

1587  
ED

**C<sub>4</sub>H<sub>5</sub>N**

**3-Butenenitrile**  
Allyl cyanide

C<sub>s</sub> (*syn*)  
C<sub>1</sub> (*gauche*)  
H<sub>2</sub>C=CH-CH<sub>2</sub>-C≡N

<i>r<sub>a</sub></i>	Å <sup>a)</sup>	<i>θ<sub>α</sub></i>	deg <sup>a)</sup>
C(3)=C(4)	1.326(7)	C(4)=C(3)-C(2) ( <i>syn</i> )	125.01(18)
C(1)≡N	1.162(7)	C(1)-C(2)-C(3) ( <i>syn</i> )	114.0(10)
C(2)-C(3)	1.508(5)	C(3)=C(4)-H(1) <sup>b)</sup>	121.8(30)
Δ(C-C) <sup>c)</sup>	0.048(8)	Δ[C(3)=C(4)-H(2)] <sup>d)</sup>	-1.1 <sup>e)</sup>
C(3)-H <sup>b)</sup>	1.085(8)	Δ[C(4)=C(3)-H(2)] <sup>d)</sup>	-1.9 <sup>e)</sup>
Δ(C-H) <sup>b) f)</sup>	0.012(15)	C-C-H <sup>b)</sup>	111.4(12)
		<i>φ</i> <sup>g)</sup>	120.0 <sup>h)</sup>
		<i>τ</i> ( <i>gauche</i> ) <sup>i)</sup>	125.5(19)
		<i>δ</i> <sup>j)</sup>	13.8(53)

The molecule exists as a mixture of the *syn* (94(18)%) and *gauche* conformers.  $\Delta E = E(\textit{gauche}) - E(\textit{syn}) = 6.2 \text{ kJ mol}^{-1}$ .  
The measurements were made at 20 and 180 °C.  
The results at 20 °C are listed.

<sup>a)</sup> Twice the estimated standard errors including a systematic error.

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

<sup>c)</sup>  $\Delta(\text{C-C}) = [\text{C}(2)-\text{C}(3)] - [\text{C}(1)-\text{C}(2)]$ .

<sup>d)</sup> Increment relative to angle C(3)=C(4)-H(1).

<sup>e)</sup> Fixed at the values from *ab initio* calculations.

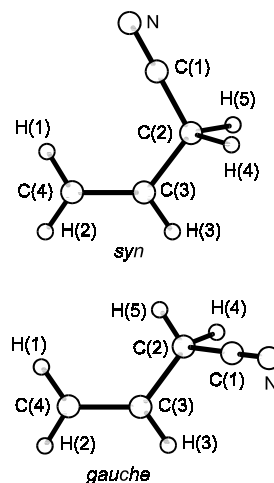
<sup>f)</sup>  $[\text{C}(2)-\text{H}] - [\text{C}(3)-\text{H}]$ .

<sup>g)</sup> Angle between projections of C(1)-C(2) and C(2)-H(4,5) on plane perpendicular to C(2)-C(3) bond.

<sup>h)</sup> Assumed.

<sup>i)</sup> Torsional angle C(1)-C(2)-C(3)=C(4) for the *gauche* conformer.

<sup>j)</sup> The root-mean-square amplitude of the torsional angle C(1)-C(2)-C(3)=C(4) for the *syn* conformer.



Schei, S.H.: J. Mol. Struct. **98** (1983) 141.