

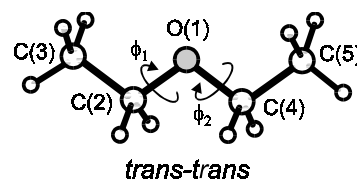
1819 **C₄H₁₀O**
ED, MW, *ab initio*
(HF/4-21G) calculations

Diethyl ether
1,1'-Oxobisethane

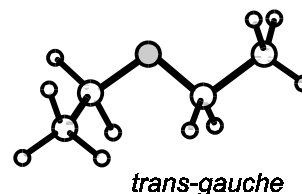
C_{2v} (trans-trans)
C₁ (trans-gauche)
H₃C–CH₂–O–CH₂–CH₃

r_g	$\text{\AA}^a)$		θ_α	$\text{deg}^a)$	
	<i>trans-trans</i>	<i>trans-gauche</i>		<i>trans-trans</i>	<i>trans-gauche</i>
O(1)–C(2)	1.419(1)	1.421(1)	C–O–C	113.5(4)	114.8(4)
O(1)–C(4)	1.419(1)	1.420(1)	O–C(2)–C(3)	108.6(1)	114.0(1)
C(2)–C(3)	1.514(2)	1.521(2)	O–C(4)–C(5)	108.6(1)	108.1(1)
C(4)–C(5)	1.514(2)	1.516(2)	O–C–H ^{b)}	110.4(9)	109.4(9)
C–H ^{b)}	1.114(2)	1.113(2)	C–C–H ^{b)}	110.5(7)	110.5(7)
			ϕ_1 ^{c)}	180 ^{d)}	76(10)
			ϕ_2 ^{e)}	180 ^{d)}	161(15)

The molecule exists as a mixture of *trans-trans* (69(8)%) and *trans-gauche* (31%) conformers with energy difference 1.3(2) kcal/mol. The structural differences between conformers were taken from *ab initio* calculations except for the dihedral angles. The temperature of the experiment was about 27 °C.



- a) Three times the estimated standard errors.
b) Average value.
c) Dihedral angle C(4)–O(1)–C(2)–C(3).
d) Assumed.
e) Dihedral angle C(2)–O(1)–C(4)–C(5).



Kuze, N., Kuroki, N., Takeuchi, H., Egawa, T., Konaka, S.: J. Mol. Struct. **301** (1993) 81.

MW

r_s	\AA	θ_s	deg	C_{2v} (trans-trans)
C(3,5)–C	1.517(5)	C–C–O	108.4(3)	
C–O	1.411(3)	C–O–C	112.1(3)	
C(3,5)–H(s)	1.092(4)	C(2,4)–C–H(s)	110.2(4)	
C(3,5)–H(a)	1.090(5)	C(2,4)–C–H(a)	110.2(5)	
C(2,4)–H	1.100(3)	H(s)–C(3,5)–H(a)	108.9(4)	
		H(a)–C(3,5)–H(a)	108.2(5)	
		C(3,5)–C–H	110.4(5)	
		H–C–O	110.0(3)	
		H–C(2,4)–H	107.6(4)	
		$\gamma^a)$	110.2(5)	
		$\delta^b)$	0.0(6)	

Atom	$a_s [\text{\AA}]$	$b_s [\text{\AA}]$	$c_s [\text{\AA}]$
C(3,5)	± 2.3722	-0.3977	0.0
C(2,4)	± 1.1711	0.5288	0.0
O	0.0	-0.2591	0.0
H(s)	± 3.2969	0.2134	0.0
H(a)	± 2.3556	-1.0368	± 0.8827
H	± 1.1885	1.1780	± 0.8878

a) The corrected C(2,4)–C–H value defined by $\gamma = 1/3 [(C-C-H(s)) + 2(C-C-H(a))]$.

b) The tilt angle of the CCH₃ group defined by $\delta = 2/3 [(C-C-H(a)) - (C-C-H(s))]$.

Hayashi, M., Adachi, M.: J. Mol. Struct. **78** (1982) 53.