

The high-pressure, vacancy-stabilized component in clinopyroxenes

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ABSTRACT

Motivated by the recent discovery of albitic clinopyroxene, we assess the molar volume systematics of vacancy-stabilized, high-pressure clinopyroxenes. Previous assessments used the Ca-Eskola component $M2(Ca_{0.5}\square_{0.5})^{M1}Al^T Si_2O_6$ (where \square denotes a vacancy) as an end-member and were limited to compositions with $\leq 50\%$ vacancies in the M2 site. The discovery of albitic jadeite calls for extension of the solid solution space toward an end-member with entirely vacant M2 sites, $M2\square^{M1}Si^T Si_2O_6$, i.e., silica in the *C2/c* pyroxene structure. Based on our new and compiled data, we fit a model for volumes of clinopyroxenes in an 11-component subsystem. We tested two different scenarios: ideal mixing and symmetric excess volumes. Ideal mixing is easily rejected, as the correlation between vacancy concentration and volume at standard conditions is clearly nonlinear. The symmetric excess volume model, however, yields an adequate fit to the data when using three excess terms (Hd-En, Hd-Di, and Hd-Jd). The estimated molar volume of the clinopyroxene-structured silica end-member, which has one octahedrally coordinated silicon atom per formula unit, is 60.77 ± 0.75 cm³/mol on a six-oxygen formula basis, slightly smaller than that of coesite (61.73 cm³/mol) but much larger than that of stishovite (41.44 cm³/mol). We also obtained a molar volume of 62.16 ± 0.75 cm³/mol for the Ca-Eskola component, modestly larger than earlier estimates extrapolated with an ideal mixing assumption from natural samples (60.52 ± 0.73 cm³/mol) or experiments (60.87 ± 0.63 cm³/mol). The proposed volume model provides a partial basis for assessing the formation conditions of vacancy-stabilized pyroxenes.

Keywords: Albitic jadeite, molar volume, vacancy-rich clinopyroxenes, high-pressure phase, Ca-Eskola