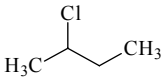
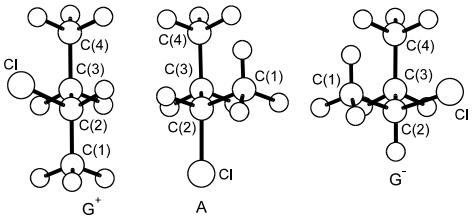
575 **C_4H_9Cl** **2-Chlorobutane** **C_1 (G^+)**
ED, *ab initio* calculations **C_1 (A)**
C_1 (G^-)

r_g	Å [a])
C(1)–C(2) [b])	1.524(3)
C(2)–C(3) [b])	1.528(3)
C(3)–C(4) [b])	1.539(3)
C–Cl	1.812(3)
C–H [b]) [c])	1.098(4)

θ_α	deg [a])
C(1)–C(2)–C(3) [b])	115.5(5)
C(2)–C(3)–C(4) [b])	113.3(5)
C(1)–C(2)–Cl	110.4(9)
C(3)–C(2)–Cl	108.43(7)
C–C(1)–H [b]) [c])	111.14(15)
H–C(3)–H	106.73 [d])
H–C(2)–Cl	116.57(19)



According to the results of HF/6-311+G(d,p) calculations, the molecule exists as a mixture of G^+ (62%), A (25%) and G^- (13%) conformers with torsional angles τ[Cl–C(2)–C(3)–C(4)] of *ca.* 60°, 180° and –60°, respectively. This conformational composition was found to fit the experimental data quite well. The differences between the corresponding parameters of the conformers were constrained in the ED analysis to the values from HF/6-311+G(d,p) calculations. The structural parameters are listed for the G^+ conformer.
The nozzle temperature was 25 °C.



[a]) Twice the estimated standard errors including a systematic error.
[b]) Differences in the C–C, C–H, C–C–C and C–C–H parameters were constrained to the values from HF/6-311+G(d,p) calculations.
[c]) Average value.
[d]) Assumed at the value from HF/6-311+G(d,p) calculations.

Aarset, K., Hagen, K., Stølevik, R.: J. Mol. Struct. **567-568** (2001) 157.

Replaces II/25C (**3**, 1776)