502 **C_4H_3N** **1-Propynyl isocyanide** **C_{3v}**
MW 1-Isocyano-1-propyne $H_3C—C\equiv C—N\equiv C$

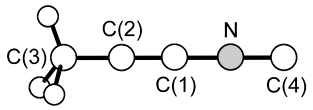
r_s	Å
C(3)–C(2)	1.4557(16)
C(2)≡C(1)	1.2159(109)
	1.2059(19) [a])
C(1)–N	1.3057(106)
	1.3157(16) [a])
N≡C(4)	1.1754(13)
H–C(3)	1.0903(14) [b])

θ_s	deg
H–C(3)–C(2)	110.71(7) [b])

r_0	Å
C(3)–C(2)	1.4541(16)
C(2)≡C(1)	1.2081(24)
C(1)–N	1.3158(17)
N≡C(4)	1.1756(6)
H–C(3)	1.0940 [b])

θ_0	deg
H–C(3)–C(2)	110.53(4)

Atom	z_s [Å]
H	–2.9341 [b])
C(3)	–2.5486
C(2)	–1.0929
C(1)	0.1230
	0.1130 [a])
N	1.4287
C(4)	2.6041



[a]) From the double substitution method.
[b]) Calculated using the assumption y_H = 1.0198 Å.

Gripp, J., Guarnieri, A., Stahl, W., Lentz, D.: J. Mol. Struct. **526** (2000) 81.