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Short communication

Heat capacity, enthalpy and entropy of Li_2CO_3 at 303.15–563.15 K

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Abstract

Measurements of the heat capacity of lithium carbonate were carried out with a heat conduction calorimeter in the temperature range of 303.15–563.15 K at atmospheric pressure. The temperature dependence of the heat capacity is

$$C_p\ (\mathrm{J\,mol^{-1}\,K^{-1}}) = 92.80 + 0.09T - 1.91 \times 10^6 T^{-2}.$$

The thermodynamic functions with reference temperature 298.15 K, calculated in the same temperature range are:

$$H_T - H_{298}\ (\mathrm{kJ\,mol^{-1}}) = -48.92 + 0.14T + 6.68 \times 10^5 T^{-2}, \quad S_T - S_{298}\ (\mathrm{J\,mol^{-1}\,K^{-1}}) = -53.73 + 0.24T - 1.55 \times 10^6 T^{-2}.$$

Keywords: Heat capacity; Lithium carbonate; Enthalpy; Entropy; Calorimetry

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1. Introduction

Lithium carbonate (Li_2CO_3) is a white, hygroscopic powder used in ceramics and porcelain glazes, varnishes, dyes, pharmaceuticals [1], in coating arc welding electrodes [2], battery alloys and in aluminium production [3].

The heat capacity of Li_2CO_3 was previously determined at 16–300 K by Brown and Latimer [4].

2. Experimental/materials and methods

The lithium carbonate was analytical reagent grade. Sample was oven-dried at 383.15 K and stored in desiccator. The mass of the sample was 3.5 ± 0.5 g.

DTA and TG measurements were performed to find any phase transitions or thermal anomaly. Lithium carbonate was stable in the whole measured temperature range.

A C80 calorimeter (SETARAM, France) was used with a heating rate of $0.5\,\mathrm{K\,min^{-1}}$, from 303.15 to 563.15 K. The calorimeter was tested with a standard sample of sapphire and the accuracy of heat capacity measurements was better than 3%. The calorimeter was calibrated electrically using the Joule-effect calibration unit supplied by Setaram.

The thermal increment method was chosen for the measurement of heat capacity. In this method the small heating step 2 K was used at each temperature. The sample is heated in a calorimeter and the heat flow detected by the heat flux transducer is directly proportional to its heat capacity. In practice, two successive tests are necessary: the first test with empty cells (measure and reference) and the second test with the sample in the measure cell, the reference cell remaining empty. Experimental conditions must be strictly identical for both tests. The heat flow deviation between two curves is directly proportional to the heat capacity of the sample.

3. Results and discussion

The experimental molar heat capacities of Li_2CO_3 are listed in Table 1.

The experimental molar heat capacity was fitted with a polynomial Eq. (1) in temperature (T). This function was further used for calculation of enthalpy and entropy and the final parameters of the polynomial equations are listed in Table 2:

$$Y(C_p, H_T - H_0, S_T - S_0) = a + b \times T + c \times T^{-2}. \tag{1}$$

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Table 1
Thermodynamic data of Li_2CO_3

T (K)	C_p (J mol^{-1} K^{-1})
303.15	99.89 ± 0.66
323.15	100.98 ± 0.88
343.15	107.69 ± 1.07
363.15	111.21 ± 1.12
383.15	115.61 ± 1.33
403.15	116.88 ± 2.48
443.15	120.05 ± 3.88
483.15	129.08 ± 1.95
533.15	132.77 ± 2.98
563.15	137.29 ± 3.23

Table 2
Parameters of polynomial equation of thermodynamic function at 303.15–563.15 K

Par.	C_p (J mol^{-1} K^{-1})	$H_T - H_0$ (kJ mol^{-1})	$S_T - S_0$ (J mol^{-1} K^{-1})
a	92.80 ± 15.13	−48.92 ± 0.73	−53.73 ± 1.89
b	0.09 ± 0.02	0.14 ± 0.01	0.24 ± 0.01
c	$(-1.91 \pm 0.82) \times 10^6$	$(6.68 \pm 0.39) \times 10^5$	$(-1.55 \pm 0.11) \times 10^6$

$T_0 = 298.15$ K.

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