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Thermodynamic properties of myo-inositol



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ABSTRACT

In the present work, the temperature dependence of heat capacity of vitamin B₈ (myo-inositol) has been measured for the first time over the range from 8 K to 340 K by precision adiabatic vacuum calorimetry. Based on the experimental data, the thermodynamic functions of the vitamin B₈, namely, the heat capacity, enthalpy $H^\circ(T) - H^\circ(0)$, entropy $S^\circ(T) - S^\circ(0)$ and Gibbs function $G^\circ(T) - H^\circ(0)$ have been determined for the range from $T \rightarrow 0$ K to 340 K. The value of the fractal dimension D in the function of multifractal generalization of Debye's theory of the heat capacity of solids was estimated and the character of heterodynamics of structure was detected. The enthalpy of combustion (-2747.0 ± 2.1) kJ·mol⁻¹ of the vitamin B₈ was measured for the first time using high-precision combustion calorimeter. The standard molar enthalpy of formation in the crystalline state (-1329.3 ± 2.3) kJ·mol⁻¹ of B₈ at 298.15 K was derived from the combustion experiments. Using combination of the adiabatic and combustion calorimetry results the thermodynamic functions of formation of the myo-inositol at $T = 298.15$ K and $p = 0.1$ MPa have been calculated. The low-temperature X-ray diffraction was used for the determination of coefficients of thermal expansion.

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1. Introduction

Myo-inositol (CAS: 87-89-8) is a sugar alcohol (isomer of glucose) widely distributed in plant and animal tissues. It is found in food, for example cereals with high bran content (buckwheat), nuts, beans, and fruit [1]. It plays an important role as the structural basis for a number of secondary messengers in eukaryotic cells, including inositol phosphates (phytic acid), phosphatidylinositol and phosphatidylinositol phosphate lipids. Inositol itself is not considered as a vitamin because it can be synthesized by the human body. On the other hand, myo-inositol was classified as a member of the vitamin B-complex (often called vitamin B₈). Patients suffering from clinical depression generally have decreased levels of inositol in their cerebrospinal fluid [2].

This work is a continuation of systematic studies of vitamins B. Earlier in the articles [3–6], we have investigated the thermodynamic properties of vitamins B_n ($n = 2, 3, 9, 12$). The goals of this work include calorimetric determination of the standard thermody-

amic functions of the myo-inositol with the purpose of describing biochemical and industrial processes with its participation.

2. Experimental

2.1. Sample

Myo-inositol was purchased from NutriVitaShop. For phase identification, an X-ray diffraction pattern of the vitamin B₈ sample was recorded on a Shimadzu X-ray diffractometer XRD-6000 (CuK_α radiation, geometry $\theta-2\theta$) in the 2θ range from 5° to 60° with scan increment of 0.02°. The water content in myo-inositol was determined by Karl Fischer titration. The water content of the compound is below the detection limit (0.05 wt%), so there is no crystallization and sorption water in the compound. The X-ray data, Karl Fischer titration and NutriVitaShop certificate led us to conclude that the myo-inositol sample studied (the content of impurities 0.1 wt%) was an individual crystalline compound (monoclinic modification, space group P2₁/c [7]).

2.2. Apparatus and measurement procedure

To measure the heat capacity C_p° of the tested substance over the range from 8 K to 340 K, a BKT-3.0 automatic precision

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