

1059
ED

C₃H₂Cl₆

1,1,2,2,3,3-Hexachloropropane

r_g	Å ^{a)}	θ_α	deg ^{a)}
C(2)–C(1,3)	1.558(16)	C(2)–C(1,3)–Cl	111.4(8)
C(1,3)–Cl	1.780(10)	C(1,3)–C(2)–Cl	108.8(4)
C(2)–Cl	1.752(18)	C–C–C	108.0(20)
C–H	1.02(8)	C–C–H	105.2(82)
		$\delta_1 = \delta_2$ ^{b)}	116.2(14)

The molecule has an all staggered *gauche* conformation without parallel Cl...Cl interactions.
The nozzle temperature was 112 °C.

^{a)} Twice the estimated standard errors.

^{b)} Torsional angles around C–C bonds, H–C–C–C; $\delta = 0^\circ$ for *anti* position.

Fernholt, L., Stølevik, R.: Acta Chem. Scand. Ser. A **29** (1975) 651.

