

DFT-B3LYP versus MP2, MP3 and MP4 calculations of the structural stability of azidoketene $O=C=CH-NNN$. Badawi, Hassan M.; Foerner, Wolfgang; Al-Saadi, Abdulaziz A. Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia. THEOCHEM (2004), 712(1-3), 131-138.

Abstract

The conformational stability of azidoketene $OCCH-NNN$ was investigated by D. Functional B3LYP and ab initio second-, third- and fourth-order Moeller Plesset calcns. with the 6-311+G** basis set. Azidoketene was predicted at the DFT-B3LYP level to have the s-cis.dblarw.s-trans conformational equil. with the s-trans ($O=C=C$ and NNN moieties are trans to each other) being the predominant low energy form, while at the MP2, MP3 and MP4 levels to have the gauche ($O=C=C$ and NNN moieties are near trans to each other) form as the min. in the potential curve of the mol. From full structural optimization of the ground and transition states at the DFT-B3LYP level, the trans-cis barrier was calcd. to be about 2 kcal/mol. The vibrational frequencies for the cis and trans conformations were computed for the gauche form at the MP2 level. The calcd. IR and Raman spectra of the mol. were plotted. Complete vibrational assignments were provided on the basis of normal coordinate calcns. for the mol.