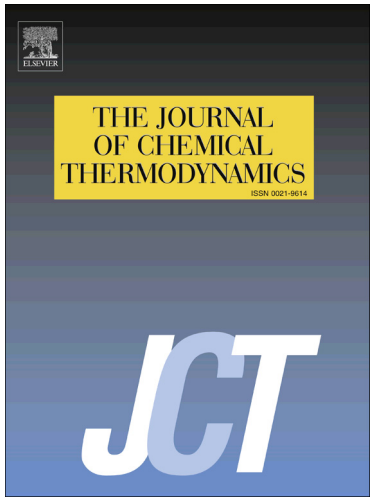

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Thermodynamic and spectroscopic properties of $KNbTeO_6$

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Abstract

In the present work, the temperature dependence of heat capacity of $KNbTeO_6$ has been measured for the first time over the range from 6 K to 332 K by precision adiabatic vacuum calorimetry. The experimental results were used to calculate standard thermodynamic functions, namely the heat capacity $C_p^{\circ}(T)$, enthalpy $H^{\circ}(T) - H^{\circ}(0)$, entropy $S^{\circ}(T) - S^{\circ}(0)$ and Gibbs function $G^{\circ}(T) - H^{\circ}(0)$, for the range from $T \rightarrow 0$ K to 332 K. The phase transitions and thermal decomposition of $KNbTeO_6$ were determined by differential scanning calorimetry. Structural changes in phase transitions were studied by high-temperature Raman spectroscopy.

Keywords: Pyrochlore; $KNbTeO_6$; Adiabatic vacuum calorimetry; Heat capacity; Thermodynamic functions; Raman spectroscopy

1. Introduction

Materials with the pyrochlore structure have been extensively studied for a range of applications including their use as adsorbents [1,2], radioactive waste form materials [3-5], as fast ion conductors [6], as Li-battery electrodes and, more recently, for photocatalytic splitting of water [7-10]. The pyrochlore structure type is also represented in a wide range of natural occurrences by the mineral group of pyrochlore, microlite, betafite and stibiconite [11].

The ideal defect pyrochlore structure has cubic symmetry (space group F*d-3m*) and stoichiometry $A_2M_2X_6X'$ where A is a large, low valent cation (*e.g.* lanthanide or alkali metal or alkaline earth cation) and M is a smaller cation that can adopt octahedral coordination (*e.g.* Ti^{4+}, Zr^{4+}, W^{6+}, Sb^{6+}). Typically X represents O^{2-} while X' may be an anion such as O^{2-}, OH^- or F^-. This work is a continuation of systematic studies of defect pyrochlore. The compound $KNbTeO_6$ is one of the phases in the materials on the basis of a tellurite glass-ceramics. In addition, this compound is used as the ion exchange phase for synthesis of series pyrochlore. Earlier in the articles [12-14], we have investigated the thermodynamic properties of $KSbWO_6$, $RbNbWO_6$, $CsTaWO_6$. The goals of this work include calorimetric determination of the temperature dependence of the heat capacity $C_p^{\circ}(T)$

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