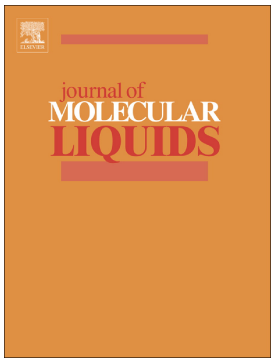

Thermodynamic behavior of charged Lennard-Jones fluids

Ivan Anashkin, Alexander Klinov

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Thermodynamic behavior of charged Lennard-Jones fluids

Ivan Anashkin, Alexander Klinov

Department of Chemical Engineering, Kazan National Research Technological University, 68 Karl Marx Str., Kazan, 420015, Russia

Corresponding author: Ivan Anashkin, e-mail: anashkin.ivan@gmail

abstract:
In the present paper one of the simplest models for the intermolecular interaction of ionic substances is used. The phase equilibrium and pVT properties in the single-phase area for the fluid with intermolecular interaction, which is described by the Lennard-Jones and Coulomb potentials, is calculated by molecular dynamics simulation. Influence of the charge on position of the Zeno line as well as on a position of the vapor-liquid equilibrium line on phase diagram is determined. It is shown that this system can be described by generalized scaling laws proposed in a series of articles Apfelbaum E.M., Vorob′ev V.S. // J. Phys. Chem. B. 112. (2008) 13064. and Apfelbaum E.M., Vorob’ev V.S. // J. Chem. Phys. 130. (2009) 214111. The expression for the dependence of properties at the critical point, the Boyle temperature and density on the charge value are proposed.

Highlights:
Phase equilibrium and the Zeno line of charged Lennard-Jones ionic fluid are calculated using molecular dynamic simulation
Dependence of the saturation line, the critical point and the Zeno line on the charge are obtained