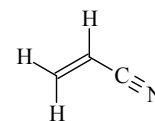


361  
MW $C_3H_3N$ 

2-Propenenitrile

Acrylonitrile

Vinyl cyanide

 $C_s$ 

$r_0$	Å
C(3)–H(t) <sup>a</sup>	1.089(1)
C(3)–H(c) <sup>a</sup>	1.087(1)
C(2)=C(3)	1.340(1)
C(2)–H	1.085(1)
C(1)–C(2)	1.432(2)
C≡N	1.159(2)

$\theta_0$	deg
C(2)=C(3)–H(t) <sup>a</sup>	119.4(1)
C(2)=C(3)–H(c) <sup>a</sup>	120.4(1)
C(3)=C(2)–H	121.8(1)
C(1)–C(2)=C(3)	122.2(1)
C–C≡N	181.0(3)

$r_s$	Å <sup>b</sup>	Å <sup>c</sup>
C(3)–H(t) <sup>a</sup>	1.097(2)	1.095(2)
C(3)–H(c) <sup>a</sup>	1.093(2)	1.091(2)
C(2)=C(3)	1.343(3)	1.340(3)
C(2)–H	1.085(2)	1.086(2)
C(1)–C(2)	1.429(4)	1.430(4)
C≡N	1.160(3)	

$\theta_s$	deg <sup>b</sup>	deg <sup>c</sup>
C(2)=C(3)–H(t) <sup>a</sup>	118.5(2)	118.7(2)
C(2)=C(3)–H(c) <sup>a</sup>	120.3(2)	120.3(2)
C(3)=C(2)–H	121.6(3)	
C(1)–C(2)=C(3)	122.5(3)	122.3(3)
C–C≡N	178.4(2)	

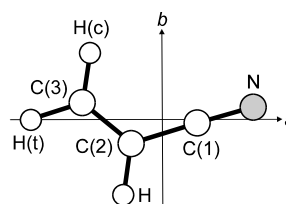
$r_{le}$	Å
C(3)–H(t) <sup>a</sup>	1.089(1)
C(3)–H(c) <sup>a</sup>	1.091(1)
C(2)=C(3)	1.342(2)
C(2)–H	1.091(2)
C(1)–C(2)	1.426(3)
C≡N	1.166(2)

$\theta_{le}$	deg
C(2)=C(3)–H(t) <sup>a</sup>	120.3 <sup>d</sup>
C(2)=C(3)–H(c) <sup>a</sup>	120.5(1)
C(3)=C(2)–H	121.8(2)
C(1)–C(2)=C(3)	122.5(3)
C–C≡N	179.6(5)

$r_m^p$	Å
C(3)–H(t) <sup>a</sup>	1.088(1)
C(3)–H(c) <sup>a</sup>	1.097(2)
C(2)=C(3)	1.333(3)
C(2)–H	1.093(4)
C(1)–C(2)	1.429(3)
C≡N	1.157(3)

$\theta_m^p$	deg
C(2)=C(3)–H(t) <sup>a</sup>	120.3 <sup>d</sup>
C(2)=C(3)–H(c) <sup>a</sup>	120.2(1)
C(3)=C(2)–H	121.7(2)
C(1)–C(2)=C(3)	122.5(5)
C–C≡N	180.7(9)

Atom	$a_s$ [Å]	$b_s$ [Å]
C(3)	–1.6874	0.3794
H(t) <sup>a</sup>	–2.7219	0.0368
H(c) <sup>a</sup>	–1.4757	1.4562
C(2)	–0.6825	–0.5065
H	–0.8653	–1.5857
C(1)	0.6878	–0.1114
N	1.8059	0.2110



<sup>a</sup>) H(t) and H(c) denote the hydrogen atoms bonded to C(3), which are *trans* and *cis* to the CN group, respectively.

<sup>b</sup>) From parent  $H_2C=CH-CN$ .

<sup>c</sup>) From parent  $H_2C=CD-CN$ .

<sup>d</sup>) Assumed.

Colmont, J.M., Wlodarczak, G., Priem, D., Müller, H.S.P., Tien, E.H., Richards, R.J., Gerry, M.C.L.: J. Mol. Spectrosc. **181** (1997) 330.

Replaces [II/25C \(3, 1109\)](#), MW