Several Hypotheses and Regularities in the Chemistry of Highly Organized Substances

Valentin Aleskowskii

Department of Chemistry, St.Petersburg State University
Universitetskii pr. 2, Petrodvoretz, St.Petersburg, 198904, Russia

SUMMARY: It was found that level of structural substance organization, amount of embodied information, and consequently, substance properties are determined by the degree of the substance polyatomicity. This substantiates the fact that both covalent and noncovalent supermolecular individuals, which are the matter of the chemistry of highly organized compounds, fulfil the same general chemical but different specific regularities. Among the former there is extended Prust's law, which was re-established by the fact of production and identification of solids with the constant composition. It was also found that formation of any individuals is due to production and realization of a certain amount of information sufficient for their structural organization. Chemical modeling of biosynthesis was chosen as the common approach for developing the processes of production and realization of information. It was shown that well-known processes of chemical buildup (CB) and molecular self-assembling (MSA) are those chemical models. The application of announced regularities has opened up a new perspective to create chemical-information technology (CIT), allowing us to produce material resources making no perturbations in the planet ecosystem.

Introduction

In 1947 S. A. Shchukarev [1], having found that popular opinion on the nature of non-stoichiometrical compounds has no real basis, established the key regularities in the chemistry of multi-atomic substances, and in fact has predicted it. We assumed that phenomenon of non-stoichiometry is due to the absence of multi-atomic compounds of a definite composition in the nature (excluding those which are the products of biosynthesis). However if the latter can be produced in the organisms then we can produce them "in glass". This was proved in 60-ties experimentally: solid compounds with definite composition were obtained and identified (the review of earlier works is given in [2]). At the same time R. B. Merrifield [3] has synthesized individual supermolecular compounds and J.-M. Lehn [4] has obtained polymolecular associates – noncovalent "mild" supermolecular chemical individuals. Study of these new objects in many

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laboratories around the world has caused the appearance of chemistry of supermolecular compounds [5] and supermolecular chemistry [6], and then chemistry of highly organized substances (HOS) has been established, generalizing both theoretical and experimental data of these complementary chemical disciplines [7]. Therewith several hypotheses were adopted and the following are among them.

Proposed General Chemical Regularities

Key Hypothesis

The state of aggregation, physical, and chemical properties of the substance depend on the level of its structural organization, which is predetermined by the degree of polyatomicity of this substance. This becomes clear when comparing low-molecular, highly- and supermolecular compounds, consisting of $10^{??}$–$10^{??}$, $10^{??}$–$10^{??}$ and greater than $10^{??}$ atoms (for example of $10^{??}$ atoms of two or several elements respectively). In a brief, nature of the substance is determined by the degree of its polyatomicity and consequently, by the amount of embodied information, i.e. property C is a function of amount of information I, or C = f(I)

Law of the Definite Proportions, Structure, Mass, and Information of Chemical Individuals

Why low-molecular individuals are formed in chemical synthesis without significant difficulties while synthesis of highly- or supermolecular solid compounds is always yielded in non-stoichiometrical compounds, comprising corresponding solid solutions? The matter is that these compounds are multi-atomic individuals, consisting of extremely huge amount of atoms. However from the multitude of atoms of two or several elements uncountable amount (for example N) of various compounds can be formed, which are practically indistinguishable one from another. Therefore the probability of formation for one of them in chemical synthesis (being a random process) P = 1/N practically equals to zero. At the same time probability of formation of the mixture of N possible compounds of these elements is P = N/N = 1. That is why in the synthesis of highly- and supermolecular multi-atomic and supermulti-atomic compounds the mixtures and solid solutions of chemical individuals but not chemical individuals are formed. They are usually assumed to be non-stoichiometric compounds [8]. Now we can draw the obvious conclusion: highly- and supermolecular chemical individuals are not formed in usual chemical reactions because of extremely low probability of their formation. In such a manner, those highly molecular and solid substances, which are in scientist's hands, are not chemical individuals. This is also proved by the fact that they do not obey Prust's law and thus the law works properly. When such is the case whether it is an appropriate time to leave

old illusions and to accept it. As the assurance in the validity of atomic-molecular theory exists there are no doubts that Prust's law should be re-established as the main law of chemistry. At the same time Shchukarev has shown that each chemical individual is the member of inconceivably huge family of innumerable multitude of related compounds (other compounds of these elements, homologues, and isomers) so that this law must be transformed into the law not only of definite proportions but also of definite structure, mass, and information. Moreover the law re-establishment in such or any other form might not be reserved for later time, because its discrimination continues to disorient both the science and technology.

Law of Individuals Formation

Formation of highly- and supermolecular individuals is, of course, not restricted in the nature. Chaos gives the way to the order in the process of the substance self-organization, when the structure and, correspondingly, certain amount of information are formed. It is known in theory of information that probability of an arbitrary event may be increased up to the limit by the cost of intake of sufficient amount of information. But what is the information? — This is the essence of the nature as a whole and of each thing separately, involved in one or the other individual structure. As a first approximation amount of information depends on the amount of those structural units, which form given structure. For example, it is discussed in [9]. During evolution, as self-organization proceeds from low-molecular to highly-molecular and then to supermolecular and even much more organized individuals — organisms, more and more multi-atomic (and consequently, more enriched with information) structures appear. So self-organization represents the process of information production and realization (IPR) in structured substances. Knowing how many atoms compose given structure and using combinatorial analysis, we can calculate number N, and according to Kholmogorov [10] can determine amount of information $I = \log N$ embodied in the given structure. For example, according to M. V. Volkenshtein [11], for polymer consisting of only 100 sections of two different types $N \cong 2^{100} \cong 10^{30}$. Using this N value in the formula we can learn that in the structure of not very multi-atomic highly molecular compound there is a great piece of information. And how much information is embodied in supermolecular compounds, consisting of more than 10^6, for example 10^{23} atoms? It seems to be easy to conclude that highly and supermolecular individuals by the content of information can be related to HOS. Obviously, to obtain HOS it is necessary to create the process where significant amount of information is produced. One of such processes is well known — it is biosynthesis. At the same time, the existence of above-mentioned CB and MSA processes as models for biosynthesis gives an indication that biosynthesis can be a prototype for artificial IPR processes. And it is not

necessary to get insight the most complex creation of the evolution. It is essential to know the principles and, if only in common, the mechanism of biosynthesis. We have started from the fact that biosynthesis is a programmable irreversible many-cyclic chemical process, occurring in the open system, where energy and substance arrive from the outside, and from where by-products and degraded energy are removed. For instance, genetic information embodied in the DNA macromolecules during biosynthesis is recorded onto many DNA copies and then onto RNA macromolecules. RNA delivers this information to the proteins. Amount of information increases with the number of DNA copies and RNA macromolecules (including the same information as each DNA has). This amount increases to a greater extension in translation processes (delivering information to proteins). It is particularly remarkable that production of information is performed by relatively simple processes of matrix biosynthesis and molecular self-assembling. Chemical models for these biological processes — CB and MSA have long been studied [5]. Thus we can state that formation of each individual is accompanied by production of a certain piece of information, which is necessary and sufficient for its structural organization. A part of this information embodied in the structure of this individual is introduced with the reagents. The greater is this part of information, the less is the energy T required for its synthesis. According to S. Ya. Frenkel [12] the matter is that $I \cdot T = \text{const}$.

Common Approach to the Individual Synthesis Organization

Individual as an object is characterized with the structure typical for it only, and consequently, with certain amount of information. Thus the goal of individual synthesis is creation of new or copying the known structure, if this individual already exists and the problem is its replication. In any case chemical modeling [5] of corresponding natural process (for example, biosynthesis) must be applied, assuming that probability to find better solution than evolution has found for billions of years is negligible. Copying the structures occurs in the processes of matrix biosynthesis, chemical model for which is above-mentioned CB method, while creation of new structures occurred by the biological self-assembling is modeled by MSA. Synthesis of individual is possible only at sufficient duration of all reactions and operations and at sufficient energy consumption. The main factors for such synthesis is amount of information I and duration τ.

Specific Regularities

Due to their polyatomicity surface of HOS is constructed from coordination unsaturated atoms that results in localization of the chemical reactions of the latter on this surface, i.e. in chemisorption. The Lengmur's theory and Shilov's conception of surface chemical compounds

describe regularities of chemisorption. Chemical parameters of HOS, in particular stoichiometrical, depend on its geometry.

Hyperbolic Dependence of HOS Properties on Their Supermolecule Size

As it was shown in the study of dispersed compounds, fibers, and films chemical activity, stability and some other properties of HOS (C) are linear function of their specific surface area s and, consequently, hyperbolic function of supermolecule size, i.e. C(s). It follows from the fact that $s = V / S = q / d$, where V is a volume, S is an area, d is a size, and q is a coefficient. Family of each HOS consists of n junior and in fact one senior member.

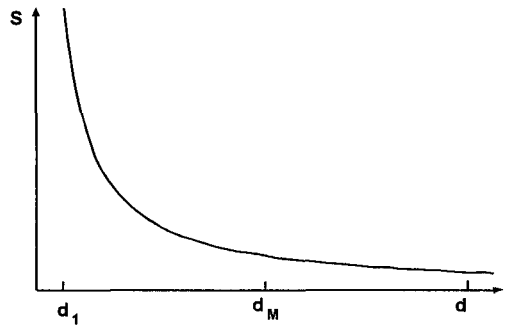

Fig. 1. Change of specific surface area s with the increase in size of solid.
d_1 is a size of first supermolecule m_1
d_m is a size of macroscopic supermolecule m_{n+1}

As it is seen from the figure, the junior members are dispersed particles, representing various compounds of the same elements, because specific surface area and, consequently, their properties are different. All other macroscopic members can be related to the senior one, having the same specific surface area that aligns their properties and makes it practically the same compound, nonetheless having no common features with the chemical individuals. If this would be known in due course the discrimination of the Prust's law would never be possible. It is also seen from this dependence that usual solid substances are supermolecular associates of multi-atomic compounds of one and the same elements, consisting of n dispersed and one macroscopic individual, i.e. of a finite amount of members: $N = n + 1$.

Core Model of Solid

Popular crystalline model of solids is extremely abstract. Such abstractness is necessary for physics, but not for chemistry of HOS, which should study any substances, not only solids, and which deals with concrete substances, having surface constructed from functional groups, but

not with abstract solids of unlimited size. Adequate model for solid supermolecule with definite composition, structure, and molecular weight [13] comes from the known theory of chemical structure at its extension for multi-atomic compounds. This is the core model [14]. Less-atomic radical R in this theory is replaced with multi-atomic core M. Dimensionality of the core D can vary from 1 to 3. Value D can be determined using formula $D = K - 1$, where K is coordination number. If $K > 4$ then the core is coordination structure. The core represents the system of atoms or atomic groups bonded one to another with covalent bonds. Periphery of the core is formed by functional groups A, B, C... Chemical bonds between the atoms in the core are relatively strong. Chemical structure of the simplest HOS is as follows.

Dimensionality of the core predetermines type of the structure independently on whether the substance is crystalline or not. Substances, having zero-, one-, two-, three-dimensional, or coordination core have the island, chain, layered, core, or coordination structures respectively, as it can be concluded from the universal structure classification [5]. Behaving as a structure-forming factor, the core provides stability and rigidity of the structure that makes it a long-lived carrier and under the certain condition – a transmitter of information. At the same time the core is a unique wave guide for electron, acoustic, and other waves that might be of a certain interest for specialists. Functional groups confer their functions on HOS, but do not predetermine will the HOS be information or semiconducting material or even solid chemical reagent, for example, a sorbent or a catalyst – this is the property of the core.

Stoichiometric Rules

Special stoichiometric rules are necessary in the HOS chemistry, because it mainly deals with the functional reactions, which proceed without core participation for the cost of functional groups only. These reactions are subjected to their own rules different from that established for low-molecular compounds. The rules are simple. The formula of supermolecular compound, consisting of three-dimensional core M and functional groups A, according to these rules is: $[M]_aA$. Here a is an amount of chemical equivalents. I.e. to introduce 1 equivalent of functional groups A in reaction we should take amount of solid reagents, containing a equivalents of M.

Applications

The possibility to produce and realize in the substance unlimited amount of information using chemical way brings close the perspective (predicted about 10 years ago) to transform technology of wealth production by the cost of non-material factor – information [15]. It is significant that IPR processes, like natural processes, make no perturbations in the biosphere. Therefore their development is the radical way to solve ecological problems. Chemical

modeling of biosynthesis promotes chemical modeling of photosynthesis and of the process of information perception and developing. Chemical model of biosynthesis is a group chemical-information process in aqueous solution, which program includes both definite and stochastic stages. Among the other variants is sol—structure process, where the role of structural units is played by the structured nanoglobules – sol particles included (in the CB process) in the system of concentric shells.

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