

The High-Pressure Structural Evolution of Olivine along the Forsterite–Fayalite Join

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Table S1a. Bond lengths (Å) and polyhedral data for Fo₁₀₀.

<i>P</i> (GPa)	0	1.22(5)	2.04(5)	2.67(5)	3.28(5)	4.82(5)	6.29(5)	7.23(5)	7.98(5)
M2-O1(Å)	2.180(5)	2.164(6)	2.165(5)	2.151(6)	2.150(5)	2.130(5)	2.132(6)	2.120(5)	2.119(5)
M2-O2(Å)	2.044(5)	2.040(6)	2.030(5)	2.035(6)	2.034(5)	2.019(5)	2.020(6)	2.008(5)	2.004(5)
M2-O3l(Å) × 2	2.215(4)	2.201(5)	2.196(4)	2.193(5)	2.190(4)	2.187(4)	2.177(5)	2.161(4)	2.162(4)
M2-O3s(Å) × 2	2.064(5)	2.059(6)	2.055(4)	2.053(6)	2.046(5)	2.033(5)	2.028(6)	2.028(5)	2.022(5)
<M2-O>	2.130	2.121	2.116	2.113	2.109	2.098	2.094	2.084	2.082
<i>V</i> (Å ³)	12.43(6)	12.31(6)	12.20(5)	12.14(2)	12.09(6)	11.91(6)	11.84(7)	11.70(5)	11.65(5)
Vol. distort.	0.0229	0.0215	0.0220	0.0222	0.0216	0.0204	0.0204	0.0196	0.0193
M1-O1(Å) × 2	2.089(3)	2.077(4)	2.074(3)	2.068(4)	2.067(4)	2.060(3)	2.051(4)	2.048(3)	2.043(3)
M1-O2(Å) × 2	2.069(3)	2.062(4)	2.062(3)	2.059(4)	2.051(3)	2.050(3)	2.043(4)	2.036(3)	2.034(3)
M1-O3(Å) × 2	2.133(3)	2.128(4)	2.122(3)	2.117(4)	2.116(3)	2.112(3)	2.104(4)	2.096(3)	2.092(3)
<M1-O>	2.097	2.089	2.086	2.081	2.078	2.074	2.066	2.060	2.056
<i>V</i> (Å ³)	11.82(4)	11.72(4)	11.67(4)	11.58(4)	11.54(4)	11.48(4)	11.34(5)	11.26(3)	11.20(4)
Vol. distort.	0.0382	0.0362	0.0354	0.0367	0.0359	0.0355	0.0360	0.0331	0.0336
T-O1(Å)	1.611(5)	1.619(6)	1.613(4)	1.619(6)	1.615(5)	1.616(5)	1.608(6)	1.608(5)	1.606(5)
T-O2(Å)	1.657(5)	1.663(6)	1.666(4)	1.656(6)	1.659(5)	1.662(5)	1.646(6)	1.663(5)	1.656(5)
T-O3(Å) × 2	1.638(5)	1.639(6)	1.636(4)	1.636(6)	1.633(5)	1.630(5)	1.629(6)	1.629(5)	1.627(5)
<T-O>	1.636	1.640	1.638	1.637	1.635	1.635	1.628	1.632	1.629
<i>V</i> (Å ³)	2.21(2)	2.22(2)	2.22(2)	2.21(2)	2.21(2)	2.20(2)	2.18(2)	2.19(2)	2.18(2)
Vol. distort.	0.0127	0.0128	0.0127	0.0143	0.0141	0.0137	0.0147	0.0144	0.0147

Table S1b. Bond lengths (Å) and polyhedral data for Fo₈₀.

P (GPa)	0	1.06(5)	1.69(5)	3.00(5)	3.71(5)	5.78(5)	7.66(5)
M2-O1(Å)	2.190(8)	2.169(5)	2.174(5)	2.167(5)	2.152(6)	2.146(7)	2.136(6)
M2-O2(Å)	2.068(9)	2.058(5)	2.050(5)	2.040(5)	2.041(6)	2.042(6)	2.020(6)
M2-O3l(Å) × 2	2.240(6)	2.224(4)	2.216(4)	2.214(4)	2.204(4)	2.198(5)	2.194(5)
M2-O3s(Å) × 2	2.053(6)	2.063(4)	2.057(4)	2.051(4)	2.052(5)	2.037(6)	2.025(6)
<M2-O>	2.141	2.134	2.128	2.123	2.118	2.110	2.099
V(Å ³)	12.60(8)	12.46(5)	12.38(5)	12.28(5)	12.19(6)	12.08(7)	11.90(6)
Vol. distort.	0.0218	0.0245	0.0236	0.0235	0.0242	0.0222	0.0210
M1-O1(Å) × 2	2.107(5)	2.091(3)	2.088(3)	2.083(3)	2.081(4)	2.061(4)	2.061(4)
M1-O2(Å) × 2	2.075(6)	2.079(3)	2.080(3)	2.077(3)	2.074(4)	2.056(4)	2.056(4)
M1-O3(Å) × 2	2.154(5)	2.149(3)	2.149(3)	2.139(3)	2.140(4)	2.120(4)	2.111(4)
<M1-O>	2.112	2.106	2.106	2.100	2.098	2.079	2.076
V(Å ³)	12.08(6)	11.94(4)	11.95(4)	11.86(4)	11.82(4)	11.51(5)	11.48(4)
Vol. distort.	0.0379	0.0418	0.0399	0.0399	0.0402	0.0392	0.0376
T-O1(Å)	1.602(8)	1.623(5)	1.617(5)	1.605(4)	1.610(5)	1.615(7)	1.603(6)
T-O2(Å)	1.661(9)	1.649(5)	1.652(5)	1.650(5)	1.651(6)	1.642(7)	1.646(6)
T-O3(Å) × 2	1.654(7)	1.638(4)	1.640(4)	1.635(4)	1.628(5)	1.630(6)	1.625(6)
<T-O>	1.643	1.637	1.637	1.631	1.629	1.629	1.625
V(Å ³)	2.24(2)	2.22(2)	2.22(2)	2.19(2)	2.19(2)	2.18(2)	2.16(2)
Vol. distort.	0.0095	0.0135	0.0120	0.0120	0.0125	0.0152	0.0136

Table 1c. Bond lengths (Å) and polyhedral data for Fo₆₂.

P (GPa)	0	0.76(5)	1.93(5)	2.86(5)	5.07(5)	7.46(5)*	8.34(5)
M2-O1(Å)	2.212(16)	2.195(15)	2.192(14)	2.201(17)	2.181(15)	2.150(12)	2.134(13)
M2-O2(Å)	2.080(17)	2.074(15)	2.072(15)	2.040(19)	2.038(17)	2.014(13)	2.033(14)
M2-O3l(Å) × 2	2.249(9)	2.257(8)	2.253(8)	2.253(10)	2.221(9)	2.220(7)	2.206(7)
M2-O3s(Å) × 2	2.079(7)	2.079(7)	2.070(6)	2.061(8)	2.048(7)	2.043(6)	2.040(6)
<M2-O>	2.158	2.157	2.152	2.145	2.126	2.115	2.110
V(Å ³)	12.81(12)	12.80(11)	12.70(10)	12.58(13)	12.30(11)	12.11(9)	12.04(9)
Vol. distort.	0.0292	0.0281	0.0284	0.0271	0.0244	0.0240	0.0245
M1-O1(Å) × 2	2.095(9)	2.101(8)	2.096(8)	2.076(10)	2.071(8)	2.064(7)	2.065(7)
M1-O2(Å) × 2	2.105(8)	2.099(7)	2.095(7)	2.103(9)	2.090(8)	2.088(6)	2.080(6)
M1-O3(Å) × 2	2.180(10)	2.163(9)	2.165(8)	2.158(11)	2.154(10)	2.123(8)	2.126(8)
<M1-O>	2.127	2.121	2.119	2.112	2.105	2.092	2.090
V(Å ³)	12.23(10)	12.14(9)	12.10(9)	12.04(11)	11.94(10)	11.72(8)	11.66(8)
Vol. distort.	0.0466	0.0454	0.0457	0.0420	0.0397	0.0395	0.0425
T-O1(Å)	1.635(10)	1.626(9)	1.619(9)	1.629(11)	1.619(9)	1.615(7)	1.614(8)
T-O2(Å)	1.657(16)	1.664(15)	1.662(14)	1.679(18)	1.663(16)	1.670(13)	1.651(13)
T-O3(Å) × 2	1.622(9)	1.622(8)	1.613(8)	1.612(10)	1.635(9)	1.614(7)	1.613(7)
<T-O>	1.634	1.634	1.627	1.633	1.638	1.628	1.626
V(Å ³)	2.20(4)	2.20(3)	2.18(3)	2.20(4)	2.22(4)	2.18(3)	2.16(3)
Vol. distort.	0.0141	0.0143	0.0134	0.0122	0.0126	0.0133	0.0152

*Data collected during decompression.