

Conformational composition of 1-butanol in matrix isolation

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IR absorption spectra of 1-butanol isolated in an argon matrix were obtained at temperatures from 10 to 50 K. The conformational behavior of 1-butanol was analyzed using the results of quantum-chemical simulation of the structure and vibrational spectra of its small clusters. We studied the conformational composition of 1-butanol in matrix isolation and showed the transformation of its structure that occurs with an increase in the matrix temperature.

Keywords: butanol, conformer, matrix isolation, infrared absorption.

1. Introduction

Alcohol molecules can exist in various conformational forms. This is due to the possibility of rotation of atoms around chemical bonds. Alcohols are characterized by three types of isomerism of dihedral angles: trans ($\approx 180^\circ$), gauche ($\approx 60^\circ$), and gauche' ($\approx -60^\circ$) conformations. The total number of possible structures can be calculated using the formula 3^N , where N is the number of structural dihedral angles in a molecule. For alcohols, these angles are CCCC, CCCO, and CCOH. As a result, an alcohol such as 1-butanol ($\text{CH}_3\text{-(CH}_2\text{)}_3\text{-OH}$) can have 27 conformers. Taking into account the properties of enantiomers (structures that are mirror images of each other), the actual number of different 1-butanol conformers is 14.

The conformational properties of alcohols and, in particular, 1-butanol have been thoroughly studied both in the gas phase and in matrix isolation, as well as by computer simulation methods [1–8]. However, these studies did not take into account the possibility of the formation of hydrogen-bonded clusters as combinations of different conformers. Considering the processes of cluster formation in normal butanol, the authors of [9–13] did not take into account the existence of different conformational forms of a butanol molecule.

The aim of this work is to study the influence of the conformational properties of 1-butanol on the processes of cluster formation, to determine the conformational composition and cluster structure of 1-butanol isolated in a low-temperature argon matrix.

2. Experimental and calculation details

To prepare the samples, we used liquid 1-butanol manufactured by Fluka with a purification degree $> 99.9\%$. Additional purification of liquid alcohol from water molecules was carried out by holding on a molecular sieve (3 Å) for 48 hours. Immediately before the preparation of the gas mixture for the deposition of the matrix, the alcohol was degassed by repeating the cycle of alternate freezing, pumping, and thawing of the sample on a standard vacuum setup. Samples for matrix isolation were prepared by mixing of 1-butanol vapor with argon (Elme Messer, purity > 99.995) under vacuum. 1-butanol vapors were obtained by natural evaporation from the surface of a liquid sample. The ratio of alcohol molecules to argon atoms, determined using a standard manometer, was 1:1000. The gas mixture was deposited onto a substrate (CsI) cooled to 10 K, which was in a closed-cycle helium cryostat (Laybold-Hareus RW2). The gas flow in the cryostat was controlled using a needle valve. The spraying rate was about 4 moles of the gas mixture per hour, which ensures the formation of a partially crystallized argon matrix. Infrared absorption spectra were recorded using a Bruker IFS 113 FTIR spectrometer. Spectral data were obtained in the range from 500 to 4000 cm^{-1} with a resolution of 0.5 cm^{-1} . To increase the signal-to-noise ratio, each spectrum was recorded as an average of 128 interferograms. The spectra were recorded at different temperatures from 10 to 50 K with a step of 5 K. At each temperature, the sample was annealed for 5 minutes.

Quantum-chemical calculations were carried out using Gaussian 09 software package [14] and ROCBS-QB3 (restricted-open-shell complete basis set-quadratic Becke3 model) complex method at B3LYP/CBSB7 level of theory. This limited open-shell method is based on the CBS-QB3 method [15] with a limited in spin wave function for direct calculations and extrapolation of the correlation energy to the CBS limit. A detailed description of it is given in [16]. This method allows one to calculate the accurate energy values and is successfully used for the conformational analysis of aliphatic monohydric alcohols [8, 17]. To eliminate restrictions on the symmetry of molecules, the *NoSymm* parameter was used in the calculations. In addition, within the framework of the standard methods of the Gaussian 09 program, strict convergence criteria and an exact numerical integration grid (*Opt = Tight*, *SCF = Conver = 9*, and *Int = Ultrafine*) were used. To take into account the argon environment when simulating the behavior of molecules in matrix isolation, we used the self-consistent interaction field (SCRf) method specified as a continuous polarized medium (PCM). GaussView software was used to visualize the data and calculation results [18].

IR absorption spectra within the framework of the ROCBS-QB3 method were calculated at the level of the B3LYP/CBSB7 theory in the harmonic approximation. Besides, anharmonic IR spectra were calculated for all structures using the B3LYP/6-311G(2d, d, p) method.

3. Results and discussion

3.1. IR absorption spectra of 1-butanol in matrix isolation

Figure 1 shows the registered IR absorption spectrum of 1-butanol isolated in an argon matrix at a temperature of 10 K. Several groups of bands can be distinguished in the spectrum. In the low-frequency part of the spectrum, there are the bands of the bending vibrations of OH, CH₃, and CH₂ groups. Since the 1-butanol molecule contains one CH₃

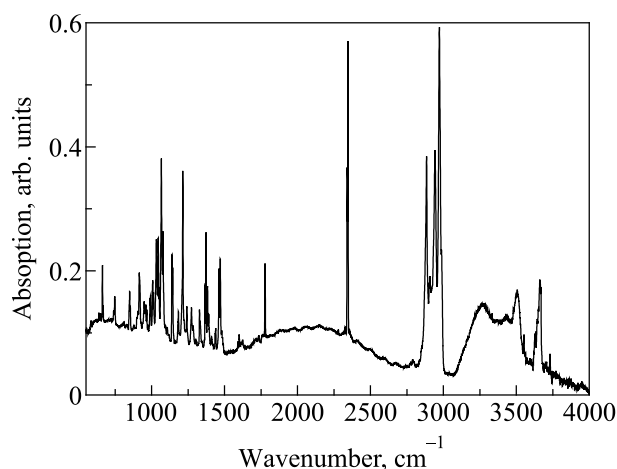


Fig. 1. Registered IR absorption spectrum of 1-butanol isolated in an argon matrix at 10 K.

and three CH₂ groups, the total number of IR absorption bands in this region is quite large, and their detailed assignment is very difficult, especially taking into account the conformational properties of the molecule under consideration. For the same reason, the region of the stretching vibrations of CH₃ and CH₂ groups (2800–3000 cm⁻¹) is not very informative. The most convenient spectral range for studying clustering processes is the region of the stretching vibrations of the hydroxyl group (3100–3800 cm⁻¹). There is only one hydroxyl group in a 1-butanol molecule, and the frequency of its stretching vibrations depends on the presence and strength of the hydrogen bond between the molecules [12, 13]. Thus, the position of the band of O–H stretching vibrations in alcohols can be used to determine the cluster structure of the sample under study, as well as its conformational composition [17]. Therefore, further in this article, we will consider only the spectral region 3100–3800 cm⁻¹ and the spectral changes that occur in this region when the temperature increases.

Figure 2 shows a part of the IR absorption spectrum of 1-butanol isolated in an argon matrix at a temperature of 10 K in the spectral region of the stretching vibrations of the hydroxyl group. As seen from Fig. 2, the spectrum in this region contains a structured band with peaks at about 3660 and 3630 cm⁻¹, as well as a broad band with maxima at 3265, 3360, 3425, and 3505 cm⁻¹. In addition, narrow bands are visible at 3550 and 3730 cm⁻¹.

Using the information known from earlier studies on IR absorption spectra of monohydric alcohols in matrix isolation [12, 13, 19–22], the 3660 cm⁻¹ band can be attributed to the vibrations of the 1-butanol monomer. The 3630 cm⁻¹ band corresponds to the vibrations of the proton acceptor molecule in the dimer, and the 3505 cm⁻¹ band corresponds to the vibrations of the proton donor molecule in the dimer. Similarly, the bands at 3425, 3360, and 3256 cm⁻¹ are assigned, respectively, to trimers, tetramers, and pentamers of 1-butanol [23, 24]. The bands at 3550 and 3730 cm⁻¹

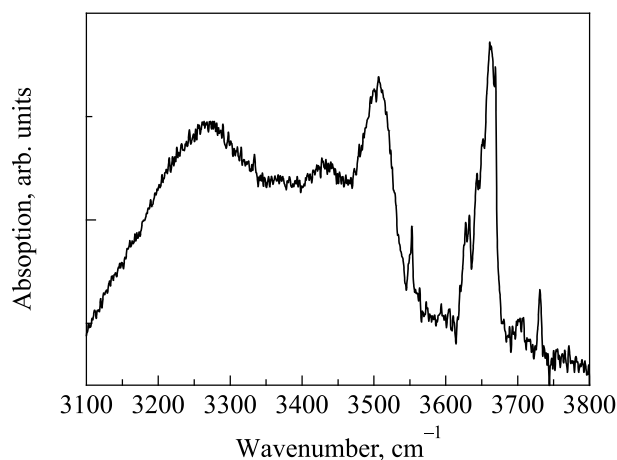


Fig. 2. IR absorption spectrum of 1-butanol in an argon matrix at 10 K in the spectral range of 3100–3800 cm⁻¹.

can be associated with the presence of water in the sample because of its incomplete purification. In this case, the 3730 cm^{-1} band corresponds to the stretching O–H vibrations of free water molecules, and the 3550 cm^{-1} band corresponds to the vibrations of those molecules that are involved in the formation of hydrogen bonds, in particular, in mixed dimers of water and 1-butanol, similar to how it was observed during the isolation of 1-propanol in an argon matrix [23].

It should be noted that already at a temperature of 10 K there are relatively large clusters — trimers, tetramers, and pentamers — in the sample. This fact is surprising, since in the experiments on the isolation of other linear alcohols in an argon matrix, the molecular sizes of which are close to the size of a 1-butanol molecule, under the same conditions (a concentration ratio of 1:1000 and a matrix deposition temperature of 10 K), mainly monomers and dimers were observed. Moreover, it was so not only for longer molecules, such as 1-hexanol [12, 19, 22], but also for 1-propanol, a molecule of which is shorter than that of 1-butanol [12]. The formation of 1-propanol clusters, consisting of three or more molecules, in an argon matrix at a temperature of 12–15 K was observed in [23], but in this case the alcohol concentration in the sample was two times higher. Apparently, such a difference in the cluster composition of similar samples can be explained by the fact that clusters of alcohol molecules are formed in the gas phase, and only after that the formed clusters, together with the argon flow, are deposited on the substrate, forming a matrix. Thus, the cluster composition of the obtained sample depends not so much on the conditions of matrix deposition as on the initial composition of the sprayed mixture [17].

When the sample is heated, noticeable changes occur in the registered IR absorption spectra in the spectral range of $3100\text{--}3800\text{ cm}^{-1}$. Figure 3 shows the temperature evolution of IR absorption spectra of 1-butanol in an argon matrix in the temperature range from 10 to 50 K. It can be seen that

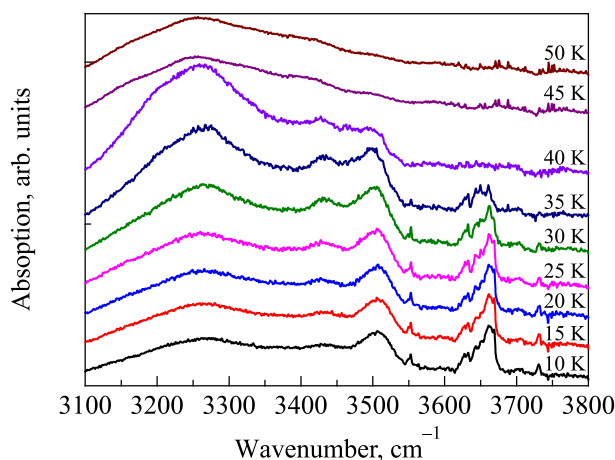


Fig. 3. Temperature evolution of IR absorption spectra of 1-butanol in an argon matrix at temperatures from 10 to 50 K in the spectral range of $3100\text{--}3800\text{ cm}^{-1}$.

with an increase in temperature, the absorption in the range $3600\text{--}3700\text{ cm}^{-1}$ decreases, while the intensity of the bands in the range $3200\text{--}3300\text{ cm}^{-1}$ increases. The absorption intensity at frequencies of $3350\text{--}3550\text{ cm}^{-1}$ first increases and then decreases. This dependence of the spectral bands let us suggest that, at the lowest temperature (10 K), the sample under study contains both 1-butanol monomers and clusters consisting of different numbers of molecules. As the temperature rises, the matrix softens, resulting in the possibility of combining individual molecules into clusters. This combining occurs gradually. First, there are a decrease in the number of monomers in the sample and a parallel increase in the number of dimers and trimers. With a further increase in temperature, dimers and trimers are combined into larger clusters, which is reflected in an increase in absorption intensity at frequencies corresponding to clusters of four, five, and more molecules. At temperatures of 45–50 K, the absorption bands of monomers are completely absent in the spectra, and at frequencies corresponding to dimers, absorption is very weak. Instead, a broad structured band with several maxima is observed, which can be attributed to the O–H vibrations in hydrogen-bonded trimers, tetramers, pentamers, and larger clusters.

3.2. Quantum-chemical simulation of 1-butanol conformers

For a more detailed assignment of the registered bands in the IR absorption spectra of 1-butanol, quantum-chemical simulation of its conformational properties was carried out. Using the ROCBS-QB3 method at the level of B3LYP/CBSB7 theory, the optimal geometries of 27 possible 1-butanol conformers were calculated. This approach has already been successfully applied to simulate the conformational behavior of 1-hexanol molecules in matrix isolation [17].

Each conformer was denoted with a symbolic code using the conventional dihedral scheme CCCC+CCCO+CCOH with capital+capital+lowercase letters for trans (T, t), gauche (G, g), and gauche' (G', g') conformers [5, 7, 8, 10]. Table 1 shows the calculated values of the relative energies ΔH of all possible conformers of 1-butanol, as well as their comparison with the results of calculations by ROCBS-QB3 method performed by the Katsikadakis group [8] and by CBS-QB3 method performed by the Moc group [7]. Since the calculations in the both works did not take into account the effect of the solvent, the difference in the values of the relative energies is quite noticeable; however, this does not affect the order of the configurations in the list according to their stability.

An interesting fact is the arrangement of the conformations of 1-butanol by groups, which are visually highlighted in Table 1. As can be seen, the stability of the conformation, according to the results of quantum-chemical simulation, is determined mainly by the dihedral angles CCCC and CCCO in alcohol molecules. Moreover, in each

Table 1. Relative energies ΔH (at 298.15 K) of 1-butanol conformers, calculated by ROCBS-QB3 (under the influence of argon environment), ROCBS-QB3 (in a vacuum) [8], and CBS-QB3 (in a vacuum) [7] methods

Conformer	ΔH , kJ/mol			
	ROCBS-QB3			CBS-QB3, in vacuum [7] ²
	in argon		in vacuum [8]	
	enantiomer ¹			
TGt	0.02	0.00	0.00	0.00
TGg	0.86	0.82	1.04	1.00
TGg'	0.90	0.87	1.21	1.13
TTt	1.00		1.27	1.21
TTg	1.14	1.18	1.57	1.51
GGt	2.03	2.07	1.95	1.72
GGg	2.72	2.64	2.82	2.59
GGg'	3.43	3.33	3.62	3.35
GTt	3.94	3.91	4.22	4.06
GTg'	4.03	3.99	4.40	4.27
GTg	4.56	4.57	4.96	4.77
GG't	6.60	6.61	6.34	6.23
GG'g'	6.94	6.91	6.84	6.74
GG'g	8.46	8.49	8.70	8.70

¹ The values of the relative energies of the corresponding enantiomers are given (obtained by replacing all gauche angles with gauche' angles and vice versa);

² Original article [7] contains values in kcal/mol which have been converted to kJ/mol to make comparison easier.

of the selected groups, the most stable conformation is the structure with the trans-angle CCOH. These most stable structures from each group are shown in Fig. 4.

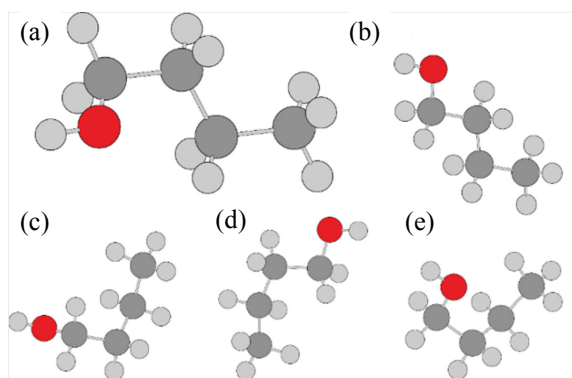


Fig. 4. Conformers of 1-butanol in an argon matrix, arranged in the order of decreasing of their stability according to two dihedral angles — CCCC and CCCO: (a) TG*; (b) TT*; (c) GG*; (d) GT*; (e) GG'*.

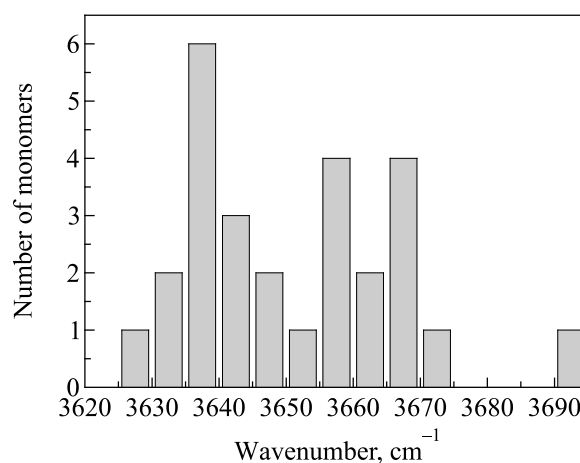


Fig. 5. The number of the 1-butanol conformers with a certain frequency of the stretching O–H vibrations in the range of 3620–3695 cm^{-1} .

Using the obtained structures and energies of conformers, for each of the 27 structures of the 1-butanol molecule, IR absorption spectra were calculated in the anharmonic approximation. Figure 5 shows the statistical distribution of the obtained vibrational frequencies in the spectral region of the stretching vibrations of the hydroxyl group. As can be seen, different conformations of 1-butanol are characterized by an IR absorption spectrum in the region of 3625–3675 cm^{-1} , and only one of the structures has an absorption band at a frequency of 3692 cm^{-1} .

At the same level of theory (B3LYP/CBSB7 by ROCBS-QB3 method), the energies of equilibrium transition structures between pairs of conformers were calculated. The obtained values can be considered as heights of energetic barriers between different conformers. The total number of possible pairs of conformers is 675, and the energies of transition structures were calculated for most of them. Their values vary from 0.315 kJ/mol to almost 24 kJ/mol depending on the number of angles and distances changing during the transition. It is known that the energy barriers lower than 5–8 kJ/mol enable conformer interconversion in inert-gas matrices [25]. According to the results of our calculations, near 30% of energy barriers appeared to be lower than 8 kJ/mol. Therefore, because of interconversions between 1-butanol conformers separated by low-energy barriers in the process of matrix deposition, the conformational composition of the sample may be essentially simpler. Moreover, some of the obtained values of the transition structures turned out to be negative, such as for the transformation of GTg' conformers into TTt, or GG't into TTg, G'Gg' into TGg, and some others. It means that they cannot exist in their initial configuration and transform into others. Comparing these unstable conformers with the results from Table 1, one can notice a good correlation — all of them are in the bottom of the “stability list” of 1-butanol conformers.

3.3. Conformational behavior of 1-butanol dimers

Besides individual 1-butanol molecules, the calculations were carried out for all possible dimeric structures of this alcohol. Since each of the two molecules can be in 27 different configurations, there are 729 possible combinations. Only one of them has no chiral properties (TTt–TTt), and all the rest are pairs of enantiomers. As shown by the example of chiral pairs of monomers, their energy characteristics differ little; although they are not the same at the considered level of theory (see Table 1). Therefore, only 365 dimers will be taken into account below. It is not very informative to give the calculated energies of all these dimers. The dependence of the stability of various structures formed by two molecules can be presented in the form of a statistical distribution. This distribution is shown in Fig. 6. The most stable structures have a relative energy close to zero, the least stable — near 19 kJ/mol. As can be seen, 1-butanol has 22 stable dimers with relative energies up to 2 kJ/mol. The most stable structure is TGt–TGg'. Both conformations that make up this dimer are, individually, one of the most likely conformers in this alcohol, according to the data in Table 1.

In addition, 18 out of the 22 mentioned stable dimers contain at least one 1-butanol conformation, which is among the top three most stable conformers. Moreover, seven of them contain two of these molecules, that is, we can talk about some dependence of the stability of the dimer structure on the monomer stability.

Another criterion for the stability of 1-butanol dimers can be the value of the hydrogen bond energy, which determines the time of cluster dissociation into two separate molecules. Figure 7 shows the statistical distribution of the hydrogen bond energy values in the dimers. This energy was calculated as the difference between the energy of the dimer and the energies of the two individual monomers.

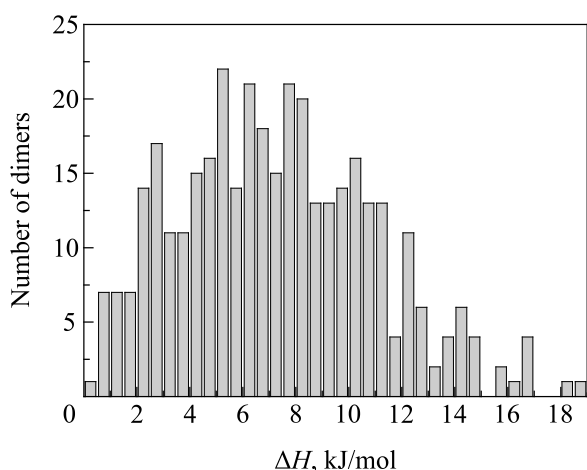


Fig. 6. Distribution of 1-butanol dimers according to the values of their relative energy ΔH .

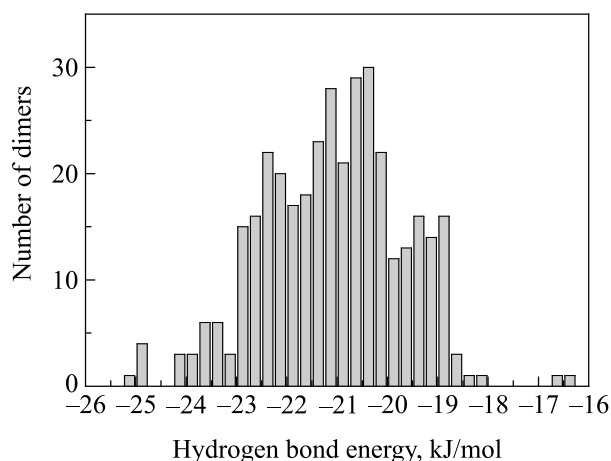


Fig. 7. Distribution of 1-butanol dimers over hydrogen bond energy values.

If we consider the relative energy values, the three most stable dimers have hydrogen bond energies of 22.46 kJ/mol (TGt–TGg'), 21.92 kJ/mol (TGt–TGg), and 21.86 kJ/mol (TGt–TG'g). At the same time, the dimer with the highest binding energy (GGg–G'G'g, 25.18 kJ/mol) is characterized by a relative energy $\Delta H = 2.41$ kJ/mol. The dimer with the lowest binding energy (GG't–TGt, 16.35 kJ/mol) has a relative energy $\Delta H = 11.81$ kJ/mol, which confirms its instability relative to other dimers under equal conditions. In general, we can say that most of the possible 1-butanol dimers have hydrogen bonds with energies from 19 to 24 kJ/mol (4.54–5.74 kcal/mol), which differs from the results obtained for dimers of other alcohols using lower levels of theory [9, 19, 20, 26].

For all 365 dimers, the IR absorption spectra were calculated in the anharmonic approximation. Figure 8 shows the statistical distribution of vibrational frequencies of the stretching O–H vibrations in these clusters [27]. As can be

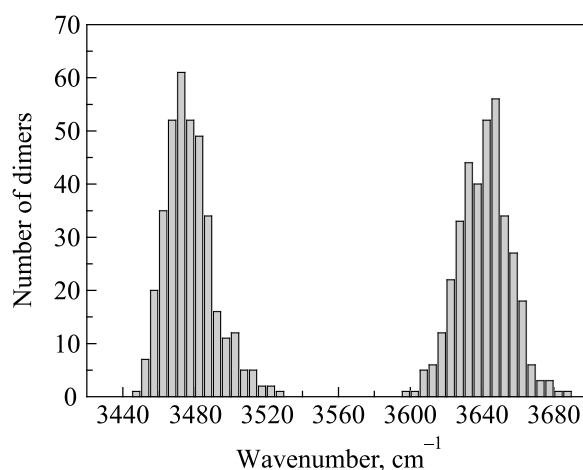


Fig. 8. The statistical distribution of O–H stretching frequencies of 1-butanol dimers.

seen, this dependence has a nonzero value in the spectral regions 3450–3530 and 3600–3690 cm^{-1} . The first of the two regions corresponds to the vibrations of a molecule that is a proton donor in a dimer, and the second one — to the vibrations of an acceptor molecule. It is noticeable that the second region coincides with the region of the corresponding vibrations of 1-butanol monomers. Thus, due to the presence of dimers in the structure of the sample, it is extremely difficult to analyze the vibrational bands of monomers in its spectra.

3.4. Analysis of the cluster composition of 1-butanol

At the same level of theory, the structures and IR absorption spectra of the chain (45 out of 19,683 possible) and cyclic (25 out of 19,683 possible) trimers were calculated. Figure 9 shows a comparison of the experimentally registered spectrum of 1-butanol in matrix isolation with the statistical distributions of the stretching vibration frequencies of different 1-butanol clusters. As can be seen, the vibrational bands of free O–H groups of dimers in the range of 3600–3700 cm^{-1} completely overlap with the vibrations of 1-butanol monomers. Besides, longer chain clusters, which contain a terminal free hydroxyl group, can also make a significant contribution to this band. The vibrations of the molecules that are donors of protons in dimers are located in the range of 3450–3525 cm^{-1} . These frequency values correlate well with the intense absorption band observed in the experimentally registered spectra at 3450–3550 cm^{-1} , which was attributed to the vibrations of 1-butanol dimers. The low-frequency side of the spectrum up to 3370 cm^{-1} contains vibrations of cyclic trimers, as well as larger clusters, for which quantum-chemical calculations were not performed yet due to their high cost. The spectral range from 3300 to 3445 cm^{-1} contains vibrations of chain trimers.

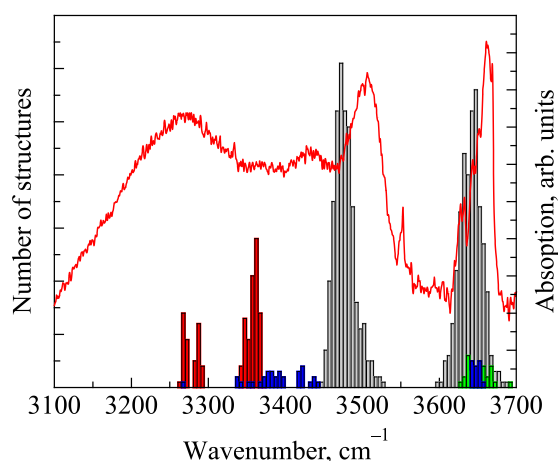


Fig. 9. (Color online) Comparison of the experimentally registered IR absorption spectrum of 1-butanol in matrix isolation at 10 K (red curve) in the range of 3100–3700 cm^{-1} with the statistical distributions of the frequencies of the stretching O–H vibrations in different 1-butanol clusters: monomers (green bars), dimers (black), chain trimers (blue), cyclic trimers (red).

4. Conclusion

The use of the ROCBS-QB3 complex method made it possible to simulate the conformational properties of 1-butanol in matrix isolation. It turned out that among all the rotational isomers of 1-butanol in an argon matrix, the most stable are those in which the CCOH angle is in the trans-conformation.

It is also shown that the cluster composition of 1-butanol in a low-temperature matrix depends on which clusters were formed in a gas mixture before its cooling and matrix deposition. As shown above, the experimentally registered IR absorption spectrum of 1-butanol isolated in an argon matrix at a temperature of 10 K can be interpreted taking into account only 4 possible cluster structures: monomers, dimers, and two types of trimers — chain and cyclic. The calculated vibrational spectra of these cluster structures almost completely overlap the experimental spectrum in the region of the stretching O–H vibrations of 1-butanol. From the behavior of the corresponding spectral bands when the matrix is heated, the conclusions about the changes in the relative amount of these structures in the sample can be drawn.

An analysis of the temperature evolution of the IR absorption spectra of 1-butanol in matrix isolation shows that heating of the sample under study to 30 K increases the proportion of clusters consisting of three or more molecules. Simultaneously the number of monomers and dimers decreases. Heating to higher temperatures is accompanied by a further increase in the number of large clusters and a decrease in the number of small ones. At 40 K, no monomers and dimers remain in the sample at all.

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Конформаційний склад 1-бутанолу в матричній ізоляції

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Зареєстровано спектри ІЧ поглинання 1-бутанолу, ізольованого в аргонній матриці при температурах від 10 до 50 К. Методами квантово-хімічного моделювання проаналізовано конформаційну поведінку 1-бутанолу, розраховано структуру та коливальні спектри його невеликих кластерів. Досліджено конформаційний склад 1-бутанолу в матричній ізоляції, показано трансформацію його структури при підвищенні температури матриці.

Ключові слова: бутанол, конформер, матрична ізоляція, інфрачервоне поглинання.