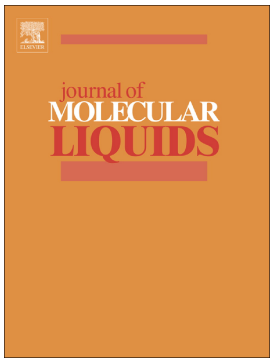

Prediction of Henry's law constant of CO2 in ionic liquids based on SEP and Sσ-profile molecular descriptors

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Prediction of Henry's law constant of CO_2 in ionic liquids based on S_{EP} and $S_{\sigma\text{-profile}}$ molecular descriptors

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Abstract: Nowadays, greenhouse gas CO_2 emissions have caused serious global warming problems. Unique properties of ionic liquids (ILs), such as negligible vapor pressure, good thermal and chemical stability, high gas dissolution capacity, etc., have made them highly promising in capturing CO_2 . Although researchers have done a lot of experimental work using ILs to capture CO_2, time-consuming and high experimental economic costs have led to a strong interest in establishing predictive models. In this work, 297 experimental data points including 16 cations and 9 anions for 34 ILs are collected and the structures of cations and anions are optimized by quantum chemistry. Then the electrostatic potential surface area (S_{EP}) and charge distribution area ($S_{\sigma\text{-profile}}$) descriptors are calculated and used to predict the Henry's law constant (HLC) of CO_2 in ILs. Three new models, namely, the multiple linear regression (MLR), support vector machine

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