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A $P2_1/c$-$C2/c$ high-pressure phase transition in $Ca_{0.5}Mg_{1.5}Si_2O_6$ clinopyroxene

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ABSTRACT

A high-pressure $P2_1/c$-$C2/c$ phase transition in a synthetic iron-free clinopyroxene of composition $Ca_{0.5}Mg_{1.5}Si_2O_6$ was observed at pressure between 3 and 5 GPa from powder diffraction data collected up to P = 14.2 GPa in a diamond anvil cell by means of synchrotron radiation. The transition is marked by a continuous decrease in a, c, and β cell parameters in the transition range and by the disappearance of reflections with $h+k$ odd. No hysteresis could be found. The spontaneous strain due to the transition occurs almost completely on the (010) plane and is described by a strong compression at a direction of 150° from the c axis and a milder expansion at 60° from the c axis. Interaction between the macroscopic cell strain and microscopic strain due to compositional heterogenities may explain the difference from the transition behavior in clinoenstatite. A third-order Birch-Murnaghan equation of state for the $C2/c$ high-pressure phase was refined giving the following parameters: V_0 = 429(2) Å^3, K = 99(7) GPa, K' = 6.5 ($w\chi^2$ = 1.3). Only minor differences are observed with other iron-free clinopyroxenes. The compressional strain in the $C2/c$ phase in the $Ca_{0.5}Mg_{1.5}Si_2O_6$ pyroxene has almost the same orientation as in diopside and in $Ca_{0.8}Mg_{1.2}Si_2O_6$ pyroxene, displaying higher compression on (010) at 140° from the c axis and suggesting a similar compressional mechanism for Ca-rich $C2/c$ clinopyroxenes.