

Structure Data of Free Polyatomic Molecules

 74
MW

CHCl₃
Chloroform
Trichloromethane

C_{3v}
CHCl₃

r_0	Å
C–H	1.096(3)
C–Cl	1.7609(2)

r_{1e}	Å
C–H	1.101(4)
C–Cl	1.758(1)

r_s	Å ^{a)}
C–H	1.102(5)
C–Cl	1.759(2)

r_m^p	Å
C–H	1.105(7)
C–Cl	1.755(2)

r_z	Å
C–H	1.081(2)
C–Cl	1.7658(2)

$r_e^{b)}$	Å
C–H	1.080(2)
C–Cl	1.760(2)

θ_0	deg
H–C–Cl	107.81(2)
Cl–C–Cl	111.08(2)

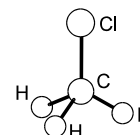
θ_{1e}	deg
H–C–Cl	107.61(14)
Cl–C–Cl	111.27(14)

θ_s	deg ^{a)}
H–C–Cl	107.70(6)
Cl–C–Cl	111.18(6)

θ_m^p	deg
H–C–Cl	107.57(22)
Cl–C–Cl	111.30(20)

θ_z	deg
H–C–Cl	108.27(2)
Cl–C–Cl	110.65(2)

$\theta_e^{b)}$	deg
H–C–Cl	108.23(2)
Cl–C–Cl	110.68(2)


^{a)} Uncertainties were not estimated in the original paper.

^{b)} Estimated by combining r_z and *ab initio* structure.

 Colmont, J.-M., Priem, D., Dréan, P., Demaison, J., Boggs, J.E.: J. Mol. Spectrosc. **191** (1998) 158.

 Replaces [II/25B\(3, 147\)](#)