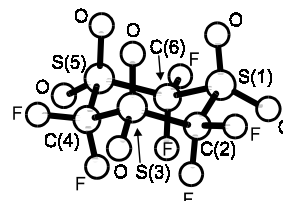
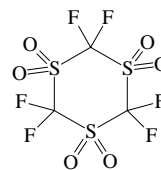


1020
ED

$\text{C}_3\text{F}_6\text{O}_6\text{S}_3$

2,2,4,4,6,6-Hexafluoro-1,3,5-trithiane 1,1,3,3,5,5-hexaoxide C_{3v}

r_a	$\text{\AA}^a)$	θ_α	$\text{deg}^a)$
C–F	1.338(4)	C–S–C	100.2(7)
S=O	1.418(2)	S–C–S	117.4(6)
C–S	1.866(4)	F–C–F	109.2(7)
		O=S=O	125.9(14)
		$\rho_1(\text{CF}_2)^b)$	4.1(12) ^{c)}
		$\rho_2(\text{SO}_2)^b)$	–0.9(7) ^{c)}
		$\theta_1^d)$	51.9(23)
		$\theta_2^e)$	60.8(23)
		$\phi^f)^g)$	62.1(14)



The nozzle temperature was 55 °C.

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

^{b)} Rocking angle.

^{c)} Axial fluorines pushed together and axial oxygens pushed apart.

^{d)} Puckering angle between the C(2)S(1)C(6) and C(2)S(3)S(5)C(6) planes.

^{e)} Puckering angle between the S(3)C(4)S(5) and C(2)S(3)S(5)C(6) planes.

^{f)} Torsional angle S–C–S–C.

^{g)} Dependent parameter.

Waterfeld, A., Weiss, I., Oberhammer, H., Gard, G.L., Mews, R.: J. Fluor. Chem. **67** (1994) 27.