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Spirals of Polysaccharides Simultaneously Rotating in Opposite Directions

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Abstract

Geometric metric models of sugar molecules and polysaccharides in spaces of various dimensions are investigated. It is shown that simplified three-dimensional models of sugar molecules and polysaccharides lead to the formation of helices with rotation in opposite directions in two mutually perpendicular planes.

Keywords: Glucose Molecules; Nucleic Acids; Polytopes; Sugar Molecules; Genetic Code

Introduction

In works [1-3], higher-dimensional models of the D-ribose molecule and its simplified three -dimensional image were constructed, based on which the geometry of nucleic acids was studied. As a result of [4,5], it was possible to establish a hidden order of interaction of nucleic acids, leading to an unambiguous correspondence of the number of nucleotides, taking into account their possible location in the space of higher dimension with the number of amino acids. In this work, D-glucose molecules and chains of these molecules are subjected to a similar analysis. It was found that pyranose molecules, when chains are formed, form spirals with simultaneous rotation in opposite directions.

Spatial models of pyranose molecules

One of the most important monosaccharides is glucose. It makes up a significant part of all biomass (cellulose, starch), found in the blood of humans and animals.

The most important aldohexose is D-glucose. The image of the molecule glucose with a closed carbon cycle (the α-D-glucose molecule) in the form of a closed polytope [6] is presented in figure 1. When depicting the polytope in figure 1, the assumption that the atoms of the carbon cycle are located in the plane was not used. Therefore, this image is suitable for any conformation of molecule α-D-glucose. In the model in figure 1, the edges corresponding to chemical covalent bonds are indicated in red. The remaining edges have only the geometric meaning of creating a convex polytope. They are marked in black. In the aggregate, each vertex of a polytope (atom or functional group) is connected with all other vertices by edges. This means that the image in question is a simplex

Figure 1: The molecule of α-D-glucose.

type polytopic. It is proved that the dimension of this polytope is 15 [6].

To obtain a three-dimensional simplified model of the molecule α-D-glucose, in figure 1 we leave only the edges corresponding to chemical covalent bonds, the edges of the external contour, and the edge connecting the atoms. We assume as a first approximation that the ring of carbon atoms is a regular pentagon with a side length of 0.15 nm (the standard length of the carbon - carbon chemical bond). Since carbon atoms exhibit tetrahedral coordination, other valence bonds of carbon atoms must be located either above the plane of the ring or below the plane of the ring. It is con-

venient to assume for further geometric analysis that the atoms of hydrogen and the hydroxyl group located in figure 1 inside the carbon ring are in space above the plane of the carbon ring. While the oxygen atom and the functional groups of the outer contour (larger) are under the plane of the carbon ring. A part of this spatial structure located under the plane of the carbon ring is shown in figure 2.

Figure 2: The part of the glucose molecule located under the carbon ring.

The length of the carbon-hydrogen and carbon-oxygen bonds is denoted by the letter a = 0.1 nm. Then the carbon - carbon bond length takes the form 1.5a. Thus, the part of the construction of the α-D-glucose molecule under the carbon ring is a pyramid with a lower base in the form of an irregular hexagon and an upper base in the form of a regular pentagon.

To determine the yet unknown geometric characteristics of the figure in figure 2, it is first necessary to find the value of the angle of inclination of the side edges of the pyramid to its base. For this, we consider separately the flat lateral faces of the pyramid in the vicinity of the oxygen atom. We double these faces and designate the vertices and some characteristic points of this structure in separate letters (Figure 3).

We denote the angle CAK by the letter φ. Given that $\angle AKC = \pi/2$ we have $CK = LS = BE = a\sin\varphi$, so *AC=CD=DE=EF=a*, AK=a cos φ. Since the carbon cycle is a regular pentagon, then $\angle AKL = \pi/2 - 54 = 126^o$. Since *CE=1.5a* and point S is middle of segment *CE* then $DS = \sqrt{a^2 - (3/4)^2 a^2} = a\sqrt{7}/4.$ From triangle DSL we have $DL = \sqrt{DS^2 - SL^2} = \frac{a}{4}\sqrt{7 - 16\sin^2\varphi}.$ Therefore, from the triangle KLD we obtain $KD = \sqrt{DK^2 + KL^2} = a\cos\varphi = AK.$ Then $\angle KDC = \varphi.$ Besides, $\sin\angle DKL = \frac{DL}{KD} = \frac{\sqrt{7 - 16\sin^2\varphi}}{4\cos\varphi}.$ Therefore,

$$\angle AKD = \angle AKL - \angle DKL = 126^o - \arcsin\frac{\sqrt{7 - 16\sin^2\varphi}}{4\cos\varphi}$$

Figure 3: The enlarged part of the side surface of the pyramid (Figure 2) in the vicinity of the oxygen atom.

From the triangle KAD we obtain $\frac{AD}{2a\cos\varphi} = \sin\frac{\angle AKD}{2}$. From here we find

$$AD = 2\cos\varphi\sin(63^o - \frac{1}{2}\arcsin\frac{\sqrt{7 - 16\sin^2\varphi}}{4\cos\varphi}). \quad (1)$$

Besides, from four-angle *AKLD* we have *KN/AK=cos* (*126^o -90^o*). Then,

$$KN = a\cos\varphi\cos 36^o = LM.AM = AN + NM = a\cos\varphi\sin 36^o + \frac{3}{4}a.$$

Therefore, $MD = DL - LM = \frac{a}{4}\sqrt{7 - 16\sin^2\varphi} - a\cos\varphi\cos 36^o.$ Thus, we find also one express for segment *AD*

$$AD = \sqrt{MD^2 + AM^2} = \left[(\frac{a}{4}\sqrt{7 - 16\sin^2\varphi} - a\cos\varphi\cos 36^o)^2 + (a\cos\varphi\sin 36^o + \frac{3}{4}a)^2\right]^{1/2} \quad (2)$$

Comparing (1) and (2) after transformations, we obtain the equation for finding the angle φ for any a

$$\sin(63^o - \frac{1}{2}\arcsin\frac{\sqrt{7 - 16\sin^2\varphi}}{4\cos\varphi}) = \left[\frac{1}{2} + \frac{3}{8}\frac{\sin 36^o}{\cos\varphi} - \cos 36^o\frac{\sqrt{7 - 16\sin^2\varphi}}{8\cos\varphi}\right]^{1/2} \quad (3)$$

Solving equation (3) numerically, we find that the angle φ = 36°. Thus, the height of the lower part of the α-D-glucose molecule is φ = 0.058778 nm, the characteristic size of the upper base is 0.243 nm, and the characteristic size of the lower base is 0.243+2acos φ = 0.405 nm.

The angle of inclination of the side edges of the lower part of the model, as follows from the solution, is different from 90. This reflects in averaged form the presence of atoms in the conformations of the α-D-glucose molecule located quite close to the equatorial plane of the molecule [7-9].

The upper part of the α-D-glucose molecule above the carbon cycle should be depicted in the form of a pentagonal prism, direct-

ing the volatile bonds from the carbon atoms of the cycle vertically upward. This is consistent with the tetrahedral coordination of atoms around a carbon atom. Thus, the α-D-glucose molecule in a simplified three-dimensional form is a pyramid in contact with the carbon cycle with hexagonal and pentagonal bases and a straight pentagonal prism. If the hydroxyl group bonded to the atom $C_{(1)}$ lies on the pentagonal base of the prism, then a simplified image of the α-D-glucose molecule (α-anomer) shown in figure 4.

Figure 4: The spatial simplified images of the α-D-glucose molecule (α-anomer).

In the molecules of other pyranoses, the atoms or functional groups partially connected to the carbon atoms of the carbon cycle partially change. In this case, the structure of the molecules, up to functional groups, remains the same for glucose molecules in the pyranose cycle carbon atoms. Therefore, the dimension of molecules such as D-mannose, D-galactose, L-fucose is also equal to 15. Three - dimensional models of these molecules will retain their appearance, images are shown in figure 4.

Monosaccharide chains

Monosaccharide molecules combine with each other thanks to the combination of two hydroxyl groups with the release of a water molecule. The remaining oxygen atom connects the remaining part of the monosaccharides. The most common chains of α-D-glucose monosaccharide residues. In some cases, the carbon atom C(2) in the cycle will be involved in the compound. Branching chains of glucose molecules occurs at the sixth carbon atom in the functional group CH2OH. Using the obtained simplified three-dimensional models of α-D-glucose molecules (-anomer), we consider in more detail these compounds in a metric image, taking into account the angles between the valence bonds.

Let two α-anomers of the α-D-glucose molecule join together, linking the carbon atom C(1) of the first α-D-molecule to the carbon atom C(4) of the second α-D-molecule (maltose). Based on the geometric image in figure 4, you can imagine a top view of this connection (Figure 5).

Figure 5: Projections of α-anomer disaccharides.

It is easy to see that the same attachment of the third α-D-glucose molecule leads to a nonlinear arrangement of molecules when viewed from above on this compound. Nonlinearity will save with the following similar connections. Thus, the chain of molecules turns to the right. However, given the three-dimensionality of the image, you should look at this connection from a different view. Figure 5a shows an image of the junction of two α-D-glucose molecules when viewed from the front. The black segments in figure 5a are the traces of the intersection of the upper bases of the prism with a plane passing through the valence bonds of the oxygen atom and carbon atoms. According to the obtained solution of equation (3), the angle between the base of the prism and the valence bond is 36 degrees both the first α-D-glucose molecule and the second α-D-glucose molecule. Thus, on the figure 5a the angle 1H $C_{(1)}$ is 36 degrees and the angle $C_{(1)}OC_{(4)}$ is 112 degrees. Since, the angle $C_{(4)}$ O_2 is 36 degrees too, so the angle between bases 1H and O_2 is 14 degrees. This means that the base of the second α-D-glucose molecule has a consequently slope to the base of the first α-D-glucose molecule to the left. It is clear that such an addition of a third α-D-glucose molecule will increase the angle of inclination of this molecule relative to the first molecule. Thus, chains of α-anomers of α-D-glucose molecules rotate simultaneously in opposite directions in perpendicular planes.

Conclusion

Three-dimensional geometric metric models of the pyranose molecule and chains of these molecules, constructed on the basis of simplification of complete higher-dimensional models of such molecules, are studied in detail. It is shown that a simplified three-dimensional model of the pyranose molecule consists of two parts of a straight pentagonal prism and a pyramid with pentagonal and hexagonal bases connected by a carbon cycle. It was found that due

to the difference in the geometric three-dimensional figures that form the sugar molecule, the spiral chains of these molecules are characterized by a seemingly paradoxical property: rotation of the figures in two perpendicular planes in opposite directions.

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