

Accepted Manuscript

Research on solubility and bio-solubility of amino acids ionic liquids

Tian Tian, Xiaoling Hu, Ping Guan, Xiaoqi Ding

PII: S0167-7322(16)33132-4
DOI: doi:[10.1016/j.molliq.2016.11.071](https://doi.org/10.1016/j.molliq.2016.11.071)
Reference: MOLLIQ 6618

To appear in: *Journal of Molecular Liquids*

Received date: 12 October 2016
Accepted date: 15 November 2016



Please cite this article as: Tian Tian, Xiaoling Hu, Ping Guan, Xiaoqi Ding, Research on solubility and bio-solubility of amino acids ionic liquids, *Journal of Molecular Liquids* (2016), doi:[10.1016/j.molliq.2016.11.071](https://doi.org/10.1016/j.molliq.2016.11.071)

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.

Research on Solubility and Bio-solubility of Amino Acids Ionic Liquids

Tian Tian, Xiaoling Hu, Ping Guan and Xiaoqi Ding*

School of Natural and Applied Science, Northwestern Polytechnical University, the Key Laboratory of Space Applied Physics and Chemistry, Ministry of Education, Xi'an 710072, China

Abstract: Herein, the synthesis of L-(+)- α -(positive butyl)-leucine ethyl ester ionic liquids with anions based on bromide (Br^-), tetrafluoroborate (BF_4^-) and hexafluorophosphate (PF_6^-) were presented. The structures and purities of these amino acids ionic liquids (AAILs) were characterized by ^1H NMR and the determinations of water content. The interaction energies of AAILs-solvents/amino acids and dipole moment of AAILs were obtained through ab initio at MP2/6-311G++(2d, p). The relationships between the solubility of AAILs and common solvents, molecular structure and the interaction energies of AAILs-solvents along with the influences of temperature and molecular structure on the bio-solubility of AAILs were discussed systematically. The results revealed that the solubility of the title AAILs increased firstly and then decreased with decreasing dielectric constant of solvent; With the dipole moment of AAILs and hydrogen bond interaction increasing, the solubility in polar solvents had a increasing trend; With the interaction energies of AAILs-solvents becoming bigger, AAILs can be easily dissolved in the solvents; The dissolution of amino acids in AAILs was largened with temperature increasing. Additional, the ease or difficulty of dissolution for amino acids in AAILs can be predicted by theoretical calculation. This prediction is consistent with the dissolution behavior of AAILs.

Keywords: amino acids ionic liquids; ab initio; interaction energies; solubility; bio-solubility

Download English Version:

<https://daneshyari.com/en/article/5409224>

Download Persian Version:

<https://daneshyari.com/article/5409224>

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