

Density functional calculations of vibrational wavenumbers and derived potential energy distributions for fluoro- and chlorocarbonyl ketenes. Badawi, H. M.; Forner, W.; Al-Saadi, A

Abstract

The structural stability and conformational behavior of fluorocarbonyl ketene and chlorocarbonyl ketene were investigated by utilizing ab initio calcns. with the 6-311++G** basis set at the d. functional (B3LYP) level. Both mol. systems were predicted to exist in the planar s-cis and s-trans conformations with a relatively high-energy barrier. Full geometrical optimization was performed at the ground and transition states in the two systems. The vibrational frequencies were computed at the DFT-B3LYP/6-311++G** level and the calcd. vibrational IR and Raman spectra of the cis-trans mixts. of fluoro- and chlorocarbonyl ketenes were plotted. Complete vibrational assignments were made on the basis of normal coordinate calcns. for both stable conformers of the mols.