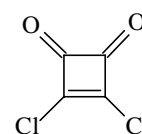


1464
MW, ED

C₄Cl₂O₂

3,4-Dichloro-3-cyclobutene-1,2-dione

C_{2v}

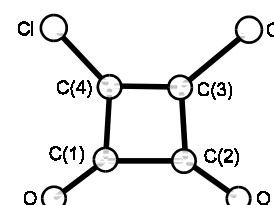


r_0	\AA^a	θ_0	deg^a
C=O	1.191(5)	C(3)=C(4)-C(1)	94.2(5)
C(3)=C(4)	1.348(6)	C(3)=C(4)-Cl	133.3(3)
C(1)-C(4)	1.513(5)	C(4)-C(1)=O	135.5(5)
C(1)-C(2)	1.569(5)		
C-Cl	1.681(3)		

The parameters have been allowed to vary within a confidence interval set at the corresponding uncertainty in the ED structure (see below).

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

Caminati, W., Fantoni, A.C., Lunelli, B., Scappini, F.: J. Mol. Spectrosc. **131** (1988) 154.



ED

r_g	\AA^a	θ_α	deg^a
C=O	1.191(2)	C(3)=C(4)-C(1)	94.1(2)
C(3)=C(4)	1.358(6)	C(3)=C(4)-Cl	133.5(6)
C(1)-C(4)	1.516(6)	C(4)-C(1)=O	135.7(7)
C(1)-C(2)	1.574(9)		
C-Cl	1.683(2)		

The nozzle temperature was 76 °C.

^a) Twice the estimated standard errors.

Hagen, K., Hedberg, K., Lunelli, B., Giorgini, M.G.: J. Phys. Chem. **92** (1988) 4313.