

1595
MW

C₄H₅N

Methyl isocyanide – acetylene (1/1)
(weakly bound complex)

C_{3v}
(effective symmetry class)
H₃C–NC · HC≡CH
H₃C–NC · DC≡CD
H₃C–NC · DC≡CH

| Isotopic species | $r_0(R_{\text{cm}})$ [Å] ^{a)} | $r_0(\text{C} \cdots \text{C})$ [Å] ^{a)} | k_s [N m ⁻¹] ^{d)} | ν_s [cm ⁻¹] ^{e)} |
|---------------------------|--|---|--|---|
| CH ₃ NC · HCCH | 5.5319(50) | 3.596(5) | 4.777 | 71.31 |
| CH ₃ NC · HCCD | 5.5940(50) | 3.598(5) | 4.801 | 70.67 |
| CH ₃ NC · DCCH | 5.4671(50) | 3.592(5) | 4.926 | 71.58 |
| CH ₃ NC · DCCD | 5.5292(50) | 3.593(6) | 4.945 | 70.95 |

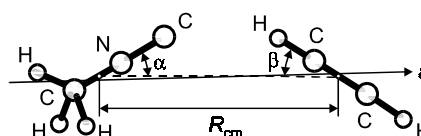
^{a)} The average angles α and β between the R_{cm} axis and the molecular symmetry axis of CH₃NC and HCCH, respectively, are both assumed to be 12°.

^{b)} Uncertainties are larger than those of the original data.

^{c)} The distance between C of the –NC group and one of the two carbon atoms of acetylene that is closer to CH₃NC.

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

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



Legon, A.C., Lister, D.G., Rego, C.A.: Chem. Phys. Lett. **189** (1992) 221.