

Structure Data of Free Polyatomic Molecules

372 MW	$\text{C}_3\text{H}_4\text{N}_2$	Cyanoacetylene – ammonia (1/1) 2-Propynenitrile – ammonia (1/1) (weakly bound complex)	C_{3v} (effective symmetry class) (large-amplitude motion) $\text{NC}-\text{C}\equiv\text{CH} \cdot \text{NH}_3$
	r_0	$\text{\AA}^{\text{a)}}$	θ_0 deg $^{\text{a)}}$
	$\text{H}\dots\text{N}^{\text{b)}}$	2.212(5)	$\varphi^{\text{c)}}$ 21.0(10)

The acetylenic proton is hydrogen bonded to the nitrogen of the NH_3 , and the intermolecular stretching force constant is 10.8 N m^{-1} .

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

^{b)} Hydrogen bond length between the hydrogen of cyanoacetylene and the nitrogen of ammonia.

^{c)} Average amplitude of the ammonia bending.

Omron, R.M., Walker, A.R.H., Hilpert, G., Fraser, G.T., Suenram, R.D.: J. Mol. Spectrosc. **179** (1996) 85.