

1236 $\text{C}_3\text{H}_6\text{Br}_2$
ED, MM calculations

1,2-Dibromopropane

C_1 (A)
 C_1 (G^-)
 C_1 (G^+)
 $\text{H}_3\text{C}-\text{CHBr}-\text{CH}_2\text{Br}$

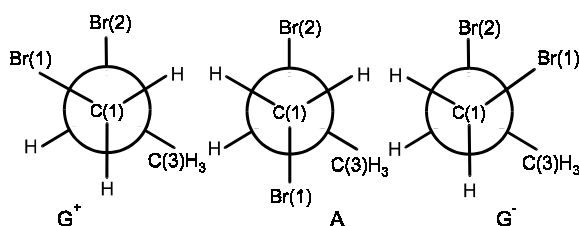
r_a	\AA^a	θ_α	deg ^{a)}
C–C	1.530(11)	C(1)–C(2)–C(3) (A) ^{b)}	109.2(24)
C–Br	1.960(7)	Br(1)–C(1)–C(2) (A) ^{b)}	110.8(14)
C–H	1.109(23)	Br(2)–C(2)–C(1) (A) ^{b)}	108.6(11)
		Br(2)–C(2)–C(3)	108.6(11)
		C(2)–C(1)–H	109.7 ^{c)}
		Br(1)–C(1)–H	111.0 ^{c)}
		C(1,3)–C(2)–H	109.0 ^{c)}
		C(2)–C(3)–H	110.0 ^{c)}
		ϕ (A) ^{d)}	165(4)
		ϕ (G^-) ^{d)}	–59(10)
		ϕ (G^+) ^{d)}	65(10)

The molecule exists as a mixture of *anti* A (85(6)%), *gauche* G^- (4%) and *gauche* G^+ (11%) conformers.

Local symmetries C_{3v} , C_s and C_s were assumed for the C– CH_3 , CH_2Br and C–CH–C groups, respectively. The lengths of all the

C–H bonds and the two C–Br bonds and the Br–C(2)–C(3) angles for all the conformers were assumed to be equal.

The nozzle was at 40 °C.



^{a)} Twice the estimated standard errors.

^{b)} Conformational differences were fixed at the values from molecular-mechanics calculations.

^{c)} Values from molecular mechanics calculations.

^{d)} Torsion angle Br–C–C–Br; $\phi = 0^\circ$ for *syn* position.

Schei, S.H., Stølevik, R.: J. Mol. Struct. **128** (1985) 171.