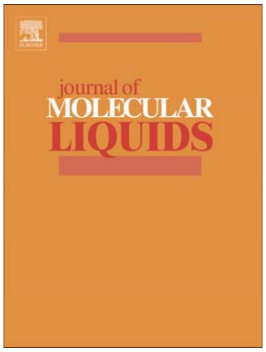

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PII: S0167-7322(16)32836-7
DOI: doi:10.1016/j.molliq.2016.12.111
Reference: MOLLIQ 6801

To appear in: *Journal of Molecular Liquids*

Received date: 21 September 2016
Revised date: 29 November 2016
Accepted date: 23 December 2016

Please cite this article as: V.S. Fundamensky, T.A. Kochina, Y.A. Kondratenko, A.A. Zolotarev, Yu.G. Vlasov, I.S. Ignatyev, Ionic liquids based on Triethanolammonium Salts of Dicarboxylic Acids (oxalic, malonic, succinic). Crystal structure and cation-anion interaction, *Journal of Molecular Liquids* (2017), doi:10.1016/j.molliq.2016.12.111

Ionic liquids based on Triethanolammonium Salts of Dicarboxylic Acids (oxalic, malonic, succinic). Crystal structure and cation-anion interaction.

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Keywords: triethanolammonium salts; triethanolamine; dicarboxylic acid; X-ray diffraction structure; IR spectra; protic ionic liquids.

Abstract

The series of ionic liquids based on triethanolammonium salts of dicarboxylic acids (oxalic, malonic and succinic) was synthesized, characterized by IR and H^1, C^{13} NMR spectroscopy, thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC). Their structure was determined by single-crystal X-ray diffraction. It was found that triethanolammonium $[(HOCH_2CH_2)_3NH]^+$ cations in salts of oxalic (**1**), malonic (**2**) and succinic acids (**3**) containing monoanions $[OOC(CH_2)_nCOOH]^-$ (n=0-2) have the *endo* conformation and the ammonium proton (H_{am}) resides inside the “lampshade” formed by three CH_2CH_2OH branches connected with nitrogen atom. The asymmetric cell of the second modification of the succinic acid salt (**4**) includes two triethanolammonium cations and a succinate dianion $[(HOCH_2CH_2)_3NH]_2{}^+[OOC(CH_2)_2COO]^{2-}$. In this salt (**4**) one CH_2CH_2OH branch of the triethanolammonium cation is rotated around the N-C bond (*endo-exo* conformation) and forms infinite TEA chains. This pattern was firstly found in organic salts of TEA. The obtained results show that different structures of triethanolammonium cations in the salts of dicarboxylic acids have significant influence on the cation-anion interaction.

Introduction

Interaction of trithanolamine (TEA) with protic acid leads to the dissociation of the acid, the proton transfer to a nitrogen atom of TEA and the formation of triethanolammonium salts known as protaranes [1]. Protatranes, consisting of bulky organic cations $[(HOCH_2CH_2)_3NH]^+$ and