

Theoretical Calculations and Analysis of Vibrational Infrared and Raman Spectra for Trifluoromethyl-

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Abstract

The conformational behavior and structure of trifluoromethylsulfonyl isocyanate were investigated by utilizing

ab initio calculations with a 6-311++G** basis set at DFT-B3LYP and MP2 levels. The results obtained

predict a single gauche conformer with the isocyanate group almost eclipsing one of the sulfonyl-oxygen bonds

(CSNC angle about 121°). The vibrational frequencies of the gauche conformer were computed at DFT-

B3LYP/6-311++G** level. Vibrational assignments were made on the basis of normal coordinate calculations.

The calculation yields structural parameters that are in good agreement with those obtained in previous

electron diffraction studies.