

## Ring inversion, structural stability and vibrational assignments of sulfolane $c\text{-C}_4\text{H}_8\text{SO}_2$ and 3-sulfolene $c\text{-C}_4\text{H}_6\text{SO}_2$ .

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### Abstract

The structural stability of sulfolane (tetrahydrothiophene1,1-dioxide) and 3-sulfolene (dihydrothiophene1,1-dioxide) was investigated by DFTB3LYP and ab initio MP2 calculations with 6-311+G\*) basis set. The calculated symmetric ring-puckering potential of 3-sulfolene at the B3LYP level is consistent with a flat minimum that corresponds to a planar ring but at the MP2 level with a double minimum with a low barrier of about 193 cal mol<sup>-1</sup> to ring planarity in reasonable agreement with experimental results. From the calculations at the two levels of theory sulfolane was predicted to exist predominantly in the *twist* conformation. The vibrational wavenumbers were calculated at the MP2/6-31G\*\* level of theory and the potential energy distributions PED among the symmetry coordinates of the normal modes were computed for the low-energy structure of the molecules. Complete vibrational assignments were provided on the basis of the calculated PED values. The experimental infrared and Raman spectra of the two molecules were compared to the calculated ones.