

1129 **C₃H₄**
MW, IR, *ab initio*
calculations

Methylacetylene
Propyne

C_{3v}
H₃C–C≡CH

r_0	Å
C(3)–H	1.0548(3) ^{a)}
C(1)–H	1.0940(4) ^{a)}
C(2)–C(3)	1.4595(5) ^{a)}
C(1)≡C(2)	1.2088(6) ^{a)}

r_s	Å
C(3)–H	1.0561(3) ^{b)}
C(1)–H	1.0895(52) ^{b)}
C(2)–C(3)	1.4586(4) ^{b)}
C(1)≡C(2)	1.2066(4) ^{b)}

r_{Δ}	Å
C(3)–H	1.0563(1) ^{b)}
C(1)–H	1.0929(3) ^{b)}
C(2)–C(3)	1.4574(1) ^{b)}
C(1)≡C(2)	1.2074(1) ^{b)}

r_m^p	Å
C(3)–H	1.0589(3) ^{b)}
C(1)–H	1.0885(5) ^{b)}
C(2)–C(3)	1.4552(5) ^{b)}
C(1)≡C(2)	1.2037(6) ^{b)}

r_e	Å
C(3)–H	1.061(1)
C(1)–H	1.089(1)
C(2)–C(3)	1.458(2)
C(1)≡C(2)	1.204(1)

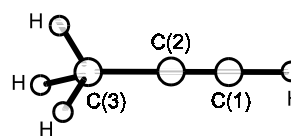
θ_0	deg
H–C(3)–C(2)	110.6(2) ^{a)}

θ_s	deg
H–C(3)–C(2)	110.6(1) ^{b)}

θ_{Δ}	deg
H–C(3)–C(2)	110.7(1) ^{b)}

θ_m^p	deg
H–C(3)–C(2)	111.12(6) ^{b)}

θ_e	deg
H–C(3)–C(2)	110.7(5)



The r_0 , r_s , r_{Δ} and r_m^p structures were all derived from the ground state molecular constants of 17 isotopomers, obtained from MW and also from IR data. The r_s structure given here uses normal propyne as parent molecule but two other parent molecules are also given in the paper. The r_{Δ} structure is obtained by fitting ground state molecular constants and isotopic changes $\Delta I_0 = I_0^i - I_0$ at the same time. An $r_{e,I}$ structure very similar in this case to the r_{Δ} structure, and not reported here, is obtained by assuming that the vibrational dependence of the inertia moments $\varepsilon = I_0 - I_e$ is isotope-independent. The r_m^p structure is deduced from ground state moments of inertia first scaled by a factor deduced from the substitution structure. The pseudo-equilibrium structure r_e reported here is elaborated from all these experimental structures, from ED structures and from several *ab initio* ones, taking into account their known deficiencies, offsets and trends.

^{a)} One standard deviation.

^{b)} Uncertainty was not given in the original paper. Here the dispersion among three substitution structures is taken as uncertainty.

Le Guennec, M., Demaison, J., Wlodarczak, G., Marsden, C.J.: J. Mol. Spectrosc. **160** (1993) 471.

See also: Pekkala, K., Graner, G., Wlodarczak, G., Demaison, J., Koput, J.: J. Mol. Spectrosc. **149** (1991) 214.