Abstract Submitted
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Binding energies of CO_2 with some ionic liquids[1] WILLIAM EUCKER, JOHN BENDLER, United States Naval Academy — Room temperature ionic liquids (RTILs), a novel class of materials with negligible vapor pressures and potentiality as benign solvents, may be an ideal chemical for carbon dioxide (CO_2) gas sequestration. *Ab initio* computational modeling was used to investigate the molecular interactions of simple RTIL anions hexafluorophosphate (PF_6^-) and tetrafluoroborate (BF_4^-) with CO_2. Electronic potential energy surface (PES) scans of a comprehensive sampling of 1:1 anion-CO_2 orientations were computed using Spartan '02 with Dunning's correlation consistent basis sets. Qualitatively, the PES scans yielded deeper, more numerous and radially closer active sites surrounding BF_4^- anion as compared with the PF_6^- anion. Quantitatively, the binding energies of 17.87 kJ/mol and 25.24 kJ/mol were extracted from the identified global energy minima for the PF_6^- and BF_4^- systems, respectively. The smaller BF_4^- anion was concluded to bind more strongly to the CO_2. However, literature-reported experimental Henry's law constants for CO_2 dissolved in imidizolium based RTILs show greater gas solvation in the PF_6^- system. The discrepancy between the energetics calculation results and the experimental solvation data will be discussed.

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