

1112
MW

$\text{C}_3\text{H}_3\text{N}$

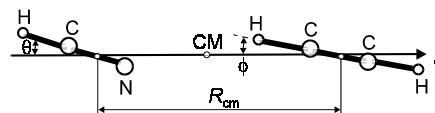
Acetylene – hydrogen cyanide (1/1)
(weakly bound complex)

$\text{C}_{\infty v}$
(effective symmetry class)
 $\text{HC}\equiv\text{CH} \cdot \text{HCN}$

Species	$r_0(R_{\text{cm}})$ [\AA] ^{a)}	$r_0(\text{N}\cdots\text{H})$ [\AA] ^{a)}	k_s [N m^{-1}] ^{b)}
$\text{HCN}\cdots\text{HCCH}$	4.645(5)	2.406(5)	4.45
$\text{HCN}\cdots\text{H}^{13}\text{CCH}$	4.623(5)	2.408(5)	4.44
$\text{H}^{13}\text{CN}\cdots\text{HCCH}$	4.664(5)	2.406(5)	4.50
$\text{HCN}\cdots\text{HC}^{13}\text{CH}$	4.667(5)	2.405(5)	4.23
$\text{HC}^{15}\text{N}\cdots\text{HCCH}$	4.625(5)	2.406(5)	4.49

r_s	\AA ^{a)}	θ_s	deg ^{a)}
R_{cm}	4.651(5)	θ ^{c)}	17.1(5)
		ϕ ^{c)}	7.8(5)

Atom	a_s [\AA]
C	-2.8199
N	-1.7161
C	1.7696
C	2.9609



A T-shaped $\text{HCN} \cdot \text{HCCH}$ dimer was reported earlier in [1]. It is found that formation of the linear form is favored by using neon first run as the carrier gas, but it is strongly relaxed to the T-shaped isomer by addition of a small amount of Ar (6%).

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

^{b)} Stretching force constant of the intermolecular bond.

^{c)} For definition see figure.

Jaman, A.I., Germann, T.C., Gutowsky, H.S., Augspurger, J.D., Dykstra, C.E.: Chem. Phys. **154** (1991) 281.

[1] Aldrich, P.D., Kukolich, S.G., Campbell, E.J.: J. Chem. Phys. **78** (1983) 3521.