

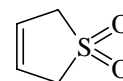
1667
MW

C₄H₆O₂S

2,5-Dihydrothiophene 1,1-dioxide

C_s

r_0	Å ^{a)}	θ_0	deg ^{a)}
S=O	1.450(10)	O=S=O	118.5(10)
C(2)–S	1.807(10)	C(2)–S–C(5)	97.7(10)
C(2)–C(3)	1.504(10)	S–C(2)–C(3)	103.0(10)
C(3)=C(4)	1.300(10)	C(2)–C(3)=C(4)	118.2(10)
C(2)–H	1.092(20)	H–C(2)–H	109.5(20) ^{b)}
C(3)–H	1.072(20)	ϕ ^{c)}	20(3)

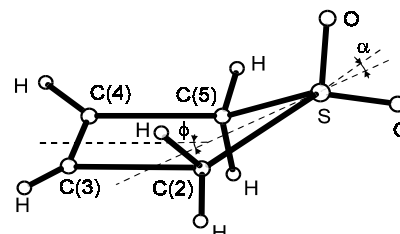


The potential function gives a barrier to ring inversion of 50(11) cm^{−1} and an equilibrium dihedral angle of ≈20°.

^{a)} Uncertainties were not estimated in the original paper.

^{b)} CH₂ maintains local C_{2v} symmetry, C(3,4)–H bonds lie on the bisector.

^{c)} Dihedral angle, see figure.



López, J.C., Lister, D.G., Villamañán, R.M., Alonso, J.L.: J. Chem. Phys. **92** (1990) 6384.