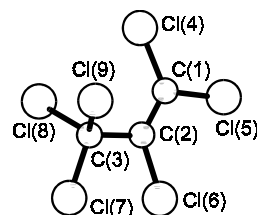


1003 **C₃Cl₆**
ED, *ab initio* calculations
(HF/6-31G*)

1,1,2,3,3,3-Hexachloro-1-propene
Hexachloropropene

C_s(*anti*)
Cl₂C=CCl–CCl₃

r_g	Å ^{a)}	θ_α	deg ^{a)}
C(1)=C(2)	1.350(13)	C–C=C	124.4(11)
C(2)–C(3)	1.536(17)	C(1)=C(2)–Cl(6)	117.7(21)
C(1)–Cl(4)	1.716(3) ^{b)}	C(2)=C(1)–Cl(4)	123.7(11) ^{c)}
C(1)–Cl(5)	1.714(3) ^{b)}	C(2)=C(1)–Cl(5)	121.5(11) ^{c)}
C(2)–Cl(6)	1.725(3) ^{b)}	C(2)–C(3)–Cl(7)	114.6(26)
C(3)–Cl(7)	1.773(3) ^{b)}	C(2)–C(3)–Cl(8)	109.9(14)
C(3)–Cl(8)	1.781(3) ^{b)}	Cl(8)–C(3)–Cl(9)	109.9 ^{d)}



No indications of a second conformer were observed, but small amounts (< 10%) of the *syn* form (C(3)–Cl eclipsing C=C) could not be excluded. The nozzle was at 351 K.

^{a)} Twice the estimated standard errors including the scale error.

^{b)} Differences between C–Cl distances fixed at the *ab initio* values.

^{c)} Difference between the C(2)=C(1)–Cl(4) and C(2)=C(1)–Cl(5) bond angles fixed at the *ab initio* value.

^{d)} Fixed at the *ab initio* value.

Hagen, K., Stølevik, R., Kaleem, H.: J. Phys. Chem. **98** (1994) 6293.