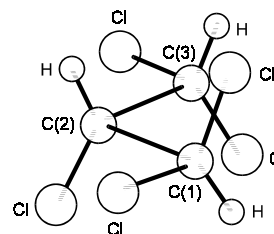


1094 **C₃H₃Cl₅**
ED, MM calculations

1,1,2,3,3-Pentachloropropane

C₁
Cl₂HC–CHCl–CHCl₂

r_a	Å ^{a)}	θ_α	deg ^{a)}
C–Cl (average)	1.774(2)	C–C–C	113.8(8)
C–C (average)	1.521(9)	C(2)–C(1)–Cl	111.8(5)
C–H	1.115 ^{b)}	C(1)–C(2)–Cl	109.8(6)
		C(2)–C(1)–H	109.4 ^{c)}
		C(1)–C(2)–H	107.3 ^{c)}
		(Cl–C–Cl) ^{d)}	123.3
		Cl–C(1)–Cl ^{e)}	109.5(2)
		H–C(1)–Cl ^{e)}	106.6(6)
		H–C(2)–Cl ^{e)}	108.3(18)
		δ_{1-2} ^{f)}	112.3(9)
		δ_{2-3} ^{f)}	123.8(11)



The molecule has a conformation which contains no parallel Cl...Cl interaction.
The nozzle temperature was 83 °C.

^{a)} Estimated standard errors.

^{b)} Estimated from radical distribution curve.

^{c)} Values from molecular mechanics calculations.

^{d)} The projection of the angle Cl–C–Cl on a plane perpendicular to the C–C bond.

^{e)} Dependent angle.

^{f)} Torsional angle around C(1)–C(2) and C(2)–C(3), respectively; $\delta = 0^\circ$ for the *anti* position of the chain H–C–C–C.

Grindheim, S., Stølevik, R.: Acta Chem. Scand. Ser. A **31** (1977) 69.