Transgenetic Cybernetics Regarding the Nucleic Acids DNA and RNA Assimilated to Cybernetic Systems with Automatic Self-organization

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Abstract
The capacity of the carbon atom to generate linear, branched and cyclic chains by linking with other carbon atoms, enables the human brain's natural neuronal networks to materialize, with living structures, the fundamental computing algorithmic structures sequence, selection and iteration in the artificial neuronal networks of artificial intelligence.
The nucleic acids DNA and RNA consist of structural units called nucleotides, which contain a purinic or pyrimidine base having the shape of a double heterocycle or a base with the shape of a heterocycle.
Analyzing the structure of the bases having the shape of a heterocycle or double heterocycle, the geometric symmetry of the double links made of a σ link and a π link can be noticed.
Setting out from F. Schrödinger's wave equation we use the function of orbital wave Ψ or orbital. In practical models, the orbitals are considered to be bounded by surfaces of the same electronic density, and within these bounds there may occur a high electron density which accounts for the particular shape of the orbitals in the modeling representation.
In our paper, the nucleic acids DNA and RNA are assimilated to cybernetic systems with automatic self-organization, by the electrons transition owing to some external actions to the orbitals geometrical shape and their distribution in space.

Key words: heterocycle, orbitals, nucleic acids, cybernetics.

1 Introduction

The object of the paper is to try to explain the "Vital Force" through the self organization of the orbitals of the C, N, H, O and P atoms under the conditions of the orbital hybridization through external energy contribution.
The problem can be solved by logical and mathematical interpretation of the simple and double bonds, of the σ and π bonds, through spatial-temporal reconfiguration of the hybrid orbitals, by which the primary entities of the living structure (the nucleic acids DNA and RNA) have been synthesized.

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The orbitals with the same main quantum number n, make up a layer. Each layer may consist of $\mathbf{n^2}$ orbitals, which differ from one another by their spatial arrangement.

For the quantum state **n=1** there corresponds an orbital of spherical symmetry, **1s,** which can be occupied at the most, by two electrons which differ through their antiparallel spin.

The quantum state **n=2** is made up of four orbitals: an orbital **2s**, which can be taken up by two electrons at the most and three orbitals **2p** (**$2p_x$, $2p_y$** and **$2p_z$**) which can be taken up by six electrons at the most.

The orbital **2s** is arranged with spherical symmetry around the atomic nucleus , being situated at a greater distance than the orbital 1s and separated from the orbital **1s** by a region where the probability of finding an electron is almost zero by a nodal surface.

The three orbital **2p** differ from the orbital **2s** through energy level, orbital shape and spatial disposition.

With the orbitals **p**, the electron density is maximum in two opposite regions, lying on either side of the nucleus; that is why the shape of these orbitals is not of spherical symmetry but bilobic, the two lobes being separated by a nodal plane that passes through the nucleus and where the likelihood of finding an electron is null.

The bounding surfaces have their centers on one of the three axes of Cartesian co-ordinates, on either side of the atomic nucleus, considered to be situated in the co-ordinates origin.

2 The Fundamental Theoretic Bases of Mathematics and Atomic-Molecular Interpretation of the Nucleic Acids DNA and RNA

2.1 Nucleic Acid Structure

D. Watson and F.H.C. Crick (Stanescu,1977) have studied the desoxyribonucleic acid, pointing out the macromolecule structure of the DNA. DNA. is a nucleic acid located in the cell nucleus, especially at the chromosomes, while RNA is found especially in the cytoplasm. The nucleic acids are macromolecular substances consisting of simple structural units called nucleotides (macronucleotides).

Each nucleotide is made up of a phosphoric radical, a sugar and a purine or pyramidine nitrogenous base. The purine bases are adenine and guanine, purine being a double heterocycle. (fig.1). The pyrimidine bases are: cytosine, thymine, uracil and methylcitosine while the pyrimidine ring is an aromatic, dinitrogenous heterocycle. (fig.2).

The sugars that enter into the structure of nucleic acids are: desoxyribose, for DNA and rybose for RNA which are pentoses, cyclic monosugars with 5 carbon atoms. (fig.1).

The phosphoric radical has three free hydroxyls of which two are esterified, so that the nucleic acids are phosphodiesters. By combining a nitrogenous base with a sugar (ribose, desoxyribose) the nucleosides are formed (fig3). The nucleotides, basic units of nucleic acids result from nucleosides phosphorylation (fig.3) .

By linking nucleotides , oligonucleotides are obtained, having up to 10 nucleotides and polynucleotides, that is nucleic acids, which have more than 10 nucleotides.

DNA contains desoxyribose as glucoside. RNA contains ribose while the pyrimidine nitrogenous base, thymine in DNA is replaced by uracil in RNA. RNA is formed of a single polynucleotidic chain and in DNA we can distinguish two parallel chains, linked up by a bond between a purine nitrogenous base and a pyramidine one.

2.2 Chains On Carbon Atoms

The carbon atom is characterized by its capacity to link up with other carbon atoms, forming chains, which can be linear, branched or cyclic (Berai, 1973, Zapan, 1973)

2.2.1 The Linear Chains

The linear chains contain carbon atoms joined in such a way each carbon atom is linked with two other carbon atoms, at most (fig. 4). The length of such a chain is varied, in principle it can be infinite.

2.2.2 The Branched Chains

The branched chains contain several carbon atom chains combined in such a way so that, besides the carbon atoms linked in a chain, there are also carbon atoms linked to three or even four carbon atoms (fig. 5).

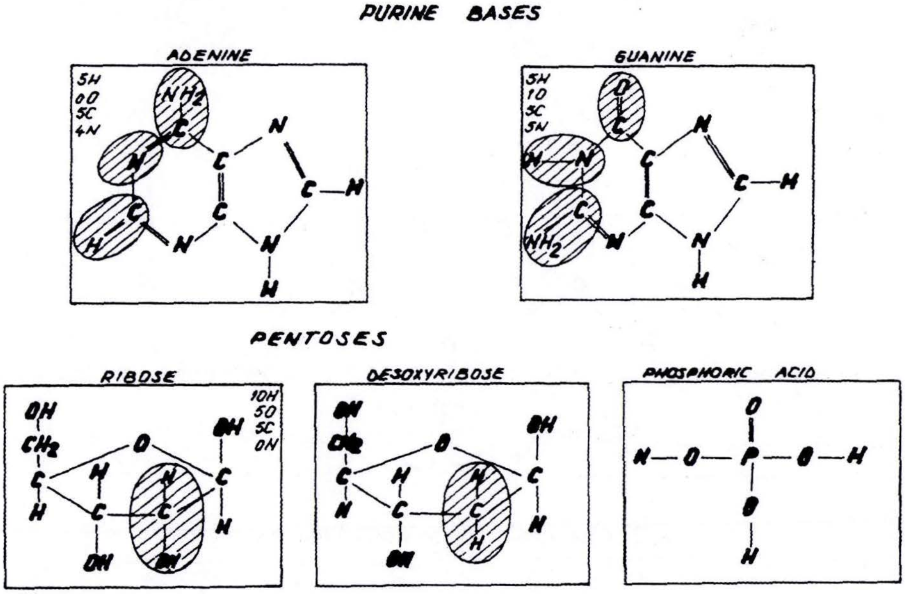

Fig.1: The main constituents of nucleic acids, purine bases and pentoses

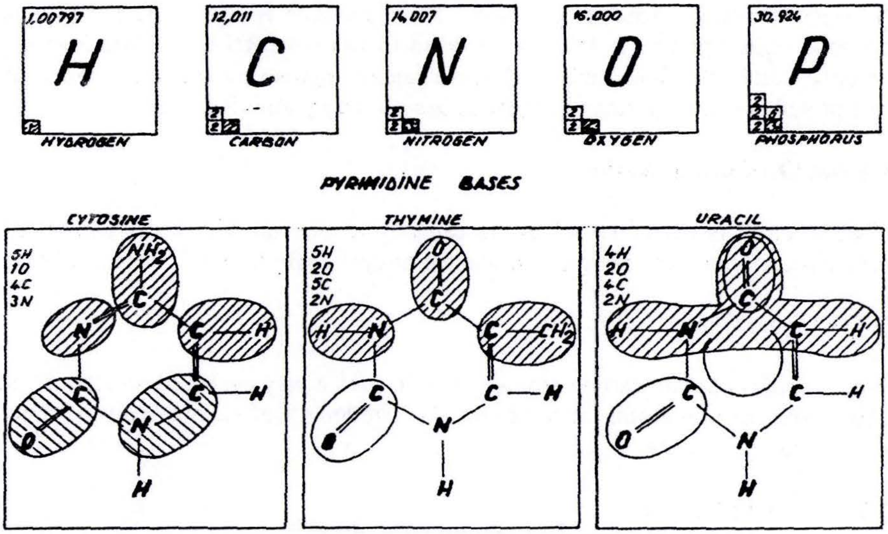

Fig.2: Pyrimidine bases

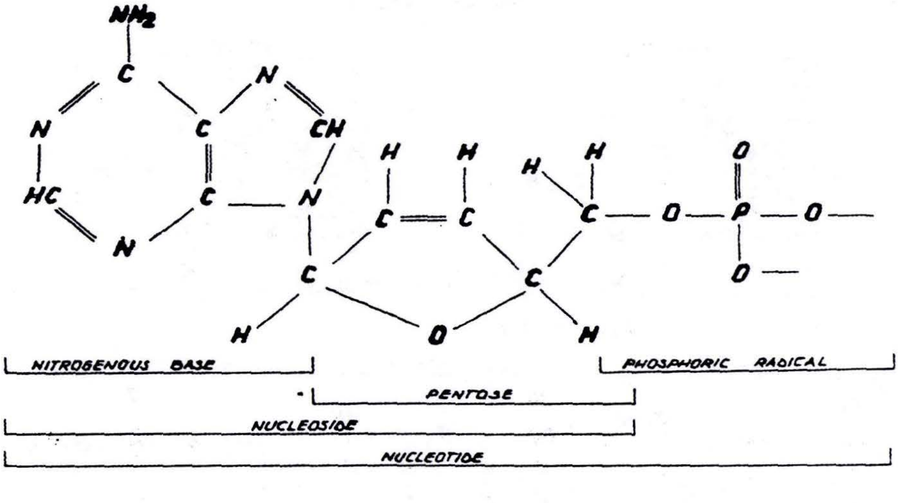

Fig.3: Chemical composition of nucleic acids

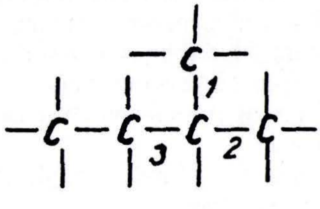

Fig.4: Linear chains

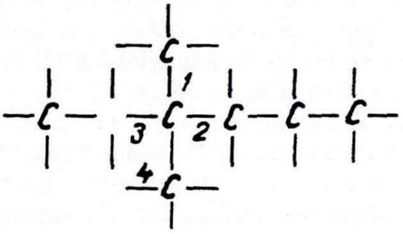

Fig.5: Branched chains

2.2.3. The Cycles

The cycles contain closed chains of carbon atoms; they are also called rings or nuclei (fug.6)

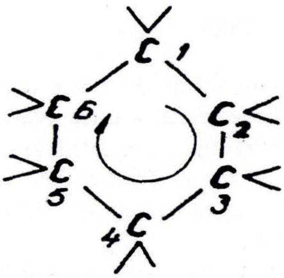

Fig.6: Closed chains, rings or nuclei

2.3. The Orbitals

Quantum mechanics relies on the principle that elementary particles (the electrons) have both the character of particles and waves, a dualism which can be expressed by L. de Broglie's relation

$$\lambda = \frac{h}{m \cdot v} \tag{1}$$

where:

λ - the wave length;
h – Plank's constant;
m – particle mass;
v – particle velocity.

The electron motion on the orbital round the nucleus generates an undulatory phenomenon, characterized by the occurrence of a tridimensional stationary wave, which defines the atomic orbital itself (a viewpoint introduced by quantum mechanics, differing from Bohr's atomic model, which considered the electron only in point of particle and therefore all the processes as the result of the motion of a negatively charged particle round the positive nucleus of the atom).

As a result of this interpretation, the classical motion equations are replaced by F. Schrödinger's (Bransden, 1980; Joachain, 1980) wave equation:

$$\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}+\frac{8\pi^2 m}{h^2}\left(E_{tot}-E_{pot}\right)\psi=0 \qquad (2)$$

where: ψ-represents the electronic wave amplitude for a point of coordinates (x,y,z);
E_{tot} – total energy;
E_{pot} – the electron potential energy.

By solving the wave equation by integration, the wave function Ψ is obtained; in order to calculate Ψ, the term E_{tot} should have certain values, called eigen values.

As the energy allowed values in Schrodinger's equation are the equivalent of the energy level of the electrons, represented by the orbitals in Bohr's relation, it means that the corresponding wave functions are the equivalent of the electronic orbitals from the classic theory in ondulatory mechanics.

The wave function ψ, termed eigen function is also called orbital wave function or orbital.

The electron energy, in the atom stationary state is precisely established, therefore according to the uncertainity principle, established by Heisenberg, the electron geometric position and its impulse cannot be ascertained simultaneously, hence its trajectory cannot be exactly determined. Only relations of probability can be determined for electrons.

In interpreting physical processes in quantum mechanics the values $|\Psi|^2$ dV represents the probability of finding the electron in a certain element of volume dV.

For the electron, the value of $|\Psi|^2$ at a given point in space is interpreted as the charge density at that point (often called probability density).

That is why the electron can be considered to be extended in a cloud of negative electricity whose density varies from place to place.

The orbitals with the same main quantum number n make up a layer. Each layer can be made up of n^2 orbitals, which differ, from one another by their spatial distribution.

The electrons taking up on orbital are characterized by quantum numbers, namely, both the three quantum numbers identifying the orbital (the main quantum number n, the azimutal quantum number l, the magnetic quantum number m) as well as the spin quantum number s, which is due to the electron rotational motion round its own axis, which gives rise to a magnetic moment of the electron.

Formulating an electronic structure is done by indicating the electrons, which are found in various orbitals, respectively by the main quantum number n followed by the secondary quantum number l, at which the electron number is noted by an index. Table 1 gives examples of occupying the orbitals with electrons.

Table 1: Occupying the orbital of the elements H, C, N, O with electrons

Nr. crt	**ELEMENT**	**LEVER n =1**	**LAYER n=2**				
			1s	**2s**	**$2p_x$**	**$2p_z$**	
1	**H**	↑					$1s^1$
2	**C**	↑↓	↑↓	↑	↑		$1s^2,2s^2,2p_x^1,2p_y^1$
3	**N**	↑↓	↑↓	↑	↑	↑	$1s^2,2s^2,2p_x^1,2p_y^1,2p_z^1$
4	**O**	↑↓	↑↓	↑↓	↑	↑	$1s^2,2s^2,2p_x^2,2p_y^1,2p_z^1$

2.3.1 Quantum States

The quantum state **n** = **1** (to which corresponds **l** = **0** and **m** = **0**) is made up of a single orbital of spherical symmetry, called **1s**. It can be taken up by two electrons, at most (**$1s^2$**), which differ, by their antiparallel spin.
The quantum state **n** = **2** is made up of four orbitals – an orbital **2s** (corresponding to **l** = **0** and **m** = **0**), which can be occupied by two electrons, at most (**$2s^2$**) and three orbitals **2p** (corresponding to **l** = **1** and **m** = **-1** or **m** = **0** or **m** = **+1**), equivalent from the power viewpoint, that is **$2p_x$, $2p_y$, $2p_z$** which can be taken up by six electrons, at most (**$2p_x^2$, $2p_y^2$, $2p_z^2$**).
The orbital **2s** is arranged with spherical symmetry round the atomic nucleus, being situated at a greater distance from the nucleus and being separated from the orbital **1s** by a region where the probability of finding an electron is almost zero, that is by a nodal surface.
The three orbitals **2p** differ from the orbital **2s** through the energy level, through the orbital shape and spatial arrangement.
The orbitals with the same main quantum number do not have the same energy. The orbital **2s** has lower energy than the orbitals **2p**, being more stable.

2.3.2 Hybrid Orbitals

In its fundamental state, the carbon atom has electronic distribution **$1s^2 2s^2 2p_x^1 2p_y^1$**.
Having 2 unmatched electrons (**$2p_x^1$ and $2p_y^1$**) it has to be bicovalent, but only in rare cases the carbon atom manifests bicovalence; especially in organic combinations, the carbon is tetracovalent.
The carbon atom tetracovalence is brought about by an electron redistribution. As a result of an intensification caused by an external action, an electron **2s** is promoted into

an orbital **2p**, the electronic configuration of the activated carbon atom becoming $\mathbf{1s^22s^12p_x^12p_y^12p_z^1}$ (fig. 7). As an outcome of this electronic **2s → 2p**, each electron of the layer **n = 2** occupies one orbital.(fig.8)

These valence orbitals become identical as regards energy and spatial distribution and are called hybrid orbitals. With hybrid orbitals, the electronic cloud density along the orbital axis is much greater than in a non-hybrid orbital; therefore the covalent link made by its interpenetration with another orbital is stronger.

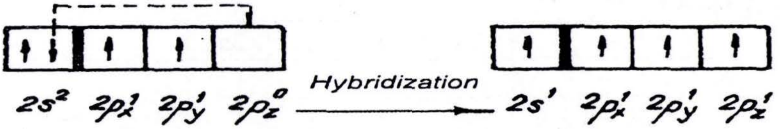

Fig.7: The transition of the electron 2s into an orbital 2p

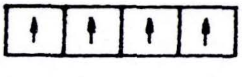

Fig.8: Hybrid orbital Sp^3

2.3.2.1 Hybridization $\mathbf{sp^3}$

When by the interpenetration of the orbital **2s** and of the three orbitals **2p**, four equivalent orbitals are obtained by equating the energy levels; the hybridization is of the type $\mathbf{sp^3}$ (fig. 7). The orbitals $\mathbf{sp^3}$ are occupied by an electron called σ; they have the same form (fig. 8), the same energy and are oriented in space in the most symmetrical way possible in relation to the nucleus, respectively turned towards the vertices of the tetrahedron forming between them equal angles (fig. 9). The hybridization of an orbital **s** and of an orbital **p** in orbital $\mathbf{sp^3}$ is shown in fig.10.

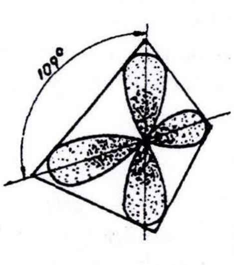

Fig.9: The spatial disposition of the four hybrid linking orbitals sp^3

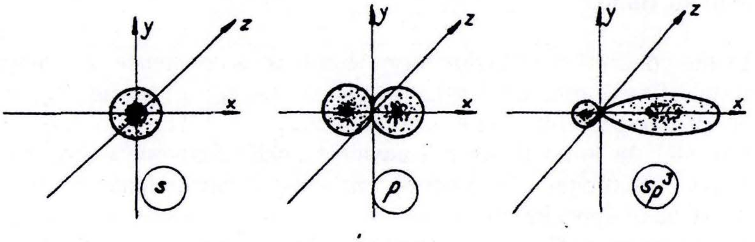

Fig. 10: The hybridization of an orbital p into a hybrid orbital sp^3

This orientation is due to the fact that the four direction orbitals having the same electric charge reject one another and thus have the tendency of taking up as distant positions as possible from one another, a requirement met only by tetrahedron arrangement.

2.3.2.2. Hybridization sp^2

When the orbital **2s** is interpenetrated by only two of the three orbitals **2p ($2p_x$ and $2p_y$)** there result three equivalent hybrid orbitals **$2p^2$**; the third orbital **$2p_z$** remains unaltered (fig. 11).

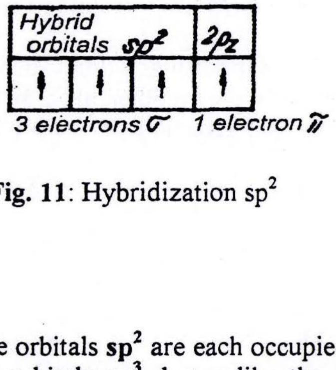

Fig. 11: Hybridization sp^2

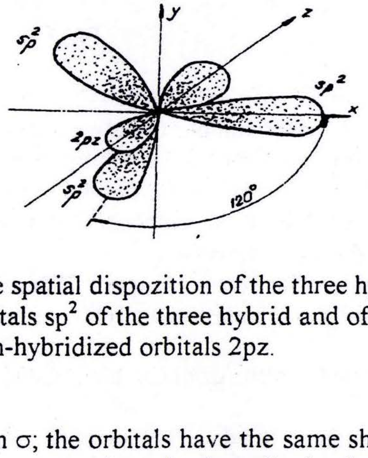

Fig. 12: The spatial dispozition of the three hybrid orbitals sp^2 of the three hybrid and of the non-hybridized orbitals 2pz.

The orbitals **sp^2** are each occupied by an electron σ; the orbitals have the same shape as the orbitals **sp^3**, but unlike the orbitals **sp^3**, they are oriented trigonally in the same plane, forming between themselves 120° (fig. 12).

The non-hybridized orbital **2p** is formed perpendicularly above and below this plane; it is occupied by an electron **π**. The **sp^2** hybridization is found with carbon combinations containing a double link.

2.4. The Covalent Bond

According to the conception in ondulatory mechanics, a covalence is achieved by the interpenetration of two orbitals, either belonging to each participating atom. The electronic clouds interpenetrate and electronic density redistribution occurs, resulting in a molecular orbital. In order to form a covalent bond, each one of the participating atoms must have an orbital occupied by one single (uncoupled) electron; the two electrons have to be of opposite spin.
The emerging molecular orbital is therefore taken up by two antiparallel spin electrons and has two nuclei. (fig.13)

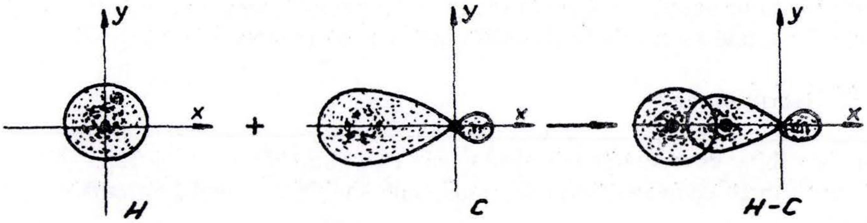

Fig.13: Linking orbital C-H

The ordinary atom covalence is given by the number of uncoupled electrons in the atom and not by total number of valence electrons.
The energy of a molecular orbital is lower than the energy of the atomic orbitals before the link was formed, therefore the molecule is more stable than the participating atoms.
The interpenetration can occur only as far as the reciprocal rejection of the atomic nuclei doesn't oppose it.
The molecular orbitals wave equation is more intricate and can be solved by approximate calculation methods.

2.4.1 The Carbon Atom Covalent Bonds

The covalent bonds, by which the carbon atom can link up with the atoms of other elements or with other carbon atoms, are of two types: σ bonds and π ones. The σ bond is made by the carbon atom in tetragonal valence state (hybridization $\mathbf{sp^3}$). For example, the **C-H** bond orbital resulting from the interpenetration of a hybrid orbital $\mathbf{sp^3}$, occupied by an electron σ, with a **1s** spherical orbital of the hydrogen atom (fig.13). This orbital shows rotation symmetry to the axis linking the nuclei of the two bound atoms.

The **C-C** bonds are made in a similar way, a hybrid orbital **sp**^{3} from a carbon atom interpenetrates a similar orbital of the other carbon atom (fig. 14). The σ bond is stable, having a relatively high linking energy and is hard to unbind.

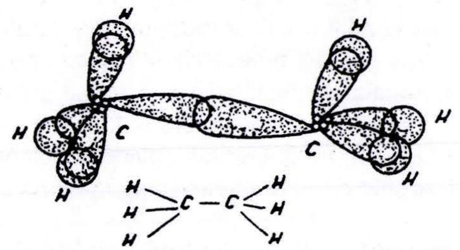

Fig.14: The formation of a bond C-C

As the pair of electrons, σ cannot be shifted easily, the orbital **s** is likely to distort with difficulty under the influence of the substituents; the bond σ is hardly polarizable. The characteristic of the bond σ is also the possibility of its free rotation round itself owing to the orbital σ rotation symmetry to the axis passing through the atom nuclei participating in the bond. The bond π is found at the compounds with multiple (double) bonds.

2.4.2 The Double Bond

The double bond is explained by the trigonal valence state in the case of hybridization **sp**^{2}. Through the three hybrid orbitals **sp**^{2}, the carbon atoms link up with two hydrogen atoms, as well as between themselves. The fourth bond from the carbon the carbon atoms is formed by the interpenetration of the non-hybridized orbitals **2p**$_z$, from each carbon atom. (fig.15)

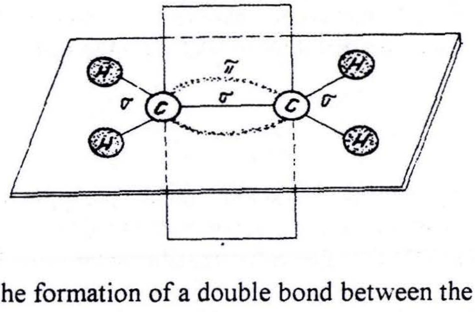

Fig. 15: The formation of a double bond between the two atoms

The resulting linking orbital is taken up by two electrons of opposite spin (the π electrons) forming the so-called π bond. The double bond is formed of a bond σ and a bond π and not of two identical bonds. Owing to the form and position of the orbitals **sp^2**, the two carbon atoms and four hydrogen atoms are found in a plane, the angles between the bonds being 120 degrees. The orbitals **$2p_z$** are perpendicular on the plane of the links σ. The linking orbital resulting from their interpenetration is made up of two parts that are in a plane perpendicular on the plane of the bonds s, above and below it; the electronic density of the bond p is null at the plane intersection (fig 15.)

As the bilobular shape of the orbitals **p** does not allow an interpenetration as profound as that of the hybridized orbitals, the bond π is less stable than the bond σ. Because of the electronic density of the bond π, above and below the bonds σ plane, the free rotation round the axis **C-C** can no longer take place; a rotation of the two halves of molecules distorts the electronic cloud π, diminishing the molecule stability.

3 Cybernetic Interpretation of The Nucleic Acids DNA and RNA

The possibility of the formation of linear and branched chains by carbon atom cohesion creates the premise of linear chains cohesion in cybernetic cycles constituted in nuclei or rings. By the alternation of carbon and nitrogen atom coalescence through alternative simple and double bonds, purine and pyrimidine nitrogen bases have been created such as adenine and guanine , respectively cytosine, thymine, uracil and methylcytosine (Wiener, 1948, Berai, 1977).

The pyrimidine ring appears in the form of dinitrogenous aromatic heterocycle, purine being a double heterocycle. But for the possibility of linear chain formation, the nucleotide linking would not have been possible in order to obtain oligonucleotides , with up to 10 nucleotides, polynucleotides (nucleic acids with more than 10 nucleotides) and heteropolymer molecules, which consist of over 200,000 nucleotides.

Analyzing the simple and double heterocycles in the nitrogenous bases, purine and pyrimidine, we can notice the alternative nature of the double covalent bonds made of link σ and π. The links σ are found in the same plane, the angles between the links being 120°. The bonds π (the orbitals) are perpendicular on the bond plane σ situated also at 120°

By closing the linear chains in a cycle, there occurs a redistribution of electronic clouds (the feedback effect) in a contour circuit, having as consequences dynamic behaviors specific to life, to which is added the composition with the orbital fields π perpendicular on the cycle plane.

4 Conclusions

The nucleic acids DNA and RNA are assimilated in the paper to cybernetic systems with automatic self-organization of the geometric shape of the orbitals and of their distribution in space through the electrons transition between the orbitals due to an external force.

The carbon atom capacity to generate linear, branched and cyclic chains by coalescing with other carbon atoms, enable the natural neuronal networks of the human brain to materialize, with living structures, the fundamental informational algorithmic structures

- the sequence, selection and iteration in the artificial neuronal networks of artificial intelligence.

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