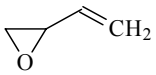
538 **C_4H_6O** **3,4-Epoxybut-1-ene** **C_1** (*anti*)
ED, MW, *ab initio* calculations
Ethenyloxirane
Vinyloxirane
C_1 (*gauche*-1)

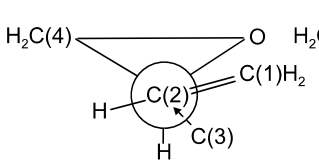


r_g	Å [a])
C–H (ring)	1.097(4)
C–H (vinyl)	1.098(4)
C(1)=C(2)	1.331(4)
C(3)–O [b])	1.436(2)
C(4)–O [b])	1.429(2)
C(3)–C(4) [b])	1.477(7)
C(2)–C(3) [b])	1.500(7)

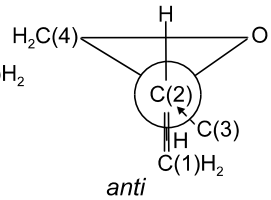
θ_α	deg [a])
C(2)–C(3)–O	115.2(19)
C(1)=C(2)–C(3)	123.1(21)
H–C–O	117(2)
H–C=C	119(3)
τ [c])	146.0 [d])

The experimental data analysis indicated the presence of *anti* (64(17)%) and *gauche*-1 conformers. The parameters are given for the *anti* conformer.
The nozzle temperature was 298 K.

[a]) Twice the estimated standard errors including a systematic error.
[b]) Differences in the C–O and in the C–C bond lengths were assumed at the values from HF/6-31G* calculations.
[c]) C(1)=C(2)–C(3)–O torsional angle from the *syn* position.
[d]) Assumed.



gauche-1



anti

Khalil, M., Shen, Q.: J. Phys. Chem. A **103** (1999) 5585.

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