

1266  
MW

**C<sub>3</sub>H<sub>6</sub>O**

**Allyl alcohol**  
2-Propen-1-ol

**C<sub>1</sub> (ac, -sc)**  
H<sub>2</sub>C=CH-CH<sub>2</sub>-OH

$r_s$	Å <sup>a)</sup>	$\theta_s$	deg <sup>a)</sup>
C(2)=C(3)	1.337(5)	C(1)-C(2)=C(3)	123.9(5)
C(1)-C(2)	1.502(2)	O-C(1)-C(2)	111.8(5)
C(1)-O	1.428(5)	H(5)-C(3)=C(2)	122.0(15)
C(3)-H(5)	1.078(10)	H(6)-C(3)=C(2)	119.8(10)
C(3)-H(6)	1.091(10)	H(7)-C(2)=C(3)	121.0(10)
C(2)-H(7)	1.092(10)	H(8)-C(1)-C(2)	107.7(20)
C(1)-H(8)	1.096(30)	H(8)-C(1)-O	113.3(15)
C(1)-H(9)	1.102(20)	H(9)-C(1)-C(2)	108.0(10)
O-H(10)	0.960(5)	H(9)-C(1)-O	107.3(10)
		H(10)-O-C(1)	107.3(10)
		C(3)=C(2)-C(1)-O	122.9(10)
		C(2)-C(1)-O-H(10)	-55.9(10)

Atom	$a_s$ [Å]	$b_s$ [Å]	$c_s$ [Å]
C(1)	-0.5612	-0.5724	0.1206
C(2)	0.7021	0.1891	0.4094
C(3)	1.8384	0.0528	-0.2727
O	-1.6567	0.2923	-0.1596
H(5)	1.8874	-0.6738	-1.0965
H(6)	2.7226	0.6206	-0.0601
H(7)	0.6253	0.9264	1.2199
H(8)	-0.2958	-1.2779	-0.7135
H(9)	-0.8201	-1.1509	1.0140
H(10)	-1.3939	0.8550	-0.8945

One conformer (ac, -sc) was assigned.

<sup>a)</sup> Uncertainties were not estimated in the original paper.

Badawi, H., Lorencak, P., Hillig, K.W., Imachi, M., Kuczkowski, R.L.: J. Mol. Struct. **162** (1987) 247.

ED, MW, *ab initio*  
calculations (4-21G)

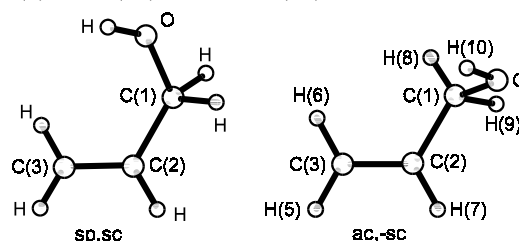
**C<sub>1</sub> (ac, -sc)**  
**C<sub>1</sub> (sp, sc)**

$r_g$	Å <sup>a)</sup>	$\theta_\alpha$	deg <sup>a)</sup>
(sp, sc) conformer		(sp, sc) conformer	
C(2)=C(3)	1.334(5)	C(1)-C(2)=C(3)	124.7(15)
C(1)-C(2)	1.500(8)	O-C(1)-C(2)	113.6(11)
C(1)-O	1.425(5)	C(3)=C(2)-C(1)-O	22(9)
(ac, -sc) conformer		C(2)-C(1)-O-H(10)	62(30)
C(2)=C(3)	1.335(5)	(ac, -sc) conformer	
C(1)-C(2)	1.496(8)	C(1)-C(2)=C(3)	125.3(15)
C(1)-O	1.431(5)	O-C(1)-C(2)	112.2(11)
for both conformers		C(3)=C(2)-C(1)-O	122(2)
C-H (average)	1.096(6)	C(2)-C(1)-O-H(10)	-62(15)
O-H(10)	1.028(27)		

At 300 K the conformer composition consists of 57(6)% (sp, sc) and 43% (ac, -sc) forms.

The vinyl moiety was assumed to be planar.

The nozzle temperature was  $\approx$  300 K.



<sup>a)</sup> Three times the estimated standard errors.

Vanhouteghem, F., Pyckhout, W., van Alsenoy, C., van den Enden, L., Geise, H.J.: J. Mol. Struct. **140** (1986) 33.