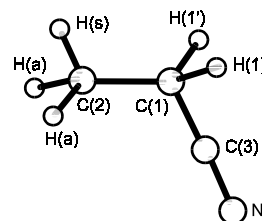


1214  
MW

$C_3H_5N$

**Propionitrile**  
Propanenitrile

$C_s$   
 $H_3C-CH_2-C\equiv N$



$r_s$	Å	$\theta_s$	deg
C(1)–C(2)	1.537(1)	C(1)–C(3)≡N <sup>a)</sup>	178.73(22)
C(1)–C(3)	1.459(1)	C(2)–C(1)–C(3)	111.98(10)
C(3)≡N	1.159(1)	C(2)–C(1)–H(1)	110.62(3)
C(1)–H	1.094(1)	C(3)–C(1)–H(1)	108.13(6)
C(2)–H(s)	1.079(18)	H(1)–C(1)–H(1')	107.19(4)
C(2)–H(a)	1.091(1)	H(a)–C(2)–H(a)	107.85(6)
		H(a)–C(2)–H(s)	108.44(124)
		H(a)–C(2)–C(1)	110.47(2)
		H(s)–C(2)–C(1)	111.08(237)
		$\tau$ <sup>b)</sup>	59.31(10) <sup>c)</sup>
		tilt (CH <sub>3</sub> ) <sup>d)</sup>	1.32(10) <sup>c)</sup>

$r_0$	Å	$\theta_0$	deg
C(1)–C(2)	1.538(12)	C(1)–C(3)≡N <sup>a)</sup>	178.67(147)
C(1)–C(3)	1.459(43)	C(2)–C(1)–C(3)	112.15(29)
C(3)≡N	1.162(42)	C(2)–C(1)–H(1)	111.44(126)
C(1)–H	1.085(4)	C(3)–C(1)–H(1)	108.90(30) <sup>c)</sup>
C(2)–H(s)	1.069(13)	H(1)–C(1)–H(1')	103.60(20) <sup>c)</sup>
C(2)–H(a)	1.099(3)	H(a)–C(2)–H(a)	110.27(30) <sup>c)</sup>
		H(a)–C(2)–H(s)	107.77(30) <sup>c)</sup>
		H(a)–C(2)–C(1)	109.37(86)
		H(s)–C(2)–C(1)	112.26(58)
		$\tau$ <sup>b)</sup>	57.60(123)

Atom	$a_s$ [Å]	$b_s$ [Å]	$c_s$ [Å]
C(1)	–0.6146	0.6548	0.0
C(2)	–1.6561	–0.4750	0.0
C(3)	0.7507	0.1391	0.0
N	1.8257	–0.2945	0.0
H(1,1')	–0.7377	1.2922	±0.8804
H(s)	–2.6596	–0.0778	0.0
H(a)	–1.5347	–1.1059	±0.8818

<sup>a)</sup> The C(3)≡N bond is bent towards the methyl group.

<sup>b)</sup> Dihedral angle H(s)–C(2)–C(1)–H(1).

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

<sup>d)</sup> Tilt angle of the axis through the center of mass of the three methyl H atoms and the C(2) atom towards the C(3)≡N group with respect to the C(2)–C(1) bond.

Heise, H.M., Lutz, H., Dreizler, H.: Z. Naturforsch. **29a** (1974) 1345.