EXAMINATION OF H₂CO-X⁺ AND NH₂CH₂COOH-X⁺ COMPLEXES [X⁺ = Li⁺, Na⁺, K⁺] USING ELECTRONIC STRUCTURE THEORY

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Infrared spectroscopy is a powerful tool for studying molecular structure as changes in the frequency and intensity of infrared transitions provide a way to probe environment effects on molecular systems. In this study we investigate how the frequency and intensity of the C=O stretch vibration of formaldehyde and glycine change upon the introduction of alkali metal cations. Specifically we focus on the complexes of Li⁺, Na⁺, and K⁺ with H₂CO and NH₂CH₂COOH. There is evidence of small changes in the harmonic C=O stretch frequency; however, the changes in intensity are much larger. For example the intensity of the C=O stretch vibration is affected by the particular alkali metal cation as well as the geometry of the complex. All calculations in this study were performed using Gaussian03 at the MP2/6-311G^{*} level of theory/basis set.