EXAMINATION OF $H_2CO–X^+$ AND $NH_2CH_2COOH–X^+$ 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 H_2CO and NH_2CH_2COOH. 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 in $H_2CO–Li^+$ is twice that in bare H_2CO. The ultimate goal of this work is to determine how the sensitivity 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.