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Ionic liquids as solutes in molecular solvents: Universal phenomenological model of interactions

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Ionic liquids (ILs) form the promising class of non-molecular universal solvents which are highly stable at room temperatures. They are nonvolatile at atmospheric pressure and such a fundamental thermophysical characteristic as the vapor pressure seems to be negligible for them. Its absence as well as the supposedly undeterminable inherent microscopic structure of ILs (it admits the usage of the quite different non-molecular models including the ionic and cluster ones) is the main obstacle to investigate, in detail, the physical mechanism of solubility. In this context, the study of neat ILs and of their dilute solutions in usual molecular solvents might provide the useful information about types of interactions between the constituent particles. One needs also the relatively simple but still rather flexible model of a pair potential to interpret adequately the above information. The main aim of present work is to argue that the novel essentially molecular approach and the respective common format of the fluctuation equation of state (FT-EOS) are able to predict the phase transitions of IL-containing solutions and/or of neat IL-solvents even in the regions of criticality. Its determinative feature is the concept and methodology of global fluid asymmetry (GFA) existing between the equilibrium or metastable phases of gas, liquid and solid at any subcritical temperatures. In this work the author intends to demonstrate that the frequent suggestion that ILs and such ionic systems as liquid metals are not subject to the Principle of Corresponding States (PCS) is most likely wrong. More accurately, both types of gas-liquid (g,l) and liquid-liquid (l,l) phase transitions either in the IL-containing solutions or in the neat molecular and ionic solvents can be analyzed and simulated (at least, preliminarily) in terms of the common finite-range Lennard-Jones potential with the given effective parameters. To estimate latter the reference measurable atmospheric isobar for each pure component might be extrapolated in the T, ρ -plane up to the limits of zero-temperature and zero-density. The respective characteristic parameters of "cold volume" v_0 ($T \rightarrow 0$) and of "ideal-plasma" temperature T_0 ($\rho \rightarrow 0$) are directly connected with the hypothesized critical parameters of thermally-unstable ILs and heavy n-alkanes, for example, as well as with the actual critical parameters of molecular solvents. In this turn, this connection provides the thermodynamically-consistent effective diameter and well-depth of the underlying LJ-interactions without any appeals to their supposedly electrostatic physical nature. In other words, since the complexity of the discussed problem is so high and the search of an adequate force-field for ILs is a quite formidable task, the use of appropriate phenomenological methodologies seems to be worthwhile. The further more detailed investigations of ILs-containing solutions may be based on such preliminary PCS-results.

Biography

Vitaly B Rogankov has completed his PhD-equivalent in 1979 and his degree of Dr. Phys.-Math. Sci. from Leningrad University in 1991. He is the Head of the Applied Physics and Electrotechnics Department. He has published more than 100 papers in reputed journals. He works actively at the present time in the area of Green Chemistry and of the relevant problems arising at the theoretical study of ionic heat-transfer and thermal-storage liquids.

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