Theoretical vibrational spectra and analyses of isocyanatoketene O=C=CH-N=C=O. Badawi, Hassan M.; Al-Saadi, Abdulaziz A. Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia. THEOCHEM (2004), 676(1-3), 35-40.

Abstract

The conformational stability of isocyanatoketene O=C=CH-N=C=O was studied by D. Functional B3LYP and ab initio second-order Moller Plesset MP2 calcns. with the 6-311 + G** basis set. Isocyanatoketene was predicted to have the s-cis s-trans conformational equil. with the s-trans being the predominant form. Full structural optimization was performed at the ground and transition states and the trans-cis barrier is .apprx.2 kcal/mol. The vibrational frequencies were computed at the DFT-B3LYP level, and the calcd. IR and Raman spectra of the cis-trans mixt. were plotted. Vibrational calcns. were also done for deuterated d1-isocyanatoketene. Reliable vibrational assignment was provided from normal coordinate calcns. for the stable conformers of the mol.