Abstract

We use *Gaussian 09* to perform density functional theory calculations for γ-butyrolactone and its dimers and trimers. The UM06 functional is used in conjunction with the 6-311++(2d,p) basis set to obtain optimized structures, and calculate binding energies for each dimer and trimer, in addition to counterpoise corrections. Structural changes are observed for each dimer and trimer species, in reference to the monomer. Infrared spectra are also calculated for both normal and deuterated species, and are compared to experimental spectra obtained in a solid nitrogen matrix. Through this comparison, it is shown that the monomer, dimer and trimer species can be differentiated experimentally, particularly in the carbonyl region. Approximate relative abundances of these species are also calculated, and the effects of photolysis and annealing on these abundances are observed.