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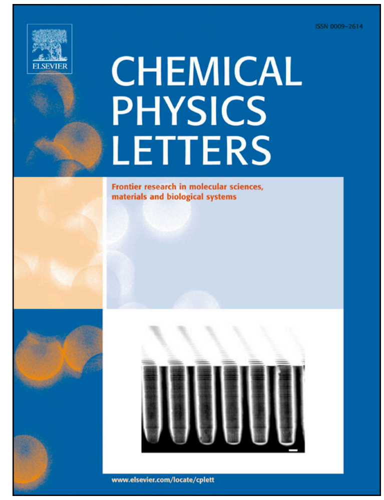

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Similarity law and critical properties in ionic systems.

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Abstract

Using molecular simulations, we determine the locus of ideal compressibility, or Zeno line, for a series of ionic compounds. We find that the shape of this thermodynamic contour follows a linear law, leading to the determination of the Boyle parameters. We also show that a similarity law, based on the Boyle parameters, yields accurate critical data when compared to the experiment. Furthermore, we show that the Boyle density scales linearly with the size-asymmetry, providing a direct route to establish a correspondence between the thermodynamic properties of different ionic compounds.

Keywords: Ionic fluids, Alkali Halides, Zeno line, Critical properties; Similarity Law.

1. Introduction

Recent advances in the theory of vapor liquid equilibrium have led to the identification of new similarity laws, which allow for alternate pathways for the determination of the critical properties of fluids [1, 2, 3, 4]. Such theories rely on the prior determination of a contour known as the Zeno line, i.e. the line for which the compressibility factor Z is equal to 1 ($Z = PV/RT = 1$), that spans the subcritical and supercritical domain of the phase diagram [5]. Remarkably, in the case of model systems (i.e. for a Van der Waals fluid and the Lennard-Jones system) [6], the Zeno line has been shown to be accurately modeled by a linear law that crosses the temperature and density axes at the Boyle temperature T_B and density ρ_B, respectively. The Boyle parameters can then be used to obtain the critical properties through the

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