Vibrational infrared and Raman spectra of chloromethyl isocyanate based on ab initio density functional calculations. Badawi, Hassan M.; Forner, Wolfgang

Abstract

The vibrational frequencies of the gauche chloromethyl isocyanate were computed at DFT-B3LYP/6-311++G** level with diffuse and polarization functions in a valence triple-zeta basis set. From the calcns., DFT in general produces better spectrum as compared to exptl. than MP2, with much less computational time and expenses. Normal coordinate calcns. were carried out and potential energy distributions PED were calcd. for the stable gauche conformer of the mol. On comparison, the PED values depend on the quality of the vibrational frequencies and on the basis set used and hence on the level of computations used.