


1702
MW

C_4H_7N

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

C_{2v}
(effective symmetry class)

(large-amplitude motion)

| Isotopic species | $r_0(R_{cm})$ [1] [Å] ^{b)} | $r_0(CC...C)$ ^{a)} [1] [Å] ^{b)} | θ_0 ° [2] [deg] | α_0 ° [2] [deg] | β_0 ° [2] [deg] |  · HCN |
|-------------------------|--|--|---------------------------|---------------------------|--------------------------|---|
| $C_3H_6 \cdot HCN$ | 4.471(5) ^{d)} 4.473(5) ^{e)} | 3.474(5) ^{d)} 3.477(5) ^{e)} | | | | |
| $C_3H_6 \cdot HC^{15}N$ | 4.492(5) ^{d)} 4.494(5) ^{e)} | 3.474(5) ^{d)} 3.476(5) ^{e)} | 12.4(1) ^{f)} | 8.9(6) ^{f)} | 8.9(6) ^{f)} | |

^{a)} Separation of the C–C bond of cyclopropane and the C of hydrogen cyanide.

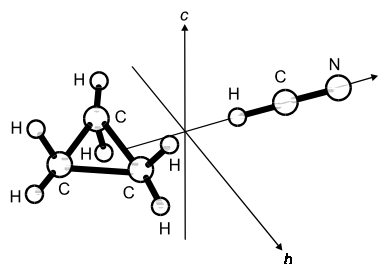
^{b)} Uncertainties for interatomic distances are about twice those of the original data.

^{c)} Average angle. For definition, see cyclopropane – hydrogen chloride (1/1) molecule.

^{d)} Obtained from I_{bb} data.

^{e)} Obtained from I_{cc} data.

^{f)} Obtained from eQq.



[1] Kukolich, S.G.: J. Chem. Phys. **78** (1983) 4832.

[2] Aldrich, P.D., Kukolich, S.G., Campbell, E.J., Read, W.G.: J. Am. Chem. Soc. **105** (1983) 5569.