

1167
MW

C₃H₄O₂

3-Oxetanone

C_{2v}

r_0	Å	θ_0	deg
C(1)–H	1.09 ^{a)}	H–C(1)–H	110 ^{a)}
C(1)–O	1.441(20)		
C(2)=O	1.222(20)		

r_s	Å	θ_s	deg
C(1)–C(2)	1.524(3)	C(1)–C(2)–C(1')	88.23(30)

Atom	a_s [Å]	b_s [Å]	c_s [Å]
C(1)	–0.469	±1.058	0.00
C(2)	0.626	0.00	0.00

The H atoms were assumed to be symmetrically placed about the O–C(1)–C(2) angles.

^{a)} Assumed.

Gibson, J.S., Harris, D.O.: J. Chem. Phys. **57** (1972) 2318.

