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Comprehensive thermodynamic study of methylprednisolone

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ABSTRACT

In the present work the temperature dependence of heat capacity for methylprednisolone has been measured for the first time over the temperature range from 6 to 350 K using by precision adiabatic vacuum calorimetry. Based on the experimental data, the thermodynamic functions of the methylprednisolone, namely, the heat capacity, enthalpy $H°(T) - H°(0)$, entropy $S°(T) - S°(0)$ and Gibbs function $G°(T) - H°(0)$ have been evaluated from the experimental values for the range from $T \to 0$ to 350 K. Standard molar enthalpy of combustion (-11898.9 ± 6.7) kJ·mol^{-1} of the methylprednisolone was measured for the first time using high-precision combustion calorimeter. The standard molar enthalpy of formation in the crystalline state (-1045.8 ± 7.3) kJ·mol^{-1} of compound at 298.15 K was derived from the combustion experiments. The standard molar enthalpy of sublimation at 298.15 K (194.5 ± 2.2) kJ·mol^{-1} was measured by using the quartz-crystal microbalance (QCM). Using combination of the adiabatic and combustion calorimetry with the result from QCM, the thermodynamic functions of the methylprednisolone at $T = 298.15$ K and $p = 0.1$ MPa have been calculated.

1. Introduction

Methylprednisolone (CAS 83-43-2) is a glucocorticoid. Methylprednisolone is used to treat many different inflammatory conditions like arthritis, lupus, psoriasis, ulcerative colitis, allergic disorders, gland (endocrine) disorders, and conditions that affect the skin, eyes, lungs, stomach, nervous system, or blood cells. The locally injected methylprednisolone delivered by chitosan-β-glycerophosphate hydrogel might be a promising treatment for facial nerve damage [1]. This work is a continuation of systematic studies of bioactive compounds. Recently [2–7], we have investigated the thermodynamic properties of vitamins and steroid hormones. Among the goals of this work is the calorimetric determination of the standard thermodynamic functions of the methylprednisolone with the further purpose of describing biochemical and industrial processes with its participation.

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2. Experimental

2.1. Sample

Methylprednisolone was purchased from company Hongsu Fan. The absence of water in Methylprednisolone was determined by Karl Fischer titration. The certificate (purity control performed by mass spectrometry (Fig. 1S) with a preliminary chromatographic separation) and Karl Fischer titration led us to conclude that the methylprednisolone sample studied (the content of impurities 0.1 wt.%) was an individual crystalline compound (Table 1S).

2.2. Apparatus and measurement procedure

To measure the heat capacity C_p^o of the tested substance in the range from 6 to 350 K a BKT-3.0 automatic precision 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 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 rising to 40 K, and was equal to ±0.2% at $T > 40$ K.