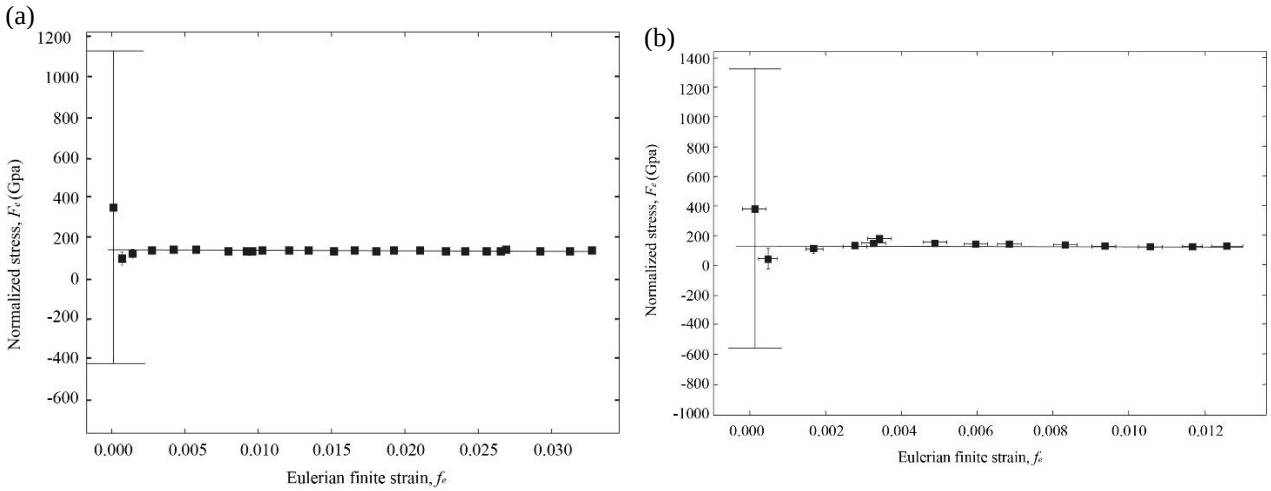

Fig. S1. Normalized pressure (F_e) vs. Eulerian finite strain (f_e) plot for a) Mg-sursassite synthetic single crystal and b) the natural sursassite sample. The solid lines are weighted linear fits to the data.

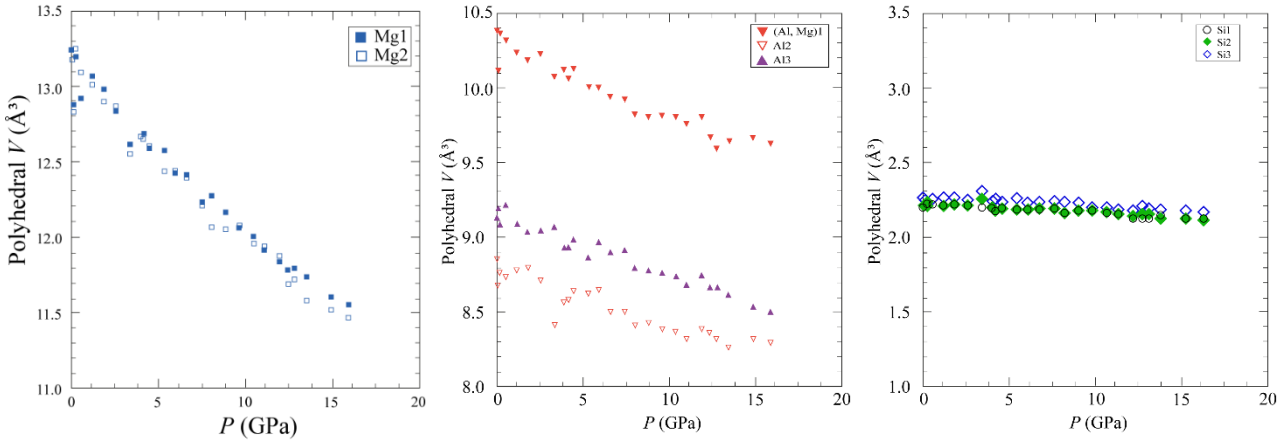

Fig. S2 Evolution with *P* of the polyhedral volume for the crystal sites in the structure. A fit of the data with BM-II EoS indicate a site compressibility of 93 GPa for Mg1 site; 86 GPa for Mg2 site; 174 GPa for (Al,Mg)1 site; 191 GPa for Al2 site; 187 GPa for Al3 site; 272 GPa for Si1 site; 247 GPa for Si2 site; 253 GPa for Si3 site.

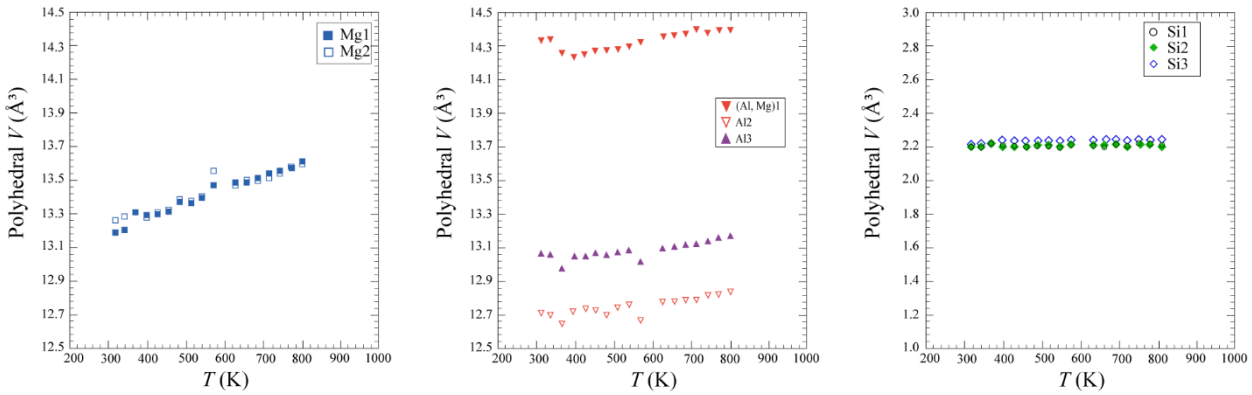

Fig. S3 Evolution with *T* of the polyhedral volume for the crystal sites in the structure.

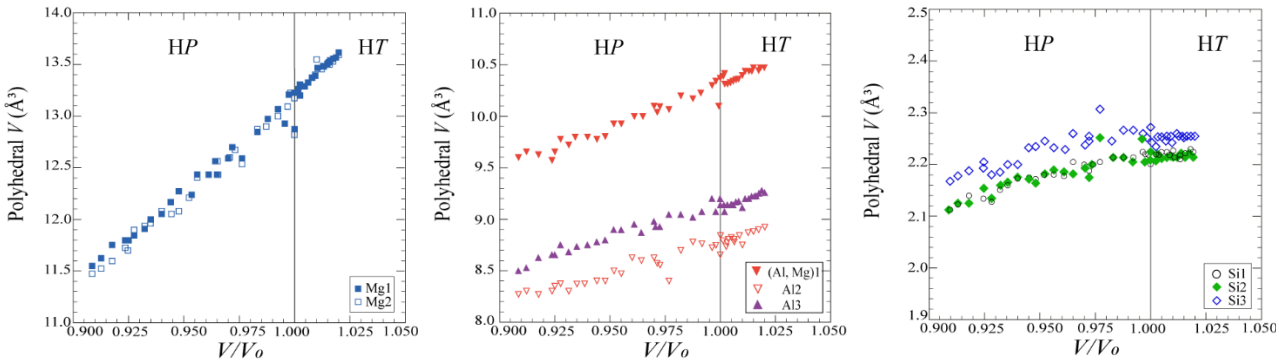

Fig S4. “Inverse relationship” of structural parameters as function of normalized volume.

Table S1. Atomic coordinates, site occupancies and equivalent displacement parameters (Å^2) of the Mg-sursassite studied in this work.

Site	*x*	*y*	*z*	Site occupancies	U_{eq}
T(1) (Si)	0.30725(13)	0.75	0.19530(12)	1	0.0047(4)
T(2) (Si)	0.29088(3)	0.75	0.80465(12)	1	0.0049(4)
T(3) (Si)	0.14574(13)	0.75	0.49096(12)	1	0.0067(4)
*M*g(1)	0.17797(17)	0.25	0.31541(16)	1	0.0098(5)
Mg(2)	0.27447(17)	0.25	0.66953(15)	1	0.0097(5)
M(1) (Al)	0.5	0	0.5	1	0.0129(5)
M(2) (Al)	0.5	0	0	1	0.0055(4)
M(3) (Al)	0	0.5	0	1	0.0055(4)
O(1)	0.2539(2)	0.5093(3)	0.4959(2)	1	0.0087(7)
O(2)	0.1905(2)	0.5198(3)	0.1712(2)	1	0.0065(7)
O(3)	0.3167(2)	0.5142(3)	0.8249(2)	1	0.0064(7)
O(4)	0.4063(3)	0.75	0.0745(3)	1	0.0063(9)
O(5)	0.4598(3)	0.75	0.3508(3)	1	0.0094(10)
O(6)	0.0874(3)	0.25	0.9270(3)	1	0.0069(10)
O(7)	0.4369(3)	0.25	0.3654(3)	1	0.0096(10)
O(8)	0.0747(3)	0.75	0.8975(3)	1	0.0060(9)
O(9)	0.0803(3)	0.75	0.6355(3)	1	0.0072(10)
O(10)	-0.0233(3)	0.75	0.3557(3)	1	0.0090(10)
O(11)	0.4072(3)	0.25	0.0701(3)	1	0.0072(10)

Table S2. Anisotropic displacement parameters (Å^2) of the Mg-sursassite studied in this work.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
T(1)	0.0048(5)	0.0050(6)	0.0045(6)	0	0.0016(4)	0
T(2)	0.0044(6)	0.0050(6)	0.0056(6)	0	0.0019(4)	0
T(3)	0.0083(6)	0.0052(6)	0.0076(6)	0	0.0040(5)	0
M(1) (Al)	0.0146(7)	0.0111(7)	0.0126(7)	-0.0012(5)	0.0039(6)	0.0013(5)
M(2) (Al)	0.0055(6)	0.0046(6)	0.0064(7)	-0.0003(5)	0.0021(5)	-0.0009(4)
M(3) (Al)	0.0059(6)	0.0043(6)	0.0062(7)	0.0000(5)	0.0019(5)	0.0001(4)
Mg(1)	0.0113(7)	0.0088(8)	0.0090(8)	0	0.0028(6)	0
Mg(2)	0.0139(8)	0.0066(7)	0.0077(8)	0	0.0021(6)	0
O(1)	0.0105(11)	0.0075(11)	0.0086(12)	0.0013(8)	0.0040(9)	0.0025(7)
O(2)	0.0063(10)	0.0052(10)	0.0068(11)	0.0008(8)	0.0006(9)	-0.0003(7)
O(3)	0.0071(10)	0.0054(10)	0.0064(11)	-0.0009(8)	0.0016(9)	0.0015(7)
O(4)	0.0050(14)	0.0066(15)	0.0076(15)	0	0.0025(12)	0
O(5)	0.0070(14)	0.0145(16)	0.0061(15)	0	0.0013(12)	0
O(6)	0.0063(14)	0.0066(15)	0.0091(15)	0	0.0044(12)	0
O(7)	0.0074(14)	0.0120(16)	0.0082(15)	0	0.0006(12)	0
O(8)	0.0069(14)	0.0049(14)	0.0075(15)	0	0.0040(12)	0
O(9)	0.0071(14)	0.0095(15)	0.0059(15)	0	0.0032(12)	0
O(10)	0.0075(15)	0.0096(16)	0.0093(16)	0	0.0017(12)	0
O(11)	0.0084(14)	0.0045(14)	0.0103(16)	0	0.0051(12)	0

Table S3. Interatomic distances (Å) selected from the structural refinement of the Mg-sursassite studied in this work.

T(1)-O(2) (×2)	1.6215(19)
-O(4)	1.641(4)
-O(5)	1.648(3)
<*T*(1)-O>	1.6332
T(2)-O(3) (x2)	1.6154(19)
-O(8)	1.649(4)
-O(9)	1.651(3)
<*T*(2)-O>	1.6327
T(3)-O(1) (x2)	1.6480(19)
-O(9)	1.657(4)
-O(10)	1.613(3)
<*T*(3)-O>	1.6415
M(1)-O(1) (×2)	2.0896(19)
-O(5) (×2)	1.979(2)
-O(7) (×2)	1.8905(18)
<*M*(1)-O>	1.9864
M(2)-O(3) (×2)	1.9094(16)
-O(4) (×2)	1.886(3)
-O(11) (×2)	1.860(3)
<*M*(2)-O>	1.8850
M(3)-O(2) (×2)	1.9224(16)
-O(6) (×2)	1.850(3)
-O(8) (×2)	1.954(3)
<*M*(3)-O>	1.9087
Mg(1)-O(1) (×2)	2.221(3)
-O(2) (×2)	2.101(3)
-O(7)	2.109(3)
-O(9)	2.397(4)
<*Mg*(1)-O>	2.1917
Mg(2)-O(1) (×2)	2.201(3)
-O(3) (×2)	2.077(3)
-O(5) (×2)	2.338(4)
-O(10) (×2)	2.081(4)
<*Mg*(2)-O>	2.1622

Table S4. Lattice parameters of natural sursassite at different pressures, collected using a 4:1 methanol:ethanol mixture as *P*-transmitting medium (*P*-uncertainty: ±0.05 GPa).

P (GPa)	*a* (Å)	*b* (Å)	*c* (Å)	*β* (°)	*V* (Å^3)
0.15	8.749(7)	5.7981(4)	9.7910(18)	109.00(5)	469.6(4)
0.56	8.713(6)	5.7971(3)	9.7845(17)	108.96(4)	467.4(3)
1.10	8.713(7)	5.7880(4)	9.7657(19)	108.90(5)	465.9(4)
1.48	8.708(6)	5.7861(4)	9.7600(17)	108.91(5)	465.2(4)
1.87	8.727(7)	5.7782(4)	9.748(2)	108.92(5)	465.0(4)
2.29	8.707(6)	5.7730(4)	9.7324(18)	108.82(5)	463.1(4)
2.60	8.676(7)	5.7744(4)	9.7328(18)	108.85(5)	461.5(4)
2.97	8.676(7)	5.7670(4)	9.7191(18)	108.82(5)	460.3(4)
3.50	8.650(7)	5.7639(4)	9.7100(18)	108.78(5)	458.4(4)
3.83	8.646(7)	5.7562(4)	9.6953(18)	108.75(5)	456.9(4)
4.24	8.617(7)	5.7559(4)	9.6943(18)	108.76(5)	455.3(4)
4.72	8.620(6)	5.7462(3)	9.6739(17)	108.72(4)	453.8(3)
5.27	8.592(9)	5.7467(4)	9.676(3)	108.68(7)	452.6(5)
5.63	8.596(10)	5.7413(4)	9.666(3)	108.59(8)	452.2(6)