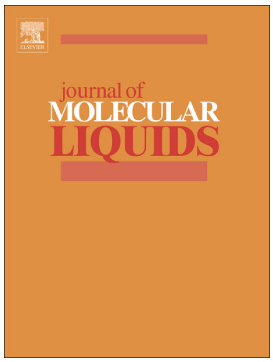

The energetics of solvation and ion-ion interactions in prospidium chloride aqueous solutions

A.V. Kustov, O.A. Antonova, N.L. Smirnova, A.A. Kladiev, A.A. Kladiev, T.V. Kudayarova, M.S. Gruzdev, D.B. Berezin

PII: S0167-7322(18)31353-9
DOI: doi:10.1016/j.molliq.2018.04.118
Reference: MOLLIQ 9021

To appear in: *Journal of Molecular Liquids*

Received date: 15 March 2018
Accepted date: 23 April 2018

Please cite this article as: A.V. Kustov, O.A. Antonova, N.L. Smirnova, A.A. Kladiev, A.A. Kladiev, T.V. Kudayarova, M.S. Gruzdev, D.B. Berezin , The energetics of solvation and ion-ion interactions in prospidium chloride aqueous solutions. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Molliq(2017), doi:10.1016/j.molliq.2018.04.118

The energetics of solvation and ion-ion interactions in prospidium chloride aqueous solutions

A.V. Kustov[1,2*], O.A. Antonova[1,2], N.L. Smirnova[1,2], A.A. Kladiev[3], A.A. Kladiev[4], T.V. Kudayarova[2], M.S. Gruzdev[1], D.B. Berezin[2]

[1] *G.A. Krestov Institute of Solution Chemistry, Russian Academy of Sciences, Russia*
[2] *Ivanovo State University of Chemistry and Technology, Ivanovo, Russia*
[3] *Biotechnological TNK company, Moscow, Russia*
[4] *Moscow State University, Moscow, Russia*

*Corresponding author.
E-mail address: kustov@isuct.ru (A. Kustov**)**

A B S T R A C T

This paper focuses on the first accurate thermochemical study of hydration and interactions of the well-established cytostatics "Prospidine" (prospidium chloride) in water. Enthalpies of solution of the drug have been determined with the isoperibol solution calorimeter at 298 and 313 K and heat capacities of solid prospidine have been obtained with the NETZSCH DSC calorimeter at 275-355 K. Standard enthalpies and heat capacities of solution, partial molal heat capacities at an infinite dilution as well as enthalpic parameters of solute-solute pair interactions have been computed using the Redlich-Rosenfeld-Meyer-type equation and discussed in terms of solute-solvent and solute-solute interactions in a liquid phase.

Keywords:
Prospidium chloride; Water; Thermochemistry of solution; Hydration; Ion-ion interactions

1. Introduction

"Prospidine" or "Prospidium chloride" (3,12-bis(3-chloro-2-hydroxypropyl)-3,12-diaza-6,9-diazoniadispyro[5,2,5,2]hexadecane dichloride, see Figure 1) is a water-soluble and low toxic cytostatic agent for treating both primary tumors and their metastases [1-3]. For many cases it allows to achieve the total disappearance of initial malignancy or at least to decrease strongly a tumor size. The mechanism of action of the drug is believed to be twofold [2,4]. The first component is connected with decreasing the cellular membrane permeability for important inorganic ions and vital organic species, which leads to the disruption of normal cell activity and evokes apoptotic cell death. The second one is in the direct binding of organic cations with DNA or RNA molecules inducing fatal cell damage and further programmable cell death.