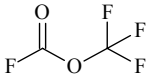
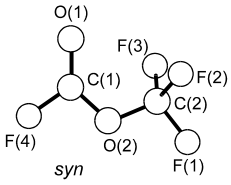
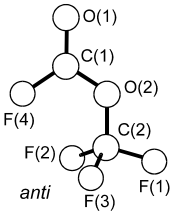
179 **$C_2F_4O_2$** **Carbonofluoridic acid trifluoromethyl ester** **C_s** assumed (*syn*)
ED, IR, *ab initio* and DFT calculations
Fluoroformic acid trifluoromethyl ester
Trifluoromethyl fluoroformate



r_a	Å [a])	θ_a	deg [a])
C=O(1)	1.188(4)	O(1)=C(1)–O(2)	130.3(16)
C–O(2) (mean)	1.364(9)	O(1)=C(1)–F(4)	123.9(20)
C(1)–O(2)	1.349(10) [b])	O(2)–C(1)–F(4)	105.8(12)
C(2)–O(2)	1.379(10) [b])	C(1)–O(2)–C(2)	117.1(7)
C–F (mean)	1.322(3)	F–C–F	108.9(7)
C(1)–F	1.321(6) [b])	tilt(CF_3) [c])	3.7 [d])
C(2)–F	1.323(5) [b])		

The molecule was found to exist mainly as a *syn* conformer with C(2)–O bond in the *syn* position with respect to the C(1)=O bond. ED intensities were not sensitive to a small amount (4%) of *anti* conformer detected in the IR spectra in Ar matrix. Local C_{3v} symmetry was assumed for the CF_3 group.
The nozzle was at room temperature.





[a]) Three times the estimated standard errors.
[b]) Differences in the C–O(2) and in the C–F bond lengths were assumed at the values from MP2/6-311G* calculations.
[c]) Angle between the C_3 axis of the CF_3 group and the O(2)–C(2) bond direction, toward the oxygen lone pair.
[d]) Assumed at the value from MP2/6-311G* calculations.

Hermann, A., Trautner, F., Gholivand, K., von Ahsen, S., Varetti, E.L., Della Vedova, C.O., Willner, H., Oberhammer, H.: Inorg. Chem. **40** (2001) 3979.