Comparison of Experimental Heat Capacity Data of Ionic Liquids with Prediction Methods and Advanced Data Analysis

Čanji, Maja
2019

Comparison of Experimental Heat Capacity Data of Ionic Liquids with Prediction Methods and Advanced Data Analysis

Student: Maja Čanji, MSc.
Supervisor: Ing. Magdalena Bendová, Ph. D.

In spite of many statements on the potential application of ionic liquids, these organic salts present both advantages and disadvantages as to their possible use in real processes. However, some of them show an application potential. This requires their thorough thermophysical characterization. For instance, reliable thermal property data seem to be significantly lacking for pure ionic liquids. Group contribution models (GCMs) are used extensively by chemical engineers to predict the physical and thermodynamic properties of components in industrial processes where little or no experimental data are available. GCMs are based on the assumption that the properties of a compound depend on the functional groups which make up its structure, and that each group provides a fixed contribution towards the properties, irrespective of the species involved. The aim of this work is a comparison of experimental heat capacity data for a series of 1-alkyl-3-methylimidazolium saccharinate ionic liquids (alkyl=butyl, hexyl, octyl, and decyl) obtained by differential scanning calorimetry with heat capacity calculated by several group contribution methods and an in silico method based on COSMO-RS[1–4]. All data, experimental and predicted, will be analyzed by means of mathematical gnostics. Based on the thermodynamics of data and theory of measurement, mathematical gnostics is a novel non-statistical approach towards data uncertainty. A critical assessment of the predicted heat capacity values will thus be carried out.

Acknowledgement

The authors gratefully acknowledge the financial support of the Czech Science Foundation under Grant No. 17-08218S.

References

1. Ge, R.; Hardacre, C.; Jacquemin, J.; Nancarrow, P.; Rooney, D. W. Heat Capacities of Ionic Liquids as a Function of Temperature at

0.1 MPa. Measurement and Prediction. *J. Chem. Eng. Data* **2008**, *53*, 2148–2153.
2. Valderrama, J. O.; Martinez, G.; Rojas, R. E. Predictive model for the heat capacity of ionic liquids using the mass connectivity index. *Thermochim. Acta* **2011**, *513*, 83–87.
3. Ahmadi, A.; Haghbakhsh, R.; Raeissi, S.; Hemmati, V. A simple group contribution correlation for the prediction of ionic liquid heat capacities at different temperatures. *Fluid Phase Equilib.* **2015**, *403*, 95–103.
4. Preiss. P.R.M.U.; Slattery. M.J.; Krossing. I. In silico prediction of molecular volumes, heat capacities and temperature dependent densities of ionic liquids. *Ind. Eng. Chem. Res.* **2009**, *48*, 2290–2296.