Title : Computational Study of CO_2 Capture by [EMI][TFSI] and [EMI][BF_4]

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ABSTRACT

The structures of Ionic liquids (ILs), 1-ethyl-methylimidazolium bis(trifluoro methylsulfonyl)imide or [EMI][TFSI] and 1-ethyl-methylimidazolium tetrafluoroborate [EMI][BF_4] and their interactions with CO_2 were investigated using DFT calculations at the B3LYP/6-311G+(2d,p) level. Compared to anion of $[TFSI]^-$ and $[BF4]^-$ has a more symmetric structure and a more evenly distributed charge. CO_2 can be captured by ILs models and structural change was observed, the C=O bond length increases slightly, and the OCO angle decreases more in $[BF_4]^-$ indicated a stronger interaction than with $[TFSI]^-$. ESP charge analysis shows the nitrogen (N) atom in EMI^+ and sulfur (S) in $[TFSI]^-$ and boron (B) in $[BF_4]^-$ in CO_2 interactions. Boron (B) charge in $[BF_4]^-$ decreases upon CO_2 binding, further supporting its stronger interaction. Infrared (IR) analysis supports these findings, showing the C=O stretching frequency shifts to a lower wavenumber (redshift), with $[BF_4]^-$ showing a larger shift than $[TFSI]^-$, reinforcing its greater binding strength with CO_2.

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