

1276 C₃H₆O₂ED, MW, *ab initio*

calculations (HF/4-21G, 6-31G**)

Ethyl formate

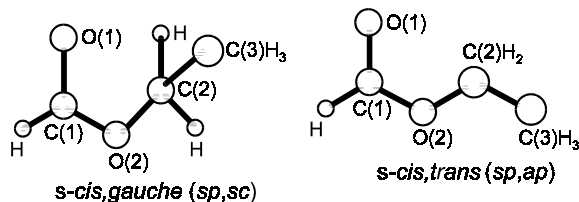
C_s (*s-cis,trans*)C₁ (*s-cis,gauche*)H₃C–CH₂–O–C(O)H

	r_g [Å] ^{a)}	r_α^0 [Å] ^{a)}	θ_α^0	deg ^{a)}
<i>s-cis,trans</i>				
C(1)=O(1)	1.213(6)	1.209(6)	O(1)=C(1)–O(2)	124.1(5)
C(1)–O(2)	1.354(6)	1.350(6)	C(2)–O(2)–C(1)	117.3(5)
O(2)–C(2)	1.465(6)	1.463(6)	O(2)–C(2)–C(3)	105.4(5)
C(2)–C(3)	1.500(6)	1.493(6)	O(1)=C(1)–H	127.3(10)
C(1)–H	1.109(12)	1.091(12)	O(2)–C(2)–H	108.6(10)
C(2)–H	1.094(12)	1.076(12)	C(2)–C(3)–H	108.7(10)
C(3)–H	1.098(12)	1.072(12)	C(2)–O(2)–C(1)=O(1)	0
			C(3)–C(2)–O(2)–C(1)	180
<i>s-cis,gauche</i>				
C(1)=O(1)	1.213(6)	1.209(6)	O(1)=C(1)–O(2)	124.4(5)
C(1)–O(2)	1.354(6)	1.351(6)	C(2)–O(2)–C(1)	117.8(5)
O(2)–C(2)	1.466(6)	1.463(6)	O(2)–C(2)–C(3)	109.7(5)
C(2)–C(3)	1.505(6)	1.501(6)	O(1)=C(1)–H	127.2(10)
C(1)–H	1.108(12)	1.090(12)	O(2)–C(2)–H	108.4(10)
C(2)–H	1.092(12)	1.075(12)	C(2)–C(3)–H	108.5(10)
C(3)–H	1.096(12)	1.071(12)	C(2)–O(2)–C(1)=O(1)	0
			C(3)–C(2)–O(2)–C(1)	81.7(5)

The compound exists as a mixture of *s-cis,trans* (61(2)%) and *s-cis,gauche* (39(2)%) conformers. Differences in similar parameters as well as conformational differences were constrained to *ab initio* values.

The nozzle temperature was 300 K.

^{a)} Estimated total errors.



Peng, Z., Shlykov, S., van Alsenoy, C., Geise, H.J., van der Veken, B.: J. Phys. Chem. **99** (1995) 10201.