

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

$r_g$	Å <sup>a)</sup>	$\theta_\alpha$	deg <sup>a)</sup>
C(1)=C(2)	1.337(20)	O(3)-C(2)=C(1)	127.3(18)
C(2)-O(3)	1.359(15)	C(1)=C(2)-H(7)	124.4(20)
C(4)-O(3)	1.427(7)	C(2)=C(1)-H(5)	125.4(20)
C(1)-H(5,6)	1.095(3)	C(2)=C(1)-H(6)	121.4(20)
C(2)-H(7)	1.095(3)	O(3)-C(2)-H(7)	108.3(7)
C(4)-H(8)	1.105(3)	C(2)-O(3)-C(4)	116.8(18)
C(4)-H(9,10)	1.110(3)	O(3)-C(4)-H(8)	105.6(7)
		O(3)-C(4)-H(9,10)	110.7(7)
		$\tau_1^b)$	0 <sup>d)</sup>
		$\tau_2^c)$	180 <sup>d)</sup>

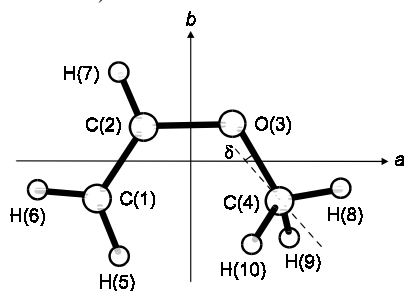
Constraints on geometrical parameters were obtained from *ab initio* calculations. The measurements were made at room temperature.

<sup>a)</sup> Three times the estimated standard errors.

<sup>b)</sup> Dihedral angle C(1)=C(2)-O(3)-C(4).

<sup>c)</sup> Dihedral angle C(2)-O(3)-C(4)-H(8).

<sup>d)</sup> Fixed.



Pyckhout, W., van Nuffel, P., van Alsenoy, C., van den Enden, L., Geise, H.J.: J. Mol. Struct. **102** (1983) 333.

See also: (ED) van den Enden, L., Geise, H.J.: J. Mol. Struct. **97** (1983) 139.

(ED) Samdal, S., Seip, H.M.: J. Mol. Struct. **28** (1975) 193.

MW

$r_s$	Å	$\theta_s$	deg
C(1)=C(2)	1.339(1)	O(3)-C(2)=C(1)	128.0(1)
C(2)-O(3)	1.350(1)	C(1)=C(2)-H(7)	121.7(1)
C(4)-O(3)	1.420(1)	C(2)=C(1)-H(5)	121.9(1)
C(1)-H(5)	1.096(1)	C(2)=C(1)-H(6)	118.3(1)
C(1)-H(6)	1.077(1)	O(3)-C(2)-H(7)	110.3(1)
C(2)-H(7)	1.086(1)	C(2)-O(3)-C(4)	116.1(1)
C(4)-H(8)	1.077(5)	O(3)-C(4)-H(8)	106.9(7)
C(4)-H(9,10)	1.102(1)	O(3)-C(4)-H(9,10)	110.3(1)
		H(8)-C(4)-H(9)	110.7(8)
		H(9)-C(4)-H(10)	108.0(1)
		H(5)-C-H(6)	119.7(2)
		$\gamma^a)$	109.1(3)
		$\delta(\text{CH}_3)^b)$	2.3(5)

Atom	$a_s$ [Å]	$b_s$ [Å]	$c_s$ [Å]
H(8)	2.3941	-0.3281	0.00
C(4)	1.3469	-0.5790	0.00
H(9,10)	1.0878	-1.1725	$\pm 0.8913$
O(3)	0.6297	0.6464	0.00
C(2)	-0.7165	0.5464	0.00
H(7)	-1.1676	1.5338	0.00
C(1)	-1.4609	-0.5668	0.00
H(5)	-1.0100	-1.5657	0.00
H(6)	-2.5329	-0.4650	0.00

<sup>a)</sup> The corrected value of the O-C-H angle, defined by  
 $\gamma = (1/3) [(O-C-H(8)) + 2(O-C-H(9))]$ .

<sup>b)</sup> The tilt angle of the methyl group, defined by  $\delta = (2/3) [(O-C-H(9)) - (O-C-H(8))]$ .

Fujitake, M., Hayashi, M.: J. Mol. Struct. **127** (1985) 21.