

## Accepted Manuscript

Theoretical study on interactions between Trifluoromethanesulfonate (Triflate) based ionic liquid and thiophene

Renqing Lü, Chongchong Wu, Jin Lin, Ye Xiao, Fang Wang, Hector De la Hoz Siegler



PII: S0167-7322(16)34122-8  
DOI: doi: [10.1016/j.molliq.2017.04.105](https://doi.org/10.1016/j.molliq.2017.04.105)  
Reference: MOLLIQ 7261

To appear in: *Journal of Molecular Liquids*

Received date: 19 December 2016

Revised date: 10 April 2017

Accepted date: 21 April 2017

Please cite this article as: Renqing Lü, Chongchong Wu, Jin Lin, Ye Xiao, Fang Wang, Hector De la Hoz Siegler, Theoretical study on interactions between Trifluoromethanesulfonate (Triflate) based ionic liquid and thiophene. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Molliq(2017), doi: [10.1016/j.molliq.2017.04.105](https://doi.org/10.1016/j.molliq.2017.04.105)

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.

## Theoretical Study on Interactions between Trifluoromethanesulfonate (Triflate) Based Ionic Liquid and Thiophene

Renqing Lü<sup>a</sup> Chongchong Wu<sup>b\*</sup> Jin Lin<sup>c</sup> Ye Xiao<sup>b</sup> Fang Wang<sup>a</sup> Hector De la Hoz Siegler<sup>b</sup>

<sup>a</sup> College of Science, China University of Petroleum (East China), 266580, Qingdao, Shandong Province, China

<sup>b</sup> Department of Chemical and Petroleum Engineering, University of Calgary, T2N 1N4, Calgary, Alberta, Canada

<sup>c</sup> College of Chemical Engineering, China University of Petroleum (East China), 266580, Qingdao, Shandong Province, China

### Abstract

Density functional theory was employed to investigate the interactions between 1-ethyl-3-methylimidazolium ([EMIM]<sup>+</sup>)/ 1-ethylpyridinium ([EPY]<sup>+</sup>)/ 1-ethyl-1-methylpyrrolidinium ([EPYRO]<sup>+</sup>)/ 1-ethyl-1-methylpiperidinium ([EPIP]<sup>+</sup>) cations and trifluoromethanesulfonate ([OTf]<sup>-</sup>) anion, as well as the interactions between trifluoromethanesulfonate ([EMIM]<sup>+</sup>[OTf]<sup>-</sup>/ 1-ethylpyridinium trifluoromethanesulfonate ([EPY]<sup>+</sup>[OTf]<sup>-</sup>/ 1-ethyl-1-methylpyrrolidinium trifluoromethanesulfonate ([EPYRO]<sup>+</sup>[OTf]<sup>-</sup>/ 1-ethyl-1-methylpiperidinium trifluoromethanesulfonate ([EPIP]<sup>+</sup>[OTf]<sup>-</sup>) and thiophene. The ionic liquids and complexes formed between [EMIM]<sup>+</sup>[OTf]<sup>-</sup>/ [EPY]<sup>+</sup>[OTf]<sup>-</sup>/ [EPYRO]<sup>+</sup>[OTf]<sup>-</sup>/ [EPIP]<sup>+</sup>[OTf]<sup>-</sup> and thiophene were analyzed by natural bond orbital, atoms in molecules, and noncovalent interaction, HOMO-LUMO overlap integral analyses, and electron density difference analysis. The calculated results show that thiophene ring is parallel to [EMIM]<sup>+</sup>/ [EPY]<sup>+</sup> ring, beneficial to  $\pi$ - $\pi$  interaction, while [EPYRO]<sup>+</sup> / [EPIP]<sup>+</sup> branched chains tend to form C-H $\cdots$  $\pi$  interactions with thiophene. The interactions between [EMIM]<sup>+</sup>/ [EPY]<sup>+</sup> / [EPYRO]<sup>+</sup> / [EPIP]<sup>+</sup> and thiophene are stronger than that of [OTf]<sup>-</sup> and thiophene proposed by interaction energy and electron density differences. The HOMO-LUMO overlap integral analyses demonstrate the different charge transfer direction and interacting nature of frontier orbitals.

\* Corresponding author.

E-mail address: [Chongchong.wu@ucalgary.ca](mailto:Chongchong.wu@ucalgary.ca); [happy.chongchongwu@gmail.com](mailto:happy.chongchongwu@gmail.com)

Download English Version:

<https://daneshyari.com/en/article/5409032>

Download Persian Version:

<https://daneshyari.com/article/5409032>

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