Computational Study of Substituent Effects and Vibrational Analysis of Formyl Haloketenes and Formyl

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Abstract

The structural stability and conformational behavior of fluoro-formyl, chloro- and formyl methyl ketene were

investigated with the 6-311++G** basis set at the Density Functional (B3LYP) level. From our calculations,

the three molecular systems were predicted to exist in the planar conformations with a relatively high energy

barrier. 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 the three molecular systems were plotted.

Complete vibrational assignments were made for the stable conformers of the molecules on the basis of

normal coordinate calculations and derived potential energy distributions.