

1041  
MW

**C<sub>3</sub>HNO**

**Ethynyl isocyanate**

**C<sub>s</sub>**  
**HC≡C–NCO**

$r_0$	Å	$\theta_0$	deg
H–C	1.057 <sup>a)</sup>	H–C≡C	180.0 <sup>a)</sup>
C≡C	1.2237(20)	C≡C–N	180.0 <sup>a)</sup>
C–N	1.3025(54)	N=C=O	170.02(93)
N=C	1.2139(60)	$\alpha$ <sup>b)</sup>	140.67(48)
C=O	1.1741(48)		

$$y [\text{Å rad}^{-2}] \quad 0.0887(66) \text{ } ^\text{c)}$$

The barrier to linearity is 537.2(54) cm<sup>−1</sup>.

Bond lengths and bond angles were thought to be functions of the ≡C–N=C= angle  $\rho = \pi - \alpha$  such that

$$r_i(\rho) = r_i(0) + y_i \rho^2$$

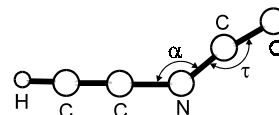
$$\tau_i(\rho) = \tau_i(0) + \tau'_i \rho.$$

In actual fitting,  $r_i(0)$  and  $\tau_i(0)$  were replaced by  $r_i^e = r_i(\rho_e)$  and  $\tau_i^e = \tau_i(\rho_e)$ , respectively.

<sup>a)</sup> Assumed.

<sup>b)</sup> See figure for definition.

<sup>c)</sup>  $y$  of the ≡C–N= bond.



Ross, S.C., Cooper, T.A., Firth, S., Kroto, H.W., Walton, D.R.M.: J. Mol. Spectrosc. **152** (1992) 152.