

1031
MW

C₃HClO

Propioloyl chloride
Propynoyl chloride

C_s
HC≡C–C(O)Cl

r_0	Å ^{a)}
C–H	1.056 ^{b)}
C≡C	1.208 ^{b)}
C–C	1.435 ^{b)}
C=O	1.207(10)
C–Cl	1.753(5)

θ_0	deg ^{a)}
H–C≡C	180.0 ^{b)}
C≡C–C	180.0 ^{b)}
C–C=O	124.9(10)
C–C–Cl	113.0(5)

r_z	Å ^{a)}
C–H	1.055 ^{b)}
C≡C	1.207 ^{b)}
C–C	1.4415(100)
C=O	1.1988(40)
C–Cl	1.7587(37)

θ_z	deg ^{a)}
H–C≡C	180.0 ^{b)}
C≡C–C	179.58(22) ^{c)}
C–C=O	125.19(30)
C–C–Cl	112.42(23)

^{a)} Uncertainties were partially estimated in the original paper.

^{b)} Assumed.

^{c)} The ethynyl group is bent away from the C–Cl bond.

Davis, R.W., Gerry, M.C.L.: Can. J. Chem. **60** (1982) 679.