Prediction of High Pressure Thermodynamic Properties of Ionic Liquids

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Thermophysical properties of compressed liquids are quantities of great interest in several physics and physical chemistry fields. Thus, many studies have been devoted to experimental measurements of the thermophysical properties of liquids and their mixtures. Significantly, temperature and pressure dependences of thermophysical properties have been investigated by experiments for hundreds of molecular systems and mixtures. The state of any fluid is something that engineering chemists often find it necessary to specify clearly. Such a specification must include the density (or specific volume) of a substance, the pressure, and the temperature. The mathematical relationship that links them is the Equation of State (EoS), which remains the basis of thermodynamics. Although many EoSs were introduced either to understand the physical background of liquids or use practical calculations instead of extensive direct measurements, there is no “universal predictive recipe,”, especially for liquids with complex inter-particle interactions. One of the most important examples of such media are ionic liquids, which are of great modern interest from the fundamental view of physical chemistry as well as prospective practical applications.

In this work, we demonstrate the possibility of calculating the high-pressure properties of ionic liquids using their thermodynamic parameters determined at ambient pressure addressing the scaling properties revealed for thermodynamic fluctuations, especially the inverse reduced density fluctuations and reduced pressure fluctuations. Our method, which led to the so-called Fluctuation Theory-based Equation of State (FT-EoS), already demonstrated its predictive capacity for density of the dataset of 80 different ILs with an overall relative absolute average deviation close to 0.14% [1] and got strict mathematical support from the theory of thermodynamic linear analysis. Its further development resulted in the predictive approach to the speed of sound’s predictions based on the pressure fluctuations [2]. By applying our method, the agreement, well-coordinated with the possibilities of the actual experimental method, is observed between experimental and predicted high-pressure speed of sound data for all collected ILs from the ILTermo database; see, for example, Fig. 1. An overall relative average absolute deviation is close to 0.85%.

REFERENCES

[1] M. Chorążewski, E.B. Postnikov, B. Jasiok et al. *Scientific Reports*, 7 (2017) 5563.

[2] E.B. Postnikov, B. Jasiok, V.V. Melent’ev et al. *Journal of Molecular Liquids*, 310 (2020) 113016.

FIGURES

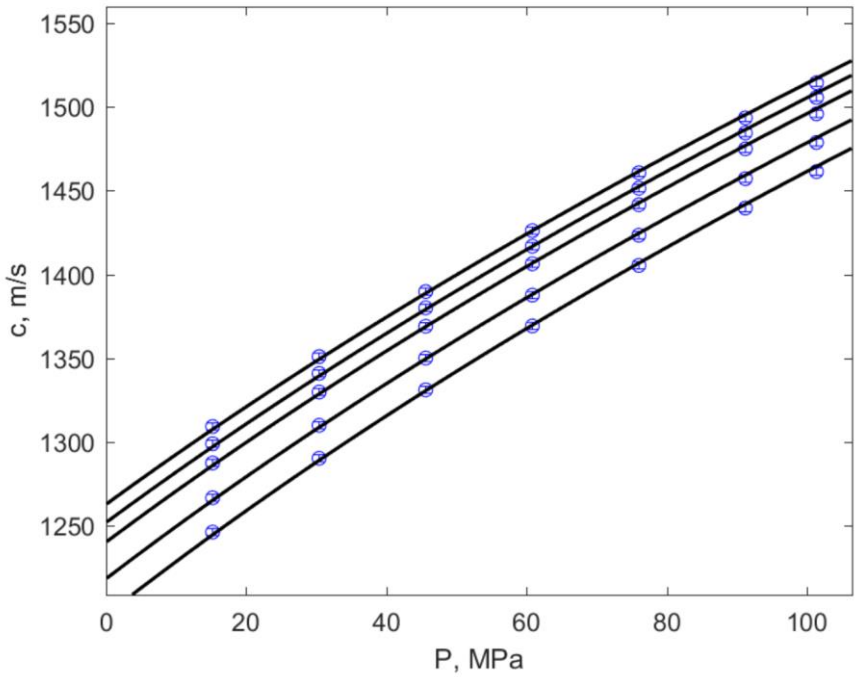

Figure 1: A comparison of the pressure dependence of the speed of sound between FT-EoS and collected experimental results for 1-ethyl-3-methylimidazolium bis((trifluoromethyl)sulfonyl)imide for (288, 292, 298, 308 and 318) K from up to down.