EVALUATION AND PREDICTION OF THE ENTHALPY OF VAPORIZATION FOR ROOM-TEMPERATURE IONIC LIQUIDS

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The enthalpy of vaporization is one of key quantities for the compounds involved in chemical production. For ionic liquids (ILs) the experimental determination of this quantity is a complicated task, but application of these compounds would require at least the estimated values of the enthalpy of vaporization. In this work we collected the experimental data on the enthalpy of vaporization for aprotic ILs published by March 2014 and proposed a number of predictive procedures for Δ_vap H_m.

The database included 89 ILs whose enthalpy of vaporization was determined mainly from their temperature-dependent vaporization into vacuum either directly or through a small orifice. The uncertainties of all the data were evaluated and the dataset of the most reliable Δ_vap H_m values for 68 ILs was obtained. With the use of the evaluated data a number of datasets for the development of correlations and additive schemes was generated. It was found that the enthalpies of vaporization for ILs correlate with density (molar volume) and surface tension. The form of the obtained equations was obtained with the use of symbolic regression. For the most effective correlations the r.m.s. deviation of the calculated values from the experimental ones was about 5 kJ·mol⁻¹.

The substitution-based incremental scheme for prediction of the enthalpy of vaporization for imidazolium, pyridinium and pyrrolidinium ILs was developed. In this scheme, the compound of interest is generated in a line of functional group substitutions starting from the base compound 1,3-dimethylimidazolium bis(trifluoromethanesulfonyl)imide. An increment corresponds to each substitution, and the resulting value is a sum of all the increments and the contribution from the base compound. The substitution-based additive scheme demonstrated the r.m.s. deviation of the calculated values from the experimental ones of 2.3 kJ·mol⁻¹, which is several times lower than that for the atom-based group contribution schemes proposed earlier [1,2].

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