

Thermal expansion of minerals in the pyroxene system and examination of various thermal expansion models

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ABSTRACT

To examine the effects of chemical composition on thermal expansion in the pyroxene mineral group, X-ray diffraction data have been collected from room temperature to ~925 °C on a chemically diverse group of 13 pyroxenes including four orthorhombic and nine monoclinic samples. Additionally, resulting unit-cell volumes computed from the XRD data have proven to be good tests for a large number of thermal expansion models; the physical model by Kroll and coworkers and the empirical one by Fei have been found to be especially useful. Modeling also has allowed the connection of present data, collected at temperatures above 25 °C, to the volume data of other workers for much lower temperatures, well below 0 °C, and also extrapolation of values for volume and thermal expansion well beyond the measurement range.

We have found for orthopyroxenes that Fe²⁺-Mg²⁺ substitution has little effect on thermal expansion coefficients for volume. For clinopyroxenes, however, greater thermal expansion occurs in Ca²⁺- (diopside, augite, hedenbergite, johannsenite) than in Li⁺- (spodumene) or Na⁺-bearing members (jadeite, aegirine, kosmochlor). Present data support the observation that differences in volume thermal expansion relate primarily to differences in expansion along the *b* crystallographic axis. This apparently is due to the greater concentration of M1 polyhedra along the *b* crystallographic axis, where expansion differences can be related to the shared O1-O1 polyhedral edge and inter-oxygen repulsion that is made easier by divalent, as opposed to trivalent, cation occupancy of the M1 crystallographic site.

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