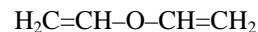


1639 $\text{C}_4\text{H}_6\text{O}$
ED, MW, IR,

Divinyl ether

C_1 (*sp,ac*)
 C_{2v} (*ap,ap*)

ab initio calculations (HF/4-21G)



r_g	\AA^a	θ_α	deg^a
C–H (average)	1.103(12)	C=C–O ^b	119(2)
C=C (average)	1.337(2)	C(5)=C(4)–O(3) ^c	124(2)
C–O (average)	1.389(2)	C=C–H (average)	115(3)
		ϕ_1 ^d	–13(6)
		ϕ_2 ^e	145(4)

The molecule exists as a mixture of *sp,ac* (80(6)%) and *ap,ap* (20%) conformers.
The nozzle temperature was 30 °C.

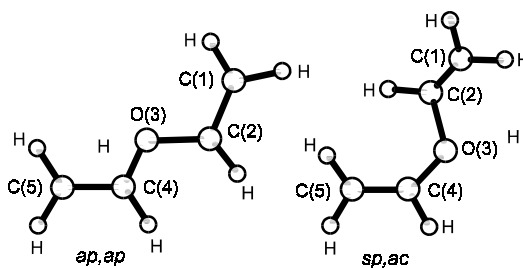
^a) Six times the estimated standard errors.

^b) All the C=C–O angle for *sp,ac* and *ap,ap* except for the C(5)=C(4)–O(3) angle for *sp,ac*.

^c) For the *sp,ac* conformer.

^d) Torsional angle C(2)–O(3)–C(4)=C(5) for the *sp,ac* conformer, $\phi_1 = 180^\circ$ for *ap,ap* conformer.

^e) Torsional angle C(1)=C(2)–O(3)–C(4) for the *sp,ac* conformer, $\phi_2 = 180^\circ$ for *ap,ap* conformer.



Pyckhout, W., van Alsenoy, C., Geise, H.J., van der Veken, B., Pieters, G.: J. Mol. Struct. **130** (1985) 335.