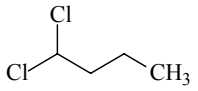
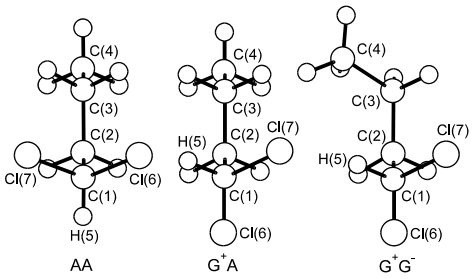
557 **$C_4H_8Cl_2$** **1,1-Dichlorobutane** **C_1** (G^+A)

ED, *ab initio* calculations



r_g	Å [a])	θ_α	deg [a])
C(1)–C(2)	1.521(4)	C(1)–C(2)–C(3)	114.4(13)
C(2)–C(3)	1.539(4)	C(2)–C(3)–C(4)	112.5(13)
C(3)–C(4)	1.546(4)	C(2)–C(1)–Cl(6)	110.4(7)
C–Cl	1.782(3)	C(2)–C(1)–Cl(7)	111.9(7)
C(1)–H	1.082(6)	C–C–H (mean)	108.9(47)
C(2)–H	1.102(6)	Cl–C(1)–Cl	109.6(5)
C(3)–H	1.117(6)		
C(4)–H	1.120(6)		



Gauche-anti (G^+A) conformer (85(40)%) was found to be the low-energy form. Certain amounts of *anti-anti* (AA) and *gauche*$^+$-*gauche*$^-$ (G^+G^-) conformers might be present. The symbols refer to torsion about the C(1)–C(2) and C(2)–C(3) bonds, *anti* (A) with H(5)–C(1)–C(2)–C(3) and C(1)–C(2)–C(3)–C(4) torsional angles of 180° and *gauche* (G^+ or G^-) with torsional angles +60° or –60°, respectively. The differences between parameters in the same conformer and between the different conformers were assumed at the values from HF/6-31G(d) calculations. The parameters are listed for the G^+A conformer.
The nozzle temperature was 23 °C.

[a]) Twice the estimated standard errors including a systematic error.

Aarset, K., Hagen, K., Stølevik, R.: J. Mol. Struct. **413-414** (1997) 241.