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The effect of Ca substitution on the elastic and structural behavior of orthoenstatite

FABRIZIO NESTOLA,* G. DIEGO GATTA,† AND TIZIANA BOFFA BALLARAN

Bayerisches Geoinstitut, Universitaet Bayreuth, Universitaetstrasse 30, D-95447, Bayreuth, Germany

ABSTRACT

A single crystal of orthopyroxene with composition $Ca_{0.07}Mg_{1.93}Si_2O_6$ (space group *Pbca*) has been investigated at high pressure and room temperature by in-situ X-ray diffraction using a diamond anvil cell. The unit-cell parameters have been determined at ten different pressures up to 10.16(5) GPa. In the pressure range investigated no evidences of phase transitions have been found. The pressure-volume data have been fitted with a third-order Birch-Murnaghan equation of state resulting in the following parameters: V_0 = 838.26(8) Å^3, K_{T0} = 110(1) GPa, K' = 6.6(4). The Ca substitution in the pure orthoenstatite $Mg_2Si_2O_6$ structure causes a slight increase in K_{T0} and a decrease in K'. The compressibility of *a*, *b*, and *c* unit-cell parameters is strongly anisotropic with a compressibility scheme $\beta_b >> \beta_c >> \beta_a$. The structure evolution as a function of pressure has been determined at five different pressures up to 6.25(5) GPa. The M2 polyhedron undergoes the largest volume variation (~7.7%), whereas the volume variation of M1 is ~6.1%. The TA and TB tetrahedral volumes decrease by about 3% and 1.2%, respectively, without a discontinuity in the pressure range investigated.

Keywords: Orthopyroxene, high-pressure, compressibility, equation of state