

1596  
MW

$C_4H_5N$

**1,3-Butadiyne – ammonia (1/1)**  
(weakly bound complex)

$C_{3v}$   
(effective symmetry class)  
 $HC\equiv C-C\equiv CH \cdot NH_3$

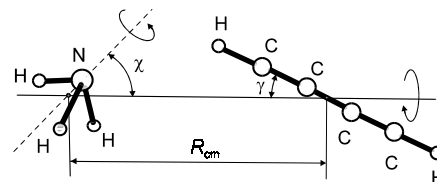
	$NH_3 \cdot HCCCCCH$	$ND_3 \cdot HCCCCCH$	$^{15}NH_3 \cdot HCCCCCH$
$r_0(R_{cm}) [\text{\AA}]$	5.306(5) <sup>a)</sup>	5.347(5) <sup>a)</sup>	5.302(5) <sup>a)</sup>
$r_0(R_{hyd}) [\text{\AA}]$ <sup>b)</sup>	2.287(5) <sup>a)</sup>	2.281(5) <sup>a)</sup>	2.286(5) <sup>a)</sup>
$k_s [\text{N m}^{-1}]$ <sup>c)</sup>	83.0	83.3	83.9
$\nu_s [\text{cm}^{-1}]$ <sup>d)</sup>	105	99	104

<sup>a)</sup> Uncertainty was not estimated in the original paper.

<sup>b)</sup>  $R_{hyd}$  is the distance between the diacetylene hydrogen and the ammonia nitrogen.

<sup>c)</sup> Stretching force constant of the intermolecular bond.

<sup>d)</sup>  $\nu_s = (2\pi c)^{-1}(k_s/\mu)^{1/2}$ .



Matsumura, K., Lovas, F.J., Suenram, R.D.: J. Mol. Spectrosc. **144** (1990) 123.