

1698
MW

C₄H₇N

Isobutyronitrile
Isopropyl cyanide

C_s
N≡C–CH(CH₃)₂

r_0	Å ^{a)}	θ_0	deg ^{a)}
C(1,2)–H	1.092 ^{b)}	C(1)–C(3)–C(2)	113.8 ^{b)}
C(3)–H	1.091 ^{b)}	φ ^{c)}	53.8(50)
C≡N	1.159 ^{b)}		
C(3)–C(4)	1.501(30)		
C(3)–C(1,2)	1.522 ^{b)}		

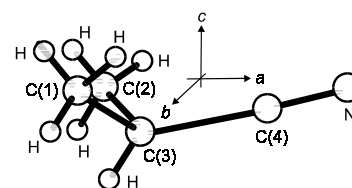
r_0	Å ^{a)}	θ_0	deg ^{a)}
C(1,2)–H	1.092 ^{b)}	C(1)–C(3)–C(2)	113.0 ^{b)}
C(3)–H	1.091 ^{b)}	φ ^{c)}	52.5(50)
C≡N	1.159 ^{b)}		
C(3)–C(4)	1.481(30)		
C(3)–C(1,2)	1.522 ^{b)}		

Two possible sets of structural parameters are given.

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

^{b)} Assumed.

^{c)} Angle between the C(1)C(3)C(2) plane and the C≡N bond.



Durig, J.R., Li, Y.S.: J. Mol. Struct. **21** (1974) 289.