THERMOPHIL: AN APPLICATION FOR IONIC LIQUIDS PROPERTY ESTIMATION

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Abstract:

Ionic liquids (ILs) are a class of neoteric solvents composed of large organic cations and organic or inorganic anions that cannot form an ordered crystal and thus remain liquid at or near room temperature. The outstanding characteristics of these fluids, and the easy manipulation of their properties due to the possibility of interchange among thousands of cations and anions, make of the ILs "designer" solvents with a wide range of foreseeable applications.

Despite the exponential focus on ILs, both by academia and industry, the availability of thermophysical properties data is still limited and with questionable quality, making difficult the development of correlations and predictive models for these properties. It was however possible after a critical analysis of the available experimental data, complemented with further data measured at our lab to propose a number of predictive methods for the thermophysical and equilibrium properties of ionic liquids.

Based on the correlations and group contribution methods developed at our research group a on-line computer application was developed for the prediction of a number of thermophysical and equilibrium properties such as density, isobaric expansivity and isothermal compressibility, viscosity, surface tension, speed of sound, ionic conductivity, heat capacity, water solubility and carbon dioxide solubility in a wide temperature range.

The application developed will be presented and it will be discussed how it can be used for Computer Aided Molecular Design of Task Specific Ionic Liquids.

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