

Structure Data of Free Polyatomic Molecules

362 MW	C₃H₃NO	Cyanoacetylene – water (1/1) 2-Propynenitrile – water (1/1) (weakly bound complex)	C_{2v} (effective symmetry class) (large-amplitude motion) HC≡C–CN · H ₂ O
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r_0 H...O ^{b)}	\AA ^{a)} 2.125(5)
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The acetylenic proton is hydrogen-bonded to the oxygen of the water, and the intermolecular stretching force constant is 9.6 N m⁻¹. The complex has a dynamical C_{2v} structure, as evidenced by the presence of two nuclear-spin modifications of the complex.

^{a)} Uncertainty was not estimated in the original paper.

^{b)} Distance between the acetylenic H and O of the water.

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