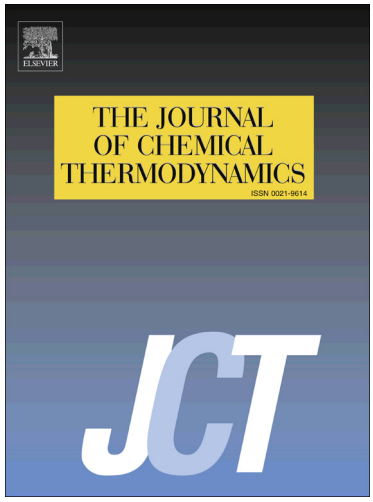

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Yunpeng Zhou, Dongmei Xu, Lianzheng Zhang, Yixin Ma, Xiaolong Ma, Jun Gao, Yinglong Wang

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Separation of thioglycolic acid from its aqueous solution by ionic liquids: Ionic liquids selection by the COSMO-SAC model and liquid-liquid phase equilibrium

Yunpeng Zhou [a], *Dongmei Xu* [a,*], *Lianzheng Zhang* [a], *Yixin Ma* [a], *Xiaolong Ma* [a], *Jun Gao* [a,*], *Yinglong Wang* [b]

[a] College of Chemical and Environmental Engineering, Shandong University of Science and Technology, Qingdao 266590, China

[b] College of Chemical Engineering, Qingdao University of Science and Technology, Qingdao 266042, China

*Corresponding author

E-mail addresses: xudongmei.cn@163.com, gao@sdust.edu.cn

Abstract: To separate thioglycolic acid (TGA) from its aqueous solution by ionic liquids (ILs), sixty imidazolium-based ionic liquids (ILs) were screened by using the COSMO-SAC model based on the evaluation of the selectivity, capacity and performance index, which were derived from the activity coefficient at infinite dilution. Meanwhile, the effects of the different anions and the alkyl chain length of the cations for the separation of TGA were analysed by the σ-profile for each component. Consequently, 1-octyl-3-methyl-imidazolium trifluoromethanesulfonate ([OMIM]OTf), 1-octyl-3-methyl-imidazolium perchlorate ([OMIM]ClO_4), 1-octyl-3-methyl-imidazolium hexafluorophosphate ([OMIM]PF_6) and 1-octyl-3-methyl-imidazolium aluminum tetrachloride ([OMIM]$AlCl_4$), were selected to extract TGA from it aqueous solution. The results revealed that the selected ILs can extract TGA effectively from its aqueous solution. The experimental liquid-liquid