

148
MW

 Cl_2O_2

Chloryl chloride

 C_s

r_0	Å
Cl–Cl	2.1966(15)
Cl=O	1.4367(8)

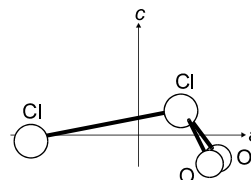
θ_0	deg
Cl–Cl=O	104.14(9)
O=Cl=O	114.96(10)

r_z	Å
Cl–Cl	2.1987(14)
Cl=O	1.4390(7)

θ_z	deg
Cl–Cl=O	104.02(8)
O=Cl=O	114.63(9)

$r_e^a)$	Å ^{b)}
Cl–Cl	2.1921(20)
Cl=O	1.4368(10)

$\theta_e^a)$	deg ^{b)}
Cl–Cl=O	104.02(10)
O=Cl=O	114.63(15)



^{a)} Approximate equilibrium parameters derived from r_z .

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

Müller, H.S.P., Cohen, E.A., Christen, D.: J. Chem. Phys. **110** (1999) 11865.