Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting information for:

Atomic and electronic structure transformations in SnS_2 at high pressures: A joint single crystal X-ray diffraction and DFT study

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Table S1. Data collection strategy at ambient pressure (no DAC). Frame width = 1.0000°, exposure time = 5.0000 seconds.

Run #	*Type*	*Start (°)*	*End (°)*	*Theta (°)*	*Kappa (°)*	*Phi (°)*	*Frames*
1	Omega	-78.00	-6.00	-19.8195	130.0000	-67.0000	72
2	Omega	-96.00	-22.00	-19.8195	-77.0000	60.0000	74
3	Omega	-48.00	53.00	-19.8195	57.0000	-180.0000	101

Table S2. Data collection strategy at high pressure. Frame width = 0.3000°, exposure time = 30.0000 seconds.

Run #	*Type*	*Start (°)*	*End (°)*	*Theta (°)*	*Chi (°)*	*Phi (°)*	*Frames*
1	Omega	-10.000	20.000	-12.500	54.726	90.000	100
2	Omega	40.000	105.000	12.500	54.726	90.000	216
3	Omega	25.000	90.000	-12.500	-54.726	90.000	216
4	Omega	40.000	70.000	12.500	-54.726	90.000	100
5	Omega	-10.000	20.000	-12.500	54.726	270.000	100
6	Omega	40.000	105.000	12.500	54.726	270.000	216
7	Omega	25.000	90.000	-12.500	-54.726	270.000	216
8	Omega	40.000	70.000	12.500	-54.726	270.000	100
9	Omega	40.000	105.000	12.500	90.000	90.000	216
10	Omega	25.000	90.000	-12.500	-90.000	90.000	216
11	Omega	40.000	105.000	12.500	90.000	270.000	216
12	Omega	25.000	90.000	-12.500	-90.000	270.000	216

Table S3. Selected results from data collection and reduction

p (GPa)	*Completeness (%)*	*Redundancy*	*Max 2θ (°)*	*R(int)*
0.0001(0)	98.3	4.70	64.33	0.0649
0.664(9)	32.8	6.35	53.17	0.0241
1.109(11)	33.3	6.42	53.26	0.0277
1.991(16)	32.6	2.58	53.46	0.0200
3.40(3)	32.8	2.56	53.71	0.0169
4.22(3)	32.1	2.48	53.85	0.0202
6.29(5)	31.3	2.38	54.21	0.0234
8.08(6)	35.6	2.94	49.68	0.0207
9.78(8)	35.6	2.89	49.91	0.0178
11.88(9)	33.3	6.43	50.02	0.0230
13.68(19)	37.1	4.77	50.08	0.0228
14.8(2)	36.1	4.70	50.11	0.0204
16.8(4)	34.0	6.78	50.22	0.0255
20(1)	32.0	2.93	50.53	0.0257

Table S4. Selected results from refinement.

p (GPa)	*Extinction*	*Uiso(S)*	*Uiso(Sn)*	*R1*	*GOF*
0.0001(0)	1.25(10)	0.0110(4)	0.0117(4)	0.0236	1.142
0.664(9)	0.85(14)	0.0096(5)	0.0078(4)	0.0210	1.257
1.109(11)	0.86(14)	0.0095(5)	0.0076(4)	0.0218	1.149
1.991(16)	0.53(9)	0.0089(5)	0.0071(4)	0.0201	1.235
3.40(3)	0.27(4)	0.0091(5)	0.0074(4)	0.0198	1.223
4.22(3)	0.23(5)	0.0087(4)	0.0067(3)	0.0159	1.383
6.29(5)	0.19(6)	0.0080(5)	0.0066(4)	0.0165	1.174
8.08(6)	0.18(6)	0.0080(5)	0.0067(4)	0.0186	1.394
9.78(8)	0.17(10)	0.0077(6)	0.0060(5)	0.0180	1.549
11.88(9)	0.06(4)	0.0086(5)	0.0073(4)	0.0171	1.264
13.68(19)	-	0.0087(5)	0.0079(3)	0.0158	1.318
14.8(2)	-	0.0097(4)	0.0087(2)	0.0138	1.422
16.8(4)	-	0.0101(6)	0.0091(3)	0.0209	1.398
20(1)	-	0.0094(6)	0.0085(3)	0.0201	1.319

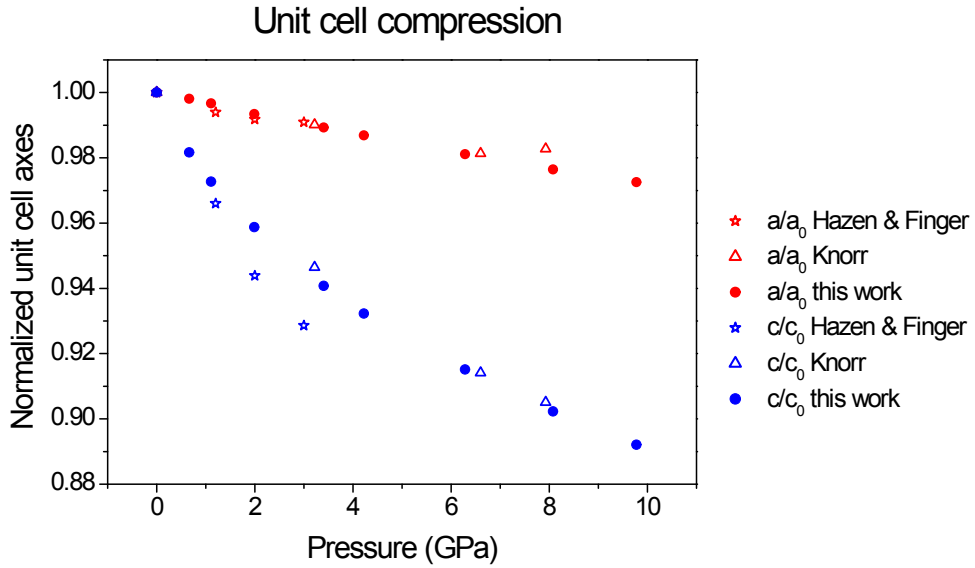

Fig. S1. Compression of unit cell axes of SnS_2 from 3 different studies (Hazen & Finger[1], Knorr *et al.*[2], and the present study). Data points for p > 10 GPa from the present study have been excluded to enable easy comparison.

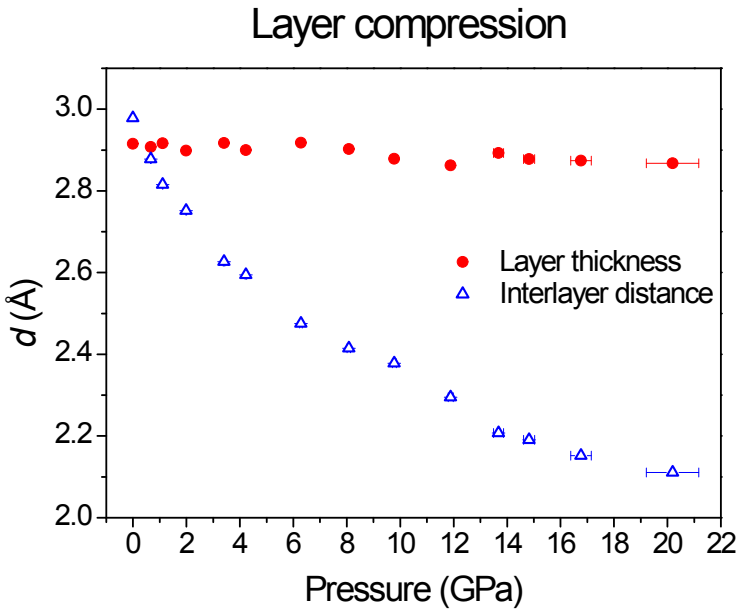

Fig. S2. Layer thickness and interlayer distance as a function of pressure. The layer thickness is defined as the distance parallel to *c* between two S-atoms on opposite sides of a S-Sn-S sandwich layer: *d*(layer) = *c* · 2z(S). In the same manner, the interlayer distance is the distance parallel to *c* between two S atoms from two consecutive layers: *d*(interlayer) = *c*(1 - 2z(S)).

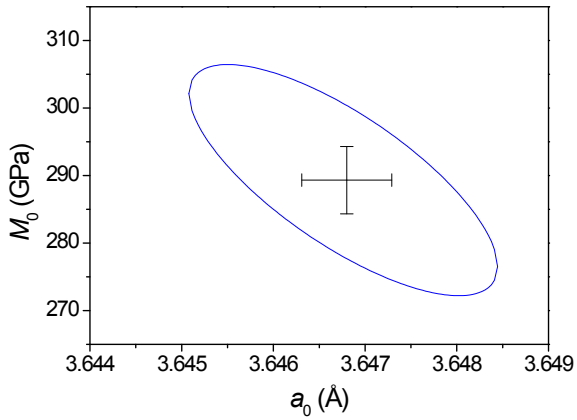

Fig. S3. Confidence ellipse for the correlation between a_0 and M_0 (3 sigma level). The crosshair indicates the fitted values and the independently determined uncertainties.

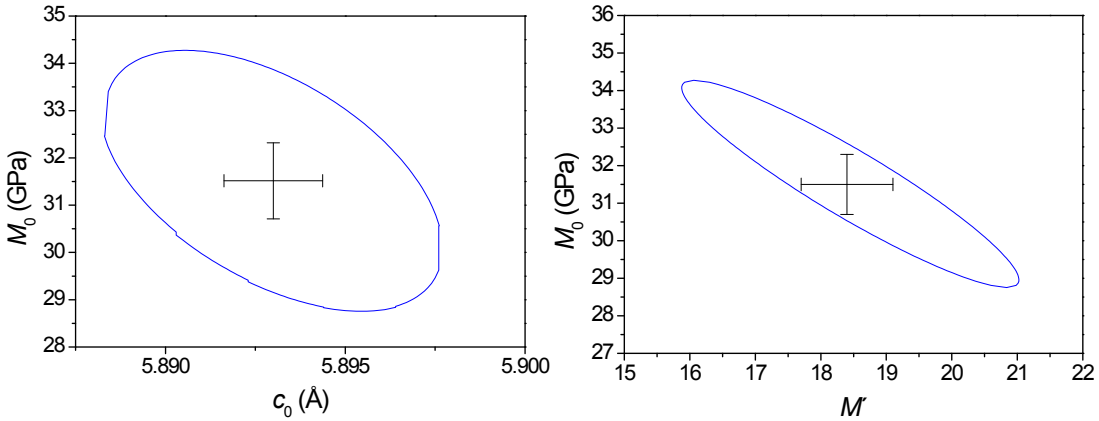

Fig. S4. Confidence ellipse for the correlation between c_0 and M_0 (left) and M_0 and M' (right) (3 sigma level). The crosshairs indicate the fitted values and the independently determined uncertainties.

Calculation of compressibilities:

$$\beta_{0T}(\parallel) = -\frac{1}{a_0}\left(\frac{\partial a}{\partial p}\right)_T = \frac{1}{\left(-a_0\left(\frac{\partial p}{\partial a}\right)_T\right)} = \frac{1}{M_{0T}(a)} \quad \text{(S1)}$$

$$\beta_{0T}(\perp) = -\frac{1}{c_0}\left(\frac{\partial c}{\partial p}\right)_T = \frac{1}{\left(-c_0\left(\frac{\partial p}{\partial c}\right)_T\right)} = \frac{1}{M_{0T}(c)} \quad \text{(S2)}$$

1. R. M. Hazen and L. W. Finger, *Am. Mineral.*, 1978, **63**, 289-292.
2. K. Knorr, L. Ehm, M. Hytha, B. Winkler and W. Depmeier, *Phys. Stat. Sol. B*, 2001, **223**, 435-440.