

1218  
MW

**C<sub>3</sub>H<sub>5</sub>NO**

**3-Hydroxypropanenitrile**  
3-Hydroxypropionitrile

**C<sub>1</sub> (*gauche*)**  
**C<sub>s</sub> (*anti* I)**  
**C<sub>1</sub> (*anti* II)**

HO-CH<sub>2</sub>-CH<sub>2</sub>-C≡N

$r_0$	Å	$\theta_0$	deg
C≡N	1.157 <sup>a)</sup>	C-C≡N	180.00 <sup>a)</sup>
C-O	1.415 <sup>a)</sup>	C-C-H	109.47 <sup>a)</sup>
C(2)-C(3)	1.538 <sup>a)</sup>	H-C-H	109.47 <sup>a)</sup>
C(1)-C(2)	1.474 <sup>a)</sup>	C-O-H	104.00 <sup>a)</sup>
C-H	1.093 <sup>a)</sup>	O-C-C <sup>b)</sup>	108.00 <sup>a)</sup>
O-H	0.970 <sup>a)</sup>	O-C-C <sup>c)</sup>	112.50 <sup>a)</sup>
		C-C-C ( <i>gauche</i> )	109.5(15)
		C-C-C ( <i>anti</i> I)	109.0(15)
		C-C-C ( <i>anti</i> II)	109.0(15)
		H-O-C-C <sup>b)</sup>	0.00 <sup>a)</sup>
		H-O-C-C <sup>c)</sup>	120.00 <sup>a)</sup>
		O-C-C-C ( <i>gauche</i> ) <sup>d)</sup>	59(3)
		O-C-C-C ( <i>anti</i> I) <sup>d)</sup>	180 <sup>a)</sup>
		O-C-C-C ( <i>anti</i> II) <sup>d)</sup>	180 <sup>a)</sup>

Atom	$ a_s $ [Å]	$ b_s $ [Å]	$ c_s $ [Å]
H(OH) <i>gauche</i>	0.74457	1.51463	imaginary
H(OH) <i>anti</i> I	2.8827	0.645	0.250

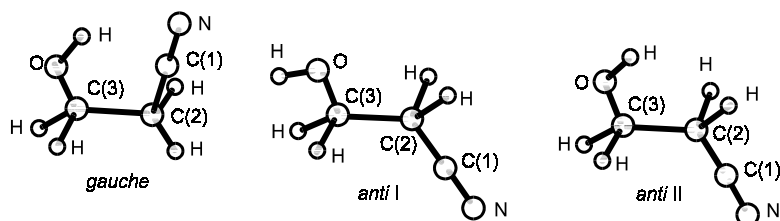
The hydrogen-bonded heavy-atom *gauche* conformation was found to be 2.7(4) kJ mol<sup>-1</sup> more stable than *anti* I and to be 7.4(24) kJ mol<sup>-1</sup> more stable than *anti* II.

<sup>a)</sup> Assumed.

<sup>b)</sup> For *anti* I.

<sup>c)</sup> For *gauche* and *anti* II.

<sup>d)</sup> From *syn* position.



Marstokk, K.-M., Møllendal, H.: Acta Chem. Scand., Ser. A **39** (1985) 15.