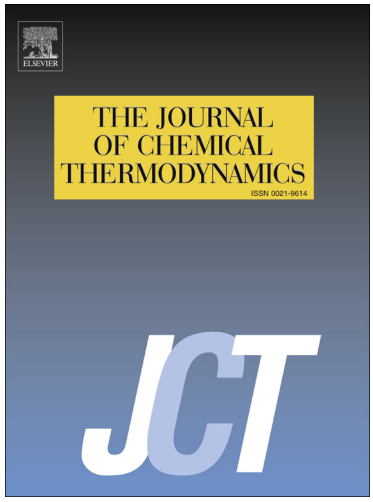

Calorimetric Study on the Interaction of Didecyldimethylammonium and Decyltrimethylammonium Cations with Native Cyclodextrins in Water

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PII: S0021-9614(16)00049-5
DOI: http://dx.doi.org/10.1016/j.jct.2016.01.027
Reference: YJCHT 4542

To appear in: *J. Chem. Thermodynamics*

Received Date: 22 October 2015
Revised Date: 24 January 2016
Accepted Date: 29 January 2016

Please cite this article as: D. Ondo, Calorimetric Study on the Interaction of Didecyldimethylammonium and Decyltrimethylammonium Cations with Native Cyclodextrins in Water, *J. Chem. Thermodynamics* (2016), doi: http://dx.doi.org/10.1016/j.jct.2016.01.027

Calorimetric Study on the Interaction of Didecyldimethylammonium and Decyltrimethylammonium Cations with Native Cyclodextrins in Water

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Abstract

The interaction of two decylammonium surfactants, didecyldimethylammonium bromide (D) and decyltrimethylammonium bromide (S), with native α-, β-, and γ-cyclodextrins (CDs) was systematically examined using the isothermal titration calorimetry (ITC). The measured heat data at five temperatures ranging from (283.15 to 318.15) K were treated simultaneously allowing the estimation of thermodynamically consistent temperature dependence of the equilibrium constant, the enthalpy and heat capacity for the formation of inclusion complexes. The heat data for D/α-CD interaction were analysed by the sequentional binding model with 1:1, 1:2 and 1:3 (D:α-CD) stoichiometries, while other surfactant-CD combinations were examined using only 1:1 and 1:2/2:1 stoichiometries. Thermodynamic quantities for complexation are discussed in terms of structural features and their temperature dependence. The enthalpy-entropy compensation analysis of selected surfactant-CD 1:1 complexes obeys a linear relationship. Due to entropical stabilization caused to a high extent by alkyl chain desolvation, the $>C_{10}$ bearing ions were found not to follow the patterns previously published on binding of other guests. The prediction of the binding thermodynamic properties of D/CD from the S/CD interaction was tested and found surprisingly accurate.

Keywords:
Didecyldimethylammonium, Decyltrimethylammonium, Water, Cyclodextrin, Inclusion complex stability, Binding thermodynamics

1. Introduction

Quaternary ammonium surfactants (QAS), are organic compounds that contain at least one surface active chemical group covalently bonded to a positively charged nitrogen. Due to their resemblance with membrane phospholipids and their likely adsorption to cell surfaces, double chain surfactants constitute a special class of QAS. One of widely used double alkyl chain ammonium cation is didecyldimethylammonium. This cation has been found to combine with chloride and propionate as biocides [1], with various anions leading to ionic liquids [2–4] or even to pharmaceutically active ingredients [5]. Given its widespread commercial use as biocide, traces of didecyldimethylammonium cation can be found in the environment where it is suspected to be toxic not only to aquatic life [6, 7]. This calls for new formulations design with biocompatible interaction partners. Good candidates for such partnership are cyclodextrins, which are agents of choice for toxicity reduction, solubility and release control [8].

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