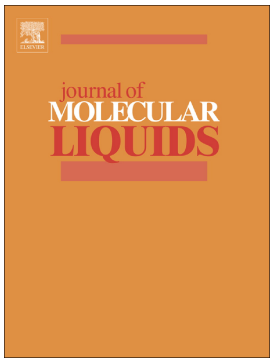

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Insights into interactions between 1-butyl-3-methylimidazolium dicyanamide and molecular solvents: γ-valerolactone, γ-butyrolactone and propylene carbonate. Volumetric properties and MD simulations

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Abstract

Experimental densities of the binary mixtures containing 1-butyl-3-methylimidazolium dicyanamide ionic liquid, $[C_1C_4im][DCA]$ and molecular solvent: γ-valerolactone (γVL) or propylene carbonate (PC) were measured at temperatures from (293.15 to 313.15) K and at a pressure of 0.1 MPa over the whole composition range. Related excess molar volumes were calculated and fitted using Redlich-Kister's polynomial equation and compared with previously measured IL + γ-butyrolactone (γBL) mixture. Obtained values are negative in the whole range of ionic liquid mole fraction and at all temperatures. Molecular dynamics simulations were applied to quantify the intermolecular interactions in pure liquids and binary mixtures, hydrogen bond, dipole-dipole and stacking interactions. Excess molar volumes obtained from MD simulations follow the trend observed in the experiment. Orientational correlations were characterized by several combined angular and distance distribution functions between first neighbour molecules. Results suggest that strength of solvent-solvent interactions plays a significant role in the observed difference in volumetric properties of these binary mixtures. Calculated hydrogen bond geometry indicates that the hydrogen bond interaction in the three molecular solvents is weak and follows the order PC > γBL > γVL.

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