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Data Processing of Experimental Results in Systems of Ionic Liquids. Pitfalls and Challenges.

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In previous work a number of physico-chemical properties of systems with ionic liquids (ILs) was presented. A group of *quasi-isomeric* 1-butyl-3-alkylimidazolium bistriflimides, where alkyl stands for pentyl, isopentyl, 3-pentyl, and cyclopentyl was selected in view of the influence that structural changes might have in tailoring the physico-chemical properties of ILs. Isobaric heat capacity, density, viscosity, electrical conductivity, or mutual solubility with water have been measured for the studied ionic liquids as a function of temperature and the effect of isomerization was clearly observed.

Raw data can in some cases be sufficient to assess the relation between the chemical structure and properties of a substance. This was *e.g.* the case for the density and heat capacity data in present series. However, to calculate some derived properties, *e.g.* the isobaric expansivity, data regressed with a suitable function are essential. In this example it was found, that the quality and adequacy of the density data correlation plays a crucial role in determining the isobaric expansivity temperature dependency. If the correlation is incorrect (which may not be evident at first sight), the derived properties often show physically nonsensical shapes. To obtain the best results, a robust linear regression along the gnostic influence function based on mathematical gnostics¹ was applied to optimize the correlation parameters for the experimental data.

In this contribution, a correlation of liquid-liquid equilibrium data in binary systems of the studied ionic liquids with water was also carried out. To correlate the data on mutual miscibility of ionic liquids with water the Non-Random Two-Liquid (NRTL)² equation was used in the following form:

$$Q = \frac{G^E}{RT} = x_1 x_2 \left(\frac{\tau_{21} g_{21}}{x_1 + x_2 g_{21}} + \frac{\tau_{12} g_{12}}{x_2 + x_1 g_{12}} \right) \quad (1)$$

where $\tau_{ij} = a_{ij}/T$ and $g_{ij} = \exp(-\alpha\tau_{ij})$. This model of excess Gibbs free

energy is based on theoretical concepts of the description of the system on the molecular level. Consequently, its parameters have a physical meaning. As opposed to empirical models, NRTL allows for a more reliable description of multicomponent systems using only binary parameters a_{ij} . However, the NRTL equation is not linear in its parameters, a non-linear optimization procedure is therefore needed. The parameter τ_{ij} is temperature-dependent, whereas parameter a_{ij} is usually fixed to a constant value. However, this often doesn't lead to a sufficiently good description of binodal curves. A temperature dependence is then used for the a_{ij} parameter, which makes the optimization more difficult. Fortunately, even simple functional forms such as a linear dependence can bring about a significant improvement in the quality of the data fitting. In this study some other forms of temperature dependency of parameter a_{ij} were also tested.

References

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