How Meaningful Is the Halogen Bonding in 1-Ethyl-3-methyl Imidazolium-Based Ionic Liquids for CO2 Capture?

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 We report on several parameters that can be used to describe the 1-ethyl-3-methyl-4,5-(X2)imidazolium cations (where X = H, Br, and I) within the Canongia-Lopez and Padua Force Field (CL&P) framework. Geometrical parameters like intramolecular distances and radial distribution functions are close to the experimental structure. Density values obtained with our force field are within the expected ones from CL&P calculations in related systems. This information is used to simulate through molecular dynamics the solubilization of CO2 by these ILs. For pure ILs, the addition of halides in position 4 and 5 promotes an enhanced hydrogen bond interaction at position 2 with the oxygen atoms in the anion. It is found that CO2 should be in the interstices of the anion-cation 3D network with longer distances than those found in other reports at ab initio levels, suggesting that halogen bond, if present, may be not the driving force interaction in these systems. Th