An investigation of structural stability and analysis of vibrational spectra of formyl ketene based on ab initio 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 (DFT-B3LYP) levels. The molecule was predicted to have the s-cis double left right arrow s-trans conformational equilibrium. Full optimization was performed at the transition state and the rotational barrier was calculated. The pi-pi interaction between the carbonyl and ketene groups was 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. (