

1594
MW

C_4H_5N

Acetylene – acetonitrile (1/1)
(weakly bound complex)

C_{3v}
(effective symmetry class)
 $H_3C-CN \cdot HC\equiv CH$
 $H_3C-CN \cdot DC\equiv CH$
 $H_3C-CN \cdot DC\equiv CD$

Isotopic species	$r_0(R_{cm}) [\text{\AA}]^a$	$r_0(N\cdots C) [\text{\AA}]^a$	$\theta_0 [\text{deg}]^a$	$k_s [\text{N m}^{-1}]$
$CH_3C^{14}N \cdot HCCH$	5.31178(200)	3.4254(20)	12.0(15)	4.70
$CH_3C^{14}N \cdot DCCH$	5.24746(200)	3.4216(20)	14(2)	4.90
$CH_3C^{14}N \cdot HCCD$	5.37395(200)	3.4270(20)	12(2)	4.63
$CH_3C^{14}N \cdot DCCD$	5.30961(200)	3.4241(20)	12(2)	4.89
$CH_3C^{15}N \cdot HCCH$	5.28135(200)	3.4257(20)		4.74

^a) Not all the uncertainties were estimated
in the original paper.

Howard, N.W., Legon, A.C.: J. Chem. Phys.
85 (1986) 6898.

