

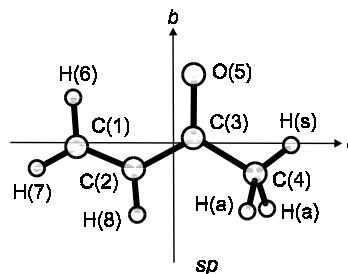
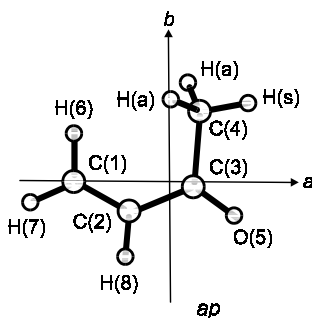
**1643**     **C<sub>4</sub>H<sub>6</sub>O**  
ED, MW, *ab initio* (HF/4-21G,  
4-21G\*\*) and MM calculations

**3-Buten-2-one**  
Methyl vinyl ketone

**C<sub>s</sub> (*ap*)**  
**C<sub>s</sub> (*sp*)**  
H<sub>2</sub>C=CH-C(O)-CH<sub>3</sub>

*ap* conformer

$r_g$	Å <sup>a)</sup>
C(1)=C(2)	1.336(3)
C(2)-C(3)	1.49(2)
C(3)-C(4)	1.52(2)
C(3)=O	1.219(3)
C(1)-H(6)	1.09(4)
C(1)-H(7)	1.09(4)
C(2)-H(8)	1.09(4)
C(4)-H(s)	1.10(4)
C(4)-H(a)	1.11(4)



$\theta_\alpha^0$	deg <sup>a)</sup>	
	<i>ap</i> conformer	<i>sp</i> conformer
C(1)=C(2)-C(3)	125.0(15)	120.6(15)
C(2)-C(3)-C(4)	118.9(15)	116.1(15)
C(2)-C(3)=O	119.7(15)	121.8(15)
C(2)=C(1)-H(6)	123(5)	120(5)
C(2)=C(1)-H(7)	121(5)	122(5)
C(1)=C(2)-H(8)	121(5)	122(5)
C(3)-C(4)-H(s)	108(5)	110(5)
C(3)-C(4)-H(a)	110(5)	110(5)
H(s)-C(4)-H(a)	109(5)	110(5)
H(a)-C(4)-H(a)	108(5)	108(5)

The molecule exists as a mixture of *ap* and *sp* conformers in the ratio 80:20. The  $r_g$  values for the *sp* conformer are essentially equal to those for the *ap* conformer.

$\Delta H = H(sp) - H(ap) = 1.07(10) \text{ kcal mol}^{-1}$ .

The nozzle temperature was 300 K.

<sup>a)</sup> Estimated total error.

de Smedt, J., Vanhouteghem, F., van Alsenoy, C., Geise, H.J., van der Veken, B., Coppens, P.:  
J. Mol. Struct. **195** (1989) 227.