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On the Properties and Structure of 2-Hydroxyethylammonium Formate Ionic Liquid

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ABSTRACT: This work reports an experimental and theoretical study on 2-hydroxyethylammonium formate (2-HEAF) protic ionic liquid. Relevant physicochemical properties, density, speed of sound, dynamic viscosity and surface tension, were measured as a function of temperature in the 298.15 to 323.15 K range. Likewise, the solubility parameter of 2-HEAF was estimated at different temperatures according to Eyring's approach. Theoretical studies using Density Functional Theory and molecular dynamic simulations were carried out for the nanoscopic characterization of the selected ionic liquid and its relationship with macroscopic properties. The interfacial behavior regarding to air interfaces was also studied using molecular dynamics simulations. The possible cytotoxicity of 2-HEAF was theoretically studied using molecular dynamics considering the interaction of this ionic liquid with model lipidic biomembranes formed by 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine. The reported results lead to a full characterization of this representative protic ionic liquid from micro and macroscopic viewpoints including toxicity issues, and thus

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