

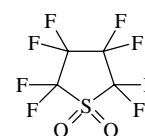
1482
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C₄F₈O₂S

Octafluorotetrahydrothiophene 1,1-dioxide

C₂

r_a	Å ^{a)}	θ_a	deg ^{a)}
C–F(average)	1.327(3)	C–S–C	93.2(10)
C–C(average)	1.556(6)	S–C–C ^{b)}	107.7(10)
S–C	1.882(7)	C–C–C ^{b)}	107.9(12)
S=O	1.427(4)	F–C–F	109.9(5)
$q^{b) c)}$	0.382(10)	C–S=O	108.2(8)
		O=S=O ^{b)}	125.9(24)
		$\tau^d)$	23.2(6)



The five-membered ring is strongly puckered and possesses the half chair conformation. The C–C bond lengths were assumed to be equal. The CF₂ groups were assumed to bisect the adjacent endocyclic bond angles; i.e. the rocking, twisting and wagging angles for the CF₂ groups were set to zero.

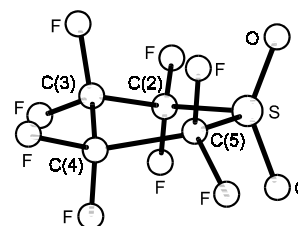
The nozzle was at room temperature.

^{a)} Three times the estimated standard errors including the scale error.

^{b)} Dependent parameter.

^{c)} Puckering amplitude; for definition see [1].

^{d)} Twist angle of the C(3)–C(4) bond about the C₂ symmetry axis.



Mack, H.-G., Oberhammer, H., Shreeve, J.M., Xia, X.-B.: J. Mol. Struct. **196** (1989) 57.

[1] Cremer, D., Pople, J.A.: J. Am. Chem. Soc. **97** (1975) 1354, 1358.