Thermodynamic properties of natural melilites

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ABSTRACT

In the present study, four samples of natural melilites were characterized using electron microprobe analysis, powder X-ray diffraction, FTIR, and Raman spectroscopy, and their thermodynamic properties were measured with a high-temperature heat-flux Tian-Calvet microcalorimeter. The enthalpies of formation from the elements were determined to be: -3796.3 ± 4.1 kJ/mol for $Ca_{1.8}Na_{0.2}(Mg_{0.7}Al_{0.2}Fe^{2+}_{0.1})Si_2O_7$, -3753.6 ± 5.2 kJ/mol for $Ca_{1.6}Na_{0.4}(Mg_{0.5}Al_{0.4}Fe^{2+}_{0.1})Si_2O_7$, -3736.4 ± 3.7 kJ/mol for $Ca_{1.6}Na_{0.4}(Mg_{0.4}Al_{0.4}Fe^{2+}_{0.2})Si_2O_7$, and -3929.2 ± 3.8 kJ/mol for $Ca_2(Mg_{0.4}Al_{0.6})[Si_{1.4}Al_{0.6}O_7]$. Using the obtained formation enthalpies and estimated entropies, the standard Gibbs free energies of formation of these melilites were calculated. Finally, the enthalpies of the formation of the end-members of the isomorphic åkermanite-gehlenite and åkermanite-alumoåkermanite series were derived. The obtained thermodynamic properties of melilites of different compositions can be used for quantitative modeling of formation conditions of these minerals in related geological and industrial processes.

Keywords: Melilite, åkermanite, gehlenite, alumoåkermanite, thermochemistry, enthalpy of formation, entropy, Gibbs free energy, Calvet microcalorimetry