A Simple Prediction Method for the Surface Tension of Ionic Liquids as a Function of Temperature

Thomas M. Koller [C, S], Corina Steininger, Michael H. Rausch and Andreas P. Fröba
Institute of Advanced Optical Technologies - Thermophysical Properties (AOT-TP), Friedrich-Alexander-University Erlangen-Nürnberg (FAU), Erlangen, Bavaria, Germany
thomas.m.koller@fau.de

Ionic liquids (ILs) are candidates as working fluids in chemical and energy engineering. An important property relevant in connection with wetting, adsorption, absorption, extraction, or mass transfer processes is the surface tension or interfacial tension. For the design of ILs with respect to a special application, simple prediction methods are recommended to handle the broad variety of ILs over a wide range of thermodynamic states. For the development of simple predictions, the large variety of structural and intermolecular effects responsible for the complex fluid behavior at the surface of ILs can often not be considered sufficiently. Proper consideration of the diverse features of ILs results in more complicated and less universal models.

The objective of the present study is to develop a simple prediction method for the surface tension of ILs as a function of temperature. Based on a database of experimental surface tension values collected from the literature, first a prediction scheme for the surface tension at a reference temperature of 298.15 K using only information on the density, molar mass, and anion type of the IL is suggested. By combination of this approach with the temperature dependence of the density, an extended prediction scheme describing the temperature dependence of the surface tension of ILs is recommended. The optimized prediction model for the surface tension allows for the prediction of about 3500 temperature-dependent experimental surface tension data of 226 different ILs with a standard deviation of about 7 %. In comparison with fluid-specific prediction methods found in literature, the developed simple empirical prediction model requires only easily accessible parameters and can be applied for ILs with arbitrary cation and anion combinations. Thus, the proposed prediction method seems to be a valuable engineering tool for the quantitative estimation of the surface tension of ILs.