

$r^a)$	Å $b)$	$\theta^a)$	deg $b)$
C(1)–C(2)	1.525(8)	C(2)–C(1)–O(4)	111.5(16)
C(2)–O(3)	1.412(14)	O(3)–C(2)–C(1)	109.4(14)
C(1)–O(4)	1.444(18)	C(1)–O(4)–C(5)	112.5(20)
O(4)–C(5)	1.337(8)	O(4)–C(5)=O(6)	126.7(20)
C(5)=O(6)	1.203(6)		<i>gauche</i> -1 <i>gauche</i> -2
C(1)–H(8)	1.102 $^c)$	$\alpha^d)$	108.8(45)      124.7(90)
O(3)–H(12)	1.18(6)	$\beta^d)$	161 $^c)$ 170 $^c)$
C(5)–H(7)	1.106 $^c)$	$\gamma^d)$	271.6(45)      299.5(45)
	<i>gauche</i> -1 <i>gauche</i> -2		
O(3)...O(6)	2.785(20)		
O(3)...O(4)	2.806(30)		

Molecule exists as a mixture of *gauche*-1 (58(1)%) and *gauche*-2 (42(1)%) conformers.

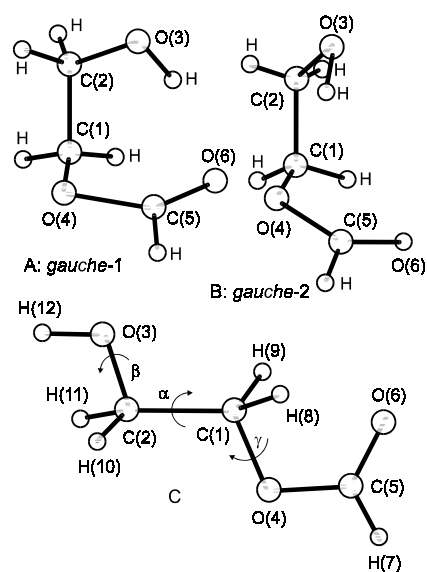
Temperature of the measurements was 110 °C.

$a)$  Unidentified, possibly  $r_a$  and  $\theta_a$ .

$b)$  Uncertainty estimates are twice or three times those of the original data.

$c)$  Assumed.

$d)$  Rotational angles are zero in the position shown in figure C.



Bijen, J.M.J.M.: J. Mol. Struct. **17** (1973) 69.