

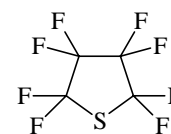
1483
ED

C₄F₈S

Octafluorotetrahydrothiophene

C₂

r_a	\AA^a	θ_a	deg^a
C–F(average)	1.338(2)	C–S–C	94.5(3)
C–C(average)	1.548(4)	S–C–C ^b	107.4(3)
S–C	1.822(4)	C–C–C ^b	106.4(4)
$q^{b) \text{ c)}$	0.403(8)	F–C–F	108.0(5)
		τ^d	25.2(5)



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.

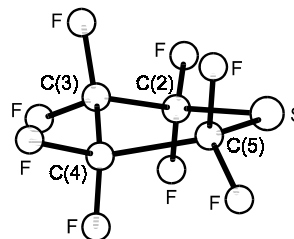
The nozzle was at room temperature.

^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.