Abstract

This thesis studies the potential photodecomposition pathways of vinyl acetate using the computational programs Gaussian and Gaussview. Fragments were optimized using UMo6/aug-cc-pVTZ as the method and basis set and their vibrational frequencies were calculated to determine their energies. These energies were then used to construct potential decomposition pathways of vinyl acetate which revealed several energetically favorable fragmentation patterns that could occur during photochemical excitation.