

1740  
MW

**C<sub>4</sub>H<sub>8</sub>O**

**3-Buten-1-ol**

**C<sub>1</sub> (conformer I)**  
H<sub>2</sub>C=CH-CH<sub>2</sub>-CH<sub>2</sub>-OH

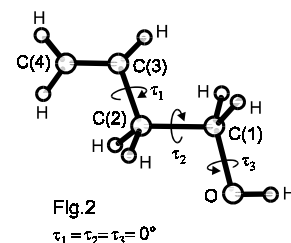
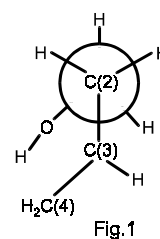
$r_0$	Å	$\theta_0$	deg
C(3)=C(4)	1.311 <sup>a)</sup>	C(4)=C(3)-C(2)	127.8 <sup>a)</sup>
C(2)-C(3)	1.496 <sup>a)</sup>	C(1)-C(2)-C(3)	111.6 <sup>a)</sup>
C(1)-C(2)	1.528 <sup>a)</sup>	C(2)-C(1)-O	112.3 <sup>a)</sup>
C-O	1.415 <sup>a)</sup>	C(1)-O-H	105.0 <sup>a)</sup>
O-H	1.150 <sup>a)</sup>	C(3,4)=C-H	121.5 <sup>a)</sup>
C(4)-H	1.090 <sup>a)</sup>	H-C(2)-H	109.48 <sup>a)</sup>
C(3)-H	1.090 <sup>a)</sup>	H-C(1)-H	109.48 <sup>a)</sup>
C(2)-H	1.093 <sup>a)</sup>	$\tau_1$ (C(1)-C(2)-C(3)=C(4)) <sup>b)</sup>	75(3)
C(1)-H	1.093 <sup>a)</sup>	$\tau_2$ (C(3)-C(2)-C(1)-O) <sup>b)</sup>	116(3) <sup>c)</sup>
		$\tau_3$ (H-O-C(1)-C(2)) <sup>b)</sup>	225(10)

<sup>a)</sup> Assumed.

<sup>b)</sup> The origins of the angles, i.e.  $\tau_1 = 0^\circ$ ,  $\tau_2 = 0^\circ$ , and  $\tau_3 = 0^\circ$ , are defined in Fig.2.

<sup>c)</sup> 64(3) from *syn*.

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ED

$r_a$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>	C <sub>1</sub> (conformers I and II)	
C(3)=C(4)	1.331(2)	C(4)=C(3)-C(2)	127.8(6)		
C(2)-C(3)	1.496(5)	C(1)-C(2)-C(3)	111.6(6)		
C(1)-C(2)	1.528(6)	C(2)-C(1)-O	112.3(5)		
C-O	1.415(2)	C(1)-O-H	103.4 <sup>b)</sup>		
O-H	1.014(8) <sup>b)</sup>	C(3)=C(4)-H	120.5(25)		
C-H	1.100(2) <sup>b)</sup>	C(4)=C(3)-H	116.1(23)		
		H-C-H	109.4(28)		
				conformer I	conformer II
		$\tau_1$ (C(1)-C(2)-C(3)=C(4)) <sup>c)</sup>	61.6(43)	94.6(87)	
		$\tau_2$ (C(3)-C(2)-C(1)-O) <sup>c)</sup>	109.3(25)	-129.0 <sup>b)</sup>	
		$\tau_3$ (H-O-C(1)-C(2)) <sup>c)</sup>	206.0 <sup>b)</sup>	142.0 <sup>b)</sup>	

The molecule exists as a mixture of the conformer I (68.6(80)%) and conformer II (31.4(80)%). The nozzle temperature was 40 °C.

<sup>a)</sup> Estimated standard errors.

<sup>b)</sup> Determined by *R*-factor optimization.

<sup>c)</sup>  $\tau = 0^\circ$  for *anti* position, as shown in Fig. 2.

Trætteberg, M., Østensen, H.: Acta Chem. Scand. Ser. A **33** (1979) 491.