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Adamantane as a Means of High Dimension, Preventing the Formation of the Beta-Amyloid

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Abstract

The structure of the adamantane molecule, which coincides with the unit cell of diamond, is constructed. It is proved that the dimension of the adamantane molecule is 9. This is more than twice the dimension of the adamantane molecule previously considered. The higher dimension of adamantane molecules indicates the higher dimension of the molecules of substances containing adamantane molecules in their composition, in particular drugs based on adamantane. In this work, it is shown that main part of adamantane itself, containing 10 active carbon atoms, can be a means of impeding the formation of beta-amyloids that play the main role in various diseases of nerve cells.

Keywords: Space; Simplex; Adamantane; Dimension; Structure

Introduction

Adamantane as a chemical compound was discovered in 1933 Landa S [1]. The adamantane molecule consists of 10 carbon atoms, repeating the arrangement of carbon atoms in the crystal lattice of diamond, and 16 hydrogen atoms, connected to carbon atoms by their unsaturated carbon atoms valence bonds. The discovery of adamantane served as an impetus for the development of the chemistry of organic polyhedranes. Adamantane derivatives have found practical application as drugs with different biological activity and for various purposes (antiviral drugs, antispasmodics, antiparkinsonian drugs, etc.): amantadine [2], memantine [3], rimantadine, tromantadine, etc. All these drugs repeat the structural group of carbon atoms, characteristic for adamantane, only the structural groups attached to the carbon atoms change. Among the inorganic and elemental-organic compounds, there are a number of structural analogues of the adamantane molecule, in which atoms of other elements act instead of carbon atoms. Moreover, between the atoms that are analogues of carbon atoms in the adamantane molecule, other atoms can be located that do not change the topological structure of the molecule. These compounds include Pb_4O_6, As_4O_6, Sb_4O_6, P_4O_{10}, P_4O_4, SiCl4, BcF_2, HgS, Ag2O, Cu2O, ZnS, Cu_2Cl [4]. Despite the wide distribution in nature of adamantane molecules and their analogues, it can be assumed that the structure of this molecule has not yet been sufficiently studied. It is well known that the elementary cell of the diamond, which makes up the main part of the adamantane molecule, was identified by various authors of three - dimensional polytopes of various forms: tetrahedron, octahedron and other polyhedrons [5]. In the future, it was found that the reason for such a variety is that the main part tof the adamantane molecule of 10 atoms has a dimension of 4, i.e. the highest dimension [6], which includes tetrahedrons, octahedrons, prisms, and pyramids as three - dimensional figures. However, due to the complexity of the image of the main part of the adamantane molecule on the plane, the composition of three - dimensional figures included in the main part of the adamantane molecule was not completely determined. This work is devoted to clarifying the result of 10 years ago, it shows that the dimension of the main part of the adamantane molecule is much higher and equal to 9.

The Structure of the Main Part of the Adamantane Molecule

Let us denote 10 atoms of the main part of the adamantane molecule by symbols $a_1,\ldots,a_{10}$. Let us take into account [6] at 6 atoms ($a_2, a_3, a_4, a_6, a_8, a_9$) out of these ten atoms are located in the centers of the flat faces of the three - dimensional cube (thin black lines in Figure 1), and each of the four remaining atoms (a_1, a_5, a_7, a_{10}) is equally removed from the three nearest centers of the flat faces of the cube and the corresponding common to these faces vertices of the cube.

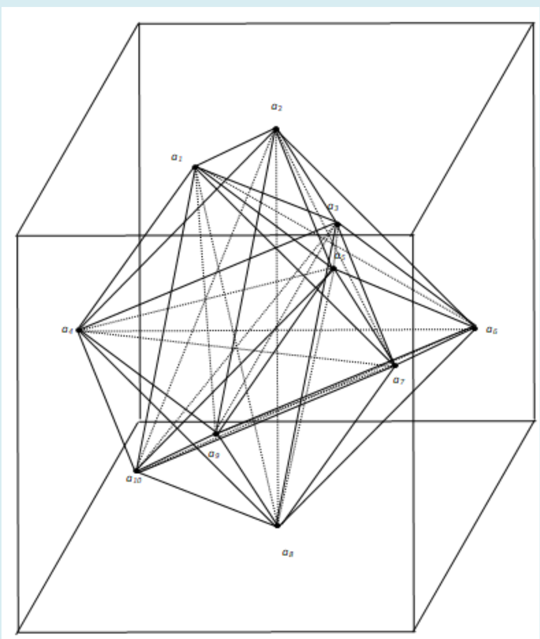

Figure 1: The structure of main part of adamantane molecule.

Let us connect with black lines the atoms equidistant from the three nearest flat faces of the cube with the centers of these flat faces of the cube. This creates edges $a_1a_2, a_1a_3, a_1a_4, a_5a_2, a_5a_6, a_5a_9, a_7a_3, a_7a_6, a_7a_8, a_{10}a_4, a_{10}a_8, a_{10}a_9$. We also connect the atoms in the centers of the flat faces of the cube closest to each other with thick black lines. This creates edges $a_2a_4, a_2a_6, a_2a_9, a_2a_3, a_3a_4, a_3a_6, a_3a_8, a_4a_8, a_4a_9, a_9a_8, a_9a_6, a_8a_6$. In addition, let's connect with thick black lines the atoms equidistant from the corresponding three nearest flat faces of the cube. This creates edges $a_1a_5, a_5a_{10}, a_5a_7, a_1a_{10}, a_1a_7, a_7a_{10}$. The total number of edges is 30. They make up the polytope shown in Figure 1.

As you can see, the polytope in Figure 1 contains a number of three - dimensional figures inside, in particular 5 tetrahedrons, 8 octahedrons, and, in addition, many prisms with triangular bases (trigonal prisms). Each octahedron forms a complex with six trigonal prisms. These prisms break down into pairs of prisms. Each pair of prisms has a rectangular face that coincides with one of the three rectangular sections of the octahedron. Therefore, 48 trigonal prisms are possible here. Each complex of an octahedron with trigonal prisms is included in the total set of such complexes, in general, forming a rather complex formation of combined three - dimensional figures. It should be noted that the combination of three - dimensional figures is a common property of higher - dimensional polytopes. To determine the dimension of polytopes of higher dimension, the Euler - Poincaré equation is usually used Poincaré [7].

$$\sum_{i=0}^{n-1}(-1)^i f_i(n) = 1+(-1)^n, \qquad (1)$$

where f_i is the number of geometric elements with the dimension i, and n is the dimension of the polytope *P*.

With a large number of elements of different dimensions included in the polytope, it is rather difficult to use equation (1). This requires an unambiguous and accurate recalculation of all elements of different dimensions. However, another way can be used, which, in particular, was used in the previous works of the author on the study of the garnet structure [8,9]. It consists in bringing it closer to the polytope, the dimension of which is determined by a simple algebraic formula, without changing the number of vertices of the polytope. This can be done, for example, by increasing the number of edges of the polytope. After all, even in simpler cases, the edges of a polytope are determined from the condition of giving the figure under study a closed convex form [8]. In this case, in Figure 1, 6 edges emanate from each vertex of the polytope to other vertices. It is enough to add edges to this figure so that 9 edges come out of each vertex, i.e. each of the 10 vertices was connected by an edge to all the other vertices of the polytope. Then the polytope takes the known form of a simplex - type polytope [8]. Additional edges in Figure 1 are indicated by thin dotted lines. The dimension of a simplex polytope is one less than the number of polytope vertices [8]. Therefore, the dimension of the polytope in Figure 1, taking into account the dotted lines, is 10 - 1 = 9.

The number of faces of different dimensions i in a simplex polytope of dimension n is determined by the formula [8,9].

$$f_i(n) = C_{n+1}^{i+1}, i = 0,1,2,\ldots,n. \qquad (2)$$

In accordance with this formula, for example, there are 20 vertices, 45 edges, ${C_{10}}^3 =$ 360 two - dimensional faces (triangles), ${C_{10}}^4 = 210$ three - dimensional faces (tetrahedrons) in the Adamantane structure. The Euler - Poincare equation (1) is valid for a simplex polytope of any dimension [8]. Therefore, it also holds for a Adamantane structure of dimension 9. This proves that the constructed Adamantane structure is a polytope.

Since adamantane molecules are included in many drugs, this indicates a higher dimension of biological processes associated with the use of these drugs.

Creation of Chemically Inert Particles from Adamantane that Prevent the Formation of Beta-Amyloid

As follows from Figure 1 [6], the main part of adamantane has carbon atoms with free valences. Atoms a_1, a_5, a_7, a_{10} each have one free valence, while atoms $a_2, a_3, a_4, a_6, a_8, a_9$ each have two free valences. Saturated valence bonds connect the atom with the $a_2, a_3, a_4,$ atoms; the a_3 atom is connected to the atoms; the a_1, a_7 atom is connected to the a_1, a_{10} atoms; the a_5 atom is connected to the a_2, a_9, a_6 atoms; the a_6 atom is connected to the a_5, a_7 atoms; the a_7 atom is connected to a_6, a_3, a_8 ; the a_8 atom is connected to the a_7, a_{10} atoms; the a_9 atom is connected to the atoms; the a_5, a_{10} atom is connected to the atoms; the a_{10} atom is connected to the a_9, a_8, a_4 atoms. Thus, the main part of the adamantane molecule has 16 unsaturated valence bonds. These bonds allow at least 16 amino acid residues to be attached to the main part of one adamantane molecule. In the amino acid residue, there are also unsaturated valence bonds (Figure 2) at the carbon atom and at the nitrogen atom, along which amino acid residues are connected to each other in protein molecules.

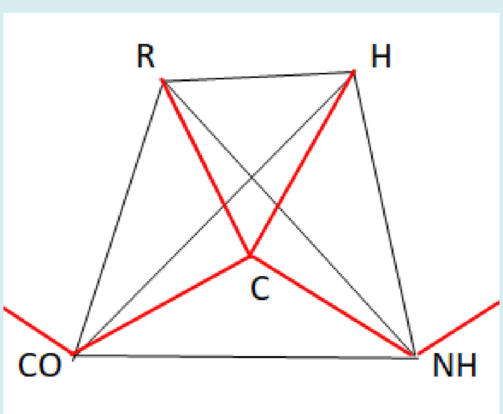

Figure 2: The structure of the residuum of the molecule amino acid.

When meeting with the main part of the adamantane molecule, one of the free valence bonds of the amino acid residue can be attached to adamantane, and the other free valence bond can be used to connect amino acid residues to each other. Thus, around the main part of the adamantane molecule, a shell is formed from amino acid residues with extinguished valence bonds. Therefore, a chemically inactive particle is formed based on the main part of the adamantane molecule. This will prevent the formation of amino acid polymer chains to form beta-amyloids.

Conclusion

It has been established that the structure of the main part of the adamantane molecule is much more complex than previously thought. The dimension of this structure is determined by reducing it to the well-known simplex polytope form. It is determined that the dimension of this polytope is 9. Adding various functional groups to the main part of the adamantane molecule only increases its dimension. Consequently, many drugs, which include adamantane molecules with different functional groups, have a higher dimension. It has been established that 10 carbon atoms in the main part of the adamantane molecule have 16 active (non-extinguished) valence bonds. At least 16 amino acid residues can join them. In this case, in addition, the amino acid residues, connecting with each other, form a chemically inert shell around the main part of the adamantane molecule. Thus, the main part of the adamantane molecule without functional groups added in various drugs can concentrate amino acid residues around itself, forming chemically inert particles, thereby preventing the creation of beta-amyloids, leading to the development of various prion diseases of nerve cells, such as Alzheimer's disease, Parkinson's disease, and other diseases [1,10-12].

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