

1527
MW

C₄H₃N

3-Butynenitrile

C_s
HC≡C–CH₂–C≡N

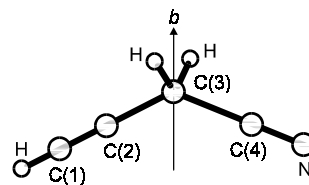
r_0	Å	θ_0	deg ^{a)}
H–C(1)	1.057 ^{b)}	H–C(3)–C(2)	111.3 ^{b)}
C(1)≡C(2)	1.207 ^{b)}	C(2)–C(3)–C(4)	112.86(210)
C(3)–C(2)	1.465 ^{b)}	C(3)–C(4)≡N	179.1(20) ^{c)}
H–C(3)	1.090 ^{b)}	C(1)≡C(2)–C(3)	180.0 ^{b)}
C(3)–C(4)	1.461(51)	H–C(1)≡C(2)	180.0 ^{b)}
C(4)≡N	1.159 ^{b)}	φ ^{d)}	122.32 ^{b)}

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

^{b)} Assumed.

^{c)} Away from H–C(1)≡C(2).

^{d)} Dihedral angle between the C(2)C(3)C(4) and HC(3)C(2) planes.



Jäger, W., Krause, H., Mäder, H., Gerry, M.C.L.: J. Mol. Spectrosc. **143** (1990) 50.