

1246
ED, MW

C₃H₆Cl₂

2,2-Dichloropropane

C_{2v}
H₃C–CCl₂–CH₃

r_g	\AA^a	θ_{av}	deg ^{a)}
C–C	1.523(4)	C–C–C	113.0(4)
C–Cl	1.799(3)	C–C–Cl	108.9(4)
C–H	1.101(5)	Cl–C–Cl	108.3(3)
		H–C–H	107.2(9)

One C–H bond of each methyl group lies on the CCC plane in the *trans* position to the most distant C–C bond. The tilt angle of the methyl groups was assumed to be zero. The measurements were made at room temperature.

^{a)} Estimated total errors.

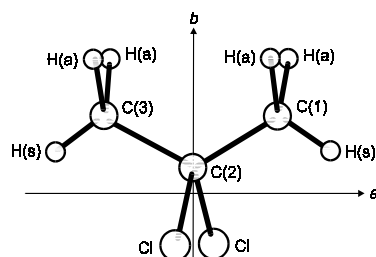
Hirota, M., Iijima, T., Kimura, M.: Bull. Chem. Soc. Jpn. **51** (1978) 1589.

MW

r_0	\AA	θ_0	deg
C–C	1.530(5)	C–C–C	112.0(1)
C–Cl	1.785 ^{a)}	C–C–Cl	108.9(1)
C–H	1.090 ^{a)}	Cl–C–Cl	109.0(1)
C...C	2.538	C–C–H	110.8(12)
Cl...Cl	2.906		

r_s	\AA	θ_s	deg
C–C	1.528(2)	C–C–C	112.4(1)
C–Cl	1.785(3)	C–C–Cl	108.9(2)
C...C	2.539	Cl–C–Cl	108.9(2)
Cl...Cl	2.904		

Atom	$a_s [\text{\AA}]$	$b_s [\text{\AA}]$	$c_s [\text{\AA}]$
C(1)	0.00	1.2568	1.2697
C(2)	0.00	0.4072	0.00
C(3)	0.00	1.2568	–1.2697
Cl(1)	1.4518	0.6312	0.00
Cl(2)	–1.4518	0.6312	0.00



^{a)} Fixed.

Takeo, H., Sugie, M., Matsumura, C.: J. Mol. Struct. **352/353** (1995) 267.