Abstract:

Vinyl acetate (VA) is examined using the computational software package Gaussian, utilizing Density Functional Theory and Multi-Configuration methods. Energetic calculations and vibrational calculations are performed on VA in each of its possible 4 conformations in the lowest energy singlet and triplet states. IR spectra are predicted that may be useful for future comparison to experimentally obtained results. The potential surfaces of the different conformations are examined as well as possible isomerizations among conformers. Additionally, the potential surfaces of several sets of bond lengths are calculated, and we show that it is likely that the molecule dissociates into radicals. Finally, we have located at least one point where it is likely that a phenomenon such as a conical intersection occurs between potential surfaces.