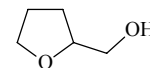


666 **C₅H₁₀O₂**ED, *ab initio*
calculations**Tetrahydro-2-furanmethanol**

Tetrahydrofurfuryl alcohol

C₁ (conformer A)**C₁** (conformer B)

r_g	Å ^{a)}	θ_a	deg ^{a)}
C(2)–O(1)	1.438(3)	C(5)–O(1)–C(2)	113.1(16)
C(2)–C(3)	1.537(4)	O(1)–C(2)–C(3)	102.9(6)
C(3)–C(4)	1.542 ^{b)}	C(2)–C(3)–C(4)	105.2(10)
C(4)–C(5)	1.539 ^{b)}	C(3)–C(4)–C(5)	100.7(16)
C(5)–O(1)	1.435 ^{b)}	C(4)–C(5)–O(1)	106.4(20)
C(2)–C(6)	1.532 ^{b)}	O(1)–C(2)–C(6)	105.5(14)
C(6)–O(7)	1.416 ^{b)}	C(3)–C(2)–C(6)	112.3(8)
O–H	0.925(12)	C(2)–C(6)–O(7)	112.9(10)
C–H (mean)	1.109(3)	C–O–H	104.8 ^{c)}
		H–C–H (mean)	108.7(16)
		O(1)–C(2)–C(3)–C(4)	330.2(20)
		C(2)–C(3)–C(4)–C(5)	34.0(18)
		C(3)–C(4)–C(5)–O(1)	334.0(34)
		C(4)–C(5)–O(1)–C(2)	8.3(44)
		C(5)–O(1)–C(2)–C(3)	13.4(36)
		O(1)–C(2)–C(6)–O(7)	307.8(22)
		C(2)–C(6)–O(7)–H	55.7 ^{c)}
		q_0 ^{d)}	9.8(3)
		f^e	85.5(64)

It was found that the molecule exists as a mixture of conformers A (84(8)%) and B (16(8)%). The most abundant conformer was found to be stabilized by hydrogen bonding. This conformer has the O–H group placed over the ring, which has a distorted $_4T^3$ conformation. The conformer B has the O–H group located outside the ring and directed towards the ring oxygen also participating in the hydrogen bond formation. Each CH₂ group was assumed to have local C_{2v} symmetry with one of the symmetry planes formed by the carbon of the CH₂ group and the two adjacent atoms, carbon or oxygen. Differences between parameters of the conformers were assumed at the values from MP2(fc)/6-311++G** calculations. The parameters are listed for conformer A. The barrier height to pseudorotation was estimated to be 2 kJ mol^{–1} by HF/6-311++G** calculations.

The nozzle temperature was 22 °C.

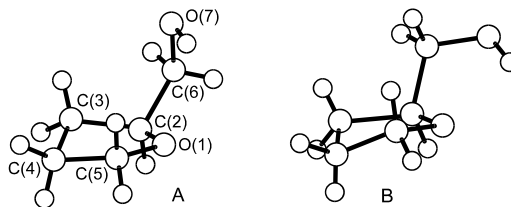
^{a)} Twice the estimated standard errors including a systematic error.

^{b)} Differences between the C–C bond lengths and between the C–O bond lengths were assumed at the values from MP2(fc)/6-311++G** calculations.

^{c)} Assumed at the *ab initio* value.

^{d)} Pseudorotation puckering amplitude.

^{e)} Pseudorotation phase angle.



Borisenko, K.B., Samdal, S., Shishkov, I.F., Vilkov, L.V.: J. Mol. Struct. **448** (1998) 29.