

1044
MW

C₃HO

3-Oxo-1,2-propadien-1-yl

C_s
H $\dot{\text{C}}$ =C=C=O

r_0	Å	θ_0	deg
C(1)–H	1.090(44)	H–C=C	156(8)
C(1)=C(2)	1.242(10)	C=C=C	157(5)
C(2)=C(3)	1.400(16)	C=C=O	135.5(17)
C(3)=O	1.186(7)		

r_s	Å	θ_s	deg
C(1)–H	1.065(18)	H–C=C	168(7)
C(1)=C(2)	1.221(3)	C=C=C	163(2)
C(2)=C(3)	1.390(5)	C=C=O	136.5(7)
C(3)=O	1.195(2)		

r_m^p	Å	θ_m^p	deg
C(1)–H	1.060(18)	H–C=C	168(7)
C(1)=C(2)	1.219(3)	C=C=C	163(2)
C(2)=C(3)	1.387(5)	C=C=O	136.5(6)
C(3)=O	1.192(2)		

Assumed to be fully *trans*.

Cooksy, A.L., Watson, J.K.G., Gottlieb,
C.A., Thaddeus, P.: J. Chem. Phys. **101**
(1994) 178.

