Abstract

This thesis is a computational study of possible fragments due to the photodecomposition of γ-butyrolactone in a matrix using Gaussian09. The geometries of these fragments were optimized in two different basis sets, and the frequencies of vibration were calculated to produce IR spectra. The energies of these fragments were compared to γ-butyrolactone and it was found that the vast majority of the fragments were much less stable than γ-butyrolactone, but there were a few that were more stable than γ-butyrolactone. The more stable fragments are expected to be seen in the IR spectrum of γ-butyrolactone during photodecomposition. These calculations for frequencies of vibrations can be used to determine the formation of fragments.