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Information Basis of Nanochemistry

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Abstract—The concepts of the information theory can be fruitfully used in nanochemistry. An asymptotic formula is presented for the number of different nanosystems of the same chemical composition. An estimate is given for the maximum value of the specific information capacity. A special attention is paid to the theoretical foundations of chemical-information synthesis. The problem of chemical replication of polyatomic systems is analyzed in the adiabatic approximation. The information aspect of operation of a configuration machine is considered.

INTRODUCTION

Nanochemistry studies systems whose dimensions in one, two, or three directions range from 1 to 100 nm. This dimension range corresponds to the limiting degree of dispersity at which a colloid system still retains one of its main properties, the heterogeneity [1]. The specificity of small systems is that the smaller particles of matter, the greater the role of surface phenomena in them [2]. Therefore, the theoretical concepts of colloid chemical are widely used in nanochemistry [3–6].

At the same time, nanofragments determine the specific properties of not only ultradisperse heterogeneous systems, but also homogeneous systems such as, e.g., glasses [7] whose properties depend on the middle-range order [8] caused by nanometer-ranged inhomogeneities [9]. Just the transitions of atoms over potential barriers in nanometer-ranged fragments [10] determine the specific abnormal low-temperature properties of glasses [11], as well as the boson peak [12–14]. Finally, nanostructures play an important role in the chemistry of highly organized substances produced by chemical-information synthesis [15–17]. All these facts demonstrate the necessity of using various theoretical concepts in nanochemistry, including the methods of the information theory [18].

Indeed, the theoretical foundations of chemical-information synthesis are being actively developed [15]. The information sense of the wave function Ψ has been established [19]. It has been shown [19–20] that the evolution of complex physical systems essentially depends on small perturbations, i.e., on signals suitable for controlling a system. In addition, the mathematically rigorous definition of the amount of syntactic information by Shannon [18] stimulates the formulation of the problem of the number of different nanosystems.

Information is not material, but it is manifested in the form of various material carriers: signs, signals, functions, etc. Different carriers can correspond to the same information. Among them, there are those providing the internal exchange of information in the course of microscopic processes. The detailed study of the mechanism of such exchange is also of principal importance for nanochemistry.

NUMBER OF DIFFERENT NANOSYSTEMS

There is no simple analytical expression to find the number G of different systems having equal chemical composition and consisting of M atoms. However, there is a simple asymptotic (at $M \to \infty$) formula

$$G \sim \exp(\beta_{\mathbf{n}} M), \quad (1)$$

where $\beta_{\mathbf{n}}$ is the specific information capacity [21] whose value depends on the chemical composition determined by vector **n**. The vector components are the relative concentrations n_i of atoms of each sort; they obey the relationship

$$\sum_i n_i = 1. \quad (2)$$

The problem of finding the number G [Eq. (1)] of different systems of equal chemical composition is closely related to the problem of recording the maximum amount $I^{(s)}$ of information. With some technical means, the amount I of recorded information can be varied only within a certain range

$$0 \le I \le I^{(s)}. \quad (3)$$

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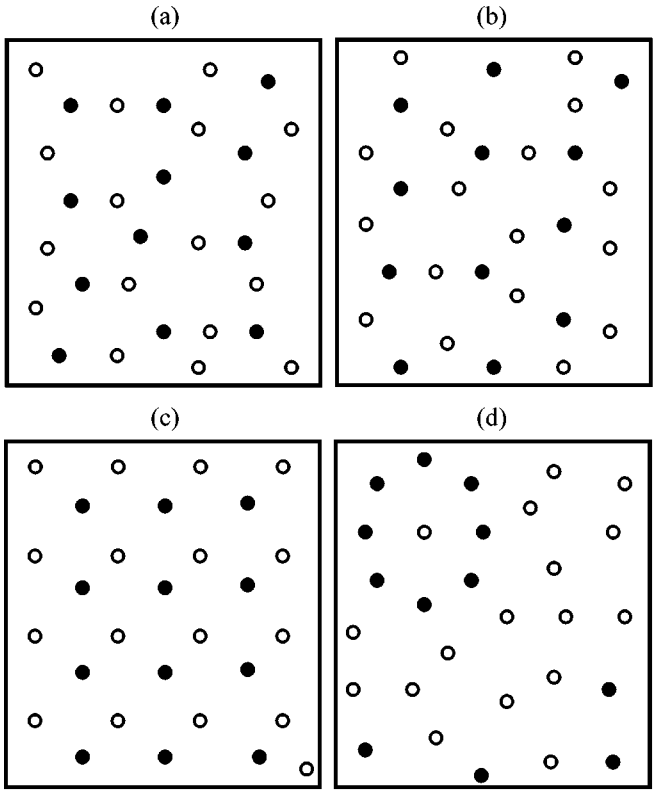

Fig. 1. Different nanofragments of equal chemical composition and locations of atomic nuclei of two kinds (denoted by *light* and *filled circles*). (a–d) For comments, see text.

According to Shannon [18], the upper limit $I^{(s)}$ is finite,

$$I^{(s)} = \log_2 G, \quad (4)$$

and, taking into account (1), is estimated as

$$I^{(s)} \sim M\beta_{\mathbf{n}}/\ln 2. \quad (5)$$

Here the quantities I and $I^{(s)}$ are expressed in bits, and $\beta_{\mathbf{n}}$ in nats [20], with the conversion factor of ln 2. According to (5), the ratio of the maximum amount of recorded information $I^{(s)}$ [Eq. (3)] to the number of atoms M is approximately equal to $\beta_{\mathbf{n}}/\ln 2$. That is why the positive parameter $\beta_{\mathbf{n}}$ [Eq. (1)] is termed the specific information capacity. This is one of matter characteristics like density, dielectric permittivity, etc.

Numerical values of $\beta_{\mathbf{n}}$ can be found from equations of quantum theory [21], but in this case a mathematically rigorous definition of "different systems" is required. We explain this notion by the example of several nanofragments of equal chemical composition (Fig. 1). Nanofragments in Figs. 1a and 1b correspond to a glassy substance, that in Fig. 1c, to a crystal, and that in Fig. 1d, to an amorphous substance. Fragments in Figs. 1a and 1c are evidently different. This is in agreement with the fact that a glass and a crystal are different substances. There is no such agreement in the case of fragments in Figs. 1a and 1b. On the one hand, they are not exactly identical [21]. It is impossible to bring the locations of their atomic nuclei in coincidence by moving one of these fragments as a whole (Fig. 1). On the other hand, the fragments in Figs. 1a and 1b correspond to glasses of equal properties: chemical composition, density, refractive index, etc. Such glasses are evidently identical.

Hence, the notions "different substances" and "different systems" are not identical. The quantity G [Eq. (1)] is the number of different systems of equal chemical composition which are not exact copies of each other. As applied to the nanofragments in Fig. 1, this means that their atomic networks cannot be brought into coincidence.[1] Different nanofragments can belong not only to different substances, but also to the same substance. Unfortunately, there are no clear criteria to unambiguously conclude whether the systems belong to different substances or to a certain single substance. For example, it is hard to say exactly how many defects should be added to an existing defect in the lower right corner of the nanofragment of a crystal (Fig. 1c) to obtain another substance.

Let us comment Eqs. (1) and (3)–(5). A question arises: When calculating G, should metastable systems with finite lifetime $t_{\max}$ be taken into account? This depends on the problem under consideration. The choice will affect only the numerical value of the parameter $\beta_{\mathbf{n}}$, but not the interrelation between the quantities in (1) and (3)–(5). Strictly speaking, the specific information capacity is a function $\beta(t_{\max}, \mathbf{n})$ of two arguments, $t_{\max}$ and $\mathbf{n}$ [21]. However, this and similar refinements cannot change the analytical form of Eqs. (1) and (3)–(5). Their versatility is caused by the fact that the number G [Eq. (1)] increases exponentially with the atom number M. This fact is not so surprising in view of a great diversity of different

[1] The criterion of coincidence of atomic networks is not always affirmative. For example, in the case of large systems, the mutual location of distant atoms can vary, due to atomic oscillations, in wide limits exceeding interatomic distances. In such situations, by exact copies are meant systems that are described within the framework of the same quasi-closed ensemble [21].

polyatomic systems. For example, even micelles exhibit polymorphism, namely, the existence of a number of structures and geometrical shapes caused by different packings of surfactant molecules [3]. Naturally, this set of substances includes not only all possible nanosystems, but also equilibrium and metastable liquids, glasses, ideal crystals, crystals with various concentration of defects of various types, polycrystals, amorphous substances, amorphous and glassy films, glass ceramics, microscopically inhomogeneous materials with information recorded in them, and many others. Finally, the set of substances under consideration explains the possibility of varying the properties of many practically used materials (e.g., glasses [7]) by changing the conditions of their preparation.

The specific information capacity $\beta_{\mathbf{n}}$ [Eq. (1)] as a function of the chemical composition **n** is bounded from both below and above:

$$0 \le \inf_{\mathbf{n}} \beta_{\mathbf{n}} \le \beta_{\mathbf{n}} \le \sup_{\mathbf{n}} \beta_{\mathbf{n}} \equiv B^{(\mathrm{I})}. \qquad (6)$$

We estimate the exact upper boundary $B^{(\mathrm{I})}$ proceeding from the number G_{gas} of different configurations realized in an ideal gas.[2] The position of each nucleus can be given approximately, with uncertainty δ, by indicating a small fragment v_0 in which a nucleus is localized (Fig. 2). We assume that each volume v_0 contains no more than one atomic nucleus. This does not restrict the generality of our approach, since the atomic nucleus coordinates are always determined experimentally with a certain error. Within the framework of the above assumptions, the number G_{gas} of different configurations is finite,

$$G_{\mathrm{gas}} = \frac{(V/v_0)!}{(V/v_0 - M)! \prod_i (Mn_i)!}, \qquad (7)$$

and equal to the number of permutations with recurrences of order V/v_0, where V is the gas volume.

Only a part of configurations of an ideal gas are realized in real polyatomic systems,[3] i.e., $G < G_{\mathrm{gas}}$. Therefore, taking into account (1), we can give the following upper estimate for $B^{(\mathrm{I})}$ [Eq. (6)]:

$$B^{(\mathrm{I})} < \frac{1}{M} \ln G_{\mathrm{gas}}. \qquad (8)$$

[2] Strictly speaking, the set of all possible physically nonequivalent atomic configurations is not countable and is a continuum [22].

[3] We remind [23] that, in an ideal gas, any atomic configuration, even crystalline, is realized with equal probability.

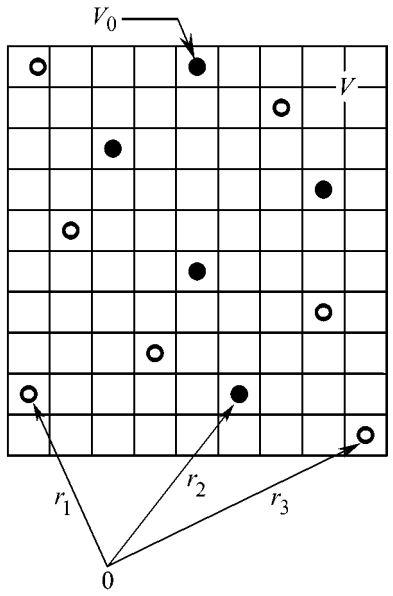

Fig. 2. One of atomic configurations realized in an ideal gas.

Substituting (7) in (8), we obtain, after transformations using Stirling's formula [24], the relationship

$$B^{(\mathrm{I})} < \left[\ln \frac{\gamma^{\gamma}}{(\gamma - 1)^{\gamma - 1}} - \sum n_k \ln n_k \right], \qquad (9)$$

where

$$\gamma = V/(M v_0), \text{ with } \gamma > 1. \qquad (10)$$

The parameter γ in Eq. (10) is equal to the ratio of the average volume per atom (V/M) to the volume v_0 of small fragments specifying, with error δ, the coordinates $\mathbf{r}_i$ of atomic nuclei (Fig. 2). Let $\gamma = 100$ and $n_1 = n_2 = \ldots = n_{10} = 1/10$. Then inequality (9) takes the form $B^{(\mathrm{I})} < 7.9$, which is in agreement with the estimate of the constant $B^{(\mathrm{I})}$ from (6),

$$B^{(\mathrm{I})} \approx 3, \qquad (11)$$

obtained beyond the framework of the ideal gas model [21].

CHOICE AND FIXATION OF STRUCTURE

Due to the permanent chaotic motion of particles, an ideal gas does not fix (does not store) a certain configuration determined in classical physics by vector **R**

$$\mathbf{R} = (\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_i, \ldots \mathbf{r}_M), \qquad (12)$$

where $\mathbf{r}_i$ are the radius vectors of the centers of the areas in which the atomic nuclei are localized (Fig. 2).

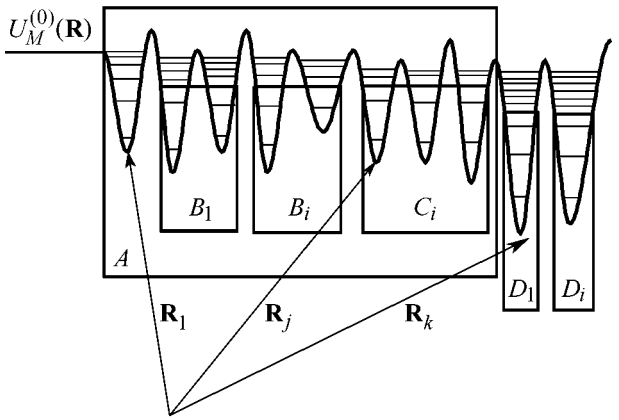

Fig. 3. Adiabatic electronic term $U_M^{(j)}(\mathbf{R})$. The rectangles A, B_i, C_i, and D_i show the potential wells determining different nanostructures $\mathbf{R}_j$ corresponding to a liquid, a glass, an amorphous substance, and a crystal. The horizontal line segments give the quantum state energies. The figure is rather conventional since, according to Eq. (12), the function $U_M^{(j)}(\mathbf{R})$ for polyatomic systems is given in a multidimensional space ($M >> 1$).

Even if, at a certain moment of time, a certain configuration (12) is chosen by measurement [25] (or self-measurement [19]), it is quickly forgotten as the system approaches the thermodynamic equilibrium. Just for this reason, a gas is never used for recording information. This is a stochastic system with zero information and maximum entropy [20].

Information is a fixed choice of a certain alternative of G possible alternatives.[4] The amount of information I in bits is determined by the right-hand side of Eq. (4). That is why it is easy to calculate I when one configuration (Fig. 2) of G possible (Fig. 1) is fixed (frozen). Such a freezing occurs in the course of vitrification [7]. Its essence, however, consists in the choice and fixation of one of G possible quasi-closed ensembles of glass [23], but not of a single configuration. Naturally, this does not influence the way of calculating I: Eq. (4) is suitable here also.

Certainly, the knowledge of the amount I of syntactic information is useful, but the number I itself does not allow us to judge the essence of information. That is why the semantic information is of particular interest. It is essential for nanochemistry that semantic information is inseparably linked with a certain structure [17]. The steric structures are fixed by interatomic and intermolecular interactions. For their adequate description, the adiabatic approximation is commonly used [27], based on the considerable difference of electrons and atomic nuclei in the mass.

At a fixed location of atomic nuclei, the internal energy of a system of M atoms is equal to the adiabatic electronic term $U_M^{(j)}(\mathbf{R})$. When the motion of atomic nuclei does not induce transitions between various electronic states, the function $U_M^{(j)}(\mathbf{R})$ can be interpreted as the potential energy of the nuclei, corresponding to the jth electronic state. In this case, the motion of nuclei proceeds in the potential field $U_M^{(j)}(\mathbf{R})$. We further resrtrict the consideration to the ground state of an electronic subsystem ($j = 0$). The corresponding adiabatic electronic term $U_M^{(j)}(\mathbf{R})$ is shown schematically in Fig. 3.

The equilibrium configurations correspond to potential wells [to minima of $U_M^{(j)}(\mathbf{R})$]. When they are realized, atomic nuclei are in the state of stable equilibrium. Therefore, just equilibrium configurations are suitable for the structure self-fixation and information recording. Like G [Eq. (1)], the number of equilibrium configurations is exponentially large. The following theorem [21] is valid for the number J of various physically nonequivalent local minima of the adiabatic electronic term $U_M^{(j)}(\mathbf{R})$ corresponding to the ground electronic state of an electrically neutral system consisting of M atoms at $M \to \infty$:

$$J \sim \exp(\alpha_{\mathbf{n}} M), \tag{13}$$

where $\alpha_{\mathbf{n}}$ is a positive parameter depending only on the chemical composition $\mathbf{n}$ [Eq. (2)].

At a low temperature, atomic nuclei practically do not overcome potential barriers around a minimum $\mathbf{R}_k$ if they are sufficiently high. Then the movement of atomic nuclei can be localized near a single minimum $\mathbf{R}_k$. The configuration $\mathbf{R}_k$ is thus fixed (frozen). In the general case, a system is described within the framework of one of G possible quasi-closed ensembles [21] allowing simultaneous localization of atomic nuclei near a number of minima (a number of potential wells) of the adiabatic electronic term $U_M^{(j)}(\mathbf{R})$ (Fig. 3). Therefore, the number G [Eq. (1)] of different systems of a fixed chemical composition does not exceed the number J [Eq. (13)] of minima:

$$G \leq J. \tag{14}$$

[4] Together with matter and energy, information is an indefinable term. According to mathematics, the primal notions (point, set, etc.) cannot be defined. With respect to them, only comments, explanations, etc., can be given. Various interpretations of the information notion are discussed in detail in [26].

A similar inequality relates the parameters $\beta_{\mathbf{n}}$ [Eq. (1)] and $\alpha_{\mathbf{n}}$ [Eq. (13)]:

$$0 \le \beta_{\mathbf{n}} \le \alpha_{\mathbf{n}} \le B \approx 3, \quad (15)$$

where B is the exact upper boundary of $\beta_{\mathbf{n}}$. The estimate of B is currently the same as that of $B^{(I)}$ [Eq. (11)] [21].

The relationships (15) give the ranges of the numerical values of parameters $\beta_{\mathbf{n}}$ [Eq. (1)] and $\alpha_{\mathbf{n}}$ [Eq. (13)]. This is useful even when discussing general methodological problems of nanochemistry. Indeed, synthesis of new nanosystems and experimental study of their properties, apparently, cannot be considered as the main goal of nanochemistry, as the number of possible nanosystems is too large. They all cannot be synthesized. Only the number G of different nanosystems of equal mass ($\sim 10^{-18}$ g) and a fixed ($\mathbf{n}$ = const, $M = 10^4$) chemical composition, with $\beta_{\mathbf{n}} = 0.02$, is $\exp(0.02 \times 10^4) \approx 7 \times 10^{86}$ according to Eq. (1). Their total mass ($\sim 7 \times 10^{68}$ g) considerably exceeds the mass of the Sun (1.984×10^{33} g [28]). Therefore, we shall always deal with individual "selected" nanosystems.

For example, the chemical assembling method [15] allows the synthesis of multilayer nanostructures as alternating, in a given order, silicon–oxygen and titanium–oxygen layers. The thickness of each layer is determined by the number of cycles of molecular layer deposition. The number of different multilayer nanostructures of equal composition is also determined by Eq. (1), but a smaller parameter $\beta_{\mathbf{n}}^{(\mathbf{i})}$ should be used in place of $\beta_{\mathbf{n}}$:

$$\beta_{\mathbf{n}}^{(\mathbf{i})} < \beta_{\mathbf{n}}. \quad (16)$$

Glasses of the SiO_2–TiO_2 system are obtained by another method, namely, by nonequilibrium cooling of a melt [29]. Naturally, such method is unsuitable for the synthesis of a multilayer nanosystem. The matter is that the probability of realization of any of multilayer nanosystems in a melt is practically zero since their fraction γ in the total number of all possible nanosystems is exponentially small according to Eq. (16):

$$\gamma \equiv [\exp(\beta_{\mathbf{n}}^{(\mathbf{i})} M)]/[\exp(\beta_{\mathbf{n}} M)] \to 0 \text{ at } M \to \infty. \quad (17)$$

Therefore, glasses are obtained, at cooling of a melt, as macroscopically isotropic systems [7].

For the synthesis of an anisotropic multilayer nanosystem, an information (program) determining the sequence of operations in the course of chemical assembling is required. That is why such syntheses are called chemical-information syntheses [15]. Their goal is to obtain highly organized chemical individuals [17] including, naturally, multilayer nanosystems.

The properties of chemical individuals are essentially different from statistically mean properties over the ensemble of all possible systems of a given composition. It is practically impossible to obtain chemical individuals accidentally. They are relatively few. They form an ensemble with a decreased configuration entropy [30]. The number of systems in this ensemble is determined by the same Eq. (1) as in case of multilayer nanosystems (16), but $\beta_{\mathbf{n}}$ should be replaced by the smaller nonnegative parameter $\beta_{\mathbf{n}}^{(\mathbf{i})}$.

The boundary between chemical individuals and other systems is not sharp. Therefore, it is appropriate to consider the problem of synthesis of chemical individuals within the framework of the more general problem of replication of an arbitrary polyatomic system.

INFORMATION ASPECT OF REPLICATION OF POLYATOMIC SYSTEMS

The carrier of full information on a system is, in particular, the system itself. It is impossible to obtain its exact copy without necessary information [21]. However, what is this information? What is its sense? First of all, data ($\mathbf{n}$, M) on the chemical composition [Eq. (2)] are required. Also, additional data are necessary to choose from a set of possible systems with a fixed chemical composition (synthesize) a system that is an exact copy of the initial system. We remind that the number G [Eq. (1)] of different polyatomic systems of equal chemical composition is exponentially large. Thus, for the replication of any nanosystem, it is insufficient to have the necessary chemical elements. An additional information is required, e.g., data on the structure $\mathbf{R}_j$ (Fig. 3).

The problem of replication would be largely solved if the procedure for reproduction of the structure $\mathbf{R}_j$ of any polyatomic system were known. Indeed, electrons adapt themselves to any configuration $\mathbf{R}$ [Eq. (12)] of atomic nuclei. Moreover, at a fixed structure $\mathbf{R}_j$, the electronic subsystem itself spontaneously and, as a rule, relatively rapidly passes form an excited state to the ground nondegenerate state. Thus, the ground state of the electronic subsystem is automatically reproduced in many cases. Sometimes, naturally, it is necessary to replicate not only the structure $\mathbf{R}_j$, but also the required state of the electronic subsystem.

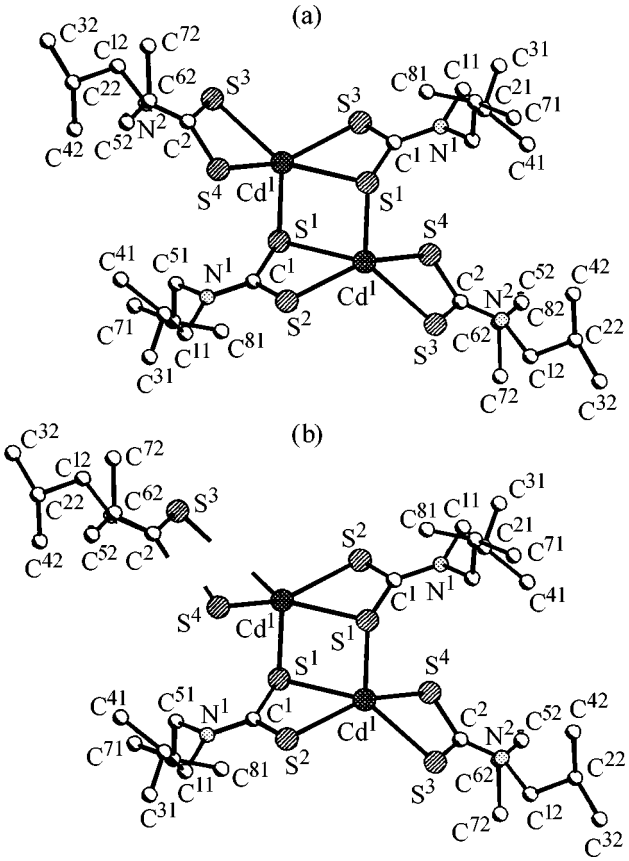

Fig. 4. (a) The dimer $[Cd(i\text{-}Bu_2NCS_2)_2]_2$ [32] and (b) two its fragments. The hydrogen atoms are not shown. The coordinates of the numbered atoms are given in [32].

But how can the fixation of a given configuration $\mathbf{R}_j$ of atomic nuclei be realized? Here, the notion of a hypothetical device, a configuration machine, is useful. In its operation, two aspects, material and ideal [31], should be distinguished. The first aspect is related to the procedure of changing along given trajectories the coordinates $\mathbf{r}_i$ (12) of the centers of areas in which the atomic nuclei are localized. The second aspect is related to the working program of the configuration machine, i.e., to information which is not material.

When the coordinates $\mathbf{r}_i$ [Eq. (12)] are known, they can be entered into the configuration machine in advance. Many works (see, e.g., [32]) are devoted to the experimental determination of $\mathbf{r}_i$. Of course, such data are available only for some of polyatomic system. They can be replaced by algorithms with the aid of which the configuration machine itself will compute the coordinates $\mathbf{r}_i$. Such algorithms are usually based on the mutual spatial correlation of atom locations [23]. The measure of algorithmic information is equal to the size (in bits) of the shortest computer program describing the tape of zeros and units as a record of a given information message [19]. There are also other useful algorithms, e.g., those programming the sequence of addition of single fragments to each other in the course of replication or describing in detail the multistage chemical-information synthesis [15]. The algorithms containing the randomizer subroutine deserve special attention. They allow adequate modeling of real chemical processes.

Since the reproduction and fixation of a given structure $\mathbf{R}_j$ is a chief job of the configuration machine, the amount of processed information is not smaller than the Shannon information amount I [18] corresponding to the carrier $\mathbf{R}_j$. The estimation of I is relatively simple. Indeed, the coordinates $\mathbf{r}_i$ are known with uncertainty δ. Therefore, they are given by a finite number of digits. The same is true for the vector $\mathbf{R}$ [Eq. (12)]. In the binary system, the vector can be represented as a certain sequence

$$\underbrace{011001100000101001000011111...}_{N}, \qquad (18)$$

consisting of finite number N of zeros and units with

$$N = kM, \qquad (19)$$

where k is the integer coefficient determined by the uncertainty δ of coordinates $\mathbf{r}_i$. According to Shannon [18], the sougth-for amount of information I (in bits) contained in sequence (18) is

$$I = \log_2 2^N = kM. \qquad (20)$$

The coefficient k [Eq. (19)] is usually of the order of 10^2. Then, according to (20), the numerical value of I, e.g., for nanosystems of $M = 10^8$ atoms, is of the order of 10^{10} bit. It is difficult to operate with so large amount of information. It is still more difficult to fix so large number, 10^8, of atomic nuclei in preset points.

This is not required when using chemical assembling [15]. In this case, the global structure $\mathbf{R}_j$ is formed by a sequence of irreversible reactions. They are localized in given regions and proceed in a strictly definite order. In other words, addition of single atoms or molecular fragments proceeds according to our program. Such manipulations form the essence of the work of a molecular assembler [33].

A question arises: Is it possible to make by molecular assembling an exact copy of any molecular system? Generally, it is not. The matter is that, in the general case, all atomic nuclei should be simultaneously fixed in given points. For example, to obtain the dimer $[Cd(i\text{-}Bu_2NCS_2)_2]_2$ (Fig. 4a) from two

isolated fragments (Fig. 4b), it is necessary, first of all, to reproduce and fix, for each of them, the same structures as in the dimer under replication. Then these fragments should be driven closer to each other. The result will be an exact copy of the dimer $[Cd(i\text{-}Bu_2NCS_2)_2]_2$. Evidently, the configuration machine can perform the above manipulations only if data on the coordinates of all atomic nuclei of the dimer are available. Without these data, the configuration machine is only able to drive the fragments closer, not maintaining the mutual location of atomic nuclei (the working regime of a molecular assembler). At such movements, the fragment configurations will change tending to equilibrium configurations, which are different from those depicted in Fig. 4b. Eventually, this will result, generally, not in the dimer $[Cd(i\text{-}Bu_2NCS_2)_2]_2$ (Fig. 4a), but in another system of the same chemical composition. This is not so striking taking into account Eq. (1).

It is quite natural that the entropy factor, caused by the exponentially large number J [Eq. (13)] of physically different nonequivalent minima of the adiabatic electronic term $U_M^{(j)}(\mathbf{R})$ (Fig. 3), impedes the microscopically reproducible synthesis of nanosystems. However, the variant multiplicity can be useful. Otherwise, there would be no information structures [34] used for information recording. The entropy factor plays an important role in formation of the middle-range order determining the functional properties of disordered systems. In particular, the unique optical and transport properties of glasses are caused by the structure of nanofragments and by their interaction. Finally, we can always hope that, among numerous [G, Eq. (1)] different nanosystems, there is a nanosystem with the required properties. Of course, its synthesis will also be hindered by the entropy factor. However, the entropy factor can be neutralized if necessary information is available.

CONCLUSION

Entropy is indeed one of fundamental notions of the modern science. The role of entropy is essential for the development of many branches of science. This cannot be said about information so far. We are at the starting stage of studying the information aspect of the microscopic mechanism of synthesis and replication of polyatomic systems. Already today, the development of chemistry sets the following problems: how to control chemical processes and how to conduct chemistry to obtain the required molecules and substances with required properties [35]. Any control implies the use of information.

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