

Abstract

This study investigates the characteristics of vinyl acetate in a coordination complex with water. Vinyl acetate was studied in its monomeric form. The aug-cc-pVTZ basis set and M06-2X functional were used. Three possible conformations of vinyl acetate were optimized, and their frequencies were calculated. After optimization, a water molecule was then added to form a complex between the two. Each complex was then optimized again, and their frequencies were again calculated. The results of this study will visually display the geometry of the optimized structures and their water complexes. Infrared spectra and tables listing binding energies of the water complexes will also be provided.