

## Structure Data of Free Polyatomic Molecules

<b>428</b> MW	<b>C<sub>3</sub>H<sub>7</sub>N</b>	<b>Propyne – ammonia (1/1)</b> (weakly bound complex)	<b>C<sub>3v</sub></b> (effective symmetry class) (large-amplitude motion) CH <sub>3</sub> C≡CH · NH <sub>3</sub>
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$r_0$	$\text{\AA}^{\text{a)}}$	$\theta_0$	$\text{deg}^{\text{a)}}$
H...N <sup>b)</sup>	2.322(5)	$\varphi^{\text{c)}}$	24.9(10)

The acetylenic proton is hydrogen-bonded to the nitrogen of the NH<sub>3</sub>, and the intermolecular stretching force constant is 6.0 N m<sup>-1</sup>.

<sup>a)</sup> Uncertainties were not estimated in the original paper.

<sup>b)</sup> Hydrogen bond length between the acetylenic hydrogen of propyne and the nitrogen of ammonia.

<sup>c)</sup> 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.