

Enthalpies of formation of pyrrhotite $\text{Fe}_{1-0.125x}\text{S}$ ($0 \leq x \leq 1$) solid solutions

FEN XU AND ALEXANDRA NAVROTSKY*

Peter A. Rock Thermochemistry Laboratory and NEAT ORU, University of California at Davis,
One Shields Avenue, Davis, California 95616, U.S.A.

ABSTRACT

Binary iron sulfides are of major interest and importance in environmental, geological, and planetary science. Oxidative high-temperature oxide melt drop-solution calorimetry in molten sodium molybdate ($3\text{Na}_2\text{O} \cdot 4\text{MoO}_3$) solvent at 975 K was applied to determine the energetics of formation of the binary iron monosulfide solid solution (pyrrhotite) ($\text{Fe}_{1-0.125x}\text{S}$, $0 \leq x \leq 1$). The enthalpies of formation from elements are consistent with earlier data in the literature, available for a few compositions. Within the experimental errors, the enthalpies of formation of the solid solution from the end-members $\text{Fe}_{0.875}\text{S}$ and FeS (ΔH_{mix} , kJ/mol) at 25 °C equal to zero. Under the assumption of random distribution of Fe vacancies, the Gibbs free energies of mixing of $\text{Fe}_{1-0.125x}\text{S}$ ($0 \leq x \leq 1$) are estimated. Our data support the two-sublattice model proposed by Waldner and Pelton (2005).

Keywords: Pyrrhotite, iron sulfides, thermodynamics, enthalpy of formation, oxidative high-temperature oxide melt solution calorimetry