

The Study of Solute–Solvent Interactions in 1-Butyl-3-Methylimidazolium Hexafluorophosphate + 2-Pyrrolidone from Volumetric, Acoustic, Optical and Spectral Properties

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Journal of Solution Chemistry **47**, 430–448 (2018)

184 Accesses | **3** Citations | [Metrics](#)

Abstract

The density (ρ), speed of sound (u) and refractive index (n_D) of [Bmim][PF₆], 2-pyrrolidone and their binary mixtures were measured over the whole composition range as a function of temperature between (303.15 and 323.15) K at atmospheric pressure. Experimental values were used to calculate the excess molar volumes (V_m^E) ($\diamond\diamond\diamond^E$), excess partial molar volumes (\bar{V}_m^E) ($\diamond\diamond\diamond^E$), partial molar volumes at infinite dilution ($\bar{V}_m^{E,\infty}$) ($\diamond\diamond\diamond^{E,\infty}$), excess values of isentropic compressibility (κ_S^E) ($\diamond\diamond\diamond^E$), free length (L_f^E) ($\diamond\diamond\diamond_f^E$) and speeds of sound (u^E) ($\diamond\diamond\diamond^E$) for the binary mixtures. The calculated properties are discussed in terms of molecular interactions between the components of the mixtures. The results reveal that interactions between unlike molecules take place, particularly through intermolecular hydrogen bond formation between the C₂–H of [Bmim][PF₆] and the carbonyl group of pyrrolidin-2-one. An excellent correlation between thermodynamic and IR spectroscopic measurements was observed. The observations were further supported by the Prigogine–Flory–Patterson (PFP) theory of excess molar volume.