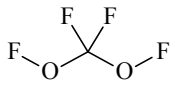
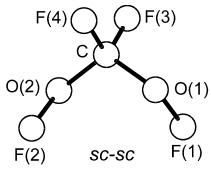
51 **CF_4O_2** **Hypofluorous acid difluoromethylene ester** **C_2** assumed (*sc-sc*)
ED, *ab initio* and DFT calculations
Difluoromethylene dihypofluorite **C_1** (*sc-ap*)
Bis(fluorooxy)difluoromethane



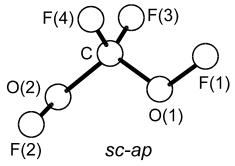
r_a	Å [a])
C–F	1.317(5)
C–O	1.387(6)
O–F	1.440(5)

θ_α	deg [a])
O–C–O	115.0(9)
C–O–F	105.7(4)
O–C–F (mean)	107.1(4)
O(1)–C–F(3)	112.1(11) [b])
O(1)–C–F(4)	102.1(11) [b])
F–C–F	113.0(9) [c])
O–C–O–F	55.3(21)

The ED intensities were reproduced best by a mixture of *sc-sc* (70(10)%) and *sc-ap* (30(10)%) conformers corresponding to $\Delta H° = H°(sc\text{-}ap) - H°(sc\text{-}sc) = 0.9(3)$ kcal mol^{-1}. Differences between the structural parameters for the *sc-sc* and *sc-ap* conformers were constrained to the values from MP2/6-31G* calculations. The dihedral angles for the *sc-ap* conformer were set to the theoretical values (O(1)–C–O(2)–F(2) = 67.8° and O(2)–C–O(1)–F(1) = 181.6°). The parameters are listed for the *sc-sc* conformer.
The nozzle was at room temperature.



sc-sc



sc-ap

[a]) Three times the estimated standard errors including a systematic error.
[b]) Difference between the O(1)–C–F(3) and O(1)–C–F(4) bond angles was assumed at the value from MP2/6-31G* calculations.
[c]) Dependent parameter.

Gobbato, K.I., Mack, H.-G., Oberhammer, H., Della Védova, C.O.: J. Am. Chem. Soc. **119** (1997) 803.