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High pressure behavior, transformation and crystal structure of synthetic iron-free pigeonite

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Abstract

A single-crystal high pressure X-ray investigation was performed up to $P = 6.5$ GPa on a synthetic clinopyroxene of composition $Ca_{0.15(1)}Mg_{1.85(1)}Si_{2.00(1)}O_6$ [$Di_{15}En_{85}$, unit-cell parameters at room pressure: $a = 9.6525(6)$Å, $b = 8.8461(2)$Å, $c = 5.2036(5)$Å, $\beta = 108.370(5)°$, $V = 421.68(4)$Å^3]. A first order $P2_1/c$-$C2/c$ displacive phase transition was found at $P = 5.1$ GPa; the transition was revealed by the disappearance of the b reflections ($h + k$ = odd) and by sharp changes in the unit-cell parameters. Reversals through the transformation show that, if present, hysteresis is smaller than 0.1 GPa. The volume variation has been described by a third-order Birch-Murnaghan equation of state with $V_0 =$ 421.68(8) Å^3, $K_{T0} = 102(2)$ GPa, and $K' = 8(1)$ for the low-symmetry phase ($P2_1/c$) and with $V_0 =$ 411.06(3) Å^3 and $K_{T0} = 108(2)$ GPa for the high-symmetry phase ($C2/c$), with K' fixed to the value obtained for the low-symmetry form. The axial compressibility shows the following scheme: $\beta_b > \beta_a \cong \beta_c > \beta_{a\sin\beta}$ for both phases. In comparison with pure clinoenstatite, $Di_{15}En_{85}$ shows a similar step in unit-cell parameters at the transition, the disappearence of hysteresis and a decrease of transition pressure and of bulk modulus.

Full intensity data sets were collected at room pressure, 2.6 and 4.5 GPa for the $P2_1/c$ phase and at $P = 6.2$ GPa for the $C2/c$ phase. A slight increase of the intensity of $h + k$ odd reflections and of the difference in the A and B chain kinking angles were observed. A comparison of the structural behavior of the $P2_1/c$ phase at high temperature and high pressure shows opposite behavior for M2-O bond lengths and O3-O3-O3 kinking angle.