

Accepted Manuscript

Estimating density of ionic liquids under very high pressure

Tatiana C. Penna, Vitor H. Paschoal, Luiz F.O. Faria, Mauro C.C. Ribeiro



PII: S0167-7322(18)32642-4
DOI: [doi:10.1016/j.molliq.2018.06.028](https://doi.org/10.1016/j.molliq.2018.06.028)
Reference: MOLLIQ 9226
To appear in: *Journal of Molecular Liquids*
Received date: 21 May 2018
Accepted date: 6 June 2018

Please cite this article as: Tatiana C. Penna, Vitor H. Paschoal, Luiz F.O. Faria, Mauro C.C. Ribeiro , Estimating density of ionic liquids under very high pressure. Molliq (2017), doi:[10.1016/j.molliq.2018.06.028](https://doi.org/10.1016/j.molliq.2018.06.028)

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.

Estimating Density of Ionic Liquids Under Very High Pressure

Tatiana C. Penna, Vitor H. Paschoal,

Luiz F. O. Faria, and Mauro C. C. Ribeiro *

*Laboratório de Espectroscopia Molecular, Departamento de Química Fundamental,
Instituto de Química, Universidade de São Paulo,
Av. Prof. Lineu Prestes 748, 05508-000, Brazil*

* e-mail: mccribei@iq.usp.br

Equation of state according to the Carnahan-Starling-van der Waals model has been proposed for ionic liquids based on the anions tetrafluoroborate, $[\text{BF}_4]^-$, hexafluorophosphate, $[\text{PF}_6]^-$, and bis(trifluoromethanesulfonyl)imide, $[\text{NTf}_2]^-$, from available volumetric data within the MPa range of pressure. Then, the equation of state is used to estimate density in the GPa range of pressure. The hard sphere part of the equation considered a binary mixture of cation and anion spheres whose diameters exhibit a satisfactory degree of transferability among different systems with a common ion. It is shown that pressure induced vibrational frequency shift, $\Delta\nu$, of the characteristic Raman band of the stretching mode of $[\text{BF}_4]^-$, $[\text{PF}_6]^-$, and $[\text{NTf}_2]^-$ collapses into a master curve when $\Delta\nu$ is plotted as a function of reduced density for each group of ionic liquids. Thus, Raman spectroscopy provides a validation test of the high-pressure extrapolation of the equation of state for ionic liquids.

Keywords: ionic liquid, density, high pressure, Raman.

Download English Version:

<https://daneshyari.com/en/article/7841979>

Download Persian Version:

<https://daneshyari.com/article/7841979>

[Daneshyari.com](https://daneshyari.com)