Theoretical Vibrational Spectra and Analyses of Isocyanatoketene O=C=CH-N=C=O

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ABSTRACT

The conformational stability of isocyanatoketene O=C=CH-N=C=O was investigated by Density Functional B3LYP and ab initio second-oreder Möller Plesset MP2 calculations with the 6-311+G** basis set. Isocyanatoketene was predicted to have the s-*cis* ⇔ s-*trans* conformational equilibrium with the s-*trans* being the predominant form. Full structural optimization was performed at the ground and transition states and the *trans-cis* barrier was calculated to be about 2 kcal/mol. The vibrational frequencies were computed at the DFT-B3LYP level, and the calculated infrared and Raman spectra of the *cis-trans* mixture were plotted. Vibrational calculations were also done for deuterated d_1-isocyanatoketene. Reliable vibrational assignment was provided on the basis of normal coordinate calculations for the stable conformers of the molecule.

Keywords: Vibrational spectra and assignments; Rotational barriers; Normal coordinate analysis; Isocyanatoketene.