

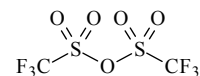
183 **C₂F₆O₅S₂**ED, *ab initio*
calculations

r_a	Å ^{a)}
C–F	1.318(3)
S=O(1,2)	1.409(3)
S–O	1.623(5)
S–C	1.848(6)

Trifluoromethanesulfonic acid anhydride

Trifluoromethanesulfonic anhydride

θ^b	deg ^{a)}
S–O–S	128.1(14)
O–S=O(1,2) (mean)	107.1(9)
O–S=O(1) ^{c)}	109.6(11)
O–S=O(2) ^{c)}	104.6(11)
O(1)=S=O(2) ^{d)}	128.0(21)
C–S=O(1,2) (mean)	105.9(11)
O–S–C	99.1(14)
F–C–F	110.4(4)
$\tau_{1,2}$ ^{e)}	99.1(14)



Two stable conformers with C₂ symmetry and different torsional angles $\tau(\text{C–S–O–S})$ (for one conformer $\tau_{1,2} = 96^\circ$, for another $\tau_{1,2} = 149^\circ$) and one with C₁ symmetry and different torsional angles ($\tau_1 = 120^\circ$, $\tau_2 = 175^\circ$) were predicted by HF/3-21G* calculations. The structure with C₂ symmetry and torsional angle of 96° is the most stable with $\Delta E = 0.4$ kcal mol^{−1} relative to each of the other conformers. According to the ED data, the dominant conformer has C₂ symmetry with $\tau_{1,2}$ of $99.1(14)^\circ$. The presence of up to 30% of the two other conformers could not be excluded. Local C_{3v} symmetry was assumed for CF₃ groups. The CF₃ groups were assumed to be staggered with respect to the SO₃ groups. The nozzle was at room temperature.

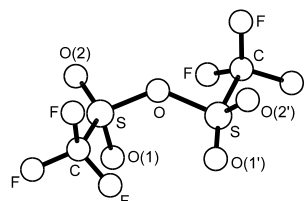
^{a)} Three times the estimated standard errors.

^{b)} Unidentified, possibly θ_a .

^{c)} Difference between the O–S=O angles was assumed at the value from HF/3-21G* calculations.

^{d)} Dependent parameter.

^{e)} C–S–O–S torsional angle, $\tau_{1,2} = 0$ in the *syn* position.



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