

1273 **C₃H₆O₂**
ED, MW, *ab initio*
calculations (4-21G)

Methyl acetate

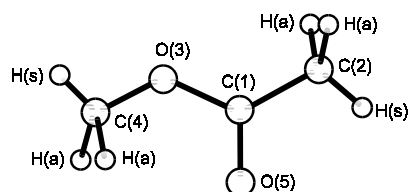
C_s (*syn*) assumed
H₃C–C(O)–O–CH₃

r_g	Å ^{a)}	θ_α^0	deg ^{a)}
C(1)–O(3)	1.360(6)	C(2)–C(1)–O(3)	111.4(9)
O(3)–C(4)	1.442(6)	C(1)–O(3)–C(4)	116.4(9)
C(1)–C(2)	1.496(6)	O(3)–C(1)=O(5)	123.1(9)
C(1)=O(5)	1.209(6)	H(s)–C(4)–O(3)	103.1(9)
C(4)–H(s) ^{b)}	1.107(18)	H(a)–C(4)–O(3)	109.1(9)
C(4)–H(a) ^{b)}	1.109(18)	H(s)–C(2)–C(1)	107.6(9)
C(2)–H(a) ^{b)}	1.112(18)	H(a)–C(2)–C(1)	107.6(9)
C(2)–H(s) ^{b)}	1.107(18)	C(1)–O(3)–C(4)–H(a)	58.1(9)
		C(4)–O(3)–C(1)=O(5)	0 ^{b)}
		C(4)–O(3)–C(1)–C(2)	180 ^{b)}

Data are in accord with a planar heavy-atom skeleton in the *syn* conformation.
The nozzle temperature was ≈ 30 °C.

^{a)} Estimated total errors.

^{b)} Assumed.



Pyckhout, W., van Alsenoy, C., Geise, H.J.: J. Mol. Struct. **144** (1986) 265.