AN INVESTIGATION OF INTRAMOLECULAR HYDROGEN BONDS AND THE SPATIAL CONFORMATIONS OF THE STEREOISOMERIC α-OXOALCOHOLS OF THE CYCLOHEXANE, PIPERIDINE, AND DECAHYDROQUINOLINE SERIES

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The influence of the conformation of the geometric isomers of 1-acetyl-4-tert-butylcyclohexan-1-ol and of 4-acetyl-1, 2-dimethyldecahydroquinoline on the nature of the intramolecular hydrogen bonds has been studied by IR spectroscopy, and on the basis of the results obtained the configurations and conformations of the geometric isomers of the 4-acyl-1, 2, 5-trimethylpiperidin-4-ols have been established.

Conformational stability of the stereoisomers of ketols of the piperidine series has been found.

It has been shown that the geometric isomers of each of the compounds studied with axially orientated acyl groups exist in solutions in the form of an equilibrium mixture of two rotameric forms. The enthalpy of an intramolecular hydrogen bond in these compounds is 0.5–0.7 kcal/mole.

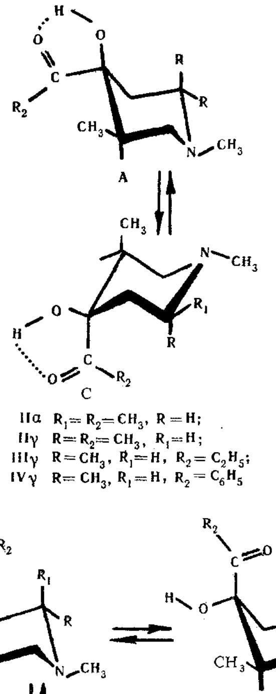
In recently-published papers, the spatial configurations of the cis and trans isomers of 1-acetyl-2-methylcyclohexan-1-ol [1], their piperidine analogs—the cis and trans isomers of 4-acetyl-1, 3-dimethylpiperidin-4-ol [2]—and the three geometric isomers of 4-acetyl-1, 2, 5-trimethylpiperidin-4-ol [3] have been investigated by spectroscopic methods.

In the present work, using methods of IR spectroscopy, we have studied the spatial conformations of 4-acetyl-1-methylpiperidin-4-ol (I) [2], the geometric isomers of 4-acetyl-1, 2, 5-trimethyl-, 4-propionyl-1, 2, 5-trimethyl-, and 4-benzoyl-1, 2, 5-trimethylpiperidin-4-ols (IIα, β, γ, IIIβ, γ, and IVβ, γ, respectively [3, 4]), and of the three geometric isomers of 4-acetyl-4-hydroxy-1, 2-dimethyldecahydroquinoline (Vα, VIα, β [5]), which were obtained by the hydration of the corresponding acetylenic alcohols [5–7].

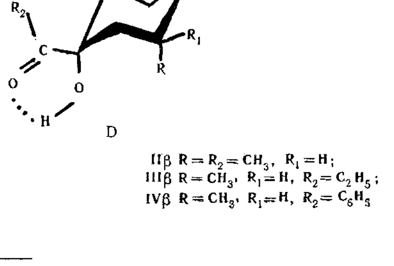
As model compounds we studied the structurally related 1-acetylcyclohexan-1-ol (VII) [8] and the cis and trans isomers of 1-acetyl-4-tert-butylcyclohexan-1-ol (VIIIα, β) and of 1-acetyl-2-methylcyclohexan-1-ol (IXα, β) [1].

The spectral method of determining the spatial orientation of the hydroxyl group in a number of cis- and trans-alkylcyclohexanols proposed previously [9–11], which is based on a consideration of the frequencies of the stretching vibrations of the C—O bonds, proved to be inapplicable to the analysis of the spectra of the compounds that we have studied. The presence of a large number of absorption bands in the frequency range from 900 to 1100 cm^{-1} together with the comparatively weak influence of the polarity of the solvent on the shift of the frequency of the $\nu_{\mathrm{C-O}}$ vibrations does not permit reliable assignments to be made in this region of the spectrum. In addition to this, taking into account the capacity of the keto alcohols studied for forming intramolecular hydrogen bonds, the nature of which must substantially depend on the conformation of the molecule, we considered it desirable to make a more detailed study of the spectral characteristics of the hydrogen bonds in compounds I, IIα, β, γ, IIIβ, γ, and IVβ, γ.

The presence in the molecules of the ketols IIα, β, γ, IIIβ, γ, and IVβ, γ of geminal carbonyl and hydroxyl groups gives the possibility of the formation of an intramolecular hydrogen bond for both the cis and the trans isomers* (the conformers **B**, **D**, and **A**, **C**, in Scheme 1).



IIα $R_1 = R_2 = CH_3$, $R = H$;
IIγ $R = R_2 = CH_3$, $R_1 = H$;
IIIγ $R = CH_3$, $R_1 = H$, $R_2 = C_2H_5$;
IVγ $R = CH_3$, $R_1 = H$, $R_2 = C_6H_5$



IIβ $R = R_2 = CH_3$, $R_1 = H$;
IIIβ $R = CH_3$, $R_1 = H$, $R_2 = C_2H_5$;
IVβ $R = CH_3$, $R_1 = H$, $R_2 = C_6H_5$

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*The specification of the cis and trans configurations is understood with respect to the mutual position of the acyl and methyl groups at the C_5 atom of the piperidine ring.

Table 1

Bands of Stretching Vibrations of the Carbonyl and Hydroxyl Groups of Stereoisomeric α-Oxoalcohols

Compound	Name	Frequency of the vibrations, cm^{-1}		
		$\nu_{C=O}$	ν_{OH} free	ν_{OH} bound
I	4-Acetyl-1-methylpiperidin-4-ol	1713	—	3485
IIγ	2e4e5e-4-Acetyl-1,2,5-trimethylpiperidin-4-ol*	1712	—	3485
IIα	2a4e5e- (or 2e4e5a)-4-Acetyl-1,2,5-trimethylpiperidin-4-ol	1707	—	3485
IIIγ	2e4e5e-4-Propionyl-1,2,5-trimethylpiperidin-4-ol	1708	—	3480
IVγ	2e4e5e-4-Benzoyl-1,2,5-trimethylpiperidin-4-ol	1669	—	3465
IIβ	2e4a5e-4-Acetyl-1,2,5-trimethylpiperidin-4-ol	1705–1720	3614	3478
IIIβ	2e4a5e-4-Propionyl-1,2,5-trimethylpiperidin-4-ol	1702–1718	3612	3474
IVβ	2e4a5e-4-Benzoyl-1,2,5-trimethylpiperidin-4-ol	1687	3608	—
Vα	trans-2a4e-4-Acetyl-4-hydroxy-1,2-dimethyldecahydroquinoline**	1709	—	3472
VIα	trans-2e4e-4-Acetyl-4-hydroxy-1,2-dimethyldecahydroquinoline	1711	—	3480
VIβ	trans-2e4a-4-Acetyl-4-hydroxy-1,2-dimethyldecahydroquinoline	1705–1717	3612	3474
VII	1-Acetylcyclohexan-1-ol	1712	—	3485
VIIIα	1e4e-1-Acetyl-4-tert-butylcyclohexan-1-ol	1710	—	3489
IXα	1e2e-1-Acetyl-2-methylcyclohexan-1-ol	1708	—	3480
VIIIβ	1a4e-1-Acetyl-4-tert-butylcyclohexan-1-ol	1704–1721	3615	3490
IXβ	1a2e-1-Acetyl-2-methylcyclohexan-1-ol	1704–1718	3612	3480

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*Here and everywhere below, the spatial arrangement of the methyl and acyl (benzoyl) groups is indicated.

**The trans linkage of the cyclohexane and piperidine rings is symbolized.

Table 2

ΔH for an Intramolecular Hydrogen Bond

Compound	Name	$\left(\frac{A_{free}}{A_{bound}}\right)$ 23°	$\left(\frac{A_{free}}{A_{bound}}\right)$ 68°	ΔH, kcal/mole
IXβ	1a2e-1-Acetyl-2-methylcyclohexan-1-ol	0.64	0.72	0.53
VIβ	trans-2e4a-4-Acetyl-1,2-dimethyldecahydroquinoline	0.50	0.56	0.51
IIβ	2e4a5e-4-Acetyl-1,2,5-trimethylpiperidine-4-ol	0.70	0.79	0.55
IIIβ	2e4a5e-4-Propionyl-1,2,5-trimethylpiperidin-4-ol	0.33	0.38	0.64

However, simple ideas based on a consideration of molecular models permit the conclusion that in the case of the conformers **B** and **C** with the axial acyl groups, the formation of intramolecular hydrogen bonds is energetically less favorable, because of steric hindrance and the mutual repulsion of the R_2 radical and the axial meta hydrogen atoms of the piperidine ring in **B** (the axial methyl group in **C**), which approach to a distance considerably less than the sum of the Van der Waals radii. In the case where $R_2 = C_6H_5$, the decrease in the steric effect destabilizing the hydrogen bond must lead to a disturbance of the coplanarity of the carbonyl group at the phenyl ring and to a loss of resonance energy connected with it. Since in the conformers **D** the steric hindrance mentioned is absent, the conversion transition **B** → **D** must correspond to a stabilization of the intramolecular hydrogen bond. Consequently, geometric isomers with the cis arrangement of the acyl and the C_5-methyl group may in principle be regarded as conformationally mobile compounds. Conversely, the corresponding trans isomers must have conformation **A** preferentially, which corresponds not only to greater thermodynamic stability of the ring but also to the formation of more stable intramolecular hydrogen bonds preventing the conversion transition **A** → **C**.

On the basis of these considerations it could have been expected that the conformational differences in the spectra of the geometric isomers studied should be shown most distinctly in the region of the stretching vibrations of the hydroxyl and carbonyl groups responsible for the formation of the hydrogen bonds.

The spectral measurements that we have performed (Table 1) have in fact enabled these differences to be clearly observed. Thus, in the spectra of solutions of the compounds **I** and **VII** and the geometric isomers **II**α, γ, **III**γ, and **IV**γ, measured at a concentration of $5 \cdot 10^{-3}$ mole/l—which excludes the possibility of the formation of intermolecular hydrogen bonds*—in the region of the stretching vibrations of the hydroxyl groups only one band of a bound hydroxyl at 3465–3485 cm^{-1} and a symmetrical carbonyl band in the 1669–1713 cm^{-1} region are observed. For the spectra of compounds **II**β and **III**β under the same conditions of measurement, the existence of a split band of the stretching vibrations of the carbonyl group with two maxima in the 1702–1720 cm^{-1} and of two bands due to the stretching vibrations of both bound (3474–3478 cm^{-1}) and free (3612–3614 cm^{-1}) hydroxyl groups is characteristic.

The considerations expounded above give every reason for establishing the predominance of the conformation with the equatorial acyl (benzoyl) group in compounds **I**, **VII**, **II**α, γ, **III**γ, and **IV**γ, which give spectra of the first type, and ascribing **II**γ, **III**γ, and **IV**γ to the geometric isomers of the trans series.* In their turn, compounds **II**β and **III**β, which give spectra of the second type, should be assigned to the geometric isomers of the cis series.

The spectral data obtained unambiguously show the conformational similarity of the model compounds **I** and **VII** and the isomers **II**α, γ, **III**γ, and **IV**γ (the **A** conformation) and the absence from their solutions of **A** $\rightleftarrows$ **C** conversion transitions.

The interpretation of the spectra of the cis isomers **II**β and **III**β is far less clear. The simultaneous presence in them of bands of the stretching vibrations of free and bound hydroxyl groups, and also the splitting of the carbonyl band can be explained not only by the possibility of the **B** $\rightleftarrows$ **D** conversion transition and the incomplete inclusion of the functional groups of the conformer **B** in an intramolecular hydrogen bond because of steric hindrance, but also by the existence of the rotational isomerism **B** $\rightleftarrows$ **E** due to the internal rotation of the axial acyl groups of the conformers **B** round the C—C axis. In this case, the formation of the sterically unhindered and more favorable rotamer **E** requires the complete rupture of the hydrogen bond in the conformer **B**.

A consideration of the spectrum of the geometric isomer **IV**β shows that, at least in this compound, the ring conversion **B** $\rightleftarrows$ **D** is excluded. In actual fact, the presence of the conformational equilibrium **B** $\rightleftarrows$ **D** should necessarily lead to the appearance in the spectrum of compound **IV**β of absorption bands of the stretching vibrations of bound hydroxyl (3465 cm^{-1}) and carbonyl (1669 cm^{-1}) groups of the conformer **D**, analogous to the bands observed in the spectrum of conformer **A** and its epimer **IV**α. Actually, in the spectrum of the geometric isomer **IV**β absorption in the region of the stretching vibrations of bound hydroxyl groups is completely absent, and a single band of a free hydroxyl (3608 cm^{-1}) is observed, while the carbonyl band with a frequency of 1687 cm^{-1}, which is typical for aromatic ketones, has an outline close to that of a dispersion band. These results show the complete absence from compound **IV**β of the hydrogen bonds of the conformers **B** and **D** and indicate the existence of **IV**β in the unitary conformation **E** with a coplanar benzoyl group.

The stability of the rotamer **E** of compound **IV**β with an axially oriented voluminous benzoyl grouping excluding the possibility of its stabilization through the formation of an intramolecular hydrogen bond appears somewhat unexpected. In view of this, we have studied the spectral characteristics of the geometric isomers of the conformationally stable oxoalcohols of the decahydroquinoline series **V**α and **VI**α, β, having a rigid trans linkage of the cyclohexane and piperidine rings which definitely exclude the possibility of the conversion of the rings. In addition to the bicyclic ketols **V**α and **VI**α, β, we also used the cis and trans

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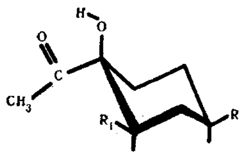
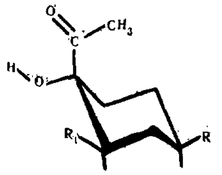
*The measurements of the spectra of the solutions showed that, at least beginning from a concentration of $1 \cdot 10^{-2}$ mole/l, there are no changes in the frequencies and relative intensities of the bands of the OH vibrations with the dilution of the solutions.

*The mutual arrangement of the acetyl and C_5 methyl groups in the geometric isomer **II**α having the cis arrangement of the C_2- and C_5-methyl groups cannot be established in the same way.

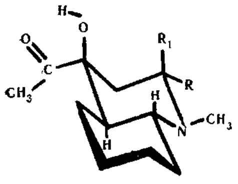
isomers of 1-acetyl-4-tert-butylcyclohexan-1-ol VIIIα, β* (Scheme 2), as models with a fixed conformation excluding conversion transitions of types A ⇄ C and B ⇄ D.



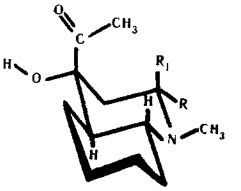
VII $R=R_1=H$;
VIIIα $R=t\text{-}C_4H_9$, $R_1=H$;
IXα $R=H$, $R_1=CH_3$



VIIIβ $R=t\text{-}C_4H_9$, $R_1=H$
IXβ $R=H$, R_1 CH_3



Vα $R=H$, $R_1=CH_3$;
VIα $R=CH_3$, $R_1=H$



VIβ $R=CH_3$, $R_1=H$

As can be seen from the results of the measurements (Table 1), in the spectra of the geometric isomers Vα, VIα, β and VIIIα, β only the same differences are observed as in the spectra of the piperidine ketols IIα, β, γ, IIIβ, γ, and IVβ, γ. As in the case of compounds IIα, γ, IIIγ, and IVγ, an unsplit carbonyl band in the 1709–1711 cm^{-1} region and a single band in the region of the stretching vibrations of bound hydroxyl groups (3472–3489 cm^{-1}) are present only for the trans isomer VIIIα and the geometric isomers of the bicyclic ketols Vα and VIα with equatorially oriented acetyl groups. In their turn, bands of free (3615 cm^{-1}) and bound (3474–3490 cm^{-1}) OH groups were observed exclusively for the cis isomer VIIIβ and the bicyclic ketol VIβ having, like compounds IIβ and IIIβ, an axially oriented acetyl group. Thus, the spectra of the model compound confirmed the conclusion that the characteristic spectral differences of the geometric isomers in all the cases considered are due not to the conversion transitions B ⇄ D but to the rotational isomerism B ⇄ E. We have observed just the same picture in the spectra of the cis and trans isomers of 1-acetyl-2-methylcyclohexan-1-ol (IXβ and IXα) (Table 1), the structures of which were considered previously [1]. The differences in the hydroxyl region of the Raman spectra of the isomers IXα, β were explained in this paper by the acid-base properties of the equatorial and axial hydroxyl groups and the more pronounced tendency to the formation of a hydrogen bond in IXβ. At the same time, the existence of conversion transitions of the type A ⇄ C and B ⇄ D was predicated [1] in solutions of both IXα and IXβ. Actually, as has now become obvious, these differences are connected with the fact that in solutions of the cis isomer IXβ there is a rotational isomerism of the type B ⇄ E which is absent in the case of IXα, existing exclusively in conformation A.

The relative stability of the rotameric forms B and E of the compounds investigated can be characterized by the value of the enthalpy of the intramolecular hydrogen bond in the isomers IIβ, IIIβ, VIβ, VIIIβ, and IXβ. With this aim, we measured the integral intensities of the ν_{OH} bands of the stretching vibrations of the free and bound hydroxyl groups in the spectra of some compounds of this type at temperatures of 23 and 68° C (Table 2). The measurements were carried out at concentrations of the solutions of $2\text{–}5 \cdot 10^{-3}$ mole/l, corresponding to the existence of only the equilibrium mixture of the two rotational isomers B and E. To a first approximation* it may be considered that the intensities of the absorption bands under consideration are, respectively, proportional to the molar fractions of these isomers (N_1 and N_2) and the ratio of the intensities determines the constant of the equilibrium B ⇄ E at the given temperature, i.e.,

$$\left(\frac{A_{OH_{free}}}{A_{OH_{bound}}}\right)_T \approx \left(\frac{N_1}{N_2}\right) = K_T.$$

The enthalpy of the hydrogen bond was evaluated from the equation [12]

$$\ln\frac{K_{T_2}}{K_{T_1}} = \frac{\Delta H}{R}\left(\frac{1}{T_1} - \frac{1}{T_2}\right).$$

As can be seen from the figure of Table 2, the magnitude of the enthalpy of the intramolecular hydrogen bond in the isomers IIβ, IIIβ, VIβ, and IXβ can be evaluated as 0.5–0.7 kcal/mole.

The values of ΔH found to the same approximation for the compounds IIβ, IIIβ, and IXβ and the model compound VIβ with a fixed conformation that have been studied proved to be extremely close.

The results obtained enable the existence of IVβ in only one rotameric form, E, to be explained. The stabilization of the rotameric form B through the formation of an intramolecular hydrogen bond with an energy of the order of 0.5–1.0 kcal/mole in this compound does not compensate the energy of the repulsion of the voluminous phenyl group by the axial meta hydrogen atoms and the loss of delocalization energy connected with a disturbance of the coplanarity of the benzene grouping which is unavoidable in this case. The calculation that we have carried out by the MO method in Hückel's approximation has shown that the rotation of the carbonyl group relative to the plane of the phenyl

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*Since, as a rule, the formation of an intramolecular hydrogen bond affects the magnitude of the integral intensity of the bands of the ν_{OH} vibrations, the ratio $A_{OH,free}/A_{OH,bound}$ is not, strictly speaking, proportional to the ratio of the molar fractions N_1/N_2. Because the change in the position of the equilibrium observed in the range of temperatures studied is small, this contribution can be neglected.

ring by 90° leads to a loss of delocalization energy by 0.36β, which corresponds to 6.5 kcal/mole, exceeding the energy of the intramolecular hydrogen bond of conformer **B** by approximately one order of magnitude. In view of this, in the case of the cis-ketol IVβ the rotameric equilibrium $\mathbf{B} \rightleftarrows \mathbf{E}$ is shifted completely in the direction of the rotamer **E**.

EXPERIMENTAL

The spectra of the compounds investigated were measured on a "Zeiss" UR-10 double-beam spectrometer with KBr (400–700 cm^{-1}), NaCl (700–2000 cm^{-1}), and LiF (2000–4000 cm^{-1}) optics in solutions in CCl_4 at concentrations of 0.005–0.001 mole/l with absorbing layer thicknesses of 0.4–0.04 cm.

The integral intensities of the bands of the stretching vibrations of the free and bound hydroxyl groups were measured at temperatures of 23 and 68° C using solutions with concentrations of 0.002–0.005 mole/l and absorbing layer thicknesses of 2.00 ± 0.02 cm. The measurements were carried out in hermetically sealed thermostatted cells and were repeated for 4–5 samples of each compound. The rate of scanning did not exceed 32 cm^{-1}/min. The spectral slit width was 8.3 cm^{-1} in the 1700 cm^{-1} region, 4.5 cm^{-1} in the 3470–3490 cm^{-1} region, and 5.7 cm^{-1} in the 3605–3615 cm^{-1} region. The linearity of the photometric scale of the instrument was checked by a published method [13]. The integral optical densities were calculated by the numerical integration of the observed distribution function $D_\nu = \ln(I_0/I)_\nu = f(\nu)$, corresponding to the experimental shape of the band cut off by the base line.

4-Acetyl-1-methylpiperidin-4-ol (I): v.w. 487, w. 565, w. 625, w. 960, w. 970, v.w. 980, s. 1060, w. 1080, s. 1115, s. 1160, s. 1190, s. 1298, v.s. 1370, s. 1387, w. 1440, w. 1455, w. 1475, v.s. 1713, v.w. 2680, s. 2700, s. 2745, s. 2768, v.s. 2805, v.s. 2925, v.s. 2945, v.w. 3400, s.sym. 3485.

2e4e5e-4-Acetyl-1, 2, 5-trimethylpiperidin-4-ol (IIγ): w. 512, w. 570, w. 607, w. 643, v.w. 675, w. 910, w. 932, w. 960, v.w. 1010, s. 1053, s. 1088, s. 1105, w. 1125, v.s. 1165, w. 1290, w. 1312, v.s. 1365, v.s. 1390, w. 1430, s. 1455, s. 1470, v.s.sym. 1712, v.w. 2620, v.w. 2660, s. 2770, v.s. 2798, v.s. 2845, s. 2880, v.s. 2920, v.s. 2940, v.s. 2965, v.w. 3090, v.s. 3400, s.sym. 3485, v.w. 3730.

2a4e5e- (or 2e4e5a-) -4-Acetyl-1, 2, 5-trimethylpiperidin-4-ol (IIα): w. 425, w. 450, w. 483, w. 510, w. 537, w. 589, v.w. 610, s. 655, w. 675, w. 912, w. 940, s. 1050, w. 1088, s. 1112, s. 1122, v.s. 1160, w. 1198, s. 1310, v.s. 1380, s. 1435, s. 1455, s. 1475, v.s.sym. 1707, w. 2770, s. 2805, s. 2835, s. 2880, v.s. 2935, v.s. 2965, w. 3000, v.w. 3400, s.sym. 3485, v.w. 3730.

2e4e5e-4-Propionyl-1, 2, 5-trimethylpiperidin-4-ol (IIIγ): s. 430, w. 515, w. 560, w. 660, w. 920, s. 955, s. 1060, s. 1100, v.s. 1145, v.s. 1168, v.s. 1312, v.s. 1350, v.s. 1390, s. 1430, v.s. 1460, v.s. 1472, v.s.sym. 1708, v.w. 2615, v.w. 2655, v.w. 2700, v.w. 2725, s. 2770, v.s. 2795, v.s. 2800, s. 2820, v.s. 2845, v.s. 2880, v.s. 2915, v.s. 2940, v.s. 2970, v.s. 2990, s.sym. 3480, v.w. 3680.

2e4e5e-4-Benzoyl-1, 2, 5-trimethylpiperidin-4-ol (IVγ): w. 410, w. 435, w. 508, v.w. 594, s. 667, w. 900, w. 913, s. 944, w. 960, s. 1051, w. 1088, s. 1100, s. 1137, v.s. 1165, v.s. 1175, w. 1295, w. 1320, s. 1355, v.s. 1389, w. 1436, s. 1459, s. 1472, v.s.sym. 1669, v.w. 2613, v.w. 2730, w. 2770, s. 2790, s. 2800, s. 2820, s. 2844, s. 2880, s. 2935, v.s. 2970, v.s. 2980, v.w. 3029, w. 3070, w. 3095, s.sym. 3465.

2e4a5e-4-Acetyl-1, 2, 5-trimethylpiperidin-4-ol (IIβ): w. 520, w. 560, w. 587, w. 625, v.w. 660, v.w. 675, w. 907, w. 922, w. 940, w. 950, w. 960, s. 1060, s. 1090, s. 1130, s. 1150, s. 1180, w. 1290, w. 1310, s. 1360, s. 1385, s. 1428, s. 1450, s. 1470, s. 1705, v.s. 1720, s. 2770, s. 2795, s. 2845, s. 2880, s. 2915, s. 2937, s. 2970, v.w. 3420, w.sym. 3478, w.sym. 3614, v.w. 3720.

2e4a5e-4-Propionyl-1, 2, 5-trimethylpiperidin-4-ol (IIIβ): w. 420, w. 510, w. 530, w. 610, w. 620, w. 640, w. 988, s. 918, w. 945, w. 960, s. 1052, s. 1093, s. 1125, s. 1165, w. 1195, w. 1293, v.s. 1368, s. 1420, s. 1440, s. 1468, v.s. 1702, v.s. 1718, w. 2770, s. 2790, s. 2845, s. 2880, v.s. 2940, v.s. 2970, s. 3070, w. 3425, s.sym. 3474, s.sym. 3612.

2e4a5e-4-Benzoyl-1, 2, 5-trimethylpiperidin-4-ol (IVβ): w. 420, w. 500, w. 510, w. 555, v.w. 590, s. 635, w. 912, s. 940, w. 960, s. 1050, w. 1065, w. 1088, w. 1100, s. 1132, v.s. 1150, v.s. 1168, v.s. 1190, w. 1290, s. 1345, v.s. 1458, w. 1468, v.s.sym. 1687, w. 2770, s. 2800, v.s. 2845, s. 2882, s. 2910, s. 2938, v.s. 2970, w. 3070, s.sym. 3608.

2a4e-4-Acetyl-4-hydroxy-1, 2-dimethyldecahydroquinoline (Vα): w. 431, v.w. 505, v.w. 526, w. 548, w. 600, w. 670, v.w. 910, v.w. 960, v.w. 1010, w. 1038, s. 1060, s. 1096, s. 1129, s. 1138, s. 1160, s. 1174, s. 1310, s. 1367, s. 1384, s. 1432, s. 1458, s.sym. 1709, w. 2670, s.w. 2770, v.s. 2799, v.s. 2860, s. 2877, v.s. 2924, v.s. 2938, w. 3000, v.s.sym. 3472.

2e4e-4-Acetyl-4-hydroxy-1, 2-dimethyldecahydroquinoline (VIα): s. 417, w. 552, s. 625, w. 920, w. 960, w. 990, w. 1040, s. 1097, s. 1130, v.s. 1162, s. 1190, w. 1290, w. 1310, s. 1344, v.s. 1369, w. 1430, s. 1459, w. 1490, s.sym. 1711, s. 2790, v.s. 2860, v.s. 2940, s. 2967, s. 2995, s.sym. 3480.

2e4a-4-Acetyl-4-hydroxy-1, 2-dimethyldecahydroquinoline (VIβ): w. 416, w. 520, w. 530, w. 540, w. 570, w. 617, v.w. 630, w. 645, w. 910, w. 932, w. 954, w. 1048, w. 1068, s. 1090, w. 1116, s. 1150, s. 1187, w. 1304, v.w. 1320, w. 1340, s. 1360, s. 1378, w. 1428, s. 1460, s.asym. 1705, 1717, v.w. 2690, v.s. 2857, v.s. 2935, s. 2970, w. 2990, v.s. 3474, v.s. 3612, v.w. 3675.

trans-1e4e-1-Acetyl-4-tert-butylcyclohexan-1-ol (VIIIα): w. 564, s. 486, w. 545, w. 614, w. 632, s. 850, s. 870, w. 935, w. 1016, s. 1050, s. 1136, s. 1192, s. 1270, w. 1323, w. 1340, v.s. 1373, s. 1392, s. 1400, w. 1439, s. 1454, w. 1480, v.s.sym. 1710, s. 2847, v.s. 2870, v.s. 2960, s.sym. 3489.

cis-1e4a-1-Acetyl-4-tert-butylcyclohexan-1-ol (VIIIβ): s. 490, w. 540. v.w. 579, v.w. 634, v.w. 637, w. 670, s. 845, w. 923, w. 935, w. 1015, s. 1060, s. 1085, s. 1123, w. 1145, s. 1179, w. 1269, w. 1275, w. 1300, w. 1328, s. 1361, s. 1376, s. 1402, w. 1428, w. 1442, s. 1460, w. 1476, w. 1489, v.s. 1704, v.s. 1721, s. 2846, s. 2870, v.s. 2912, v.s. 2960, v.w. 3420, w. 3490, s. 3609, s. 3638, v.w. 3720.

1-Acetylcyclohexan-1-ol (VII): v.w. 517, w. 608, v.w. 897, v.w. 918, w. 970, s. 1048, s. 1160, v.w. 1190, w. 1285, w. 1332, w. 1360, w. 1370, w. 1390, w. 1476, s.sym. 1712, s. 2855, s. 2865, v.s. 2938, w. 3000, w. 3030, v.w. 3400, s.sym. 3485.

trans-1e2e-1-Acetyl-2-methylcyclohexan-1-ol (IXα): v.w. 460, w. 475, w. 510, w. 603, v.w. 630, v.w. 635, w. 650, w. 928, v.w. 1050, w. 1095, s. 1160, v.w. 1192, w. 1310, w. 1330, v.s. 1368, s. 1388, s. 1455, v.s.sym. 1708, s. 2860, v.s. 2930, v.w. 3390, s. 3480.

cis-1a2e-1-Acetyl-2-methylcyclohexan-1-ol (IXβ): v.w. 490, w. 555, w. 595, w. 650, w. 920, w. 938, w. 1000, v.w. 1040, s. 1050, s. 1095, s. 1130, s. 1150, s. 1180, s. 1195, w. 1240, w. 1315, s. 1360, s. 1390, s. 1420, s. 1455, s. 1470, s. 1704, v.s. asym. 1718, s. 2860, v.s. 2945, s.sym. 3480, s.sym. 3612.

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