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Thermodynamic properties of methylprednisolone aceponate

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ABSTRACT

In the present work, temperature dependence of heat capacity of methylprednisolone aceponate has been measured for the first time over the range from 7 K to 346 K by precision adiabatic vacuum calorimetry. Based on the experimental results, the thermodynamic functions of the methylprednisolone aceponate, 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/K → 0–333. The enthalpy of combustion (−14304.4 ± 9.1) kJ·mol^{-1} of the methylprednisolone aceponate was determined for the first time using high-precision combustion calorimeter. The standard molar enthalpy of formation in the crystalline state (−1465.3 ± 9.8) kJ·mol^{-1} of compound at 298.15 K was derived from the combustion experiments. Using a combination of the adiabatic and combustion calorimetry results the thermodynamic functions of formation of the folic acid dihydrate at T = 298.15 K and p = 0.1 MPa have been calculated.

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1. Introduction

Methylprednisolone aceponate (CAS: 86401-95-8) is a non-halogenated diester of 6α- methylprednisolone. The introduction of two ester groups results in a molecule with increased lipophilicity and enhanced penetration into skin. Estimations of anti-inflammatory activity in humans suggest that it is a protein glucocorticosteroid. In humans its atrophogenic potential, as assessed by skin thinning and telangiectasia, appears lower than, or similar to, that of other agents belonging to this class such as betamethasone valerate and mometasone furoate [1].

This work is a continuation of systematic studies of bioactive compounds. Earlier in the articles [2–6], we have investigated the thermodynamic properties of vitamins and hydrocortisone acetate. It should be noted that the temperature dependence of the heat capacity of the steroid hormones has not been studied previously. The goals of this work include calorimetric determination of the standard thermodynamic functions of the methylprednisolone aceponate (steroid hormone) with the purpose of describing biochemical and industrial processes with its participation.

2. Experimental

2.1. Sample

Methylprednisolone aceponate was purchased from Fluka. For phase identification, an X-ray diffraction pattern of the methylprednisolone aceponate sample was recorded on a Shimadzu X-ray diffractometer XRD-6000 (CuKα radiation, geometry θ-2θ) in the 2θ range from 5° to 60° with scan increment of 0.02°. The absence of water in methylprednisolone aceponate was determined by Karl Fischer titration. The X-ray data, certificate (purity control performed by mass spectrometry) and Karl Fischer titration led us to conclude that the methylprednisolone aceponate sample studied (the content of impurities 0.1 wt%) was an individual crystalline compound (trigonal modification [7]).

2.2. Apparatus and measurement procedure

To measure the heat capacity C_p° of the tested substance in the range from 7 K to 346 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

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