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Solubility of Carbon Dioxide in Imidazolium-based Ionic Liquids by Molecular Dynamics Simulations

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ABSTRACT FOR ORAL PRESENTATION

Ionic Liquids (ILs) are organic salts with a melting point below 100 °C. They promise a wide range of opportunities especially as solvents for reaction and material processing, as extraction media or as working fluid in mechanical applications. The knowledge of physical properties of the ILs is often an essential necessity for these applications. Often the experimental measurements are difficult and for the various combination of anions and cations not possible to perform. This is why simulation techniques will become important to explore this interesting field.

1-Alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide $[C_n mim][NTf_2]$ with n = 2,4,6,8 were studied by molecular dynamics (MD) simulations because recently systematic measurements of the infinite dilution properties for a number of gases, including methane, carbon dioxide and noble gases have been reported. We have developed a force field for this class of ILs which has shown good agreements with experimental date for various properties.[1]

By applying the Bennett's overlapping distribution method (ODM), as well as the Widom's particle insertion technique we determine excess chemical potentials and solubilities which are in excellent agreement with available experimental solubility data for a large temperature range from 300 K up to 500 K. The simulations reveal the experimental observed "anomalous" temperature dependence of CO_2-solubility represented by counter-compensation negative enthalpies and entropies of solvation. By systematically varying the interaction-strength of CO_2 we show that the dominating negative solvation entropy is not due to the cavity effects but introduced by both favourable Coulomb and van-der-Waals interactions. Finally we demonstrate that molecular dynamics simulations are able to predict Henry-coefficients for a wide range of gases in ILs [2-3] and we also can explain the mechanism of solvation for these systems.

REFERENCES

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