

1775 **C₄H₉Cl**
ED, *ab initio* calculations
(HF/6-31G*)

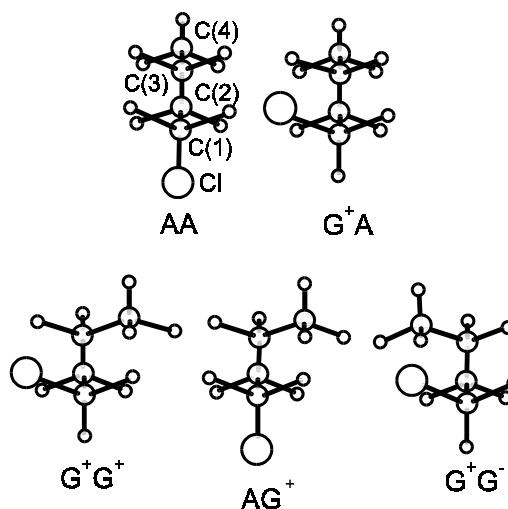
1-Chlorobutane
Butyl chloride

C₁ (GA, GG, AG)
C_s (AA)
H₃C–CH₂–CH₂–CH₂Cl

r_g	Å ^a	θ_α	deg ^a
C(1)–C(2)	1.519(3)	C(1)–C(2)–C(3)	114.3(6)
C(2)–C(3)	1.530(3)	C(2)–C(3)–C(4)	112.0(6)
C(3)–C(4)	1.543(3)	C–C–Cl	112.3(5)
C–Cl	1.800(4)	C–C(1)–H	111.1(18)
C(1)–H	1.097(5)	C–C(2)–H	108.9(18)
C(2)–H	1.107(5)	C–C(3)–H	109.5(18)
C(3)–H	1.121(5)	C–C(4)–H	110.7(18)
C(4)–H	1.108(5)	Cl–C(1)–C(2)–C(3)	59(4)
		C(1)–C(2)–C(3)–C(4)	168(17)

The compound exists as a mixture of AA (13(12)%), G⁺A (60(13)%), AG⁺ (12(16)%), G⁺G⁺ (12(13)%) and G⁺G[−] (3(8)%) conformers, where the first and the second symbols refer to torsions about the C(1)–C(2) and C(2)–C(3) bonds, respectively. The symbols refer to *anti* (A) with the torsion angle of about 180° and *gauche* (G⁺ and G[−]) with torsion angles of about +60° and −60°, respectively. Differences between the same set of parameters, C–C, C–H, C–C–C and C–C–H in the same conformer and those between different conformers were all fixed at the *ab initio* values.

Parameters are given for the GA conformer.
The nozzle temperature was 18 °C.



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

Aarset, K., Hagen, K., Stølevik, R., Sæbø, P.C.: Struct. Chem. **6** (1995) 197.

See also: Fagerland, S., Rydland, T., Stølevik, R., Seip, R.: J. Mol. Struct. **96** (1983) 339.

MW

C_s (AA)
C₁ (GA, AG)

θ_0 [deg] ^a	AA	GA	AG
Cl–C(1)–C(2)	109.73(20)	113.7(5)	108.1(5)
C(1)–C(2)–C(3)	110.08(20)	113.0(5)	114.7(5)
C(2)–C(3)–C(4)	113.58(20)	108.6(5)	114.9(5)
τ_1 ^b		63.2(5)	
τ_2 ^c			62.5(5)

³⁵ Cl [Å]	AA	GA	AG
<i>a</i> ₀	2.1418	1.7823	2.0563
<i>b</i> ₀	0.2044	0.4527	0.2158
<i>c</i> ₀	0.0	0.1134	0.1261

^a) Uncertainties were not estimated in the original paper.

^b) Dihedral angle Cl–C(1)–C(2)–C(3).

^c) Dihedral angle C(4)–C(3)–C(2)–C(1).

Melandri, S., Favero, P.G., Damiani, D., Caminati, W., Favero, L.B.: J. Chem. Soc. Farad. Trans. **90** (1994) 2183.