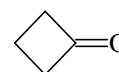


1651
ED, MW

C₄H₆O

Cyclobutanone

C_s



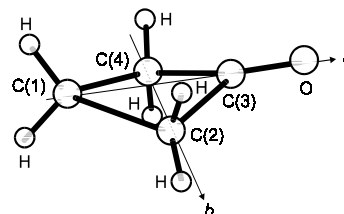
r_g	\AA^a	θ_α	deg^a
C=O	1.202(2)	C(2)–C(1)–C(4)	90.3(4)
C–H (average)	1.100(4)	H–C–H (average)	105.9(16)
C(1)–C(2)	1.567(5)	β^b	7.3(37)
C(2)–C(3)	1.534(3)		

Puckering motion was included in the analysis. The C=O bond is assumed to be on the bisector of the C(2)–C(3)–C(4) angle.

The measurements were made at room temperature.

^a) Three times the estimated standard errors including a systematic error.

^b) $\beta = (1/2)[C(1)–C(2)–C(3)] - \mu$, where μ is the angle between the HC(2)H plane and the C(1)–C(2) bond.



Tamagawa, K., Hilderbrandt, R.L.: J. Phys. Chem. **87** (1983) 5508.

MW

r_s	\AA	θ_s	deg
C=O	1.204(6)	H–C(2)–H	109.2(2)
C(2)–H	1.099(3)	tilt (C(2)H ₂) ^a	4.6(8)

^a) Tilt angle of the C(2)H₂ group towards the carbonyl group, i.e. the angle between the HC(2)H plane and the bisector of the C(1)–C(2)–C(3) angle.

Stigliani, W.M., Laurie, V.W., Scharpen, L.H.: J. Mol. Spectrosc. **62** (1976) 85.

MW

C_s^a

r_0	\AA	θ_0	deg
C=O	1.201(10)	H–C(2,4)–H	112.5(15)
C(2,4)–H	1.110 ^b	H–C(1)–H	112.9(15)
C(1)–H	1.089(20)		

r_s	\AA	θ_s	deg
C(3)–C	1.527(3)	C(2)–C(3)–C(4)	93.1(3)
C(1)–C	1.556(2)	C(3)–C–C	88.0(3)
		C(2)–C(1)–C(4)	90.0(2)

Atom	$a_s [\text{\AA}]$	$b_s [\text{\AA}]$	$c_s [\text{\AA}]$
O	1.796	0.0	0.0
C(3)	0.5900	0.0	0.0
C(2,4)	–0.4607	± 1.1085	0.0
H	–0.326	± 1.675	± 0.923
C(1)	–1.5520	0.0	0.0
H	–2.184	0.0	± 0.908

^a) Deviates slightly from C_{2v}.

^b) Assumed.

Bauder, A., Tank, F., Günthard, H.H.: Helv. Chim. Acta **46** (1963) 1453.

Scharpen, L.H., Laurie, V.W.: J. Chem. Phys. **49** (1968) 221.

UV

State ^{a)}	A ¹ A ₂	B ¹ B ₂
Reference	[1]	[2]
<hr/>		
Height of barrier to planarity (cm ⁻¹)		
S ₁₉ (b ₁) ^{b)}	1550	
S ₂₀ (a ₂) ^{c)}	112	255

Vibrational analysis of ultraviolet spectra.

The molecular structure in all states is slightly non-planar, through ring puckering and/or with the O atom out of the plane of the ring.

^{a)} State assignments based on theory and analogy.

^{b)} Vibrational overtones fitted to energies calculated from model double potential minimum potentials in symmetrized displacement-coordinate 19 (carbonyl out-of-plane wag).

^{c)} Ditto, coordinate 20 (ring-puckering). A barrier height of 7.6(2) cm⁻¹ for this vibration has also been deduced for the ground state from MW and far IR data [3].

[1] Moule, D. C.: Can. J. Phys. **47** (1969) 1235.

[2] Momicchioli, F., Baraldi, I., DiLonardo, G.: J. Chem. Soc., Faraday Trans. II, **71** (1975) 791.

[3] Sharpen, L. H., Laurie, V. W.: J. Chem. Phys. **49** (1968) 221.