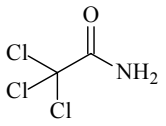
214 **$C_2H_2Cl_3NO$** **2,2,2-Trichloroacetamide** **C_1**

ED, DFT calculations

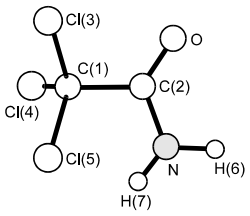
r_g	Å [a])
C=O	1.213(3)
C–N	1.347(4)
C–C	1.591(5)
N–H(6)	1.033(8)
N–H(7)	1.032 [c])
C–Cl(3)	1.761(2)
C–Cl(4)	1.775 [c])
C–Cl(5)	1.789 [c])

θ_α	deg [a])
O=C–N	127.7(6)
C–C–N	114.1(9)
C–N–H(6)	117.0 [b])
C–N–H(7)	123.2 [b])
C–C–Cl(3)	109.5(1)
C–C–Cl(4)	106.4 [c])
C–C–Cl(5)	112.1 [c])
Cl(3)–C–Cl(4)	109.1 [c])
Cl(3)–C–Cl(5)	108.3 [c])



According to the analysis of ED data by using a dynamic model and the results of B3LYP/6-31+G** calculations, the molecule exists as a perpendicular conformer with τ[Cl(4)–C(1)–C(2)–N] = 90°. This conclusion did not agree with the results of HF/6-311G** calculations, which predicted existence of a *syn* conformer. The amide fragment was assumed to be planar in the ED analysis.
The nozzle was at about 160 °C.

[a]) Estimated standard errors including a systematic error.
[b]) Assumed at the *ab initio* value.
[c]) Differences between similar parameters were assumed at the values from B3LYP/6-31+G** calculations.



Samdal, S., Seip, R.: J. Mol. Struct. **413-414** (1997) 423.