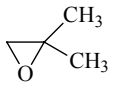
562 **C_4H_8O** **2,2-Dimethyloxirane** **C_s** (see comment)
MW



r_0	Å
C(2)–C(3)	1.474(10)
C(3)–O	1.438(1)
C(1)–C(2)	1.512(5)
C(3)–H	1.083 [a])
C(1)–H	1.09 [a])
C(2)–O	1.445(10) [b])

θ_0	deg
C(3)–C(2)–C(1)	119.65(40)
O–C(3)–C(2)	59.47(44)
C(2)–C(3)–H	119.20 [a])
C(2)–C(1)–H	109.40 [a])
C(1)–C(2)–C(1')	116.41(63) [b])
O–C(2)–C(1)	114.20(48) [b])
O–C(2)–C(3)	59.03(34) [b])
C(2)–O–C(3)	61.50(45) [b])
O–C(3)–C(2)–C(1)	102.03(77)
O–C(2)–C(3)–H	103.20 [a])
C(3)–C(2)–C(1)–H	0.00 [a])
H'–C(1')–C(2)–C(1)–H	120.0 [c])

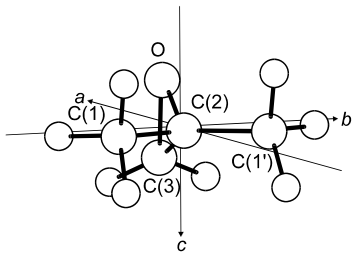
r_s	Å
C(2)–C(3)	1.444(6)
C(3)–O	1.437(2)
C(1)–C(2)	1.522(3)
C(2)–O	1.419(7)

θ_s	deg
C(3)–C(2)–C(1)	120.81(28)
O–C(3)–C(2)	59.03(37)
C(1)–C(2)–C(1')	114.42(33)
O–C(2)–C(1)	114.00(39)
O–C(2)–C(3)	60.26(21)
C(2)–O–C(3)	60.70(35)
O–C(3)–C(2)–C(1)	101.82(62)

$r_{\Delta 0}$ [d])	Å
C(2)–C(3)	1.478(10)
C(3)–O	1.445(4)
C(1)–C(2)	1.518(5)
C(3)–H	1.083 [a])
C(1)–H	1.09 [a])
C(2)–O	1.445(11) [b])

$\theta_{\Delta 0}$ [d])	deg
C(3)–C(2)–C(1)	119.53(40)
O–C(3)–C(2)	59.11(50)
C(2)–C(3)–H	119.20 [a])
C(2)–C(1)–H	109.40 [a])
C(1)–C(2)–C(1')	116.21(63) [b])
O–C(2)–C(1)	115.48(52) [b])
O–C(2)–C(3)	59.92(40) [b])
C(2)–O–C(3)	61.41(44) [b])
O–C(3)–C(2)–C(1)	102.64(85)
O–C(2)–C(3)–H	103.20 [a])
C(3)–C(2)–C(1)–H	0.00 [a])
H'–C(1')–C(2)–C(1)–H	120.0 [c])

Atom	a_s [Å]	b_s [Å]	c_s [Å]
C(2)	–0.1591	0.0	0.0799
C(3)	1.1544	0.0	0.6790
O	0.9929	0.0	–0.7494
C(1,1')	–0.9796	±1.2797	0.00



G_{18} symmetry group applies when the internal rotation of two CH_3 groups is taken into account.

[a]) Assumed.
[b]) Dependent parameter.
[c]) C_{3v} symmetry of the methyl group is assumed.
[d]) Use is made of only the differences in rotational constants between the normal and isotopic species.

Hartwig, H., Dreizler, H.: J. Mol. Struct. **406** (1997) 1.