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

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Abstract

The series of ionic liquids based on triethanolammonium salts of dicarboxylic acids (oxalic, malonic and succinic) was synthesized, characterized by IR and ^1H , ^{13}C 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 $[(\text{HOCH}_2\text{CH}_2)_3\text{NH}]^+$ cations in salts of oxalic (**1**), malonic (**2**) and succinic acids (**3**) containing monoanions $[\text{OOC}(\text{CH}_2)_n\text{COOH}]^-$ ($n=0-2$) have the *endo* conformation and the ammonium proton (H_{am}) resides inside the “lampshade” formed by three $\text{CH}_2\text{CH}_2\text{OH}$ 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 $[(\text{HOCH}_2\text{CH}_2)_3\text{NH}]_2^+[\text{OOC}(\text{CH}_2)_2\text{COO}]^{2-}$. In this salt (**4**) one $\text{CH}_2\text{CH}_2\text{OH}$ 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 triethanolamine (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]. Protaranes, consisting of bulky organic cations $[(\text{HOCH}_2\text{CH}_2)_3\text{NH}]^+$ and

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