

## Structural mechanisms of solid solution and cation ordering in augite-jadeite pyroxenes: II. A microscopic perspective

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### ABSTRACT

Infrared spectra of ordered ( $P2/n$ ) and disordered ( $C2/c$ ) pyroxenes belonging to the join augite-jadeite were investigated at room temperature in the range 70–1400  $\text{cm}^{-1}$ . The spectra change as a function of composition and the phase transition  $P2/n \rightarrow C2/c$  produces an increase in band widths. The autocorrelation function quantified changes in line widths due to these effects. Phonons at low frequencies are very sensitive to both changes in composition and degree of order and are indicative of a non-ideal mixing behavior for the  $C2/c$  solid solution. Phonons at high frequencies depend on the average composition of the samples and not on local configurational changes related to the order-disorder transition. High degrees of local heterogeneity were suggested by the  $\Delta_{\text{corr}}$  values of the  $C2/c$  omphacites at intermediate compositions. This effect is most evident in the low frequency region of the spectra, corresponding to modes involving, primarily, the M cations. The changes in frequency due to ordering,  $\Delta\omega$ , and the change in line widths  $\delta(\Delta_{\text{corr}})_{100-200}$  for the spectral region 100–200  $\text{cm}^{-1}$  and  $\delta(\Delta_{\text{corr}})_{210-800}$  for the range 210–800  $\text{cm}^{-1}$  have been used to characterize the state of local order at different compositions. The spectra yield information related to the local structural states of augite-jadeite pyroxenes, down to a unit-cell length scale, which may then be compared with the average structure determined by X-ray diffraction studies of the same samples.