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Supporting information for article:

Isothermal equation of state and high-pressure phase transitions of synthetic meridianiite (MgSO4·11D2O) determined by neutron powder diffraction and quasielastic neutron spectroscopy

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Table S1

Refined unit-cell parameters of $MgSO_4 \cdot 11D_2O$ as a function of pressure.

T (K)	P (MPa)	*a* (Å)	*b* (Å)	*c* (Å)	α (°)	β (°)	γ (°)	V (Å^3)
Fortes *et al*., (2008)								
Uncertainty in T = ± 0.05 K, in P = n/a (ambient).								
240	0.1	6.7495(1)	6.8115(1)	17.2920(3)	88.135(1)	89.491(1)	62.687(1)	705.97(1)
Experiment 1: PEARL/HiPr, 2008								
Uncertainty in T = ± 1 K, in P ≈ 5 %								
240	192	6.735(1)	6.776(1)	17.269(3)	88.38(2)	89.60(2)	62.60(2)	699.4(3)
240	248	6.735(1)	6.769(1)	17.260(3)	88.40(1)	89.59(2)	62.57(1)	698.1(3)
240	257	6.732(2)	6.764(2)	17.255(4)	88.42(2)	89.56(2)	62.57(2)	697.1(3)
240	260	6.733(2)	6.760(2)	17.251(4)	88.47(2)	89.60(2)	62.53(2)	696.5(3)
240	496	6.721(1)	6.728(1)	17.225(2)	88.70(1)	89.60(1)	62.39(1)	690.0(1)
240	773	6.710(1)	6.691(1)	17.191(3)	88.97(1)	89.63(2)	62.23(2)	682.8(2)
Experiment 2: PEARL/HiPr, 2009								
Uncertainty in T = ± 1 K, in P ≈ 5 %								
240	514	6.7234(4)	6.7250(4)	17.224(1)	88.733(5)	89.578(6)	62.339(5)	689.59(8)
Experiment 3: OSIRIS, 2011								
Uncertainty in T = ± 0.1 K, in P = 0.3 %.								
240	48.0	6.7479(2)	6.8036(2)	17.2850(6)	88.175(3)	89.509(3)	62.650(2)	704.48(2)
240	103.5	6.7453(2)	6.7947(2)	17.2767(5)	88.246(2)	89.524(3)	62.606(2)	702.69(2)
240	149.7	6.7430(2)	6.7867(2)	17.2680(5)	88.306(2)	89.519(3)	62.584(2)	701.16(2)
240	200.2	6.7390(2)	6.7784(2)	17.2647(5)	88.340(2)	89.530(3)	62.550(2)	699.55(2)
240	252.0	6.7366(2)	6.7694(2)	17.2554(5)	88.397(2)	89.532(3)	62.523(2)	697.84(2)
240	305.5	6.7325(2)	6.7603(2)	17.2515(5)	88.460(2)	89.556(2)	62.497(2)	696.18(2)
240	351.0	6.7292(2)	6.7533(2)	17.2450(5)	88.502(2)	89.561(2)	62.468(2)	694.69(2)
240	409.8	6.7252(2)	6.7430(2)	17.2399(5)	88.569(2)	89.566(3)	62.461(2)	692.99(2)
240	451.8	6.7254(2)	6.7367(2)	17.2311(5)	88.607(2)	89.561(3)	62.439(2)	691.88(2)
240	499.8	6.7236(2)	6.7295(2)	17.2242(5)	88.661(2)	89.566(3)	62.404(2)	690.48(2)
240	550.0	6.7218(1)	6.7218(1)	17.2184(3)	88.709(1)	89.582(2)	62.371(1)	689.08(1)

Pressure calibration using a revised equation of state for Pb

The Pb equation of state employed in this work was derived from a synthesis of literature values for the ambient-pressure thermal expansivity, and ultrasonic determinations of the temperature dependence of the bulk modulus and its first pressure derivative (see overleaf). The principal improvement in our implementation of this equation of state over that described previously (Fortes *et al*., 2007, 2012) lies in the robust propagation of errors.

The pressure is determined using a 3rd-order Birch-Murnaghan equation of state,

$$P_{V,T} = \frac{3}{2} K_{0,T}\left(x^{7/3} - x^{5/3}\right)\cdot\left[1 + \frac{3}{4}\left(K'_{0,T} - 4\right)\left(x^{2/3} - 1\right)\right]$$

where $x = V_{0,T} / V_{P,T}$; and the unit-cell volume, $V_{0,T}$, the isothermal bulk modulus, $K_{0,T}$, and its first pressure derivative, $K'_{0,T}$, are found from temperature dependent polynomials; The second pressure derivative of the bulk modulus, $K''_{0,0}$, is assumed to be independent of temperature.

$V_{0,T} = V_{0,0} + aT + bT^2$	$V_{0,0}$	121.41813 ± 0.00013 Å^3
	a	$1.05822 \pm 0.00007 \times 10^{-2}$ Å^3 K^{-1}
	b	$3.493 \pm 0.004 \times 10^{-6}$ Å^3 K^{-2}
$K_{0,T} = K_{0,0} + cT + dT^2$	$K_{0,0}$	41.725 ± 0.009 GPa
	c	$-2.544 \pm 0.004 \times 10^{-2}$ GPa K^{-1}
	d	$-2.76 \pm 0.24 \times 10^{-6}$ GPa K^{-2}
$K'_{0,T} = K'_{0,0} + eT$	$K'_{0,0}$	5.39 ± 0.25
	e	0.0011 ± 0.001 K^{-1}

In a typical high-pressure experiment carried out on PEARL using the Paris-Edinburgh press, it is usual to obtain an uncertainty of ~ 0.05 % in the Pb unit-cell volume and ~ 0.3 % in temperature; the propagated error in the pressure is then approximately 3 %.

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Our previous application of the Pb equation of state is given in:

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SUPPLEMENTARY MATERIAL

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