

r_0	\AA^a		θ_0	deg^a	
	<i>anti</i>	<i>gauche</i>		<i>anti</i>	<i>gauche</i>
C–C	1.526 ^b	1.526 ^b	C–O–H	106.0(20)	106.0(20)
C–H	1.095 ^b	1.095 ^b	C–C–O	109.5(10)	110.1(10)
C–O	1.43 ^b	1.43 ^b	C–C–H	109.5 ^b	109.5 ^b
C–Cl	1.80(2)	1.80(2)	C–C–C	109.5(10)	110.1(10)
O–H	0.956 ^b	0.956 ^b	C–C–Cl	109.5(10)	110.1(10)
			τ_1^c	178.0(20)	68.0(20)
			τ_2^d	62.0(20)	64.5(20)
			τ_3^e	175.0(20)	176.5(20)

Two conformer were observed. For both conformers the O atom is *gauche* with respect to the C(2)–C(3) bond and the hydroxyl H is *anti* with respect to the C(1)–C(2) bond. In one conformer Cl is *anti* with respect to C(1)–C(2) and *gauche* in the other.

^a) Uncertainties were not estimated in the original paper except for τ .

^b) Assumed.

^c) Dihedral angle Cl–C(3)–C(2)–C(1).

^d) Dihedral angle O–C(1)–C(2)–C(3).

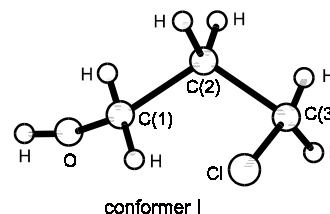
^e) Dihedral angle H–O–C(1)–C(2).

Fuller, M.J., Wilson, E.B., Caminati, W.: J. Mol. Spectrosc. **96** (1982) 131.

ED

r_a	\AA^a	θ_a	deg^a
C–C	1.531(3)	C–C–O	106.1(7)
C–H	1.122(6)	C–C–C	111.3(11)
C–O	1.422(4)	C–C–Cl	112.4(5)
C–Cl	1.806(4)	τ_1^b	120.8(32)
O–H	0.976(17)	τ_2^c	108.5(48)

C_1 (conformers I, II and III)



The following three conformers have been detected (possibly at room temperature):

1) 63.6(82)% (conformer I):

Cl–C(3) is *gauche* to the C(1)–C(2) bond,

O–C(1) is *gauche* to the C(2)–C(3) bond,

O–H and Cl are on different sides of the CCC plane forming a long Cl...O distance.

2) 19.5(48)% (conformer II):

The same as 1), but O–H and Cl are on the same side of the CCC plane forming a short Cl...O distance.

3) 16.9(46)% (conformer III):

Cl–C(3) is *anti* to the C(1)–C(2) bond, O–C(1) is *gauche* to the C(2)–C(3) bond.

^a) Twice the estimated standard errors.

^b) Angle between the ClCC and the CCC planes; effective torsional angle from *anti* (conformer I).

^c) Angle between the CCC and the CCO planes; effective torsional angle from *anti* (conformer I).

Bastiansen, O., Brunvoll, J., Hargittai, I.: Kem. K zlemen. **37** (1972) 379.

Bastiansen, O., Brunvoll, J., Hargittai, I.: "Molecular Structures and Vibrations", Ed.: S.J. Cyvin, Elsevier, Amsterdam, London, New York, **1972**, chapter 18/II, p. 330.