

1118
MW

C₃H₃NO

Fulminic acid – acetylene (1/1)
(weakly bound complex)

C_s
(effective symmetry class)
HCNO · HC≡CH

$$\frac{r_0}{R_{\text{cm}}} \quad \text{\AA}^{\text{a)}} \\ 3.77(1)$$

Two structural forms are consistent with the spectroscopic data. For both of these forms the molecular axes of fulminic acid and acetylene are approximately between perpendicular (T-shaped) and parallel orientations. One form appears to be hydrogen-bonded with an acetylenic hydrogen-oxygen distance of 2.41 Å. Consideration of H–H van der Waals distances in the second form indicates that the hydrogen-bonded structure is likely the observed form.

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

Gillies, C.W., Gillies, J.Z., Lovas, F.J., Suenram, R.D., Hebert, K.: 47th Ohio State Univ. Int. Symp. Mol. Spectrosc., Columbus, Ohio, 1992, RB08.