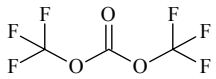
336 **$C_3F_6O_3$** **Carbonic acid bis(trifluoromethyl) ester** **C_{2v}** assumed

ED, IR, *ab initio* and DFT calculations

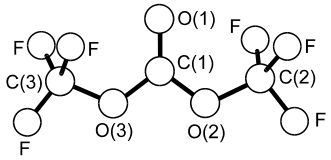
Bis(trifluoromethyl) carbonate



r_a	Å [a])	θ_a	deg [a])
C=O(1)	1.188(9)	O(1)=C(1)–O(2)	128.5(15)
C–O (mean)	1.377(5)	O(2)–C(1)–O(3)	103.1(22)
C(1)–O(2)	1.365(6) [b])	C(1)–O(2)–C(2)	116.5(7)
C(2)–O(2)	1.389(6) [b])	F–C–F	110.2(7)
C–F	1.315(3)	tilt(CF_3) [c])	4.6(21)

The molecule was found to exist as a *syn-syn* conformer with C–O bonds in the *syn* positions with respect to the C(1)=O bond. A small amount (1%) of *syn-anti* conformer detected in the IR spectra in Ar matrix was ignored in the ED analysis. 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]) Differences in the C–O(2) 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–C bond direction, toward the oxygen lone pair.

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.