

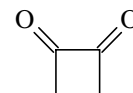
1564
MW

C₄H₄O₂

1,2-Cylobutanedione

C_{2v}

r_0	Å ^{a)}	θ_0	deg
C=O	1.215 ^{b)}	H-C-H	110.5 ^{c)}
C(1)-C(2)	1.567(3)		
C(2)-C(3)	1.527 ^{b)}		
C(3)-C(4)	1.556 ^{b)}		
C-H	1.095 ^{b)}		



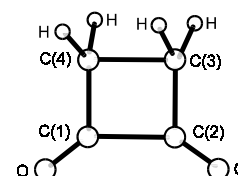
The C=O extension was assumed to bisect the internal angle of the ring.

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

^{b)} Assumed.

^{c)} With bisector of angle H-C-H coincident with that of angle C(2)-C(3)-C(4).

Legon, A.C.: J. Chem. Soc., Faraday Trans. II **75** (1979) 651.



ED, MW

r_α^0	Å ^{a)}	θ_α^0	deg ^{a)}
C=O	1.191(2)	H-C-H	108.2(17)
C(1)-C(2)	1.574(16)	C-C-H	114.4(5)
C(2)-C(3)	1.549(14)	C(1)-C(2)=O	135.9(10)
C(3)-C(4)	1.544(14)	C(1)-C(2)-C(3)	89.5(2)
C-H	1.096(8)		

The nozzle temperature was 100 °C.

^{a)} Twice the estimated standard errors.

Hagen, K., Hedberg, K.: J. Am. Chem. Soc. **103** (1981) 5360.