Internet Electronic Journal of Molecular Design **2003**, *2*, 000–000
BioChem Press http://www.biochempress.com

A Connection between Shcherbak's arithmetical and Yang's 28-gon polyhedral "views" of the genetic code

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Received xxx; Preprint published xxx; Accepted xxx ; Published xxx

Internet Electron. J. Mol. Des. **2003**, *1*, 000–000

Abstract

Motivated by the recent work by Shcherbak , we have analysed the nucleon content of the four ribosides, the discrete building blocks of RNA, and also the nucleon content of the four nitrogenous bases of DNA. In both cases, the total nucleon sum is the *immediate* neighbour of a number divisible by Shchebak's 037. Now, calling for a formal "borrowing" process, of just *one* nucleon from hundreds, as in Sherbak's work, we have, first, true divisibility by 37 and, second, the result of dividing these nucleon total sums by 37 gives us numbers which appear to be equal or simply related to the characteristic numbers of the 28-gon model of the genetic code, recently introduced by Yang. We give to the connection between these two apparently unrelated works a concrete numerical form, invoquing Euler's equation for polyhedra in three dimensions, as suggested by Yang. Also, we make some remarks connected with the (many) observed occurences of this particular number and its variants in biology and in the physical world.

Method. Simple reckoning of nucleon-sums in the basic building-blocks of life and some tools from linear algebra.

Results. A connection between the remarkable (arithmetical) analysis of the genetic code by Shcherbak based on the use of nucleons as digital signs in amino acids, and the polyhedral (topological) model of the genetic code, based on the 28-gon model, by Yang.

Keywords. Genetic code, nucleon-number, nucleic acids, Shcherbak's 037, divisibility test

In this short paper, which follows a recent one [1], we propose a numerical connection between the beautiful arithmetical approach to the genetic code by Shcherbak, [2], based on the use of the *nucleon numbers-as-digital-signs*, and involving a distinguished (prime) number, Shcherbak's *Prime Quantum* 37, which appears to occupy a central role in his work, and the recent theory by Yang, [3], a topological approach, to classify the amino acids and based on a particular polyhedron, the quasi-28-gon or *ikosicaioctagon*. The first author has shown clearly that the genetic machinery appears to "know", and possibly use in some way, the decimal system[1] [4]. He says for example in [2] that ""decimalization" is superposed perfectly onto the numerous exact balances of the nucleons as well as onto the semantic symmetry of the triplets, with zero acting as a special number". Also, he supposed that nature could have selected the *nucleons* (protons and neutrons in the atomic nuclei) as digital *signs* for the amino acids. In [2], many (striking) and remarkable *exact balances* involving the *nucleon*s sums of amino acids standard blocks (which are the same for all 20 amino acids) and/or side-chains (which are variable), in specific (and different) sets, are given. Moreover, the digital notations of the balanced sums acquire the beautiful and unique form aaa (a=1, 2, …, 9)[2],

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[1] Computers doing arithmetic using the decimal mode are well known, as the Remington Rand Univac LARC (1960), which has been qualified by Charles Cole as "a marvel or, may be, a monster" who also says "The LARC was the first "supercomputer," and demonstrated the exciting promise of computing as a scientific tool ". May be, Nature could have tamed the "economy" of energy and solved many complex wiring problems in three dimensional space.

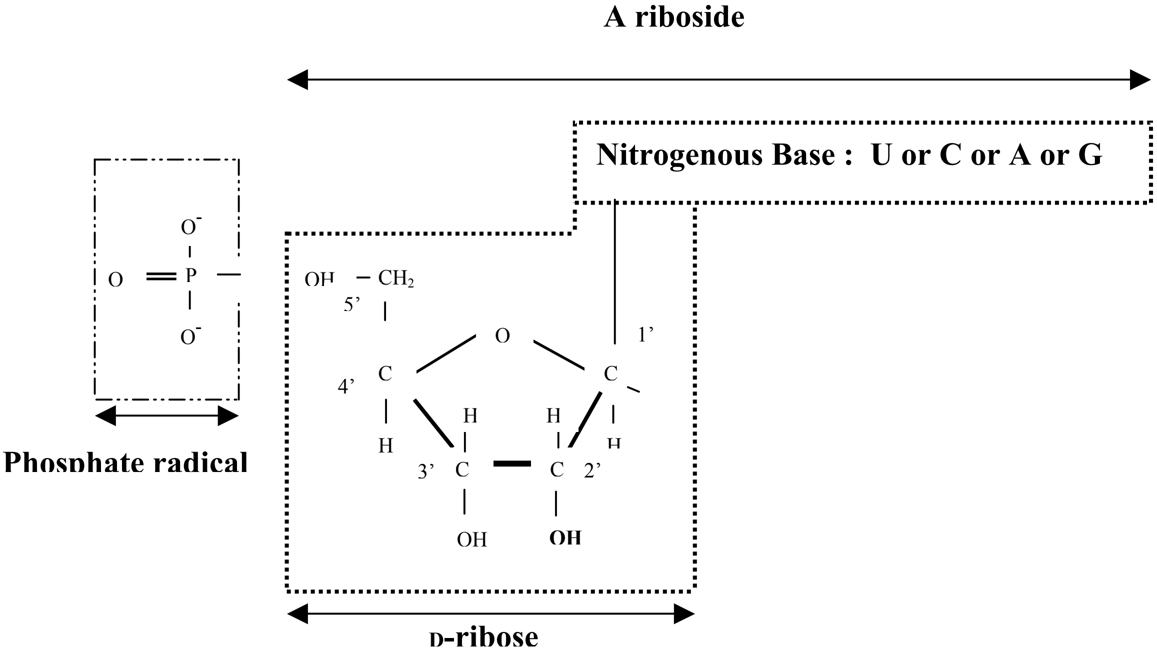
[2] The multiplication table for the sequence k×37, of multiples of 37,with k a multiple of 3 is:

such a form being the consequence of the *divisibility criterion* by 37 (more precisely 037, to emphazise a three-digit nature, see Ref.[2]). It is important to note that the specific sets, mentioned above, are intimately linked to symmetry, more precisely and essentially Rumer's symmetry, [2], (see also [1]). Without a "partitioning" of the 64-codons set according to this symmetry (and some of its extensions), it would be difficult, to "see" these striking and beautiful balanced sums. In this respect, we have constructed recently a concrete group theoretical framework for these sets, in reference [1], involving discrete symmetry groups like Klein's four group V and the dihedral group D_8. It is worth mentioning that, in the work by Shcherbak, call is made for a borrowing (formal) action of just one nucleon to reveal for example the beautiful Pythagorean relation and some balances. Shcherbak was also concerned mainly with the nucleon content of the amino acids and, as a possible consequence of his ressults, he proposed that the existence of the *divisibility criterion feature* could possibly simplify (see footnote 2) an hypothetical "computing process" in some organelles functioning as bio-computers. Now recently, Yang in [3], used a completely different approach, based on a (topological) rearrangment of the genetic code table by using the regularity in the four nitrogenous bases U (uracil), C (cytosine), A (adenine) and G (guanine) through a *determinative measure* of chemical regularity, he associates to the sp^2 N-atom-number in these bases. Concretely, this gives U=0, C=1, G=2 and A=3 symbolized in the succession UCGA. Althoug there exist a competing succession, UCAG (see [4], [1] and also in the ending remarks below), which fits well the monotonic size gradation of the bases and based on their atomic content, Yang choosed to use the first suucession to rearrange the codon table according to a spherical polyhedral symmetry model. Importantly for what follows, Yang, in a note (note 3) of his figure 5, showed that for the icosikaioctagon or 28-fon, one has a polygon with 28 faces, 16 vertices and 42 edges, in agreement with the famous Euler formula for the sphere v-e+f-2=0. In the following, we make an attempt to bring together these two views of the genetic code by (i) extending Shcherbak's analysis to the whole set of the RNA-components constituted by the *ribosides*. We extract the number 37, from the total nucleon sum in all four ribosides, as the result of the divisibility test, as applied to a number with more than three-digits, of this sum, by 37, that is itself, at the sole condition to call for an analogous "borrowing" of just one nucleon, see below, and (ii) by examining the consequences of adding in our analysis the contribution of the four DNA-bases, T (thymine), C (cytosine), A (adenine) and G (guanine), this time *without* their deoxy-sugar. By considering together the two contributions, that is the four RNA-components or ribosides and the four DNA-components alone, we arrive at a numerical "fitting" with the Icosikaioctagon model, 28-gon model, introduced recently by Yang [3], see above, in the sense that the number of faces, vertices and edges of the 28-gon appear simply related to the result of division of the total sum of nucleons in all ribosides, the one in all DNA-bases and their sum, respectively, by 37.

Let us we begin by asking whether it is possible to find (if any) some manifestation of the *divisibility-by-37-property* in the components of the nucleic acids. Shcherbak, in [2], has already touched the point (briefly) in his paper by computing nucleon-sums in the components of DNA (individual bases, *without* sugar) and found: A+T=259 and C+G=260=259+1. (T and A, on the one hand, and C and G, on the other, are two Watson-Crick pairs.) The number 259 is, first, divisible by 37 and also a member of the triad {259, 592, 925} in which all members are obtained by permutations and all divisible by 37. He also noted that uracil (an RNA component) has 111 (=3×37) nucleons. This is fine, but let us see things otherwise. Consider, first, the RNA

(1+1+1)×37=111, (2+2+2)×37=222, (3+3+3)×37=333, (4+4+4)×37=444, (5+5+5)×37=555, (6+6+6)×37=666, (7+7+7)×37=777, (8+8+8)×37=888, (9+9+9)×37=999. One has in all cases that aaa/37 is just a+a+a.

components, the four nitrogenous bases U (uracil; 4, 2, 2, 3), C (cytosine; 4, 3, 1, 4), A (adenine; 5, 5, 0, 4) and G (guanine; 5, 5, 1, 4), where the numbers in a parenthesis refer to the content in carbon (nn=12), nitrogen (nn=14), oxygen (nn=16) and hydrogen (nn=1) atoms, respectively, and nn stands for nucleon number. The nucleon content of the four bases is U: 111, C=110, A=134 and G=150. Here, we have only that U+C=111+110=221 or 222-1. (In the french edition of his famous text book "Biology of the gene", Watson replaces a double bond inside the cytosine ring by a single bond at the price of adding one hydrogen atom, in which case one would have U+C=222, exactly, which is 6×37.) As for A+G, there is nothing interesting. Now, let us consider, as a *unit*, the "flag", the base, *and* the "flag-ship", the D-ribose sugar, to which the base is attached in real RNA-sequences. Russian chemist Nikolaïev, in chapter two (Part 3) of his book "Principles of chemical-physics processes", [5], describes the ribose sugar as a kind of π-electron *insulator*, because it does not harbor conjugated-bonds and there are π-electrons inside the bases. In this way, one could imagine the ribose sugar as an element of some larger (hypothetic) bio-hardware set. We do not consider, here, the phosphate group (radical), which normally links together two consecutives ribosides in ribonucleic acid (RNA), because its inclusion is not constructive, here, but it must be remembered that the true nucleotide "unit" inside the polypeptide RNA-chain comprises a base, a D-ribose and a phosphate group. In the case we consider, we have the entities, termed *nucleosides*, or *side-chains*, *uridine* or uracil riboside (9, 2, 6, 12) with molecular weight (m.w.) 244.20, *cytidine* or cytosine riboside (9, 3, 5, 13), m.w. 243.22, *adenosine* or adenine riboside (10, 5, 4, 13), m.w. 267.24 and *guanosine* or guanine riboside (10, 5, 5, 13), m.w. 283.24. We show, in the figure below, the situation



We have therefore for the total number of nucleons, an integer number, uridine: 244, cytidine: 243, adenosine: 267 and guanosine: 283. Comparing with the nucleon content of the bases (see above), we have that the D-ribose-sugar part is the same for all the four bases and has the value 133, to be compared with the value obtained from the general nucleoside brut formula: $C_5O_4H_9$ + base. (These are well known molecules with appearance as white or almost white cristalline powders, and are available in the pharmaceutical market.) Adding now all the above four values for the ribosides, we obtain the interesting number 1037 or, equivalently, 999+38 which is *almost* divisible[3] by 37. Similarly to what has been done by Shcherbak (see [2]), one could make some kind of formal "borrowing", of just *one* nucleon (hydrogen atom nucleus), from some base among the four or something else, to reach a remarkable result. In Shcherbak's treatment, the borrowing of juste *one* nucleon, by the block, from the side chain, of just one amino acid, proline, is necessary in order to satisfy the marvelous Pythagorean relation in the amino acid-set belonging to the degeneracy IV series (see [2]). Shcherbak explains this as a possible working *trick* of an hypothetical bio-computing processes of organelles inside the living cell. Concerning proline, it is well known from biochemistry textbooks that this amino acid has a great tendency to "break" the helices. In view of the following discussion, it is interesting to note that the proportion of the amino acid proline in kinked helices, as given by Kumar and Bansal, [6], studying a whole database of 1131 α-helices, rise to 3.7% (a tenth fraction of 37), when its value in, in the middle regions, remains very small. The *propensities* given by the above authors for proline, in their Table 3, in *all* cases considered (short, long) are the smallest among all amino acids; it is the most avoided amino acid in middle α-helices. This phenomenon of increased occurrence of proline is thought to be one of the (multiple) factors enhancing protein thermostability. All these facts could contribute to the special "position" of this amino acid. Returning to our four nitrogenous bases and, invoquing what we may tentatively call Shcherbak's "Borrowing Principle", we have found by searching together with the untiring Google that, possibly, there could be a "mechanism" by which we could achieve a true borrowing and thus true divisibilty by 37 of the total number of nucleons in the four side chains considered above. Indeed, the phenomenon of *water mediated base pairs*, discovered by Holbrook et al. in 1991, [7], and more recently quantitatively studied by Schneider and his collaborators [8], including a quantum mechanical *ab initio* treatment and molecular dynamics simulations, seems to us a potential candidate. As a matter of fact, in this system, comprising a cytosine, an uracil and a water molecule there are two kinds of bonds. The first one consists of an hydrogen, H42 of cytosine, which is H-bonded to an oxygen, O4 of uracil, and the second one consists of an hydrogen, H3 of uracil, a nitrogen, N3 of cytosine, both linked by hydrogen bonds to a tighly associated water molecule in a triangular shape (see the Figures. in [8]). It is well known that, in the H-bonding phenomenon, a hydrogen atom is shared between two other atoms, a donor and an acceptor. Loosly

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[3] In fact, 38 is obtained by applying the divisibility test, for a more than 3-digit number, to 1037 (see [2]): 1037→001+037=038.

speaking, we could say that the hydrogen atom is “half” on the donor and “half” on the acceptor. In the theory of resonances, it is well founded to speack about “half” bonds: in benzene, for example, a good image would be that each carbon atom inside the 6-membered ring makes 1.5 bonds with the carbons in either side of it. (This is true also for the ozone molecule with three hydrogen atoms.) In our case, we could apply these ideas to the WUC-system. The results of the authors of reference [8] indicate that “the WUC-complex is a structurally autonomous building block of RNA structure with a high degree of cooperativity”. Now, here, we could re-consider more precisely what was undertaken above and consider that uracil, in his H-bonding relation with the water molecule has only 2.5 hydrogen atoms (nucleons) in place of 3 and cytosine, in his H-bonding relation with the oxygen atom of uracil, has only 3.5 hydrogen atoms (nucleons) in place of 4. In this case, by re-computing the nucleon sums, we have 243.5 for uridine, 243.5 for cytidine and evidently no change for adenosine and guanosine. Suming again, gives 1037-1=1036 for the total nucleon sum, which is, first, divisible by 37 (1036/37=28) because the divisibility test is 001+036=037 and second, it could be written 999+37. One could push things further by computing the *mean value* of the nucleon number in the four nucleosides. One has 1036/4=259, which is 7×37 and an “ideal” *mean codon* (3 bases + 3 sugars) would have 3×7×37=(7+7+7)×37=777 nucleons: Shcherbak call this process “*integer division by addition*”, see foootnote 2. For the division of 1036 by 37, one has (see [2]):

$$\frac{1036}{37} = \frac{999+037}{37} = \frac{999}{37} + \frac{037}{37} = (9+9+9) + (010) = (9+9+9) + (1) = 27 + 1 = 28. \qquad (1)$$

Finally, we turn to the four DNA-bases (without the D-sugar) T (thymine), C (cytosine), A (adenine) and G (guanine), mentioned at the begening of this section, which are the DNA-components, with nucleon numbers 125, 110, 134 and 150, respectively. The grand total nucleon sum is computed as 259+260=519. Here also, by invoquing the “Borrowing Principle”, for one nucleon, the sum becomes divisible by 37 and one has (519-1)/37=5+1+8=14, just half the preceeding result, which was connected with the RNA-components. Now, adding *both* contributions from RNA *and* DNA, one obtains 28+14=42. In connection with the latter sum, it is interesting to note that, Yang, [9], in his note 3, explains that for the Icosikaioctagon, or 28-gon, of the genetic code one has, as mentioned above, 28 *faces*, 16 *vertices* and 42 *edges*, fitting the Euler characteristic relation for dimension three. As a matter of fact, re-writing our sum as 28+(14+2)-42-2=0 shows the close relation with Euler’s equation. Using a fancy (but suggestive) picture, we could say that we have simply “borrowed” a zero, that is nothing (-2+2=0), from the “vacuum” of numbers, much like the electron-positron pairs appearing spontaneously from the true physical vacuum, and inserted it in the first equation (28+14=42) to reveal the second. We have therefore that the charachteristic numbers of the 28-gon could be simply related to the total nucleon-number in the ribosides, in the DNA-nucleobases and in their sum, divided by 37.

Let us end this short paper with two remarks. First, in [1], we have found this particular number, 37, as the common ratio of, traces *and* matrix-norms, between two kinds of matrices for the 64 codons, one encoding the "size" (or H-bond-number) of these codons as the concatenation of the individual sizes (or H-bond-numbers) of the constituting bases and the other encoding the "size" (or H-bond-number) of the codons as the sum of the sizes (or H-bond-numbers) of the constituting bases, using a completely different approach with respect to the present work. Let us, very briefly, recall the main results and make an important remark. The bases U, C, A and G are represented either by their "size": U=1, C=2, A=3 and G=4, computed from their atomic content according to Rosen's formula (see [1] and the references therein), giving a monotonic function[4], or by their H-bond number: U=A=2, C=G=3. The choice for the "size", corresponds therefore to the succession UCAG in both cases, ours and Rosen's; when the latter is translated in the binary notation U=00, C=01, A=10 and G=11, it identifies with the Gray code labelling of the four bases considered by Swanson, in his seminal work in 1984, [9]. Next, we define the following elementary 2×2 matrices (see [1])

$$B = \begin{pmatrix} U & C \\ A & G \end{pmatrix}, \quad e = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \tag{2}$$

The matrices encoding the "sizes" of the 16 base-doublets are given by

$$\mathbf{D} = \mathbf{B} \otimes \mathbf{e} + \mathbf{e} \otimes \mathbf{B} \tag{3}$$

Where the symbol ⊗ stands fot the Kronecker product. The first term gives the contribution of the first base, the second the one for the second base, and finally **D** gives all the contribution-sums in one equation. The consequences of Equ.(3) have been examined in [1]. Here, we consider only the matrices for the 64 codons, and we define for them, as explained above, two kinds of matrices: (i)

$$\mathbf{C} = \mathbf{B} \otimes \mathbf{e} \otimes \mathbf{e} + \mathbf{e} \otimes \mathbf{B} \otimes \mathbf{e} + \mathbf{e} \otimes \mathbf{e} \otimes \mathbf{B} \tag{4}$$

and (ii)

$$\mathbf{C}^{\mathbf{concat}} = 100 \times (\mathbf{B} \otimes \mathbf{e} \otimes \mathbf{e}) + 10 \times (\mathbf{e} \otimes \mathbf{B} \otimes \mathbf{e}) + \mathbf{e} \otimes \mathbf{e} \otimes \mathbf{B} \tag{5}$$

The matrix in Equ.(4), an 8×8 matrix with 64 elements, gives the size-number *or* H-bond number of the 64 codons, as the sum of the contributions of the first, second and third bases, respectively, with respect with their appearance in the equation from left to right. As for matrix (5), it gives the *concatenation* of the sizes-numbers or H-bond-numbers of the bases, in place of their sum. Therefore, this process allows us to assign to each codon a *three-digit* number, obtained by

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[4] In fact, our choice is shifted by one unit with respect to Rosen's choice (see [1]).

concatenating the size-numbers or H-bond-numbers, of its constituting bases, and this for all the 64 codons. Interestingly, the definition (5), is equivalent to the Kronecker product with concatenation introduced in [10] in order to take into account the *non-commutativity* of the bases in the codons; for example, codons in the form XXY, XYX and YXX must be labelled differently. By concatenating, rather than multiplying, all codons are assigned, each, a distinct number, which is not the case using defintion in (4), where there is a numeric "*degeneracy*", see below. The definition in Equ.(5) could be viewed as a matrix counterpart of the writing of ordinary numbers in (true) decimal notation by using arabic numerals. Next, we use, as in [1], a tool from linear algebra consituted by the *matrix-norm* notion, which captures the essential notions of size and distances in vector spaces, to compare the above matrices, (4) and (5), between themselves. Also, we invoque the trace which is a matrix-invariant quantity. From the many existing norms, we have found fruitful to use the well known 1-norm and ∞-norm. In practice, the 1-norm, $||\mathbf{A}||_1$, of a matrix A is equal to the *maximum column sum* and the ∞-norm, $||\mathbf{A}||_\infty$, is equal to *the maximum row sum* (see [1] for the mathematical definition and a justification for its use. The result is the following (see also [1]): the ratio between *like* quantities (traces, 1-norms and ∞-norms) in $\mathbf{C}^{\mathbf{concat}}$ and those in **C**, in *both* cases, (U=1, C=2, A=3, G=4) and (U=A=2, C=G=3), is exactly equal to 37. Let us quickly precise, also in connection with the corresponding result in [1], that this result is in fact previsible or a build-in outcome, rather than a "proof" for this number. We think that the "derivation" obtained in the main part of this paper, may appear more interesting. Rather, we consider the couple of Equs.(4) and (5), together with their "ratios" of traces, 1-norms and ∞-norms, as a matrix "couterpart" of the beautiful (partial) multiplication table mentioned in footnote 2. It seems to us that these equations constitute a matrix framework for the codon, adapted to swhat we called in this paper Shcherbak's arithmetic. As a brief visualization, take for example the first choice: U=1, C=2, A=3 and G=4. By computing explicitly Equs.(4) and (5), we have for **C** (see Equ.(22) in [1]):

$||\mathbf{C}||_1 = 6+3\times8+3\times10+12,$

$||\mathbf{C}||_\infty = 9+3\times10+3\times11+12$

and for $\mathbf{C}^{\mathbf{concat}}$:

$||\mathbf{C}^{\mathbf{concat}}||_1 = 222+(224+242+422)+(244+424+442)+444$

and

$||\mathbf{C}^{\mathbf{concat}}||_\infty = 333+(334+343+433)+(344+434+443).$

(note the numerical degeneracies in **C**, mentioned above). In the last two norms, the individual numbers in the triplets of 3-digit numbers (in parenthesis) are not divisible by 37 but their sum is; recall that abc+cab+bac=3×37×(a+b+c). We see therefore that the ratio between respective norms in $\mathbf{C}^{\mathbf{concat}}$ and **C** leads exactly to 37, and similarly for the other choice (H-bonding). Finally, displaying the 64 codons matrix in Equ.(5), shows that, besides the four codon-numbers in the form aaa (with a=1,2,3,4), the remaining 60 codons could be grouped in 20 triplets of codons according to the Gamow's partitioning of the genetic code table (see [1] and also [2]). We shall report more on this last point, in a (near) future paper.

Our second, and last remark, is connected with a curious multiple occurence of Shcherbak's number, more exactly 37 or some of its negative power of ten multiples, in various areas in biology and physics. As a few examples in biology, besides the example we already gave above when discussing the importance of proline (3.7% proline-residues in the kink region), we have that the formation of a peptide bond (the condensation reaction) produces a system, constituted by two amino acids *and* a water molecule, exhibiting a net dipole moment evaluated to 3.7 Debye ([11]). Also, the vertebrate mitochondrial genome, which is structured as two circular strands, the heavy strand and the light strand, encodes for exactly 37 genes, of which 28 are in the heavy strand. We cannot leave biology without evoquing the more than 50 years old famous α-helix Model of Pauling, Corey and Branson, (see the rubrique "news and views" in [13]), with 3.7 amino acid residues per helix turn. Perutz, who elucidated the X-ray structure explains in 1951 that his reflexion "appears to exclude all models exept the 3.7 helix residue of Pauling, Corey and Branson with which it is in perfect concord". In the physical area, let us look at the fundamental atomic constituent of life hydrogen, carbon, nitrogen and oxygen. The terrestrial quantities of these atoms have certainly their origin in the stellar furnaces, billions of years ago, and have been produced by the so called CNO cycle which concerns stars with a mass ≥1.1 solar mass and involves carbon as a catalyst and also nitrogen and oxygen as well as their isotopes. Now, the terrestrial abundances of some of these isotopes, which are well known, [12], are the following C^{13}: 1.11% (3×0.37), N^{15}: 0.37% and O^{17}: 0.037%. (It is well known that the (precise) value for C^{13} has recently much helped the "palanteo-biologists" to estimate the "time" for the beginning of life on Earth. Also, it is used, as a technique, in medecine to detect the presence of bacterial infections.) Finally, the Earth's atmosphere contains about 0.037% or 370 ppm carbon dioxyde (CO_2) by volume. This is at least curious and thought provocative and, may be, this arithmetico-physical phenomenon goes beyond the sole biological area. The organelles in the living cell, functioning as bio-computers, as suggested by Shcherbak, could be only tiny parts of the gigantic computer, the Universe, in which we live.

The author acknowledges Dr. Ovidiu Ivanciuc for his kind invitation to participate to the Internet Electronic Conference on Molecular Design.

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Biography

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