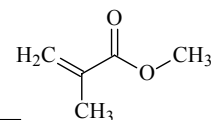


649 **C₅H₈O₂**ED, *ab initio*
calculations**Methyl 2-methyl-2-propenoate**Methyl methacrylate
2-Methyl-2-propenoic acid methyl esterC_s assumed (*s-anti*)C_s assumed (*s-syn*)

r_g	Å ^{a)}	θ_α	deg ^{a)}
C(2)=C(3)	1.341(6)	C(3)=C(2)-C(1)	121.2(7)
C(1)-O(4)	1.348(5)	C(3)=C(2)-C(7)	123.3(9)
C(2)-C(7)	1.505(2) ^{b)}	C(2)-C(1)-O(4)	113.3(8)
C(1)-C(2)	1.494(2) ^{b)}	C(2)-C(1)=O(6)	123.4(7)
C(1)=O(6)	1.209(3)	C(1)-O(4)-C(5)	116.8(9)
O(4)-C(5)	1.433(3)	C(2)=C(3)-H(8)	121.8 ^{c)}
C(3)-H(8)	1.098(4) ^{d)}	C(2)=C(3)-H(9)	120.9 ^{c)}
C(3)-H(9)	1.101(4) ^{d)}	O(4)-C(5)-H(10)	104.7(13) ^{e)}
C(5)-H(10)	1.105(4) ^{d)}	O(4)-C(5)-H(11)	109.5(13) ^{e)}
C(5)-H(11)	1.107(4) ^{d)}	C(2)-C(7)-H(13)	109.4(13) ^{e)}
C(7)-H(13)	1.109(4) ^{d)}	C(2)-C(7)-H(14)	109.7(13) ^{e)}
C(7)-H(14)	1.110(4) ^{d)}	C(1)-O(4)-C(5)-H(11)	60.5 ^{c)} ^{f)}
		C(3)=C(2)-C(7)-H(14)	120.7 ^{c)} ^{f)}

The molecule was found to exist as a mixture of *s-anti* (64(17)%) and *s-syn* conformers. Differences between the structural parameters of *s-anti* and *s-syn* conformers were assumed at the values from HF/6-31G** calculations. The parameters are listed for the *s-anti* conformer.

The nozzle temperature was 25 °C.

According to HF/6-31G** calculations, the *s-anti* conformer is more stable than the *s-syn* conformer by 0.32 kcal mol⁻¹.

^{a)} Three times the estimated standard errors.

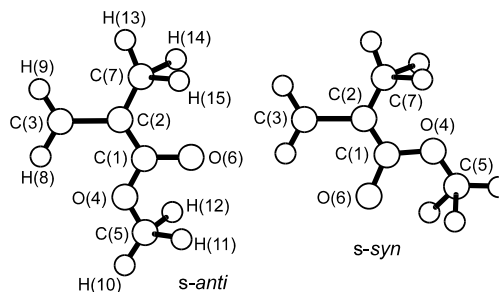
^{b)} Difference between the C(2)-C(7) and C(1)-C(2) bond lengths was assumed at the value from HF/6-31G** calculations.

^{c)} Assumed at the value from HF/6-31G** calculations.

^{d)} Differences in the C-H bond lengths were assumed at the values from HF/6-31G** calculations.

^{e)} Differences among the O(4)-C(5)-H(10), O(4)-C(5)-H(11), C(2)-C(7)-H(13) and C(2)-C(7)-H(14) bond angles were assumed at the values from HF/6-31G** calculations.

^{f)} Measured from the *syn* position.



Tsuji, T., Ito, H., Takeuchi, H., Konaka, S.: J. Mol. Struct. **475** (1999) 55.