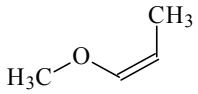
561 **C_4H_8O** **(*Z*)-1-Methoxy-1-propene** **C_1**

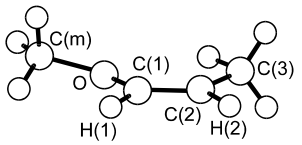
ED, *ab initio* calculations

(*Z*)-Methyl 1-propenyl ether



r_a	Å [a])	θ_a	deg [a])
C(1)=C(2)	1.340(3)	C(2)=C(1)–O	120.1(8)
O–C [b])	1.395(3)	C–O–C	117.2(13)
Δ(O–C) [c])	0.051 [d])	C(1)=C(2)–C(3)	124.6(6)
O–C(1)	1.370(6)	H–C–H [b])	109.9(8)
O–C(m)	1.421(6)	C=C–H(1)	122.4 [d])
C(2)–C(3)	1.518(3)	C=C–H(2)	116.8 [d])
C–H(methyl)	1.101(3) [e])	tilt(OCH_3) [f])	3.3 [d])
C–H(vinyl)	1.091(3) [e])	tilt(CCH_3) [g])	0.7 [d])
		τ [h])	161.2(45)

The molecule was found to exist as a single conformer. Local C_{3v} symmetry was assumed for the methyl groups. It was assumed that the C(m)H_3 group is staggered with respect to the O–C(1) bond, one H–C(3) bond is eclipsed with respect to the C(1)=C(2) bond, and the dihedral angle O–C(1)=C(2)–C(3) is 0° (*syn*). The potential barrier at the exactly planar *anti* conformation of the C=C–O–C skeleton (τ = 180°) was determined to be 0.20(10) kcal mol^{-1}. This experimental result reproduced well the value from MP2/6-31G* calculations (V_0 = 0.11 kcal mol^{-1}).
The nozzle was at room temperature.



[a]) Three times the estimated standard errors.
[b]) Mean value.
[c]) [O–C(m)] – [O–C(1)].
[d]) Constrained to the value from MP2/6-31G* calculations.
[e]) Difference between the C–H(methyl) and C–H(vinyl) bond lengths was assumed at the *ab initio* value.
[f]) Tilt angle between the C_3 axis of the methyl group and the O–C(m) bond direction, away from the C(1) atom.
[g]) Tilt angle between the C_3 axis of the methyl group and the C(2)–C(3) bond direction, away from the C(2)=C(1) bond.
[h]) C=C–O–C torsional angle from the *syn* position.

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