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Raman spectroscopy of (Ca,Mg)$MgSi_2O_6$ clinopyroxenes

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ABSTRACT

The Raman spectra of eight clinopyroxenes synthesized along the join diopside-clinoenstatite (Di-Cen, $CaMgSi_2O_6$-$Mg_2Si_2O_6$) were measured. The splitting of the 670 cm^{-1} mode of the A_g symmetry, observed in the composition $Di_{52}En_{48}$ to clinoenstatite, was interpreted as evidence of a $C2/c$-$P2_1/c$ phase transition. The transition was also revealed by deviation from the linear dependence of the peak position vs. composition and by the appearance of several new peaks in the samples richer in clinoenstatite.

Analysis of peak positions vs. structural changes suggests that for the M2 polyhedron, in which Ca substitution for Mg occurs, a different deformation mechanism acts in Ca richer and poorer $P2_1/c$ pyroxenes, and that Ca richer $P2_1/c$ pyroxenes deform with the same mechanism as $C2/c$ pyroxenes. The frequency of the peak at 670 cm^{-1} was found to change linearly with the kinking angle of the tetrahedral chains for $C2/c$ and of the B chain for $P2_1/c$, whereas the position of the peak ascribed to the A chain was little affected by the kinking angle.

Peak broadening in $C2/c$ Ca-rich homogeneous pyroxenes was interpreted to be a consequence of the positional disorder of the Ca and Mg in the M2 cavity: peak broadening increases with increasing Mg content for peaks assigned to M2-O vibrations, but it changes little for peaks assigned to chain bending, which suggests that cation substitution in the M2 cavity occurs with little interaction with the silicate chain. Furthermore peak broadening was observed in intermediate pyroxenes as a consequence of mottled textures, antiphase domains, and compositional inhomogeneity.

Keywords: Pyroxene, Raman spectroscopy, peak position and structure, diopside-clinoenstatite, peak broadening, microstructures