Two rotors potential scans and vibrational assignments for dihalomethylsulfonyl isocyanates

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**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.