

1322
MW

C₃H₇N

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

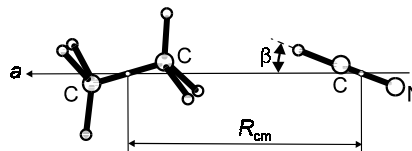
C_{3v}
(effective symmetry class)
H₃C–CH₃ · HC≡N
H₃C–CH₃ · DC≡N

Isotopic species	$r_0(\langle R_{\text{cm}}^2 \rangle^{1/2})$ [Å]	$r_0(\text{C} \cdots \text{C})$ [Å]	β_{av} [deg]	k_s [N m ⁻¹] ^{a)}	ν_s [cm ⁻¹] ^{b)}
C ₂ H ₆ · HCN	5.0379(10)	3.7609(10)	17.25(10) ^{c)}	2.392	53.39
C ₂ H ₆ · DCN	4.9840(10)	3.7610(10)	16.47(13)	2.553	54.63

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

^{b)} $\nu_s = (2\pi c)^{-1}(k_s/\mu)^{1/2}$.

^{c)} Uncertainty is larger than those of the original data.



Legon, A.C., Wallwork, A.L., Warner, H.E.: Chem. Phys. Lett. **191** (1992) 97.