

An investigation of structural stability and analysis of vibrational spectra of formyl ketene based on ab initio calculations. Badawi, H. M.; Forner, W.; Al-Saadi, A.

Abstract

The conformational behavior and structural stability of formyl ketene were studied by using ab initio calcns. with 6-311++G** basis set at RHF and d. functional (DFT-B3LYP) levels. The mol. was predicted to have the s-cis s-trans conformational equil. Full optimization was performed at the transition state and the rotational barrier was calcd. The π - π 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 calcd. rotational barrier. Complete vibrational assignments were made from normal coordinate calcns. for both stable conformers of the mol.