**Analyzing the Experimental Thermodynamic Data for Ionic Liquids and their Study as Thermal Energy Storage Materials.**

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2018

Dostupný z http://www.nusl.cz/ntk/nusl-387537

# Analyzing the Experimental Thermodynamic Data for Ionic Liquids and their Study as Thermal Energy Storage Materials

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The aim of this work is to characterize a series of 1-alkyl-3-methyl-imidazolium saccharinate ionic liquids (alkyl standing for butyl, hexyl, octyl, and decyl),[1] analyze the experimental data, and assess their potential application in thermal energy storage.[2]

The characterization of this series of ionic liquids was carried out experimentally by measurements of heat capacity using the differential scanning calorimetry (DSC) and of density by the oscillating-tube densitometry. The experimental data were then analyzed by means of the advanced data analysis methods based on mathematical gnostics.[3] Mathematical gnostics is a novel non-statistical approach to data uncertainty. As such it enables us to evaluate the measurement uncertainty of statistically non-significant data sets containing as few as four datapoints and identify unreliable or outlying data.[4] Also, using a robust regression algorithms along a gnostic influence function, functional dependencies and structure-property patterns can be reliably determined. Modelling based on the COSMO-RS[5] model was used to predict density and heat capacity[6] for the studied ILs and compared with the experimental data.

## References

1. Tonova, I.; Svinyarov, I.; Bogdanov, M.G. Hydrophobic 3-alkyl-1-1methylimidazolium saccharinates as extraction for L-lactic acid recovery. *Sep. Purif. Technol.* **2014**, *125*, 239–246.
2. Mehrkes,. A.; Karunanithi, A. T. Optimal design of ionic liquids for thermal energy storage. *Comput. Chem. Eng.* **2016**, *93*, 402–412.
3. Wagner, Z.; Bendova, M.; Rotrekl, J.; Velisek, P.; Storch, J.; Uchytil, P.; Setnickova, K.; Reznickova, J. Advanced analysis of isobaric heat capacities by mathematical gnostics. *J. Solut. Chem.* **2017**, *46*, 1836–183.
4. Kovanic, P.; Humber, M.B. The economics of information – Mathematical gnostics for data analysis book pp 717 [on-line], 2015. Avail-

able online at http://www.math-gnostics.eu/books [cit 2018-05-15] (5 September 2015)

5. Klamt, A. A Conductor-like screening model for real solvent: A new approach to the quantitative calculation of solvation phenomena. *J. Phys. Chem. A.* **1995**, *95*, 2224–2235.

6. 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.