

Theoretical vibrational spectra and potential scans for trichloromethylsulfonyl isocyanate.

Badawi, H. M.; Forner, W.; Oloriegbe, Y. S

Abstract

The conformational stability and structure of trichloromethylsulfonyl isocyanate were investigated by utilizing ab initio calcns. The computations were carried out at DFT-B3LYP/6-311++G** and MP2/6-311++G** levels. The calcn. predicted the stability of a single gauche conformer for this mol. at ambient temp. The vibrational frequencies of the gauche conformer were computed at DFT-B3LYP/6-311++G** level with diffuse and polarization functions in a valence triple-zeta basis set. Normal coordinate calcns. were carried out and the potential energy distributions PED were calcd. for the stable gauche conformer of the mol. The calcd. vibrational frequencies were compared to those obtained exptl. for similar mols.