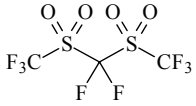
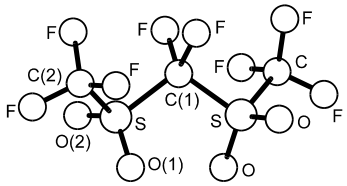
339 **$C_3F_8O_4S_2$** **Difluorobis[(trifluoromethyl)sulfonyl]methane** **C_2**

ED, *ab initio* calculations



r_a	Å [a])	θ [b])	deg [a])
C–F (mean)	1.323(2)	S–C–S	110.0(8)
C(1)–F	1.339(5) [c])	F–C(1)–F	110.5 [d])
C(2)–F	1.318(3) [c])	C–S–C	103.8(7)
S=O	1.420(2)	C(1)–S=O (mean)	109.1(8)
S–C (mean)	1.869(3)	C(1)–S=O(1)	110.5(9) [c])
S–C(1)	1.876(4) [c])	C(1)–S=O(2)	107.7(9) [c])
S–C(2)	1.862(4) [c])	C(2)–S=O	106.6(8)
		O=S=O [e])	120.3(22)
		F–C(2)–F	110.4(3)
		$\tau(CF_3)$ [f])	8(3)
		$\tau_{1,2}$ [g])	143(2)

Two stable conformers with C_2 symmetry ($\tau_{1,2}$ = 155° (most stable) and $\tau_{1,2}$ = 87°, ΔE=3.7 kcal mol^{-1}) and one with C_1 symmetry (τ_1 = 96° and τ_2 = 196°, ΔE = 2.3 kcal mol^{-1}) were predicted by HF/3-21G* calculations. The ED data identified a single conformer with C_2 symmetry, and the populations of the two other conformers were estimated to be less than 10%. Local C_{3v} symmetry was assumed for the CF_3 groups.
The nozzle was at room temperature.



[a]) Three times the estimated standard errors.
[b]) Unidentified, possibly θ_a.
[c]) Differences between the corresponding parameters were assumed at the *ab initio* values.
[d]) Assumed at the value from *ab initio* calculations.
[e]) Dependent parameter.
[f]) Torsional angle of the CF_3 group; $\tau(CF_3)$ = 0° when the CF_3 group is staggered with respect to the bonds around the S atom.
[g]) C–S–C–S torsional angle, 0° for the *syn* position.

Haist, R., Mack, H.-G., Waterfeld, A., Gard, G.L., Oberhammer, H.: J. Mol. Struct. **380** (1996) 213.