure code in cif	sp8038	mnjtrt	mn0311	mnjt04	mnjt12
CCDC Deposition No	755025	755026	755027	755028	755029
Temperature/ K	150	298	298	298	298
Pressure/ GPa	0	0	1.5	2.5	0
Crystal data					
Chemical formula	[Mn ₁₂ O ₁₆ (^t BuCH ₂ CO ₂) ₁₆ (H ₂ O) ₄].xMeNO ₂ .yCH ₂ Cl ₂				
<i>x, y</i>	1, 1	1,1	0.75, 0.5	0, 0	1,1
<i>M_r</i>	2898.94	2911.68	2853.96	2765.71	2911.68
<i>a, b, c</i> (Å)	15.8368 (4), 16.4179 (5), 27.3955 (7)	16.099 (4), 16.702 (4), 27.570 (6)	15.3530 (11), 15.5310 (11), 26.7020 (12)	15.0148 (19), 15.1418 (19), 26.7583 (19)	16.0888 (10), 16.6899 (10), 27.5390 (17)
α, β, γ (°)	76.817 (2), 78.1610 (10), 78.264 (2)	76.585 (4), 78.042 (4), 77.809 (4)	76.669 (5), 76.441 (5), 78.069 (5)	76.184 (9), 76.208 (8), 79.415 (8)	76.5270 (10), 78.0850 (10), 77.7050 (10)
<i>V</i> (Å ³)	6695.5 (3)	6950 (3)	5943.8 (7)	5685.1 (11)	6930.0 (7)
Radiation type	Mo <i>K</i> α	Synchrotron X-ray, $\lambda = 0.47800$ Å			
μ (mm ⁻¹)	1.17	0.34	0.40	0.41	0.34
Crystal size (mm)	0.66 × 0.41 × 0.35	0.2 × 0.2 × 0.1	0.2 × 0.2 × 0.1	0.2 × 0.2 × 0.1	0.2 × 0.2 × 0.1
Data collection					
Diffractometer	Bruker Smart Apex diffractometer	Bruker APEXII diffractometer			
Absorption correction	Multiscan (SADABS)				
<i>T_{min}, T_{max}</i>	0.525, 0.663	0.594, 0.744	0.649, 0.744	0.646, 0.744	0.599, 0.744
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	52152, 26597, 20068	68279, 27434, 19784	32067, 4879, 3177	12135, 3426, 2067	68385, 27186, 16773
<i>R_{int}</i>	0.041	0.043	0.070	0.078	0.050
θ_{\max} (°)	26.4	17.3	15.5	13.5	17.3
Refinement					
$R[F^2 > 2\sigma(F^2)],$ $wR(F^2), S$	0.053, 0.145, 1.04	0.081, 0.269, 1.12	0.108, 0.256, 1.04	0.110, 0.286, 1.03	0.082, 0.275, 1.12
No. of reflections	26597	27434	4879	3426	27186
No. of parameters	1442	997	775	746	997
No. of restraints	0	4866	1849	1839	4866
$\Delta\rho_{\max}, \Delta\rho_{\min}$ (e Å ⁻³)	0.94, -0.60	0.99, -0.80	0.55, -0.40	0.49, -0.46	1.06, -0.70

Table S2. Crystallographic data.

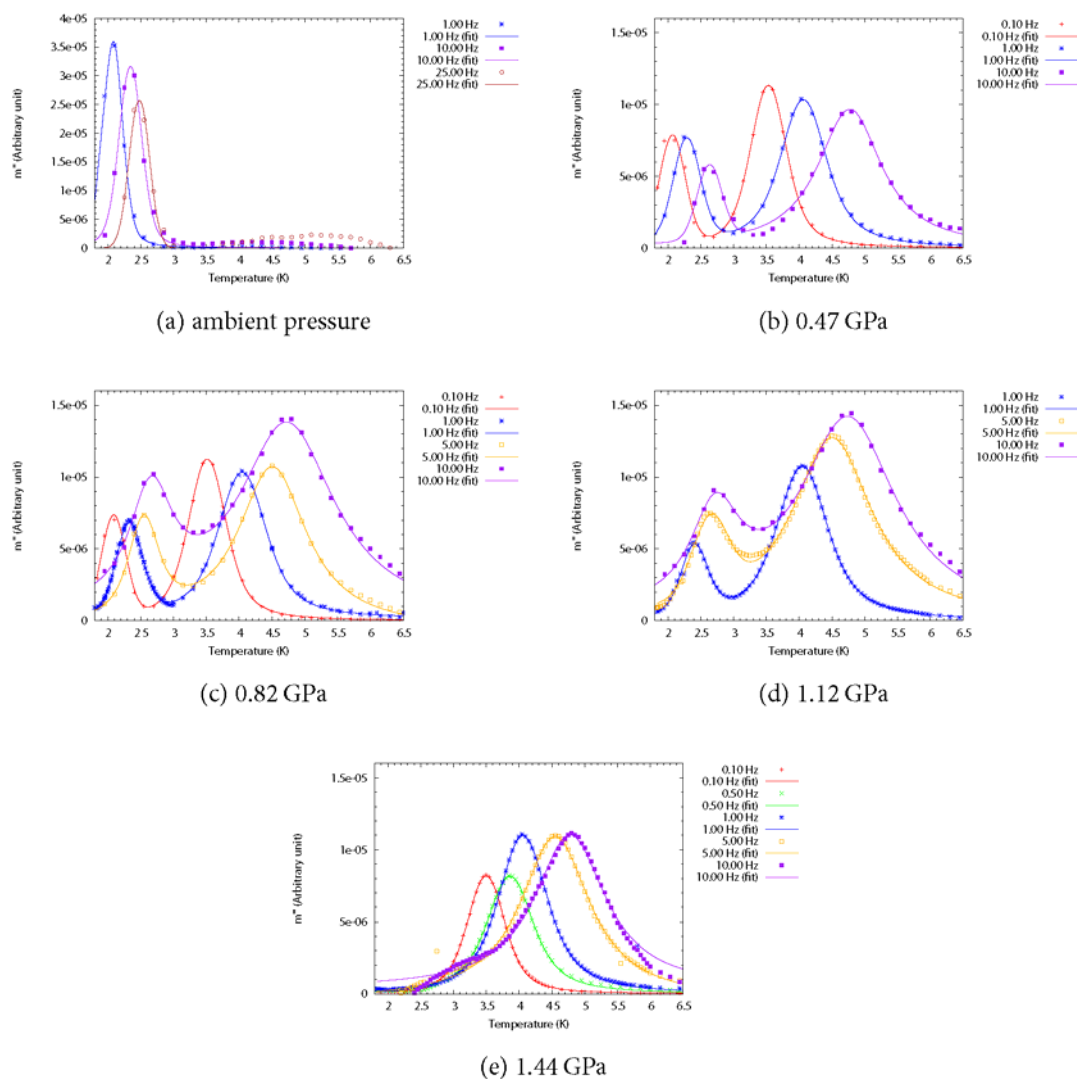


Figure S1. Frequency dependent AC susceptibility data, m'' versus T , at various pressures from ambient to 1.44 GPa.