DFT and MP2 vibrational spectra and assignments for gauche N-methyleneformamide CH2=N-CHO

Author(s): Badawi HM

Source: JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM **Volume:** 617 **Pages:** 9-15

Abstract: The conformational behavior of N-methyleneformamide CH2=N-CHO was investigated by DFT-B3LYP and MP2 calculations with 6-311 + G** basis set. The molecule was predicted by both levels to exist predominantly in the non-planar gauche structure as a result of pronounce repulsive interaction between the carbonyl oxygen and the lone-pair on the nitrogen that overcame the conjugation between the C=N and C=O moieties. The vibrational frequencies were computed at the DFT-B3LYP and the MP2 levels and the calculated infrared and Raman spectra of the molecule in the gauche conformation were plotted. On comparison there was no significant change in the calculated vibrational line intensities of the infrared spectra by both levels. In the Raman spectra of the molecule the line intensity of some skeletal modes of the heavy atoms were noticed to significantly change as going from DFT to MP2 calculations. Complete vibrational assignments were made on the basis of normal coordinate calculations for the molecule.