

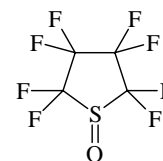
1481
ED

C₄F₈OS

Octafluorotetrahydrothiophene 1-oxide

C₁

r_a	Å ^{a)}	θ_a	deg ^{a)}
C–F(average)	1.337(2)	C–S–C	89.4(4)
C–C(average)	1.553(5)	S–C–C ^{b)}	110.2(4)
S–C	1.903(4)	C–C–C ^{b)}	106.5(6)
S=O	1.464(5)	F–C–F	108.9(4)
$q^{b) \text{ } c)}$	0.403(8)	C–S=O	104.3(11)
		$\tau^d)$	24.6(5)



The five-membered ring is strongly puckered and possesses the half chair (C₂) 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.

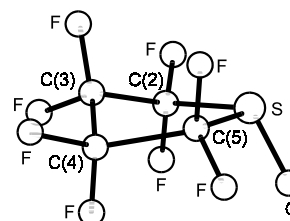
The nozzle was at room temperature.

^{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.