THE STRUCTURE OF WATER AND ITS STUDY BY THE STRUCTURAL TEMPERATURE METHOD

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Abstract

The main part of the human body consists of water, and water plays the role of a favorable environment for all biochemical processes in the body. The beneficial or harmful effects of chemical substances entering the body are determined by their interaction with water. The use of harmful substances for the health of the body should be low enough. , the goal is to detect chemical substances that can be useful to the body. Considering that the main solvent in the human body is water, we can say that chemical substances that structure water should be detected. The main problem facing pharmacologists is to identify chemical substances that have a positive or negative effect on the structure of water in a short time. consists of. The physical quantity that accurately determines the effect of substances on the structure of water is structural temperature. Therefore, the concept of structural temperature and the development of its theory are of great importance for pharmacology. In the presented work, the main properties of water, its structure and the importance of structural temperature were discussed in detail. Finally, it should be noted that the determination of structural temperature is the most perfect method for the preparation of pharmacological substances in a short period of time.

Keywords: Water, structure of water, structural models, structural temperature.

Water is the most common unusual and strangest substance in nature. K. E. Siokovsky said that if the Earth is the cradle of humanity, the world ocean is also the cradle of life on earth. We owe our life and existence to water, which is universal matter and which we carry in our bodies. It is known that all organs and tissues of the human body, which contain 70% water, contain water, for example, bones of the skeleton 25%, living tissues 30%, liver, brain, skin, heart, lungs, etc. 75-80%, blood consists of 83% water. The special role of water in the life activity of a living organism is not only that it is a component of cells and tissues, but also that it is a favorable environment for all biochemical processes. Compared to other liquids, almost all properties of water are unusual, that is, abnormal. The unusual properties of water help it perform a number of functions in living organisms. Water, as a medium, performs very important functions such as transporting substances in the body through osmosis and diffusion, protecting cells and organs, and protecting the body from cold and heat due to its high heat capacity and evaporation heat. Water has the ability to absorb high-energy radiation and plays a major role in energy transfer in living organisms. The point is that it is impossible to find any property of water that is not unusual. In other words, depending on the temperature, pressure and other factors, the change of a certain property of water results in the formation of organic liquids, molten metals, liquefied inert gases, etc. differs in that its properties change depending on those factors. In liquids other than water, these changes are similar and can be explained on the basis of general physical considerations. It can be said that the biological functions are mainly aimed at regulating or dispersing the structure of water. It can be considered that the study of life, although simplified, means the study of water at different structural levels [1]. Many models have been given by different researchers to study the structure and properties of water. The classification of these models allows us to conclude that the main reason for the formation of water structure is the presence of intermolecular hydrogen bonds. The basis of modern ideas about the structure of water was mentioned in the work of Bernal and Fowler, who put forward a two-structure model of liquid water, and was later developed by many researchers. According to Bernal and Fowler, in water there are associates and relatively free molecules consisting of a large number of molecules connected to each other through hydrogen bonds. As the temperature decreases, the size of clusters in water increases and the amount of free water molecules decreases. The network of hydrogen bonds in water is random. In this network, the interbond angles differ randomly, not according to a certain regularity. While in a crystal (ice) the neighboring molecules around each molecule are arranged in the same order, in water the molecules around each molecule are arranged in a random order. For this reason, the structure of the random network cannot be determined by X-ray structural analysis. Therefore, it is impossible to determine the structure of water, that is, the state of all molecules, experimentally. Therefore, researchers currently use other methods to determine the structure of water and, above all, modeling methods [2]. It should be noted that so far about 20 structural models of water have been given. The real picture of the structure of water consists of a network of random four-coordinated hydrogen bonds. As a result of external influences, the network can change in two ways:

1) the lengths of connections change without changing the structure

2) the structure changes, but the lengths of the bonds remain constant.

An increase in the length of hydrogen bonds when temperature increases is considered the first type of change and is characteristic of all substances, including water. However, the second type of change in water plays a greater role. At low temperatures, the structure of water is more regular, that is, the angles between the hydrogen bonds in the space lattice differ less from the tetrahedral angle. Therefore, the mesh is more patterned, has a lower density and is difficult to deform. As the temperature increases, water changes its structure and is reorganized. At this time, along with the change of the angles between the connections, the nature of the connection between the nodes of the network changes. At low temperatures, the structure of various modifications of ice remains stable in a certain finite temperature interval, and then, when passing from one discrete structure to another, despite the reorganization of the network, eventually hydrogen bonds from the network structure change continuously with temperature. Taking into account this, water anomalies can be explained. The substance added to water changes the structure of water, and as a result, the degree of water intervention and participation in water processes changes. Note that the structure of water is the average kinetic energy (temperature) of water molecules, the energy of intermolecular hydrogen bonds, the density, length, distribution configuration, etc. of these bonds. is determined by a set of many such molecular design parameters. One of the parameters characterizing the effect of a substance on the structure of water is "structure temperature". This parameter characterizing the properties of water solutions was introduced and used by Bernal and Fowler in the first half of the 20th century. Bernal and Fowler defined structural temperature as follows: a) Any substance introduced into water changes the structure of water, and as a result, any physical or physico-chemical property of water changes. b) On the other hand, that property of water can change with the change of temperature. If this change is small, any parameter characterizing the water can be changed as desired by increasing or decreasing the water temperature. c) It follows from the above two statements that for any aqueous solution with concentration c'- there is such a temperature T'- that the physical property of pure water taken at that temperature is the same as that physical property of aqueous solution with concentration c'- at room temperature. Bernal and Fowler called the T'- temperature the structural temperature. Although it seems simple and understandable at first glance, the concept of structural temperature in the sense defined by Bernal and Fowler has several shortcomings. First, the physical meaning of structural temperature in Bernal and Fowler's sense is not so clear. Then, from the point of view of physics, the mechanisms by which any property of the solution can be changed by the substance introduced into the water or as a result of the change in temperature can be different. Thus, when solute molecules are introduced into the solvent, a new structure is formed, which is determined by the interaction between the solvent and solute molecules and the size of the solute molecule. In both cases, the resulting new structures may not be adequate to each other, even if they have the same macro-properties. The structure temperature in the sense of Bernal and Fowler also depends on which temperature is chosen, such as room temperature, which leads to further uncertainty. In this sense, the structural temperature cannot always be determined. This makes structural temperature meaningless in the sense of Bernal and Fowler [3]. For all these and a number of other reasons, the concept of structural temperature in the sense of Bernal and Fowler did not find its development and was almost forgotten. The concept of structural temperature was again used by Uberreiter in the 70s of the 20th century. It is one of the many empirical formulas known for the temperature dependence of the viscosity of liquids

$$\eta(T) = A \cdot e^{\frac{B}{T-T_0}} \tag{1}$$

Using Vogel's formula, he calculated the parameter T_0 for pure water, a number of polymers and aqueous solutions of organic compounds of low molar mass. Here,$\eta(T)$ the density of the liquid at temperature T, and A and B are constants whose physical meanings will be explained a little later. As can be seen from Vogel's formula, T_0 is the temperature at which the viscosity of the liquid becomes infinitely large. In this regard, Uberreiter named T_0- structuring or structural temperature and gave a new meaning to the concept of structural temperature [4]. Note that Vogel's formula was obtained with the help of theoretical considerations for the temperature dependence of the viscosity of liquids

$$\eta(T) = \eta_0 e^{\frac{\Delta G}{RT}} \tag{2}$$

It is very similar to the Frenkel-Eyring formula. Here ΔG is the free energy of the viscous flow of liquid molecules, R is the universal gas constant,η_0 and is the viscosity at infinitely high temperatures. Comparison of formulas (1) and (2) shows that the constant A in Vogel's formula is equal to -η_0. And B is a quantity that has a certain relationship with the activation energy of viscous flow ΔG. Experiments show that the viscosity of water at small changes in temperature agrees very well with the values calculated by the Frenkel-Eyring formula. So, at this time, the degree of reliability of the approximation curve passing through the experimental points, in other words, the correlation coefficient of the line is quite high and almost equal to unity. However, during relatively large changes in temperature, the viscosity of the liquid begins to differ more and more from the values calculated by the Frenkel-Eyring formula.The real physical reason why the viscosity of water begins to differ from the values calculated by the Frenkel-Eyring formula during large temperature changes is that the temperature dependence of the activation free energy of viscous flow is not only

$$\Delta G(T)= \Delta H - T\Delta S \qquad (3)$$

not in the form, but it can also be in a very complicated way due to the dependence of ΔH and ΔS on temperature:

$$\Delta G(T)= \Delta H(T) - T\Delta S(T) \qquad (4)$$

Such dependence on temperature appears due to the fact that some interactions of a different nature and which can lead to structuring are not taken into account in the Frenkel-Eyring theory. Considering all these interactions together, by writing T-T' instead of T in the denominator of the super-exponential fraction in the formula (3), the experimental points can be brought onto the curve expressed by the Frenkel-Eyring formula. This new added limit T' is called the structural temperature. From the form of the input and, as we will see a little later, its numerical value, it is clear that the structure temperature is a fictitious parameter. However, it is well known that fictitious parameters also play an important role in solving a number of problems in science. In this sense, the issue was not in the exact calculation of the structural temperature of the liquid, but in knowing in which direction and how much the structural temperature changes due to the effect of the substance added to the liquid [5]. If the structural temperature of the liquid has increased due to the influence of any substance, then when cooling that liquid, the temperature at which the viscosity is infinitely large will arrive sooner, that is, the liquid will be structured more quickly. From this point of view, it can be said that the increase in the structural temperature of the liquid due to the effect of any dissolved substance and other physical parameters means its structuring compared to the pure liquid as a result of this effect. Likewise, it can be said that the decrease in structure temperature is equivalent to the collapse of the structure of the liquid. Let's note that liquids with a structural temperature equal to zero, that is, the temperature dependence of viscosity can be expressed quite well by the Frenkel-Eyring formula, are called free liquids, and vice versa, liquids with a certain internal structure, that is, a non-zero structural temperature, are called non-free liquids. It should be noted that the structure temperature and viscosity do not always change in the same way depending on the concentration. In other words, the increase and decrease of the viscosity of the solution does not yet allow us to give a definite opinion about the structural change. This change determines the structural temperature in a single value. Since most of the body is made up of water, when scientists are preparing pharmacological substances, they study the effect of these substances on the structure of water. Detecting this effect in a short period of time is one of the main issues ahead. The most effective and fastest method in this matter is the determination of the structure temperature. We will present the study of structural temperature through various methods in the next works.

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