THERMODYNAMIC FUNCTIONS OF SOME ALKALINE EARTH METAL BOROSILICATES

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Alkaline earth metal borosilicates are used in modern technologies, particularly in the creation of low-temperature ceramic materials, liquid crystal matrices, sensors, and glass ceramics. The introduction of boron oxide in varying concentrations imparts multifunctionality to borosilicate glasses. Boron-containing compounds are also used in medical practice, the construction industry, and in magneto-optical components of devices.

This work is devoted to a comparative analysis of experimental and theoretical thermodynamic constants, the correlation of IR frequencies with the structure of oxides and composites based on them. The theoretical values of the studied systems were calculated by the ion increment method [1], and also obtained using the quantum-chemical software package Gaussian16 and methods of electron density functional theory and semi-empirical approximation [2].

By studying the bifurcation of the Na_2SiO_3 - B_2O_3 components, the composition of a new composite was determined: Na_2O - 41.2%, SiO_2 - 42%, B_2O_3 - 16.8%, the formula of which was assumed to be $Na_4Si_2O_6 \cdot B_2O_3$. This composite was synthesized using the solid-phase method at a temperature of 900 °C. The resulting glass was X-ray amorphous and transparent. The composition of the obtained substance was analyzed by IR spectroscopy. The thermodynamic data of the composite, according to the ion increment and quantum chemistry methods, are as follows:

Formula	Calculation method	$-\Delta_f H^0_{298}$, kJ/mol	$-\Delta_f G^0_{298}$, kJ/mol	S^0_{298}, J/mol·K	$C_p{}^0_{298}$, J/mol·K
$Na_4Si_2O_6 \cdot B_2O_3$	Ion increment	3985.55	4132.90	281.14	312.59
	PM3MM	3575.14	3758.03	613.49	276.55

The methods used show good agreement between the results obtained, with the exception of entropy, which, according to the semi-empirical method, indicates that the system under consideration is twice as disordered.

1. Aldabergenov M.K., Balakaeva G.T., Ospanova A.S., and Chekimbaev A.F. Calculation of the Standard Thermodynamic Functions of Borosilicates // Russian Journal of Physical Chemistry A. 2000. Vol. 74, Nr. 8. P. 1368.

2. Frisch M.J., Trucks G.W., Schlegel H.B., et al. Gaussian16, Revision A.03, Wallingford: CT, 2016.