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Optimization of the thermodynamic properties and phase diagrams of P_2O_5-containing systems

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P_2O_5 is an important oxide component in the late stage products of numerous igneous rocks such as granites and pegmatites. Typically, P_2O_5 combines with CaO and crystallizes in the form of apatite, while in volatile-free conditions, Ca-whitlockite is formed. In spite of their interest, the thermodynamic properties and phase diagrams of P_2O_5-containg systems are not well known yet. In the case of the pure P_2O_5 for example, no experimental thermodynamic data are available for the liquid and the O and O' solid phases. As a result, we re-evaluated all the thermodynamic and phase diagram data of the P_2O_5 unary system [1]. Optimization of the thermodynamic properties and phase diagrams of the binary P_2O_5 systems was then performed including the Li_2O-, Na_2O-, MgO-, CaO-, BaO-, MnO-, FeO-, Fe_2O_3-, ZnO-, Al_2O_3-, and SiO_2-P_2O_5 [2] systems. All available thermodynamic and phase equilibrium data were simultaneously reproduced in order to obtain a set of model equations for the Gibbs energies of all phases as functions of temperature and composition. In particular, the Gibbs energy of the liquid solution was described using the Modified Quasichemical Model [3-5] implemented in the FactSage software [6]. Thermodynamic modeling of the Li_2O-Na_2O-K_2O-MgO-CaO-FeO-Fe_2O_3-Al_2O_3-SiO_2 system, which include many granite-forming minerals such as nepheline, leucite, pyroxene, melilite, feldspar and spinel is currently in progress.

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