Microwave Spectrum, Conformation and Intramolecular Hydrogen Bonding of 2-Oxiraneethanol

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The microwave spectra of 2-oxiraneethanol and one deuterated species (hydroxyl group) have been investigated in the 26.0–39.0 GHz spectral region at about 0 °C. One conformer with a six-membered intramolecular hydrogen bond formed between the hydrogen atom of the hydroxyl group and the oxygen atom of the oxirane ring has been assigned. This rotamer is estimated to be at least 2 kJ mol^{-1} more stable than any other rotameric form of the molecule. Ab initio computations have been made for three selected conformations at the 6-31G* and MP2/6-31G* levels of theory.

Several alcohols with six-membered internal hydrogen (H) bonds have been investigated in the free state in recent years by microwave (MW) spectroscopy and electron diffraction (ED). Rather varied results have been obtained in these studies: In 3-aminopropanol[1] only one conformer with a O–H $\cdots$ N six-membered ring was identified in a MW study and presumed to be considerably more stable than further rotameric forms. The conformer with a O–H $\cdots$ O hydrogen bond was likewise found to be the most stable rotameric form of 3-methoxypropanol.[2] The one conformer identified for butane-1,3-diol[3] is also stabilized by a O–H $\cdots$ O hydrogen bond, but it is quite likely that other rotameric forms with the same kind of H bonds coexist in this case.[3] 3-Chloropropanol exists as a mixture of three conformers according to an ED investigation.[4] One of these, present to an extent of about 16%, contains an internal O–H $\cdots$ Cl hydrogen bond. The other two, more stable, conformers have no H bond.[4] The last-mentioned two conformers were later assigned in a MW study[5] which failed to find the H-bonded rotamer. Similarly, 3-fluoropropanol[6] also exists as a mixture of three conformers, two without and one with a six-membered H bond between the H atom of the hydroxyl group and the fluorine atom, as shown by MW spectroscopy. The H-bonded rotamer is not the most stable form of this compound.[6] Interestingly, HOCH$_2$CF$_2$CF$_2$H, which can have rotamers stabilized with six- or five-membered O–H $\cdots$ F internal H bond, prefers a conformer with a five-membered intramolecular H bond.[7]

4-Pentenol, 4-pentynol and 2-cyclopropaneethanol may in a way be said to be able to form intramolecular H bonds that are similar to the six-membered bonds in the aforementioned compounds. One conformer stabilized with O–H $\cdots$ πH bond was identified both in 4-pentenol[8]

and in 4-pentynol[9] by ED. The H-bonded rotamer seen for each of these[8,9] exists together with other forms which are not stabilized by internal H bonding. Very recently, 2-cyclopropaneethanol[10] was shown to possess a O–H $\cdots$ pseudo-π electron H-bonded conformer as its most stable form in a joint MW and ED investigation. Two further non H-bonded rotamers were found to coexist in this case with the more stable H-bonded rotamer.[10]

Several α-hydroxyoxirane derivatives have previously been studied by MW spectroscopy.[11] In these studies[11] it has been found that two different H-bonded conformers exist with a small energy difference. In one of these, the H atom of the hydroxyl group forms a H bond with the pseudo-π electrons along the edge of the ring, while in the second conformation the H atom of the hydroxyl group is bonded to the oxygen atom of the ring.

No studies of free β-hydroxy oxirane derivatives have been reported, and this was one motivation to carry out the present work. The title compound, which is the simplest β-hydroxy oxirane derivative and therefore the natural starting point, may possess three conformations which are stabilized by six-membered intramolecular H bonds, as shown in Fig. 1. Rotamers I and II have O–H $\cdots$ O hydrogen bonds, while the pseudo-π electrons along the C–C edge act as acceptor in III. I differs from II in that the H bond is formed from the side of the oxirane ring in I (the C1–C2–C3–C4 chain of atoms is near 120° from syn), whereas it is formed form above the oxirane ring in II (the C1–C2–C3–C4 chain of atoms is near 30° from syn). It is shown in this study that 2-oxiraneethanol prefers conformer I.

Experimental

The compound was synthesized as described by Brown and Lynch[12] with one minor difference: The reaction was
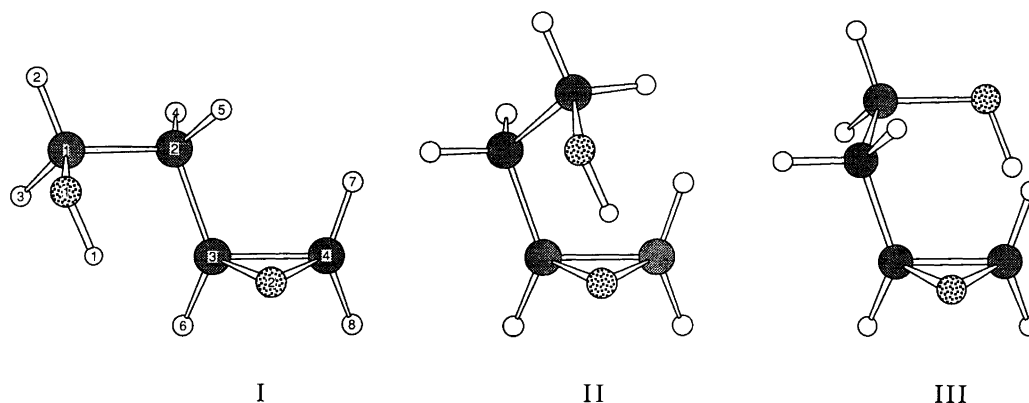

I   II   III

Fig. 1. Three conformations of 2-oxiraneethanol which possess intramolecular H bonds. I and II have a H bond to the oxygen atom of the oxirane ring, while III has a H bond to the pseudo-π electrons along the C3–C4 edge of the ring. Only I was found experimentally and is at least 2 kJ mol^{-1} more stable than II.

allowed to proceed for about 10 days. The compound was purified by preparative gas chromatography before use. The spectra were studied between 26.0 and 39.0 GHz at approximately 0°C using the Oslo spectrometer which is described in Ref. 13. Lower temperatures, which would have increased the MW spectral intensities, could not be employed owing to insufficient vapour pressure of the compound. The pressure was in the 2–6 Pa range during the spectral measurements. The accuracy is presumed to be better than ±0.10 MHz. Deuteration of the hydroxyl group was made by conditioning the wave guide with heavy water and then introducing the normal sample.

Results

Ab initio *calculations*. The calculations were made at the 6-31G* and MP2/6-31G* levels of theory using the Gaussian 90 program package[14] running on the Cray-Y-MP/464 computer in Trondheim. 2-Oxiraneethanol has three axes of internal rotation. Consequently, a large number of conformations is possible for this molecule. It has not been possible to make computations for all of them. Calculations were restricted to conformers I, II and III shown in Fig. 1. Rotamers I and II were selected because they are the two conformations that may form O–H ··· O internal H bonds. III was chosen because the most stable form of 2-cyclopropaneethanol was found to have a H bond involving the pseudo-π electrons of the ring.[10]

The geometries of the three conformations were fully optimized. They were found to be stable, as no imaginary vibrational frequencies were computed for any of them[15] using the 6-31G* basis set. (Calculation of vibrational frequencies has not been implemented at the MP2/6-31G* level.) The geometries and other parameters of interest obtained in the MP2/6-31G* computations are listed in Tables 1 and 2. All values in these two tables were only slightly different from those found with the 6-31G* calculations (not reported herein).

Microwave spectrum and assignment. Not unexpectedly, a rather weak MW spectrum was observed for this molecule in spite of the fact that rather large values are predicted (Table 2) for the principal-axes dipole moment components for each of the three forms. For example, the peak absorption coefficients of the high-J ^bQ-type ground-state transitions, which are the strongest lines observed in the spectrum, are roughly 1.5×10^{-7} cm^{-1}. The weakness is presumably caused mainly by a large value for the partition function at 0°C, as the intensities are inversely proportional to it.[16]

According to the ab initio results in Table 2, conformer I was predicted to be the most stable form of 2-oxiraneethanol, and a search for this rotamer was thus made first. I was predicted to have its largest dipole moment components along the a- and b-intertial axes (Table 2). The high-J b-type Q-branch transitions were thus predicted to be the strongest transitions in the spectrum. The approximate frequencies of these lines were predicted using the rotational constants shown in Table 2. These transitions were found after some searching. The rather weak high-K_{-1} ^aR-branch transitions were then found using a low Stark voltage which only modulated transitions with fast Stark effects. Low-$K_{-1}a$-type R-branch and low-J ^bR-branch lines were then immediately found. Attempts to find high-J ^bR- and ^aQ-branch transitions failed, presumably because they are too weak. No c-type transitions were identified, although the spectral positions of the strongest ones of them could presumably be predicted accurately. This is in accord with the fact that a small dipole moment component along the c-inertial axis is predicted in the ab initio computations (Table 2). Ultimately, a total of 70 transitions were measured.* A selected portion of the spectrum is shown in

Table 1. Structures[a] of conformations **I**, **II** and **III** of 2-oxiraneethanol obtained by MP2/6-31G* *ab initio* computations.

	Conformation		
	I	**II**	**III**
Bond lengths/pm			
O1–H1	97.5	97.6	97.1
C1–O1	142.0	142.0	142.6
C1–H2	109.3	109.3	109.2
C1–H3	110.2	110.1	110.0
C1–C2	152.7	152.5	152.3
C2–H4	109.7	109.8	109.7
C2–H5	109.5	109.5	109.4
C2–C3	150.5	150.9	150.3
C3–H6	109.1	109.1	109.3
C3–C4	146.4	146.5	146.9
C3–O2	145.3	145.2	143.8
C4–H7	108.7	108.6	108.8
C4–H8	108.7	108.7	108.8
Angles/°			
C1–O1–H1	106.3	105.1	107.1
O1–C1–H2	106.1	106.2	106.2
O1–C1–H3	111.4	111.6	105.5
O1–C1–C2	111.7	112.2	112.2
C1–C2–H4	110.6	110.3	109.8
C1–C2–H5	108.1	107.6	109.4
C1–C2–C3	111.3	114.4	111.9
C2–C3–H6	116.0	115.3	115.9
C2–C3–C4	122.6	123.6	121.5
C2–C3–O2	115.5	117.1	116.5
C3–C4–H7	119.0	120.3	119.0
C3–C4–H8	120.2	119.6	120.2
Dihedral angles/°			
H1–O1–C1–H2	191.5	−67.4	−58.2
H1–O1–C1–H3	74.9	176.6	−174.2
H1–O1–C1–C2	−48.2	57.4	65.8
O1–C1–C2–H4	193.8	53.2	56.5
O1–C1–C2–H5	−48.4	169.8	−174.5
O1–C1–C2–C3	72.8	−67.8	−64.0
C1–C2–C3–H6	76.9	166.4	−62.4
C1–C2–C3–C4	−126.0	−39.1	91.7
C1–C2–C3–O2	−57.5	30.8	160.4
C2–C3–C4–H7	−1.4	1.0	0.6
C2–C3–C4–H8	−155.1	−153.1	−152.9

[a]Atom numbering given in Fig. 1.

Table 2. Selected MP2/6-31G* parameters of conformations **I**, **II** and **III** of 2-oxiraneethanol.

	Conformation		
	I	**II**	**III**
Rotational constants/MHz			
A	7195.9	6241.2	7730.7
B	2569.2	2826.7	2265.0
C	2130.9	2386.2	1910.9
Dipole moment[a]/10^{-30} C m			
μ_a	8.35	7.80	2.30
μ_b	10.61	9.52	1.21
μ_c	0.43	5.30	5.57
Principal axis coordinates of the H1 atom[b]/pm			
$|a|$	87.6	84.8	125.5
$|b|$	138.7	135.8	143.6
$|c|$	7.8	38.9	40.2

Energy difference[c]/kJ mol^{-1}

$E_{II} - E_{I} = 2.1$ 　　　　　 $E_{III} - E_{I} = 9.6$

Hydrogen-bond parameters [b,d,e] **of conformer I**

H1···O2 202.8	O1···C3 261.6
O1···C4 306.1	O1···O2 285.6
∠O1–H1···O2 141.4	∠O1–H···C3 108.0
∠O1–H1,C3–O2[f] 57.7	

Sum of van der Waals radii[g]/pm

H···O 260	O···O 280	O···C[h] 310

[a]1 debye = $3.335\ 64 \times 10^{-30}$ C m. [b]Atom numbering given in Fig. 1. [c]The total energy of conformer I was computed to be $-802\ 808.40$ kJ mol^{-1}. [d]Distances in pm; angles in degrees. [e]Calculated from the structure of I given in Table 1. [f]Angle between O1–H1 and C2–C3 bonds. [g]Taken from Ref. 22. [h]van der Waals radii of carbon taken to be 170 pm as for the half-thickness of aromatic molecules.[22]

Table 3. The spectroscopic constants (*A*-reduction, *I*[r]-representation)[17] obtained by a least-squares fit are listed in Table 4.

Unfortunately, the dipole moment of this compound could not be determined because the low-*J* transitions were too weak.

One vibrationally excited state was assigned, as shown in Table 5. Relative intensity measurements made as described in Ref. 18 yielded 105(20) cm^{-1} for this normal mode. *Ab initio* computations with the 6-31G* basis set predict 84 cm^{-1} for the lowest torsional vibration. Attempts to assign additional excited state transitions

failed, presumably because of the weakness and rather crowded nature of the spectrum.

The *ab initio* computations predict a small energy difference of only 2.1 kJ mol^{-1} between I and II (Table 2). Conformation II is predicted to possess dipole moment components along the *a*- and *b*-inertial axes, which in both cases are close to those calculated for I (Table 2). Searches for this rotamer amongst the weak unassigned transitions were made next using the rotational constants of Table 2 for predicting the strongest transitions in this hypothetical spectrum. However, no assignments could be made for this conformation.

Conformation III is predicted to have a sizable μ_c, but is predicted to be 9.6 kJ mol^{-1} less stable than I (Table 2). Attempts to find this rotamer were also unsuccessful.

The spectrum of the deuterated species (hydroxyl group) of I was studied to locate with certainty the position of the H atom of the said group. The assignment of

Table 3. Selected transitions of the ground-state MW spectrum of conformer I of 2-oxiraneethanol.

Transition $J''_{K''-1,K''+1} \leftarrow J'_{K'-1,K'+1}$	Observed frequency[a]/MHz	Obs. − calc. freq./MHz
$7_{0,7} \leftarrow 6_{0,6}$	30 585.67	0.01
$7_{1,6} \leftarrow 6_{1,5}$	32 816.42	0.07
$7_{1,7} \leftarrow 6_{0,6}$	32 139.96	−0.03
$7_{3,4} \leftarrow 6_{3,3}$	32 021.26	−0.07
$8_{0,8} \leftarrow 7_{0,7}$	34 691.84	0.04
$8_{0,8} \leftarrow 7_{1,7}$	33 137.38	−0.10
$8_{2,6} \leftarrow 7_{2,5}$	37 579.77	−0.03
$8_{4,4} \leftarrow 7_{4,3}$	36 471.72	−0.05
$8_{4,5} \leftarrow 7_{4,4}$	36 462.35	0.05
$8_{7,1} \leftarrow 7_{7,0}$	36 371.92	0.00
$8_{7,2} \leftarrow 7_{7,1}$	36 371.92	0.00
$9_{0,9} \leftarrow 8_{1,8}$	37 668.57	−0.03
$9_{4,5} \leftarrow 9_{3,6}$	35 202.24	0.06
$11_{4,8} \leftarrow 11_{3,9}$	36 134.58	0.03
$13_{3,11} \leftarrow 13_{2,12}$	32 475.38	−0.07
$14_{3,12} \leftarrow 14_{2,13}$	34 213.18	−0.02
$14_{4,11} \leftarrow 14_{3,12}$	37 179.33	0.02
$16_{2,14} \leftarrow 16_{1,15}$	31 225.83	−0.04
$17_{4,13} \leftarrow 17_{3,14}$	26 747.79	−0.04
$18_{2,16} \leftarrow 18_{1,17}$	38 688.95	0.06
$18_{4,14} \leftarrow 18_{3,15}$	26 068.52	−0.13
$20_{3,17} \leftarrow 20_{2,18}$	32 710.70	−0.10
$20_{5,15} \leftarrow 20_{4,16}$	37 050.95	0.01
$22_{4,17} \leftarrow 22_{3,18}$	27 172.80	−0.02
$22_{5,17} \leftarrow 22_{4,18}$	33 893.14	0.00
$23_{5,18} \leftarrow 23_{4,19}$	32 735.22	0.00
$24_{5,19} \leftarrow 24_{4,20}$	32 041.40	−0.05
$26_{5,21} \leftarrow 26_{4,22}$	32 451.98	0.15
$28_{5,23} \leftarrow 28_{4,24}$	35 626.68	0.05
$29_{6,23} \leftarrow 29_{5,24}$	38 457.81	−0.02
$31_{6,25} \leftarrow 31_{5,26}$	37 866.06	−0.01
$32_{6,26} \leftarrow 32_{5,27}$	38 641.29	−0.02

[a] ± 0.10 MHz.

Table 4. Spectroscopic constants[a,b] of the ground vibrational state of the parent and the deuterated (hydroxyl group) species of conformer I of 2-oxiraneethanol.

Species:	Parent	Deuterated
No. of transitions:	70	41
R.m.s. dev.[c]/MHz:	0.058	0.049
A_0/MHz	7427.3508(76)	7224.580(17)
B_0/MHz	2475.1509(44)	2470.2876(80)
C_0/MHz	2061.4669(44)	2043.7109(80)
Δ_J/kHz	1.279(35)	1.409(69)
Δ_{JK}/kHz	−5.401(25)	−4.909(67)
Δ_K/kHz	14.73(39)	11.94(82)
δ_J/kHz	0.25551(76)	0.2635(18)
δ_K/kHz	0.994(32)	0.884(78)

[a] A-reduction I^r-representation.[17] [b] Uncertainties represent one standard deviation. [c] Root-mean-square deviation.

of them belong to further conformations, in particular rotamer II, remains. The fact that all the strongest transitions of the spectrum were assigned to rotamer I, together with the *ab initio* prediction that μ_a and μ_b of each of rotamers I and II should be roughly the same (Table 2), is a strong indication that I is indeed the most stable form of the molecule. Moreover, the strongest unassigned lines have less than 50% of the intensity of the strongest assigned ones. This allows us to estimate conservatively that I is a least 2 kJ mol^{-1} more stable than the hypothetical conformation II, a finding that is in agreement with the *ab initio* result (Table 2).

Structure. A full structure of 2-oxiraneethanol cannot be obtained from only the two isotopomers studied in this work. Assumptions have to be made to derive a *plausible* structure from which deductions can be made. The high-level MP2/6-31G* structure (Table 1) is suggested as a plausible structure for conformer I for the following reasons: It can be seen from Table 2 that the structure of I yields rotational constants that are 3–4% away from the experimental values (Table 4). The principal-axis coordinates of H1 are in fair agreement with experiment, as mentioned above. Moreover, comparison of the com-

Table 5. Spectroscopic contants[a,b] of the first excited torsional state of the parent species of conformer I of 2-oxiraneethanol.

No. of transitions:	32
R.m.s. dev.[c]/MHz	0.083
A_v/MHz	7413.079(19)
B_v/MHz	2474.810(16)
C_v/MHz	2064.151(16)
Δ_J/kHz	1.60(12)
Δ_{JK}/kHz	−5.957(77)
Δ_K/kHz	16.4(11)
δ_J/kHz	0.2714(19)
δ_K/kHz	0.897(84)

[a-c] Comments as for Table 4.

this spectrum was rather straightforward. The resulting spectroscopic constants obtained from 41 transitions are listed in Table 4. Kraitchman's substitution coordinates[19] for H1 were then calculated as $|a| = 55.53(6)$ pm, $|b| = 135.21(3)$ pm and $|c| = 30.92(11)$ pm. The large *b*-coordinate is close to the value obtained in the computations (Table 2), while a larger discrepancy exists for the *a*- and *c*-coordinates. Interestingly, a similar difference was found for the *a*-coordinate of 3-methoxypropanol,[2] which has a structure that resembles that of rotamer I of the title compound. It has been pointed out[20] that substitution coordinates are often quite unreliable for H atoms in cases where large-amplitude motions are involved, as is indeed the case for conformer I.

The conformational composition. The assignments reported above for the ground and one vibrationally excited state of I include all the strongest transitions, and many weak ones too. However, many relatively intense transitions remain unaccounted for. Many of these lines undoubtedly belong to vibrationally excited states of I which could not be assigned. The possibility that some

puted structural parameters (Table 1) of conformations I–III with accurate experimental structures of similar molecules[21] reveals no large differences.

Discussion

There can be no doubt that internal H bonding is a major reason why 2-oxiraneethanol prefers conformer I. The reason why rotamer I is preferred to II is much more difficult to say, but it is possible that repulsion between non-bonded atoms is more prevalent in the latter conformation. I and II are thought to be more stable than III because the oxygen atom is a better H bond acceptor than are the pseudo π-electrons along the C3–C4 bond.

Most bond angles and distances of conformer I shown in Table 1 take rather normal values. However, the dihedral angles reveal the influence of H bonding: The H1–O1–C1–C2 dihedral angle is about 12° smaller than the normal dihedral angle of 60° from syn. This brings the H atom of the hydroxyl group into closer proximity with the oxygen atom, thereby strengthening the H bond. Similar swings of about 10° have been seen in the other compounds possessing six-membered H bonds.[1–3,5,6] The large C1–C2–C3–C4 dihedral angle (76.9°), the small C1–C2–C3–C4 and C1–C2–C3–O2 dihedral angles of −126.0 and −57.5°, respectively, also help to bring the H of the hydroxyl group into close contact with the oxygen atom of the ring.

Another unusual dihedral angle is the O1–C1–C1–C3 angle, which is about 73° from syn, 13° larger than 'normal'. Similar observations have been made for 3-methoxypropanol[2] [75(4)°], butane-1,3-diol[3] [77.0°], 3-aminopropanol[1] [76.6°] and in the H-bonded conformer of 3-fluoropropanol[6] [77(2)°]. The widening of this dihedral angle is suggested to be caused by repulsive effects that arise when the compact six-membered internal H bond is formed. The fact that I is the most stable conformation of 2-oxiraneethanol indicates that its internal H bond is so strong that it more than compensates for the strain the somewhat unusual dihedral angles may cause.

Moreover, the H bond of conformer I is characterized by having the O2···H1 non-bonded distance about 60 pm shorter than the sum of the van der Waals radii[22] of hydrogen and oxygen (Table 2). The O1–H1···O2 angle is about 141°, while approximately 180° would have produced an ideal H-bond interaction. These two parameters are close to their counterparts in 3-methoxypropanol,[2] which has a H bond that is actually quite similar to that of conformation I.

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