

**Conformational stability and normal coordinate analyses of imidoylketene OCCH-CHNH.** Badawi, Hassan M.; Al-Saadi, Abdulaziz A. Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia. *Journal of Molecular Structure* (2006), 784(1-3), 259-264.

### **Abstract**

The conformational and structural stability of imidoylketene  $O=C=CH-CH=NH$  were investigated by DFT-B3LYP and ab initio MP2 calcns. with the 6-311+G\*\* basis set. From the calcns. imidoylketene was predicted to exist predominantly in a mixt. of trans-anti (the CCCN dihedral angle is  $180^\circ$ ) and cis-anti (the CCCN dihedral angle is  $0^\circ$ ) 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 calcns. The equil. const. for the trans.tautm.cis conformational conversion of the two anti forms of imidoylketene was calcd. to be 0.4432 kcal/mol that corresponds to an equil. mixt. of about 31% cis-anti and 69% trans-anti at 300 K. The vibrational frequencies were computed at the DFT-B3LYP level and the IR and Raman spectra of the mol. were calcd. Complete vibrational assignments were made on the basis of normal coordinate analyses.