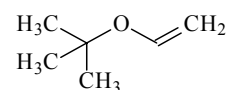


750 C₆H₁₂OED, *ab initio*
calculations**2-(Ethenyloxy)-2-methylpropane***t*-Butyl vinyl ether**C₁**

r_a	\AA^a	θ_a	deg^a
C=C	1.322(9)	C=C-O	122.9(15)
O-C(2)	1.445(10)	C-O-C	117.5(11)
O-C(5)	1.368(10)	C-C-C	111.6(7)
C-C	1.529(2)	H-C-H (methyl)	109.1(8)
C-H(methyl)	1.100(3) ^c	C=C-H	121.0 ^b
C-H(vinyl)	1.090(3) ^c	tilt(<i>t</i> -butyl) ^d	5.1(4)
		τ^e	166.6(46)

Local C_{3v} symmetry was assumed for the *t*-butyl and methyl groups. Staggered position with respect to the O-C(5) bond was assumed for the *t*-butyl group. The molecule was found to exist as a single conformer. The potential barrier at the exactly planar *anti* conformation of the C=C-O-C skeleton ($\tau = 180^\circ$) was determined to be 0.15(10) kcal mol⁻¹. This experimental result reproduced well the value from MP2/6-31G* calculations ($V_0 = 0.12$ kcal mol⁻¹).

The nozzle was at room temperature.

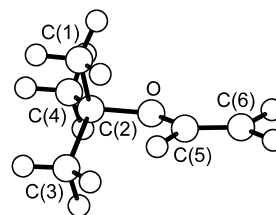
^a) Three times the estimated standard errors.

^b) Assumed at the value from MP2/6-31G* calculations.

^c) Difference between the C-H(methyl) and C-H(vinyl) bond lengths was assumed at the *ab initio* value.

^d) Tilt angle between the C₃ axis of the *t*-butyl group and the O-C(2) bond direction, away from C(5).

^e) C=C-O-C(2) torsional angle from the *syn* position.



Leibold, C., Oberhammer, H.: J. Am. Chem. Soc. **120** (1998) 1533.