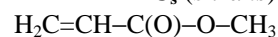


1659 C₄H₆O₂ED, MW, *ab initio*

calculations (HF/4-31G*)

Methyl acrylate

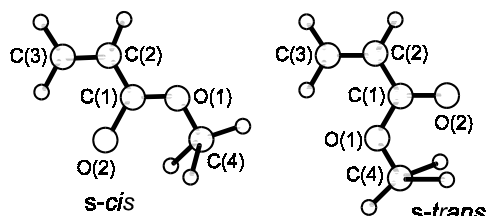
Methyl 2-propenoate

C_s (s-*cis*)**C_s (s-*trans*)**

r_z	Å ^{a)}	θ_z	deg ^{a)}
C(2)=C(3)	1.332(7)	C(1)–C(2)=C(3)	120.3(8)
C(1)–C(2)	1.480(6)	C(2)–C(1)=O(2)	126.1(5)
C(1)=O(2)	1.207(2)	C(2)–C(1)–O(1)	110.3(3)
C(1)–O(1)	1.345(3)	C(1)–O(1)–C(4)	116.4(5)
O(1)–C(4) ^{b)}	1.434(3)	C(1)–O(1)–C(4)–H	–60.5 ^{c)}
C–H (mean)	1.079(5)		

At room temperature (23 °C) the molecule exists in a conformational equilibrium of two forms, *s-cis* and *s-trans*, in the ratio of 67(11):33. Conformational differences of structural parameters were fixed at *ab initio* values.

The parameters are given for the *s-cis* conformer.



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

^{b)} Dependent parameter; difference between O(1)–C(4) and C(1)–O(1) was fixed at the *ab initio* value.

^{c)} Assumed.

Egawa, T., Maekawa, S., Fujiwara, H., Takeuchi, H., Konaka, S.: J. Mol. Struct. **352/353** (1995) 193.