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Ca-Zn solid solutions in *C*2/*c* pyroxenes: Synthesis, crystal structure, and implications for Zn geochemistry

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ABSTRACT

The effect of Zn substitution on a series of clinopyroxenes along the join $CaZnSi_2O_6$-$Zn_2Si_2O_6$ was studied. The pyroxenes were synthesized at $P = 4–5$ GPa and $T = 1000–1200$ °C by a multi-anvil apparatus. SEM-EDS and XRD analysis showed complete solid solution; all of the samples have the *C*2/*c* space group. No miscibility gap between clino- and orthopyroxene nor phase transition to the $P2_1/c$ space group was found. Moreover, the cell volume of Ca-Zn pyroxenes decreases less than expected from the decrease of the average cation size for the substitution of Zn for Ca.

The crystal structures of three synthetic pyroxenes of composition $(Ca_{0.5}Zn_{0.5})ZnSi_2O_6$, $(Ca_{0.3}Zn_{0.7})ZnSi_2O_6$, and $(Ca_{0.2}Zn_{0.8})ZnSi_2O_6$ were refined by single-crystal X-ray diffraction ($R_{4\sigma}$ between 3 and 4.5%). It was observed that the Ca-Zn substitution occurs in the M2 polyhedron, with a sub-site splitting of Zn in a position at approximately 0.7 Å from Ca. In this position, Zn retains a highly distorted fourfold coordination; moreover, the tetrahedral chain configuration is little changed along the series, and the M1 polyhedral size increases with Zn substitution in M2.

An implication of the present work is the interpretation of the partitioning of Zn between clinopyroxene and melt. The distribution coefficients of Zn and Co are quite different in rocks of the same composition, despite their very similar ionic radius, and the difference is related to the preference of Zn for the M2 site, where Zn may find a suitable atomic coordination.

Keywords: Clinopyroxene, high pressure, X-ray diffraction, trace elements, Zn