Vibrational infrared and raman spectra and density functional calculation of C-S rotational barrier in vinyl sulfonyl chloride and fluoride

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Abstract: The structure and conformational stability of vinyl sulfonyl chloride and fluoride were investigated using ab initio calculations at DFT-B3LYP/6-311 + +G** level. From the calculations the molecules were predicted to exist predominantly in the nonplanar gauche conformations with the vinyl C=C group being nearly eclipsing one of the sulfonyl S=O groups as a result of significant conjugation between the two moieties. The asymmetric potential function for the internal rotation was determined for the molecule. The vibrational frequencies were computed. Normal coordinate calculations were carried out and potential energy distributions were calculated for the two molecules in the gauche conformation.