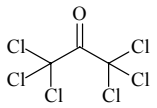
333 **C_3Cl_6O** **1,1,1,3,3,3-Hexachloro-2-propanone** **C_2**
ED, *ab initio* calculations
Hexachloroacetone

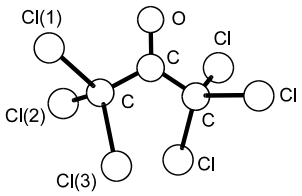


r_g	Å [a])
C–C [b])	1.590(10)
C=O	1.202(11)
C–Cl [b])	1.772(3)
C–Cl(1) [c])	1.764(3)
C–Cl(2) [c])	1.777(3)
C–Cl(3) [c])	1.775(3)

θ_α	deg [a])
C–C–C	123.5(11)
C–C–Cl [b])	109.5(3)
C–C–Cl(1) [c])	108.2(3)
C–C–Cl(2) [c])	106.0(3)
C–C–Cl(3) [c])	114.2(3)
Cl(1)–C–Cl(2) [d])	111.8(3)
Cl(1)–C–Cl(3) [d])	107.8(3)
Cl(2)–C–Cl(3) [d])	109.0(3)
C–C=O [d])	118.2(5)
Cl(1)–C–C=O	31.6(12)

The molecule was found to exist as a single conformer with C_2 symmetry, in contradiction to the conclusions from the previous ED study [1]. According to the results of MP2/6-311+G(2d) calculations, the potential barrier V_0 in the eclipsed position of the CCl_3 groups (C_{2v} molecular symmetry) was estimated to be 5.17 kcal mol^{-1}.
The nozzle temperature was 573 K.

[a]) Twice the estimated standard errors including a systematic error.
[b]) Average value.
[c]) Differences in the C–Cl and C–C–Cl parameters were constrained to the values from *ab initio* calculations.
[d]) Dependent parameter.



Johansen, T.H., Muren, S., Hagen, K.: J. Mol. Struct. **567-568** (2001) 113.
[1] Andersen, P., Astrup, E.E., Borgan, A.: Acta Chem. Scand. A **28** (1974) 239.

Replaces II/25C (**3**, 1005)