Abstract

Vinyl Acetate is examined using the computational chemistry software *Gaussian 16*. This study focused on the trans-cis conformation and the cis-cis conformation of vinyl acetate. Energetic and Vibrational calculations were performed on vinyl acetate in both the lowest singlet and triplet states. Excited state optimizations were also performed on these states which led to the formation of fragments and radicals. These molecules energies were compared to vinyl acetate. Twelve excited states of vinyl acetate were calculated and plotted on a graph along with their respective multiplicities in order to determine the swapping of multiplicities and crossing between different excited states.