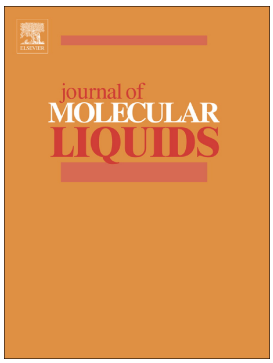

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A theoretical guide for screening ionic liquid extractants applied in the separation of a binary alcohol-ester azeotrope through a DFT method

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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][BF_4] 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][BF_4]-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

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