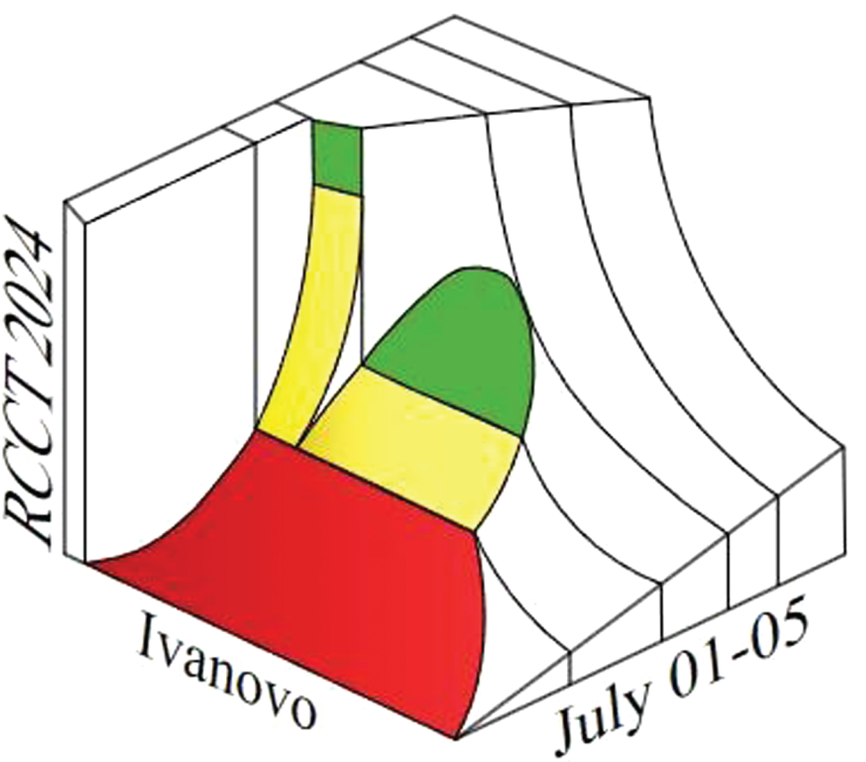
XXIV International Conference on Chemical Thermodynamics in Russia

July 1-5, 2024
Ivanovo, Russia



RCCT-2024

BOOK OF ABSTRACTS

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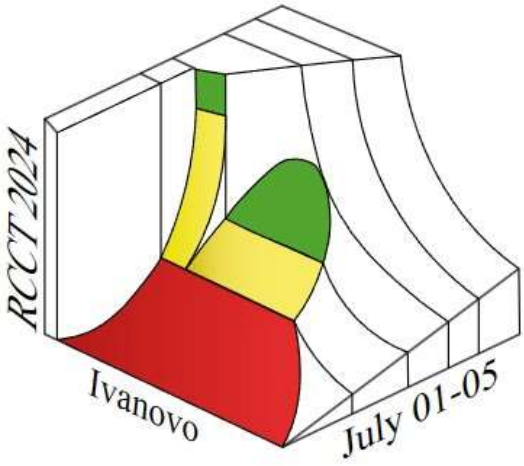

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BOOK OF ABSTRACTS

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CALCULATION OF THE THERMODYNAMIC PROPERTIES IN THE $SrO-TiO_2-ZrO_2$ SYSTEM BASED ON THE SEMI-EMPIRICAL APPROACHES USING THE HIGH TEMPERATURE MASS SPECTROMETRIC DATA

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The materials based on the $SrO-TiO_2-ZrO_2$ system are promising for a wide range of practical applications. For instance, the $SrO-TiO_2-ZrO_2$ ceramics is of significant interest for the development of nuclear reactor core melt traps and for modeling of the accident scenarios at nuclear power plants to prevent their consequences [1]. Moreover, the $SrO-TiO_2-ZrO_2$ system is characterized by unique electrochemical properties due to the formation of the perovskite-type phases [2] and may be used to obtain highly active solid base catalysts [3].

In the present study, the vaporization processes and thermodynamic properties of the $SrO-TiO_2-ZrO_2$ system, including the binary $SrO-ZrO_2$ and TiO_2-ZrO_2 systems, were studied by the Knudsen effusion mass spectrometric (KEMS) method [1, 4]. The samples in the system under consideration were synthesized by the solid-state method based on the $SrCO_3$, TiO_2, and $ZrO(NO_3)_2 \bullet 2H_2O$ as initial components with the maximum annealing temperature of 1723 K for at least 20 hours. The samples obtained were characterized by X-ray phase and X-ray fluorescence analyses. The KEMS study was carried out using an MS-1301 mass spectrometer at an ionizing voltage of 30 V from a tungsten twin effusion cell [4]. The vaporization of the samples of the $SrO-TiO_2-ZrO_2$ system was observed at temperatures above 1900 K, with the main vapor species being Sr, O, TiO, and TiO_2. The experimental data obtained by KEMS enabled the temperature dependences of the partial pressures of the vapor species as well as the SrO activities in the $SrO-TiO_2-ZrO_2$ system to be determined.

The thermodynamic properties in the $SrO-ZrO_2$ system described in [1], in the TiO_2-ZrO_2 system obtained in the present study, and in the $SrO-TiO_2$ system derived earlier [5] allowed the excess Gibbs energies in the $SrO-TiO_2-ZrO_2$ system to be calculated by the semi-empirical Kohler, Toop, Redlich-Kister, and Wilson methods. The excess Gibbs energy values calculated in the system under study showed negative deviations from the ideal behavior at the temperature 2100 K. The calculated values of the SrO и TiO_2 activities were compared with the experimental data, demonstrating a reasonable agreement. Discrepancies between the results obtained using various semi-empirical methods were discussed.

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