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Biological and Chemical Research, 211-228 | Science Signpost Publishing

Unitary Symmetry of Atoms, Molecules, Codons, Mixtures and Its Applications in Chemistry, Genetics, Pharmacology and Early Diagnosis of Diseases

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Received: May 15, 2017 / Accepted: June 12, 2017 / Published: August 25, 2017

Abstract:

Nature is conservative in two main hypostases. **The first** is the combination of elements of one level of development of matter with the formation of a set of objects of the next, more complex, level of development of matter, which, in turn, is the initial set of elements for forming compounds of the next, more complex level of matter development.

This process with small transformations of a homeostatic character occurs in all natural and civilizational areas of development - from quarks to philology.

The second basic, conservative hypostasis of Nature is the parallelism of general regularities, manifested in the formation of each of the levels of development of matter, i.e. such features as homology (gradualness), hierarchy of interactions of elements in complex objects, normal distribution, symmetry, periodicity, etc. are repeated in a number of details and in physical objects and processes, and in chemical objects and processes, and in biological processes ... And even in philology and economics.

> If the **physicist Murray Gell-Mann** (He was awarded a Nobel Prize in Physics in 1969 for his contributions and discoveries concerning the classification of elementary particles and their interactions) knew all this, ...
>
> If chemists, biologists, physicians and educators understood, ...

Then in the early 60s of the last century, solving the inverse problem of combinatorics (representing a proton and a neutron in the form of a combination of invented quark-elements), **Murray would understand** that chemistry is a

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classical variant of the direct combinatorial problem - the nuclei of atoms consist of combinations Protons and neutrons with repetitions, the atoms consist of combinations of nuclei and electrons with repetitions, the molecules consist of atoms with repetitions and permutations.

Then Murray would understand that between protons and neutrons in nuclei, between nuclei and electrons, between electrons in atoms, between atoms in molecules, as well as between molecules in stationary mixtures (particles in plasma and reagents of chemical reactions), there exists Hierarchy of interactions, some of which can be compensated under certain conditions.

Then Murray would understand that combining elements of one level of matter development with the formation of a set of objects of the next, more complex level of matter development leads to the formation of two types of homologous series - homologies, formed as a result of replacing one element in a combinatorial object with another element from a certain set, which I call **homology of substitution,** and homologies, formed as a result of attaching a constant particle or a constant group of particles to a base formation (such as the length of a carbon chain). Such homology series can be called **the homology of adjunction.**

Then Murray would understand that the combinatorial sequences of homology of substitution can be divided into several groups of two-link homologies, when considering which, in certain physical conditions, compensation for some weak interactions appears in the space of physical parameters.

Then Murray would understand that in the relations of a physical parameter for combinatorial two-link homologous objects, the manifestation of compensation for certain interactions leads to the invariance of the relations of the physical parameter. And the symmetry corresponding to these invariants is Unitary Symmetry.

But Murray was a physicist, a narrow specialist in the field of elementary particles!

And **Chemists did not know** what combinatorics was, they did not know the theory of groups, they did not know that in addition to the homologous series formed by the principle of addition, there are homologous series formed by the principle of substitution. And, of course, they did not know how some interactions between the electrons and the nucleus in the atom and between the electrons in the molecule can be easily compensated.

Chemists were carried away by nonmeasurable (adjustable) coefficients in quantum models and by additive methods of estimating physical parameters.

About biologists and physicians and can not speak. In their knowledge, they are very far from the physical interpretations of combinatorics and group theory.

I'm in my article tries popular to talk about what is the basis of notions of unitary symmetry and its **critical applications in chemistry, genetics, pharmacology and diagnosis of diseases.**

1. Geometric Symmetry and Unitarian Symmetry. Similarities and Differences

1.a. Geometric Symmetry

A geometric shape of the object is symmetric if it can be divided into two or more identical pieces that are arranged in an organized fashion. This means that an object is symmetric if there is a geometrical transformation that moves individual pieces of the object but doesn't change the overall shape [1].

The symmetry in geometric space implies that:

- it is considered a **single object**
- **no physical fields** that could affect the shape of the object
- symmetry is manifested in keeping the shape of the object at different movements of the object **as a whole in the space of geometric coordinates** (+ time)
- invariants have to be **completely accurate**

1.b. Unitary (Parametric) Symmetry

The object on which I discovered a unitary symmetry represents the entire class of molecules, for example, halogenated methane. Fig. 1 shows the entire combinatorial set of compounds with the general formula $Y_oH_jF_kCl_mBr_nI_p$, where Y_o - subgroup carbon atoms, or other complex atomic structure.

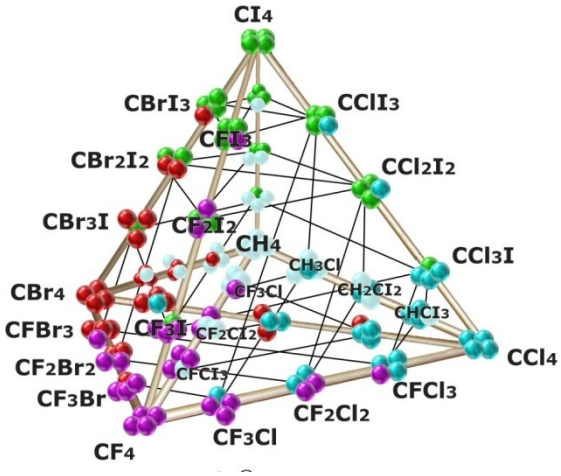


Fig.1. The structure of the homologous series of molecules with the general formula $Y_oH_jF_kCl_mBr_nI_p$, where Y_o - subgroup carbon atoms, or other complex atomic structure. The structure of the homologous series turned out to be the weight diagram that corresponds to the irreducible representations of the group SU (5).

In our case, a group of halogenated methane can be regarded as a kind of **Hyperobject**. Considering the Hyperobject is no longer in the geometric space, and in the space of its physical or chemical parameters, we can discover a change of its "form". But it turns out that there are certain constant relation for certain "parts of the Hyperobject"

The physical meaning of the constant relations lies in the fact that during the transition from one part of the "Hyperobject." (molecules) to another part of the Hyperobject strong interaction between electrons and the nucleus are still strong, but with "weak" differing from each other. This difference can be considered as a small correction "± additive" and it can be compensated when finding certain relations for the subgroup of neighboring atoms. (see Table 1):

Table 1. The system of equations for the replacement F-H. Before each chemical compound in order to save space omitted designations of some physical or chemical parameter of the molecule $CH_{4-n-m}X_nY_m$ (X,Y = F,Cl,Br,I . Or in a more general form $Y_oH_jF_kCl_mBr_nI_p$, here Y=C,Si,Ge,Sn,Pb). For some parameters, for which the geometric symmetry of the molecule does not play a big role, the equation with (*) and without ( ) can be combined.

Replacement: F ⟷ H	
1	CF3C1 - CF3Br = CH3C1 - CH3Br
1*	CHF2C1 - CHF2Br = CH2FC1 - CH2FBr
2	CF3Br - CF3I = CH3Br - CH3I
2*	CHF2Br - CHF2I = CH2FBr - CH2FI
3	CF3C1 - CF3I = CH3C1 - CH3I
3*	CHF2C1 - CHF2I = CH2FC1 - CH2FI
4	CF2C12 - CF2Br2 = CHFC12 - CHFBr2 = CH2C12 - CH2Br2
5	CF2C12 - CF2I2 = CHFC12 - CHFI2 = CH2C12 - CH2I2
6	CF2Br2 - CF2I2 = CHFBr2 - CHFI2 = CH2Br2 - CH2I2
7	CFC13 - CFBr3 = CHC13 - CHBr3
8	CFBr3 - CFI3 = CHBr3 - CHI3
9	CFI3 - CFC13 = CHI3 - CHC13

So the symmetry in the space of physical parameters of the objects (unitary symmetry) means that:

- it is considered a set of objects formed by one or more combinatorial operations over a number of homologous elements

- the original elements and the final formation of which are dealt with **under the force fields** and the corresponding hierarchy of energy interactions between all the elements of objects.
- symmetry is manifest in the form of **conservation of certain relationships** between combinatorial objects if we replace one element of the original homologous series ("ligand") to another member of the same series.
- **invariants are approximate,** but almost always more accurate in comparison with the experimentally measured due to the numerous intersections of homologous replacement series, which is mathematically expressed in solving a system of linear equations.
- one of the most important properties of the system of equations consists in the possibility of determining the values of the physical parameter of the entire group of combinatorial objects only over a small number of experimental values, i.e. **can be predicted**.

We can change the name of the physical space as you like. Hyperobject elements will change their location relative to each other. But compensatory ratios will remain the same. This is a remarkable property is the basis of unitary symmetry.

The above views are the basis for constructing a system of linear equations, which is in violation of the selected approximation exact symmetry describes all relations on the set of the parameter in question closed class of molecules.

For any molecule, one can select the corresponding family of homologous molecules (Hyperobject) and find the corresponding Unitarian symmetry invariants.

The main advantage of the system of invariants is the ability to calculate the values of the physical or chemical parameter for the entire "Hyperobject" only by a small number of experimental data. In doing so, **we obtain self-consistent values** on the set of molecules "Hyperobject"

This section is described in more detail and popularly in [2], the theoretical justification is given in [3] and [4]. Examples are given in [5].

2. Chemical Applications

2.a. Combinatorial System of Chemical Elements

The nuclei of atoms are the simplest objects in combinatorial chemistry. They are merely combinations of two nucleons with 2-3 repetitions of a proton (isotones) or neutrons (isotopes). An analysis of the hierarchy of interactions between nucleons in nuclei, which has been studied in detail, leads to an

understanding of the essence of unitary nuclear symmetry.For them, there are also invariants of the unitary symmetry. This, for example, invariants mirror nuclei (See Fig 2 upper graph).

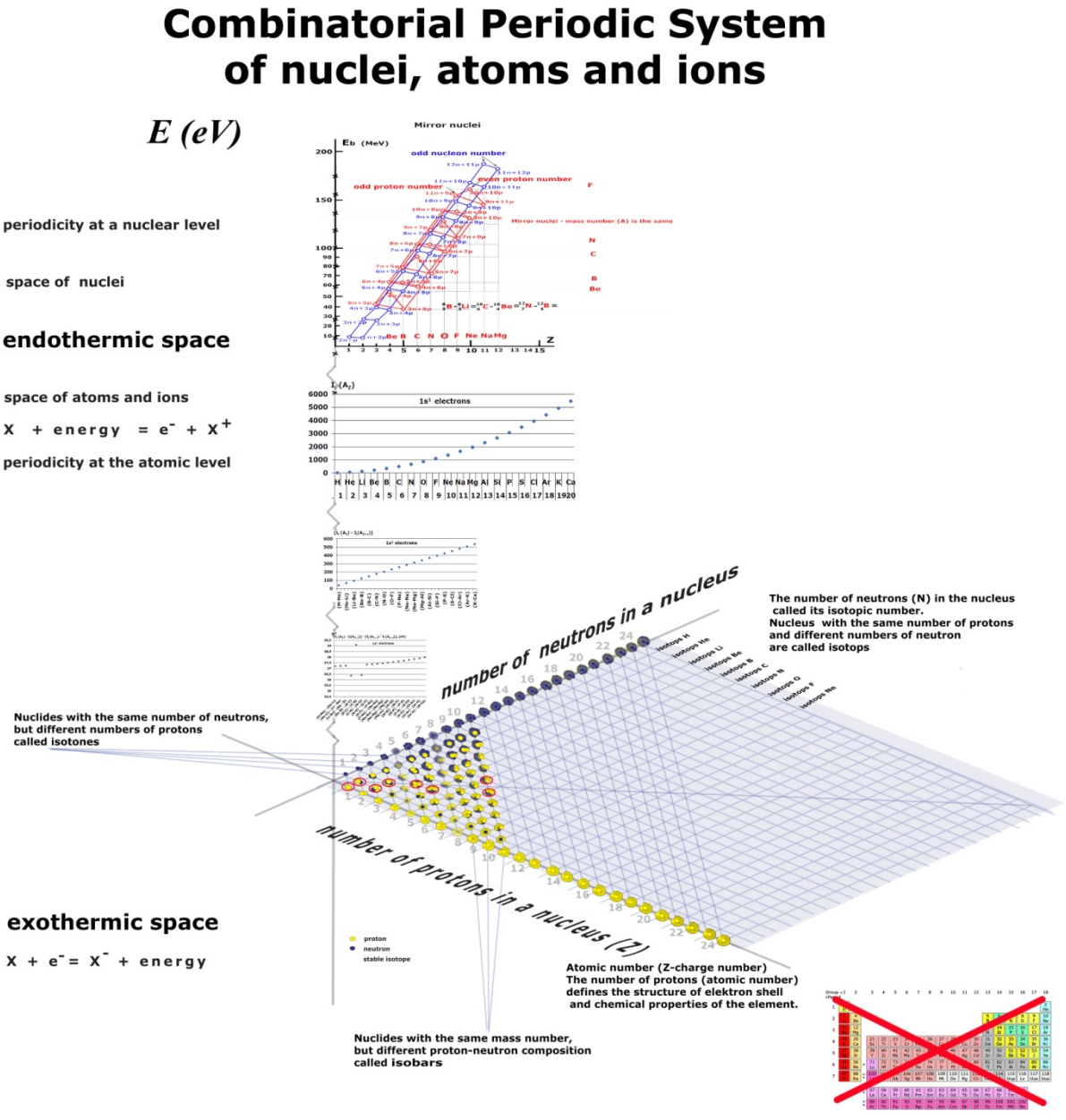


Fig.2. Combinatorial nuclei system of chemical elements, chemical elements itself and and ions. Here is one example of invariants for some mirror nuclei: $^{8}_{5}B - ^{8}_{3}Li = ^{10}_{6}C - ^{10}_{4}Be = ^{12}_{7}N - ^{12}_{5}B =$

They are located in the region of high energies. The energy range is 10-200 MeV.

Below are the energy space of the electrons in the atom. The third graph below shows Ionisation Energies (eV) of $1s^1$ electrons vs Z for atoms Z = 1 - 20. The energy range is 1000 -6000 eV. The second graph below shows the Ionisation Energies difference between the values of the $1s^1$ electron of two neiboring elements - $[I_i (A_Z) - I_i(A_{Z+1})]$, (eV) vs Z for atoms Z = 1 - 20. The energy range is 100 -600 eV. The Ionisation Energies difference between the values of the $1s^1$ electron of two groups of the neiboring elements - $[I_i (A_Z) - I_i(A_{Z+1})] - [I_i (A_{Z+1}) - I_i (A_{Z+2})]$, (eV).

As can be seen from the Fig. 2 the almost linear dependence:

$$[I_i (A_Z) - I_i(A_{Z+1})] - [I_i (A_{Z+1}) - I_i (A_{Z+2})] \text{ vs } [Z_i (A_Z) - Z_i(A_{Z+1})] - [Z_i (A_{Z+1}) - Z_i (A_{Z+2})]$$

$$\text{i.e. } [I_i (A_Z) - I_i(A_{Z+1})] - [I_i (A_{Z+1}) - I_i (A_{Z+2})] = \text{const} \quad (1)$$

here A is a chemical element.

Moreover, for the first two (apart from the nucleus) electrons constant in equation (1) is approximately equal to 27 eV, (two 1S electrons). It has previously been shown [6] that for third - tenth electrons this constant is about 7 eV (2S and 2P electrons), and for 11 - 15 electrons - about 3 eV. The experimental data are taken from [7].

The main thing is that these laws are easily detected "suspicious" (dropping out of the general trend) values for the differences of the ionization potentials (see Fig.2):

$$\{[\mathbf{I(Be) - I(B)] - [I(B) - I(C)]\},}$$

$$\mathbf{\{[I(B) - I(C)] - [I(C) - I(N)]\},}$$

$$\mathbf{\{[I(C) - I(N)] - [I(N) - I(O)]\}}$$

Ionization Energies for Be, B, C, N, and O atoms need to be refined.

Thus, for physical and chemical discrete objects, the combinatorial energy space can be constructed. It includes all the nuclei of atoms, the atoms and ions themselves. Moreover, the entire space consists of two spaces - a subspace where the energy expended (the upper part in Fig.2):

$$X + \text{energy} \rightarrow e^- + X^+ \quad (2)$$

and the subspace where the energy is released (the lower part of Fig. 2)

$$X + e^- \rightarrow X^- + \text{energy} \quad (3)$$

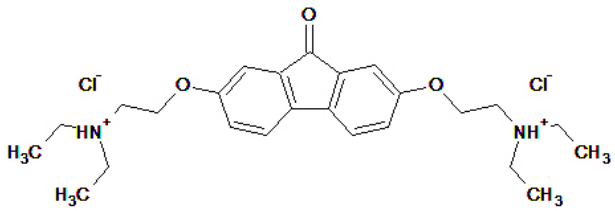
In its entirety, and a visual representation Combinatorial Periodic System differs from the well-known Periodic table of elements on the following parameters:

1. by **paradigm of natural evolution**, inherent to most objects of Nature - "a combination - selection - fixing"

2. by paradigm of natural existence, inherent in all objects of Nature - energy, with the consideration of discrete objects to the **hierarchy of energy interactions** of the particles to be combined in the formation of these objects
3. by representation of objects within a **mathematically formalized description of periodic law** as a system of simple equations representing conservation laws
4. by representation of objects in an explicit form the of **law of conservation of unitary symmetry,** not only for nuclei of atoms, the atoms themselves atoms and their isotopes, isobars and isotones but for atoms and ions as well.
5. by demonstration the functionality of the systems using **only the experimental data** (for example, the photoelectron spectra), without the use of approximations and assumptions of quantum mechanics.
6. 6. the present system is a ready-made **template when creating a New Database** for the nuclei, atoms and ions in place of the obsolete and overflowing with erroneous values the NIST base [6].
7. the present system is a ready **template when creating a new chemistry course**, which was built on the basis of Zipping and Spiralization of Educational information [9].

In addition, the represented system is much "smarter" as widespread Periodic table of chemical elements of the past two centuries.

The use of the notions of unitary symmetry of molecules is shown above using halomethanes as an example. For more complex molecules studied by pharmacologists, one can also use such representations. For example, for some chemicals may need to find New Stereoisomer form and. **predict such Multy Stereoisomer compounds.** For example, for such a compound as Tilorone:



may be the best in terms of biochemical activity of homologs, where CH_3 replaced by CH_2F group, CHF_2, CF_3 (the example unfounded in terms of Biochemistry). **Prediction of biochemical activity of such compounds are also part of the problem of unitary symmetry of molecules.**

2.b. Combinatorial System of Mixtures

As mixtures, both mixtures of molecules in a stationary state, as well as mixtures of atoms, ions, radicals and molecules can act at a certain time during the course of physical or chemical processes. In this

case, the "discrete objects" will be the proportion of the components. Fig. 3 shows the homology of the system for the five-component mixtures.

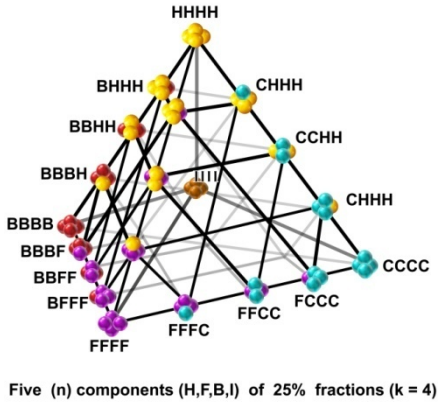


Fig.3. The structure of the homologous series of mixtures. The structure of the homologous series turned out to be the weight diagram that corresponds to the irreducible representations of the group SU (5). In order not to overload the graphic not all combinations shown here. Designations of the components - (H, F, B, I) - are chosen specifically to emphasize the commonality with Fig. 1.

The corresponding system of invariants is presented in Table. 2.

Table 2. The system of equations for the replacement of 25% fraction of F component on the same fraction of component H. Before each chemical compound in order to save space omitted designations of some physical or chemical parameter of the mixtures.

Replacement F ----- H	
1	**FFFC - FFFB = HHHC - HHHB**
2	**HFFC - HFFB = HHFC - HHFB**
3	**FFFB - FFFI = HHHB - HHHI**
4	**HFFB - HFFI = HHFB - HHFI**
5	**FFFC - FFFI = HHHC - HHHI**
6	**FFCC - FFBB = HFCC - HFBB = HHCC - HHBB**
7	**FFCC - FFII = HFCC - HFII = HHCC - HHII**
8	**FFCC - FFII = HFBB - HFII = HHBB - HHII**
9	**FCCC - FBBB = HCCC - HBBB**
10	**FBBB - FIII = HBBB - HIII**
11	**FIII - FCCC = HIII - HCCC**

As to the chemical process, the reactants can be represented as a curved line in a certain system of homology components. This opens up the possibility of describing the chemical reactions in the paradigm of combinatorics and the unitary symmetry of the mixtures.

As emphasized earlier [2], [7], [8]:

1. All physical property values for the entire class of combinatorial mixtures can be calculated using only a few experimental values

2. The values thus obtained will be mutually agreed upon

3. Erroneous values are easily identified, **thanks to the self-consistency (mutual intersection) homologous series.**

3. Genetic Applications

The building blocks of DNA and RNA are the set of five nitrogenous bases. These nitrogenous bases are adenine (A), uracil (U), guanine (G), thymine (T), and cytosine (C). These nitrogenous bases are the original discrete elements. The standard combinatorial problem implies the choice of combinatorial operations. Geneticists initially solved the reverse combinatorial problem - they were looking for combinatorial operations to match such a set of nitrogenous bases that would overlap the synthesis of 20 amino acids. Such a combinatorial operation turned out to be "Combinations with repetitions and permutations."

The complete homology structure is shown in Fig.4.

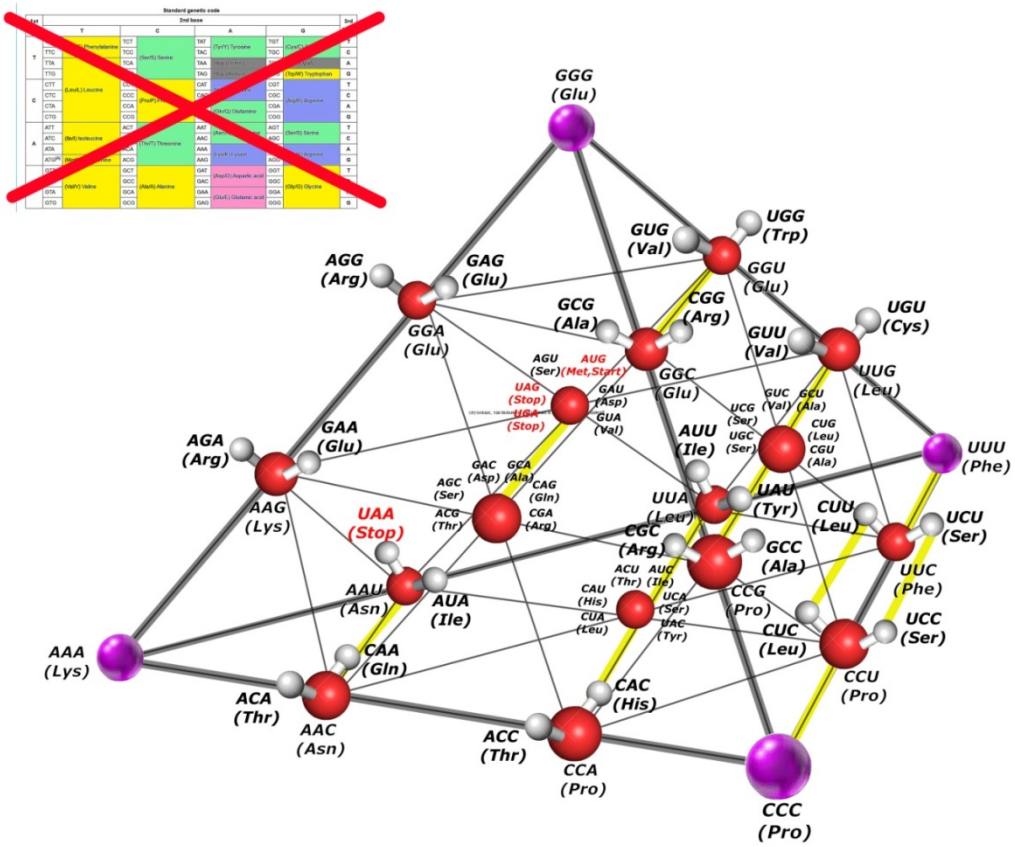


Fig.4. Combinatorial codons system of homologous series. Codons, specify which amino acid (in brackets) will be added next during protein synthesis. Yellow lines show the "related" transitions from one codon to another codon while replacing (C - U).

Given the above paradigm, the well-known archaic RNA codon table [10] should be replaced by the structure shown in Fig. 4. The possible transitions for the RNA bases are presented in Fig. 5.

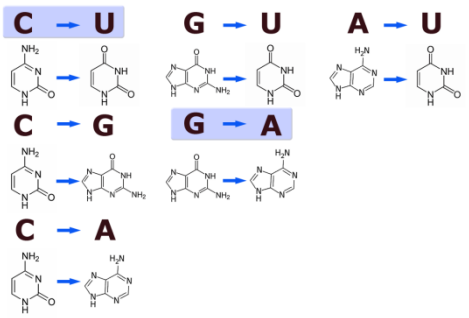


Fig.5. All the possible replacement of one nitrogenous base to the other. Shaded two changes relating to the "true" purine and "true" pyrimidine transitions. Adenine and guanine belong to the double-ringed class of molecules called purines Cytosine, thymine, and uracil are all pyrimidines.

By analogy with simpler molecules (combinatorial objects) for which the transition from one object to another, we observed invariance relations of a certain parameter (see. Table 1 in [2]), it would be logical to assume the existence of a certain invariance and in the case of biological combinatorial objects - codons.

In the form of invariants, these transitions look as shown in Fig.6.

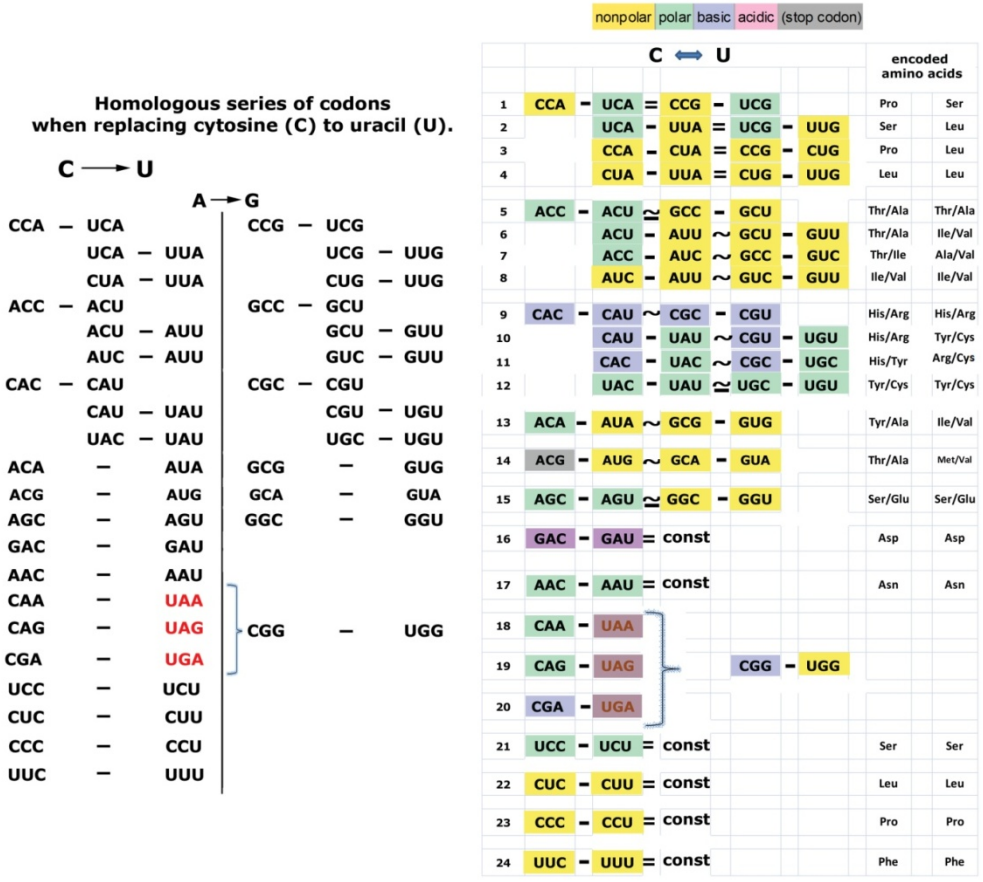


Fig. 6. Homologous series of codons. Stop codons (left) highlighted in red . Rihgt: All possible - equivalent and not equivalent - the replacement of one codon to another in a gene. In order to save space in front of each codon omitted a symbol of A, which characterizing the physical, chemical or biological parameter of both the codon and amino acid encoded by them. Sign (-), (=), (~) and the approximate equality are yet conditional and require strict biochemical and genetic interpretation.

Yellow lines in the above structure (see Fig.4) shows the transitions between codons (replacement C - U), in which the difference in quantity (may be qualitative) characteristics (A) for these codons should be preserved:

$$A (CUC - Leu/L) - A (CUU - Leu/L) = A (UCC - Ser/S) - A (UCU - Ser/S)$$

In this form, Nature programmed multiple mutational processes that have led to a huge variety of classes, species of flora and fauna. And ethnicities.

Why is this idea better known conventional artificial and primitive table in [10]

- **First**, a representation of Codon Systematic **is in line with the combinatorial mechanism of evolution** of the Material World.
- **Second** , this form **includes the presentation and image Homology in genetics** - general scientific predictive mechanism for the evolution of the Material World .

Third, combinatorial homologous series of codons shows **very interesting mutational and biochemical patterns** in which geneticists have yet to understand .

4. Pharmacological Applications

Once researchers identify promising compound for development, they analyze and conduct experiments in order to collect information on:

- How it is absorbed, distributed, metabolized, and excreted
- Its potential benefits and mechanisms of action
- The best dosage
- The best way to give the drug (such as by mouth or injection)
- Side effects (often referred to as toxicity)
- How it affects different groups of people (such as by gender, race, or ethnicity) differently
- How it interacts with other drugs and treatments
- Its effectiveness as compared with similar drugs

And almost on each of these stages the Unitary symmetry of the combinatorial chemical entities can increase the efficiency of solving the problems listed above.

All living things in Nature exist in two main hypostases - metabolism and homeostasis in the form of processing all coming from the outside and not recycled to save the biochemical balance in the body.

And the metabolism and homeostasis of an animal depends on a combination of age and sex hormones. In humans, this dependence is especially pronounced in the manifestation of secondary sexual characteristics and corresponding physiology and psychology. Therefore, before the "cure" a person, need to determine that a person is in a "norm", i.e. to start to solve the pharmacological problem of "key (medicine) - lock (disease)"- we need to determine a specific pharmaceutical drug appropriate to metabolism and homeostasis of a particular organism.

Fig. 7 shows how identification of the person (patient) in the paradigm of "age-a combination of sex hormones" should occur.

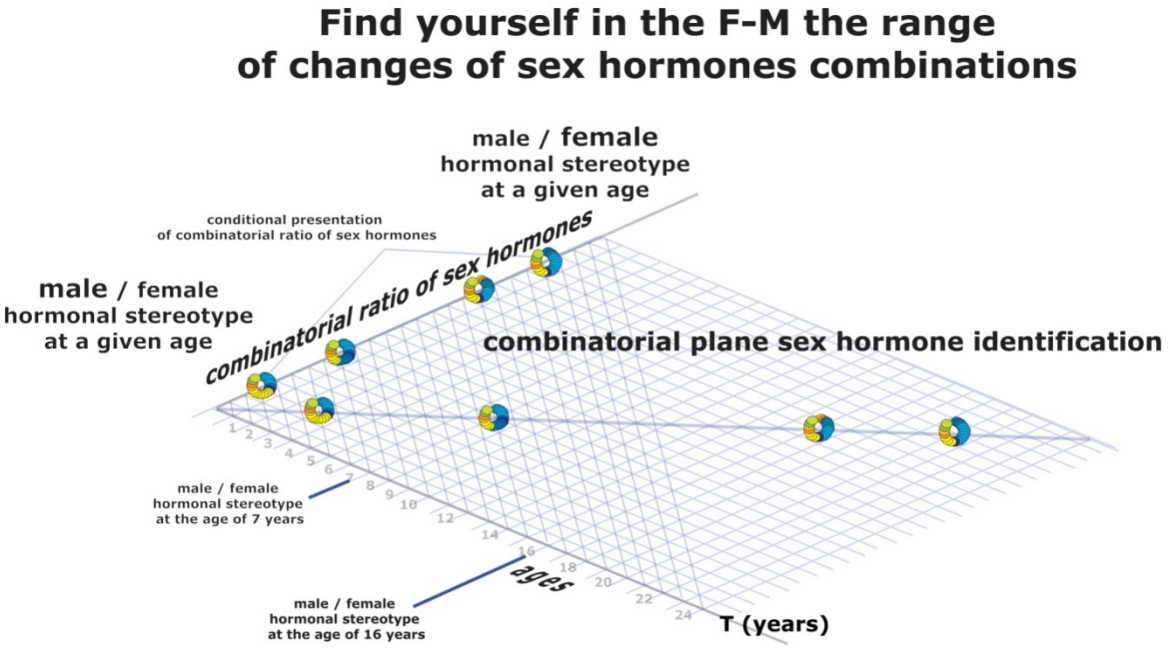


Fig.7. Identification of the person (patient) in the paradigm of "age - a combination of sex hormones". The process of the formation of the **Hormonal Passport**.

Excess male or female sex hormones in the mixture indicates either a genetic disorder of the equilibrium composition of the sex hormones to a certain ethnic group, or of a serious disease of sex glands.

The limitation of the "repetition" of the same hormones in the mixtures is the determination of "norm" for every age, i.e., construct a "normal line" (straight or curved, as in the case of the nuclei of atoms, where the number of repetitions of the nucleon was limited to natural conditions by a small number). So, combinatorial representation of the human body problem is the composition of a mixture of sex hormones for a particular age, which can be called **"Hormonal passport".**

Having understood and accepting this sub-paradigm, we can use the representation of Unitary symmetry of mixtures with the corresponding invariant- equations for creating both personal and population databases of hormonal passports. The process is described in more detail in [11].

5. Early Prediction of Disease Applications

It is known [12] that are hormones humoral (blood-borne) regulators of certain processes in various organs and systems: **hormone** is any member of a class of signaling molecules produced by glands in multicellular organisms that are transported by the circulatory system to target distant organs to regulate **physiology and behaviour**, including **sexual orientation**.

Of particular interest, it seems to me, is the problem of finding a relationship **"composition of the mixture of hormones - a pathology"**. In this case it is necessary to consider as mixtures the **blood, lymph and urine.**

With respect to our body the **blood** plays the role of **"materials supplier"** to all tissues (arterial) and **"waste transporter"** to waste outputting organs, which may be collected all over the body (venous).

Lymph acts as a **waste collector** from all nooks of our body. Function of the lymph - returning proteins, water, salts, metabolites and toxins from the tissues into the blood. **Urine** is a liquid, by which **all water-soluble metabolites derive out of the body.**

If from the entire set of hormones - 57:

- identify and group them on the basis of " the place of the synthesis "
- identify and group them on the basis of possible participation in the formation of pathology
- generate within each group the appropriate number of combinations of hormones with an appropriate number of repetitions
- identify those that correspond to the homeostasis of the human body
- opt for this kind of mixtures of certain physical parameters (e.g. The dielectric constant (ε_r), permeability (μ_r) and electrical conductivity (σ_r)) accurately determines the mix of human hormones (as in fingerprinting)
- calculate the physical parameters for all real mixtures in equations such as those presented in Table. 2

• measure the physical parameters of the particular mixture of hormones, consult your doctor, the patient,

We in the space **"the mix of sex hormones, the patient's age, the composition of the synthesis of hormones from the place (L) (the value of a physical parameter of the mixture, corresponding to a given composition and the appropriate attribution of certain pathologies mixture"),** can obtain the characteristic point (see. Fig. 9).

Tracking hormonal composition over time will allow to predict the development of the pathology in time.

I assume that the pathology is born and develops in different gender stereotypes in different ways.

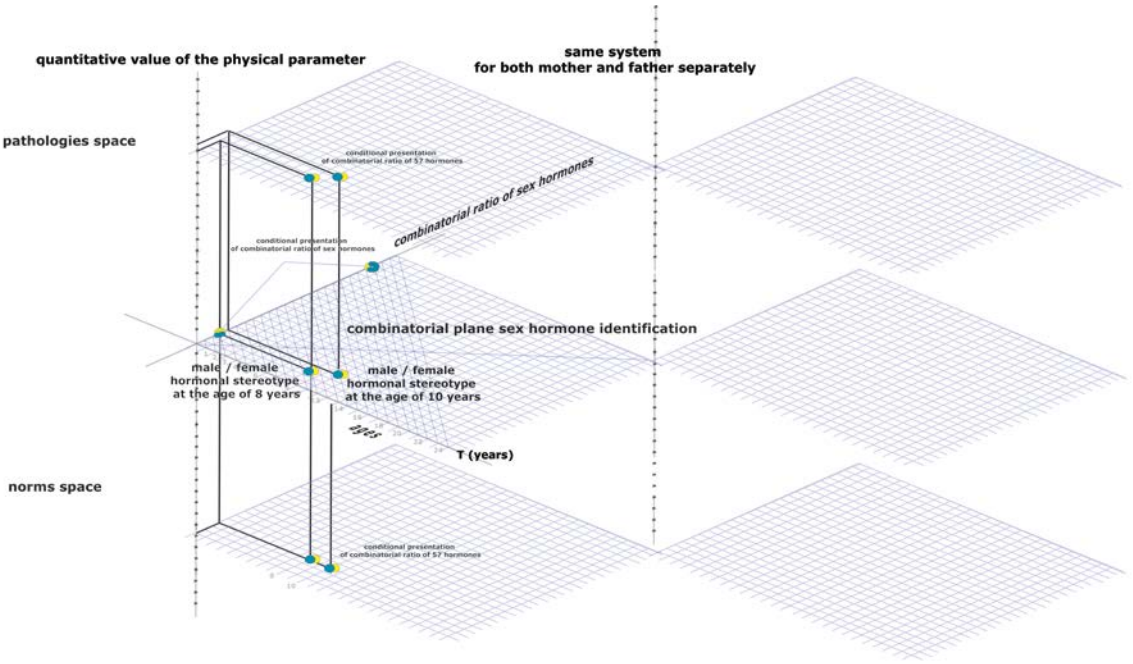


Fig.9. Combinatorial homology diagnostic system "composition of the mixture of sex hormones, the patient's age, the composition of the synthesis of hormones from producer ***(L)*** - pathology" for one of the 18 hormone producers. To the right is shown the ability to compare the combinatorial structure of the patient with the same combinatorial structure parent hormones.

According to the accumulated experimental data which corresponds age sexual determinant (the patient with the characteristic composition of the sex hormones) in "**NORM**":

• it is possible to calculate the "mixtures course" (the evolution of the mixture) over time, on relevant invariants (Table 2 type) i.e., predict the emergence and development of disease.

• reaction of the mixture on the pharmacological and physical therapy impact

The prediction accuracy is determined by accuracy of measuring concentrations of components of the mixture.

Note that this analysis be carried out as for a blood hormones mixtures and for mixtures of hormones in urine and lymph. This will significantly improve the diagnostic accuracy of pathological changes and their temporal orientation.

Very interesting is the problem of correlation of hormones mixtures invariants of children and their parents.

One of the main tasks at this stage is to learn how to create a combinatorial system of a mixture of 57 hormones with a limited number of repetitions and the corresponding system of Unitarian symmetry invariants. This process is described in more detail in [13].

6. Conclusions

The paradigm of "**a set of elements - a combination of elements - combinatorial homology - homology invariants - the system of equations for the invariants - finding a physical parameter for the entire class combinations for a limited number of experimental values"** is the prevailing paradigm of Natural phenomena - from elementary particles through the nucleus, atoms, simple molecules, complex molecules in consideration with their individual and as mixtures.

Moreover the mixture can be regarded as a state of equilibrium and the kinetic embodiment. In the latter case, the mixture passes through the stages, for example by dissociation from the parent molecule through the formation of radicals, and their formation of stable products.

Considered paradigm radically changes both the research itself, and natural science education process [9].

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