Two rotors potential scans and vibrational assignments for dihalomethylsulfonyl isocyanates

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Source: SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY **Volume:** 58 **Issue:** 5 **Pages:** 983-997

Abstract: The conformational behavior and structural stability of dichloro and difluoromethyl-sulfonyl isocyanates were investigated by quantum mechanical DFT and ab initio calculations. The 6-311 + + G** basis set was employed to include polarization and diffuse functions in the calculation at B3LYP and MP2 levels. The molecules were found to exist in a mixture of trans-gauche and gauche-gauche conformations at ambient temperatures. From the calculations the isocyanate NCO moiety was predicted to nearly eclipse one of the sulfony S=O bonds in the two stable conformers of both molecules. The potential scans for the rotations of the:two NCO and CX2H rotors were calculated from which the rotational barriers could be estimated. The vibrational frequencies, potential energy distributions, IR intensities as well as depolarization ratios were calculated.