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-order Möller Plesset MP2 calculations with the 6-311+G** basis set. Isocyanatoketene was predicted to have the \( \text{s-cis} \Leftrightarrow \text{s-trans} \) conformational equilibrium with the \( \text{s-trans} \) 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 \( \text{d}_1 \)-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.