AN INVESTIGATION OF STRUCTURAL STABILITY AND ANALYSIS OF VIBRATIONAL SPECTRA OF FORMYL KETENE BASED ON AB INTIO CALCULATIONS

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ABSTRACT

The conformational behavior and structural stability of formyl ketene were investigated by utilizing ab initio calculations with 6-311++G** basis set at restricted Hartree Fock (RHF) and Density Functional (B3LYP) levels. The molecule was predicted to have the s-cis ⇔ s-trans conformational equilibrium. Full optimization was performed at the transition state and the rotational barrier was calculated. The π-π interaction between the carbonyl and ketene groups were found to stabilize the planar s-cis and s-trans conformers only with a relatively high rotational barrier. The vibrational frequencies were computed at the RHF and DFT-B3LYP levels and the zero-point corrections were included into the calculated rotational barrier. Complete vibrational assignments were made on the basis of normal coordinate calculations for both stable conformers of the molecule.

Keywords: Vibrational spectra and assignments. Rotational barriers. Formyl ketene.