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High-pressure $P2_1/c$-$C2/c$ phase transitions in clinopyroxenes: Influence of cation size and electronic structure

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ABSTRACT

The high-pressure behavior of the clinopyroxenes kanoite $Mn_{0.9}Mg_{1.1}Si_2O_6$, $MnSiO_3$, and $CrMgSi_2O_6$ (all space group $P2_1/c$) was studied by single-crystal X-ray diffraction in a diamond-anvil cell at room temperature. Phase transitions from $P2_1/c$ to $C2/c$ clinopyroxene were found and reversed at 5.06 ± 0.14 GPa for kanoite, 2.905 ± 0.005 GPa in $MnSiO_3$, and 3.60 ± 0.03 GPa in $CrMgSi_2O_6$. The phase transitions are first-order in character and are accompanied by a volume decrease of approximately 2.3%. The structure of high-pressure $C2/c$ kanoite was determined from single-crystal X-ray intensity data collected at 5.20 GPa, and is very similar to that of high-pressure (HP) $C2/c$-ferrosilite. Although the space group $C2/c$ is the same as for the high-temperature (HT) kanoite form, the two phases have significantly different structures. The silicate chains are extremely kinked in HP kanoite while they are almost straight in HT kanoite. Compared with the transition pressure of clinoenstatite-clinoferrosilite, the new data suggest that the effective ionic radii of M1 and M2 cations do not exclusively control the transition pressure and that the HP $C2/c$ clinopyroxenes with Cr^{2+} and Fe^{2+} gain additional stabilization energy from crystal field effects.