

1197
ED, MW

C₃H₅ClO

2-(Chloromethyl)oxirane
Epichlorohydrin

C₁ (*gauche*-1)
C₁ (*gauche*-2)

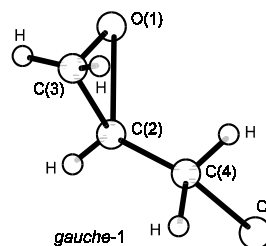
r_a	Å ^{a)}	θ_a	deg ^{a)}
C–H	1.095(5)	C(4)–C(2)–O	114(1)
C(2,3)–O	1.442(3)	C–C–C	119(1)
C(2)–C(3)	1.475(8)	C–C–Cl	108.9(7)
C(2)–C(4)	1.523(7)	τ (Cl–C–C–O) ^{b)} (<i>gauche</i> -2)	–150(10)
C–Cl	1.798(2)	τ (Cl–C–C–O) ^{b)} (<i>gauche</i> -1)	78(10)

The molecule exists as a mixture of *gauche*-2 (67(12)%) and *gauche*-1 (33(12 %) conformers. The nozzle temperature was 67 °C.

^{a)} Three times the estimated standard errors.

^{b)} $\tau = 0^\circ$ for *syn* position.

Shen, Q.: J. Mol Struct. **130** (1985) 275.



MW

r_0	Å ^{a)}	θ_0	deg ^{a)}
C(2,3)–H	1.082 ^{b)}	φ_1 ^{c)}	58.125 ^{b)}
C(2,3)–O	1.436 ^{b)}	φ_2 ^{d)}	54.65 ^{b)}
C(2)–C(3)	1.471 ^{b)}	φ_3 ^{e)}	21.9 ^{b)}
		φ_4 ^{f)}	21.9 ^{b)}
<i>gauche</i> -1		<i>gauche</i> -1	
C(2)–C(4)	1.513 ^{b)}	C(2)–C(4)–H	109.45 ^{b)}
C(4)–H	1.092 ^{b)}	C(2)–C(4)–Cl	109.45 ^{b)}
C(4)–Cl	1.765(10)	τ ^{g)}	54.02(300)
<i>gauche</i> -2		<i>gauche</i> -2	
C(2)–C(4)	1.522(10)	C(2)–C(4)–H	109.45 ^{b)}
C(4)–H	1.092 ^{b)}	C(2)–C(4)–Cl	110.97(100)
C(4)–Cl	1.767(10)	τ ^{g)}	–70.21(300)
<i>cis</i>		<i>cis</i>	
C(2)–C(4)	1.522(10)	C(2)–C(4)–H	109.45 ^{b)}
C(4)–H	1.092 ^{b)}	C(2)–C(4)–Cl	110.94(100)
C(4)–Cl	1.794(10)	τ ^{g)}	173.22(300)

^{a)} Uncertainties were not estimated in the original paper.

^{b)} Assumed.

^{c)} Angle between C(2,3)–H and the ring plane.

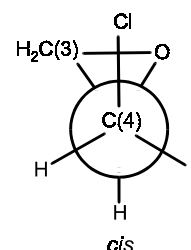
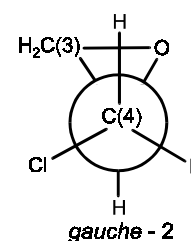
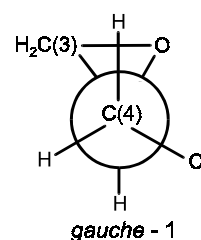
^{d)} Angle between C(2)–C(4) and the ring plane.

^{e)} Angle between C(2)–C(3) and the HCH plane.

^{f)} Angle between C(2)–C(3) and the HC(2)C(4) plane.

^{g)} Dihedral angle H–C(2)–C(4)–Cl; $\tau = 0^\circ$ for *syn* position.

C₁ (*gauche*-1)
C₁ (*gauche*-2)
C₁ (*cis*)



Mohammadi, M.A., Brooks, W.V.F.: J. Mol. Spectrosc. **73** (1978) 353 (*gauche*-1).

Mohammadi, M.A., Brooks, W.V.F.: J. Mol. Spectrosc. **78** (1979) 89 (*gauche*-2, *cis*).