

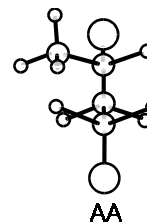
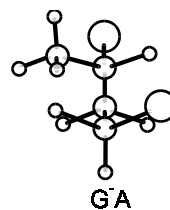
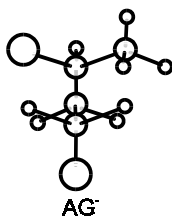
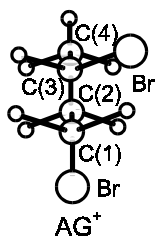
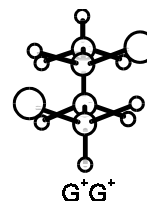
1720 C₄H₈Br₂

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

1,3-Dibromobutane

 C₁ (all conformers)
 H₂BrC–CH₂–CHBr–CH₃

r_g	Å ^a	θ_α	deg ^a
C(1)–C(2)	1.518(6)	C(1)–C(2)–C(3)	115.3(16)
C(2)–C(3)	1.521(6)	C(2)–C(3)–C(4)	111.6(16)
C(3)–C(4)	1.526(6)	C(2)–C(1)–Br	112.2(9)
C(1)–Br	1.963(6)	C(2)–C(3)–Br	109.8(9)
C(3)–Br	1.974(6)	C–C–H (average)	111.5(51)
C–H (average)	1.082(11)		



This molecule may in principle exist as a mixture of nine different conformers; five of them (G⁺G⁺(60(23)%) AG⁺(<1%), G⁻A (36(22)%), AG⁻(<1%), and AA(4(9)%)) were included in the analysis. The first and second symbols refer to torsion about the C(1)–C(2) and C(2)–C(3) bonds, respectively. The symbols refer to *anti* (A) with a torsion angle of about 180° and *gauche* (G⁺ and G⁻) with torsion angles of about +60° and –60°, respectively. Only the average values for C–C, C–Br, C–H, C–C–C, C–C–Br and C–C–H were refined in the least-squares analysis; the differences between the values for these parameters in the same conformer and those between different conformers were fixed at the corresponding *ab initio* values.

Parameters are given for the predominant G⁺G⁺ conformer.

The nozzle temperature was 23 °C.

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

Aarset, K., Hagen, K., Stølevik, R.: J. Phys. Chem. **99** (1995) 11089.