

1109
MW

C₃H₃N

2-Propenenitrile

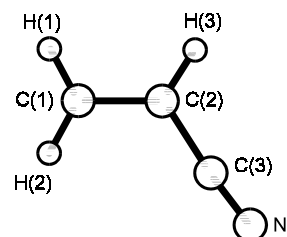
Acrylonitrile
Vinyl cyanide

C_s
H2C=CH-C#N

r_s	Å	θ_s	deg
C(3)≡N	1.1637(30)	C(1)=C(2)–C(3)	122.6(3)
C(2)–C(3)	1.4256(30)	C(1)=C(2)–H(3)	121.7(5)
C(1)=C(2)	1.3389(30)		
C(2)–H	1.0863(50)		

Costain, C. C., Stoicheff, B. P.: J. Chem. Phys. **30** (1959) 777.

r_e	Å ^{a)}
C(2)–C(3)	1.432(3)
C(1)=C(2)	1.337(4)



^{a)} Uncertainties were not estimated in the original paper.

Demaison, J., Cosleou, J., Bocquet, R., Lesarri, A.G.: J. Mol. Spectrosc. **167** (1994) 400.

ED, MW

r_g	Å ^{a)}	θ_α	deg ^{a)}
C(3)≡N	1.167(4)	C(1)=C(2)–C(3)	121.7(5)
C(2)–C(3)	1.438(3)	C(1)=C(2)–H(3)	122.0(20)
C(1)=C(2)	1.343(4)	C(2)–C(3)≡N ^{b)}	178.2(10)
C(1)–H	1.114(7)	H(1)–C(1)=C(2)	118.0(31)
		H(2)–C(1)=C(2)	119.0(26)

The molecule is planar.

The measurements were made at room temperature.

^{a)} Estimated limits of error.

^{b)} The N atom is *anti* to the C(1) atom.

Fukuyama, T., Kuchitsu, K.: J. Mol. Struct. **5** (1970) 131.