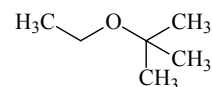
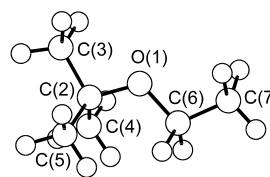


754  
MW**C<sub>6</sub>H<sub>14</sub>O*****t*-Butyl ethyl ether**  
2-Ethoxy-2-methylpropane**C<sub>s</sub>**

$r_0, r_s$	Å <sup>a)</sup>	$\theta_0, \theta_s$	deg <sup>a)</sup>
C(6)–O <sup>b)</sup>	1.423(4)	C–O–C	119.4(8)
C(6)–C(7) <sup>b)</sup>	1.512(3)	C(7)–C(6)–O <sup>b)</sup>	108.2(3)
C(2)–C(3)	1.495(6)	C(3)–C(2)–O	105.9(6)
C(2)–C(4,5)	1.565(6)	C(4,5)–C(2)–O	110.5(6)
C(2)–O	1.417(16)	C(3)–C(2)–C(4,5)	110.7(4)
		C(5)–C(2)–C(4)	108.4(6)
		$\delta(\text{tilt})$ <sup>c)</sup>	3.0(8)

Atom	$a_s$ [Å]	$b_s$ [Å]	$c_s$ [Å]
C(2)	−0.8632	<sup>d)</sup>	0.0
C(3)	−1.70843	1.2906	0.0
C(4,5)	−1.1662	−0.8050	±1.2596
O	0.4641	0.4978	0.0
C(6)	1.51605	−0.4719	0.0
C(7)	2.83208	0.2810	0.0



The structural analysis indicates that the lowest energy form of the molecule is the completely extended conformer with C<sub>s</sub> symmetry. The bulkiness of the *t*-butyl group causes the C–O–C angle to be 6° to 7° larger than that found in most other ethers.

<sup>a)</sup> Twice the estimated standard errors.

<sup>b)</sup>  $r_s$ .

<sup>c)</sup> Tilt angle is defined as  $(2/3)\{[C(4,5)–C(2)–O] – [C(3)–C(2)–O]\}$ .

<sup>d)</sup> Imaginary value.

Suenram, R.D., Lovas, F.J., Pereyra, W., Fraser, G.T., Walker, A.R.H.: J. Mol. Spectrosc. **181** (1997) 67.

[II/25D \(3, 2357\)](#)