

**VIBRATIONAL ASSIGNMENTS AND DERIVED POTENTIAL ENERGY
DISTRIBUTIONS FOR TRI- AND DIFLUOROMETHYL KETENE BY
DENSITY FUNCTIONAL CALCULATIONS**

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ABSTRACT

The structures of 3,3,3-trifluoromethyl ketene and 3,3-difluoromethyl ketene were studied by utilizing ab initio calculations with 6-311++G** basis set at Density Functional (B3LYP) level. Full optimization was performed for both molecules at their ground and transition states. Energy optimization of the systems under investigation shows that the trifluoromethyl ketene exists only in the *cis* conformation (fluorine atom eclipses the ketene group). The difluoromethyl ketene was predicted to have two stable conformations; the *cis* (hydrogen atom eclipses the ketene group) and the *gauche* (fluorine atom eclipses the ketene group) form. The conformational stability of the molecules was found to be mainly governed by electrostatic and molecular orbital interaction in the systems. The vibrational frequencies were computed and complete assignments were provided on the basis of normal coordinate calculations and comparison with similar molecules. The potential energy distributions (PED) among symmetry coordinates were derived for the stable conformations of the two molecules.

Keywords: Vibrational spectra and assignments; Rotational barriers; Trifluoromethyl ketene; Difluoromethyl ketene.