

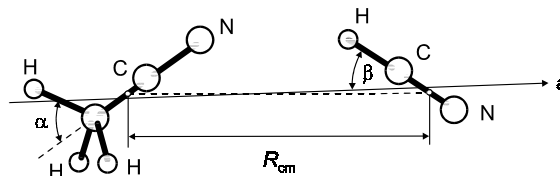
1155
MW

$\text{C}_3\text{H}_4\text{N}_2$

Hydrogen cyanide – acetonitrile (1/1)
(weakly bound complex)

C_{3v}
(effective symmetry class)
 $\text{H}_3\text{C}-\text{C}\equiv\text{N} \cdot \text{HC}\equiv\text{N}$
 $\text{H}_3\text{C}-\text{C}\equiv\text{N} \cdot \text{DC}\equiv\text{N}$

Species	α_{av} [deg]	β_{av} [deg]	$\langle R_{cm}^2 \rangle^{1/2}$ [Å]	$r_0(\text{N}\dots\text{C})$ [Å]	k_s [N m ⁻¹]
$\text{CH}_3\text{C}^{14}\text{N} \cdot \text{HC}^{15}\text{N}$	13(1)		5.1364(1)	3.272(2)	9.51
$\text{CH}_3\text{C}^{15}\text{N} \cdot \text{HC}^{14}\text{N}$		11.5(5)	5.0848(1)	3.272(2)	9.61
$\text{CH}_3\text{C}^{14}\text{N} \cdot \text{DN}^{15}\text{N}$	13(1)		5.0787(2)	3.270(2)	10.2



Howard, N.W., Legon, A.C.: J. Chem. Soc., Faraday Trans. II **83** (1987) 991.