

Supplementary

Table S1a. Structur refinement details for OEn at ambient conditions.

	R626	R638	Mg#100 OEn R545	R598	R623
Chemical formula	Mg _{0.958} (Si _{1.019} Al _{0.007})O ₃	Mg _{0.966} (Si _{1.016} Al _{0.005})O ₃	Mg _{0.990} (Si _{1.005} Al _{0.005})O ₃	Mg _{0.940} (Si _{0.956} Al _{0.005})O ₃	Mg _{0.935} (Si _{0.974} Al _{0.001})O ₃
crystal size (mm ³)	0.30 × 0.12 × 0.12	0.12 × 0.06 × 0.07	0.10 × 0.04 × 0.03	0.20 × 0.09 × 0.08	0.60 × 0.30 × 0.25
Space group	Orthorhombic, <i>Pbca</i>	Orthorhombic, <i>Pbca</i>	Orthorhombic, <i>Pbca</i>	Orthorhombic, <i>Pbca</i>	Orthorhombic, <i>Pbca</i>
<i>a</i> (Å)	18.2218(4)	18.2181(4)	18.2201(3)	18.2235(3)	18.2182(10)
<i>b</i> (Å)	8.8107(2)	8.8100(2)	8.8111(2)	8.81060(10)	8.8140(4)
<i>c</i> (Å)	5.17640(10)	5.17660(10)	5.17500(10)	5.17730(10)	5.1753(2)
<i>V</i> (Å ³)	831.05(3)	830.85(3)	830.79(3)	831.27(2)	831.02(7)
<i>Q</i> _{calcd} (g cm ⁻³)	3.210	3.211	3.211	3.209	3.210
<i>Z</i>	8	8	8	8	8
<i>T</i> (K)	293	293	293	293	293
absorption coe.	0.568	0.568	0.568	0.567	0.568
Range of <i>hkl</i>	-19 ≤ <i>h</i> ≤ 30	-30 ≤ <i>h</i> ≤ 30	-24 ≤ <i>h</i> ≤ 26	-30 ≤ <i>h</i> ≤ 30	-18 ≤ <i>h</i> ≤ 30
	-14 ≤ <i>k</i> ≤ 14	-14 ≤ <i>k</i> ≤ 14	-12 ≤ <i>k</i> ≤ 12	-14 ≤ <i>k</i> ≤ 14	-14 ≤ <i>k</i> ≤ 14
	-8 ≤ <i>l</i> ≤ 8	-8 ≤ <i>l</i> ≤ 8	-7 ≤ <i>l</i> ≤ 7	-8 ≤ <i>l</i> ≤ 8	-8 ≤ <i>l</i> ≤ 8
Total refls.	7602	22791	15583	15508	7360
Unique refls.	2010	2014	1270	2006	2007
Observed refl.	1459	1636	1075	1864	1871
<i>F</i> _o > 2(<i>F</i> _o)					
<i>R</i> _{int}	0.0573	0.0398	0.0294	0.0204	0.0247
<i>R</i> ₁ ^a	0.0331	0.0264	0.0214	0.0186	0.0229
<i>wR</i> ₂ ^b	0.0911	0.0743	0.0583	0.0512	0.0613
Goodness-of-fit	1.079	1.152	1.052	1.065	1.106
Refined parameters	93	93	95	95	95
restraints	0	0	0	0	0

$$^a R_1 = (\sum ||F_o| - |F_c||) / \sum |F_o|. \quad ^b wR_2 = \{\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]\}^{1/2}.$$

Table S1b. Structur refinement details for OEn at ambient conditions.

Al-bearing OEn	
R624	R608
$\text{Mg}_{0.925}(\text{Si}_{0.967}\text{Al}_{0.037})\text{O}_3$	$\text{Mg}_{0.933}(\text{Si}_{0.962}\text{Al}_{0.031})\text{O}_3$
$0.18 \times 0.10 \times 0.09$	$0.22 \times 0.12 \times 0.10$
Orthorhombic, <i>Pbca</i>	Orthorhombic, <i>Pbca</i>
18.2128(4)	18.2139(4)
8.7902(2)	8.7995(2)
5.17460(10)	5.17410(10)
828.43(3)	829.27(3)
3.274	3.271
8	8
293	293
0.583	0.583
$-33 \leq h \leq 35$	$-20 \leq h \leq 30$
$-11 \leq k \leq 17$	$-14 \leq k \leq 14$
$-10 \leq l \leq 10$	$-8 \leq l \leq 8$
10,308	7643
2824	2004
2049	1711
0.0573	0.0300
0.0341	0.0235
0.0833	0.0603
1.043	1.095
96	96
3	3

Table S2. Atomic coordinates, occupancy, and displacement parameters for OEn at ambient conditions.

		Mg#100 OEn				Al-bearing OEn		
		R626	R638	R545	R598	R623	R624	R608
Mg1	<i>x</i>	0.37687(4)	0.37686(3)	0.37685(3)	0.37694(2)	0.37682(2)	0.37755(2)	0.37726(2)
	<i>y</i>	0.51339(7)	0.51328(6)	0.48684(6)	0.51362(3)	0.51310(3)	0.51416(5)	0.51376(4)
	<i>z</i>	0.35884(12)	0.35897(10)	0.35860(10)	0.35880(5)	0.35868(5)	0.35626(8)	0.35701(7)
	<i>U</i> _{iso}	0.00742(17)	0.00740(13)	0.00683(17)	0.00691(8)	0.00603(8)	0.00704(10)	0.00694(10)
	occupancy	0.964(3)	0.969(3)	0.953(3)	0.978(2)	0.959(2)	0.947(2)	0.956(2)
Mg2	<i>x</i>	0.37584(3)	0.37584(3)	0.37584(3)	0.37581(2)	0.37584(2)	0.37594(2)	0.37593(2)
	<i>y</i>	0.65405(7)	0.65398(5)	0.65396(5)	0.65390(3)	0.65389(3)	0.65392(5)	0.65388(4)
	<i>z</i>	0.86593(12)	0.86519(9)	0.86574(10)	0.86579(5)	0.86582(5)	0.86404(8)	0.86445(7)
	<i>U</i> _{iso}	0.00571(16)	0.00557(12)	0.00547(16)	0.00496(8)	0.00462(8)	0.00526(10)	0.00517(10)
	occupancy	0.975(3)	0.978(3)	0.960(3)	0.973(2)	0.966(2)	0.964(2)	0.964(2)
SiA (TA)	<i>x</i>	0.27166(2)	0.27168(2)	0.27168(2)	0.27160(2)	0.27169(2)	0.27154(2)	0.27159(2)
	<i>y</i>	0.34145(5)	0.34142(4)	0.34155(4)	0.34161(2)	0.34156(2)	0.34170(3)	0.34171(3)
	<i>z</i>	0.05020(9)	0.94989(7)	0.04999(7)	0.04978(4)	0.05026(4)	0.04854(6)	0.04903(5)
	<i>U</i> _{iso}	0.00525(10)	0.00500(8)	0.00395(14)	0.00373(6)	0.00323(7)	0.00431(8)	0.00394(8)
	occupancy	0.975(3)	0.979(3)	0.954(3)	0.973(2)	0.965(2)	0.963(2)	0.963(2)
SiB (TB)	<i>x</i>	0.47366(2)	0.47366(2)	0.47355(2)	0.47363(2)	0.47357(2)	0.47345(2)	0.47343(2)
	<i>y</i>	0.33739(5)	0.33740(4)	0.33734(4)	0.66263(2)	0.33734(2)	0.66279(3)	0.66275(3)
	<i>z</i>	0.20161(9)	0.20159(7)	0.79841(8)	0.79855(4)	0.79834(4)	0.80078(6)	0.80011(5)
	<i>U</i> _{iso}	0.00491(10)	0.00493(8)	0.00373(13)	0.00372(6)	0.00319(7)	0.00450(8)	0.00390(8)
	occupancy	0.971(3)	0.977(3)	0.951(3)	0.971(2)	0.965(2)	0.930(7)	0.894(9)
AlB	<i>x</i>						0.47345(2)	0.47343(2)
	<i>y</i>						0.66279(3)	0.66275(3)
	<i>z</i>						0.80078(6)	0.80011(5)
	<i>U</i> _{iso}						0.00450(8)	0.00390(8)
	occupancy						0.033(7)	0.067(10)
O1A	<i>x</i>	0.18336(7)	0.18338(5)	0.18346(5)	0.18336(3)	0.18341(3)	0.18312(4)	0.18327(4)
	<i>y</i>	0.33992(14)	0.34001(11)	0.34023(11)	0.34011(6)	0.34014(6)	0.34005(9)	0.34011(8)
	<i>z</i>	0.0356(2)	0.03524(18)	0.03459(19)	0.03455(10)	0.03463(10)	0.03372(15)	0.03377(14)
	<i>U</i> _{iso}	0.0061(2)	0.00612(15)	0.0072(2)	0.00613(10)	0.00574(10)	0.00708(14)	0.00694(14)
O2A	<i>x</i>	0.31094(7)	0.31101(5)	0.31099(5)	0.31091(3)	0.31096(3)	0.31090(4)	0.31099(4)
	<i>y</i>	0.50241(14)	0.50238(11)	0.50230(11)	0.49756(6)	0.50242(6)	0.49692(9)	0.49715(8)
	<i>z</i>	0.04310(2)	0.04344(19)	0.04352(19)	0.04312(10)	0.04343(10)	0.04178(16)	0.04216(14)
	<i>U</i> _{iso}	0.00800(2)	0.00776(16)	0.0087(2)	0.00717(10)	0.00687(10)	0.00844(14)	0.00790(13)

O3A	<i>x</i>	0.30311(7)	0.30311(5)	0.30311(5)	0.30312(3)	0.30319(3)	0.30298(4)	0.30304(4)
	<i>y</i>	0.22273(14)	0.22267(11)	0.22250(11)	0.22290(6)	0.22264(6)	0.77714(10)	0.77718(8)
	<i>z</i>	0.8315(2)	0.83143(19)	0.83176(19)	0.83081(10)	0.83158(10)	0.82963(16)	0.83013(13)
	<i>U</i> _{iso}	0.0078(2)	0.00789(16)	0.0087(2)	0.00730(10)	0.00685(10)	0.00825(15)	0.00787(14)
O1B	<i>x</i>	0.56252(7)	0.56253(5)	0.56240(6)	0.56247(3)	0.56242(3)	0.56270(4)	0.56257(4)
	<i>y</i>	0.34022(14)	0.34017(10)	0.34039(10)	0.34020(6)	0.34033(6)	0.66039(9)	0.66010(8)
	<i>z</i>	0.80000(20)	0.80018(18)	0.80021(19)	0.80061(10)	0.80022(10)	0.80272(15)	0.80201(14)
	<i>U</i> _{iso}	0.00620(20)	0.00622(15)	0.0070(2)	0.00630(10)	0.00593(10)	0.00728(14)	0.00706(14)
O2B	<i>x</i>	0.43281(7)	0.43289(5)	0.43275(6)	0.43283(3)	0.43278(3)	0.43275(5)	0.43275(4)
	<i>y</i>	0.48321(14)	0.51650(11)	0.48308(11)	0.51673(6)	0.48311(6)	0.51615(9)	0.51654(8)
	<i>z</i>	0.6898(2)	0.68953(19)	0.68887(19)	0.68928(10)	0.68895(10)	0.68850(16)	0.68852(13)
	<i>U</i> _{iso}	0.00770(20)	0.00754(16)	0.0083(2)	0.00757(10)	0.00699(10)	0.00849(14)	0.00816(14)
O3B	<i>x</i>	0.44747(7)	0.44757(5)	0.44753(6)	0.44753(3)	0.44757(3)	0.44722(5)	0.44736(4)
	<i>y</i>	0.30449(14)	0.30460(11)	0.19500(12)	0.30475(6)	0.30492(6)	0.30634(9)	0.30584(8)
	<i>z</i>	1.10360(20)	1.10336(18)	0.60388(19)	1.10380(10)	1.10371(10)	1.10720(15)	1.10597(13)
	<i>U</i> _{iso}	0.00780(20)	0.00781(16)	0.0086(2)	0.00705(10)	0.00649(10)	0.00839(15)	0.00818(14)

Table S3a. The Si-O bond distances (Å) and tetrahedral volume (Å³) of OEn.

Mg#100 OEn					Al-bearing OEn (low-Al)		Mg#100 OEn	Al-bearing OEn (high-Al)
Hydrous					Hydrous		Anhydrous	Hydrous
	R626	R638	R545	R598	R623	R624	R608	[37]
								[23]
Si1-O2A	1.5890(13)	1.5892(10)	1.5875(11)	1.5881(6)	1.5886(6)	1.5897(9)	1.5896(8)	1.5860
Si1-O1A	1.6109(13)	1.6106(10)	1.6095(11)	1.6101(6)	1.6099(6)	1.6123(8)	1.6107(8)	1.6145(19)
Si1-O3A	1.6445(13)	1.6443(10)	1.6443(11)	1.6459(5)	1.6456(5)	1.6438(8)	1.6449(7)	1.6400(18)
Si1-O3A	1.6638(13)	1.6636(10)	1.6651(11)	1.6643(5)	1.6640(6)	1.6630(8)	1.6631(7)	1.6642(18)
<i>V</i> _{SiA(TA)}	2.180	2.179	2.177	2.179	2.179	2.180(8)	2.179	2.176
Si2-O2B	1.5877(13)	1.5894(10)	1.5884(11)	1.5892(5)	1.5884(6)	1.5964(9)	1.5930(8)	1.6076(19)
Si2-O1B	1.6195(13)	1.6192(10)	1.6192(11)	1.6191(6)	1.6185(6)	1.6257(9)	1.6238(8)	1.6459(20)
Si2-O3B	1.6754(13)	1.6737(10)	1.6748(11)	1.6752(5)	1.6743(6)	1.6781(9)	1.6752(8)	1.6885(19)
Si2-O3B	1.6756(13)	1.6764(10)	1.6766(11)	1.6765(5)	1.6766(6)	1.6804(9)	1.6793(8)	1.6851(19)
<i>V</i> _{SiB(TB)}	2.246	2.247	2.247	2.248	2.246	2.269	2.259	2.238

Table S3b. The M-O bond distances (Å) and octahedral volume (Å³) of OEn.

	Mg#100 OEn				Al-Bearing OEn (low-Al)			Mg#100 OEn	Al-Bearing OEn (high-Al)
	Hydrous				Hydrous			Anhydrous	Hydrous
	R626	R638	R545	R598	R623	R624	R608	[37]	[23]
M1-O2A	2.0061(14)	2.0057(11)	2.0071(11)	2.0056(6)	2.0060(6)	2.0019(9)	2.0027(8)	2.0070	1.9867(20)
M1-O1A	2.0225(13)	2.0240(11)	2.0265(11)	2.0264(6)	2.0260(6)	2.0203(9)	2.0230(8)	2.02	2.0090(20)
M1-O2B	2.0432(13)	2.0420(11)	2.0444(11)	2.0433(6)	2.0445(6)	2.0324(9)	2.0367(8)	2.049	2.0045(19)
M1-O1B	2.0627(14)	2.0619(11)	2.0632(11)	2.0618(6)	2.0625(6)	2.0556(9)	2.0582(8)	2.063	2.0346(20)
M1-O1A	2.1487(13)	2.1490(10)	2.1505(11)	2.1488(6)	2.1500(6)	2.1459(9)	2.1484(8)	2.146	2.1333(20)
M1-O1B	2.1655(13)	2.1659(10)	2.1685(11)	2.1683(6)	2.1686(6)	2.1582(9)	2.1624(8)	2.162	2.1334(19)
V_{M1}	11.769	11.768	11.801	11.784	11.792	11.669	11.719	11.756	11.352
M2-O2B	1.9936(14)	1.9927(11)	1.9899(11)	1.9914(6)	1.9901(6)	1.9917(9)	1.9910(8)	1.9860	1.9981(20)
M2-O2A	2.0333(14)	2.0312(11)	2.0290(11)	2.0345(6)	2.0296(6)	2.0359(9)	2.0328(8)	2.032	2.0566(19)
M2-O1B	2.0552(13)	2.0553(11)	2.0537(11)	2.0579(6)	2.0542(6)	2.0530(9)	2.0539(8)	2.057	2.0563(19)
M2-O1A	2.0923(14)	2.0897(11)	2.0877(11)	2.0910(6)	2.0875(6)	2.0992(9)	2.0944(8)	2.096	2.1279(20)
M2-O3A	2.2865(14)	2.2866(11)	2.2861(11)	2.2870(6)	2.2868(6)	2.2867(9)	2.2871(8)	2.297	2.2846(20)
M2-O3B	2.4445(14)	2.4464(11)	2.4420(11)	2.4411(6)	2.4441(6)	2.4002(9)	2.4160(8)	2.45	2.3139(20)
V_{M2}	12.450	12.437	12.408	12.439	12.416	12.345	12.371	12.472	12.254

Table S4a. Unit cell parameters of Mg#100 OEn (R598) under high pressure.

P(GPa)	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)	<i>V</i> (Å ³)
0	18.2235(3)	8.8106(1)	5.1773(1)	831.26(2)
1.34	18.166(1)	8.7657(10)	5.159(3)	821.50(12)
4.12	18.071(2)	8.6891(14)	5.1243(3)	804.61(10)
6.32	17.996(2)	8.6323(15)	5.0994(3)	792.19(9)
8.45	17.931(2)	8.5837(14)	5.0785(3)	781.66(9)
10.37	17.877(2)	8.5412(14)	5.0600(4)	772.63(10)
11.66	17.855(3)	8.5187(25)	5.0556(6)	768.95(17)
13.22	17.871(6)	8.502(5)	5.0355(13)	765.08(34)

Table S4b. Structure refinement details for the Al-bearing enstatite (R608) under high pressure.

P(GPa)	0.00010	1.72	4.56	7.07	8.45	10.00
<i>a</i> (Å)	18.2139(4)	18.114(5)	18.014(4)	17.930(4)	17.915(10)	17.859(6)
<i>b</i> (Å)	8.7995(2)	8.7530(36)	8.6694(25)	8.6106(28)	8.5733(33)	8.5484(19)
<i>c</i> (Å)	5.1741(10)	5.1562(8)	5.1180(6)	5.0905(7)	5.0771(11)	5.0632(7)
<i>V</i> (Å ³)	829.28(3)	817.50(26)	799.29(18)	785.90(20)	779.80(36)	772.98(40)
Range of <i>hkl</i>	-20 ≤ <i>h</i> ≤ 30	-19 ≤ <i>h</i> ≤ 19	-19 ≤ <i>h</i> ≤ 19	-19 ≤ <i>h</i> ≤ 19	-19 ≤ <i>h</i> ≤ 19	-19 ≤ <i>h</i> ≤ 19
	-14 ≤ <i>k</i> ≤ 14	-8 ≤ <i>k</i> ≤ 8	-8 ≤ <i>k</i> ≤ 8	-8 ≤ <i>k</i> ≤ 8	-8 ≤ <i>k</i> ≤ 8	-8 ≤ <i>k</i> ≤ 8
	-8 ≤ <i>l</i> ≤ 8	-4 ≤ <i>l</i> ≤ 4	-4 ≤ <i>l</i> ≤ 4	-4 ≤ <i>l</i> ≤ 4	-4 ≤ <i>l</i> ≤ 4	-4 ≤ <i>l</i> ≤ 4
Unique refl.	2004	318	306	515	597	643
Observed refl. <i>F</i> _o > 2σ (<i>F</i> _o)	1711	198	206	342	404	301
2θ _{max} (°)	55.68	42.52	42.62	47.04	53.90	42.60
<i>R</i> _{int}	0.030	0.089	0.064	0.092	0.089	0.103
<i>R</i> ₁	0.024	0.061	0.056	0.068	0.073	0.106
<i>wR</i> ₂	0.060	0.123	0.118	0.131	0.180	0.264
GooF	1.093	1.078	1.055	1.127	1.083	1.131
Refined parameters	96	46	46	46	46	46
	3	3	3	3	3	3

Table S5. Structural refinement details of Al-bearing OEn (R608) at high pressure.

Radiation type	AgK α				
Pressure (GPa)	1.72				
Temperature (K)	298				
Composition	Mg _{1.865} Al _{0.061} Si _{1.924} O ₆				
Space group	orthorhombic, <i>Pbca</i>				
Lattice parameters	$a = 18.114(5)$, $b = 8.753(4)$, $c = 5.1562(8)$				
	$\alpha = \beta = \gamma = 90^\circ$				
Volume (Å ³)	817.5(5)				
Z	8				
ρ_{calcd} (g cm ⁻³)	3.318				
Range of hkl	$-19 \leq h \leq 19$, $-8 \leq k \leq 8$, $-4 \leq l \leq 4$				
μ (mm ⁻¹)	0.591				
Total reflections	1646				
Unique reflections	318				
R_{int}	0.1192				
R_1	0.0637				
wR ₂	0.1426				
Goodness-of-fit	1.032				
Refined parameters	46				
restraints	3				
Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}	occupancy
SiA	0.2710(2)	0.3417(6)	0.0462(9)	0.0074(15)	0.968(17)
SiB	0.4727(2)	0.3372(6)	0.8015(10)	0.0099(15)	0.944(17)
AlB	0.4727(2)	0.3372(6)	0.8015(10)	0.0099(15)	0.058(10)
Mg(M1)	0.3761(3)	0.6563(7)	0.8615(11)	0.0060(17)	0.933(15)
Mg(M2)	0.3778(3)	0.4851(7)	0.3548(12)	0.0084(17)	0.939(15)
O1A	0.1835(5)	0.3404(13)	0.0310(20)	0.008(2)	1
O2A	0.3105(6)	0.5028(13)	0.0410(20)	0.011(3)	1
O3A	0.3034(5)	0.2233(12)	0.8250(20)	0.008(2)	1
O1B	0.5631(5)	0.3389(12)	0.8040(20)	0.009(2)	1
O2B	0.4326(5)	0.4844(13)	0.6910(20)	0.011(3)	1
O3B	0.4477(6)	0.1944(14)	0.6140(20)	0.017(3)	1

Radiation type	AgK α				
Pressure (GPa)	4.56				
Temperature (K)	298				
Composition	Mg _{1.865} Al _{0.061} Si _{1.924} O ₆				
Space group	orthorhombic, <i>Pbca</i>				
Lattice parameters	$a = 18.018(3)$, $b = 8.6654(18)$, $c = 5.1169(5)$				
	$\alpha = \beta = \gamma = 90^\circ$				
Volume (Å ³)	798.9(2)				
Z	8				
ρ_{calcd} (g cm ⁻³)	3.395				
Range of hkl	$-19 \leq h \leq 19$, $-8 \leq k \leq 8$, $-4 \leq l \leq 4$				
μ (mm ⁻¹)	0.605				
Total reflections	1628				
Unique reflections	307				
R_{int}	0.1020				
R_1	0.0576				
wR ₂	0.1224				
Goodness-of-fit	1.077				
Refined parameters	46				
restraints	3				
Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}	occupancy
SiA	0.2711(2)	0.3416(5)	0.0414(7)	0.0087(13)	0.989(15)
SiB	0.4726(2)	0.3370(5)	0.8038(8)	0.0076(13)	0.921(16)
AlB	0.4726(2)	0.3370(5)	0.8038(8)	0.0076(13)	0.056(10)
Mg(M1)	0.3763(2)	0.6574(6)	0.8586(10)	0.0047(15)	0.930(13)
Mg(M2)	0.3779(2)	0.4833(6)	0.3508(9)	0.0063(15)	0.940(13)
O1A	0.1831(5)	0.3390(12)	0.0242(18)	0.010(2)	1
O2A	0.3103(5)	0.5062(12)	0.0368(17)	0.009(2)	1
O3A	0.3040(5)	0.2227(11)	0.8241(17)	0.007(2)	1
O1B	0.5623(5)	0.3379(11)	0.8081(18)	0.006(2)	1
O2B	0.4331(5)	0.4843(11)	0.6874(19)	0.010(2)	1
O3B	0.4459(5)	0.1911(11)	0.6136(19)	0.008(2)	1

Radiation type	AgK α				
Pressure (GPa)	7.07				
Temperature (K)	298				
Composition	Mg _{1.865} Al _{0.061} Si _{1.924} O ₆				
Space group	orthorhombic, <i>Pbca</i>				
Lattice parameters	<i>a</i> = 17.9353(8), <i>b</i> = 8.610(3), <i>c</i> = 5.094(5)				
	$\alpha = \beta = \gamma = 90^\circ$				
Volume (Å ³)	786.6(7)				
Z	8				
ρ_{calcd} (g cm ⁻³)	3.448				
Range of hkl	-19 ≤ <i>h</i> ≤ 19, -8 ≤ <i>k</i> ≤ 8, -4 ≤ <i>l</i> ≤ 4				
μ (mm ⁻¹)	0.614				
Total reflections	1721				
Unique reflections	342				
<i>R</i> _{int}	0.1320				
<i>R</i> ₁	0.0698				
w <i>R</i> ₂	0.1437				
Goodness-of-fit	1.117				
Refined parameters	46				
restraints	3				
Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}	occupancy
SiA	0.2711(2)	0.3428(6)	0.0411(9)	0.0029(14)	1
SiB	0.4729(2)	0.3378(7)	0.8038(9)	0.0102(14)	0.90(2)
AlB	0.4729(2)	0.3378(7)	0.8038(9)	0.0102(14)	0.061(11)
Mg(M1)	0.3763(3)	0.6579(8)	0.8574(11)	0.0036(16)	1
Mg(M2)	0.3782(3)	0.4822(8)	0.3508(11)	0.0063(18)	1
O1A	0.1820(6)	0.3411(15)	0.021(2)	0.009(3)	1
O2A	0.3105(6)	0.5094(15)	0.034(2)	0.009(3)	1
O3A	0.3031(6)	0.2204(13)	0.824(2)	0.007(2)	1
O1B	0.5618(5)	0.3401(15)	0.808(2)	0.005(2)	1
O2B	0.4342(6)	0.4870(15)	0.681(2)	0.012(3)	1
O3B	0.4462(6)	0.1911(14)	0.617(2)	0.007(3)	1

Radiation type	AgK α				
Pressure (GPa)	8.45				
Temperature (K)	298				
Composition	Mg _{1.865} Al _{0.061} Si _{1.924} O ₆				
Space group	orthorhombic, <i>Pbca</i>				
Lattice parameters	$a = 17.941(11)$, $b = 8.561(4)$, $c = 5.0771(14)$				
	$\alpha = \beta = \gamma = 90^\circ$				
Volume (Å ³)	779.8(6)				
Z	8				
ρ_{calcd} (g cm ⁻³)	3.478				
Range of hkl	$-19 \leq h \leq 19$, $-8 \leq k \leq 8$, $-4 \leq l \leq 4$				
μ (mm ⁻¹)	0.620				
Total reflections	1843				
Unique reflections	404				
R_{int}	0.1547				
R ₁	0.0758				
wR ₂	0.1850				
Goodness-of-fit	1.077				
Refined parameters	46				
restraints	3				
Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}	<i>occupancy</i>
SiA	0.2710(3)	0.3432(5)	0.0381(9)	0.0098(14)	0.991(16)
SiB	0.4729(3)	0.3389(5)	0.8071(9)	0.0076(14)	0.923(17)
AlB	0.4729(3)	0.3389(5)	0.8071(9)	0.0076(14)	0.061(10)
Mg(M1)	0.3764(3)	0.6573(6)	0.8539(11)	0.0032(15)	0.904(16)
Mg(M2)	0.3778(4)	0.4820(6)	0.3472(11)	0.0107(17)	0.965(17)
O1A	0.1818(7)	0.3391(12)	0.024(2)	0.011(2)	1
O2A	0.3077(7)	0.5114(11)	0.031(2)	0.007(2)	1
O3A	0.3041(7)	0.2233(12)	0.820(2)	0.013(3)	1
O1B	0.5624(7)	0.3376(11)	0.811(2)	0.008(2)	1
O2B	0.4340(8)	0.4850(12)	0.685(2)	0.017(3)	1
O3B	0.4446(7)	0.1878(11)	0.611(2)	0.009(2)	1

Radiation type	AgK α
Pressure (GPa)	10
Temperature (K)	298
Composition	Mg _{1.865} Al _{0.061} Si _{1.924} O ₆
Space group	orthorhombic, <i>Pbca</i>
Lattice parameters	$a = 17.859(6)$, $b = 8.5484(19)$, $c = 5.0632(7)$ $\alpha = \beta = \gamma = 90^\circ$
Volume (Å ³)	773.0(3)
Z	8
ρ_{calcd} (g cm ⁻³)	3.509
Range of hkl	$-19 \leq h \leq 19$, $-8 \leq k \leq 8$, $-4 \leq l \leq 4$
μ (mm ⁻¹)	0.625
Total reflections	1450
Unique reflections	301
R_{int}	0.1558
R_1	0.1063
wR ₂	0.2642
Goodness-of-fit	1.131
Refined parameters	46
restraints	3

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}	occupancy
SiA	0.2701(5)	0.3432(8)	0.0399(14)	0.016(3)	0.96(3)
SiB	0.4725(5)	0.3377(8)	0.8088(15)	0.018(3)	0.96(3)
AlB	0.4725(5)	0.3377(8)	0.8088(15)	0.018(3)	0.059(11)
Mg(M1)	0.3764(5)	0.6587(9)	0.8542(17)	0.009(3)	0.89(2)
Mg(M2)	0.3783(6)	0.4830(9)	0.3461(18)	0.019(3)	0.98(2)
O1A	0.1822(12)	0.3396(17)	0.024(3)	0.015(4)	1
O2A	0.3074(12)	0.5139(18)	0.029(3)	0.017(4)	1
O3A	0.3048(11)	0.2209(17)	0.816(3)	0.017(4)	1
O1B	0.5621(10)	0.3368(15)	0.822(3)	0.009(4)	1
O2B	0.4339(12)	0.4861(18)	0.682(3)	0.023(4)	1
O3B	0.4462(12)	0.1881(16)	0.626(4)	0.018(4)	1

Table S6. Estimation for water in olivine according to partitioning coefficient.

	P (GPa)	T (°C)	D _{water} *	Mg-end OEn (ppm) #	Al-bearing OEn (ppm) #	Olivine calculated (ppm)	Total (60ol40en)	Total (80ol20en)
MFSH	5	1175	0.58	515		888	739	813
		1250	0.28	515		1839	1310	1574
MFASH	7.5	1175	0.78		978	1254	1033	1199
		1250	1.01		978	968	976	970

MFSH: MgO–FeO–SiO₂–H₂O. MFASH: MgO–FeO–Al₂O₃–SiO₂–H₂O. * D_{water} is from *Ferot and Balfan-*

Casanova [24]. # Water content was measured by SIMS from this study.