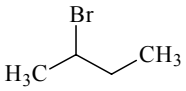
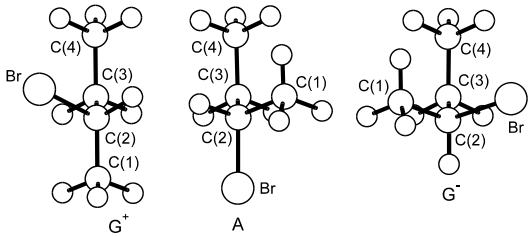
572 **C_4H_9Br** **2-Bromobutane** **C_1 (G^-)**
ED, *ab initio* **C_1 (G^+)**
calculations **C_1 (A)**

r_g	Å [a])
C(1)–C(2) [b])	1.526(4)
C(2)–C(3) [b])	1.530(4)
C(3)–C(4) [b])	1.540(4)
C–Br	1.982(5)
C–H [b]) [c])	1.111(8)

θ_α	deg [a])
C(1)–C(2)–C(3) [b])	112.5(16)
C(2)–C(3)–C(4) [b])	114.6(15)
C(1)–C(2)–Br	110.1(16)
C(3)–C(2)–Br	109.30(13)
C–C(1)–H [b]) [c])	107.67(30)
H–C(3)–H	106.61 [d])
H–C(2)–Br	114.65(43)



According to the results of the ED analysis, the molecule exists as a mixture of *anti* (A) and *gauche* (G) conformers in the ratio of 1:9. The relative amounts of the two *gauche* conformers, G^- and G^+, with torsional angles τ[Br–C(2)–C(3)–C(4)] of about –60° and 60°, respectively, were calculated by the HF/6-311+G(d,p) method to be 17% and 73%, respectively. 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.