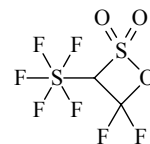


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ED $C_2HF_7O_3S_2$ **(4,4-Difluoro-2,2-dioxo-1,2 λ^6 -oxathiethan-3-yl)-
pentafluorosulfur(VI)** C_1

4,4-Difluoro-3-(pentafluorothio)-1,2-oxathietane 2,2-dioxide

r_a	\AA^a	θ_a	deg^a
C–F	1.327(6)	S(2)–C(3)–C(4)	85.6(14)
S(2)=O(2,3)	1.406(3)	C(3)–C(4)–O(1)	98.2(26)
C–O	1.41[2] ^b	C(4)–O(1)–S(2)	95.5(19)
C–C	1.52[2] ^b	O(1)–S(2)–C(3)	80.7(12)
S–F (mean)	1.571(3)	F–C(4)–F	107.7(28)
S(2)–O(1)	1.647(12)	O(2)=S(2)=O(3)	117.0(41)
S(2)–C(3)	1.792(15)	S(5)–C(3)–H	112.0 ^c
S(5)–C(3)	1.841(14)	F(3)–S(5)–F(4)	89.3(3)
C(3)...O(1)	2.232(21)	S(2)–C(3)–S(5)	118.3(9)
C–H	1.10 ^c	C(4)–C(3)–S(5)	117.8(18)
		τ^d	23.4(19)
		wag(CF ₂) ^e	4.0[20] ^b
		wag(SO ₂) ^e	4.0[20] ^b
		ϕ^f	1.2(42)



Local C_{4v} symmetry was assumed for the SF₅ group.
The nozzle was at room temperature.

^a) Three times the estimated standard errors including a systematic error.

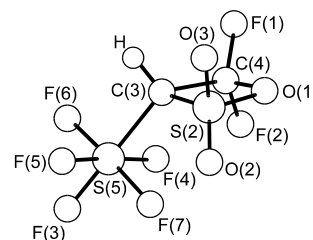
^b) Set to value for similar molecules, varied within the given range.

^c) Assumed.

^d) H–C–S–F(6) torsional angle from the *syn* position.

^e) Wagging angle towards O(1).

^f) Puckering angle between the CSO and CCO planes.



Gard, G.L., Terjeson, R.J., Oberhammer, H.: J. Mol. Struct. **443** (1998) 205.