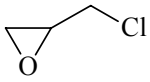
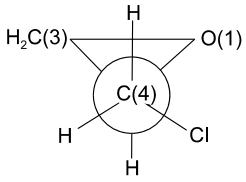
376 **C_3H_5ClO** **2-(Chloromethyl)oxirane** **C_1** (*gauche*-1)
MW, *ab initio* calculations **C_1** (*gauche*-2)



r_0 Å [a])

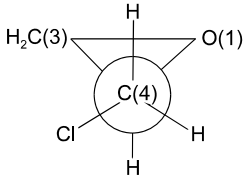
	gauche-1	*gauche*-2
Cl–C(4)	1.7914(50)	1.7900(50)
C(4)–C(2)	1.4962 [b])	1.5007 [b])
C(2)...X [c])	0.7963 [b])	0.7892 [b])
O...X [c])	0.9207 [b])	0.9396 [b])
C(4)–H	1.0910 [b])	1.0904 [b])
C(2)–H	1.0883 [b])	1.0879 [b])
C(3)–H	1.0870 [b])	1.0867 [b])



gauche-1

θ_0 deg [a])

	gauche-1	*gauche*-2
Cl–C(4)–C(2)	110.64(50)	109.98(50)
Cl–C(4)–H	107.63 [b])	108.04 [b])
C(4)–C(2)–H	115.63 [b])	115.83 [b])
C(4)–C(2)...X [c])	123.15 [b])	122.58 [b])
C(2)...X...C(3) [c])	134.64 [b])	136.19 [b])
C(2)...X...O [c])	112.68 [b])	111.90 [b])
X...C(3)–H [c])	121.89 [b])	121.89 [b])
Cl–C(4)–C(2)–H [d])	303.28(100)	62.52(100)
C(4)–C(2)...X...C(3) [c]) [d])	90.0 [b])	90.0 [b])
C(2)...X...C(3)–H [c]) [d])	90.0 [b])	90.0 [b])



gauche-2

Two *gauche* conformers, *gauche*-1 and *gauche*-2, were detected.

[a]) Uncertainties were not estimated in the original paper.
The H–C(3)–H plane was assumed to be perpendicular to the ring plane, with the angle bisectors collinear.
[b]) Assumed at the *ab initio* values.
[c]) X denotes the ring center.
[d]) Dihedral angle.

Heineking, N., Grabow, J.-U., Merke, I.: J. Mol. Struct. **612** (2002) 231.
Replaces II/25C (**3**, 1197), MW