

1820
ED

C₄H₁₀O

***t*-Butyl alcohol**
2-Methyl-2-propanol

C_s assumed
HO-C(CH₃)₃

r_g	Å ^{a)}	θ_α	deg ^{a)}
O-H	1.016(14)	C-O-H	108(3)
C-O	1.446(4)	C-C-C	110.9(2)
C-C	1.529(2)	H-C-H	108.5(5)
C-H	1.117(2)	δ ^{b)}	3.1(5)
		τ_3 ^{c)}	0 ^{d)}
		τ_4 ^{e)}	12(3)

The nozzle temperature was 21 °C.

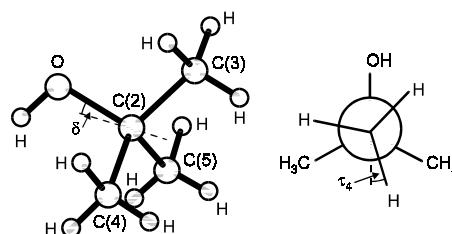
^{a)} 2.6 times the estimated standard errors including a systematic error.

^{b)} Tilt angle of the *t*-butyl group. See figure. This angle is positive when the symmetry axis of the *t*-butyl group tilts towards the alcoholic H atom.

^{c)} Dihedral angle C(3)-C(2)-O-H, $\tau_3 = 0^\circ$ when the O-H bond is *anti* to the C(2)-C(3) bond.

^{d)} Assumed.

^{e)} Torsional angle of the C(4)H₃ group, defined as zero when it takes a staggered conformation about the O-C bond. $\tau_5 = -\tau_4$.



Suwa, A., Ohta, H., Konaka, S.: J. Mol. Struct. **172** (1988) 275.