

**DENSITY FUNCTIONAL CALCULATIONS OF VIBRATIONAL
WAVENUMBERS AND DERIVED POTENTIAL ENERGY
DISTRIBUTIONS FOR FLUORO- AND
CHLOROCARBONYL KETENE**

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ABSTRACT

The structural stability and conformational behavior of fluorocarbonyl ketene and chlorocarbonyl ketene were investigated by utilizing ab initio calculations with the 6-311++G** basis set at the Density Functional (B3LYP) level. Both molecular 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 calculated vibrational infrared and Raman spectra of the *cis-trans* mixtures of fluoro- and chlorocarbonyl ketene were plotted. Complete vibrational assignments were made on the basis of normal coordinate calculations for both stable conformers of the molecules.

Keywords: Vibrational spectra and assignments; Rotational barriers; Fluorocarbonyl ketene; Chlorocarbonyl ketene.