Abstract

Density functional theory was used to study the decomposition of γ-Butyrolactone. Gaussian 09w was used to calculate the relaxed potential of each interatomic bond. Singlet and triplet state optimizations were computed and then the change in molecular energy was calculated as each bond was lengthened. The change in geometrical shape and ability of a bond to be broken was assessed. Lengthening of the carbonyl carbon α-carbon was shown have the least effect on molecular energy and therefore most likely to break first.