

1072
MW

C₃H₂O

Methyleneketene
1,2-Propadien-1-one

C_s
H₂C=C=CO

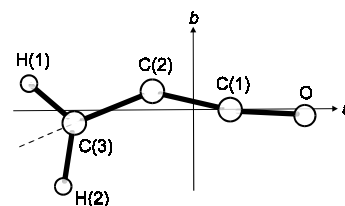
r_s	Å ^{a)}	θ_s	deg ^{a)}
C(3)–H(1)	1.094(2)	H(1)–C(3)=C(2)	117.18(12)
C(3)–H(2)	1.094(2)	H(2)–C(3)=C(2)	120.95(16)
C(2)=C(3)	1.3219(8)	C(1)=C(2)=C(3)	144.5(15)
C(1)=C(2)	1.3196(77)	C(2)=C(1)=O	169.4(35)
C(1)=O	1.1831(17)		

Atom	$ a_s $ [Å]	$ b_s $ [Å]
O	1.7706	–0.0774
C(1)	0.6028	±0.0050
C(2)	–0.6609	0.3187, 0.3286 ^{a)}
C(3)	–1.8988	–0.1629
H(1)	–2.7196	0.5581
H(2)	–2.0810	–1.2434

^{a)} r_s coordinates derived from moment equations (two values arise due to the indeterminacy of the sign of b for the C(1) nucleus).

Brown, R.D., Champion, R., Elmes, P.S., Godfrey, P.: J. Am. Chem. Soc. **107** (1985) 4109.
See also: Brown, R.D., Godfrey, P.D., Champion, R., McNaughton, D.: J. Am. Chem. Soc. **103** (1981) 5711.

r_0	Å	θ_0	deg
C(3)–H	1.0940(20)	1/2[H–C–H]	60.91(15)
C(2)=C(3)	1.3220(7)	C(2)=C(3)–M ^{a)}	178.08(6)
C(1)=C(2)	1.3307(60)	C(1)=C(2)=C(3)	143.5(10)
C(1)=O	1.1621(15)	C(2)=C(1)=O	169.4(30)



The dotted line is the bisector of the angle H–C–H.

Semirigid bender model is used to derive structural parameters.

^{a)} C(3)–M denotes the bisector of H–C(3)–H.

Brown, R.D., Godfrey, P.D., Champion, R.: J. Mol. Spectrosc. **123** (1987) 93.