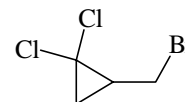


r_a	\AA^a	θ_α	deg^a
C–H	1.095(19)	C(4)–C(2)–C	117.5(13)
C–C ^b	1.496(14)	C–C–Br	110.5(19)
$\Delta(\text{C–C})^b$	0.041(36)	Cl–C–Cl	111.9(6)
C(2)–C(4)	1.543(32)	H–C–H	109.0 ^d
C–Cl	1.752(6)	C(4)–C(2)–H	110.0 ^d
C–Br	1.950(13)	C(2)–C(4)–H	111.4 ^d
		ϕ (<i>gauche</i> -1) ^c	116.2(56)
		ϕ (<i>gauche</i> -2) ^c	–132.7(76)



The molecule is found to exist as about equal amounts of the *gauche*-1 and *gauche*-2 (55(11)%) conformers. There is no evidence for the presence of a *syn* conformer, but small amounts (up to 10%) of this form cannot be excluded.

The nozzle temperature was 65 °C.

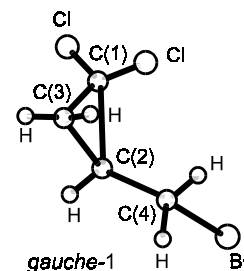
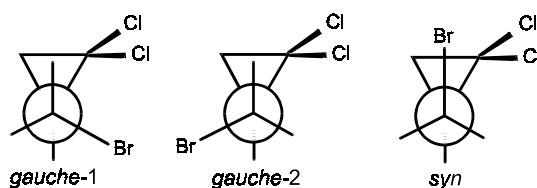
^a) Twice the estimated standard errors including a systematic error.

^b) $0.5[(\text{C}(1)\text{--}\text{C}(2)) + (\text{C}(2)\text{--}\text{C}(3))]$. C(1)–C(2) and C(1)–C(3) bond lengths were assumed to be equal.

^c) $(\text{C}(2)\text{--}\text{C}(3)) - (\text{C}(1)\text{--}\text{C}(2))$.

^d) Assumed.

^e) C–C torsion angles between C–Br and the three-membered ring; $\phi = 0^\circ$ for the *syn* position; a positive value of ϕ corresponds to a clockwise rotation of the C–Br bond in the Newman projections shown in the figure.



Shen, Q., Hagen, K.: J. Mol. Struct. **158** (1987) 347.