

1073
MW

C₃H₂O

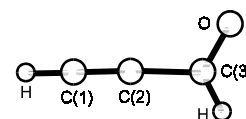
Propynal
Propiolaldehyde

C_s
HC≡C–C(O)H

r_s	Å	θ_s	deg
C(1)–H	1.0553(50)	C(2)–C(3)=O	123.9(3)
C(3)–H	1.1064(50)	C(2)–C(3)–H	113.9(5)
C(1)≡C(2)	1.2089(30)	C(1)≡C(2)–C(3) ^{a)}	178.4(5)
C(2)–C(3)	1.4446(30)	H–C(1)≡C(2)	180.0(5)
C(3)=O	1.2150(30)		

^{a)} Towards the aldehyde hydrogen.

Costain, C.C., Morton, J.R.: J. Chem. Phys. **31** (1959) 389.



ED, MW

r_g	Å ^{a)}	θ_α	deg ^{a)}
C(1)–H	1.085(7)	C(2)–C(3)=O	124.2(2)
C(3)–H	1.130(6)	O=C(3)–H	122.1(8)
C(1)≡C(2)	1.211(6)	C(1)≡C(2)–C(3) ^{b)}	178.6(3)
C(2)–C(3)	1.4527(23)		
C(3)=O	1.214(5)		

The molecule is planar.

The measurements were made at room temperature.

^{a)} Estimated limits of error.

^{b)} The C≡C bond is in the *anti* position to the C=O bond.

Sugié, M., Fukuyama, T., Kuchitsu, K.: J. Mol. Struct. **14** (1972) 333.

UV

State	\tilde{A}^1A''
Energy [eV]	3.244
r_0 [Å]	
C(1)–H	1.091
C(1)≡C(2)	1.238
C(3)=O	1.325

Estimates from vibrational frequencies and Clark's or Badger's rules.

Brand, J.C.D., Callomon, J.H., Watson, J.K.G.: Discuss. Faraday Soc. **35** (1963) 175.

Brand, J.C.D., Chan, W.H., Liu, D.S., Callomon J.H., Watson, J.K.G.: J. Mol. Spectrosc. **50** (1974) 304.