

1087
MW

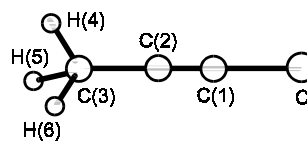
C₃H₃Cl

1-Chloro-1-propyne

C_{3v}
H₃C–C≡CCl

r_{av}	Å
C(1)≡C(2)	1.2013(18)
C(2)–C(3)	1.4611(10)
C–Cl	1.6428(15)
C–H	1.1033(54)

θ_{av}	deg
H–C–H	108.44(20)



Atom	a_{av} [Å]	c_{av} [Å]
Cl	−1.6176	0.0
C(1)	0.0252	0.0
C(2)	1.2265	0.0
C(3)	2.6877	0.0
H(4)	3.0737	0.0
H(5,6)	3.0737	±0.8950

Cox, A.P., Ellis, M.C., Perrett, T.: J. Chem. Soc., Faraday Trans. **88** (1992) 2611.