INFLUENCE OF FLUOROSUBSTITUTION ON THE HEAT CAPACITY OF ALIPHATIC ALCOHOLS

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In this paper, the principle of corresponding states was applied in a comparative analysis of the temperature dependencies of the isobaric heat capacities of aliphatic alcohols and their fluorosubstituted analogues. For the heat capacity, both experimental data from the literature and simulated data, obtained using artificial neural networks, were applied. The isobaric heat capacity for aliphatic alcohols in absolute values over a wide temperature range at constant pressure is smaller than that for the corresponding fluorosubstituted analogues. The comparison of the heat capacity data on the aliphatic alcohols and their fluorosubstituted analogues with the heat capacity of water, for which there is a hydrogen bond network, and comparison of the corresponding data with the heat capacity of hydrogen peroxide, where there are hydrogen bonds, but the network is absent, indicates that the change in the physical properties of alcohols upon fluorosubstitution is associated with the hydrogen bond density.

Keywords: *Aliphatic alcohols; Fluorosubstituted alcohols; Water; Hydrogen peroxide; Heat capacity; Principle of corresponding states*
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INTRODUCTION

The study of the thermodynamic properties of fluorosubstituted monohydric aliphatic alcohols in comparison with their unsubstituted analogues is one of the essential problems of the up-to-date physics of liquids and liquid systems. The comparison of the thermodynamic properties of liquids within one homologous series and the substitution series, obtained by substituting hydrogen atoms with fluorine atoms in their molecules, enables the analysis of the characteristics of the mechanisms of molecular processes that occur in fluorosubstituted liquids. Such research is now relatively scarce and sometimes contradictory.

At the same time, the fluorosubstituted alcohols are currently widely used in pharmacology and organic synthesis as specific solvents and cosolvents, components of high-temperature heat carriers, lubricants, and adhesives, in the manufacture of pesticides and polymeric materials [1]. Fluorosubstituted alcohols continue to master new scopes of application, in particular, they are used in biotechnology for peptides stabilization [2], enzymes biomodification [3], change of the protein macromolecules structure [4], modification of the lipid membranes properties [5], as well as for modulation of the nicotinic acetylcholine receptors function [6], the mechanosensitive channel of small conductance, KcsA channels and potassium channels Kv1.3 [7,8], etc. However, despite the widespread use of fluorosubstituted alcohols in various industries, their thermodynamic properties remain poorly studied.

Thermodynamic coefficients of individual liquids allow analyzing the intermolecular bond energy, to relate the microscopic and macroscopic parameters of the system state with the changes in the molecular structure of the liquid. The analysis of literature sources has shown that the low-molecular representatives of homologous series (such as 2,2,2-trifluoroethanol and 1,1,1,3,3,3-hexafluoropropan-2-ol), which have found wide use in the chemical industry and biochemical engineering as specific solvents, can be considered as the best studied fluorosubstituted alcohols. As an example, in [9] the quantum-chemical calculations at the Gaussian M-062x/6-31+g (d,p) level were applied to determine the standard enthalpy, entropy, and heat capacity for various fluorosubstituted alcohols, emphasizing the importance of vibrational and rotational contributions to the specified properties. In [10] the authors provided new experimental data on the surface tension for 1H,1H-perfluoroalcohols of $CF_3(CF_2)_nCH_2OH$ (n=0-5) type, supplemented by molecular dynamics simulation to determine the phase equilibria and bulk properties, including the enthalpy of vaporization.

Papers [11-13] are devoted to the helical conformation of fluorosubstituted hydrocarbon chains, what can be explained by the fact that the fluorocarbon chains, due to steric repulsion of fluorine atoms, acquire a stable helical shape, but not the usual linear zigzag conformation of aliphatic alcohols. The manifestation of the steric effect is a change in the bond length and the valence angle between the carbon skeleton and halogen, thus causing tension in the

intramolecular structure and its change: the zigzag structure of the aliphatic alcohol molecule turns into a helical arrangement of fluorine atoms in the fluorosubstituted alcohol molecule. The steric hindrance of the substituent atom can affect the formation of hydrogen bonds and significantly reduce the acidic properties of alcohols. The reason for this is the negative inductive effect (–I-effect) inherent in the strong electron-withdrawing fluorine substituent [13].

The transition from aliphatic alcohols to their fluorosubstituted analogues must affect the nature of intermolecular hydrogen bonds [14]. In [11], the quantum-chemical calculations, based on the semiempirical molecular orbital theory Parametric Method 3 (PM3), were applied to study the structural and thermodynamic properties of the formation of monomers (n=1-14, 34), dimers (n=1-14, 34), trimers and tetramers (n=1-8) of fluorosubstituted alcohols of the type $C_nF_{2n+1}CH_2CH_2OH$ at the air-water interface. From the analysis of the enthalpy, entropy, and Gibbs energy of the clusterization, it was concluded that the dimerization of fluorosubstituted alcohols at the air-water interface occurs in case, when the number of hydrocarbon links in the alcohol skeleton exceeds 6, while for the ordinary alcohols this number of the homologous series is 11. Such studies contribute to a deeper understanding of the surface and thermodynamic properties of fluorosubstituted alcohols, which is of crucial importance for practical applications. For this purpose, we have compared the thermodynamic properties of the studied alcohols with the corresponding properties of water, for which there is a continuous network of hydrogen bonds, and with the properties of hydrogen peroxide, for which the hydrogen bonds exist, but do not form a network.

At the present stage of predicting the thermodynamic properties of halogen-substituted organic compounds from the point of view of their molecular structure, special attention is paid to the application of artificial neural networks. As is well known, neural networks require reliable experimental data, and the quality of their prediction is higher the more relevant data are available within the homologous series. However, the fluorosubstituted alcohol heat capacity remains insufficiently studied experimentally today. These studies are aimed at clarifying the change in the molecular structure of the liquid at its transition from aliphatic alcohols [15,16] to their fluorosubstituted analogues. Explanation of the fluorosubstituted alcohol stabilizing properties at the molecular level, as well as comparison of the saturated acids stabilizing properties with physical mechanisms [17], remains an urgent task of condensed matter physics, which is important for modern biomedicine.

The object of this paper is to compare the temperature dependences of the isobaric heat capacity of liquid aliphatic alcohols within the same homologous series with the properties of their fluorosubstituted analogues using available experimental data and data obtained from artificial neural networks.

TECHNIQUE FOR THE ALCOHOL HEAT CAPACITY CALCULATION BY THE PRINCIPLE OF CORRESPONDING STATES

Utilizing the principle of corresponding states [18,19], the authors used the data for aliphatic alcohols, their fluorosubstituted analogues, water, and hydrogen peroxide, which are presented in up-to-date reference books [20,21], experimental databases [22-27], and databases simulated by artificial neural networks [28,29], or calculated by up-to-date statistical methods [30]. The theoretical foundations of simulations using artificial neural networks are presented in [31,32], and the examples of the artificial neural networks application for simulating the thermodynamic and transport properties of liquids are given in [33-35].

The utilized simulation approach [28] includes quantum-chemical calculations based on conformer analysis to determine the most stable structure of the molecule. In this case, optimization of the molecules spatial structure, comparison of the molecules energy levels and analysis of the relationship between the structure of the molecule and the property of the substance were carried out. The database [28] contains thermodynamic, physico-chemical, transport, spectral, biomedical, and other properties, as well as molecular descriptors. Both basic molecular descriptors, indicating the relative number of different atoms in a molecule, the structure of the molecule and the type of chemical bonds in the molecule, and special quantum-chemical descriptors, in particular topological ones (about 2000 descriptors in total), were used. The predicted data were compared with the experimental data, if available.

Note that the experimental data on the temperature dependences of isobaric heat capacity for the fluorosubstituted alcohols, as well as their critical parameters, are practically absent in the literature today. Therefore, for the fluorosubstituted alcohols, the simulations by artificial neural networks [28,29] were used. It should be noted that over the past 10 years, the simulation methods, based on artificial intelligence, have achieved significant development, thus allowing calculations of physical quantities with an error that is close to those occurring when these quantities are determined in the up-to-date experimental studies [28].

The principle of corresponding states [18,19] was used to compare the properties of aliphatic alcohols with those of their fluorosubstituted analogues. The isobaric heat capacity $C_P = T \cdot (\partial S / \partial T)_P = (\partial H / \partial T)_P$ was made dimensionless using critical values of temperature, density, and pressure:

$$C_r = \left(\frac{\partial H}{\partial T} \right)_P \cdot \frac{T_C \rho_C}{P_C} . \tag{1}$$

Here S is entropy, H is enthalpy, both referred to a mass unit (or to the number of moles) of the liquid; T_C, P_C, ρ_C are the critical values of temperature, pressure, and density, respectively. By the content of this dimensionlessness,

the enthalpy has the energy dimensionality, which is provided by the combination of critical parameters $P_C / \rho_C = P_C \cdot V_C$.

The temperature dependences of the heat capacity as well as the critical parameters were taken from literature sources [20-24] or simulated using the artificial neural networks [28,29]. Table 1 presents the utilized values of the studied liquids critical parameters.

Table 1. Critical parameters of aliphatic alcohols, their fluorosubstituted analogues, water, and hydrogen peroxide with their CAS identification

Substance	CAS	T_C, K	P_C, kPa	$\rho_C \cdot 10^4$, m³/mol
methanol	67-56-1	519.368	8012.12	1.15
ethanol	64-17-5	515.071	6137.06	1.69
propanol-1	71-23-8	535.940	5197.28	2.24
butanol-1	71-36-3	560.307	4452.95	2.77
pentanol-1	71-41-0	583.979	3839.56	3.34
hexanol-1	111-27-3	610.024	3425.08	3.89
heptanol-1	111-70-6	628.259	3095.95	4.43
octanol-1	111-87-5	646.665	2888.66	4.97
nonanol-1	143-08-8	662.673	2510.61	5.51
3F-ethanol-1	75-89-8	499	4863	2.04
5F-propanol-1	422-05-9	511	3862	2.56
7F-butanol-1	375-01-9	522	3199	3.07
9F-pentanol-1	355-28-2	536	2550	3.62
11F-hexanol-1	423-46-1	549	2263	4.15
13F-heptanol-1	375-82-6	563	1942	4.65
15F-octanol-1	307-30-2	582	1685	5.15
17F-nonanol-1	423-56-3	604	1515	5.69
water	7722-18-5	647.1	22064	0.563
hydrogen peroxide	7722-84-1	727.98	22000	0.777

TEMPERATURE DEPENDENCES OF THE ALCOHOL ISOBARIC HEAT CAPACITY ALONG THE LIQUID–VAPOR COEXISTENCE CURVE

Let us consider the temperature dependences of the isobaric heat capacity of aliphatic alcohols and their fluorosubstituted analogues applying the principle of corresponding states. For the alcohols we studied, the literature lacks both experimental data on the temperature dependences of the heat capacity and the values of the critical parameters that are necessary when applying the principle of corresponding states. In the view of the availability of only simulated data for the fluorosubstituted alcohols under study (Table 1), the data, simulated by the same technique [28,29] for both aliphatic alcohols and their fluorosubstituted analogues, are used in the paper.

Our analysis have shown that for aliphatic alcohols the difference between the simulated data on heat capacity [28] and similar data, but obtained experimentally [15, 36], generally increases with an increase in the number of carbon atoms. We estimated the relative deviation $\delta = C_P - \tilde{C}_P$ $\delta = C_P - \tilde{C}_P$ of the simulated heat capacity value $\tilde{C}_P$ from the experimental value C_P at the same temperature as $\Delta = 2 \cdot (C_P - \tilde{C}_P)/(C_P + \tilde{C}_P)$. The maximum relative deviation $\Delta_{max} = 2 \cdot (C_P - \tilde{C}_P)/(C_P + \tilde{C}_P)$ on the side of higher temperatures varied from 0.5% for ethanol to 9% for nonanol (see Table 2). At the same time, the arithmetic mean absolute deviation $\bar{\delta}$ and relative deviation $\bar{\Delta}$ for each alcohol at equidistantly selected temperatures are at least half their maximum values $\left|\delta_{max}\right|$ and $\left|\Delta_{max}\right|$, respectively.

Table 2. Modulus of the maximum absolute $\left|\delta_{max}\right|$ and relative $\left|\Delta_{max}\right|$ deviations of the simulated data on the heat capacity of aliphatic alcohols from the similar data obtained experimentally

Substance	Modulus of maximum absolute deviation $\left|\delta_{max}\right|$, J/(mol·K)	Modulus of maximum relative deviation $\left|\Delta_{max}\right|$
ethanol	0.678	0.0049
propanol-1	1.69	0.0089
butanol-1	6.50	0.0255
pentanol-1	20.9	0.0671
hexanol-1	22.8	0.0723
heptanol-1	26.7	0.0666
octanol-1	39.2	0.0885
nonanol-1	42.8	0.0883

The critical parameters of fluorosubstituted alcohols were obtained by artificial neural networks [28,29]. The temperature dependences of the dimensionless isobaric heat capacity C_r according to (1) on the reduced temperature $\tau = T / T_C$ for the aliphatic alcohols and their fluorosubstituted analogues are presented in Fig. 1 and 2, respectively.
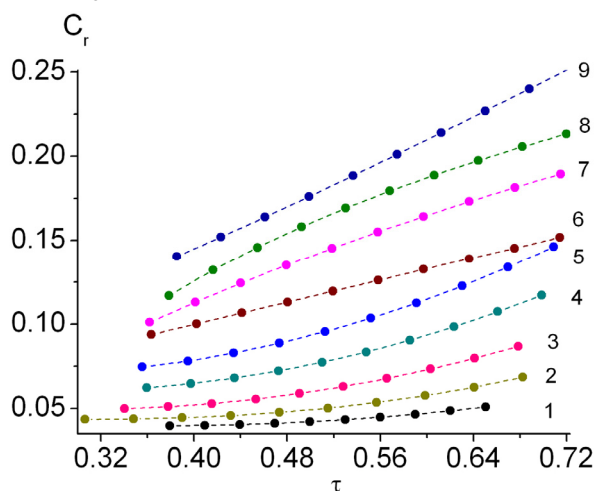

Figure 1. Temperature dependences of the reduced isobaric heat capacity of aliphatic alcohols in the liquid phase along the liquid–vapor coexistence curve: 1 – methanol, 2 – ethanol, 3 – propanol, 4 - butanol, 5 – pentanol, 6 – hexanol, 7 – heptanol, 8 – octanol, 9 - nonanol
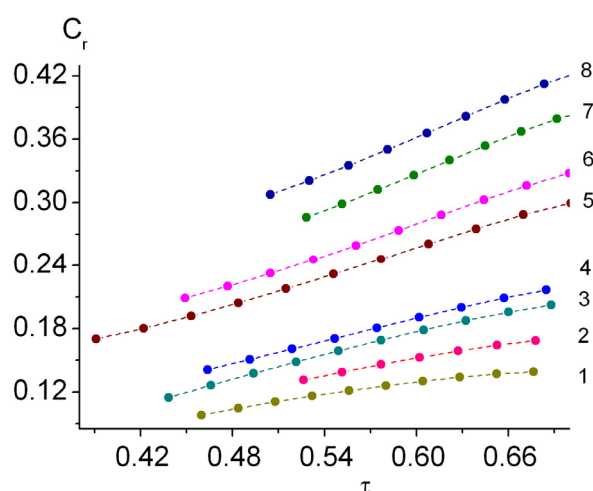
Figure 2. Temperature dependences of the reduced isobaric heat capacity of fluorosubstituted alcohols in the liquid phase along the liquid–vapor coexistence curve: 1 – 3F-ethanol, 2 – 5F-propanol, 3 - 7F-butanol, 4 – 9F-pentanol, 5 – 11F-hexanol, 6 – 13F-heptanol, 7 – 15F-octanol, 8 – 17F-nonanol

The analysis of Fig. 1 and 2 shows that the temperature dependences of the isobaric heat capacity for aliphatic alcohols and their fluorosubstituted analogues are monotonic, but under certain conditions have inflection points. Moreover, in a wide temperature range along the liquid-vapor coexistence curve, the isobaric heat capacity of the aliphatic alcohols is almost half the isobaric heat capacity of the fluorosubstituted alcohols. Fig. 3 presents the temperature dependences of the reduced isobaric heat capacity for some pairs aliphatic alcohol – its fluorosubstituted analogue.
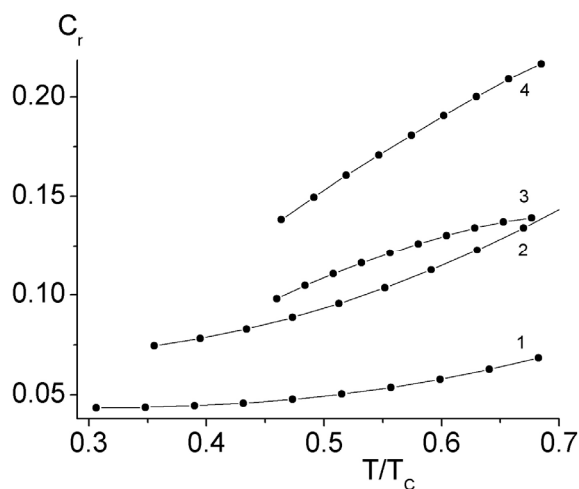

Figure 3. Temperature dependences of the reduced isobaric heat capacity of liquids along the liquid–vapor coexistence curve: 1 – ethanol, 2 – pentanol, 3 – 3F-ethanol, 4 – 9F-pentanol

As Figure 3 shows, curves 1 and 2, which correspond to aliphatic alcohols, have a positive second derivative of the heat capacity with respect to temperature, while curves 3 and 4, which correspond to fluorosubstituted alcohols, have a negative corresponding derivative. Our research has shown that for ethanol $(\partial^2 C_r / \partial T^2)_P > 0$, while for trifluoroethanol $(\partial^2 C_r / \partial T^2)_P < 0$; in the vicinity of the melting temperature for hexanol $(\partial^2 C_r / \partial T^2)_P < 0$, while for 11F-hexanol $(\partial^2 C_r / \partial T^2)_P > 0$. Such features of the behavior of fluorosubstituted alcohols as compared to the aliphatic alcohols may indicate to structural differences of the alcohols in the liquid state under study. The research described in [11,12,13] indicates the significant differences according to which the molecules of fluorosubstituted alcohols can be located more densely due to the helical conformation of the fluorosubstituted hydrocarbon chains. In our opinion, this may occur due to the destruction of a certain number of hydrogen bonds.

DISCUSSION OF RESULTS

To understand the reasons for significant difference in the values of the isobaric heat capacities of the studied alcohols, the attention should be payed to the influence of hydrogen bonds on the value of the heat capacity of liquids along the liquid–vapor coexistence curve. For this purpose, we use the principle of corresponding states to compare the heat capacity of water, in which there is a continuous network of hydrogen bonds, with that of hydrogen peroxide, where the hydrogen bonds exist, but their continuous network is absent. Fig. 4 shows the temperature dependences of the isobaric heat capacity of water and hydrogen peroxide along the liquid–vapor coexistence curve, calculated according to the principle of corresponding states. The indicated curves have minimums at the temperature of 36°C (T/T_C=0.477) for water and 155°C (T/T_C=0.558) for hydrogen peroxide. The minima in the temperature dependences of the heat capacities of water, hydrogen peroxide, and a number of other substances having a small molar mass [21,22,23,24] indicate the emergence of molecules associates [15] at the temperatures lower than those of the minima. At the same time, for the aliphatic alcohols [15,28] and their fluorine-substituted analogues [28] the minima in the temperature dependences of the heat capacities do not occur. Below the temperatures of the indicated minima, the temperature dependence of the isobaric heat capacities of water and hydrogen peroxide along the liquid–vapor coexistence curve is anomalous as compared to other liquids. When the temperatures are above the indicated minima, the heat capacities of the indicated liquids increase as the temperature grows, as it is shown in Fig. 3 for the studied alcohols.
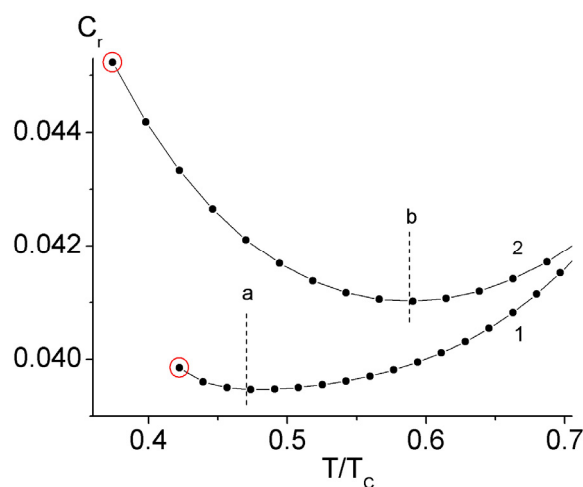

Figure 4. Temperature dependences of the reduced isobaric heat capacity of liquids along the liquid-vapor coexistence curve:
1 – water, 2 – hydrogen peroxide; a - minimum for water, b - minimum for hydrogen peroxide. Circles indicate the triple points

The analysis of Fig. 4 leads to the conclusion that the reduced heat capacity of water exceeds the reduced heat capacity of hydrogen peroxide due to the presence of a continuous network of hydrogen bonds in water. Therefore, it can be assumed that for the fluorosubstituted alcohols, where most of the hydrogen atoms are replaced by fluorine atoms, the hydrogen bonds are less dense, thus resulting in higher values of the reduced isobaric heat capacity (Fig. 3, curves 3 and 4).

Unlike the aliphatic alcohols, the temperature dependences of the isobaric heat capacity of their fluorosubstituted analogues have opposite signs of the second derivative of the heat capacity with respect to the temperature. According to [15], the curves of the temperature dependences of the alcohols heat capacity can have an inflection point associated with the breaking of hydrogen bonds above the inflection temperature. The breaking of the aliphatic alcohol hydrogen bonds corresponds to such inflection points [15] for which $(\partial^2 C_r / \partial T^2)_P > 0$ is below the inflection temperature, while $(\partial^2 C_r / \partial T^2)_P < 0$ is above the inflection temperature. Note, that for the corresponding aliphatic thiols, in whose molecules instead of the oxygen atom there is a heavier sulfur atom, the curves of the temperature dependences of the heat capacity do not have inflection points [15].

Thus, the opposite sign of the second derivative of the heat capacity with respect to the temperature for the aliphatic alcohols and their fluorosubstituted analogues indicates that for the fluorosubstituted alcohols there exists a hydrogen bond breaking dynamics.

CONCLUSIONS

Using the principle of corresponding states, a comparative analysis of the temperature dependences of the isobaric heat capacity of aliphatic alcohols and their fluorosubstituted analogues was carried out in the wide temperature range along the liquid–vapor coexistence curve.

On the basis of literature experimental data and the simulations, performed by artificial neural networks, it is shown that homologous series of aliphatic alcohols and their fluorosubstituted analogues have differences in reduced caloric properties.

It is shown that in a wide temperature range along the liquid–vapor coexistence curve, the reduced isobaric heat capacity of fluorosubstituted alcohols is almost twice as high as the corresponding value of the aliphatic alcohols, which the authors attribute to a decrease in the number of hydrogen bonds in the fluorosubstituted alcohols as compared with the aliphatic ones.

Unlike the aliphatic alcohols, for their fluorosubstituted analogues the second derivative of the heat capacity with respect to temperature along the liquid-vapor coexistence curve is opposite in sign, which indicates to the dynamics of hydrogen bond breaking upon fluorosubstitution in aliphatic alcohols.

Conflict of interest
The authors declare the absence of any conflict of interest related to the research presented in this manuscript.

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ВПЛИВ ФТОРЗАМІЩЕННЯ НА ТЕПЛОЄМНІСТЬ АЛІФАТИЧНИХ СПИРТІВ

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Із використанням принципу відповідних станів у статті проведено порівняльний аналіз температурних залежностей ізобарної теплоємності аліфатичних спиртів та їх фторзаміщених аналогів. Для теплоємності використані як літературні експериментальні дані, так і симульовані дані, отримані за допомогою штучних нейронних мереж. Ізобарна теплоємність для аліфатичних спиртів за абсолютними величинами в широкому температурному інтервалі при сталому тиску є меншими, ніж для відповідних фторзаміщених аналогів. Порівняння даних теплоємності аліфатичних спиртів та їх фторзаміщених аналогів із теплоємністю води, для якої існує сітка водневих зв'язків, із відповідними даними для перекису водню, де є водневі зв'язки, але сітка відсутня, вказує на те, що зміна фізичних властивостей спиртів при фторзаміщенні пов'язана зі щільністю водневих зв'язків.

Ключові слова: *аліфатичні спирти; фторзаміщені спирти; вода; перекис водню; теплоємність; принцип відповідних станів*