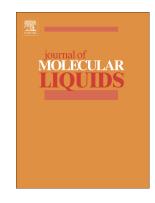
### Accepted Manuscript

Thermodynamic behavior of charged Lennard-Jones fluids

Ivan Anashkin, Alexander Klinov

PII:	S0167-7322(17)30497-X
DOI:	doi: 10.1016/j.molliq.2017.03.113
Reference:	MOLLIQ 7148
To appear in:	Journal of Molecular Liquids
Received date:	5 February 2017
Accepted date:	30 March 2017



Please cite this article as: Ivan Anashkin, Alexander Klinov, Thermodynamic behavior of charged Lennard-Jones fluids. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Molliq(2017), doi: 10.1016/j.molliq.2017.03.113

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

## **ACCEPTED MANUSCRIPT**

#### 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

1

Download English Version:

# https://daneshyari.com/en/article/5408550

Download Persian Version:

https://daneshyari.com/article/5408550

Daneshyari.com