

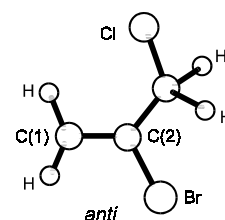
1133 **C₃H₄BrCl**
ED, MM calculations

2-Bromo-3-chloro-1-propene

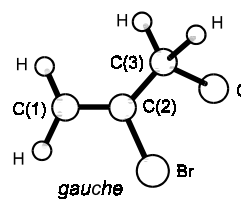
C_s (*anti*)
C₁ (*gauche*)
H₂C=CBr–CClH₂

<i>r_a</i>	Å ^{a)}	<i>θ_α</i>	deg ^{a)}
C(1)=C(2)	1.360(14)	C–C=C (<i>gauche</i>)	126.0(10)
C(2)–C(3)	1.491(16)	Δ(C–C=C) ^{b)}	2.4 ^{c)}
C–Br	1.911(11)	C=C–Br (<i>gauche</i>)	122.1(30)
C–Cl	1.803(9)	Δ(C=C–Br) ^{b)}	–0.8 ^{c)}
C–H (average)	1.139(30)	C–C–Cl (<i>gauche</i>)	112.3(26)
		Δ(C–C–Cl) ^{b)}	0.7 ^{c)}
		C(2)=C(1)–H	120.7(62)
		C(2)–C(3)–H	112.8(42)
		<i>φ</i> ^{d)}	119.5(63)
		<i>τ</i> (<i>gauche</i>) ^{e)}	109.4(26)

There is a mixture of two conformers in the gas phase with the halogen atoms *anti* or *gauche* to each other. The measurements were made at 20, 90, and 187 °C; results at 20 °C are listed. Amount of *anti* form at 20 °C: 48(11)%. $\Delta E = E(\textit{gauche}) - E(\textit{anti}) = 3(1) \text{ kJ mol}^{-1}$.



- ^{a)} Twice the estimated standard errors including a systematic error.
^{b)} The difference quantities (*anti*) – (*gauche*).
^{c)} Estimated from molecular mechanics calculations.
^{d)} Angle between projections of C–Cl and C–H bonds on a plane perpendicular to C–C bond.
^{e)} Torsional angle Br–C–C–Cl of *gauche* form; $\tau = 0^\circ$ for the planar *anti* form.



Søvnik, O.I., Schei, S.H., Stølevik, R., Hagen, K., Shen, Q.: J. Mol. Struct. **116** (1984) 239.