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Thermodynamic properties of the Tschermak solid solution in Fe-chlorite: Application to natural examples and possible role of oxidation

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ABSTRACT

The standard-state thermodynamic properties of 14 Å Fe-amesite [$Fe_4Al_4Si_2O_{10}(OH)_8$] were calculated from the reequilibration experiments of Parra et al. (2005) and natural data bearing on the Fe-Mg partitioning between chlorite and chloritoid over a wide range of pressure (*P*), temperature (*T*), and rock composition. The combination of these data with the three-site mixing model and thermodynamic properties of daphnite proposed by Vidal et al. (2001) led us to reappraise the evolution of the Margules parameter W^{G}_{AlFe} with pressure and temperature. The new data [$H^{0}f_{Fe\text{-}Am} = -7\,607\,460$ J/mol, $S^{0}_{Fe\text{-}Am} = 514.8$ J/(mol·K), $V^{0}_{Fe\text{-}Am} = 20.90$ J/bar, $W^{G}_{AlFe} = 1200 - 31T + 0.7(P - 1)$] are compatible with all the natural data and reequilibration experiments, and in fair agreement with the results of synthesis. They are used to calculate the compositional evolution of chlorite with *T*, *P*, or a_{O2} at different bulk-system compositions. The calculated phase relations and chlorite compositions are compared with previous experiments conducted in the FeO-Al_2O_3-SiO_2-H_2O system. The addition of the Fe-amesite end-member increases the number of equilibria that can be calculated for any natural assemblage involving chlorite. Two independent equilibria are obtained for natural (Fe-Mg)-chlorite-quartz or diaspore assemblages. It is therefore possible to estimate metamorphic conditions for high-variance assemblages from the composition of chlorite. We discuss the reliability of such *P*-*T* estimates using natural chlorites occurring in low-pressure and low-temperature or medium- to high-pressure and temperature samples. Assuming that the proposed model and thermodynamic parameters are correct, these various natural data suggest that $X_{Fe^{3+}}$ [$= Fe^{3+}/(Fe^{2+} + Fe^{3+})$] in metamorphic chlorites is low (<0.1), whereas it can be as high as 0.3 in Si- and Mg-rich chlorites formed at low-*P*-*T* conditions.