Theory of three-electrone bond in the four works with brief comments.

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I express my deep gratitude to my son, Bezverkhniy Vitaliy Volodymyrovich, for participation in the development of the theory (some parts as a co-author), and for his invaluable contribution to the English translation.

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1. Bezverkhniy V. D. Structure of the benzene molecule on the basis of the three-electron bond. http://vixra.org/pdf/1606.0152v1.pdf

2. Bezverkhniy V. D. Experimental confirmation of the existence of the three-electron bond and theoretical basis ot its existence. http://vixra.org/pdf/1606.0151v1.pdf

3. Bezverkhniy V. D. A short analysis of chemical bonds. http://vixra.org/pdf/1606.0149v2.pdf

4. Bezverkhniy V. D., Bezverkhniy V. V. Supplement to the theoretical justification of existence of the three-electron bond. http://vixra.org/pdf/1606.0150v1.pdf

Note 1. Three-electrone bond it is an existing particle (object).

Three-electrone bond it is an existing bond, not a mathematical or physical model. And if the three-electron bond exist, then:

1) We can represent the one true formule of benzene (p. 3 - 5 Structure of the benzene molecule on the basis of the three-electron bond. http://vixra.org/pdf/1606.0152v1.pdf).

One of the drawbacks of the resonance theory is that resonance structures do not exist in reality, and their objectification is a mistake. And assuming the existence of three-electron bond, we can represent the real formula of benzene, aromatic compounds, carboxylate anion, ozone, oxygen, etc. (p. 19-29 Structure of the benzene molecule on the basis of the three-electron bond. http://vixra.org/pdf/1606.0152v1.pdf).

2) We can simply and clearly explain the increase in the multiplicity of benzene from 1.5 to 1.67 by MO method calculations give a value of 1.67, but Pauling from resonant structures, which is logical (2 and 4 of the electron) gave 1.5.
If the multiplicity is greater than 1.5 (eg 1.67), since the communication multiplicity in classical chemistry correlates with the amount of the bonding electrons (even if it is average) like:
2 electron multiplicity 1;
4 electron multiplicity 2;
6 electrons multiplicity 3;
thene in benzene at a multiplicity of 1.67 in six (6) aromatic bonds as it further appears 1 electron:
$1.67 - 0.17 = 1.5$
$6 * 0.17 = 1.02$
At the three-electron bond in benzene and interaction through a simple explanation of the cycle - the cycle just a little compressed.

3) We can check experimentally: if the three-electron bond and interaction through the cycle are real, then it logically follows the bending real chemical bond density in benzene into benzene.
It is important that the maximum density of the chemical bond will be shifted to the center of the benzene cycle link, which is what we are seeing in the atomic force microscopy images (AFM) pentacene (p. 1-2 Experimental confirmation of the existence of the three-electron bond and theoretical basis of its existence. http://vixra.org/pdf/1606.0151v1.pdf).

4) Experimental predicted effects: anti-aromatic system (core system) should be flat in order to make it through the interaction cycle. Therefore, to obtain photos and AFM antiaromatic cyclobutadiene cyclooctatetraene must be on a special matrix to consolidate their atoms to make the system perfect planarity (to make it through the interaction cycle), and after that, take a picture AFM permission. And if anti-aromatic photo is received, then we should see a shift of three-electron bonds outside the cycle, and, the picture will be in pentatsene but the loop (p. 4–5 Experimental confirmation of the existence of the three-electron bond and theoretical basis of its existence. http://vixra.org/pdf/1606.0151v1.pdf).

And if think ... ... reflect the existence of three-electron bond directly from the theory of resonance (resonance structures do not exist, in reality there is something average between them - and now think that should really be the basis of this, some real structure? .. of course the three-electron bond !!!).

The theory of three-electron bond accepted for granted the existence of three-electron bonds (one axiom), everything else is derived logically.

The need to introduce three-electron bond in the description of the benzene molecule can be understood (to some extent) reading the book (Chapter IX "Chemistry") Loren R. Graham. Science, Philosophy, and Human Behavior in the Soviet Union, Columbia University Press, 1987.

Short and interesting in Chapter IX "chemistry" of this book Loren R. Graham describes the concept of resonance theory in chemistry (description of the benzene molecule), as well as its criticism of the Soviet period.

Loren R. Graham - Professor at MIT (USA) on the big Material of actually analyzes full of dramatic story of the interaction of dialectical materialism and Soviet scients in the period from 1917 to mid-80s.
Provides a links to the original works.

Here is a quote Pauling:
"We can say ... that the molecule can not be satisfactorily represented by any particular structure of the valence bond and stop trying to tie its structure and properties of the structure and properties of other molecules. But, using valence bond structures as a basis for discussion, we are using the concept of resonance can give an explanation of the properties of the molecule, directly and simply in terms of other properties of the molecules. For us, convenient, for practical reasons, talk about the resonance of molecules among several electronic structures. "

Here's another quote Academician Koptyuga:
British journalist: "If you look at the history of science after the Revolution, you will see several cases of political interference in the fundamental research ... What do you think, could this happen again? "
Academician V. Koptiug, Chairman of the Siberian Branch of the USSR: "You see, this is a very complex issue ...
When in the past with philosophical positions criticized the concept of resonance in chemistry ... is, from my point of view, it is true.
But when a general philosophical position of trying to solve major scientific problems, such as whether genetics science or pseudoscience, it was a mistake. "
TV interview BBC, November 8, 1981.

Who loves the history of chemistry (of benzene) is very interesting and informative.

"Now the question is how to explain the existence of the three-electron bond in benzene and other molecules and ions from the point of view of quantum theory. It stands to reason that any placement of three electrons on the same atomic or molecular orbital is out of the question. Therefore it is necessary to lay the existence of three-electron bond in molecules in reality as an axiom. In this case the three-electron bond in benzene can be actually considered a semi-virtual particle. A real particle, such as an electron, exists in the real world for indefinitely long time. Virtual particles exist for the time which is insufficient for experimental registration (strong interactions in atomic nuclei). So we shall call the three- electron bond which really exists for indefinitely long time only in molecules and ions a semi-virtual particle.

The three-electron bond as a semi-virtual particle has certain characteristics:
its mass is equal to three electronic masses,
its charge is equal to three electronic charges,
it has half-integer spin (plus, minus 1/2)
and a real spatial extension.

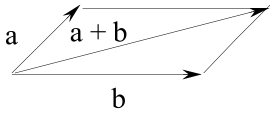
That is, our semi-virtual particle (the three-electron bond) is a typical fermion.

Fermions are particles with half-integer spin; they follow the Fermi-Dirac statistics, and have appropriate consequences, such as the Pauli exclusion principle etc. An electron is a typical fermion, and therefore such distribution in atomic and molecular orbitals is accepted (calculated). It follows that the three-electron bond in benzene is a real fermion in benzene, so quantum calculations can be extended to the molecule of benzene (and other systems) with the use of corresponding fermion (i.e. three-electron bond as a particle) instead of the electron in calculations. Then everything shall be made as usual: the Pauli exclusion principle, distribution in MO, binding and disintegrating MO, etc."

(p. 4–5 Experimental confirmation of the existence of the three-electron bond and theoretical basis of its existence. http://vixra.org/pdf/1606.0151v1.pdf).

Note 2. Chemical bond - it is the interaction of fermions.

Following from the above, interaction of two three-electron bonds in benzene (or rather interaction of three pairs) through the cycle is a typical interaction between two fermions in a molecule at a distance of 2,4 Å which is similar to the interaction of two electrons at the chemical bond formation.



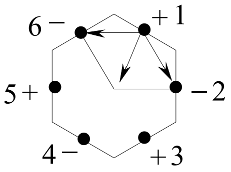


figure 3

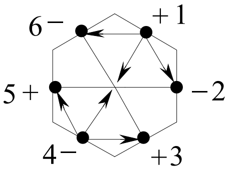
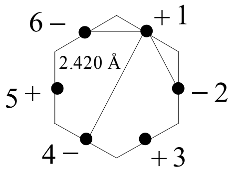


figure 4



$L_{1-2} = L_{1-6} = 1.210$ Å

$L_{1-4} = 2.420$ Å

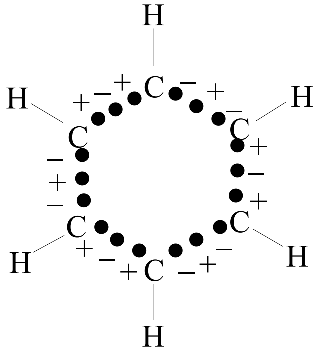


figure 1

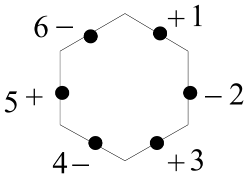
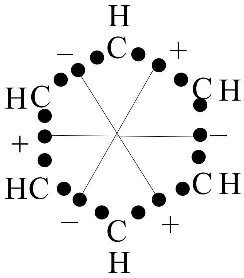
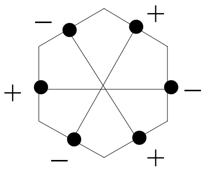


figure 2

" + " - upward spin

" − " - downward spin





" + " - the spin directed up

" − " - the spin directed down

Quantum sustem of unpaired number of fermions is itself a fermion, is a classic, so three elctrons is typical fermion who will behave appropriately (just an ordinary electron is a fermion).

This is something interestin about fermions:
"Composite fermions
In addition to elementary fermions and bosons, nonrelativistic composite particles made up of more fundamental particles bound together through a potential energy are composite fermions or bosons, depending only on the number of elementary fermions they contain:

A composite particle containing an even number of elementary fermions is a boson. Examples:
A meson contains two fermion quarks and is a boson.
The nucleus of a carbon-12 atom contains six protons and six neutrons (all fermions) and is also a boson.
A composite particle containing an odd number of elementary fermions is a fermion. Examples:
A baryon contains three quarks and is therefore a fermion.
The nucleus of a carbon-13 atom contains six protons and seven neutrons and is therefore a fermion.
The number of bosons within a composite particle made up of simple particles bound with a potential has no effect on whether the composite particle is a boson or a fermion.

In a quantum field theory, the situation is more interesting. There can be field configurations of bosons that are topologically twisted. These are coherent states that behave like particles, and they can be fermionic even if all the elementary particles are bosons. This situation was discovered by Tony Skyrme in the early 1960s, so fermions made of bosons are named Skyrmions.

Fermionic or bosonic behavior of a composite particle (or system) is seen only at large distances (compared to the size of the system). At proximity, where spatial structure begins to be important, a composite particle (or system) behaves according to its constituent makeup. For example, two atoms of helium cannot share the same space if it is comparable by size to the size of the inner structure of the helium atom itself (~10^−10 m) —despite bosonic properties of the helium atoms. Thus, liquid helium has finite density comparable to the density of ordinary liquid matter."

http://www.newworldencyclopedia.org/entry/Fermion

Note 3. Alternative description of the chemical bond.

Description of the chemical bond using the π- and σ-bond this is one of the alternative description. The correct and fair description of the chemical bond there is description of multiple bonds with the help of bent bonds (Pauling, in 1930 years).

At symposium (London, 1958) Pauling categorically stated: "There may be chemists who believe that it is extremely important innovation was the introduction of σ, π-description for the double or triple bond and conjugated systems instead of describing via bent bonds. I would argue that σ, π-description is less satisfactory than the description by means of curved links that this innovation is only transitory and will soon wither away."

Pauling was right, the theory of valence bonds, which used σ, π-description chemical bonding, lost its leading position.

(https://ru.wikipedia.org/wiki/ Теория_изогнутой_химической_связи).

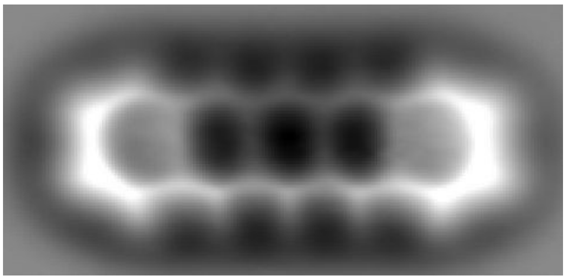
"Two different explanations for the nature of double and triple covalent bonds in organic molecules were proposed in the 1930s. Linus Pauling proposed that the double bond results from two equivalent tetrahedral orbitals from each atom,[7] which later came to be called banana bonds or tau bonds.[8] Erich Hückel proposed a representation of the double bond as a combination of a σ-bond plus a π-bond.[9][10][11] The Hückel representation is the better-known one, and it is the one found in most textbooks since the late-20-th century. There is still some debate as to which of the two representations is better,[12] although both models are mathematically equivalent. In a 1996 review, Kenneth B. Wiberg concluded that "although a conclusive statement cannot be made on the basis of the currently available information, it seems likely that we can continue to consider the σ/π and bent-bond descriptions of ethylene to be equivalent.[2] Ian Fleming goes further in a 2010 textbook, noting that "the overall distribution of electrons [...] is exactly the same" in the two models.[13]" https://en.wikipedia.org/wiki/Bent_bond

This double bond is 2 equivalent σ-bond (π-bond is not present).

Becouse of this, description bonds with σ- and π-bonds is first method of description, description bonds with bent bonds is second method of description, description bonds with three-electron bonds is third method of description. The correctness of the theory verified compliance of the experimental facts and predictions of new effects.

Theory of three-electron bond predict in aromatic interesting effect: anti-aromatic system (core system) should be flat in order to make it through the interaction cycle. Therefore, to obtain photos and AFM antiaromatic cyclobutadiene cyclooctatetraene must be on a special matrix to consolidate their atoms to make the system perfect planarity (to make it through the interaction cycle), and after that, take a picture AFM permission. And if anti-aromatic photo is received, then we should see a shift of three-electron bonds outside the cycle, and, the picture will be in pentatsene but the loop (p. 4–5 Experimental confirmation of the existence of the three-electron bond and theoretical basis of its existence. http://vixra.org/pdf/1606.0151v1.pdf).

As well as the curvature of bonds into pentacene is observed on the photo AFM.



But other than that if you use the three-electron bond in benzene at once solved a lot of problems:

1. Drawn real structure of the benzene molecule (and this is already an achievement).

2. Are explained easily and clearly aromaticity of benzene and antiaromaticity cyclobutadiene. It becomes obvious why at 4n + 2 aromatic and at 4n antiaromatic.
(p. 4–5 Structure of the benzene molecule on the basis of the three-electron bond. http://vixra.org/pdf/1606.0152v1.pdf).

3. Simply calculated delocalization energy of benzene (58,416 kcal / mol)
p. 11. Structure of the benzene molecule on the basis of the three-electron bond. http://vixra.org/pdf/1606.0152v1.pdf).

4. Easily and clearly explains the increase in the multiplicity of benzene from 1.5 to 1.66 (due to the interaction between the three electron bonds through a series of benzene slightly compressed). P. 11, 15,14. Structure of the benzene molecule on the basis of the three-electron bond (http://vixra.org/pdf/1606.0152v1.pdf).

5. Easy and simple to explain the difference of external and internal signals of protons in [18]-annulene p. 20–21 Structure of the benzene molecule on the basis of the three-electron bond (http://vixra.org/pdf/1606.0152v1.pdf).
6. You can picture structure of furan, thiophene, pyrrole, naphthalene, anthracene, graphite, oxygen, ozone, carboxylate anion and other organic and non-organic compounds. P. 19–29 Structure of the benzene molecule on the basis of the three-electron bond (http://vixra.org/pdf/1606.0152v1.pdf).

<u>And still need to clearly understand that the existence of two-electron chemical bond does not follow from fundamental interactions. But must follow!!!</u>

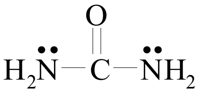
Therefore, the chemical bond and does not appear "on the tip of the pen", and introduced explanation exchange interaction and the like, since it is clear and proven that a purely Coulomb interaction (electromagnetic) is not sufficient to describe chemical bond (where there is more than one electron). By the way one-electron bond is displayed "on the tip of the pen."

Think ... with chemical bonding distance between the electrons (couple) should be the maximum that was the least the Coulomb repulsion between them and at the same time the electrons need to be concentrated in the middle of chemical bond to make it existed! With the chemical bond and the two-electron three-electron all hard. Therefore, when a breakthrough in theoretical terms in this direction chemistry waiting for great things (you will agree that this chemistry is still an empirical science, and quantum mechanical calculations are not very used experimenters, such as synthetic organic chemistry, etc.).

Note 4. Urea molecule.

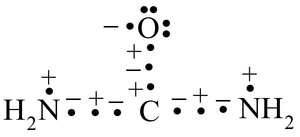
Look at the picture which shows the urea molecule with the calculations.

Classic structure



$H_2\ddot{N}-C(=O)-\ddot{N}H_2$

Real structure



$L_{C\text{-}N} = 1.33$ Å, $L_{C\text{-}O} = 1.27$ Å (8)

Multiplicity C−N = 1

Multiplicity C−N (L=1.33 Å) = 1.686

Multiplicity C−O = 2

Multiplicity C−O (L=1.27 Å) = 1.486

$E_{C\text{-}N} = 291.834$ kj/mole

$E_{C\text{-}N}$ (L = 1.33 Å) = 523.790 kj/mole

$E_{C\text{-}O} = 728.538$ kj/mole (for $R_2C{=}O$)

$E_{C\text{-}O}$ (L = 1.27 Å) = 496.940 kj/mole

$E_1 = E_{C\text{-}O} + 2E_{C\text{-}N} = 1312.206$ kj/mole

$E_2 = E_{C\text{-}O} + 2E_{C\text{-}N} = 1544.520$ kj/mole

$\Delta E = E_2 - E_1 = 1544.520$ kj/mole $- 1312.206$ kj/mole $= 232.314$ kj/mole

So, the energy gain for a real urea molecule (with three-electron bonds) as compared to the classic structure makes 232.314 kj/mole (55.487 kcal/mole). Calculations for other molecules may be done in the same way.

This example illustrates why the three-electron bonds appear at all: it proves to be that the three-electron bonds are “more poor” by energy and formation of three-electron bonds is energetically more advantageous (See calculations on page 30 on this link: Structure of the benzene molecule on the basis of the three-electron bond.

http://vixra.org/pdf/1606.0152v1.pdf).

The multiplicity of C-N bonds in the molecule of urea - 1.686. Think, this mean the C-athom connected with two atoms of nitrogen (urea) bonds with a multiplicity of approximately 1.7, fold that is one of the C-N bond is almost 2. Are classical structure transmits real formula of urea molecules?

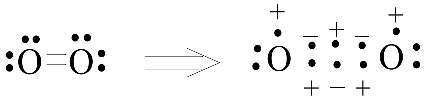
The multiplicity of C-O bond (urea) of approximately 1.5. That is the classic formula of urea (to which all accustomed to in the school and at university) almost not reflects the real structure of the urea.

Naturally, the explanation of the conjugation of the unshared pair of electrons of nitrogen with C-N bond are right. But classical formule (without arrows) does not show the structure of the molecule.

And note that the corresponding resonance structure (in which a multiplicity of the C-N bond - 2) can be written, but of course you can not write a resonance structure in which the two C-N bond have multiplicity 2.

Note 5. Oxygen.

Without regard of three electrone bond its impossible to portray oxygen molecule that has a multiplicity of connection 2 and two unpaired electrones. This experimental fact that multiplicity ob bond in the oxygen molecule is equal to two, and at the same time there are 2 unpaired electrones (Oxygen molecule has paramagnetic properties, it is an experimental fact, the multiplicity of bond correlates with the energy of bond, with IR spectra and the like, and there is no doubt that the multiplicity of oxygen molecule is two).



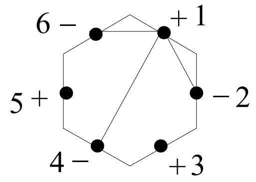
"Generally, the octet rule defines the state of the three-electron bond, that is, the distribution of the electrons, the energy of their interaction with each other and other unpaired electrons, the fact and the extent of belonging of the three-electron bond electrons to one or another atom." (p. 28, 32. Structure of the benzene molecule on the basis of the three-electron bond. http://vixra.org/pdf/1606.0152v1.pdf).

This fact is yet another confirmation of the existence of three-electrone bond.

Note 6. **Chemical bond - is a new indivisible particles,** electrons, in which the are entangled in quantum state.

The existence of large aromatic monocycles has been proved impossible based on interaction of three-electron bonds through the cycle at distances between the bonds (through the cycle) greater than 3.5 Å due to the lack of energy interaction (the length of chemical bonds is in the range of distances 0.74 Å – 3.5 Å).

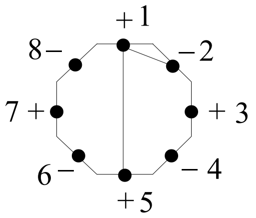
L_{c-c} = 1.397 Å



$L_{1-2} = L_{6-1}$ = 1.210 Å

L_{1-4} = 2.420 Å

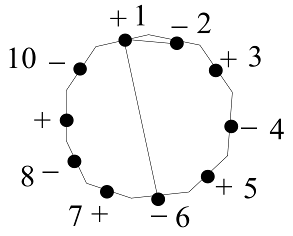
L_{c-c} = 1.410 Å



$L_{1-2} = L_{8-1}$ = 1.303 Å

L_{1-5} = 3.404 Å

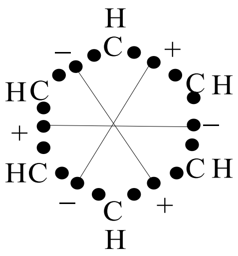
L_{c-c} = 1.400 Å

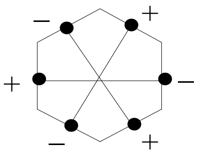


$L_{1-2} = L_{10-1}$ = 1.331 Å

L_{1-6} = 4.309 Å

The chemical bond (two-electron and three-electron) is considered on the assumption that the electrons in a chemical bond can be regarded as being in an entangled quantum state, that is, the chemical bond is seen as a new "indivisible" particle.



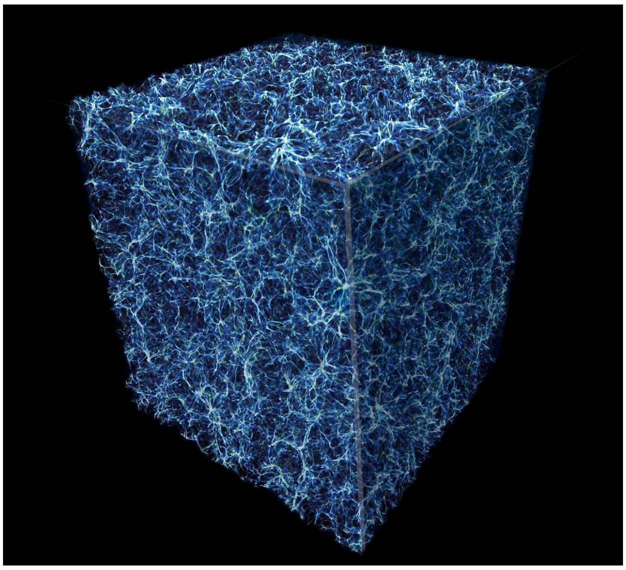


" + " - the spin directed up
" − " - the spin directed down

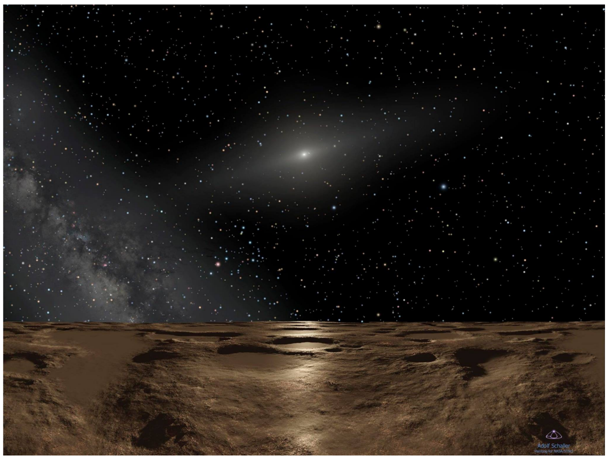
There has been provided an algorithm for calculating the two-electron chemical bond "on the tip of the pen" (Bezverkhniy V. D., Bezverkhniy V. V. Supplement to the theoretical justification of existence of the three-electron bond. http://vixra.org/pdf/1606.0150v1.pdf).

Note 7. Model of the Interfering Universe.

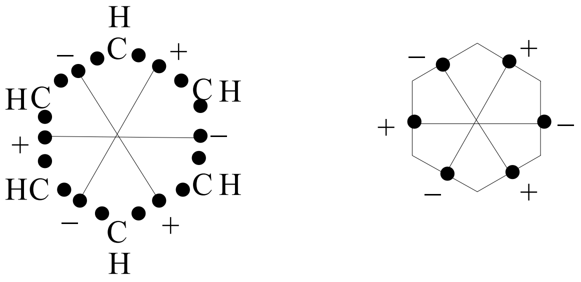
Model of the Interfering Universe, a perfect union of the microcosm and macrocosm.



1. foto. This graphic represents a slice of the spider-web-like structure of the universe, called the "cosmic web." These great filaments are made largely of dark matter located in the space between galaxies. Credit: NASA, ESA, and E. Hallman (University of Colorado, Boulder.



2. foto. How the solar system looks from Sedna. As seen from Sedna, the Sun would form somewhat of an isosceles triangle with Spica to the lower right and Antares to the lower left. NASA, ESA and Adolf Schaller - Hubble Observes Planetoid Sedna.



" + " - the spin directed up

" − " - the spin directed down

3. foto. Structure of the benzene molecule on the basis of the three-electron bond. http://vixra.org/pdf/1606.0152v1.pdf

"Now, let's try to explain the possibility of interaction of electrons and other particles, which are in an entangled quantum state, what presupposes the existence of any distance between them, for example, 1 m, or 1000 km, it is not essential, the distance can be arbitrarily long. And this distance does not affect the entangled quantum system, the particles of which miraculously know the characteristics of each other. To do this we'll have to simulate our Universe. So, let's imagine our infinite Universe as a finite (for convenience of description) object, such as an ordinary cube. Now let's imagine this cube empty of matter, space-time, and in general of any fields and other characteristics, there is no matter, and, in principle, anything. Now, let's "insert" an electron in the cube, and at once in the Universe there will appear space-time, weight, variety of fields (gravitational, electromagnetic, and so on), energy and other characteristics. After the electron appeared in the Universe, it came to life, and was born in principle. And now let's specify that the electron is not simply located in the Universe and has specific location and spot size, and its fields (electromagnetic, gravitational, and other existing and unknown) occupy and fill the whole Universe, the entire space-time continuum, our whole infinite Universe. Now let's step by step fill our cube (our Universe) with all elementary particles that exist in the Universe. And there is one condition that must be followed: each elementary particle occupies entirely and completely the whole Universe by its fields, energy and other characteristics, that is each particle completely fills (literally) all the infinite Universe, but at the same time it has certain coordinates (the most probable place of elementary particle detection).

With this description, our Universe, which is infinite in all senses (spatial, energy, time, etc.), will represent a giant interference of any and all elementary particles, a model of the "Interfering Universe". And now the main thing: since each elementary particle occupies (fills) the whole Universe (and at the same time is in a particular place with certain coordinates (its most probabilistic definition in this point, or more precisely in this region of space)), then there is nothing unusual in the fact that when forming an entangled quantum state each elementary particle "knows" the characteristics of its partner in a quantum state. Elementary particles "know" everything about all the other elementary particles since they fill the same Universe (it is their common home). They (elementary particles) constantly interact, interfere, but depending on their characteristics and the characteristics of their partners (coordinates, mass, energy, field, distances between the peak densities of detection, wave characteristics, etc.) form stable bonds (most varied and not only energy) only with certain partner particles.

... In the interfering Universe, all elementary particles "know everything" about all the other elementary particles (since they are in the same Universe), but not all of them are suitable for all in terms of formation of various bonds (in energy and other senses). Therefore, only those particles interact, which have a well-defined set of characteristics for each other and for specific types of interactions. And our world forms as a result of such interactions." (p. 5 — 6 http://vixra.org/pdf/1606.0150v1.pdf).

Defining a multiplicity of bond.

Nothing prohibits to give a definition of the multiplicity of bond:

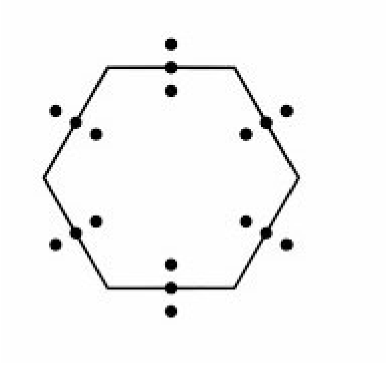
the multiplicity of bond is the energy of bond expressed in dimensionless units.

Hückel rule (4n + 2) for aromatic systems can be written in a different form, in the form of 2n where n - unpaired number. So, we have: 2, 6, 10, 14, 18, etc. This is also true for the electron shells in the atom and aromatic systems. The principle of the interaction of fermions always one, everywhere.

I note that the three-electron bond to describe the benzene molecule used even W.O. Kermak, R. Robinson and J. J. Thomson at the beginning of the 20th century. Here are links to their works:

1. Thomson, J. J. Philosophical Magazine, 1921, 41, 510-538.
2. W.O. Kermak and R. Robinson, J. Chem. Soc. 427 (1922).

Benzene molecule with three-electron bond. W.O. Kermak and R. Robinson, J. J. Thomson.



But since it is not taken into account the spin of electrons, we have already started cyclooctatetraene problems and therefore the description of the benzene molecule by a three-electron proved unsuccessful.

Using the three-electron bond with multiplicity of 1.5 and take account of the spin of each electron leads to very good results in the description of the benzene molecule and explain the aromaticity in general. With the help of three-electron bond with multiplicity of 1.5 can be represented by a real formula of many organic and inorganic molecules without the aid of virtual structures.

Theory of three-electrone bond in the four works:

1. Bezverkhniy V. D. Structure of the benzene molecule on the basis of the three-electron bond. http://vixra.org/pdf/1606.0152v1.pdf

2. Bezverkhniy V. D. Experimental confirmation of the existence of the three-electron bond and theoretical basis ot its existence. http://vixra.org/pdf/1606.0151v1.pdf

3. Bezverkhniy V. D. A short analysis of chemical bonds. http://vixra.org/pdf/1606.0149v2.pdf

4. Bezverkhniy V. D., Bezverkhniy V. V. Supplement to the theoretical justification of existence of the three-electron bond. http://vixra.org/pdf/1606.0150v1.pdf