

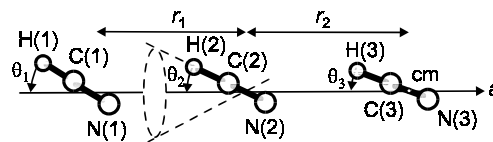
1127  
MW

$C_3H_3N_3$

**Hydrogen cyanide trimer**  
(weakly bound complex)

$C_{\infty v}$  (linear form)  
(effective symmetry class)  
 $HC\equiv N \cdot HC\equiv N \cdot HC\equiv N$

$r_s$	$\text{\AA}^a$	$\theta_s$	deg $^a$
H(1)–C(1)	1.0612(10)	$\theta_1$	12.60(20) $^b$
C(1)≡N(1)	1.1273(10)	$\theta_2$	8.55(20) $^b$
H(2)–C(2)	0.9528(10)		
C(2)≡N(2)	1.2363(10)		
H(3)–C(3)	1.1295(10)		
C(3)≡N(3)	1.1422(10)		
$r_1^c$	4.3888(10)		
$r_2^c$	4.4012(10)		



$r_0$	$\text{\AA}^a$	Atom	$a_s [\text{\AA}]$
$r_1^c$	4.357(5)	H(1)	–5.9998
$r_2^c$	4.431(5)	C(1)	–4.9386
		N(1)	–3.8113
		H(2)	–1.5409
		C(2)	–0.5881
		N(2)	0.6482
		H(3)	2.7145
		C(3)	3.8440
		N(3)	4.9862

$^a$ ) Uncertainties were not estimated in the original paper.

$^b$ ) Average value.

$^c$ ) See figure for definition.

Ruoff, R.S., Emilsson, T., Klots, T.D., Chuang, C., Gutowsky, H.S.: J. Chem. Phys. **89** (1988) 138.

IR

$r_0$	$\text{\AA}$
$R_{cm}$	3.73(1)

Structure was calculated from the rotational constants given by [1]. The distance between the centers of mass of the monomer units is designated as  $R_{cm}$ . The assumption was made that the structure of the HCN monomer unit is identical to that of the free molecule. The actual orientation of the HCN units in the trimer is not determinable with the existing data.

[1] Jucks, K.W., Miller, R.E.: J. Chem. Phys. **88** (1988) 2196.

$C_{3h}$  (cyclic form)

