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Quantitative Description of the Course of Chemical Evolution

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Abstract

Several variants of the quantitative description of the degree of complexity of the molecular structure are proposed. Complexity descriptors that allow quantitatively estimating the degree of evolutionary development of the chemical system are selected. A set of various descriptors is necessary to consider the various stages of chemical evolution from the synthesis of simplest organic molecules to the formation of supramolecular structures. The latter is especially important for tracking the evolutionary transition from the world of complex organic molecules to the world of living matter.

Keywords: Complexity of molecular structures; Molecular evolution; Descriptors; Quantitative description of evolution; Restrictions on the freedom of movement of objects in the chemical world

Introduction

A meaningful definition of the process of evolutionary development of the chemical world is given in the monograph [1] by E.M. Galimov. It differs significantly from the general insubstantial definition of evolution as the unfolding in time of any change in objects of the material, social and spiritual world. In [1] it was first proposed to define evolution as a spontaneous formation of more complex structures and properties of material objects from simpler objects by imposing restrictions on possible motions of these simpler objects. This definition of evolution is most suitable for describing the development processes in the physical and chemical world. In this paper, we will understand evolution only as such processes.

Further deepening of the molecular evolution concept was carried out in [2]. Specification of mechanisms of the evolution of organic molecules was done on the basis of methods of molecular modeling [3-5]. In [6] general regularities of the development of matter were revealed at the stages of nuclear, atomic and molecular evolution, up to the formation of supramolecules. In the same paper, physical conditions for the inhibition of evolution at the end of one stage and the transition to a qualitatively new stage of the development of matter were found.

All these features of the evolutionary process were considered on a qualitative level. However, at a conference devoted to the problems of the evolution of the early Earth and the biosphere [7], E.M. Galimov suggested that it is possible to reveal the general law of the evolutionary motion of matter. Naturally, the law must be a quantitative one in order to become a predictive tool for science. Such a law has not yet been revealed, but from Galimov's definition of evolution it follows that it must be based on a quantitative description of the complexity of material objects' structures.

In this paper, the task is to find suitable characteristics of the complexity of molecular structures to quantify the degree of evolutionary development of the chemical world. In [8] several approaches of quantitative description of the dynamic features of complex organic molecules were found. This experience extends not only to stationary electronic and vibrational states of molecules, but also to processes of chemical transformations. Therefore, the corresponding computer procedures may be used to achieve the goal set here. However, this apparatus is extremely complex, therefore, it cannot be used directly. On the basis of this apparatus, it is necessary to form integral generalized characteristics of the molecular structure complexity that are convenient for the rapid tracking of evolutionary events in the molecular world. Such characteristics can be similar to descriptors that are used in the QSAR system to track the molecular structure-activity correlation. A number of variants of these descriptors are necessary for considering various aspects of chemical evolution, such as increasing or suppressing the propensity of the participants in the system to join the reaction, the propensity to run photochemical reactions, and the propensity to form supramolecules. The latter is especially important, since the transition from the world of complex organic molecules to the world of living matter goes through biopolymers and supramolecules.

Various descriptors are offered, integrally reflecting different physical and chemical values of objects. It is assumed that these descriptors are additive ones. One can use the kinetic curves, as suggested in [4], but loaded with a certain descriptor. For instance, concentration of a component of the reaction mixture may be multiplied by the descriptor value of its molecule. Thus, the researcher of evolution will obtain a clear quantitative description of the historical process for a concrete chemical system.

The strategy of finding useful and speaking descriptors is based on the ideas of the most progressive evolutionists of the biochemical level. They believe that the goal of chemical evolution is the acquisition of specific functions by chemical objects [9]. We call such functions properties or activities. For example, an enzyme has the function of recognizing only a specific substrate and catalyzing of only one specific reaction. It is quite clear that such a function can arise only in an object with a very complex and original internal structure. For example, in may occur in a high-molecular protein. On the other hand, simple hydrocarbons are ready to participate in almost any organic reactions. Their functions are blurred. Therefore, the task is to find characteristics of the complexity as well as uniqueness of the chemical structure.

The Method of Searching for Descriptors

The construction of suitable descriptors is based on the calculation of physical properties of molecular structures. The algorithm of each such calculation is constructed as a summation of the properties of the structural elements of the molecule and on the account of the repeatability of identical elements. The latter reflects the well-known fact that the translation of identical atoms, bonds and atomic groups along the backbone of the molecule does not lead to the original properties of a large molecule.

The efficiency of the obtained descriptors is checked by comparatively simple molecules in order to compare the parameters of the complexity of molecules along the homologous series or a series of successive reactions. Simple structures will make it possible to see clearly whether the descriptors reflect the fact of the complication of structures that is clear to the chemist without any calculations. If successful, it will be possible to apply the found descriptors to complex model systems where evolutionary development takes place.

Below, for each descriptor, an algorithm for its calculation and illustrative examples of its application to relatively simple molecular structures are given.

Descriptor of Protons Mobility on the Outer Surface of a Molecule

In the equilibrium configuration, we calculate the moment of inertia I_0 of all the H atoms in the molecule. This is the norm of the inertia tensor of the proton coat of the molecule in the principal axes of inertia of the given fur. Heavy atoms are not included in this calculation, so as to not obscure the proton part of I_0 by large contributions from the skeleton of the molecule.

For each normal vibration, we find the most shifted configuration of the whole proton collective. We get a new value of I. It is important that this value depends on the displacements of all the atoms of the molecule. The proton coat obediently follows the oscillations of the skeleton and at the same time fluctuates itself.

The difference abs $(I - I_0)$ characterizes the average mobility of all protons in a given oscillation. This allows us to estimate the average possibility of a molecule to enter into various organic reactions by throwing some of its protons into a new potential well. Such are the ideas [8] about the physical content of the act of chemical transformation.

The descriptor is sum total of abs $(I - I_0)$ in all normal vibrations of the molecule. Thus, this descriptor includes all the complexity of the molecular structure. The more a molecule has normal vibrations, the more it has a chance to enter into some kind of reaction. However, the independent mobility of each proton in each normal vibration is also important. For example, in the folded structure of a globular protein, hydrophobic amino acid residues are hidden within the globule and cannot react with external agents. Therefore, for such amino acid residues, it makes no sense to calculate their contribution to this descriptor. But for protons of the active center of the enzyme, on the contrary, it is necessary to take into account all atoms that are turned inward into the cavity of the active center.

The Complexity of the Graph of the Valence Bonds of the Molecule

This descriptor is directly related to the complexity and originality of the internal structure of the molecule. We calculate it as follows.

For each coordinate of the valence bond stretching, we add the inverse masses of two bonds atoms multiplying by the reciprocal length of this bond. This characteristic is divided by the number of such bonds in the graph of the molecule. Then we find the sum of all such characteristics over all different bonds of the molecule.

The reciprocal masses of atoms characterize the mobility of a given bond in oscillations. That is, they have some connection to the possibility of participating in chemical transformations. The inverse length of the bond characterizes the importance of this bond in the overall structure of the molecule. The similarity of many valence bonds reduces the degree of originality of the structure. For example, the complexity of a true crystal is close to zero, as is its evolutionary potential.

The Complexity of the System of Natural Vibrational Coordinates

In the matrix of the kinetic energy of the molecule, the diagonal element related to the stretching of the valence bond is multiplied by the reciprocal length of this bond. We find out all similar bonds and divide the obtained characteristic by the number of these bonds. The diagonal element of any angular coordinate is divided by the number of such elements. The obtained characteristics are added together. It makes a general characteristic of the complexity and originality of the system of vibrational coordinates.

We expect that these two last descriptors will work particularly well when they are counted for a protein that already forms a secondary structure by including a few sulfur bridges and hydrogen bonds between distant regions of the primary structure of the protein. A homogeneous system of peptide bonds in the skeleton of the protein will give an almost zero contribution to these descriptors.

Activity in the IR spectrum

This is the sum of the absolute intensities over all normal vibrations of the molecule. It characterizes the behavior of the molecule in its contacts with the external environment and with the field of thermal radiation. This activity of the molecule has to do with photochemistry.

Descriptors Working Capacity

We present the results of calculations performed on a material of simple organic compounds. Table 1 shows the descriptors for individual compounds.

Chemical compound	Chemical formula	Protons mobility	Graph complexity	Vibrational coordinates complexity	IR activity
Hydrogen	H_2	3.72	2.18	2.18	0
H_2O monomer	H_2O	5.67	0.61	3.44	194.9
Methane	CH_4	22.44	0.27	0.65	66.9
Ethane	C_2H_6	41.42	0.31	1.697	64.8
Ethylene	C_2H_4	23.30	0.42	4.57	67.6
Acetylene	C_2H_2	13.01	0.725	1.09	117.1
Propane	C_3H_8	63.86	0.79	5.35	109.4
Propylene	C_3H_6	53.2	2.27	18.37	95.1
Allene	C_3H_4	32.53	0.35	4.73	86.4
Methyl-acetylene	C_3H_4	34.5	1.79	3.56	86.5
Butane	C_4H_{10}	87.3	0.49	5.10	150
Isobutane	C_4H_{10}	106.4	1.25	3.13	124.7
Methyl-allene	C_4H_{10}	74.2	0.93	12.0	110.5
Butadiene	C_4H_6	53.81	1.03	7.46	125.6
Dimethylacetilene	C_4H_6	57.26	0.413	1.91	59.54
Transbutene	C_4H_8	73.66	0.94	4.396	99.75
Hexane	C_6H_{14}	150.3	0.34	3.33	231.3
Cyclohexane	C_6H_{12}	129.8	0.11	0.61	240.8
Benzene	C_6H_6	66.8	0.21	0.763	85.5
Toluene	C_7H_8	94.9	0.732	3.7	102.6

Octane	C_8H_{18}	141.8	0.139	3.29	282.4
Isooctane	C_8H_{18}	202.3	0.079	0.49	184.1
Styrene	C_8H_8	115.0	0.88	12.2	163.2
Diphenyl	$C_{12}H_{10}$	126.9	0.249	0.939	151.7
Cyclohexyl-cyclohexane	$C_{12}H_{22}$	266.6	0.058	0.98	450.4

Table 1: Descriptors of the complexity of isolated organic molecules.

Let's pay attention to Octane and Isooctane in Table 1. An octane number is used for estimating the quality of car fuel. Octane burns quickly, but not so fast as to explode in engine cylinders. IsoOctane easily detonates because his entire hydrogen coat is very compact and exposed to the oxidizer. Everything lights up instantly and it turns out an explosion. The mobility descriptor H is exactly what it reflects. In all other senses, IsoOctane is simpler than Octane.

Our next task is to see what happens to the complexity of structures in the process of chemical transformations. We are not currently engaged in chemical kinetics and do not follow the dynamics of evolutionary changes in the chemical system. Table 2 compares the complexity of the initial participants of the chemical reaction with the complexity of the final products.

The reaction or result of a transformation chain	Reaction equation	Protons mobility before and after reaction	Graph complexity	Vibrational coordinates complexity
Methane + Methane = Ethane + Hydrogen	CH_4+ CH_4 = C_2H_6 + H_2	44.88 45.14	0.54 2.49	1.30 3.877
Ethane + Methane = Propane + H_2	C_2H_6 + CH_4 = C_3H_8 + H_2	63.86 67.58	0.58 2.97	2.347 7.53
Ethylene + Methane = Propylene + H_2	C_2H_4+ CH_4 = C_3H_6 + H_2	45.74 56.92	0.69 4.45	5.22 20.55
Acetylene + Methane = Methyl-acetylene + H_2	C_2H_2 + CH_4 = C_3H_4 + H_2	35.45 38.22	0.995 3.97	1.74 5.74
Methyl-acetylene + Methane = Dimethyl-acetylene + H_2	C_3H_4 + CH_4= C_4H_6 + H_2	56.94 60.98	2.06 2.593	4.21 4.09
Acetylene + 2 Methane = Dimethyl-acetylene + 2H_2	C_2H_2 + 2CH_4= C_4H_6 + 2H_2	57.89 64.7	1.265 4.773	1.95 6.27
Propane + Methane = Butane + H_2	C_3H_8 + CH_4 = C_4H_{10} + H_2	86.3 91.02	1.06 2.67	6.0 7.28
Ethane + Ethane = Butane + H_2	C_2H_6 + C_2H_6 = C_4H_{10} + H_2	82.84 91.02	0.62 2.67	3.39 7.28
Allene + Methane = Methyl-allene + H_2	C_3H_4 + CH_4 = C_4H_{10}+ H_2	54.97 77.92	0.62 3.11	5.38 14.18
2 Ethylene = Butadiene + H_2	2 C_2H_4= C_4H_6 + H_2	46.6 57.53	0.84 3.21	9.14 9.64
Ethylene + 2 Methane = Transbutene +2H_2	C_2H_4+2CH_4= C_4H_8 + 2H_2	68.18 81.1	0.96 5.3	5.87 8.756
Propane + Methane = Isobutane + H_2	C_3H_8 + CH_4 = C_4H_{10} + H_2	86.3 106.4	1.06 1.25	6.0 3.13
Propane + Propane = Hexane + H_2	C_3H_8 + C_3H_8 = C_6H_{14}+ H_2	127.72 154.02	1.58 2.52	10.7 5.51

Butane +2 Methane = Hexane + H_2	C_4H_{10}=$2CH_4$ = C_6H_{14} + H_2	132.18 154.02	4.85 2.52	9.46 5.51
3 Ethane = Hexane + $2H_2$	$3C_2H_6$= C_6H_{14}+ $2H_2$	124.26 157.74	0.93 4.7	5.09 7.69
2 Isobutane = Isooctane + H_2	$2C_4H_{10}$ = C_8H_{18} + H_2	212.8 206.02	2.50 2.259	6.26 2.67
2 Butane = Octane + H_2	$2C_4H_{10}$ = C_8H_{18}+ H_2	174.6 145.52	0.98 2.319	10.2 5.47
Benzene + Methane = Toluene + H_2	C_6H_6 + CH_4 = C_7H_8 + H_2	89.24 98.62	0.48 2.912	1.413 5.84
Hexane + Ethane = Octane + H_2	C_6H_{14} + C_2H_6 = C_8H_{18} + H_2	191.72 145.52	0.65 2.319	5.027 5.47
2 Propane + Ethane = Octane + 2 H_2	$2C_3H_8$ + C_2H_6 = C_8H_{18} + 2 H_2	169.14 149.24	1.89 4.499	12.397 7.65
Benzene + Ethylene = Styrene + H_2	C_6H_6 + C_2H_4 = C_8H_8 + H_2	90.1 138.3	0.63 3.06	5.333 14.38
2 Benzene = Diphenyl + H_2	$2C_6H_6$= $C_{12}H_{10}$ + H_2	133.6 130.62	0.42 2.429	1.526 3.119
2 Cyclohexane = Cyclohexyl-cyclohexane + H_2	$2C_6H_{12}$= $C_{12}H_{22}$+ H_2	300.6 270.3	0.68 2.24	6.66 3.16

Table 2: Changing the descriptors of the complexity of molecules in chemical transformations.

In Table 2, we draw attention to the various possibilities for constructing a complex structure via simpler ones. In [6] it was shown on a qualitative level that Nature is inclined to use ready-made complex structures for constructing even more complex objects. Of small objects, a large object is much more difficult to assemble. It seems that the complexity descriptors fully confirm this observation.

A Fragmentary Method for Computing Descriptors

When we turn to the structures of polypeptides and proteins, it will not be advisable to calculate each complex structure and its vibrational states anew. We suggest using the previously developed technique [10] for fragmentation of the vibrational equation of a complex molecule and extending this technique to the process of descriptors calculating.

Let's take into account that we construct each fragment as an artificial molecular structure which consists of a skeleton atom and some well-known radical. For instance, the fragment C-CH3 is a methyl-radical, connected to a carbon of some molecular skeleton. To obtain a complete ethane, we merge two such fragments. Our program removes two spare atoms C and constructs a correct spatial structure H3C-CH3.

So, we prepare fragments of a complex molecule. Their complexity can be characterized using descriptors. Then we connect the fragments using standard programs. A structure arises where there are all the vibrational coordinates, except for the coordinate of the relative rotation of the fragments around the common bond. This coordinate can be restored if desired. Then the descriptors of a finite complex structure can be accurately calculated by the method described above. But we can perform an approximate calculation without taking into account the internal relative rotation of the fragments in the final structure. Let us compare these descriptors with the result of a simple summation of the descriptors of individual fragments that have entered the final structure. Table 3 shows the results of this comparison.

Chemical fragment or compound	Chemical formula	Protons mobility	Graph complexity	Vibrational coordinates complexity	IR activity
C-Methyl	$C-CH_3$	18.4	0.49	1.64	31.4
C-Vinyl	$C-C_2H_3$	21.4	0.64	10.1	87.2
C-Phenyl	$C-C_6H_5$	54.5	0.37	1.75	73.9
Toluene without inner rotation	C_7H_8	94.2	0.73	3.26	107.1
Toluene with inner rotation	C_7H_8	94.9	0.73	3.7	102.6
Styrene without inner rotation	C_8H_8	111.9	0.88	11.74	163.3
Styrene with inner rotation	C_8H_8	115.0	0.88	12.2	163.2

Table 3: Descriptors of fragments and finished molecules composed of fragments.

Table 3 shows that the idea of fragmentary calculation of descriptors is fully justified if the fragments have essentially different internal structures. When connecting homogeneous fragments, the complexity descriptors of the connection graph and the complexity of the vibrational coordinates will acquire overestimated values, since the repeatability of identical bonds in the final structure will not be taken into account. But this difficulty is easily circumvented by a small complication of calculation programs.

Application of Descriptors on the Example of Water Oligomers

In this series of calculations, we are looking for a path to really complex chemical compounds, up to proteins with their secondary structure. In the protein α-helix, the internal turns of the peptide skeleton are firmly fastened to the regular structure by their hydrogen bonding. And we should take into account the physical and chemical features of the hydrogen bond.

It turns out that even with the wide swings of the proton entering the hydrogen bond, it is very reluctant to react with external molecules. That simply because the proton is hidden inside the molecule, and does not stand out, as in the hydrogen coat of any hydrocarbon.

In hydrocarbons, we calculated the mobility descriptor of all H atoms in all molecular vibrations. This gave a generalized idea of the reaction potential of the molecule in all possible reactions of addition or isomerization. In accordance with [8], this mobility of protons also relates to the decomposition reactions. But in compounds with hydrogen bonds, we exclude the protons of these bonds from the calculation of this descriptor. We leave in calculation only external protons, ready to enter into various reactions. The remaining descriptors are calculated in the same way as in hydrocarbons.

When describing the "reactions" of oligomerization of water, there is also one feature, reflected in the tables 4-5. When the molecule of water enters the associate after the collision, nothing is released except the binding energy. Therefore, the reaction formulas in the tables 4-5 look simpler than in the table 2 for hydrocarbons, where two molecules are connected to a larger one, and H_2 molecule is necessarily released.

From these tables 4-5 it is clear that the descriptors behave somewhat capricious. This is perfectly understandable, since the ways of coupling the next water molecule to the water associate are not always the same. In general, from all the series of calculations, hydrocarbons and water oligomers, it is clear that different descriptors behave intelligently and from different aspects allow evaluating the evolutionary value of both substances and reactions involving these substances.

We note that during oligomerization the water IR spectrum changes differs from the spectrum of the dimer that is included in dense water or ice. The fact is that the kinks of the hydrogen bonds are responsible for the fairly wide range of their protons motions. In dense water, such wide fluctuations run into steric hindrances. Just now we are building models that are suitable only for describing phenomena in sparse water vapor, where oligomers fly almost freely. To construct descriptors for the evolutionary behavior of water associates, these models are more adequate, since ice is a crystal. And crystal growth has nothing to do with Galimov's evolution.

Chemical compound	Chemical formula	Protons mobility without H-bonds	Graph complexity	Vibrational coordinates complexity	IR activity
H_2O monomer	H_2O	5.67	0.61	3.44	194.9
H_2O dimer	$(H_2O)_2$	29.9	0.95	6.61	586.1
H_2O trimer	$(H_2O)_3$	47.1	0.53	3.59	905.4
H_2O tetramer	$(H_2O)_4$	79.5	0.37	2.61	1129
H_2O pentamer	$(H_2O)_5$	97.8	0.28	2.85	1353

Table 4: Descriptors of water and its oligomers.

Chemical reaction	Chemical formula	Protons mobility before and after reaction	Graph complexity	Vibrational coordinates complexity	IR activity
2 H_2O monomer = H_2O dimer	$H_2O + H_2O = (H_2O)_2$	11.34 29. 9	1.22 0.95	6.88 6.61	389.8 586.1
H_2O dimer + H_2O = H_2O trimer	$(H_2O)_2 + H_2O = (H_2O)_3$	35.57 47.1	1.56 0.53	10.1 3.59	781 905.4
H_2O trimer + H_2O = H_2O tetramer	$(H_2O)_3 + H_2O = (H_2O)_4$	52.77 79.5	1.14 0.37	7.03 2.61	1100 1129
H_2O tetramer + H_2O = H_2O pentamer	$(H_2O)_4 + H_2O = (H_2O)_5$	85.17 97.8	0.98 0.28	6.05 2.85	1323.9 1353

Table 5: Behavior of Water descriptors in oligomerization processes.

It can be seen from Tables 4 and 5 that the behavior of descriptors in the oligomerization of water is quite predictable, since the complexity of these simple compounds can be estimated at a glance.

Approximate Calculation of Descriptors

When moving to the main task - to assess the complexity of protein structures – we will have to deal with 20 different structures of amino acid residues. We do not have exact data on the force fields of these various compounds. Therefore, we are forced to confine ourselves to approximate estimates of the vibration frequencies and displacements of the atoms in these compounds. It makes sense to check how much we will be mistaken in the descriptor estimates if we borrow the coordinates of the atoms from the data obtained by means of ChemOffice programs. The power constants can be assigned only to diagonal cells of potential energy matrices, being guided by the correlation [8] between the bond length and the value of the power constant. We will carry out a check on the material of the compounds already studied. Let's compare the exact values of the descriptors from Table 1 with approximate values given in Table 6.

Chemical compound	Chemical formula	Protons mobility	Graph complexity	Vibrational coordinates complexity	IR activity
Methane	CH_4	22.44 24.67	0.27 0.27	0.65 0.65	66.9 81
Ethane	C_2H_6	41.42 42.62	0.31 0.31	1.69 1.69	64.8 94.2
Ethylene	C_2H_4	23.30 26.4	0.42	4.57	67.6 102

Acetylene	C_2H_2	13.01 13.03	0.725	1.09	117.1 113
Propane	C_3H_8	63.86 65.7	0.79	5.35	109.4 123
Propylene	C_3H_6	53.2 54.6	2.27	18.37	95.1 125
Allene	C_3H_4	32.53 36.36	0.35	4.73	86.4 99.3
Methyl-acetylene	C_3H_4	34.5 39	1.79	3.56	86.5 100
Octane	C_8H_{18}	141.8 147.7	0.139	3.29	282.4 288.7
Isooctane	C_8H_{18}	202.3 209.7	0.079	0.49	184.1 295

Table 6: Exact and approximate values of descriptors.

On the example of the compounds given in Table 6, it is clear that the exact and approximate calculation of the descriptor of the mobility of the H atoms yields very close values. The activity of the compounds in the IR spectra is estimated in an approximate calculation much worse. Therefore, in complex compounds, an approximate calculation of this descriptor will be less suitable for analyzing the complexity of their behavior in electromagnetic fields. The descriptors of the complexity of the bond system and vibrational coordinates are always calculated exactly, since their values do not depend on the force and electro-optical fields of the molecule. Therefore, turning to the analysis of such complex compounds as proteins, we can use very approximate calculations of three descriptors to assess the complexity of these compounds.

Applying Descriptors During Modeling of a Primitive Genetic Code

In [11], we had modified the scenario [1,3] of the spontaneous emergence of primitive genetic code in the world of amino acids, nitrogen bases and ATP. In the same paper the physical quality of various "syllables" of the polypeptide "text" [12] was added. It leads to a gradual complication of polypeptide structures during the evolution of the chemical world. The complication is due to the fact that adjacent amino acid residues with complex radicals exert stronger resistance to the destructive effect of thermal motion. The results of computer imitation are shown in Table 7.

Such an experiment was carried out for the simple world of amino acids where particles collide during thermal motions. Collisions lead to autocatalytic grows of polypeptide chains (in computer algorithm they are allowed to grow up to ten links). On the other hand, thermal motion randomly demolishes long chains containing weak syllables. The computer program counts historical time in steps, i.e. as facts of productive reactions among random collisions in the chaotic world. It was shown that polypeptide chains tend to lengthen spontaneously, get decomposed, grow again, and become thereby complicated in the informational aspect. In Table 7, complexity descriptor is the vibrational coordinates complexity. Other details of the experiment are given in [11].

It is significant that in composing and decomposing peptide chains, our algorithm ignores the complexity of the resulting texts. Full information on the complexity of any material randomly yielded by the program is counted as a side effect. Table 7 lists two parameters: the average complexity of all chains containing ten links and the average complexity of all amino acids that remain free.

Number of steps	Number of chains with ten links	Average complexity descriptor of chains with ten links	Average complexity descriptor of remaining amino acids
51	0	–	15.0 ± 10.3
107	0	–	14.8 ± 9.9
168	0	–	14.3 ± 9.8
232	0	–	13.3 ± 9.6
290	0	–	12.8 ± 9.4
349	0	–	13.1 ± 9.4
405	0	–	13.6 ± 9.8
458	0	–	11.4 ± 8.4
514	1	175.1	12.5 ± 9.6
557	3	168.5 ± 24.3	12.1 ± 9.4
588	4	176.8 ± 25.8	12.0 ± 10.0
626	5	183.0 ± 22.4	12.0 ± 8.6

Table 7: Dynamics of the accumulation of polypeptide chains and their complication at the simplification of the remaining unusable amino acid material.

Conclusion

On the material of simple organic compounds and water oligomers it was shown that the evolutionary development of a chemical system can be fully quantified with the help of proposed generalized integral descriptors. Simple molecular structures are easily evaluated by their complexity. The found descriptors in their behavior do not contradict the expert's opinion about the relative changes in the complexity of molecules in chemical transformations. This allows us to use similar descriptors for a quantitative valuation of the chemical world evolution. In particular, it has been shown that taking into account the interaction between radicals of amino acid residues makes it possible to confidently model the complication of the world of polypeptides and polynucleotides during the evolution of the primary genetic code.

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