

**Conformational stability and normal coordinate analyses of
imidoylketene $O=C=CH-CH=NH$**

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Abstract

The conformational and structural stability of imidoylketene $\text{O}=\text{C}=\text{CH}-\text{CH}=\text{NH}$ were investigated by DFT-B3LYP and ab initio MP2 calculations with the 6-311+G** basis set. From the calculations imidoylketene was predicted to exist predominantly in a mixture of *trans-anti* (the CCCN dihedral angle is 180°) and *cis-anti* (the CCCN dihedral angle is 0°) conformations with the *trans-anti* being the lower energy form. The two *anti* conformations were predicted to have a comparable relative stability with the C-C rotational barrier of about 9-10 kcal/mol at DFT-B3LYP and MP2 calculations. The equilibrium constant for the *trans* \Leftrightarrow *cis* conformational conversion of the two *anti* forms of imidoylketene was calculated to be 0.4432 that corresponds to an equilibrium mixture of about 31% *cis-anti* and 69% *trans-anti* at 300 K. The vibrational frequencies were computed at the DFT-B3LYP level and the infrared and Raman spectra of the molecule. Complete vibrational assignments were made on the basis of normal coordinate analyses and isotopic substitution of imidoylketene.

Keywords: Conformational stability; Vibrational spectra and assignments; imidoylketene.