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Local Ion Hydration Structure in Aqueous Imidazolium-Based Ionic Liquids: The Effects of Concentration and Anion Nature

Marina V. Fedotova^{*1}, Sergey E. Kruchinin¹, and Gennady N. Chuev²

¹*G.A. Krestov Institute of Solution Chemistry, the Russian Academy of Sciences, Akademicheskaya st., 1, Ivanovo, 153045 Russia*

²*Institute of Theoretical and Experimental Biophysics, the Russian Academy of Sciences, Institutskaya st., Pushchino, Moscow Region, 142290 Russia*

**Email address: hebrus@mail.ru (M. V. Fedotova)*

The effects of concentration and anion nature on the ion hydration structure in aqueous imidazolium-based ionic liquids (IL), [EMIM][EtSO₄], [EMIM][Cl], and [EMIM][Gly], were studied using integral equation theory in the one- and three-Dimensional Reference Interaction Site Model (1D- and 3D-RISM) approaches. The concentration behavior of ion hydration has been examined for the [EMIM][EtSO₄]-water mixture. It was found that the main concentration effect is in significant dehydration of both the cation and the anion with increasing IL content from 0.005 M to 4.714 M. At the same time, at low IL content all ions under study are well hydrated with stronger interactions between the anions and water in comparison with the cation and water. The obtained data indicate strengthening of anion-water interactions in the sequence [EtSO₄]⁻ < [Gly]⁻ < [Cl]⁻.

Key words: ionic liquid; aqueous solution; ion; hydration structure

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