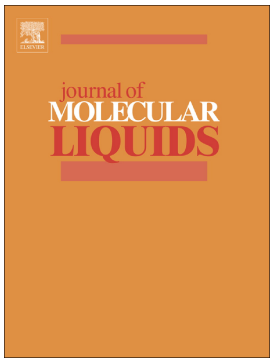


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# Deconvolution of conformational equilibria in methimazolium-based ionic liquid ion pair: infrared spectroscopic and computational study

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Abstract.

Deconvolution of conformational equilibria in ionic liquids is a challenging task. Infrared spectroscopy coupled with computational simulations is a powerful tool to characterize the interactions and conformational equilibria in ionic liquids. Herein, this approach is employed to study methimazolium-based ionic liquids. Electronic, structural and vibrational properties of the ion pair consisting of a methimazolium cation and a bis(trifluoromethanesulfonyl)imide ($Tf_2N$) anion are analyzed via the density functional theory (DFT) method using the hybrid B3LYP functional, while experimental IR study is performed for the corresponding bulk ionic liquid. DFT predicts that two lowest energy conformers are nearly degenerate in energy, suggesting that both structures are present in the bulk phase. Two intense peaks at 2848 $cm^{-1}$ and 2915 $cm^{-1}$ in the IR spectrum—which are assigned to the cation NH stretching vibrations of the two lowest-energy conformers—lend experimental support to this interpretation. Natural bond analysis and