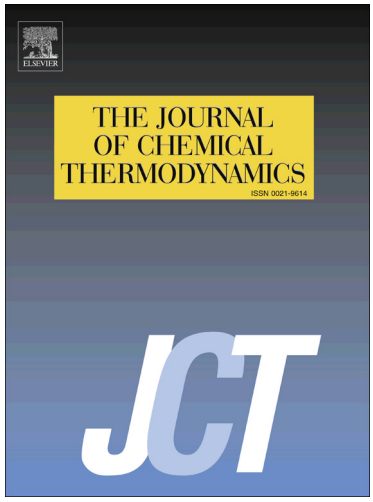

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Further Development of the Predictive Models for Physical Properties of Pure Ionic Liquids: Thermal Conductivity and Heat Capacity

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Efficient, fast and accurate heat transfer units design is currently a 'hot topic' due to the demand for more approachable and high-performance-ability materials. This is usually performed by the prediction of physical properties coupled with sufficient structure searching (for example with genetic algorithm). Ionic liquids have been found to be prospective replacement materials in this case; however, the predictive capabilities of existing models still remain poor which affects their practical application significantly. It has also been observed that for some quaternary-phosphonium based carboxylate ILs, the models fail, particularly, for thermal conductivity and heat capacity predictions. The impact of electronic structure on the heat capacity was confirmed by DFT calculations, and this was also included in further refinement. The aim of this work is to assess the predictive capabilities of existing models for thermal conductivity and heat capacity, with further improvements based on more accurate investigated structure characterization (DFT) and reparameterization (group contribution methodology). The ILs chosen for the initial study are trihexyl(tetradecyl)phosphonium-based carboxylate derivatives.