Simple Prediction of Physical Properties of Ionic Liquids: The Residual Volume Approach.

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A new method for the prediction of fundamental physical properties of ionic liquids (ILs) is proposed. The *residual volume approach* allows the estimation of density, viscosity and ionic conductivity of unknown ILs, using a simple linear correlation between a given property and newly defined substituent parameters – β^X. The proposed method has been developed for the density estimation of 50 *n*-alkyl substituted imidazolium and tetraalkylamonium ILs homologous series and has been extended for the estimation of viscosity and ionic conductivity which also correlate linearly with the corresponding β^X. In addition, the parameters β^X are temperature and pressure independent, which allows the prediction of these values at any temperature and pressure. The results demonstrate the influence of *n*-alkyl substituents on the property changes, which show the possibility for fine-tuning density, viscosity and ionic conductivity of ILs by slight variation in the structure of a given anion-cation combination.

References

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