

1039
MW, IR

C_3HN

2-Propenenitrile
Cyanoacetylene

$C_{\infty v}$
 $HC\equiv C-C\equiv N$

r_e	\AA
H-C	1.0624(5)
$C\equiv C$	1.2058(5)
C-C	1.3764(5)
$C\equiv N$	1.1605(5)

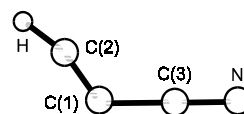
The equilibrium rotational constants B_e for six isotopomers are derived from the corresponding B_0 values by using α_i parameters obtained by *ab initio* calculations and checked against experimental values. These B_e values are then fitted to yield the equilibrium structure.

Botschwina, P., Horn, M., Seeger, S., Flügge, J.: Mol. Phys. **78** (1993) 191.

UV

C_s

State	\tilde{A}^1A''
r_e [\AA]	
C(2)-H	(1.08) ^{a)}
$C(1)\equiv C(2)$	1.25
C(1)-C(3)	1.40
$C\equiv N$	(1.159) ^{b)}
θ_0 [deg]	
$C(1)\equiv C(2)-H$	164
$C(2)\equiv C(1)-C(3)$	143
$C(1)-C(3)\equiv N$	180



^{a)} Assumed.

^{b)} The ground state value was assumed to hold in the excited state.

Job, V.A., King, G.W.: J. Mol. Spectrosc. **19** (1966) 155.