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An order-disorder model for omphacitic pyroxenes in the system jadeite-diopside-hedenbergite-acmite, with applications to eclogitic rocks

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Abstract

A new thermodynamic model for sodic pyroxenes involving jadeite-diopside-hedenbergite-acmite is presented. This model allows for ordering of Mg, Al, Fe^{2+}, and Fe^{3+} on the M1 sites, with coupled Na and Ca ordering on the M2 sites. It is calibrated on the basis of experiments in three chemical subsystems together with available information on ordering in different pyroxenes and on the limited calorimetric data. Central to the determination of the parameters of the model is the use of relationships among the end-member Gibbs energies and the interaction energies in the various possible non-independent sets of end-members. An important aspect of this model, which uses the symmetric formalism, is that Fe-Mg (FM) and Al-Fe^{3+} (AF') mixing is not assumed to be ideal. The model accounts successfully for the experiments at both 600 °C and at higher temperatures involving ordered and disordered pyroxenes coexisting with albite and quartz in NCMAS, NCFAS, NF'AS systems as well as the available calorimetry. It is also able to predict the positions and slopes of tielines in coexisting jadeite + omphacite and omphacite + augite found in nature at lower temperatures. Although the model requires a large number of energy parameters, some of these are not critical to the behavior of the model, while for others the constraints from experiment, calorimetry, ordering state and solvi lead to very limited allowable combinations. The model places some restrictive constraints on the shape of the phase relations in the jadeite–augite–acmite system. Petrological applications of the model are illustrated via a phase diagram example for a MORB bulk composition eclogite.

Keywords: Thermodynamics, omphacite, activity-model, eclogite, phase equilibria, metamorphic petrology, mixing properties