

1525
MW

C₄H₃N

2-Propynyl isocyanide
3-Isocyano-1-propyne

C_s
HC#C-CH2-N=C

r_0	Å ^{a)}	θ_0	deg ^{a)}
C–H (CH)	1.057 ^{b)}	H–C–H	109.4 ^{b)}
C≡C	1.207 ^{b)}	C–C–H	111.3 ^{b)}
C–C	1.465 ^{b)}	C–C–N	113.2(5)
C–H (CH ₂)	1.090 ^{b)}		
C–N	1.416(5)		
N=C	1.166 ^{b)}		

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

^{b)} Assumed.

McNaughton, D., Romeril, N.G., Lappert, M.F., Kroto, H.W.: J. Mol. Spectrosc. **132** (1988) 407.