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Senior Project Title: The Effect of Hydration on the Vibrational Spectrum of CTAHS
Major: Chemistry
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Abstract

The geometries and vibrational frequencies for the SO3 stretch of CTAHS were calculated at the MP2/6-311+G(d, p) level of theory in implicit solvation. These properties are studied as a function of increasing and decreasing anion-cation distances. Harmonic frequency calculations were carried out by increasing and decreasing the distance of the hydrogen sulfate anion from CTA in steps of 0.5 Å and 0.25 Å from the optimal geometry distance respectively. Vibrational frequencies decrease and increase from the optimal geometry distance for the normal and flipped configuration, however, frequencies barely change at all increasing distances. Despite the limited anion-cation interactions, the small changes may be influenced by the implicit solvation field. The calculations help to explain the effects of hydration on the vibrational frequencies of the bisulfate anion introduced with the cationic reverse micelle CTA+ and assigning the different bands for the CTA+ and HSO4- contact pair in the spectra from experimental data.