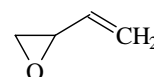


1649
MW

C₄H₆O

2-Ethenyloxirane
3,4-Epoxy-1-butene

C₁



r_0	Å ^{a)}	θ_0	deg ^{a)}
C(1)–H(1)	1.085 ^{b)}	H(1)–C(1)–H(2)	118.0 ^{b)}
C(1)–H(2)	1.086 ^{b)}	H(3)–C(2)–C(3)	116.7 ^{b)}
C(2)–H(3)	1.090 ^{b)}	C(1)=C(2)–C(3)	124.3 ^{b)}
C(3)–H(4)	1.085 ^{b)}	H(4)–C(3)...M ^{c)}	121.7 ^{b)}
C(4)–H(5)	1.085 ^{b)}	H(5)–C(4)–H(6)	116.7 ^{b)}
C(4)–H(6)	1.085 ^{b)}	α ^{d)}	57.5(10)
C(1)=C(2)	1.336 ^{b)}	β ^{e)}	20.65 ^{b)}
C(3)–C(4)	1.472 ^{b)}	τ ^{f)}	–4.9(20)
C(3)–O	1.436 ^{b)}		
C(4)–O	1.436 ^{b)}		
C(2)–C(3)	1.480(10)		

C(2)C(3)H(4) and H(5)C(4)H(6) planes were assumed to be perpendicular to the plane of the epoxy ring. The H₂C=CH fragment was assumed to be planar.

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

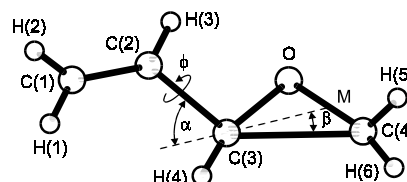
^{b)} Assumed.

^{c)} For definition of M, see figure.

^{d)} Angle between the C(2)–C(3) bond and the C(3)C(4)O plane.

^{e)} Angle between the C(3)–C(4) bond and the C(2)C(3)H(4) plane.

^{f)} Torsional angle C(1)=C(2)–C(3)...M; $\tau = 0^\circ$ for the *anti* position. The positive direction is shown by the arrow.



Ikeda, T., Sastry, K.V.L.N., Curl, R.F.: J. Mol. Spectrosc. **56** (1975) 411.