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BOOK OF ABSTRACTS

St Petersburg University

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Abstracts are presented in the author's edition with minimal technical corrections.

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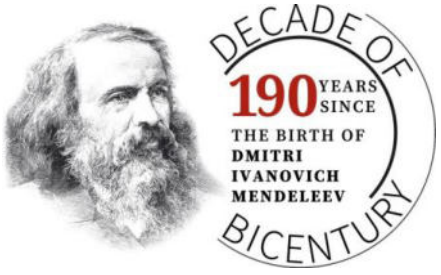

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PECULIARITIES OF COORDINATION OF WATER MOLECULES IN MIXTURES OF IONIC LIQUIDS AND WATER, CONTAINING Al^{3+} CATION

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Electrolytes based on solutions of aluminum salts in ionic liquids (ILs) can be used in metal-ion batteries. These salts exist usually in a form of the crystalline hydrates, i.e. contain sufficient amount of water. As a result, one has mixed "IL – water" solvents, and water cannot be removed from the aluminum solvation shell by standard dehydration procedures [1, 2]. Earlier the mixtures of IL [bmim]Cl (1-butyl-3-methylimidazolium chloride, $C_8H_{15}N_2Cl$) and aluminum chloride ($AlCl_3$) with different water amount were investigated [3]. The existence of different solvate complexes of Al^{3+} with Cl^- in considered systems was detected. In addition, the characteristic times of exchange processes were estimated according to NMR data. It was demonstrated that the Al^{3+} cation can strongly hold more than 6 H_2O molecules in its nearest surroundings.

This work is an extension of the study of the state of water molecules in triple systems "aluminum salt/IL/water", namely: $Al(NO_3)_3$*nH_2O in EAN (ethylammonium nitrate) and $AlCl_3$*nH_2O in EACl (ethylammonium chloride).

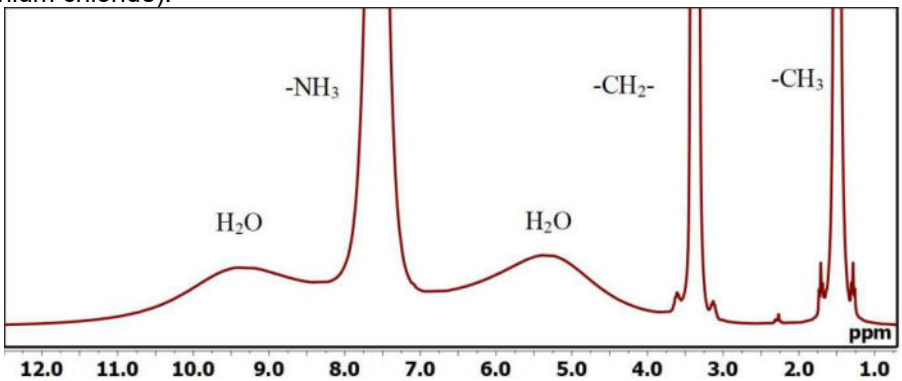

Figure 1. The ^1H spectrum (300 MHz) for the "$Al(NO_3)_3$ – EAN – H_2O" mixture at 298 K.

The samples were prepared by mass method using crystalline hydrates of aluminum chloride and aluminum nitrate. Due to low commercial availability, EAN and EACl ionic liquids have been synthesized. The composition and purity of the synthesized ILs were controlled by ^1H and ^{14}N NMR. Water content in the solutions was changed using a standard drying procedure under low pressure at 80°C and controlled by ^1H spectra.

NMR measurements were carried out using Bruker Avance III 500 MHz Spectrometer at 500 MHz for ^1H nuclei, 130 MHz for ^{27}Al nuclei, and 36 MHz for ^{14}N nuclei in the temperature range between 293 and 363 K (with increment 10 K). Some preliminary measurements of ^1H spectra were also made by Bruker DPX 300 MHz Spectrometer at 300 MHz. In all studied solutions several water lines were recorded (see the example in Fig. 1). In order to interpret the obtained experimental data quantum chemical calculations were performed by Gaussian 09 Revision D.01 [4].

References

[1] *J. Mol. Liq.* **2019**, *278*, 239.
[2] *Magn. Reson. Chem.* **2021**, *60(2)*, 221.
[3] *J. Phys. Chem. Lett.* **2023**, *14*, 9324.
[4] Gaussian 09, Revision D.01. Gaussian, Inc., Wallingford CT, **2013**.

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