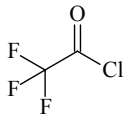
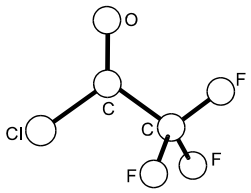
166 **C_2ClF_3O** **Trifluoroacetyl chloride** **C_s** assumed
ED

r_a	Å [a])	θ_α	deg [a])
C=O	1.186(4)	C–C=O	126.2(8)
C–C	1.533(6)	C–C–Cl	110.9(5)
C–F	1.329(2)	Cl–C=O	123.1(7)
C–Cl	1.742(4)	F–C–F	108.7(2)



The CF_3 group is staggered with respect to the C–Cl bond. Local C_{3v} symmetry was assumed for this group. The experimental parameters were reproduced by HF/3-21G* and HF/6-31G* calculations.
The nozzle was at room temperature.



[a]) Three times the estimated standard errors.

Gobbato, K.I., Leibold, C., Centeno, S., Della Védova, C.O., Mack, H.-G., Oberhammer, H.: J. Mol. Struct. **380** (1996) 55.