

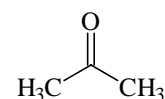
1265
MW

C₃H₆O

Propanone
Acetone

C_{2v}

r_s	Å	θ_s	deg
C–C	1.507(3)	C–C–C	117.2(4)
C=O	1.222(3)	H–C–H	108.8(10)
C–H	1.085(10)	ϕ^a	119.9
		tilt(CH ₃) ^b	1.35



Atom	a_s [Å]	b_s [Å]	c_s [Å]
C(methyl)	± 1.2864	-0.6960	0.00
H(s)	± 2.1198	-0.0012	0.00
H(a)	± 1.3551	-1.3240	± 0.8821
C	0.00	0.0893	0.00
O	0.00	1.3112	0.00

^a) Angle between the symmetry axes of the CH₃ groups.

^b) Tilt angle.

Nelson, R., Pierce, L.: J. Mol. Spectrosc. **18** (1965) 344.

ED, MW

r_g	Å ^a)	θ_z	deg ^a)
C–C	1.520(3)	C–C–C	116.0(3)
C=O	1.214(4)	H–C–H	108.4(5)
C–H	1.103(3)	O=C–C	122.0(3)
		tilt (CH ₃) ^b	2.0(5)

The effect of internal rotation is taken into account in the vibrational correction to the observed moments of inertia.

The measurements were made at room temperature.

^a) Estimated limits of error. Those for the distances are not given in the original paper.

^b) The tilt angle between the CH₃ axis and the C–C bond.

Iijima, T.: Bull. Chem. Soc. Jpn. **45** (1972) 3526.

See also: Kato, C., Konaka, S., Iijima, T., Kimura, M.: Bull. Chem. Soc. Jpn. **42** (1969) 2148.

Hilderbrandt, R.L., Andreassen, A.L., Bauer, S.H.: J. Phys. Chem. **74** (1970) 1586.