Regular Solution Site-Mixing Model for Chlorites

R. K. Stoessell

Department of Earth Sciences, University of New Orleans, New Orleans, Louisiana 70148

Abstract: Activity expressions are presented for a six end-member, regular solution, site-mixing model for chlorites. The end members are ideal 14-Å chlorites for which experimental stability data are lacking. Estimates were made of the standard state 25 ° C and 1 bar molar 3rd law entropies, volumes, and the Maier-Kelley heat capacity coefficients. Experimental stability data from the literature for 14-Å chlorites were used with different sets of exchange energies, for cations on adjacent sites, to compute estimates of the standard state chemical potentials of the end members at 25 ° C and 1 bar. More experimental data are needed for an adequate definition of the exchange energies and the standard state chemical potentials. The model was applied to diagenesis in clastic reservoirs. Aqueous activity ratios of Mg^{2+}:Fe^{2+} were computed as an equilibrium function of the corresponding molar ratios in authigenic chlorites. The aqueous activity ratio was independent of the chlorite Al content at a constant molar ratio of Mg^{2+}:Fe^{2+} in the chlorite. The model predicts a wide range of molar Mg^{2+}:Fe^{2+} ratios in authigenic chlorites in equilibrium with reservoir fluids. Trends in these molar ratios should be independent of the Al content in the chlorites. The model can be applied directly to 7-Å chlorites when experimental data become available to estimate the various thermodynamic parameters of the 7-Å end members.

Key Words: Chlorite • Diagenesis • Free energy of formation • Solid solution • Stability

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