

1645 **C₄H₆O**
ED, MW, vibrational
spectroscopy, *ab initio*
calculations (HF/4-21G)

2-Methyl-2-propenal
Methacrylaldehyde

C_s (*ap*)
C_s (*sp*)
H₂C=C(CH₃)-C(O)H

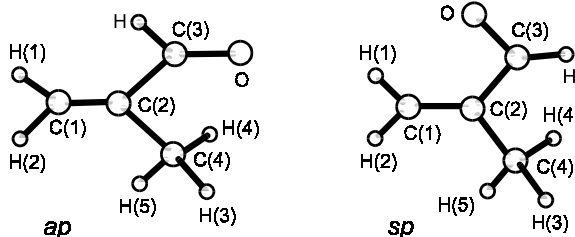
ap conformer

	r_g [Å] ^{a)}	r_α^0 [Å] ^{a)}	θ_α^0	deg ^{a)}
C(1)=C(2)	1.347(3)	1.343(3)	C(1)=C(2)-C(3)	118.5(5)
C(2)-C(3)	1.487(6)	1.485(6)	C(1)=C(2)-C(4)	124.7(5)
C(2)-C(4) ^{b)}	1.512(6)	1.509(6)	C(3)-C(2)-C(4)	116.8(5)
C(3)=O	1.217(3)	1.211(3)	C(2)-C(3)=O	122.9(5)
C(3)-H ^{b)}	1.121(40)	1.101(40)	H(1)-C(1)=C(2) ^{b)}	121.3(40)
C(1)-H(1) ^{b)}	1.097(40)	1.090(40)	H(2)-C(1)=C(2) ^{b)}	121.9(40)
C(1)-H(2)	1.095(6)	1.087(6)	C(2)-C(3)-H ^{b)}	114.9(40)
C(4)-H(3,4) ^{b)}	1.108(40)	1.084(40)	O=C(3)-H	122.2(40)
C(4)-H(5) ^{b)}	1.135(40)	1.083(40)	C(2)-C(4)-H(3) ^{b)}	109.6(40)
			C(2)-C(4)-H(5)	111.8(40)
			H(3)-C(4)-H(5) ^{b)}	109.6(40)
			C(1)=C(2)-C(3)=O	180

sp conformer

	r_g [Å] ^{a)}	r_α^0 [Å] ^{a)}	θ_α^0	deg ^{a)}
C(1)=C(2)	1.347(3)	1.344(3)	C(1)=C(2)-C(3)	118.1(5)
C(2)-C(3)	1.492(6)	1.491(6)	C(1)=C(2)-C(4)	124.4(5)
C(2)-C(4) ^{b)}	1.512(6)	1.509(6)	C(3)-C(2)-C(4)	117.5(5)
C(3)=O	1.217(3)	1.210(3)	C(2)-C(3)=O	123.7(5)
C(3)-H ^{b)}	1.124(40)	1.101(40)	H(1)-C(1)=C(2) ^{b)}	120.0(40)
C(1)-H(1) ^{b)}	1.094(40)	1.088(40)	H(2)-C(1)=C(2) ^{b)}	121.9(40)
C(1)-H(2)	1.093(6)	1.087(6)	C(2)-C(3)-H	114.9(40)
C(4)-H(3,4) ^{b)}	1.114(40)	1.090(40)	O=C(3)-H	122.2(40)
C(4)-H(5) ^{b)}	1.136(40)	1.084(40)	C(2)-C(4)-H(3) ^{b)}	108.8(40)
			C(2)-C(4)-H(5)	111.5(40)
			H(3)-C(4)-H(5) ^{b)}	111.5(40)
			C(1)=C(2)-C(3)=O	0

The molecule exists as a mixture of *sp* and *ap* conformers in the ratio 89(3):11(3). The nozzle temperature was 303 K.



^{a)} Estimated total errors.

^{b)} Dependent parameter. Difference between the refined and the corresponding dependent parameter was fixed at the *ab initio* value.

Wang, Y., de Smedt, J., Coucke, I., van Alsenoy, C., Geise, H.J.: J. Mol. Struct. **299** (1993) 43.

MW

 C_s (*ap*)

r_0	Å	θ_0	deg
C(1)=C(2)	1.349(16)	C(1)=C(2)–C(3)	114.56(115)
C(2)–C(3)	1.470(13)	C(1)=C(2)–C(4)	123.66(124)
C(2)–C(4)	1.518(13)	C(2)–C(3)=O	123.18(90)
C(3)=O	1.217(16)	H(1)–C(1)=C(2)	121.46 ^{a)}
C(3)–H	1.108 ^{a)}	H(2)–C(1)=C(2)	119.58 ^{a)}
C(1)–H(1)	1.086 ^{a)}	C(2)–C(3)–H	115.09 ^{a)}
C(1)–H(2)	1.086 ^{a)}	C(2)–C(4)–H(5)	109.47 ^{a)}
C(4)–H	1.090 ^{a)}	H(3)–C(4)–H(5)	109.47 ^{a)}

^{a)} Assumed.Durig, J.R., Qiu, J., Dehoff, B., Little, T.S.: Spectrochim. Acta A **42** (1986) 89.