

Accepted Manuscript

A theoretical guide for screening ionic liquid extractants applied in the separation of a binary alcohol-ester azeotrope through a DFT method

Hong Li, Peng Zhou, Ji Zhang, Dongyang Li, Xingang Li, Xin Gao



PII: S0167-7322(17)34617-2

DOI: <https://doi.org/10.1016/j.molliq.2017.12.049>

Reference: MOLLIQ 8345

To appear in: *Journal of Molecular Liquids*

Received date: 3 October 2017

Revised date: 5 December 2017

Accepted date: 11 December 2017

Please cite this article as: Hong Li, Peng Zhou, Ji Zhang, Dongyang Li, Xingang Li, Xin Gao , A theoretical guide for screening ionic liquid extractants applied in the separation of a binary alcohol-ester azeotrope through a DFT method. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Molliq(2017), <https://doi.org/10.1016/j.molliq.2017.12.049>

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.

A theoretical guide for screening ionic liquid extractants applied in the separation of a binary alcohol-ester azeotrope through a DFT method

Hong Li^a, Peng Zhou^a, Ji Zhang^a, Dongyang Li^a, Xingang Li^a, Xin Gao^{a,*}

^a School of Chemical Engineering and Technology, National Engineering Research Center of Distillation Technology, Collaborative Innovation Center of Chemical Science and Engineering (Tianjin), Tianjin University, Tianjin 300072, China

ABSTRACT Although imidazolium-based ionic liquids (ILs) serve as potential extractants in the separation of a binary alcohol-ester azeotrope through extractive distillation [1, 2], the interaction mechanism at the molecular level is still not yet understood. In this work, we aim to screen the optimal extractant from four different ILs [BMIM][OAc], [BMIM][Cl], [EMIM][Br] and [OMIM][BF₄] for the separation of binary azeotropic system of methanol-dimethyl carbonate (DMC). A DFT quantum chemistry calculation method is employed to investigate the separation mechanism of an azeotrope with ILs. The most stable configurations of the complexes containing different ILs with methanol and DMC are obtained. The calculation results of the interaction energies illustrate the interactions between ILs and methanol are much stronger than that between ILs and DMC, while a decreasing trend is presented for the interaction energies: complex [BMIM][OAc]-methanol > [BMIM][Cl]-methanol > [EMIM][Br]-methanol > [OMIM][BF₄]-methanol and the complexes ILs-DMC share the same order. The differences in the interactions determine the competence of the azeotrope elimination, which is consistent with experimental results. Finally, the

* Corresponding author. Tel: +86-022-27404701(X.G.); Fax: +86-022-27404705(X.G.).
E-mail: gaixin@tju.edu.cn (Xin Gao).

Download English Version:

<https://daneshyari.com/en/article/7843240>

Download Persian Version:

<https://daneshyari.com/article/7843240>

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