

1245 **C₃H₆Cl₂**
ED, MM calculations

1,3-Dichloropropane

C₂ (GG)
C_{2v} (AA)
C₁ (AG)
H₂ClC–CH₂–CClH₂

r_a	Å ^{a)}	θ_α	deg ^{a)}
C–H	1.118(6)	C–C–C	112.9(5)
C–C	1.529(4)	C–C–Cl	111.6(1)
C–Cl	1.796(3)	C(1)–C(2)–H	108.8 ^{b)}
		C(2)–C(1)–H	109.9 ^{b)}
		H–C(1)–Cl	107.8(1) ^{c)}
		H–C(1)–H	108.3(1) ^{c)}
		H–C(2)–H	108.0(7) ^{c)}
		$\varphi^d)$	120.0 ^{e)}
		δ (<i>gauche</i>) ^{f)}	114.2 (6)

Three conformers GG (73(4)%), AG (24(4)%) and AA (less than 10%) were detected.

The nozzle temperature was 38 °C.

^{a)} Estimated standard errors.

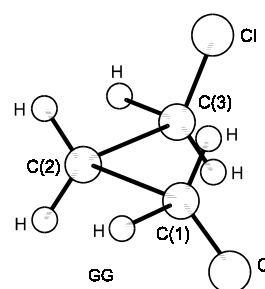
^{b)} Calculated value for GG by molecular mechanics calculations.

^{c)} Dependent parameter.

^{d)} The projection of the H–C(1)–H angle on a plane perpendicular to the C(1)–C(2) bond.

^{e)} Assumed.

^{f)} Torsional angle Cl–C–C–C, defined as zero at the *anti* conformation.



Grindheim, S., Stølevik, R.: Acta Chem. Scand. Ser. A **30** (1976) 625.