



The Dimension and Life

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Abstract

It is proved that water molecules, as the basis of living organisms and the source of the origin of life, have the highest dimension. Various types of biomolecules with the highest dimension are listed. The possibility of memory of water about the presence of toxic substances in it is analyzed analytically.

Keywords: Water Molecules; Biomolecules; Dimension; Memory of Water; Atomic Orbital

Introduction

Life began in water and continues in water. Water is matter and the matrix of life. Water is not only outside of us, but also inside us. Every living organism is 80% water. Recent studies [1-3] show that as a result of the interaction of water with pyrite FS_2 , there is a possibility of the appearance of protocells LUCA in water layers on the surface of minerals, including on the surface of nanodiamonds, which can form under terrestrial conditions at moderate temperatures and pressures [4]. All biomolecules ultimately evolved from a protocell that emerged over 4.5 billion years ago. The author's works [5-11] prove that various biomolecules in nature have the highest dimension. This article proves that the water molecules themselves, from which biomolecules originated in contact with minerals, have the highest dimension. Thus, the highest dimension of biomolecules is a consequence of the highest dimension of water molecules. Water has the ability to adjust its structure to the structure of substances that are in it or border it. As an illustration of this property, the process of restructuring of water to match the structure of cyanide compounds dissolved in water is considered.

The structure of water

The water molecule has a peculiar shape. Oxygen in the second energy level p orbital has one quantum cell with a pair of electrons

with opposite spins and two quantum cells with one electron in each of them. These two electrons combine with two electrons of the hydrogen atoms to form a covalent chemical bond. In addition, the oxygen atom has one more pair of electrons at the second energy level in the s orbital. The hydrogen atoms, which donated their two electrons to form a bond, remain sufficiently distant from the oxygen atom and have a positive charge $+$. Unshared electron pairs of the oxygen atom of the outer energy level naturally have a negative charge $-$. Conventionally, the shape of a water molecule can be represented as shown in figure 1.

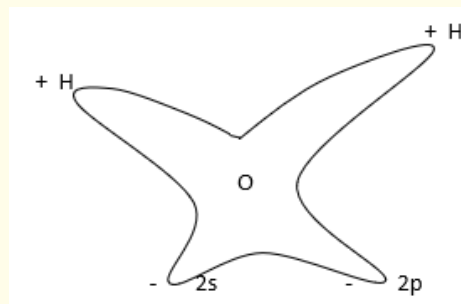


Figure 1: The shape of a water molecule.

It is obvious that positively charged protons of other water molecules can join the orbitals with negative charges of the second energy level of the oxygen atom. The result is a tetrahedral structure with a center (Figure 2).

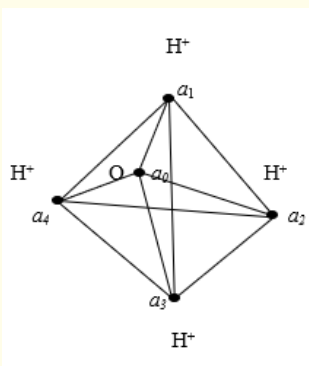


Figure 2: The tetrahedral structure with a center of molecules water with joined two protons.

The tetrahedron with a center on figure 2 has 5 vertices $a_0 \div a_4$, 10 edges $a_0a_1, a_0a_2, a_0a_3, a_0a_4, a_1a_2,$

$a_3a_1, a_1a_4, a_4a_2, a_2a_3, a_4a_3,$ 10 two - dimensional faces $a_3a_4a_1, a_1a_3a_2, a_1a_4a_2, a_2a_3a_4, a_1a_0a_3, a_1a_0a_2,$

$a_0a_4a_1, a_0a_4a_2, a_0a_3a_2, a_0a_3a_4,$ 5 three-dimensional faces $a_3a_4a_1a_2, a_0a_1a_3a_2, a_1a_4a_2a_0, a_3a_4a_1a_0, a_3a_4a_0a_2.$

To determine the dimension of a tetrahedron with a center, it is sufficient to use the Euler-Poincaré equation [12]:

$$\sum_{i=0}^{n-1} (-1)^i f_i(P) = 1 + (-1)^{n-1}. \tag{1}$$

There n is dimension of a polytope P , f_i is the number of elements with dimension i in the polytope P .

In this case $f_0 = 5, f_1 = 10, f_2 = 10, f_3 = 5.$

Substituting the obtained values into equation (1), we obtain, i.e. Euler-Poincaré's equation for a tetrahedron with a center holds for $n = 4$. This proves that a tetrahedron with a center has dimension 4.

The existence of a tetrahedral distribution of hydrogen atoms in the network of hydrogen bonds of water molecules is proved by the methods of computer experiment [13-15]. However, the possibility

of the existence of non-tetrahedral dimers is noted. This is quite natural since hydrogen bonds do not differ in strength and chaotic rearrangements of the network of hydrogen bonds are possible in water. However, the tetrahedral distribution of hydrogen atoms in the structure of water is predominant. It should be remembered that oxygen atoms are in the center of the tetrahedron, and the tetrahedron with the center has dimension 4 (this is not mentioned in all works on the structure of water). Note that this is significant if we remember the statement that life originated in water.

The dimensions of biomolecules

In biomolecules, you can find many examples of compounds in the form of a tetrahedron with a center, that is, similar to the structure of a water molecule (for example $CH_4, NH_4, PO_4,$ etc). All of them have a dimension of 4. The most important representatives of biomolecules are molecules of carbohydrates, proteins, lipids, nucleic acids. When depicting biomolecules, schematic planar images of Fisher and Haworth [16-18] are usually used. But they do not reflect the real spatial structure of biomolecules. In 2016, the author proposed spatial images of biomolecules in the form of polytopes [19], the dimension of which is determined by the Euler-Poincaré equation (1). Since the concept of a functional group is widely used in organic compounds, when determining the structure of biomolecules and their dimensions, not only individual atoms, but also functional groups can be located at the vertices of the corresponding polytope. This is how the concept of the functional dimension of a biomolecule was introduced. As a result, the functional dimensions of many biomolecules were determined. In particular [6,10], the functional dimension of the simplest carbohydrate monosaccharide aldose (with three carbon atoms) turned out to be 5, as well as the dimension of the tartaric acid molecule. The functional dimension of the D-ribose molecule is 12. The functional dimension of the α -D-glucose molecule is 15. The functional dimension of any amino acid is 4, as is the dimension of phosphoric acid. Biomolecules connecting in series with each other form chains: polysaccharides, polypeptides, nucleic acids. Geometrically, they represent chains of polytopes of the highest dimension. Additional bonds between sections of the chain or between different polymer chains with the help of hydrogen bonds or metal ions (iron, calcium, magnesium, zinc) lead to the formation of polytopes of even greater dimension. Such conformations of biomolecules play a very important role in living organisms, organizing the processes necessary for the vital activity of organisms. It has just been established [5,7-9] that the bond of nucleic acids by means of a hydrogen bond

of nitrogenous bases leads to the formation of a polytope of hereditary information of dimension 13, characterized by a powerful flow of information exchange between the elements of this polytope. This makes it possible to explain the existence of the so-called epigenetic process of the transfer of hereditary information, which is not associated with a change in the sequence of genes.

The memory of water

There is no doubt about the existence of a certain relaxation time required for the water to return to its original state after the cessation of external influences, for example, a magnetic or electric field [20-23]. Let us try to explain the existence of the memory of water about the chemical compounds dissolved in it, which are essential for the life of biological organisms. Let such compounds be cyanide compounds. It is well known that hydrocyanic acid HCN and its salts are strong poisons. The toxic effect of these compounds is that the ions CN⁻ formed in their solution inhibit the reduction of oxygen by the most important respiratory enzyme, cytochromoxidation, in the tissue cells of living organisms [17,24]. Ions CN⁻ react with the oxidized form of cytochrome oxidase and form a complex compound with a trivalent iron atom of enzyme [Fe(CN)₆]³⁻. As a result of the overlapping of the orbitals of the complexing agent Fe³⁺ by the ligands CN⁻ and the hybridization of the orbitals, the ion [Fe(CN)₆]³⁻ has octahedral coordination (Figure 3). Geometrically, this ion is an octahedron with a center.

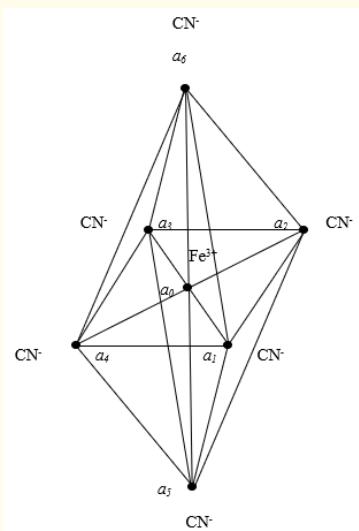


Figure 3: Geometric structure of the ion [Fe(CN)₆]³⁻.

The functional dimension of this ion is 4. The octahedron with a center on figure 3 has 7 vertices $a_0 \div a_6$, ($f_0 = 7$); 18 edges $a_0a_1, a_0a_2, a_0a_3, a_0a_4, a_0a_5, a_0a_6, a_1a_2, a_2a_3, a_3a_4, a_1a_4, a_6a_1, a_6a_2, a_6a_3, a_6a_4, a_1a_5, a_3a_2, a_5a_3, a_4a_5, (f_1 = 18)$; 20 two-dimensional faces $a_0a_6a_1, a_0a_6a_2, a_0a_3a_6, a_0a_6a_4, a_1a_0a_5, a_5a_0a_2, a_3a_0a_5, a_0a_4a_5, a_1a_0a_2, a_2a_3a_0, a_4a_0a_3, a_1a_0a_4, a_5a_2a_1, a_3a_3a_2, a_5a_3a_4, a_5a_1a_4, a_6a_2a_1, a_6a_3a_2, a_6a_3a_4, a_6a_1a_4, (f_2 = 20)$; 9 three-dimensional faces $a_0a_4a_1a_5, a_0a_1a_5a_2, a_3a_5a_2a_0, a_3a_4a_5a_0, a_1a_4a_0a_6, a_0a_1a_2a_6, a_3a_6a_0a_2, a_0a_4a_3a_6, a_1a_4a_2a_5a_3a_6, (f_3 = 9)$.

Substituting the obtained numbers $f_i (i = 0 \div 3)$ into equation (1), we obtain,

$$7 - 18 + 20 - 9 = 0,$$

i.e. the Euler-Poincaré equation holds for $n = 4$. This proves that the octahedron is centered, that is, ion [Fe(CN)₆]³⁻ has dimension 4. In this compound, each pair of electrons 2s of the nitrogen atom in each of the six ions CN⁻ occupies one of the six vacant quantum cells of the ion Fe³⁺. The ion Fe³⁺ has two vacant quantum cells in orbit 3d, one vacant quantum cell in orbit 4s and three vacant quantum cells in orbit 4p. Hybridization of the orbitals sp^3d^2 takes place. It has been experimentally established [25] that anions CN⁻ bind most strongly with cations Fe³⁺ in comparison with other ions or molecules in the stoichiometric series in terms of the strength of interaction with the complexing agent. The strong bond of ions CN⁻ with cations Fe³⁺ disrupts the redox processes in cytochrome oxidase, consisting in the transfer of electrons to copper atoms and then to oxygen. As a result, the ions H⁻ formed in the body during the decomposition of proteins, carbohydrates and amino acids do not react with oxygen to form water. The concentration of ions H⁺ in the body increases sharply, which leads to poisoning of the body. Obviously, in this way, the degree of poisoning will be determined by the concentration of ions CN⁻ in the solution. They are formed during the dissociation of hydrocyanic acid or its salts. Moreover, hydrocyanic acid dissociates weakly, and the dissociation of salts goes almost to the end. The dissociation of hydrocyanic acid as a result of the formation of ions H⁺ slows down the dissociation of water. An increase in the concentration of hydrocyanic acid leads to a decrease in the degree of dissociation of both hydrocyanic acid and water. Indeed, the concentration of ions and molecules in solution is determined by the relations:

$$\begin{aligned} [H^+] &= c_{H_2O}\alpha_{H_2O} + c_{HCN}\alpha_{HCN}, [OH^-] = c_{H_2O}\alpha_{H_2O}, [CN^-] = c_{HCN}\alpha_{HCN}, \\ [H_2O] &= c_{H_2O}(1 - \alpha_{H_2O}), [HCN] = c_{HCN}(1 - \alpha_{HCN}). \end{aligned} \quad (2)$$

There are α_{H_2O} – degree of dissociation of water, α_{HCN} – degree of dissociation of hydrocyanic acid, c_{H_2O} – concentration of water before dissociation, c_{HCN} – concentration of hydrocyanic acid before dissociation. Substituting relations (2) into the equations for the dissociation constants:

$$K_{H_2O} = \frac{[H^+][OH^-]}{[H_2O]}, K_{HCN} = \frac{[H^+][CN^-]}{[HCN]}, \quad (3)$$

Taking into account that the degrees of dissociation are small compared to unity, we obtain

$$\begin{aligned} K_{H_2O} &= c_{H_2O}\alpha_{H_2O}^2 + c_{HCN}\alpha_{HCN}\alpha_{H_2O}, \\ K_{HCN} &= c_{H_2O}\alpha_{H_2O}\alpha_{HCN} + c_{HCN}\alpha_{HCN}^2. \end{aligned} \quad (4)$$

Solving system (4) with respect to $\alpha_{HCN}, \alpha_{H_2O}$, taking into account that the mass fractions of water x_{H_2O} and acid x_{HCN} satisfy the conditions $x_{H_2O} + x_{HCN} = 1, x_{HCN} \ll 1$, we obtain

$$\alpha_{H_2O} = \frac{K_{H_2O}}{\sqrt{\rho(K_{H_2O}/\mu_{H_2O} + x_{HCN}K_{HCN}/\mu_{HCN})}}, \alpha_{HCN} = \frac{K_{HCN}}{K_{H_2O}}. \quad (5)$$

There are ρ – solution density, μ – molecular weight.

Relations (2), (5) make it possible to calculate the degree of dissociation and ion concentration for a given initial concentration of hydrocyanic acid. In particular, taking the values of the dissociation constants $K_{H_2O} = 10^{-14}$ mol/l, $K_{HCN} = 4.79 \cdot 10^{-10}$ mol/l at very low concentrations of hydrocyanic acid ($x_{HCN} \rightarrow 0$), we find $\alpha_{H_2O} = 10^{-8}, \alpha_{HCN} = 4.79 \cdot 10^{-4}$. At a lethal concentration of hydrocyanic acid [24] $x_{HCN} = 1.4 \cdot 10^{-6}$ these values are equal $\alpha_{H_2O} = 10^{-10}, \alpha_{HCN} = 4.6 \cdot 10^{-4}$. Thus, the dissociation of water in solutions of hydrocyanic acid and its salts is insignificant, and the degree of dissociation of hydrocyanic acid weakly depends on its concentration. From (2), (5) it follows that despite a decrease in the degree of dissociation of hydrocyanic acid with an increase in its concentration, the concentration of ions CN^- increases proportionally x_{HCN} .

When any substances are dissolved, the solvent molecules are strongly influenced by the molecules of the dissolved substance. In this case, the solvent molecules are modified. It was shown [26] that the water molecules surrounding the ions of the dissolved sub-

stance are under the influence of forces equivalent to a pressure of 50,000 atmospheres. In the process of hydration, molecules of hydrated water [27] pass into an excited state with vibrations of nuclei relative to new acquired positions that differ from unexcited positions. The nature of the fluctuations is determined by the nature of the hydrated ion. This is how the nature of the hydrated ion is transferred to the water molecules in its environment. Due to the excited vibrations, water molecules become more deformable and polarizable. It is these properties that put the ion CN^- on the first place in the spectrochemical series of the activities of ions and the forces of their interaction with the complexing agent. The greater the polarizability of the particle, the stronger its bond with the complexing agent. The greater the deformability of the molecule, the easier it is for the molecule to “fit” into the particular relief of the enzyme (in this case, cytochrome oxidase). The network of hydrogen bonds in water has the ability to transfer perturbations external to the network to the entire volume of the solution, while maintaining the stability of the structure of the H-network [28]. The phenomenon of negative solvation is associated with this property [29], i.e. an increase in the mobility of solvent molecules near ions. All this indicates that the excitation created by ions CN^- with an increase in concentration is transferred to almost all water molecules in solution. After dilution of this solution, the acquired properties of water are retained for some time, which is necessary for the relaxation of the H-bond network. The characteristic time for a change in the properties of water in the absence of external influences on it is, according to experiments [30], several tens of minutes. While the characteristic time for the absorption of ions and water molecules into the tissue cells of living organisms is fractions of a second [31]. It follows from this that water molecules, having changed under the influence of ions CN^- , even after dilution of water, can retain their activity and, instead of ions CN^- , take their place as ligands around the complexing agent Fe^{3+} in the cytochrome oxidase enzyme, firmly binding with it. In this case, a pair of electrons 2s of the oxygen atoms in the water molecule is transferred to the vacant orbitals 3d, 4s, 4p of the iron atom of the complexing agent. Here, too, an octahedron with a center of dimension 4 is formed around the iron atom, and the violation of redox processes in cytochrome oxidase is preserved.

Conclusion

It has been proven that the molecules of living organisms have the highest dimension (more than three) [6,10,19]. This is confirmed by the data of calculating the dimensions of molecules of

various carbohydrates, proteins, nucleic acids and other biomolecules. Water molecules, which are known to average 80% of the mass of any living organism, also have the highest dimension. Since it is believed that biomolecules were formed in the process of evolution from the LUKA protocell more than 4.5 billion years ago in layers of water on the surface of minerals [1-4], apparently the higher dimension of biomolecules is a consequence of the higher dimension of water molecules. The highest dimension of water molecules is a consequence of the electronic structure of the atoms of the water molecule and the processes of hydration around the ions of mineral substances in water and on the surface of minerals. In this case, it should be taken into account that the elementary cells of minerals also have a higher dimension [10] and water during hydration changes its structure complementary to the vicinity of mineral ions.

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