

1724 $\text{C}_4\text{H}_8\text{Cl}_2$
ED, *ab initio* calculations
(HF/6-31G*)

1,4-Dichlorobutane

C_2 ($\text{G}^-\text{G}^-\text{G}^-$)
 C_1 (G^-AA)
 S_2 (G^+AG^-)
 $\text{H}_2\text{ClC}-\text{CH}_2-\text{CH}_2-\text{CClH}_2$

r_{g}	\AA^{a}	θ_{α}	deg^{a}
C(1)–C(2)	1.523(3)	C–C–C	116.3(6)
C(2)–C(3)	1.530(3)	C–C(1)–Cl	112.2(4)
C–Cl	1.802(3)	C–C(1)–H	112.3(34)
C(1)–H	1.108(7)	C–C(2)–H	109.1(24)
C(2)–H	1.104(7)	τ_1^{b}	59(22)
		τ_2^{c}	–59(22)
		τ_3^{c}	–52(17)

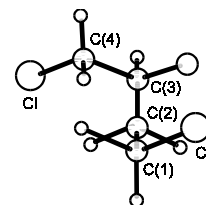
The molecule exists as a mixture of the conformers: G^-AA (25(12)%), $\text{G}^-\text{G}^-\text{G}^-$ (33(12)%), G^+AG^- (21(12)%), G^-AG^- (10(6)%), AG^-G^+ (7(11)%), $\text{G}^+\text{G}^+\text{G}^+$ (>1(6)%), AAA (4(9)%). The symbols refer to *anti* (A) and *gauche* (G^+ or G^-) dihedral angles at C(1)–C(2), C(2)–C(3) and C(3)–C(4) bonds. The differences between corresponding bond lengths and bond angles of the different conformers and the torsion angles for the G^-AG^- , AG^-G^+ , $\text{G}^+\text{G}^+\text{G}^+$ and AAA conformers were fixed at the *ab initio* values. The parameters are given for the $\text{G}^-\text{G}^-\text{G}^-$ conformer. The nozzle was at 60 °C.

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

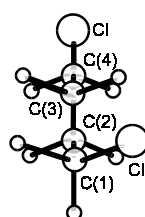
^b) Torsional angle Cl–C(1)–C(2)–C(3).

^c) Torsional angle C(2)–C(3)–C(4)–Cl.

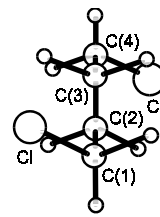
^d) Torsional angle C(1)–C(2)–C(3)–C(4).



$\text{G}^-\text{G}^-\text{G}^-$



G^-AA



G^+AG^-

Aarset, K., Hagen, K., Stølevik, R.: J. Phys. Chem. **98** (1994) 5249.