

THERMAL EFFECTS OF CAESIUM ACETATE SOLVATES DISSOLUTION AND THE RELATIONSHIP OF STRUCTURE AND PROPERTIES

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Submitted work is part of a major study of water-electrolyte systems containing alkali metal acetates. It is devoted to obtaining enthalpy characteristics of the dissolution processes of caesium acetate solvates by calorimetry. Recently, the development of chemistry of highly concentrated aqueous solutions has received a new impetus – this is due both to the search for environmentally friendly electrolytes in new generation batteries (water-in-salt WIS systems) and to the intensive study and application of inorganic ionic liquids (ionic liquids IL) [1,2]. Salts of alkaline or alkaline earth metals with a non-toxic counterion and high solubility in water are ideally suited as objects for creating such systems. One of them is caesium acetate. However, CsOAc has an extremely high hygroscopicity, which makes it difficult to work with it and prepare mixtures based on it. At the same time, CsOAc forms solvates with acetic acid of various compositions, which are less hygroscopic and easy to obtain.

We suppose that systems based on caesium acetate solvates can be considered promising for creating highly concentrated mixtures with the properties of WIS or IL. Because the availability of additional acetate ions in such systems promotes the binding of free water molecules, which will make it possible to achieve the WIS state at lower salt concentrations.

The physicochemical properties of the known caesium acetate solvates are practically not represented in the literature. As a result of this work, the thermal effects of the process of dissolution of solid caesium acetate and its solvates CsOAc·HOAc, 3CsOAc·5HOAc in water were obtained: the enthalpy of dissolution, the energy of crystalline lattices, and the enthalpy of ions hydration. Using quantum calculations, enthalpy characteristics of the intermediate processes of gaseous ions formation were obtained, which made it possible to estimate the hydration energy of the hydroxonium ion. The resulting thermal effects correlate with the structural features of the solid solvates.

1. Shigang C., Rong L., John H., et al. // Effect of cation size on alkali acetate-based ‘water-in-bisalt’ electrolyte and its application in aqueous rechargeable lithium battery. *Applied Materials Today*. 20. 2020.

2. Maria R., Jeremy I., David G., et al. // Concentrated mixed cation acetate “water-in-salt” solutions as green and low-cost high voltage electrolytes for aqueous batteries. *Energy Environ. Sci.*, 2018.

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