

MATRIX ISOLATION FTIR ANALYSIS OF WEAKLY-BOUND COMPLEXES OF WATER WITH γ -LACTONES

ANNABELLE N CARNEY, KENNETH C MOGAURO, EMILY M WEAVER, 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 weakly-bound complexes of γ -lactones with water is presented. In this study, matrix isolation FTIR and computational methods were used to examine stable 1:1 complexes of γ -butyrolactone, γ -valerolactone, and Angelica lactone complexes with water. These five-membered heterocycles contain multiple regions that could serve as binding sites for a single water molecule including two chemically distinct oxygen atoms and a π -cloud. Matrix isolation FTIR experiments identified several peaks that were not associated with isolated water or lactone, implying the bands are due to weakly-bound complexes of the two. In addition to normal water, D₂O and HDO complexes with the lactones were also observed. The spectra can be interpreted with the aid of computational chemistry. In this work, multiple density functional theories along with MP2 calculations were used to find minimum energy configurations and vibrational structure of the complexes that can be directly compared to our spectra. Possible interpretations of the experimental and computational results are presented.