

WEAKLY-BOUND COMPLEXES OF γ -BUTYROLACTONE AND WATER: A MATRIX ISOLATION FTIR AND COMPUTATIONAL ANALYSIS.

ANNABELLE N CARNEY, JOSH NEWBY, *Chemistry, Nazareth College, Rochester, NY, USA.*

The interaction preferences of water with small molecules has been an area of interest for many years as we endeavor to better understand solvation at the molecular scale. Here, a study of the 1:1 weakly-bound complexes of γ -butyrolactone (GBL) with water is presented. GBL is a five-membered heterocycle that contains two distinct regions that could serve as binding sites for a single water. Matrix isolation FTIR experiments identified several peaks that were not associated with isolated water or GBL, implying the bands are due to weakly-bound complexes of the two. In addition to normal water, the spectra of D₂O and HDO complexes with GBL were also recorded. These spectra were interpreted with the aid of computational chemistry. In this work, multiple density functional theories and MP2 calculations were used to find minimum energy configurations and vibrational structure of the complexes. Possible interpretations of the experimental and computational results will be presented here.