

**DFT-B3LYP versus MP2, MP3 and MP4 calculations of the
structural stability of azidoketene O=C=CH-NNN**

Hassan M. Badawi^{*}, Wolfgang Förner and Abdulaziz A. Al-Saadi

**Department of Chemistry, King Fahd University of Petroleum & Minerals,
Dhahran 31261, Saudi Arabia**

^{*} Author to whom correspondence should be addressed.

ABSTRACT

The conformational stability of azidoketene OCCH-NNN was investigated by Density Functional B3LYP and ab initio second-, third- and fourth-order Möller Plesset calculations with the 6-311+G** basis set. Azidoketene was predicted at DFT-B3LYP level to have the *s-cis* \leftrightarrow *s-trans* conformational equilibrium 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 minimum in the potential curve of the molecule. From full structural optimization of the ground and transition states at DFT-B3LYP level, the *trans-cis* barrier was calculated 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 calculated infrared and Raman spectra of the molecule were plotted. Complete vibrational assignments were provided on the basis of normal coordinate calculations for the molecule.

Keywords: Vibrational spectra and assignments; Rotational barriers; Normal coordinate analysis; Azidoketene.