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Thermodynamic properties of myo-inositol

A.V. Knyazev [a,*], V.N. Emel'yanenko [b,c,*], A.S. Shipilova [a], D.H. Zaitsau [c], M.I. Lelet [a], S.S. Knyazeva [a], E.V. Gusarova [a], M.A. Varfolomeev [b]

[a] Lobachevsky University, Gagarin Prospekt 23/2, 603950 Nizhni Novgorod, Russia
[b] Department of Physical Chemistry, Kazan Federal University, Kremlevskaya Str. 18, 420008 Kazan, Russia
[c] Department of Physical Chemistry and Department, Science and Technology of Life, Light and Matter, University of Rostock, Dr.-Lorenz-Weg 1, D-18059 Rostock, Germany

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ABSTRACT

In the present work, the temperature dependence of heat capacity of vitamin B_8 (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 B_8, namely, the heat capacity, enthalpy $H°(T)–H°(0)$, entropy $S°(T)–S°(0)$ and Gibbs function $G°(T)–H°(0)$ have been determined for the range from $T \to 0$ 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 B_8 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 B_8 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.

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 B_8). 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 thermodynamic 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 B_8 sample was recorded on a Shimadzu X-ray diffractometer XRD-6000 (CuK_α radiation, geometry θ–2θ) 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 $P2_1/c$ [7]).

2.2. Apparatus and measurement procedure

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

* Corresponding authors at: Department of Physical Chemistry, Kazan Federal University, Kremlevskaya Str. 18, 420008 Kazan, Russia. Tel.: +49-381-498-6499; fax +49-381-498-6524 (V.N. Emel'yanenko); Tel.: +7-831-462-32-34; fax +7-831-434-50-56 (A.V. Knyazev).

E-mail addresses: knyazevav@gmail.com (A.V. Knyazev), vladchimic@tut.by (V.N. Emel'yanenko).

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adiabatic vacuum calorimeter with discrete heating was used. The calorimeter design and the operation procedure were described earlier [8]. The calorimeter was tested by measuring the heat capacity of high-purity copper and reference samples of synthetic corundum and K-2 benzoic acid. The analysis of the results showed that relative standard uncertainty of the heat capacity of the substance at helium temperatures was within ±2%, then it decreased to ±0.5% as the temperature was increase to 40 K, and was equal to ±0.2% at $T > 40$ K.

An isoperibol bomb calorimeter described previously [9] was used for the measurements of energies of combustion of the myo-inositol. The solid sample of compound was weighed with a microbalance of 10^{-6} g resolution. We used small polyethylene pieces prepared from commercial 1 mL ampoules (Fa. NeoLab, Heidelberg, Germany). This was employed as an auxiliary material in order to achieve complete combustion. The combustion products were examined for carbon monoxide (Dräger tube) and unburned carbon, but none was detected. The energy equivalent of the

Table 1
Experimental values of isobaric heat capacities ($J \cdot K^{-1} \cdot mol^{-1}$) of myo-inositol, M = 180.156 $g \cdot mol^{-1}$. p^o = 0.1 MPa.

T/K	C_p^o/$J \cdot K^{-1} \cdot mol^{-1}$	T/K	C_p^o/$J \cdot K^{-1} \cdot mol^{-1}$	T/K	C_p^o/$J \cdot K^{-1} \cdot mol^{-1}$
Series 1		14.08	3.897	28.59	14.60
8.37	0.774	14.35	4.078	30.38	16.06
8.40	0.780	14.63	4.226	31.42	16.86
8.51	0.803	14.91	4.431	32.38	17.74
8.64	0.841	15.19	4.618	33.35	18.40
8.77	0.885	15.47	4.810	34.31	19.30
8.91	0.930	15.75	4.990	35.28	20.02
9.05	0.977	16.04	5.208	36.25	20.70
9.20	1.034	16.32	5.400	37.23	21.47
9.34	1.096	16.61	5.588	38.21	22.22
9.50	1.162	16.90	5.795	39.19	22.99
9.65	1.224	17.20	5.990	40.18	23.66
9.81	1.296	17.49	6.202	41.16	24.37
9.98	1.381	17.78	6.394	42.15	25.13
10.17	1.467	18.08	6.622	43.15	25.81
10.39	1.577	18.37	6.852	44.14	26.63
10.59	1.677	18.67	7.060	45.14	27.34
10.81	1.817	18.97	7.278	46.17	28.07
11.05	1.945	19.27	7.496	47.17	28.86
11.28	2.084	19.57	7.721	48.17	29.58
11.52	2.218	19.87	7.949	49.18	30.39
11.76	2.363	20.46	8.428	50.18	31.12
12.00	2.535	21.33	9.104	51.20	31.92
12.25	2.700	22.21	9.711	53.79	33.97
12.50	2.861	23.10	10.41	54.97	34.90
12.75	3.034	24.00	11.09	55.99	35.65
13.01	3.189	24.90	11.77	57.01	36.49
13.27	3.362	25.81	12.44	58.03	37.34
13.53	3.524	26.73	13.12	59.05	38.14
13.81	3.727	27.66	13.84	60.07	38.87
61.10	39.73	110.53	80.42	208.19	155.1
62.12	40.52	113.53	82.88	212.26	158.0
63.15	41.35	116.54	85.33	216.41	161.2
64.17	42.18	119.54	87.73	220.48	164.0
65.20	43.06	122.54	90.16	224.57	167.1
66.23	43.91	125.55	92.54	228.65	170.1
67.26	44.68	128.56	94.96	232.72	173.2
68.29	45.54	131.58	97.38	236.81	176.2
69.32	46.48	134.60	99.81	240.91	179.3
70.38	47.25	137.62	102.1	245.00	182.3
71.85	48.53	140.65	104.5	249.09	185.2
73.87	50.14	143.68	106.9	253.18	188.2
75.89	51.78	146.71	109.2	257.27	191.3
77.91	53.41	149.74	111.6	261.36	194.4
78.79	54.18	152.78	113.9	265.46	197.6
79.80	55.07	155.81	116.2	269.55	200.6
80.92	56.01	158.85	118.6	273.64	203.7
Series 2		161.89	120.9	277.73	206.6
79.15	54.64	164.97	123.2	281.90	210.0
81.14	56.14	168.01	125.5	285.98	212.8
83.15	57.79	171.06	127.7	290.07	215.9
85.15	59.59	174.10	130.0	294.15	219.0
87.15	61.09	177.15	132.3	298.22	222.0
89.15	62.93	180.20	134.4	303.01	226.0
91.14	64.62	183.25	136.7	308.39	230.0
93.14	66.21	186.30	138.9	313.76	234.0
95.13	67.80	189.35	141.2	319.12	237.9
97.12	69.47	192.40	143.5	324.46	241.9
99.11	71.03	195.46	145.6	329.77	246.0
101.58	73.24	198.52	147.8	335.05	250.1
104.56	75.65	201.57	150.1	340.30	253.9
107.54	78.02	204.63	152.3		

$u_r(C_p°(T))$ = ±2% ($5 < T \langle 2\,0)$ K; ±0.5% ($20 < T \langle 4\,0)$ K; ±0.2% ($T > 40$ K), $u(T)$ = 0.01 K, $u_r(p)$ = ±1% (level of confidence = 0.68).