Thermal Conductivity of Ionic Liquids- Measurement and Prediction

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For ionic liquids (ILs), potential fields of application have strongly increased in recent years. Due to an almost unlimited number of potential combinations of cations and anions, ILs can be tailored to a specific application. Yet, for identifying their usefulness, e.g., as solvents, electrolytes, lubricants or heat transfer fluids, knowledge about their physical and chemical properties is required. Of course, the properties of every conceivable IL cannot be obtained by carrying out appropriate measurements, since this would represent a substantial investment. An alternative approach, where the composition of an IL exhibiting a given set of properties can be predicted, would be very useful. For overcoming this limit, quantitative prediction methods with reasonable certainty must be developed. Yet, all prediction methods can only be as accurate as the experimental data used for the evaluation of their performance. Although many physicochemical properties including equilibrium and transport properties of ILs have been studied extensively, there still exists a lack of reliable data. In particular, only limited information on the thermal conductivity, which represents a key property for the engineering design of processes, is available in literature for ILs. The major aim of the present work was to provide accurate and reliable data for the thermal conductivity of a set of pure ILs selected by the criterion of differing molecular weight in the range from 170 to 400 $g \times mol^{-1}$. In detail, [EMIM] (1-ethyl-3-methylimidazolium)-based ILs having the anion [NTf_2] (bis(trifluoromethyl-sulfonyl)imide), [OAc] (acetate), [$N(CN)_2$] (dicyanamide), [$C(CN)_3$] (tricyanomethide), [$MeOHPO_2$] (methyl-phosphonate), [$MeSO_3$] (methansulfonate)[$EtSO_4$] (ethylsulfate), and [$OcSO_4$] (octylsulfate) were selected, and in addition, ILs with the [NTf_2]-anion having the cation [OMA] (trioctylmethylammonium) and [BBMIM] (1,3-dibutyl-2-methylimidazolium). Measurements were performed in the temperature range between 273 K and 333 K by a stationary guarded parallel plate instrument with a total measurement accuracy of 3 % (k = 2). For all ILs, the temperature dependence of the thermal conductivity can well be represented by a linear equation. For the [EMIM]-based ILs, an approximately linear increase of the thermal conductivity with decreasing overall molar mass is found, showing a root-mean-square deviation of 1.4 % at 293.15 K. This result implies the possibility to set up a simple prediction method for the thermal conductivity of ionic liquids based on the same cation, and thus a convenient simplification in the acquisition of this property for the enormous amount of ionic liquids available.