

1817  
MW

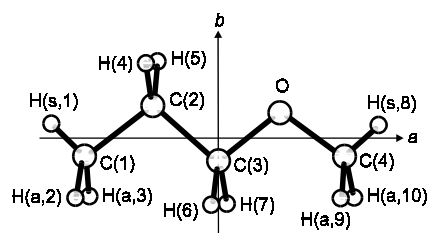
**C<sub>4</sub>H<sub>10</sub>O**

**Methyl propyl ether**

**C<sub>s</sub> (*trans-trans*)**  
**H<sub>3</sub>C–CH<sub>2</sub>–CH<sub>2</sub>–O–CH<sub>3</sub>**

$r_s$	Å	$\theta_s$	deg
C(1)–C(2)	1.530(4)	C–C–C	111.8(13)
C(2)–C(3)	1.516(15)	C–C–O	108.8(9)
O–C(3)	1.408(15)	C–O–C	112.0(14)
O–C(4)	1.413(4)	C(2)–C(1)–H(s)	111.0(4)
C(1)–H(s)	1.091(5)	C(2)–C(1)–H(a)	111.0(3)
C(1)–H(a)	1.093(4)	H(a)–C(1)–H(s)	108.0(6)
C(2)–H	1.094(2)	H(a)–C(1)–H(a)	107.6(4)
C(3)–H	1.107(6)	C(1)–C(2)–H	110.3(4)
C(4)–H(s)	1.086(8)	C(3)–C(2)–H	108.7(13)
C(4)–H(a)	1.099(4)	H–C(2)–H	107.1(2)
		C(2)–C(3)–H	109.6(24)
		O–C(3)–H	110.9(25)
		H–C(3)–H	107.1(5)
		O–C(4)–H(s)	107.4(5)
		O–C(4)–H(a)	111.1(3)
		H(s)–C(4)–H(a)	109.7(8)
		H(a)–C(4)–H(a)	107.9(4)
		$\gamma_1^a$	111.0(4)
		$\delta_1^b$	0.0(5)
		$\gamma_4^a$	109.9(4)
		$\delta_4^b$	2.5(5)

Atom	$a_s$ [Å]	$b_s$ [Å]	$c_s$ [Å]
C(1)	–2.4966	–0.3040	0.0
C(2)	–1.2110	0.5262	0.0
C(3)	0.0239	–0.3508	0.0
O	1.1663	0.4730	0.0
C(4)	2.3617	–0.2797	0.0
H(s,1)	–3.3778	0.3392	0.0
H(a;2,3)	–2.5476	–0.9479	±0.8819
H(4,5)	–1.1792	1.1792	±0.8796
H(6,7)	0.0122	–1.0085	±0.8906
H(s,8)	3.1882	0.4246	0.0
H(a;9,10)	2.4245	–0.9236	±0.8882



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

<sup>b</sup>) The tilt angle of the CH<sub>3</sub> group defined by  $\delta = 2/3 [(X-C(1,4)-H(a)) - 2(X-C(1,4)-H(s))]$ ,  
X = O or C.

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