# Review.
# Benzene on the basis of the three-electron bond.

## Theory of three-electron 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.

**Abstract:** Using the concept of three-electron bond we can represent the actual electron structure of benzene and other molecules, explain specificity of the aromatic bond and calculate the delocalization energy. Gives theoretical justification and experimental confirmation of existence of the three-electron bond. It was shown, that functional relation $y = a + b/x + c/x^2$ fully describes dependence of energy and multiplicity of chemical bond from bond distance.

**Keywords:** benzene, three-electron bond, semi-virtual particle, fermion, entangled quantum state, Interfering Universe.

## Content:

# 1. INTRODUCTION.

Chemical bond has been always a basis of chemistry. Advancement of chemical science can be considered as evolution, development of concepts about chemical bond. Aromatic bond is fundamental basis of organic chemistry. Concept of three-electron bond in benzene molecule enable to explain specificity of aromatic bond. It also becomes apparent, why planar molecules with 6, 10 etc. electrons (according to Hückel rule 4n + 2) must be aromatic, and planar molecules with 4, 8 etc. electrons cannot be aromatic by definition.

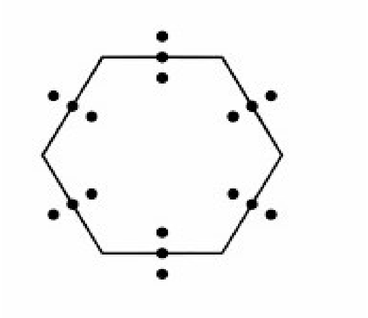
Description of chemical bond, that is given by quantum theory, especially in terms of method of molecular orbitals, is just a mathematical model. This model is an approximate representation of molecules and its bonds, whereas quantum-mechanical calculations of organic molecules require considerable simplifications and are extremely complicated.

Concept of three-electron bond and developed mathematical relations in this work are rather simple, illustrative and give exact results of different values (bond multiplicity, chemical bound energy, delocalization energy of benzene). One must clearly imagine, that three-electron bond is joint interaction of three electrons with relative spins, that results in new type of chemical bond ($A\overset{\uparrow\downarrow\uparrow}{\bullet\bullet\bullet}A$, $A\overset{\uparrow\downarrow\uparrow}{\bullet\bullet\bullet}B$). This bond type, three-electron bond, makes possible to describe real molecules of organic and inorganic compounds without invoking virtual structures, which do not exist in real terms.

Using of three-electron bond before description of benzene molecule enables to determine delocalization energy of benzene in an elementary way, understand why multiplicity of C-C bond of benzene is more than 1.5 and to understand the main point of aromatic bond in general, which is appeared to be rather illustrative. Besides, for determination of delocalization energy it is not required to select reference structures. Delocalization energy follows from the concept of aromaticity of benzene and its structure on the basis of three-electron bond.

I note that the three-electron bond to describe the benzene molecule used W.O. Kermak, R. Robinson and J. J. Thomson at the beginning of the 20th century [5, 6].

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, 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.

## 2. STRUCTURE OF THE BENZENE MOLECULE ON THE BASIS OF THE THREE-ELECTRON BOND.

### 2.1. RESULTS AND DISCUSSION.

Supposing that the chemical bond between two atoms can be established by means of three electrons with oppositely oriented spins (↑↓↑) the structure of the benzene molecule can be expressed as follows (see figure 1 and figure 2):

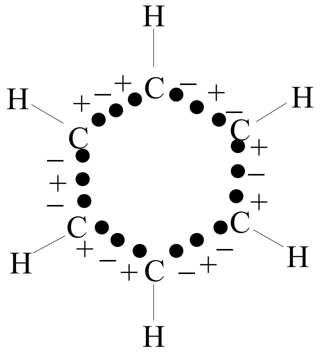


figure 1

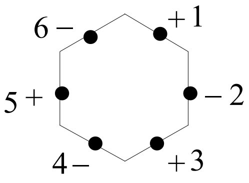


figure 2

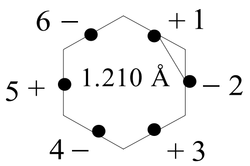
" + " - upward spin
" _ " - downward spin

It is interesting to point out that spins of central electrons on opposite sides have an opposite orientation (see figure 2). Now let us consider in detail the interaction of six central electrons between themselves. They will be itemized as shown in figure 2. As the spin of electron 1 and those of electrons 2 and 6 are oppositely oriented (see figure 2) (1 (+), 2 (-), 6 (-)), electron 1 will be attracted to electrons 2 and 6 respectively. Let’s indicate that the distance between electrons 1 and 6 or 1 and 2 is equal to 1.210 Å which can be easily shown taking into account the distance between atoms of carbon in benzene to be 1.397 Å and the angle between carbon atoms amount to 120 degrees. Let us compare the distance between electrons 1 and 6 and 1 and 2 bond lengths in ethane, ethylene and acetylene [7]:

$H_3C—CH_3$ $L_{C–C} = 1.543$ Å

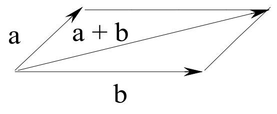
$H_2C{=}CH_2$ $L_{C=C} = 1.338$ Å

$HC{\equiv}CH$ $L_{C\equiv C} = 1.205$ Å



$L_{1-2} = 1.210$ Å

As we observe, the distance between central electrons 1 and 2 and 1 and 6 of the benzene molecule is approximately equal to that between carbon atoms in the acetylene molecule, therefore, the interaction between electrons 1 (+) and 2 (-) and 1 (+) and 6 (-) has to be rather considerable. Let us express the attraction with arrows. According to summing up vectors the resultant vector will be directed to the centre, which means that electron 1 under the influence of electrons 2 and 6 will move to the centre (figure 3):



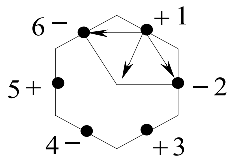


figure 3

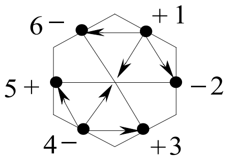
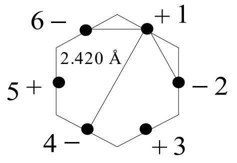


figure 4



$L_{1-2} = L_{1-6} = 1.210$ Å

$L_{1-4} = 2.420$ Å

If we take a look at electron 4 we see the similar situation with it (figure 4) and it will also move to the centre and, more importantly, its spin and that of electron 1 will be oppositely oriented, i.e. electron 1 (+) and electron 4 (-) will be attracted through the cycle. Electrons 6 (-) and 3 (+) and electrons 2 (-) and 5 (+) will interact similarly. The distance between electrons 1 and 4 in benzene is equal to 2.420 Å. It is interesting, that this distance is twice as much than distance between electrons 1 and 2, or between electrons 1 and 6 (1.210 Å · 2 = 2.420 Å). This interaction through the cycle constitutes the essence of the delocalization of electrons, of course together with a three-electron bond. Since besides the three-electron bond in the benzene molecule there is an interaction through the cycle, meaning that the benzene nucleus undergoes a kind of compression it is clear that the c-c bond multiplicity in benzene will exceed 1.5.

So, the aromatic system is a cyclic system with three-electron bonds where an interaction of central electrons through the cycle is observed. In the benzene molecule there are three interactions through the cycle - pairwise between electrons 1 (+) and 4 (-), 2 (-) and 5 (+), 3 (+) and 6 (-), as shown in figure 5:

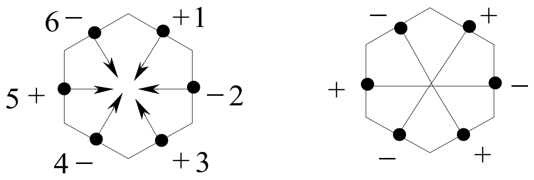
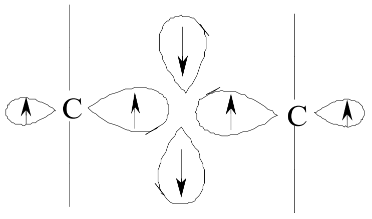
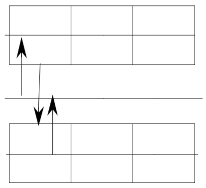


figure 5

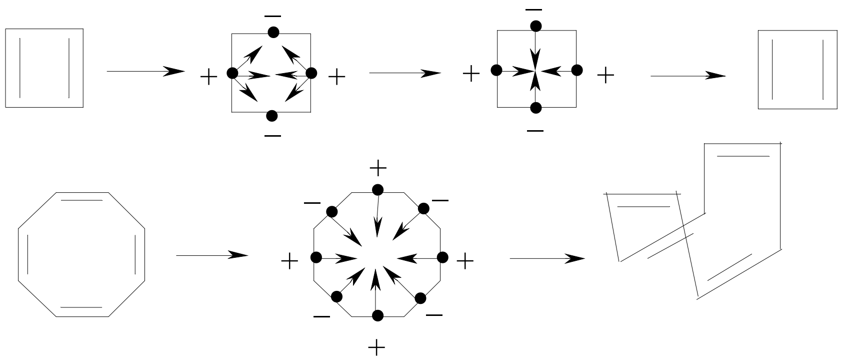
Carbon atoms in benzene are sp²-hybridized. The three-electron bond between carbon atoms in the benzene molecule can be represented as follows:





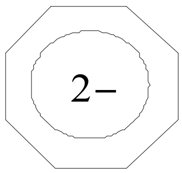
multiplicity = 3/2 = 1.5

Carbon atoms in benzene have an octet equal to 8 (3 + 3 + 2 = 8). It should be pointed out that due to the largest distance from the atoms nuclei the central electrons of the three-electron bond are supposed to be the most mobile compared to other electrons of the three-electron bond. The interaction of central electrons with opposite spins through the cycle can easily explain why cyclobutadiene and cyclooctatetraene are not aromatic compounds:



As we see both in cyclobutadiene and cyclooctatetraene, electrons interacting through the cycle have the same spins and, clearly, will be repulsed, therefore there will be no interaction through the cycle and the molecule will not be aromatic. In cyclobutadiene at the expense of small distance it causes the appearance of antiaromatic properties, and in cyclooctatetraene there is a possibility of formation of non-planar molecule, where interaction of central electrons becomes impossible and molecule losing the interaction through the cycle loses also three-electron bonds, that results in a structure, in which single and double bonds alternate.

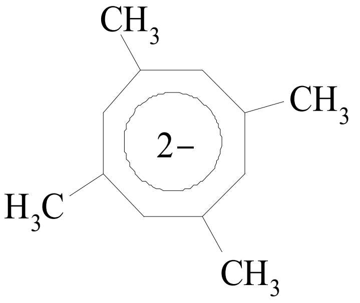
Explanation, that cyclooctatetraene is non-aromatic, because it is non-planar and does not hold water, insomuch as dianion of cyclooctatetraene is aromatic and has planar structure [8], [9].



Planar

X-ray crystal structure analysis determined crystal structure of potassium salt of dianion 1,3,5,7-tetramethylcyclooctatetraene [10], [11].

Octatomic cycle is planar with lengths of C-C bonds nearly 1.41 Å.



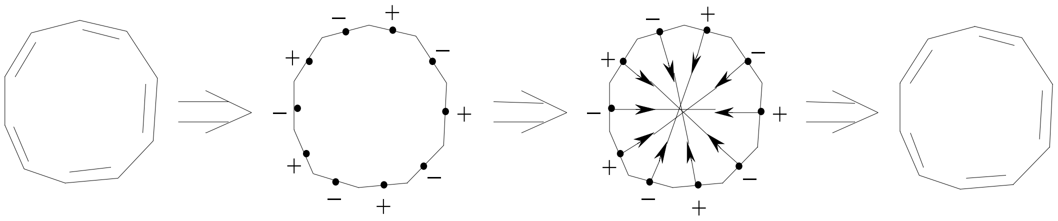
$L_{\text{c-c}} \approx 1.41$ Å

Planar

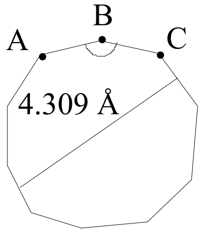
From the mentioned above we can make a conclusion: cyclooctatetraene conforms to the shape of bath tub not because of high angular pressure (15°) at planar structure, but because by interaction through the cycle central electrons of three-electron bonds have equal spin and will push away. Thus for energy reduction cyclooctatetraene conforms to the shape of bath tub and becomes non-planar, that disables interaction of central electrons.

Cyclobutadiene represents rectangular high reactivity diene [8, p. 79].

It is also interesting to observe cyclodecapentaene (cis-isomer [10]-annulene).



n = 10



n = 10

$\angle$ ABC = 144 $^{o}$C

Lc-c = AB = BC = 1.400 Å

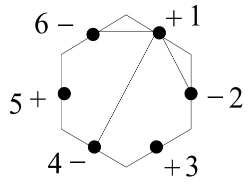
Whereas central electrons of three-electron bonds have opposite spins, then interaction through the cycle is possible. But distances between central electrons on opposite sides, which interact through the cycle, are extremely long (4.309 Å if accept Lc-c = 1.400 Å for regular decagon), angular pressure is high (24°) and that's why stabilization at the expense of interaction through the cycle at such long distance will be low and cannot cover energy consumption for creation of planar molecule.

Cyclodecapentaene was received in the form of crystalline substance at - 80°C. On spectrums $^{13}$C-NMR and $^{1}$H-NMR it was determined, that compound is non-planar and is olefin, that is logical on the basis of long distance between central electrons [8, p. 84], [12].

Lets draw our attention to the fact that in going from benzene to cyclooctatetraene and to cyclodecapentaene distance increases not only between central electrons on the opposite sides (interaction through the cycle), but also between neighboring central electrons.

Lets show it on figure.

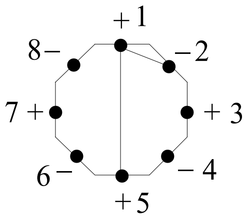
Lc-c = 1.397 Å



$L_{1-2} = L_{6-1} = 1.210$ Å

$L_{1-4} = 2.420$ Å

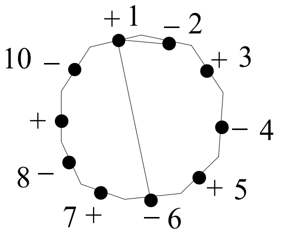
Lc-c = 1.410 Å



$L_{1-2} = L_{8-1} = 1.303$ Å

$L_{1-5} = 3.404$ Å

Lc-c = 1.400 Å



$L_{1-2} = L_{10-1} = 1.331$ Å

$L_{1-6} = 4.309$ Å

As we can see distance between neighboring central electrons 1 and 2 in benzene makes up 1.210 Å, in regular octagon 1.303 Å, and in regular decagon 1.331 Å (almost as distance between carbon atoms in ethene molecule). That is by going from benzene to regular octagon and decagon not only angular pressure (0°, 15°, 24°) and distance between central electrons increase, which are situated on the opposite sides (2.420 Å; 3.404 Å; 4.309 Å), as well as distance between neighboring central electrons 1 and 2 (1.210 Å; 1.303 Å; 1.331 Å), that causes considerable weakening of interaction through the cycle in regular decagon. That's why regular hexagon (benzene) is ideal aromatic system. As angular pressure is equal to zero, distances between central electrons both neighboring and situated on the opposite sides are minimal (accordingly 1.210 Å and 2.420 Å). I.e. interaction through the cycle will be maximal. By going to regular decagon these advantages will be lost. That's why cyclodecapentaene is olefin.

Let us note for comparison that if we take Lc-c = 1.400 Å for the planar cyclooctatetraen, we will have L(1-5) = 3.380 Å, L(1-2) = L(8-1) = 1.293 Å which vary just slightly from the above mentioned distances between the central electrons at Lc-c = 1.410 Å.

By means of the interaction through the cycle together with the three-electron bond, aromaticity of coronen, [18]-annulene, naphthalene and other organic substances can be explained (see conclusion).

Now let's pass to the definition of delocalization energy of benzene. It is easy to show, that relation multiplicity = f(L) and E = f(L), where multiplicity is multiplicity of bond, L – length of bond in Å, E – energy of bond in kj/mole will be described by function $y = a + b/x + c/x^2$ for any types of bond (C-C, C-N, C-O, C-S, N-N, N-O, O-O, C-P).

We shall consider ethane, ethylene and acetylene to be initial points for the c-c bond.

For lengths of bonds let us take the date [7]:

| | | |
|---|---|---|
| $H_3C-CH_3$ | $H_2C=CH_2$ | $HC\equiv CH$ |
| $L_{c-c} = 1.543$ Å | $L_{c=c} = 1.338$ Å | $L_{C\equiv C} = 1.205$ Å |

As usual, the C-C bond multiplicity in ethane, ethylene and acetylene is taken for 1, 2, 3.

For energies of bonds let us take the date [7, p. 116]:

| | | |
|---|---|---|
| $H_3C-CH_3$ | $H_2C=CH_2$ | $HC\equiv CH$ |
| $E_{C-C} = 347.9397$ kj/mole | $E_{C=C} = 615.489$ kj/mole | $E_{C\equiv C} = 812.278$ kj/mole |

The given bond energies (according to L. Pauling) are bond energy constants expressing the energy that would be spent for an ideal rupture of these bonds without any further rebuilding of the resulting fragments. That is, the above mentioned energies are not bond dissociation energies.

Having performed all necessary calculations we obtain the equation:

$$c - \text{c bond multiplicity} = -0.06040343 - \frac{5.67787529}{L} + \frac{11.28562201}{L^2} \qquad (1)$$

$$\text{E of c} - \text{c bonds} = -2221.34518418 + \frac{5065.62912191}{L} - \frac{1699.18638789}{L^2} \qquad (2)$$

From these equations we find:

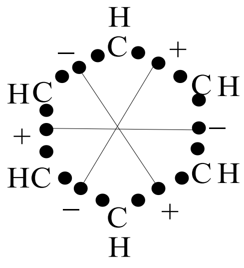
c–c benzene multiplicity (L = 1.397 Å) = 1.658

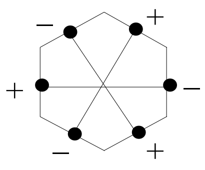
c–c graphite multiplicity (L = 1.42 Å) = 1.538 ≈ 1.54

Ec–c benzene (L = 1.397 Å) = 534.0723 kj/mole

Ec–c graphite (L = 1.42 Å) = 503.3161 kj/mole

Being aware that the benzene has the three-electron bonds and also the interaction through the cycle, we can calculate the interaction through the cycle energy.





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

For this purpose we have to determine the energy of the "clean" three-electron bond, that is of the bond with a 1.5 multiplicity and to do that we shall solve the equation:

$$1.5 = -0.06040343 - \frac{5.67787529}{L} + \frac{11.28562201}{L^2} \qquad (3)$$

from the equation we find L = 1.42757236 Å.

So, if the benzene molecule had a "clean" three-electron bond with a 1.5 multiplicity the c-c bond length would be L = 1.42757236 Å.

Now let us determine the energy of the "clean" three-electron bond with a 1.5 multiplicity knowing its length L = 1.42757236 Å:

$$Ec - c\,(L = 1.42757236\ \text{Å}) = -\,2221.34518418 + \frac{5065.62912191}{1.42757236} - \frac{1699.18638789}{(1.42757236)^2}$$

$Ec - c\ (L = 1.42757236\ \text{Å}) = 493.3097$ kj/mole

Taking into account that the benzene c-c bond energy with a 1.658 multiplicity is equal to Ec-c benzene = 534.0723 kj/mole, the difference will make:

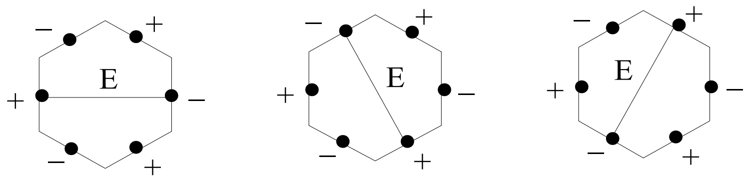
$\Delta E = 534.0723$ kj/mole – 493.3097 kj/mole = 40.7626 kj/mole.

40.7626 kj/mole is the energy of interaction through the cycle per one c-c bond. Therefore, the energy of interaction through the cycle will be two times higher:

$E_1 = 40.7626$ kj/mole · 2 = 81.5252 kj/mole (19.472 kcal/mole)

It is clear that the three interactions through the cycle present precisely the working benzene delocalization energy which is:

$E = 3E_1 = 3 \cdot 81.5252$ kj/mole = 244.5756 kj/mole (58.416 kcal/mole)



$3 \cdot E = 244.5756$ kj/mole

It is also possible to calculate the benzene molecule energy gain in comparison with the curved cyclohexatriene (let us assume that energy of C-H bonds in these molecules is similar). For this we calculate the sum of energies of single and double c-c bonds in cyclohexatriene:

$E_2 = 3E_{c-c} + 3E_{c=c} = 2890.286$ kj/mole

The energy of six benzene c-c bonds with a 1.658 multiplicity is equal to:

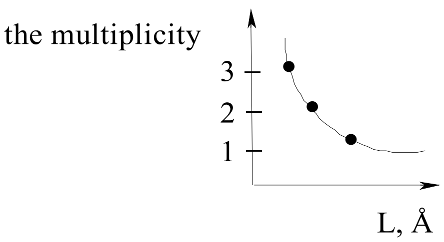
$E_3 = 6 \cdot 534.0723$ kj/mole $= 3204.434$ kj/mole

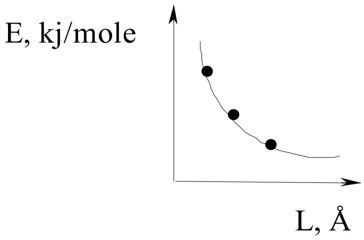
Therefore, the gain energy of benzene compared to cyclohexatriene will amount to:

$E = E_3 - E_2 = 3204.434$ kj/mole – 2890.286 kj/mole = 314.148 kj/mole (75.033 kcal/mole).

## 2.2. EXPERIMENTAL.

Let's show more detailed calculation of ratios for our mathematical relations. Let's consider relation Multiplicity = f(L) and E = f(L) for C-C bonds, where multiplicity is multiplicity of bond, L – length of bond in Å, E – energy of bond in kj/mole.





As initial points for the given bonds we will use ethane, ethene and acetylene**.**

For the length of bonds let us take the findings [7]:

$H_3C{-}CH_3$ $H_2C{=}CH_2$ $HC{\equiv}CH$

$L_{C-C} = 1.543$ Å $L_{C=C} = 1.338$ Å $L_{C\equiv C} = 1.205$ Å

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If we have two variants and we received the set of points and we marked them on the plane in the rectangular system of coordinates and if the present points describe the line equation y = ax + b that for choose the coefficients a and b with the least medium-quadratic deflection from the experimental points, it is needed to calculate the coefficients a and b by the formulas:

$$a=\frac{\left(\sum (x\cdot y)-\left(\sum x\cdot\sum y\right)/n\right)}{\left(\sum x^{2}-\left(\sum x\right)^{2}/n\right)} \tag{4}$$

$$b=\left(\sum y\right)/n-a\left(\sum x\right)/n \tag{5}$$

n-the number of given values x or y.

If we want to know how big is the derivative, it is necessary to state the value of agreement between calculated and evaluated values y characterized by the quantity:

$$r^{2}=\frac{\left[\sum (x\cdot y)-\left(\sum x\cdot\sum y\right)/n\right]^{2}}{\left(\left[\sum x^{2}-\left(\sum x\right)^{2}/n\right]\left[\sum y^{2}-\left(\sum y\right)^{2}/n\right]\right)} \tag{6}$$

The proximity of $r^2$ to one means that our linear regression coordinates well with experimental points.

Let us find by the method of selection the function $y = a + b/x + c/x^2$ describing the dependence multiplicity = f(L) and E = f(L) in best way, in general this function describes this dependence for any chemical bonds.

Let us make some transformations for the function $y = a + b/x + c/x^2$, we accept

$X = 1/x$,

$$\mathrm{Y} = \frac{(y - y_1)}{(1/x - 1/x_1)}, \quad b_1 = \mathrm{b} + \mathrm{c}/x_1,$$

than we'll receive: $Y = b_1 + cX$, that is the simple line equality, than

$$c = \frac{\left(\sum (1/x \cdot Y) - \left(\sum (1/x) \cdot \sum Y\right)/n\right)}{\left(\left(\sum 1/x^2\right) - \left(\sum (1/x)\right)^2/n\right)} \tag{7}$$

$$b_1 = \left(\sum Y\right)/n - c\left(\sum (1/x)\right)/n \tag{8}$$

n–the number of given value Y.

Let us find a from the equality: $\sum y = na + b\sum(1/x) + c\sum(1/x^2)$, (9)

when n = 3.

Let us find now multiplicity = f(L) for C─C, C═C, C≡C.

Table 1. Calculation of ratios for relation Multiplicity = f(L).

| | 1/x | $1/x^2$ | $\frac{(y - y_1)}{(1/x - 1/x_1)}$ | $\frac{((1/x)(y - y_1))}{(1/x - 1/x_1)}$ | x (L, Å) | y (multiplicity) |
|---|---|---|---|---|---|---|
| | | | | | 1.543 | 1 |
| | 0.74738416 | 0.55858308 | 10.07089756 | 7.52682927 | 1.338 | 2 |
| | 0.82987552 | 0.68869338 | 11.00186391 | 9.13017751 | 1.205 | 3 |
| ∑ | 1.57725967 | 1.24727645 | 21.07276147 | 16.65700678 | 4.086 | 6 |

$1/x_1 = 0.64808814$ $x_1 = 1.543$ $y_1 = 1$

$\Sigma(1/x^2) = 1.66729469$ $\Sigma(1/x) = 2.22534781$ when n = 3

c = 11.28562201 b = - 5.67787529 a = - 0.06040343

$$\text{Therefore the multiplicity of c} - \text{c bonds} = -\,0.06040343 - \frac{5.67787529}{L} + \frac{11.28562201}{L^2} \quad (1)$$

Let us find from the equation:

Multiplicity C−C (ethane) = 1. Multiplicity C═C (ethylene) = 2.

Multiplicity C≡C (acetylene) = 3.

Multiplicity C−C (graphite) (L = 1.42 Å) = 1.538 ≈ 1.54.

Multiplicity C−C (benzene) (L = 1.397 Å) = 1.658.

As we can see the multiplicity C−C of benzene bond is 1.658 it is near the bond order of 1.667 calculated by the method MO [8, p. 48].

It should be noted that the a, b, c coefficients for this $y = a + b/x + c/x^2$ function in case of using three pairs of points ($x_1$, $y_1$), ($x_2$, $y_2$) and ($x_3$, $y_3$) are defined explicitly; actually, they (the coefficients) are assigned to these points. In that way we find these coefficients for working further with the equation. For making certain that this dependence $y = a + b/x + c/x^2$ describes well the Multiplicity = f(L) and E = f(L) functions it will take only to perform correlation for four or more points. For example, for the dependence Multiplicity = f(L) for C-C bonds we should add a fourth point ($L_{C–C}$ = 1.397 Å, Multiplicity = 1.667) and obtain an equation with $r^2 = 0.9923$ and the coefficients a = - 0.55031721, b = - 4.31859233, c = 10.35465915.

As it is difficult, due to objective reason, to define four or more points for the Multiplicity = f(L) and E = f(L) equations for a separate bond type, we will find the a, b, c coefficients using three points (as a rule they are the data for single, double and triple bonds). The dependences obtained in such a way give good results as regards the bond multiplicity and energies.

We'll find the dependence E = f(L) for the C−C bonds

$$y = a + b/x + c/x^2 \qquad X = 1/x \qquad Y = \frac{(y - y_1)}{(1/x - 1/x_1)}$$

$$b_1 = b + c/x_1 \qquad Y = b_1 + cX$$

As usual:

$$c = \frac{\left(\sum(1/x\cdot Y) - \left(\sum(1/x)\cdot\sum Y\right)/n\right)}{\left(\left(\sum 1/x^2\right) - \left(\sum(1/x)\right)^2/n\right)} \tag{7}$$

$$b_1 = \left(\sum Y\right)/n - c\left(\sum(1/x)\right)/n \tag{8}$$

n–the number of given value Y.

Let us calculate a from the equation $\sum y = na + b\sum(1/x) + c\sum(1/x^2)$, (9)

when n = 3.

Table 2. Calculation of ratios for relation E = f(L).

| | 1/x | 1/x² | $\frac{(y-y_1)}{(1/x-1/x_1)}$ | $\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$ | x (L, Å) | y (E, kj/mole) |
|---|---|---|---|---|---|---|
| | | | | | 1.543 | 347.9397 |
| | 0.74738416 | 0.55858308 | 2694.46159281 | 2013.79790195 | 1.338 | 615.4890 |
| | 0.82987552 | 0.68869338 | 2554.29339132 | 2119.74555296 | 1.205 | 812.2780 |
| ∑ | 1.57725967 | 1.24727645 | 5248.75498413 | 4133.54345491 | 4.086 | 1775.7067 |

$1/x_1 = 0.64808814$ $x_1 = 1.543$ $y_1 = 347.9397$

$\Sigma(1/x^2) = 1.66729469$ $\Sigma(1/x) = 2.22534781$ when n = 3

c = - 1699.18638789 b = 5065.62912191 a = - 2221.34518418

$$\text{E of c} - \text{c bonds} = -2221.34518418 + \frac{5065.62912191}{L} - \frac{1699.18638789}{L^2} \tag{2}$$

Let us calculate from the equation:

Ec–c (ethane) = 347.9397 kj/mole

Ec═c (ethylene) = 615.4890 kj/mole

Ec≡c (acetylene) = 812.2780 kj/mole.

## 2.3. CONCLUSION.

As we can see, three-electron bond enables to explain aromaticity, find delocalization energy, understand aromatic bonds specificity. Aromatic bond in benzene molecule is simultaneous interaction of three pairs of central electrons with opposite spins through the cycle. But whereas central electrons are the part of three-electron bond, then it is practically interaction of six three-electron bonds between themselves, that is expressed in three interactions through cycle plus six three-electron bonds. We shouldn't forget in this system about important role of six atom nucleuses, around which aromatic system is formed. Properties of nucleuses especially their charge will influence on properties of aromatic system.

Finally, postulates of the three-electron bond theory (TBT) can be presented:

1) A chemical bond between two atoms may be established by means of three electrons with oppositely oriented spins (↑↓↑).

$$\overset{\uparrow\downarrow\uparrow}{A\bullet\bullet\bullet A} \quad \overset{\uparrow\downarrow\uparrow}{A\bullet\bullet\bullet B}$$

2) The electron shell of each atom in the stable molecule, ion, radical should have such a number of electrons which corresponds to the octet. A deviation from the octet results in an instability of a particle.

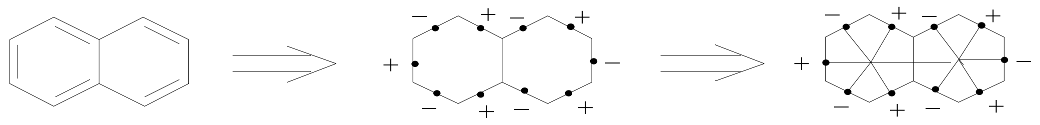
3) The state of the three-electron bond is determined by the octet rule.

4) The number of electrons participating in the chemical bond should be maximal and it's then that the energy of the system will be minimal. Taking into consideration para 5 and 2.

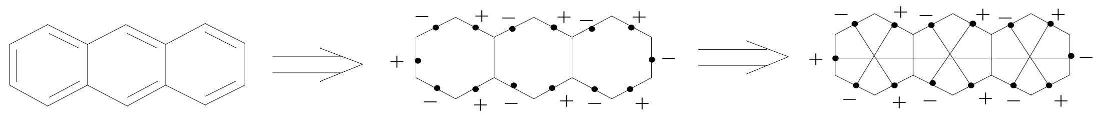
5) In the course of establishing of the chemical bond electrons (their spins) are located in such a way that enables the interaction (attraction) to be maximal.

6) The aromatic bond is a three-electron bond in flat cyclic systems with a specific interaction of electrons through the cycle.

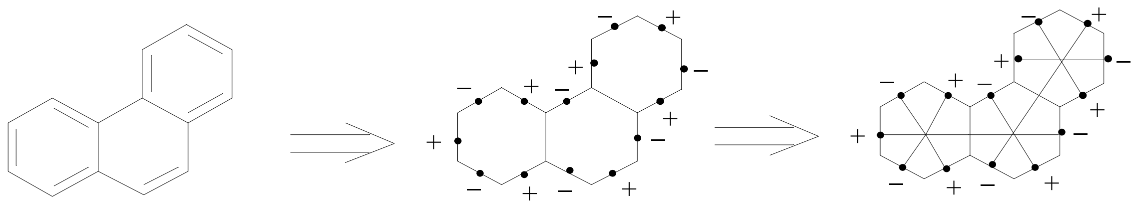
It is easy to show, that using three-electron bond one can explain paramagnetization and structure of oxygen molecule, structure of carboxylate anion, ozone, naphthalene and other organic and non-organic compounds. Let’s bring for the example structures of some compounds in terms of three-electron bond.



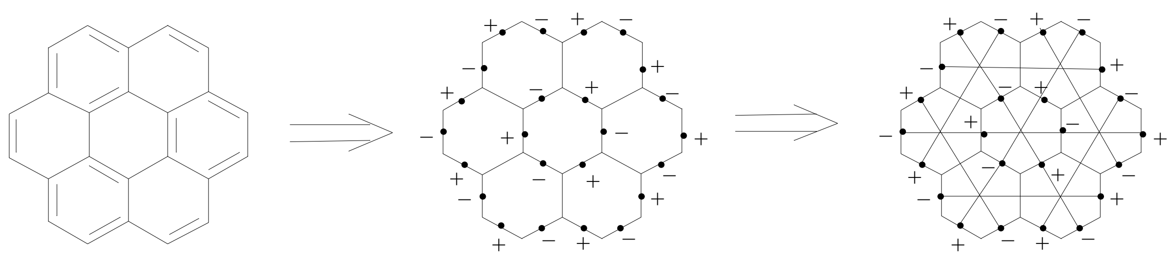
Naphthalene



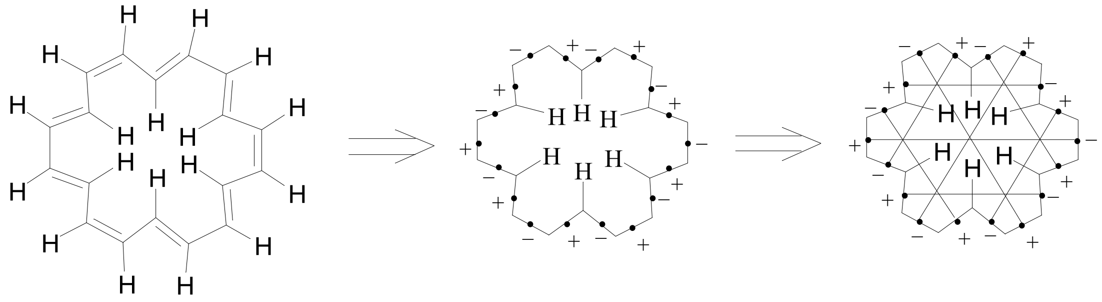
Anthracene



Phenanthrene



Coronene



[18]-Annulene

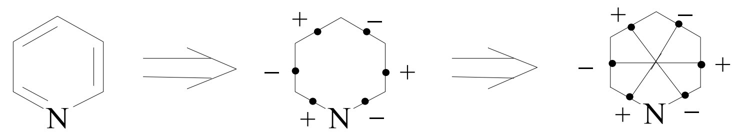
It is interesting to note extreme symmetry of structures of naphthalene, anthracene, coronene and [18]-annulene, that is typical for the majority of aromatic compounds in general.

By the example of [18]-annulene it is possible to illustrate interaction through the cycle of central electrons of three-electron bonds. Interacting through the cycle, it shifts to the centre in the direction of inner atoms of hydrogen thus increasing electron density within the cycle and decreasing outside the cycle. And that’s why outside protons (12 H) will give signals in the area of weaker field (reduction of electron density), and inner (6 H) will give signals in the area of stronger field (increase of electron density). Thus this is observed in reality [13]. It also should be noted that inner protons bracing central electrons strengthen interaction through the cycle, and so stabilize aromatic system. But interaction through the cycle is decisive.

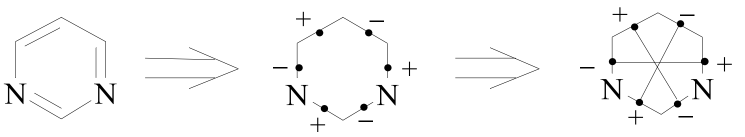
If aromatic system does not have inner protons, then outside protons will give signals in the area of weaker field (one of the features of aromatic compounds).

It is clear that in case of antiaromatic systems when there is no interaction (attraction) through the cycle, because central electrons have similar spins and push away, change in electron density in the centre of the cycle and outside the cycle will be reverse to aromatic systems.

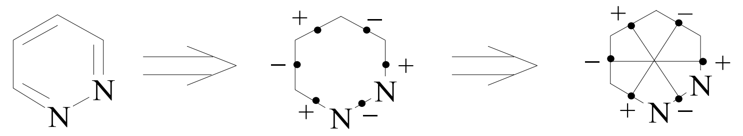
Further we will continue demonstration of construction of organic and inorganic compounds.



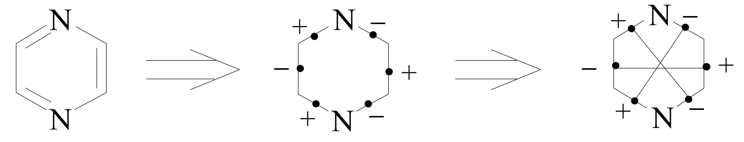
Pyridine



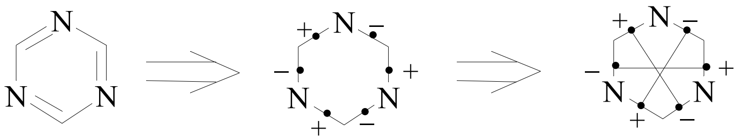
Pyrimidine



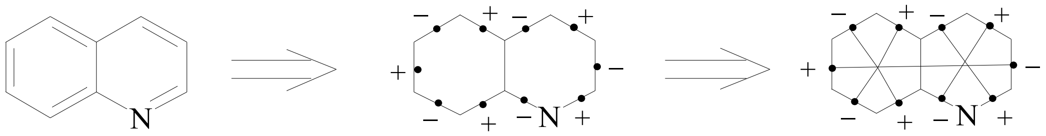
Pyridazine



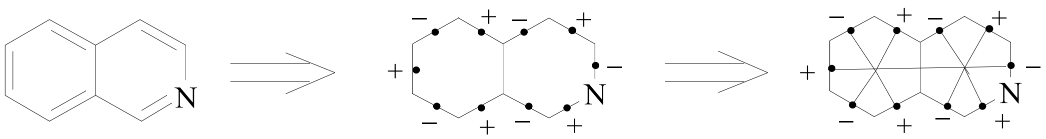
Pyrazine



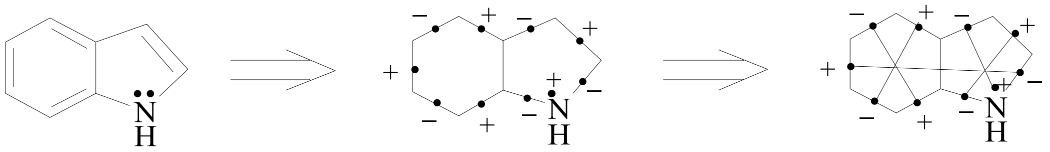
1,3,5-Triazine



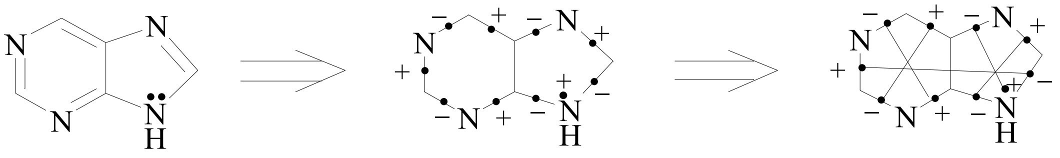
Quinoline



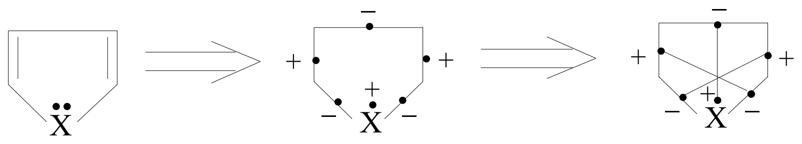
Isoquinoline



Indole

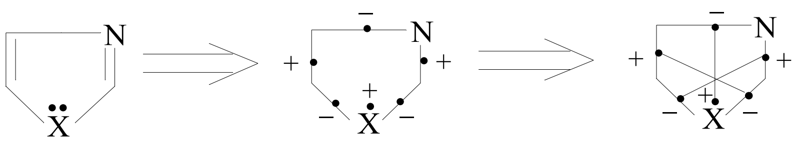


Purine



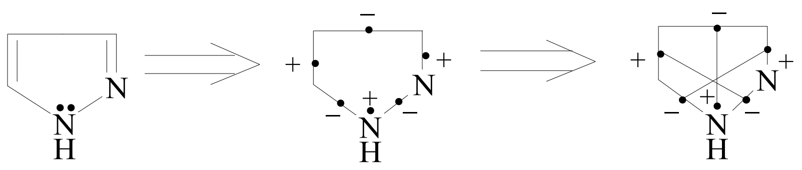
X = O, S, NH

Furan, thiophene, pyrrole

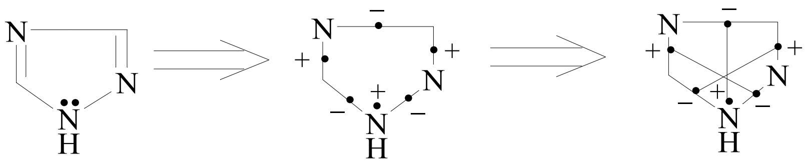


X = O, S, NH

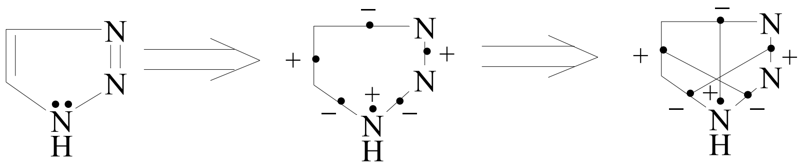
Oxazole, thiazole, imidazole



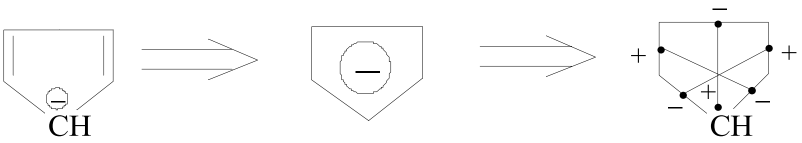
Pyrazole



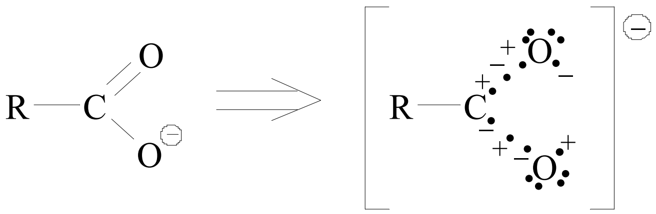
1,2,4-Triazole



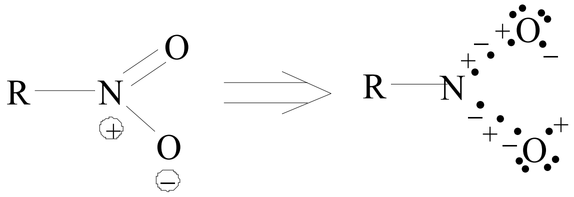
1H-1,2,3-Triazole



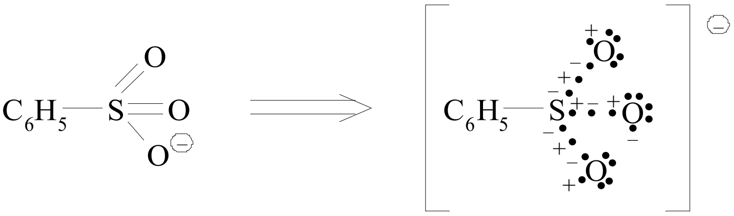
Cyclopentadienyle anion



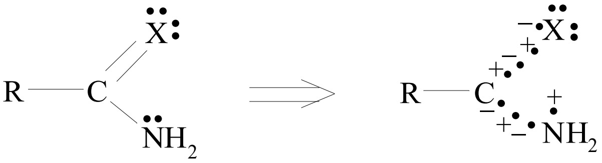
Carboxylate anion



Nitro compounds

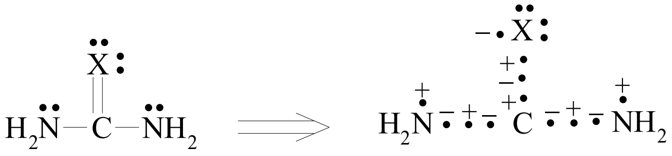


Sulfonate anion



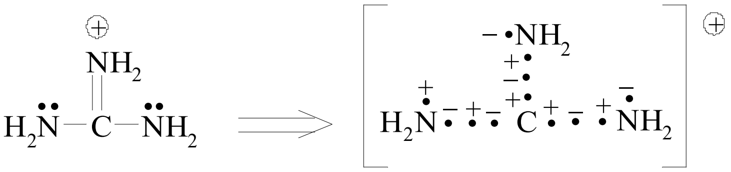
X = O, S

Organic acid amides and thioamides

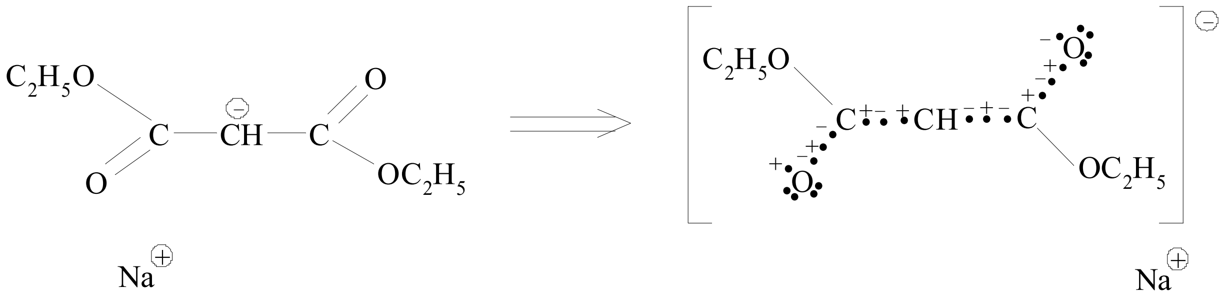


X = O, S

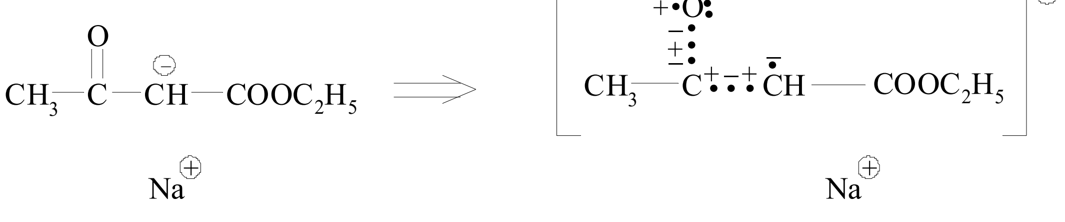
Urea and thiourea



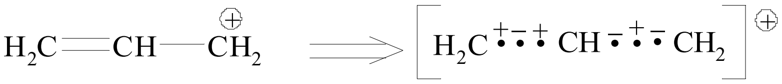
Guanidinium cation



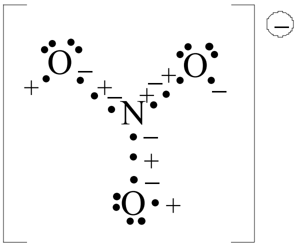
Sodium malon ether



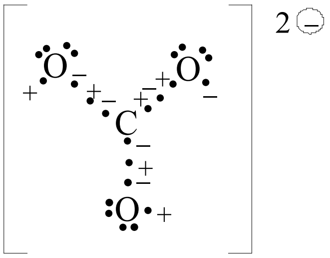
Sodium acetoacetic ether



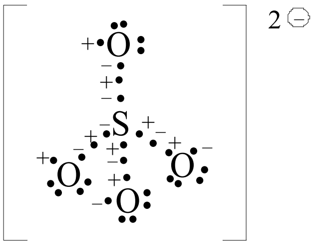
Alyle cation



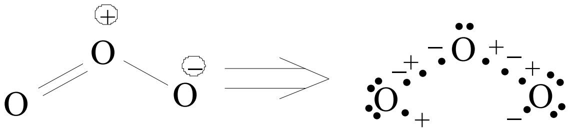
Nitrate anion



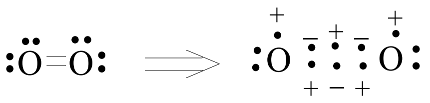
Carbonate anion



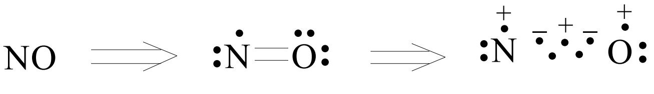
Sulfate anion



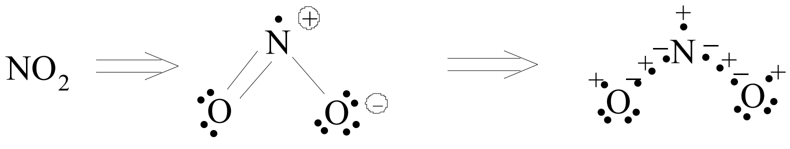
Ozone



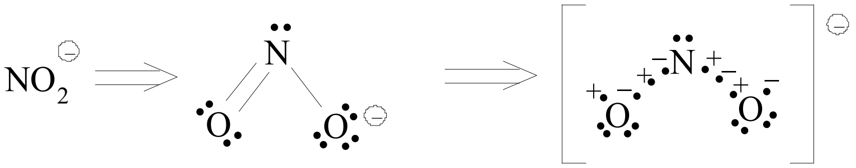
Oxygen, paramagnetic molecule



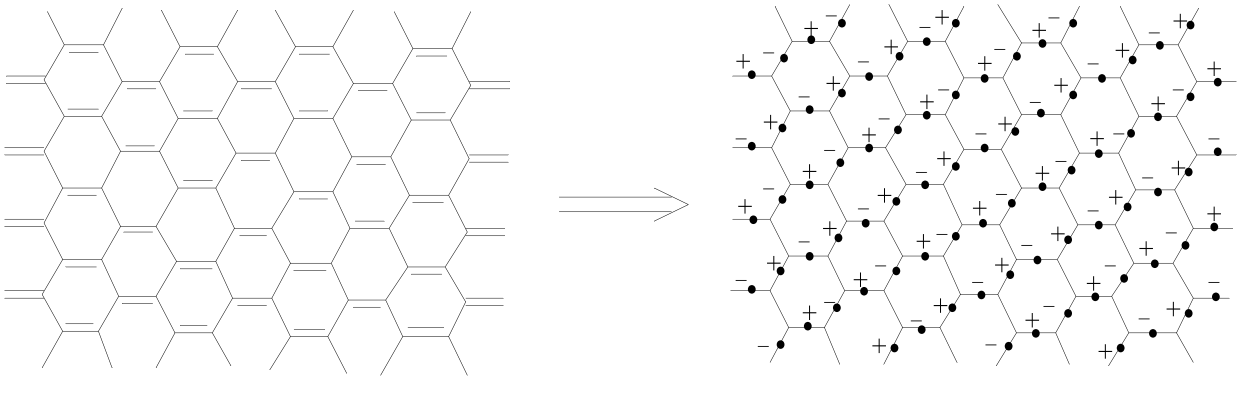
Nitrogen monoxide, paramagnetic molecule



Nitrogen dioxide, paramagnetic molecule



Nitrite anion



Graphite

As we can see with the help of three-electron bond structures of abovementioned molecules and ions are described simply and obviously by one structures, which represents the real distribution of electrons (electron density) in molecules (ions).

Author knowingly did not consider a question about kinds of forces, that make electrons to attract with opposite spins, because it is a subject of a separate consideration. All the more so, because based on famous postulate (attraction of two electrons with opposite spins) concept of localized chemical bond follows. Explaining aromatic bond in benzene molecule, interaction of central electrons is strange on such long distances (2.420 Å). But taking into account, that electrons can show wave-like behaviour and shift to the center of benzene cycle under the influence of neighbouring central electrons, this interaction looks very truly.

The fact of the distance between the graphite layers being 3.35 Å (the C-C bond length inside the layer making 1.42 Å) [14] may serve as an indirect confirmation of the possibility of interaction of the electrons through the cycle in benzene. This causes a weak bond between the layers and, as a result, the ability of the layers to shift relative to each other. Since the distance between the central electrons in benzene is less and makes 2.420 Å (in case of an interaction through the cycle), we should expect a stronger interaction.

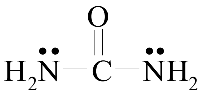
It is clear that, by increasing of cycle, distance between central electrons (both neighboring and through the cycle) will increase, and that's why interaction energy through the cycle will decrease, and by certain distance benefit from aromaticity of system will be lower, than energy consumption for creation of planar equilateral polygon (as in the case of cyclodecapentaene). Therefore existence of large aromatic monocycles will depend on relation of these two values.

With the help of equations $E = a + b/L + c/L^2$ and multiplicity $= a + b/L + c/L^2$ we can analyze different types of chemical bonds, calculate their multiplicity and energy on the basis of experimental data about bonds distances.

The tables 3 and 4 below show the a, b and c coefficients for these equations for the bonds prevailing in the organic chemistry (C-C, C-O, C-N, C-S, N-N, N-O, O-O). The coefficients have been calculated similarly to the C-C bonds. Using them it is possible to calculate the bonds multiplicity and their energy (bond energy constants) for the most part of organic molecules, both aromatic and non-aromatic ones. It makes it possible to calculate the aromatic compounds delocalization energy.

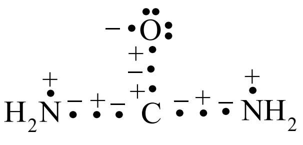
It is also possible to calculate the real molecules energy gain compared to their classic structures. To do this, it is necessary to subtract the total of the classic structure bond energies from the total of the real structure bond energies (the bond energy is calculated with the $E = a + b/L + c/L^2$ equation). Let us illustrate the above taking the urea molecule as an example (leaving out of consideration the N-H bonds):

Classic structure



$$H_2\ddot{N}-\overset{\overset{O}{\|}}{C}-\ddot{N}H_2$$

Real structure



$L_{C\text{-}N} = 1.33$ Å, $L_{C\text{-}O} = 1.27$ Å (14)

Multiplicity C−N = 1

Multiplicity C−O = 2

$E_{C\text{-}N}$ = 291.834 kj/mole [7, p.116]

$E_{C\text{-}O}$ = 728.538 kj/mole (for $R_2C{=}O$) [7, p.116]

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

Multiplicity C−N (L=1.33 Å) = 1.686

Multiplicity C−O (L=1.27 Å) = 1.486

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

$E_{C\text{-}O}$ (L = 1.27 Å) = 496.940 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. The energetic advantageousness is also the reason of the deviation of the multiplicity of the three-electron bonds from 1.5 which takes place due to either the interaction of the three-electron bonds among themselves (for example, in the benzene molecule) or the interaction of the three-electron bonds with the unpaired electrons located in atoms making the bond (urea molecule). Cases are possible when the bond multiplicity is changed due to the simultaneous influence of the above mentioned effects.

It should be also noted that the octet rule holds true in three-electron bond structures. Thus, in the urea molecule the three-electron bond electrons interact partially with the unpaired electrons located in the atoms of oxygen and nitrogen. As a result the three-electron bond electrons do not fully belong to the carbon atom and so the carbon atom octet makes 8 and not 9 (one should not also forget that the electronegativity of the atoms of oxygen (3.5) and nitrogen (3) is higher than the electronegativity of the atom of carbon (2.5)).

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.

And finally, here are the values of the a, b, c coefficients in the tables 3 and 4 for the Multiplicity = f(L) and E = f(L) equations.

Table 3. Multiplicity = a + b/L + c/L² equation coefficients for some types of bonds.

| Type of bond | a | b | c |
|---|---|---|---|
| C-C | -0.06040343 | -5.67787529 | 11.28562201 |
| C-O | 26.03252883 | -72.46498138 | 52.43899244 |
| C-N | 0.63817306 | -7.56455294 | 11.91384503 |
| C-S | 55.33256579 | -198.81807222 | 181.87538814 |
| N-N | 0.96407492 | -6.68791795 | 9.79339013 |
| N-O | 46.00756377 | -123.75637485 | 84.79763896 |
| O-O | 23.89786759 | -66.85172754 | 48.79304255 |
| C-P | 28.76548555 | -109.46128312 | 107.52805439 |
| Multiplicity - bond multiplicity,<br>L – bond length in Å. | | | |

Table 4. E = a + b/L + c/L² equation coefficients for some types of bonds.

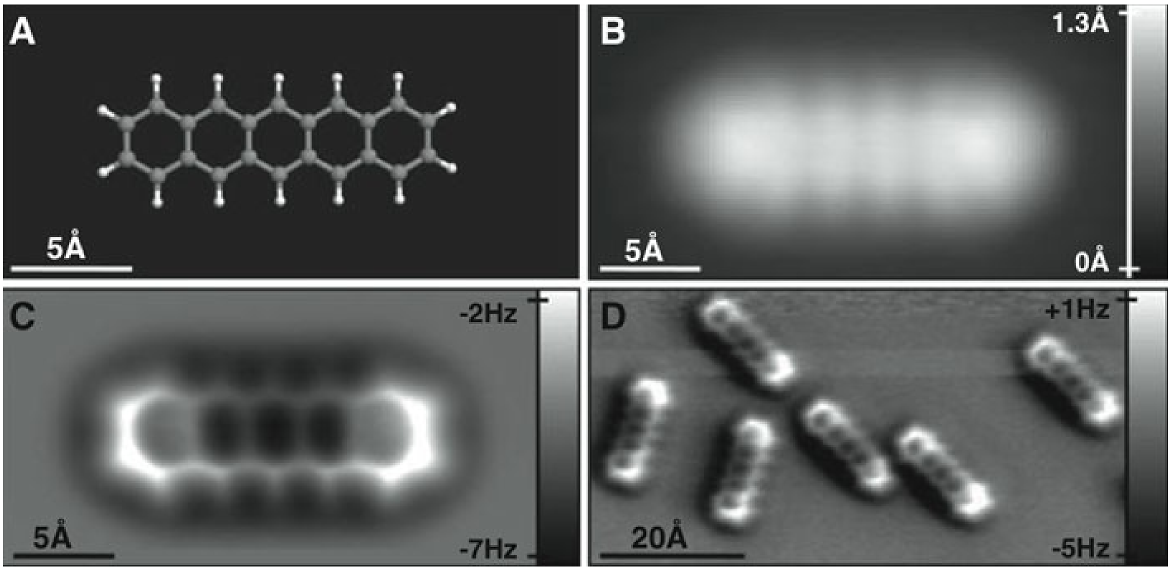
| Type of bond | a | b | c |
|---|---|---|---|
| C-C | -2221.34518418 | 5065.62912191 | -1699.18638789 |
| C-O | 11420.81052442 | -31359.17576343 | 22207.04265404 |
| C-N | -2332.69568587 | 4450.61712191 | -866.48412671 |
| C-S | -27772.64385690 | 90244.55278987 | -71414.57485742 |
| N-N | 7067.14065437 | -20274.81508318 | 14878.53765631 |
| N-O | -6564.31416262 | 15895.54907490 | -8769.11638979 |
| O-O | 10590.40848780 | -29935.02909385 | 21430.93279023 |
| E – bond energy in kj/mole,<br>L – bond length in Å. | | | |

# 3. EXPERIMENTAL CONFIRMATION OF THE EXISTENCE OF THE THREE-ELECTRON BOND AND THEORETICAL BASIS OF ITS EXISTENCE.

## 3.1. RESULTS AND DISCUSSION.

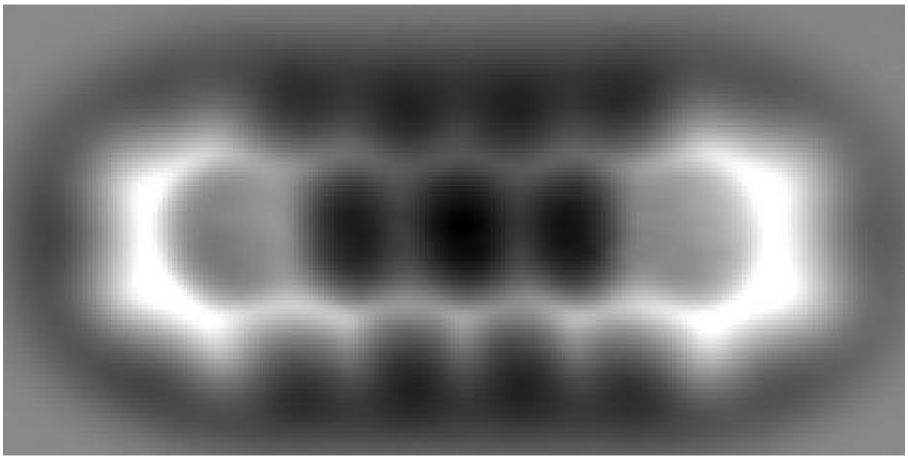
Three-electron bond in benzene is classic, "direct", along the axis of the bond, but not in the form of "banana bond" [1]. Due to real interaction through the cycle the bond should deviate slightly from the axis, possibly by 0.1 Å – 0.2 Å, somewhat shift a little to the centre of the cycle. This shift is very slight as compared to "banana bond".

Let us consider the picture of the molecule of pentacene [15]:



Using an atomic force microscope (AFM), it is possible to obtain such photos of molecules and actually to study individual molecules and their bonds; and this particular is needed to determine the presence of the three-electron bond.

Molecule of pentacene is the most representative, see photo



where the displacement of the chemical bond (or rather the bond path) to the centre of the extreme cycles is clearly shown, which should be observed according to the three-electron bond theory (TBT) and the interaction through the cycle.

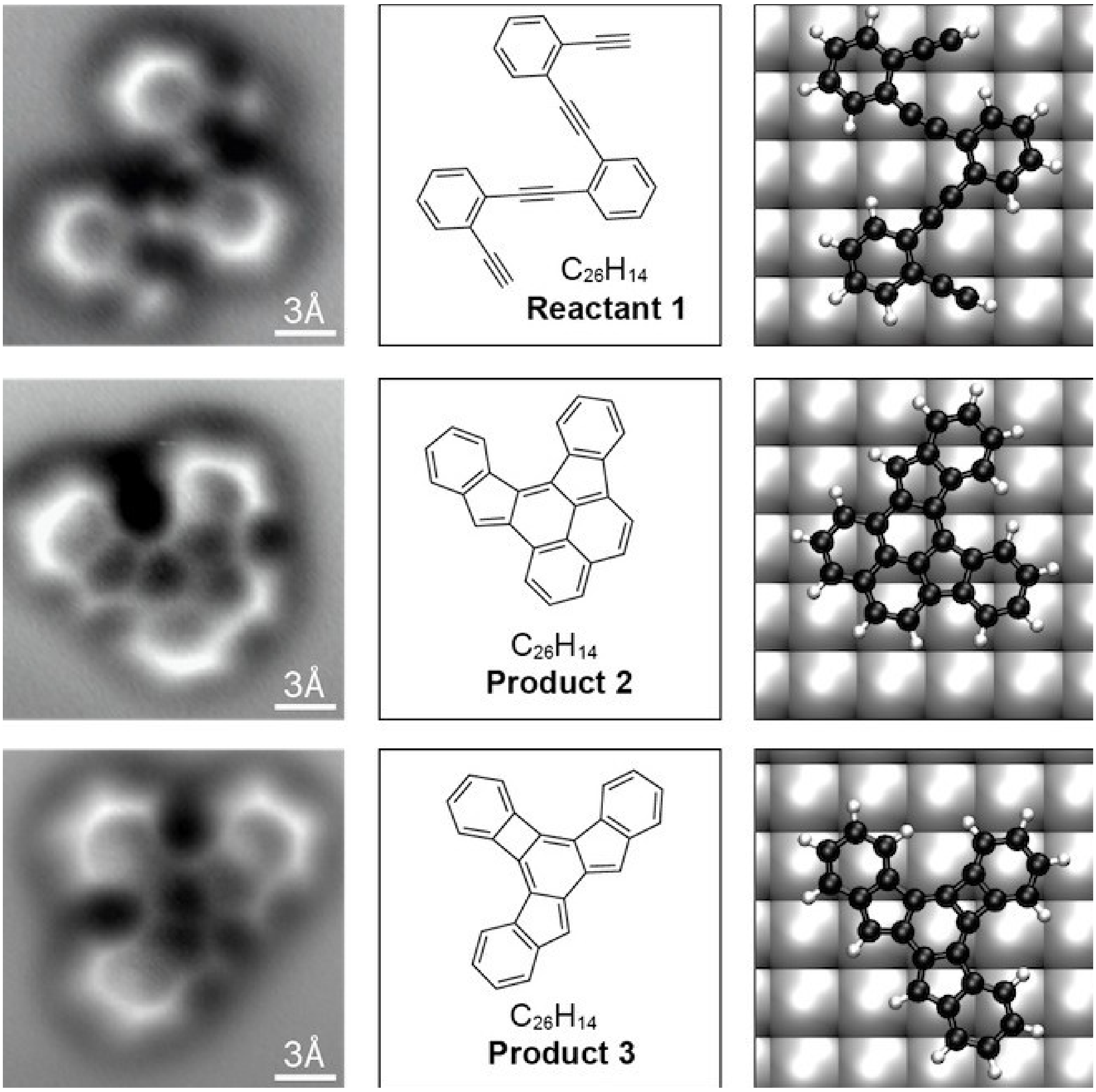
Formulae of naphthalene and anthracene are presented at p. 19 [1] according to the TBT. The molecule of pentacene will have a similar structure according to the three-electron bond theory.

Displacement of the chemical bond in the inner cycles of pentacene cannot be detected at the photo, which is logical taking into account the interaction of central electrons of the three-electron bond of inner cycles, because neighbouring central electrons act in opposite directions; so the shift to the centre of cycles is minimal or absent.

Distribution of the intensity of chemical bond in pentacene visible in the photo can be logically explained by addition of electron densities, or broadly speaking by addition of the number of electrons involved in chemical bond. Electron density near the carbon atom is not less than in the centre of the chemical bond, so there is no protrusion of the centre of the chemical bond to the centre of the cycle (regardless of the presence of three-electron bond), which is understandable considering two three-electron bonds near the carbon atom, and therefore two neighbouring electrons with opposite spins will interact with each other.

We shall see no protrusion of the centre of the chemical bond to the centre of the cycle in similar photos of antiaromatic systems. The whole image should be similar to the image of pentacene but with a shift of the chemical bond "out of the cycle".

If one consider the following molecules



the following conclusions can be drawn [16]:

See photo Reactant 1 – it is clearly shown how the triple acceptor bond pulls electron density from the benzene ring, and thus the chemical bonds of the corresponding carbon atoms will not be (or too much lesser extent will not be) drawn to the centre of the benzene cycle or so to speak "will neither bend no strain", as we can see in the photo.

See photo Product 2 - it is clearly shown two benzene nuclei and one naphthalene nucleus.

The situation is repeated where the displacement of chemical bonds (three-electron bonds) to the centre of cycles is possible; it occurs and can be clearly seen in the photo. Where interaction (pumping) of electron density occurs in the result of conjugation with double bonds, we shall see no shift of the chemical bond to the centre of the cycle. Therefore, the displacement of chemical bonds of outer sides of benzene and naphthalene is clearly visible, however this effect is not observed for inner sides.

See photo Product 3 - it is similar to the Product 2, we just have three benzene nuclei, and the shift of chemical bonds of outer sides of benzene rings is clearly visible, however this effect is not observed for inner sides involved in conjugation.

Analysis of images made in techniques of atomic force microscopy (AFM) of high resolution in pentacene and other aromatic systems shows that according to predictions, aromatic three-electron bond is deflected to the centre of aromatic nuclei, which clearly confirms the fact of existence of three-electron bond in benzene, pentacene and other aromatic systems. It also confirms the existence of this bond in carboxylate anions and other similar ions and molecules.

AFM images of benzene can be presented on the basis of pentacene image, and if it exists, or if it is received at the appropriate resolution, it will be another confirmation of real existence of the three-electron bond.

There is no doubt that AFM images of cyclobutadiene (planar) and cyclooctatetraene (planar) or of any other planar antiaromatic system, when received at the appropriate resolution, will be another confirmation of the interaction through the cycle in aromatic and antiaromatic systems. It should be noted that the deviation of chemical bond in antiaromatic systems will be "from the cycle", similarly to pentacene, but in the opposite direction.

But there is a nuance as for antiaromatic systems: an antiaromatic system (system of nuclei) should be planar in order to have the interaction through cycle [1, p. 5 – 6]. If the system is not planar, it will be a transition into the “bath” in cyclooctatetraenyl (four double bonds), a transition into the diradical in cyclobutadiene (double bond and two unpaired electron, the nuclei system shall be planar and not a square). Then the AFM image shall show the appropriate structure, ie double bonds plus unpaired electrons in cyclooctatetraene and cyclobutadiene.

Therefore, to obtain AFM images of antiaromatic cyclobutadiene and cyclooctatetraene, it is necessary to consolidate their atoms on a special matrix for achieving a perfect planarity of the system, and only then to pick AFM images of appropriate resolution, if it is possible. Undoubtedly, this AFM image will confirm the interaction of three-electron bonds through the cycle.

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.

Then, there will be three fundamental interactions (between fermions) in chemistry:

electron - electron;

electron - fermion-three-electron bond;

fermion-three-electron bond - fermion-three-electron bond;

the calculation of which should ideally lead to the calculation of any system. 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. By the way, two-electron bonds, four-electron bonds and six-electron bonds can be studied as typical bosons following the Bose-Einstein statistics.

## 3.2. CONCLUSION.

Construction of diagrams showing how electrons gravitate (in explaining the interaction through the cycle, etc.) is an attempt to explain the quantum interaction of electrons by using methods of classical chemistry [1, p. 4 – 5]. It is clear that electrons do not gravitate towards each other (gravitational interaction is neglected), but on the contrary, if they gravitate, a force should exist, as well as an equation for the calculation of this force. In nature, there are only four fundamental interactions:

1. Gravity.
2. Electromagnetic (most important for chemistry).
3. Strong.
4. Weak.

With neglect of gravitational interaction, it is only electromagnetic interaction and broadly speaking, Coulomb attraction and repulsion in the molecule (or rather between electrons and nuclei).

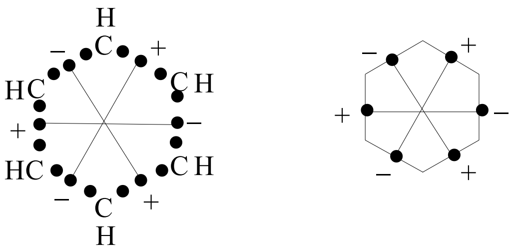
Quantum mechanics defines what such a chemical bond. Without quantum mechanics it is impossible. Classical concepts to explain what the chemical bond is impossible (and this despite the existence of four fundamental interactions). It is obvious that when the chemical bond formation quantum effects are important. That is, to form a chemical bond is not enough to have two specific atoms with unpaired electrons and the four fundamental interactions, but still need these two atoms placed at a certain distance where quantum effects "help" form a chemical bond. Without quantum effects these baselines (atoms and fundamental interactions) is not enough to form a chemical bond. It is obvious that when the chemical bonds forming, important not only the properties of atoms and fundamental interactions but also the structure of the space-time at distances of several angstroms (scale chemical bond). Quantum effects of the space-time begin to affect the interaction of atoms (the house begins to affect the interaction between residents), without it, explaining the formation of a chemical bond is impossible.

# 4. SUPPLEMENT TO THE THEORETICAL JUSTIFICATION OF EXISTENCE OF THE THREE-ELECTRON BOND.

## 4.1. RESULTS AND DISCUSSION.

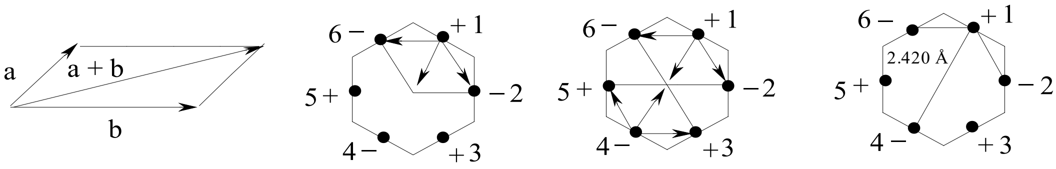
Consider and try to explain the interaction scheme of chemical bonds in the benzene molecule [1, p. 2-5, 10-11]. The interaction of two three-electron bonds in a molecule of benzene at a distance of 2.42 Å (on opposite sides) can be explained if we consider these two three-electron bonds as two particles (two fermions) in an entangled quantum state. That is, these two fermions are in an entangled quantum state. Quantum entanglement is a quantum mechanical phenomenon, in which the quantum states of two or more fermions or bosons prove to be interconnected [17-21]. And surprisingly, this interconnection remains at virtually any distance between the particles (when there are no other known interactions). It should be realized that the entangled quantum system is in fact an "indivisible" object, a new particle with certain properties (and the particles of which it is composed should meet certain criteria). And most importantly, when measuring the spin (or other property) of the first particle we will automatically unambiguously know the spin (property) of the second particle (let's say we get a positive spin of the first particle, then the spin of the second particle will always be negative, and vice versa). Two particles in an entangled state prove to be bound by an "invisible thread", that is, in fact, they form a new "indivisible" object, a new particle. And this is an experimental fact.

As for the benzene molecule [1, p. 2-11], if we consider the interaction of all six three-electron bonds as an entangled quantum state of six fermions (three-electron bonds), then the definition of the spin of one of the fermions automatically implies the knowledge of all the spins of the other five fermions, and in closer inspection it means the knowledge of the spins of all 18 benzene electrons that form all the six C-C bonds. In fact, on this basis, the benzene molecule can be used to study the entangled quantum states of electrons (fermions).



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

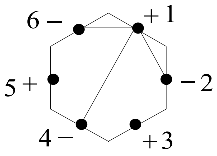
One can realize that the interaction of three-electron bonds in a molecule of benzene at a distance of 2.42 Å is significant on the basis of the fact that the bond length in a molecule of iodine (I-I) is about 2.66 Å. Therefore, it is reasonable to assume that the energy interaction of the three-electron bonds (or central electrons) at distances between them of 2.42 Å will be significant.



$L_{1-2} = L_{1-6} = 1.210$ Å
$L_{1-4} = 2.420$ Å

In addition, the length of chemical bonds in the general case is in the approximate range of 0.74 Å – 3.5 Å. The value of 3.5 Å, in principle, restricts the existence of large monocyclic aromatic systems such as of cyclodecapentaene.

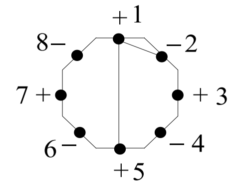
Lc-c = 1.397 Å



$L_{1-2} = L_{6-1} = 1.210$ Å

$L_{1-4} = 2.420$ Å

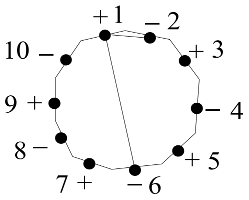
Lc-c = 1.410 Å



$L_{1-2} = L_{8-1} = 1.303$ Å

$L_{1-5} = 3.404$ Å

Lc-c = 1.400 Å

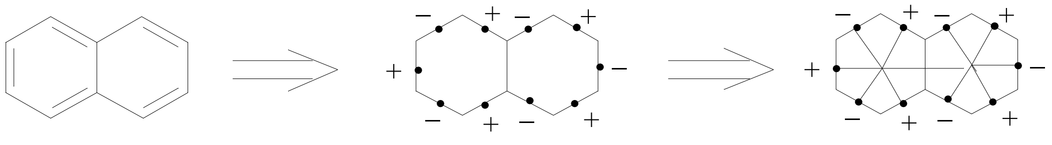


$L_{1-2} = L_{10-1} = 1.331$ Å

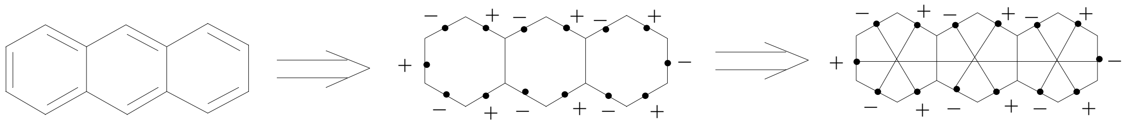
$L_{1-6} = 4.309$ Å

Since the distance between the opposite bonds is equal to 4.31 Å, i.e., there is no significant interaction between the three-electron bonds (or electrons located on opposite sides of the cycle) and thus there won't be stabilization of the cycle because the distance is more than 3.5 Å, that is longer than the "longest chemical bond". Without this interaction energy, it will be impossible to stabilize a large monocyclic aromatic system, in which the cyclic strain will substantially increase.

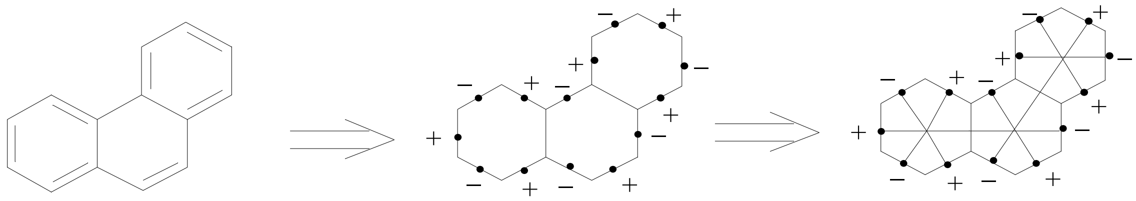
In other systems such as naphthalene, anthracene, tetracene, pentacene, and the like, the longest interaction between two three-electron bonds of different cycles (longer than 3.5 Å) will also be insignificant in terms of formation of a chemical bond [1, p. 19-20, 22, 23].



Naphthalene



Anthracene



Phenanthrene

Three-electron bonds will exist in such systems (system stabilization due to of the core of six-membered rings), but there will be no significant interaction between specific bonds over long distances (in energy terms). But this does not mean that these three-electron bonds will not interact in any way. Quite the contrary, they will certainly interact, and this interaction will lead to the formation of an entangled quantum state, which in fact will determine the type of the electron spin (or the three-electron bond). Moreover, in general, in the two-electron chemical bond, the electrons can also be regarded as being in an entangled quantum state, which actually determines their spins.

The fact that electrons during the formation of chemical bonds are in an entangled quantum state, is very important for chemistry and quantum mechanical bond calculations. For example, when calculating the two-electron chemical bond of a hydrogen molecule, it will no longer be necessary to consider the movement of two electrons in general, i.e. as independent and virtually any relative to one another.

And we will know for sure that in an entangled quantum state, these two electrons can be considered actually bound by an "invisible thread" with a certain length, that is, two electrons are connected and form a new "indivisible" particle. That is, the movement of two electrons in the field of cores can be described by the movement of a point located in the middle of the "invisible thread" (or in the center of a new particle, or in the center of mass, and so on), what should greatly simplify the quantum mechanical calculations.

The length of the "invisible thread" will definitely be much less than the sum of the covalent radii of hydrogen atoms, and it is this length that will determine the Coulomb repulsion between the two electrons. The length of the "invisible thread" between electrons in various chemical bonds should not greatly differ, and perhaps it will be a constant for all, without exception, chemical bonds (meaning two-electron bonds), maybe it will be another constant.

The three-electron bond can also be seen as an entangled quantum state in which there are three electrons. Then the length of the "invisible thread" between electrons will be different from that of the two-electron bond. You can also expect that for all, without exception, three-electron bonds the distance between electrons will be the same that is constant.

All types of chemical bonds (two-electron, three-electron, four-electron, five-electron, six-electron, and so on) can be seen as an entangled quantum state, in which there are electrons involved in chemical bonding. And interestingly, all entangled particles behave as they should according to the quantum theory, that is, their characteristics remain uncertain until the moment of measurement. From this point of view (the quantum mechanical point), it becomes clear the cause of failure to calculate chemical bonds "on the tip of the pen" with attempts to calculate the speed and energy of electrons and other characteristics. But these characteristics of electrons of the chemical bond (a chemical bond is a quantum entangled system, which contains electrons of the bond) cannot be determined in principle, because it is so constituted the quantum world. Logically, that what is impossible to determine is impossible to calculate in principle, what is confirmed by the history of quantum chemical calculations. That is, all attempts to calculate characteristics of electron chemical bond (speed, power, and so on) were doomed to failure from the beginning. Therefore, in our opinion, it would be more correct to consider the chemical bond as a certain new "indivisible" particle, with well-defined characteristics and spatial extension, which we called a "semi-virtual particle" [2, p. 5-8]. In particular chemical substance the chemical bond is really indivisible. In addition, such semi-virtual particle is a fermion for the three-electron bond and other bonds with an unpaired number of electrons and total half-integral spin. And the semi-virtual particle will be a boson for the two-electron bonds and other bonds with a paired number of electrons and total integral or zero spin. And the characteristics of a semi-virtual particle (as an integral), we can calculate. These are the characteristics of a semi-virtual particle, such as energy, spatial extension, length, and so on, that are very important for chemistry.

Calculations of a hydrogen molecule will actually come to the solution of the movement of one point in the field of two protons, which is similar to the solution of a task for the hydrogen molecular ion $H_2$ + [22-28]. And we can expect that finally the two-electron chemical bond will be calculated "on the tip of the pen”. Besides that, an entangled quantum state clearly demonstrates that the chemical bond is real and that it is neither an abstraction, nor a convenient concept used to describe and explain. Two electrons indeed form a chemical bond (which is a new particle), and they really "know each other's spins", and are in an entangled quantum state. This means that these two electrons forming a chemical bond and connected by an "invisible thread" have their own well-defined characteristics. And this bond (or this thread) is real, but not in terms of energy (if the energy of such bond really exists and is not equal to zero, then its value cannot be compared with the energies of chemical bonds).

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.

## 4.2. CONCLUSION.

Based on the foregoing, we can conclude that our Universe, our world more precisely, is an interference pattern of each and every particle in the Universe. Now the wave-particle duality of particles, probabilistic interpretation of quantum mechanical phenomena and other quantum effects of the microcosm become intuitively clear. For example, why there is a non-zero probability of finding an electron, which rotates in a specific hydrogen atom (which is in a particular laboratory), for example, on the Moon.

And it is both on the Moon and on the Sun, as well as anywhere in the space of our Universe; it really fills (takes) the whole Universe. But its presence in a particular area, "the density of presence", so to speak (probability of detection), is different at different points of the space.

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.

# 5. A SHORT ANALYSIS OF CHEMICAL BONDS.

Nothing prohibits to give a definition of the multiplicity of bond: the multiplicity of bond is the energy of bond expressed in dimensionless units.

## 5.1. RESULTS AND DISCUSSION.

We'll find the dependence Multiplicity = f (L) and E = f (L) using function $y = a + b/x + c/x^2$ for C-O bonds, where the multiplicity — is multiplicity of bond, L – length of bond in Å, E – energy of bond in kj/mole.

For the length of bonds let us take the findings:

| | | | |
|---|---|---|---|
| $H_3C{-}OH$ | Lc-o = 1.434 Å | (29) | Multiplicity = 1 |
| $H_2C{=}O$ | Lc-o = 1.206 Å | (29) | Multiplicity = 2 |
| $C{\equiv}O$ | Lc-o = 1.12823 Å | (30) | Multiplicity = 3 |

$$Y = \frac{(y - y_1)}{(1/x - 1/x_1)}$$

$y = a + b/x + c/x^2$ $\quad X = 1/x$

$b_1 = b + c/x_1$ $\quad Y = b_1 + cX$

$$c = \frac{\left(\sum(1/x \cdot Y) - \left(\sum(1/x) \cdot \sum Y\right)/n\right)}{\left(\left(\sum 1/x^2\right) - \left(\sum(1/x)\right)^2/n\right)}$$

$$b_1 = \left(\sum Y\right)/n - c\left(\sum(1/x)\right)/n$$

n–the number of given value Y.

Let us find a from the equality: $\Sigma y = na + b\Sigma(1/x) + c\Sigma(1/x^2)$, when $n = 3$

Table 1. Calculation of ratios for relation Multiplicity = f(L) for C-O bond.

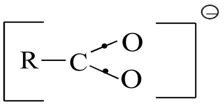
| | 1/x | $1/x^2$ | $\frac{(y-y_1)}{(1/x-1/x_1)}$ | $\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$ | x (L, Å) | y (multiplicity) |
|---|---|---|---|---|---|---|
| | | | | | 1.43400 | 1 |
| | 0.82918740 | 0.68755174 | 7.58510526 | 6.28947368 | 1.20600 | 2 |
| | 0.88634410 | 0.78560586 | 10.58234503 | 9.37959905 | 1.12823 | 3 |
| $\sum$ | 1.71553149 | 1.47315760 | 18.16745029 | 15.66907273 | 3.76823 | 6 |

$1/x_1 = 0.69735007$ $x_1 = 1.43400$ $y_1 = 1$

$\Sigma(1/x^2) = 1.95945472$ $\Sigma(1/x) = 2.41288156$

$c = 52.43899244$ $b = -72.46498138$ $a = 26.03252883$

$$\text{Multiplicity (C-O)} = 26.03252883 - \frac{72.46498138}{L} + \frac{52.43899244}{L^2}$$



Let us calculate from the equation:

$HCOO^{\ominus} Na^{\oplus}$ Lc-o = 1,27 Å (31) Multiplicity (L=1.27 Å) = 1.486

$NH_3^{\oplus} CH_2COO^{\ominus}$ Lc-o = 1,26 Å (31) Multiplicity (L=1.26 Å) = 1.551

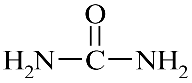
$CO_3^{2-} K_2^{2+} 3H_2O$ Lc-o = 1,29 Å (32) Multiplicity (Lc-o = 1.29 Å) = 1.370

$CO_3^{2-} Ca^{2+}$

O=CO Lc-o = 1.162 Å (33) Multiplicity (Lc-o = 1.162 Å) = 2.507

So as we see, as expected theory of three-electrone bond, frequency of C-O bond in carboxylate anion is equal to 1.5. In carbonate anion frequency of C-O is equal to 1.37, while the carbon dioxide is equal to 2.5, which correlates well with the classical ideas.

In urea C-O multiplicity of bonds equal to about 1.5, and C-N is approximately 1.7 (as shown below).



$H_2N-\overset{\overset{\displaystyle O}{\|}}{C}-NH_2$ Lc-o = 1.27 Å (34)

Multiplicity (Lc-o = 1.27 Å) = 1.486 ≈ 1.5 Multiplicity C−N = 1.686

Now let's find the dependence E = f (L) для C−O bonds.

For the bonds energy let's take the date:

| | | | |
|---|---|---|---|
| C−O | Lc-o = 1.434 Å | Ec-o = 351.708 kj/mole | (35) |
| C=O (for $H_2C=O$) | Lc-o = 1.206 Å | Ec-o = 686.668 kj/mole | (35) |
| C≡O | Lc-o = 1.12823 Å | Ec-o = 1071.773 kj/mole | (30) |

Table 2. Calculation factors for dependency E = f(L) for C-O bond.

| | 1/x | 1/x² | $\frac{(y-y_1)}{(1/x-1/x_1)}$ | $\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$ | x (L, Å) | y (E, kj/mole) |
|---|---|---|---|---|---|---|
| | | | | | 1.43400 | 351.708 |
| | 0.82918740 | 0.68755174 | 2540.70685895 | 2106.72210526 | 1.20600 | 686.668 |
| | 0.88634410 | 0.78560586 | 3809.98813722 | 3376.96049318 | 1.12823 | 1071.773 |
| ∑ | 1.71553149 | 1.47315760 | 6350.69499617 | 5483.68259844 | 3.76823 | 2110.149 |

$1/x_1 = 0.69735007$ $x_1 = 1.43400$ $y_1 = 351.708$

$\Sigma(1/x^2) = 1.95945472$ $\Sigma(1/x) = 2.41288156$

c = 22207.04265404 b = - 31359.17576343 a = 11420.81052442

$$Ec\text{-}o = 11420.81052442 - \frac{31359.17576343}{L} + \frac{22207.04265404}{L^2}$$

Let us find from the equation:

E (L = 1.434 Å) = 351.708 kj/mole

E (L = 1.206 Å) = 686.668 kj/mole

E (L = 1.12823 Å) = 1072.542 kj/mole

O=CO Lc-o = 1.16213 Å (36)

E (L = 1.16213 Å) = 879.596 kj/mole = 210.088 kcal/mole

O=CO Lc-o = 1.162 Å E (average) = 192 kcal/mole D = 127 kcal/mole (37)

E (L = 1.162 Å) = 880.257 kj/mole = 210.246 kcal/mole

$NH_3^{\oplus}—CH_2COO^{\ominus}$ Lc-o = 1.26 Å E(L = 1.26 Å) = 520.383 kj/mole

HCO−OH Lc-o = 1.41 Å D ~ 90 kcal/mole (33)

E (L = 1.41 Å) = 350.243 kj/mole = 83.654 kcal/mole

$H_3C-OH$ Lc-o = 1.434 Å D ~ 90 kcal/mole (33)
E (L = 1.434 Å) = 351.708 kj/mole = 84.004 kcal/mole

$CH_3CO-OH$ Lc-o = 1.43 Å D ~ 90 kcal/mole (33)

E (L = 1.430 Å) = 351.038 kj/mole = 83.844 kcal/mole

So we can see the binding energy calculated from the equation for C-O bond nice correlated with experimental data.

We'll find the dependence Multiplicity = f (L) and E = f (L) for C−N bonds.

For the bonds energy let's take the date (35):

| | |
|---|---|
| C−N | E = 291.834 kj/mole |
| C=N | E = 615.489 kj/mole |
| C≡N (for HC≡N) | E = 866.709 kj/mole |

For lengths of bonds let us take the date:

| | | |
|---|---|---|
| $CH_3-NH_2$ | ($L_{C\text{-}N}$ = 1.4714 Å) | (38) |
| HC≡N | ($L_{C\equiv N}$ = 1.157 Å) | (29) |
| C=N | ($L_{C=N}$ = 1.28 Å) | (39) |

We'll find the dependence Multiplicity = f (L)

Table 3. Calculation coefficients for dependence Multiplicity = f (L) for C-N bond.

| | 1/x | $1/x^2$ | $\frac{(y-y_1)}{(1/x-1/x_1)}$ | $\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$ | x (L, Å) | y (Multiplicity) |
|---|---|---|---|---|---|---|
| | | | | | 1.4714 | 1 |
| | 0.78125000 | 0.61035156 | 9.84008359 | 7.68756531 | 1.2800 | 2 |
| | 0.86430424 | 0.74702181 | 10.82957888 | 9.36005089 | 1.1570 | 3 |
| ∑ | 1.64555424 | 1.35737337 | 20.66966247 | 17.04761620 | 3.9084 | 6 |

$1/x_1 = 0.67962485$ $x_1 = 1.4714$ $y_1 = 1$

$\Sigma(1/x^2) = 1.81926331$ $\Sigma(1/x) = 2.32517908$

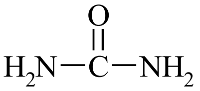
c = 11.91384503 b = - 7.56455294 a = 0.63817306

$$\text{Multiplicity (C-N)} = 0.63817306 - \frac{7.56455294}{L} + \frac{11.91384503}{L^2}$$

Let us find from the equation:

$C(N_3)_3^{\oplus}$ $SbCl_6^{\ominus}$ $L_{C-N}=1{,}34$ Å (32) Multiplicity (L = 1.34 Å) = 1.628

$C(NH_2)_3^{\oplus}$ $CO_3^{\ominus}$ $L_{C-N}=1{,}34$ Å

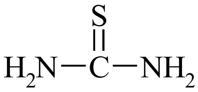


$H_2N-\overset{\overset{\displaystyle O}{||}}{C}-NH_2$

$L_{C-N}=1{,}33$ Å

$L_{C-O}=1{,}27$ Å

(34) Multiplicity ($L_{C-N}$= 1.33 Å) = 1.686



$H_2N-\overset{\overset{\displaystyle S}{||}}{C}-NH_2$

$L_{C-N}=1{,}33$ Å

$L_{C-S}=1{,}71$ Å

(34) Multiplicity ($L_{C-N}$= 1.33 Å) = 1.686

We'll find the dependence E = f (L) for C-N bonds.

Table 4. Calculation coefficients for dependence E = f (L) for C-N bond.

| | 1/x | 1/x² | $\frac{(y-y_1)}{(1/x-1/x_1)}$ | $\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$ | x (L, Å) | y (E, kj/mole) |
|---|---|---|---|---|---|---|
| | | | | | 1.4714 | 291.834 |
| | 0.78125000 | 0.61035156 | 3184.79225580 | 2488.11894984 | 1.2800 | 615.489 |
| | 0.86430424 | 0.74702181 | 3112.82707944 | 2690.42962786 | 1.1570 | 866.709 |
| ∑ | 1.64555424 | 1.35737337 | 6297.61933524 | 5178.54857771 | 3.9084 | 1774.032 |

$1/x_1 = 0.67962485$ $x_1 = 1.4714$ $y_1 = 291.834$

$\Sigma(1/x^2) = 1.81926331$ $\Sigma(1/x) = 2.32517908$

c = - 866.48412671 b = 4450.61712191 a = - 2332.69568587

$$E\ (C\text{-}N) = -2332.69568587 + \frac{4450.61712191}{L} - \frac{866.48412671}{L^2}$$

E (L = 1.33 Å) = 523.790 kj/mole

We'll find the dependence Multiplicity = f (L) and E = f (L) for C−S bonds. Firstly we'll find the dependence Multiplicity = f (L).

For lengths of bonds let us take the date:

| | | | |
|---|---|---|---|
| $H_3C-SH$ | Multiplicity = 1 | L = 1.818 Å | (40) |
| $H_2C=S$ | Multiplicity = 2 | L = 1.6108 Å | (41) |
| $C\equiv S$ | Multiplicity = 3 | L = 1.53492 Å | (30) |

In the molecule CS multiplicity equal to 3, what confirming the spectral data of the compounds CS, HCP, CP (30), (42), namely the frequency of fluctuations and constant anharmonicity (ωexe), what for C≡P and C≡S bond are almost identical:

| | | | |
|---|---|---|---|
| CS | $L_{c\text{-}s}$ = 1.53492 Å | D = 169.6 kcal/mole | $\omega e = 1285.08\ cm^{-1}$<br>$\omega exe = 6.46\ cm^{-1}$ |
| CP | $L_{c\text{-}p}$ = 1.5583 Å | D = 122 kcal/mole | $\omega e = 1239.67\ cm^{-1}$<br>$\omega exe = 6.86\ cm^{-1}$ |
| $H-C\equiv P$ | $L_{c\text{-}p}$ = 1.5421 Å<br>$L_{c\text{-}H}$ = 1.0667 Å | | $\nu_1 = 3216.9\ cm^{-1}$<br>$\nu_2 = 1278.4\ cm^{-1}$<br>$\nu_3 = 674.7\ cm^{-1}$ |

Table 5. Calculation coefficients for dependence Multiplicity = f (L) for C-S bond.

| | 1/x | $1/x^2$ | $\frac{(y-y_1)}{(1/x-1/x_1)}$ | $\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$ | x (L, Å) | y (Multiplicity) |
|---|---|---|---|---|---|---|
| | | | | | 1.81800 | 1 |
| | 0.62080954 | 0.38540448 | 14.13337066 | 8.77413127 | 1.61080 | 2 |
| | 0.65149975 | 0.42445193 | 19.71516575 | 12.84442560 | 1.53492 | 3 |
| ∑ | 1.27230929 | 0.80985641 | 33.84853640 | 21.61855688 | 4.96372 | 6 |

$1/x_1 = 0.55005501$ $x_1 = 1.81800$ $y_1 = 1$

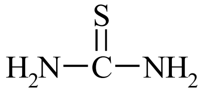
$\Sigma(1/x^2) = 1.11241692$ $\Sigma(1/x) = 1.82236429$

$c = 181.87538814$ $b = - 198.81807222$ $a = 55.33256579$

$$\text{Multiplicity (C-S)} = 55.33256579 - \frac{198.81807222}{L} + \frac{181.87538814}{L^2}$$

Let us find from the equation:

$CS_3^{2-}$ Lc-s = 1,71 Å (32) Multiplicity (Lc-s = 1.71 Å) = 1.263



$$H_2N-\overset{\overset{S}{||}}{C}-NH_2$$

$L_{C-S} = 1{,}71$ Å

$L_{C-N} = 1{,}33$ Å (34)

Multiplicity (C-S) = 1.263 Multiplicity (C-N) = 1.686

S=C=S Lc-s = 1.5529 Å (42)

Multiplicity (Lc-s = 1.5529 Å) = 2.722

In general, we see that oxygen sulfur analogs behave quite as expected:

a) thiourea and thiocarbonates anion have slightly lowered frequency of C-S bond (compared to the C-O) (1.263 to 1.507, and 1.263 to 1.370), due to more efficient delocalization of electrons on the sulfur atom is greater (compared to an oxygen atom );

b) carbon disulfide compared with carbon dioxide multiplicity of C-S bond slightly higher than the frequency of the C-O bond (2.7 against 2.5 in carbon dioxide) that can be explained by coupling undivided pair of electrons sulfur and oxygen with a double bond and therefore more coupling in the case of sulfur atom.

We’ll find the dependence E = f (L) for C−S bonds.

For energies of bonds let us take the date:

C−S L = 1.818 Å E = 259.594 kj/mole (35)

C=S L = 1.6108 Å E = 728.538 kj/mole (35)

C≡S L = 1.53492 Å E = 709.606 kj/mole (30)

Table 6. Calculation coefficients for dependence E = f (L) for C-S bond.

|  | 1/x | $1/x^2$ | $\frac{(y-y_1)}{(1/x-1/x_1)}$ | $\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$ | x (L, Å) | y (E, kj/mole) |
|---|---|---|---|---|---|---|
|  |  |  |  |  | 1.81800 | 259.594 |
|  | 0.62080954 | 0.38540448 | 6627.75936908 | 4114.57621622 | 1.61080 | 728.538 |
|  | 0.65149975 | 0.42445193 | 4436.03058434 | 2890.07282747 | 1.53492 | 709.606 |
| ∑ | 1.27230929 | 0.80985641 | 11063.78995342 | 7004.64904369 | 4.96372 | 1697.738 |

$1/x_1 = 0.55005501$ $x_1 = 1.81800$ $y_1 = 259.594$

$\Sigma(1/x^2) = 1.11241692$ $\Sigma(1/x) = 1.82236429$

c = - 71414.57485742 b = 90244.55278987 a = - 27772.64385690

$$E\ c\text{-}s = -27772.64385690 + \frac{90244.55278987}{L} - \frac{71414.57485742}{L^2}$$

Let us find from the equation:

SC=S Lc-s = 1.5529 Å E (L = 1.5529 Å) = 726.729 kj/mole = 173.576 kcal/mole

Ec-s (average) = 128 kcal/mole (37)

We’ll find the dependence Multiplicity = f (L) and E = f (L) for N−N bonds.

For energies of bonds let us take the date:

N−N E = 160.781 kj/mole (35)

N=N E = 418.000 kj/mole (43)

N≡N E = 945.333 kj/mole (44)

For lengths of bonds let us take the date:

$H_2N-NH_2$ L = 1.4530 Å (45)

HN=NH L = 1.2300 Å (46)

N≡N L = 1.0976 Å (47)

Firstly we'll find the dependence Multiplicity = f (L)

Table 7. Calculation coefficients for dependence Multiplicity = f (L) for N−N bond.

|  | 1/x | $1/x^2$ | $\frac{(y-y_1)}{(1/x-1/x_1)}$ | $\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$ | x (L, Å) | y (Multiplicity) |
|---|---|---|---|---|---|---|
|  |  |  |  |  | 1.4530 | 1 |
|  | 0.81300813 | 0.66098222 | 8.01430493 | 6.51569507 | 1.2300 | 2 |
|  | 0.91107872 | 0.83006443 | 8.97474845 | 8.17670231 | 1.0976 | 3 |
| ∑ | 1.72408685 | 1.49104665 | 16.98905339 | 14.69239737 | 3.7806 | 6 |

$1/x_1 = 0.68823125$ $x_1 = 1.4530$ $y_1 = 1$

$\Sigma(1/x^2) = 1.96470890$ $\Sigma(1/x) = 2.41231809$

c = 9.79339013 b = - 6.68791795 a = 0.96407492

$$\text{Multiplicity (N-N)} = 0.96407492 - \frac{6.68791795}{L} + \frac{9.79339013}{L^2}$$

We'll find the dependence E = f (L) for N-N bonds.

Table 8. Calculation coefficients for dependence E = f (L) for N-N bond.

|  | 1/x | $1/x^2$ | $\frac{(y-y_1)}{(1/x-1/x_1)}$ | $\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$ | x (L, Å) | y (E, kj/mole) |
|---|---|---|---|---|---|---|
|  |  |  |  |  | 1.4530 | 160.781 |
|  | 0.81300813 | 0.66098222 | 2061.43150049 | 1675.96056951 | 1.2300 | 418.000 |
|  | 0.91107872 | 0.83006443 | 3520.57842393 | 3207.52407428 | 1.0976 | 945.333 |
| ∑ | 1.72408685 | 1.49104665 | 5582.00992443 | 4883.48464379 | 3.7806 | 1524.114 |

$1/x_1 = 0.68823125$ $x_1 = 1.4530$ $y_1 = 160.781$

$\Sigma(1/x^2) = 1.96470890$ $\Sigma(1/x) = 2.41231809$

$c = 14878.53765631$ $b = - 20274.81508318$ $a = 7067.14065437$

$$E\ (N\text{-}N) = 7067.14065437 - \frac{20274.81508318}{L} + \frac{14878.53765631}{L^2}$$

Let us find from the equation:

$N_2^{\oplus}$ L = 1,116 Å, Multiplicity = 2.835, E = 846.001 kj/mole

experimentally found E = 843.26 kj/mole (48)

As we see in the latter case are almost the same value of energy of equation identified and obtained experimentally.

We'll find the dependence Multiplicity = f (L) for N−O bonds.

For lengths of bonds let us take the date:

| | | | |
|---|---|---|---|
| $NH_2{-}OH$ | $L_{N\text{-}O}$ = 1,453 Å | (49) | Multiplicity = 1 |
| $CH_3{-}NO_2$ | $L_{N\text{-}O}$ = 1,224 Å | (38) | Multiplicity = 1.5 |
| NO | $L_{N\text{-}O}$ = 1,1507 Å | (48) | Multiplicity = 2.5 |

Table 9. Calculation coefficients for dependence Multiplicity = f (L) for N-O bond.

| | 1/x | 1/x² | $\frac{(y-y_1)}{(1/x-1/x_1)}$ | $\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$ | x (L, Å) | y (Multiplicity) |
|---|---|---|---|---|---|---|
| | | | | | 1.4530 | 1.0 |
| | 0.81699346 | 0.66747832 | 3.88312664 | 3.17248908 | 1.2240 | 1.5 |
| | 0.86903624 | 0.75522398 | 8.29623106 | 7.20972544 | 1.1507 | 2.5 |
| ∑ | 1.68602970 | 1.42270230 | 12.17935770 | 10.38221452 | 3.8277 | 5.0 |

$1/x_1 = 0.68823125$ $x_1 = 1.4530$ $y_1 = 1.0$

$\Sigma(1/x^2) = 1.89636455$ $\Sigma(1/x) = 2.37426095$

$c = 84.79763896$ $b = - 123.75637485$ $a = 46.00756377$

$$\text{Multiplicity (N-O)} = 46.00756377 - \frac{123.75637485}{L} + \frac{84.79763896}{L^2}$$

$N_2O$ L (N−N) = 1.1282 Å (50)

L (N−O) = 1.1843 Å

Multiplicity (N−O) (L = 1.1843 Å) = 1.969 ≈ 1.97

Multiplicity (N−N) (L = 1.1282 Å) = 2.730

$NO_3^-$ L (N−O) = 1.243 Å (51)

Multiplicity (N-O) (L = 1.243 Å) = 1.328 ≈ 1.33

We'll find the dependence E = f (L) for N−O bond.

For energies of bonds let us take the date:

N−O E = 221.900 kj/mole (52)

N=O E = 607.086 kj/mole (52)

NO L = 1.15070 Å E = 626.847 kj/mole (48)

N−O L = 1.453 Å ($NH_2$−OH) (49)

Lengths L when N=O Multiplicity = 2 calculated by the formula:

$$\text{Multiplicity (N-O)} = 46.00756377 - \frac{123.75637485}{L} + \frac{84.79763896}{L^2}$$

$$2 = 46.00756377 - \frac{123.75637485}{L} + \frac{84.79763896}{L^2}$$

$44.00756377\ L^2 - 123.75637485\ L + 84.79763896 = 0$

$L = 1.18208253$ Å

The value of $L = 1.63007893$ Å is not considered as the basis of bond lengths, it is clear that this multiplicity <1.

So, N=O Multiplicity = 2 $L = 1.18208253$ Å

N−O $L = 1.453$ Å $E = 221.900$ kj/mole

N=O $L = 1.18208253$ Å $E = 607.086$ kj/mole

NO $L = 1.1507$ Å $E = 626.847$ kj/mole

Table 10. Calculation coefficients for dependence $E = f(L)$ for N−O bond.

| | 1/x | $1/x^2$ | $\frac{(y-y_1)}{(1/x-1/x_1)}$ | $\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$ | x (L, Å) | y (E, kj/mole) |
|---|---|---|---|---|---|---|
| | | | | | 1.45300000 | 221.900 |
| | 0.84596462 | 0.71565614 | 2442.00695125 | 2065.85148606 | 1.18208253 | 607.086 |
| | 0.86903624 | 0.75522398 | 2239.68925320 | 1946.37112471 | 1.15070000 | 626.847 |
| ∑ | 1.71500086 | 1.47088013 | 4681.69620445 | 4012.22261077 | 3.78578253 | 1455.833 |

$1/x_1 = 0.68823125$ $x_1 = 1.4530$ $y_1 = 221.900$

$\Sigma(1/x^2) = 1.94454237$ $\Sigma(1/x) = 2.40323211$

$c = -8769.11638979$ $b = 15895.54907490$ $a = -6564.31416262$

$$E\ (\text{N-O}) = -6564.31416262 + \frac{15895.54907490}{L} - \frac{8769.11638979}{L^2}$$

Let us find from the equation:

$CH_3—NO_2$ $L_{N-O} = 1{,}224$ Å $E\ (L = 1.224\ Å) = 569.050$ kj/mole

We’ll find the dependence Multiplicity = f (L) for C−P bond.

$H_2P{-}CH_3$ $L_{c-p}$ = 1.858 Å (53) Multiplicity = 1

$(CH_3)_3P{=}CH_2$ $L_{c=p}$ = 1.640 Å (54) Multiplicity = 2

$H{-}C{\equiv}P$ $L_{c\equiv p}$ = 1.5421 Å (42), (55) Multiplicity = 3

$L_{c\equiv p}$ = 1.54 Å (55)

$L_{c\equiv p}$ = 1.5421 Å (42)

Table 11. Calculation coefficients for dependence Multiplicity = f (L) for C−P bond.

| | 1/x | $1/x^2$ | $\frac{(y-y_1)}{(1/x-1/x_1)}$ | $\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$ | x (L, Å) | y (Multiplicity) |
|---|---|---|---|---|---|---|
| | | | | | 1.8580 | 1 |
| | 0.60975610 | 0.37180250 | 13.97761468 | 8.52293578 | 1.6400 | 2 |
| | 0.64846638 | 0.42050864 | 18.14005571 | 11.76321621 | 1.5421 | 3 |
| ∑ | 1.25822247 | 0.79231114 | 32.11767039 | 20.28615199 | 5.0401 | 6 |

$1/x_1 = 0.53821313$ $x_1 = 1.8580$ $y_1 = 1$

$\Sigma(1/x^2) = 1.08198452$ $\Sigma(1/x) = 1.79643561$

c = 107.52805439 b = - 109.46128312 a = 28.76548555

$$\text{Multiplicity (C-P)} = 28.76548555 - \frac{109.46128312}{L} + \frac{107.52805439}{L^2}$$

Let we see O-O bonds.

For lengths of bonds let us take the date:

$O_3$ Lo-o = 1.2717 Å (56)

$O_2$ Lo-o = 1.20735 Å (57)

$H_2O_2$ Lo-o = 1.452 Å (58)

For energies of bonds let us take the date (59)

$O_2 = 2O$ $119.11 \cdot 4.184 = 498.356$ kj/mole

$O_3 = O_2 + O$ $25.6 \cdot 4.184 = 107.110$ kj/mole - this dissociation energy

O−O $E = 33.2 \cdot 4.187 = 139.008$ kj/mole (60)

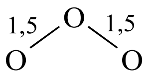
But energy O-O bond at 1.5 multiplicity we find the following manner:

$O_3 = O_2 + O$ 107.110 kj/mole

$O_2 = O + O$ 498.356 kj/mole

$O_3 = O + O + O$ 498.356 kj/mole + 107.110 kj/mole

If these three oxygen atoms forming a molecule of ozone

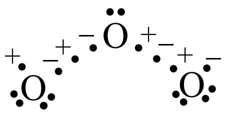


then this energy is released from the two formed three-electron bonds, so

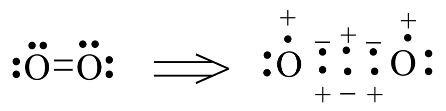
$$302.733 = \frac{(498.356 + 107.110)}{2}$$

Eo-o when multiplicity 1.5 = 302.733 kj/mole

HO−OH Multiplicity (O-O) = 1



Multiplicity (O-O) = 1.5



Multiplicity (O-O) = 2

Multiplicity O-O bond in the molecule of oxygen equal to 2, despite two three-electron bond as is the interaction of unpaired electrons on the oxygen atoms with three-elecron bond that follows a compliance rules of octet.

$H_2O_2$ Lo-o = 1.452 Å Multiplicity = 1 E = 139.008 kj/mole

$O_3$ Lo-o = 1.2717 Å Multiplicity = 1.5 E = 302.733 kj/mole

$O_2$ Lo-o = 1.20735 Å Multiplicity = 2 E = 498.356 kj/mole

Table 12. Calculation coefficients for dependence Multiplicity = f (L) for O−O bond.

| | 1/x | $1/x^2$ | $\frac{(y-y_1)}{(1/x-1/x_1)}$ | $\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$ | x (L, Å) | y (Multiplicity) |
|---|---|---|---|---|---|---|
| | | | | | 1.45200 | 1.0 |
| | 0.78634898 | 0.61834472 | 5.12065557 | 4.02662230 | 1.27170 | 1.5 |
| | 0.82826024 | 0.68601502 | 7.16563335 | 5.93500920 | 1.20735 | 2.0 |
| ∑ | 1.61460922 | 1.30435975 | 12.28628893 | 9.96163149 | 3.93105 | 4.5 |

$1/x_1 = 0.68870523$ $x_1 = 1.452$ $y_1 = 1.0$

$\Sigma(1/x^2) = 1.77867464$ $\Sigma(1/x) = 2.30331446$

c = 48.79304255 b = - 66.85172754 a = 23.89786759

$$\text{Multiplicity (O-O)} = 23.89786759 - \frac{66.85172754}{L} + \frac{48.79304255}{L^2}$$

Table 13. Calculation coefficients for dependence E = f (L) for O−O bond.

| | 1/x | $1/x^2$ | $\frac{(y-y_1)}{(1/x-1/x_1)}$ | $\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$ | x (L, Å) | y (E, kj/mole) |
|---|---|---|---|---|---|---|
| | | | | | 1.45200 | 139.008 |
| | 0.78634898 | 0.61834472 | 1676.75866772 | 1318.51747088 | 1.27170 | 302.733 |
| | 0.82826024 | 0.68601502 | 2574.95601441 | 2132.73368486 | 1.20735 | 498.356 |
| ∑ | 1.61460922 | 1.30435975 | 4251.71468213 | 3451.25115574 | 3.93105 | 940.097 |

$1/x_1 = 0.68870523$ $x_1 = 1.452$ $y_1 = 139.008$

$\Sigma(1/x^2) = 1.77867464$ $\Sigma(1/x) = 2.30331446$

$c = 21430.93279023$ $b = -29935.02909385$ $a = 10590.40848780$

$$E\ (O\text{-}O) = 10590.40848780 - \frac{29935.02909385}{L} + \frac{21430.93279023}{L^2}$$

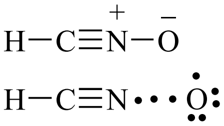
HCNO $L_{C\text{-}H} = 1.0266$ Å (61)

$L_{C\text{-}N} = 1.1679$ Å

$L_{N\text{-}O} = 1.1994$ Å

Multiplicity ($L_{C\text{-}N} = 1.1679$ Å) = 2.897

Multiplicity ($L_{N\text{-}O} = 1.1994$ Å) = 1.772



$H-C\equiv\overset{+}{N}-\overset{-}{O}$

$H-C\equiv N\cdots\dot{\underset{\cdot\cdot}{O}}:$

HNCO $L_{H\text{-}N} = 0.987$ Å (61) H−N=C=O

$L_{N\text{-}C} = 1.207$ Å

$L_{C\text{-}O} = 1.171$ Å

Multiplicity ($L_{N\text{-}C} = 1.207$ Å) = 2.549

Multiplicity ($L_{C\text{-}O} = 1.171$ Å) = 2.392

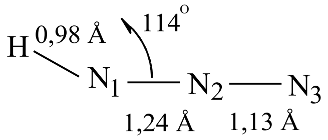
HNCS $L_{H\text{-}N} = 0.988$ Å (61) H−N=C=S

$L_{N\text{-}C} = 1.216$ Å

$L_{C\text{-}S} = 1.560$ Å

Multiplicity ($L_{C\text{-}N} = 1.216$ Å) = 2.475

Multiplicity ($L_{C\text{-}S} = 1.560$ Å) = 2.620



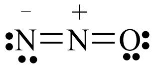
Multiplicity ($L_{N1-N2}$ =1.24 Å) = 1.940 (MO ~ 1.65) (62)

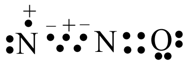
Multiplicity ($L_{N2-N3}$ =1.13 Å) = 2.715 (MO ~ 2.64)

$[N_1—N_2—N_3]^{\ominus}$

Multiplicity (N-N) ($L_{N-N}$ =1.18 Å) = 2.330 $L_{N-N}$ ~ 1.18 Å (62)

$N_2O$ ⟹





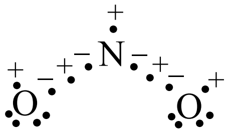
L (N−N) = 1.1282 Å (50)

L (N−O) = 1.1843 Å

Multiplicity ($L_{N-N}$ = 1.1282 Å) = 2.730

Multiplicity ($L_{N-O}$ = 1.1843 Å) = 1.969

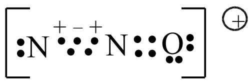
$NO_2$ ⟹



$L_{N-O}$ = 1.197 Å (63)

Multiplicity (N−O) (L = 1.197 Å) = 1.802

$N_2O^{\oplus}$



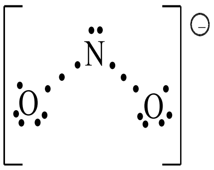
L (N−N) = 1.154 Å (50)

L (N−O) = 1.185 Å

Multiplicity ($L_{N-N}$ = 1.154 Å) = 2.523

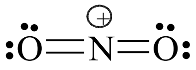
Multiplicity ($L_{N-O}$ = 1.185 Å) = 1.959

$NO_2^{\ominus}$



L (N−O) = 1.236 Å (64)

Multiplicity (N−O) = 1.388 ≈ 1.39



$:\ddot{O}=\overset{\oplus}{N}=\ddot{O}:$

$L_{N\text{-}O}$ = 1.200 Å (50)

Multiplicity (N−O) = 1.765

## 5. 2. CONCLUSION.

As exemplified in many chemical bonds (C-N, C-O, C-S, N-N, N-O, O-O) using the equation $y = a + b/x + c/x^2$ to describe the multiplicity dependence = f(L) and E = f(L) (where multiplicity - is multiplicity of bond, L - length of bond in Å, E - energy of bond in kj/mole), gives good results and determine the multiplicity of power relations in many organic and inorganic compounds. In fact, to determine the multiplicity or energy of bond we can known length of the bonds must solve simple quadratic equation. Conversely, knowing the multiplicity or energy or bond can determine its length (again solving basic equation). This method is simple, but gives good results when analyzing the chemical bonds that are nice to coincide with the experimental data or other theoretical calculations.

# 6. COMMENTS.

## 6.1. THREE-ELECTRON BOND IT IS AN EXISTING PARTICLE (OBJECT).

Three-electron 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 [1, p. 3 – 5]. 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. [1, p. 19 - 29].

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 electrons multiplicity 1;
4 electrons 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 [2, p. 1-2].

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 [2, p. 4–5].

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 Loren R. Graham "Science, Philosophy, and Human Behavior in the Soviet Union" [65].

Short and interesting in chapter IX "Chemistry" of this book Loren R. Graham [66] 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." [65, p. 3].

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 ...

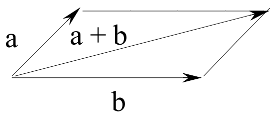
When in the past with philosophical positions criticized the concept of resonance in chemistry ... is, from my point of view, it is true.

But when a general philosophical position of trying to solve major scientific problems, such as whether genetics science or pseudoscience, it was a mistake." [65, p. 1].

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

## 6.2. CHEMICAL BOND – IT IS THE INTERACTING 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.



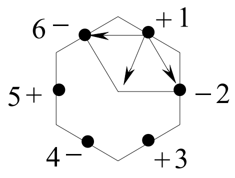


figure 3

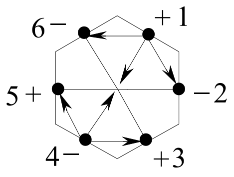
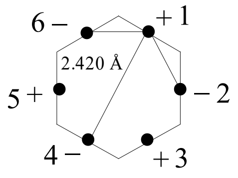


figure 4



$L_{1-2} = L_{1-6} = 1.210$ Å

$L_{1-4} = 2.420$ Å

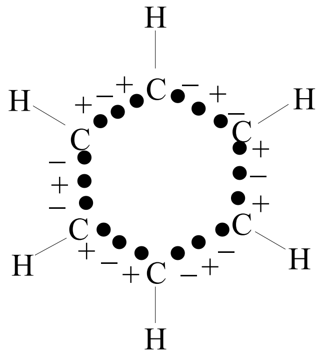


figure 1

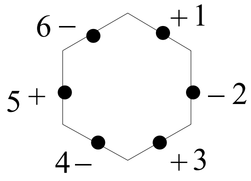
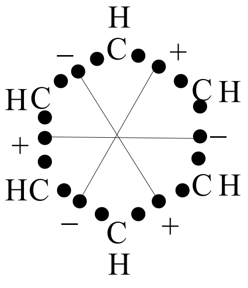
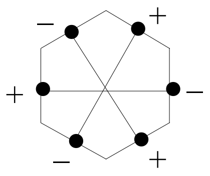


figure 2

" + " - upward spin

" – " - downward spin





" + " - the spin directed up

" – " - the spin directed down

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. And now, need to remember J.W. Linett with Double Quartet Theory [72]. J.W. Linett was right. Just need take to the point, that chemical bond is interaction of fermions (here they are doublets) with oppositely directed spins, and the fact, that octet (single atom, and, in general, the atoms form a chemical bond) consists of the sum of the electrons on the different levels s-, p-, d- (for a single atom), etc.

Consider an atom: then in the s-levels of interaction two fermions (1 (+) and 1 (-)), on the p-levels are also interacting two fermions (3 (+, -, +) and 3 (-, +, -)) two fermions (5 (+, -, +, -, +) and 5 (-, +, -, +, -)) to similarly interact d-level. But all these fermions are composed of different number of electrons for the s-levels are 1 (+) electron, p-level is 3 electrons (+, -, +) for the d-level is 5 electrons (+, -, +, - +). Huckel rule clearly defines the number of electrons is to always get a fermion (so n-unpaired number, 2n). Given the number of electrons at different levels (s-, p-, d-) we obtain the total number of electrons corresponding to the octet rule (2, 8, etc.). What is particularly important to minimize the repulsion between the electrons needed to separate fermion consisted of electrons whose spins have a different direction (ie neighboring electrons have opposite spins, for example, for fermions composed of three electrons, we have: 1 (+), 2 (- ), 3 (+). Naturally, the two interacting fermions are oppositely directed back 1 (+) and 2 (-).

Now consider the benzene. As it was shown in [1] in benzene exists between carbon atoms three-electron bond (a fermion), which interacts with the other through a series of three-electron bond (with another fermion). If we apply the idea of Linnet six of p-electrons in benzene, then benzene will be the spirit of the interaction of fermions (or two doublets): (3 (+, -, +) and 3 (-, +, -)). If we take the more general case, all the 18 electrons of benzene and then we have two interaction fermions, each of which consists of 9 electrons (9 (+) and 9 (-)). Naturally, these two fermions placed in a field of six carbon nuclei.

We now turn to the chemical bonds of different multiplicity.

Consider a single two-electron bond: we have interaction between two fermions, ie, two electrons (1 (+) and 2 (-)).

Dual four-electron bond should be considered as a combination of two single two-electron bonds. And here it is impossible not to recall the idea of Pauling on the description of multiple bonds by means of bent bonds [68, 69]. Consider the double bond as the interaction between two fermions prohibits that two electrons with opposite spins (curved bond) is a boson. In principle, the double bond can be viewed as the interaction of two bosons, which are due to the repulsive give two equivalent curved bonds (bosons tend to occupy one energy level).

Triple six-electron bond can be described by Pauling as a combination of three curved single bonds, and using ideas Linnet (which in our opinion is more true) as the interaction between two fermions (two three-electron bonds, two doublets) which have opposite spins (3 (+, - +) and 3 (-, +, -)). Here, as in the benzene six electrons interact, but now they are placed between two carbon atoms (benzene between six carbon atoms). This description is supported by its triple bond less "unsaturated" and more specific properties as compared with a double bond.

From the above it should be clear that the formation of octet, aromatic systems in general and chemical bonds is the interaction of fermions in various different environments, which leads to a variety of chemical systems.

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.

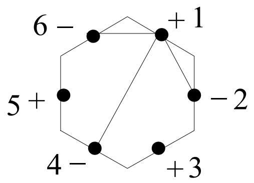
Fermionic or bosonic behavior of a composite particle (or system) is seen only at large distances (compared to the size of the system). At proximity, where spatial structure begins to be important, a composite particle (or system) behaves according to its constituent makeup. For example, two atoms of 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." [67].

## 6. 3. CHEMICAL BOND – IS A NEW INDIVISIBLE PARTICLES.

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).

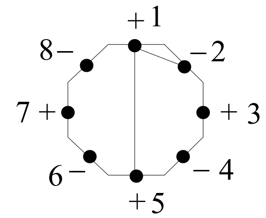
Lc-c = 1.397 Å



$L_{1-2} = L_{6-1} = 1.210$ Å

$L_{1-4} = 2.420$ Å

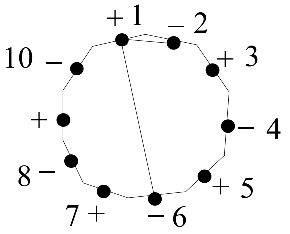
Lc-c = 1.410 Å



$L_{1-2} = L_{8-1} = 1.303$ Å

$L_{1-5} = 3.404$ Å

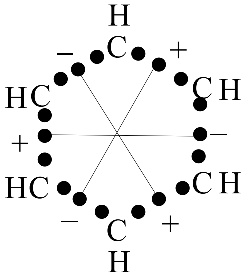
Lc-c = 1.400 Å

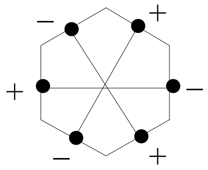


$L_{1-2} = L_{10-1} = 1.331$ Å

$L_{1-6} = 4.309$ 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" [3].

## 6. 4. ALTERNATIVE DESCRIPTION OF THE CHEMICAL BOND.

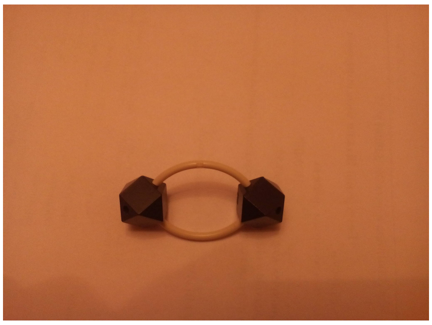
Description of the chemical bond using the π- and σ-bond this is one of the alternative description. The correct and fair description of the chemical bond there is description of multiple bonds with the help of bent bonds (Pauling, in 1930 years).

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." [68].

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

"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]" [69].

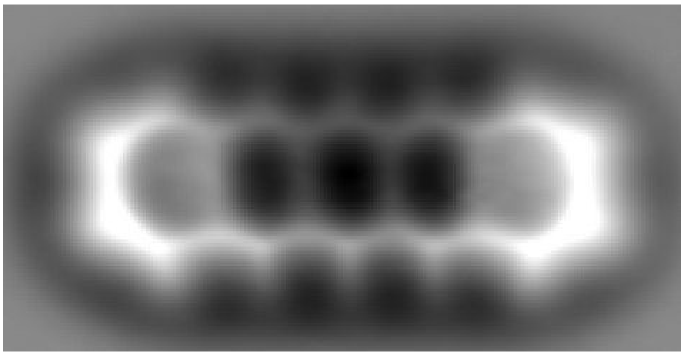
This double bond is 2 equivalent σ-bond (π-bond is not present).



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 [2, p. 4–5].

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) [1, p. 5].
2. Are explained easily and clearly aromaticity of benzene and antiaromaticity cyclobutadiene. It becomes obvious why at 4n + 2 aromatic and at 4n antiaromatic [1, p. 4–5].
3. Simply calculated delocalization energy of benzene (58,416 kcal/mol) [1, p. 11].
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) [1, p. 11, 15,14].
5. Easy and simple to explain the difference of external and internal signals of protons in [18]-annulene [1, p. 20–21].
6. You can picture structure of furan, thiophene, pyrrole, naphthalene, anthracene, graphite, oxygen, ozone, carboxylate anion and other organic and non-organic compounds [1, p. 19–29].

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

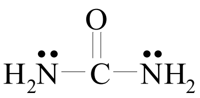
Therefore, the chemical bond and does not appear "on the tip of the pen", and introduced explanation exchange interaction and the like, since it is clear and proven that a purely Coulomb interaction (electromagnetic) is not sufficient to describe chemical bond (where there is more than one electron).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

## 6. 5. UREA MOLECULE.

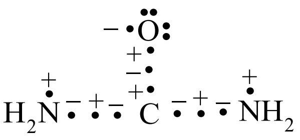
Look at the picture which shows the urea molecule with the calculations.

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 (14)

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.

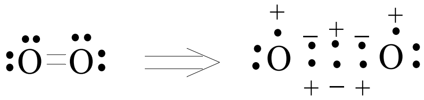
The multiplicity of C-N bonds in the molecule of urea - 1.686. Think, this mean the C-athom connected with two atoms of nitrogen (urea) bonds with a multiplicity of approximately 1.7, fold that is one of the C-N bond is almost 2. Are classical structure transmits real formula of urea molecules?

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.

## 6. 6. OXYGEN.

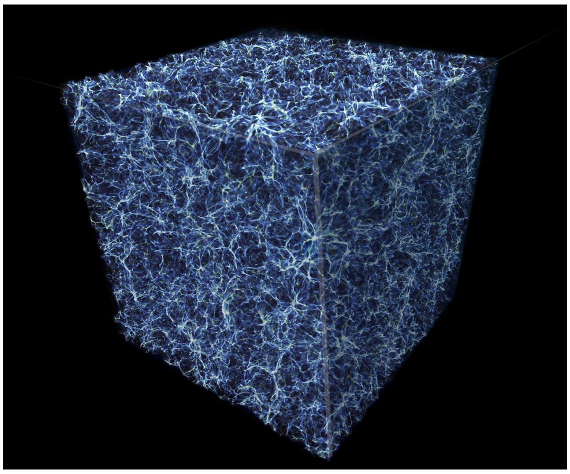
Without regard of three-electron bond its impossible to portray oxygen molecule that has a multiplicity of connection 2 and two unpaired electrones. This experimental fact that multiplicity ob bond in the oxygen molecule is equal to two, and at the same time there are 2 unpaired electrones (oxygen molecule 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).



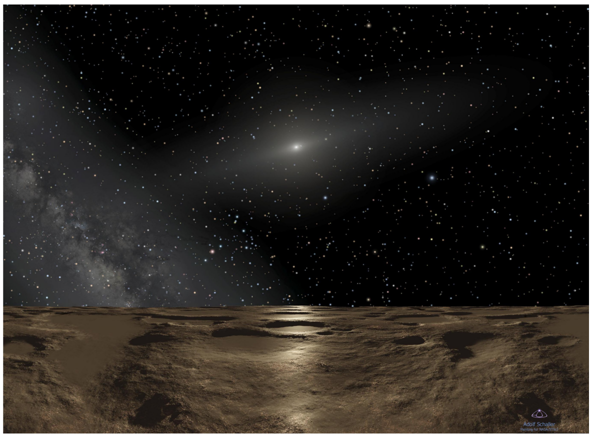
"Generally, the octet rule defines the state of the three-electron bond, that is, the distribution of the electrons, the energy of their interaction with each other and other unpaired electrons, the fact and the extent of belonging of the three-electron bond electrons to one or another atom." [1, p. 28, 32]. This fact is yet another confirmation of the existence of three electrone bond.

## 6. 7. MODEL OF THE INTERFERING UNIVERSE.

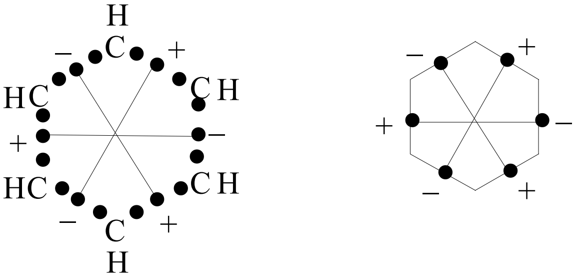
Model of the Interfering Universe, a perfect union of the microcosm and macrocosm.



1 photo. 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 [70].



2 photo. 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 [71].



" + " - the spin directed up

" – " - the spin directed down

3 photo. Benzene on the basis of the three-electron bond [1, p. 5].

These three photos illustrate to some extent, the model of the Interfereing Unuverse also demonstrate the unity of the microcosm of macrocosm.

"... 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." [3, p. 7].

## 6. 8. The reason of the formation of the chemical bond.

The reason for the formation of the chemical bond is still not clear, in fact, there is no physical justification, as it was at the time of N. Bohr, since the formation of a chemical bond does not follow from the four fundamental interactions. Just imagine, a chemical bond "does not understand" that it can not be explained normally and quietly exists... A full explanation of the chemical bond can only be provided by quantum mechanics (in the future), classical approaches simply do not work.

To understand this, it is necessary not to forget what L. Pauling did [27, 73], namely Pauling analyzed the interaction of the hydrogen atom and the proton in the entire range of lengths (he admitted that the hydrogen atom and $H +$ on the approach are preserved and showed that the bond is not formed in this case (since there is no exchange interaction or resonance by Pauling)). Only one of the above-mentioned facts actually destroys the classical approach (attraction and repulsion by Coulomb) to explaining the chemical bond. There inevitably follows that the chemical bond is a quantum-mechanical effect and no other.

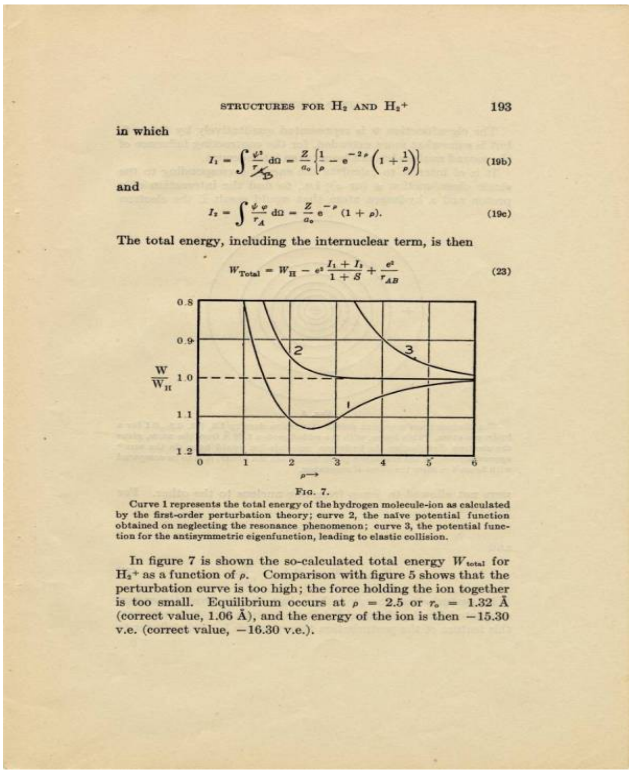
Imagine a system with two protons and one electron, but if it is treated as a hydrogen atom and a proton, then the bond can not form over the whole range of lengths. But, as Burrau showed [23], the bond in $H2 +$ is formed (if we consider the system as two protons and one electron), and no one particularly doubts this, since $H2 +$ exists. I particularly emphasize that there is only one electron (there is no inter-electronic repulsion, etc.).

After this fact, further discussions can not be continued, they do not make sense (especially to apply this to the explanation of two-electron bond or aromatic, this is a slightly different level of complexity). But nevertheless, it should be noted that quantum mechanics introduced the concept of "exchange interaction", which had no physical justification (since no fundamental interactions are altered in the interchange of electrons, but should, if a bond is formed) explained the chemical bond (more accurately, "disguised" chemical bond into the quantum-mechanical effect of the "exchange interaction"), by this, confirming that the chemical bond is indeed a quantum-mechanical effect.

The science of chemical bonding is only at the beginning of it's journey, and it is for today's students to make the most significant contribution to the theory of chemical bonding. And this will lead to fundamental changes in understanding both chemistry and physics.

On the basis of modern concepts of quantum mechanics, chemical bond can not be explained, fundamental assumptions are needed in quantum mechanics itself ...

On the photo page (p. 193) from the work of L. Pauling "The application of the quantum mechanics to the structure of the Hydrogen molecule and Hydrogen molecule-ion and to related problems" [27]:



STRUCTURES FOR $H_2$ AND $H_2^+$ 193

in which

$$I_1 = \int \frac{\psi^2}{r_{\cancel{A}B}} d\Omega = \frac{Z}{a_0}\left\{\frac{1}{\rho} - e^{-2\rho}\left(1 + \frac{1}{\rho}\right)\right\} \qquad (19b)$$

and

$$I_2 = \int \frac{\psi\,\varphi}{r_A} d\Omega = \frac{Z}{a_0} e^{-\rho}(1 + \rho). \qquad (19c)$$

The total energy, including the internuclear term, is then

$$W_{\text{Total}} = W_{\text{H}} - e^2\frac{I_1 + I_2}{1 + S} + \frac{e^2}{r_{AB}} \qquad (23)$$

FIG. 7.

Curve 1 represents the total energy of the hydrogen molecule-ion as calculated by the first-order perturbation theory; curve 2, the naïve potential function obtained on neglecting the resonance phenomenon; curve 3, the potential function for the antisymmetric eigenfunction, leading to elastic collision.

In figure 7 is shown the so-calculated total energy $W_{\text{total}}$ for $H_2^+$ as a function of $\rho$. Comparison with figure 5 shows that the perturbation curve is too high; the force holding the ion together is too small. Equilibrium occurs at $\rho = 2.5$ or $r_0 = 1.32$ Å (correct value, 1.06 Å), and the energy of the ion is then $-15.30$ v.e. (correct value, $-16.30$ v.e.).

## 6. 9. Chemical bond and A. Einstein's special theory of relativity.

The concept of three-electron bonds outputs chemical bond issue on a completely different level. And there is no doubt that in due course there will be an experimental confirmation of the existence of a three-electron link and a theoretical justification (quantitative), which will show the chemical bond from a completely different angle of view.

When describing the behavior of electrons in atoms or molecules, it is often assumed that the electrons move in a conservative field. But using the special theory of relativity it is easy to show that this is not so. Moreover, it follows from this that when the electrons move, the field in the molecule can not in principle be a conservative field by definition.

But if the field is not a conservative field, then our understanding and description of the chemical bond are not very good (then how do we explain and describe the chemical bond... ).

Here is the standard proof present in university textbook on physics [74]:

The interaction of fixed charges (point) is completely described by the Coulomb's law:

$$F = k\,(q1*q2)/r^2$$

q1-------r----------q2

Let us consider the interaction of two point charges, which are at rest in the coordinate system K1.

However, in another coordinate system K2, moving relative to K1, these charges move with identical speed and their interaction becomes more difficult. Since, due to the motion of charges, the electric field at each point of space is variable (E = (k*q)/r^2, E — the electric field) and therefore a magnetic field is generated in the system K2 (there is no magnetic field in the K1 system, since the electric field is constant). We remember that an alternating electric field generates a magnetic field and an alternating magnetic field generates an electric field.

Coulomb's law is insufficient to analyze the interaction of moving charges, and this is due to the relativistic properties of space and time and the relativistic equation of motion (the Coulomb's law has nothing to do with it). This follows from the following considerations.

Relativistic equations of motion:

$$dp/dt = F \quad (1)$$

Is invariant and has the same form in all inertial frame of reference. So in the coordinate system K2, which moves rectilinearly and uniformly with respect to K1:

$$dp2/dt2 = F2 \quad (2)$$

The left-hand sides of equations (1) and (2) include purely mechanical quantities (the behavior of which is known when passing from one coordinate system to another). Consequently, the left-hand sides of equations (1) and (2) can be related by some formula. But then the right parts of these equations (the equations of force) are related. Such a bond is conditioned the requirement of relativistic invariance of the equation of motion. Since speed enter the left-hand sides of equations (1) and (2), we conclude that the interaction of moving charges depends on the speed of motion and does not reduce to the Coulomb force.

Thus it is proved that the interaction of moving charges is realized not only by Coulomb force, but also by the force of another nature, called magnetic.

Let's note, Coulomb field is conservative, the magnetic field is not conservative.

A. Einstein's theory of relativity is one of the most fundamental and large theories in physics and there is no need to wait for some grandiose discovery to take place and theory of relativity will suddenly become incorrect. This will never happen. Will be just a little more another interpretation of the theory of relativity "aside" of quantum mechanics. And there will be a fusion of the theory of relativity and quantum mechanics and then things that now seem paradoxical, that of quantum mechanics, that in the theory of relativity will acquire a reasonable and visual explanation. And yes, we will understand more deeply both quantum mechanics and the theory of relativity. Nothing super principled will happen, there will only be an "extension of the territory of understanding" that in quantum mechanics that in the theory of relativity. We can assume that some scientific theories that are now more like science fiction than science after the confluence of quantum mechanics and the theory of relativity will be strictly moved into the realm of fantasy. The unification of quantum mechanics and the theory of relativity is inevitable, since both are fudamental in their areas (within their limits, micro- and macro world), and these areas must unite. This is inevitable, and it's only a matter of time. Ahead an interesting time ...

## 6. 10. Heisenberg's uncertainty principle and chemical bond.

Heisenberg's uncertainty principle:

$$\Delta x * \Delta p \geq \hbar/2$$

The Heisenberg uncertainty principle is one of the most fundamental principles of quantum mechanics [75]. If the uncertainty principle is incorrect, then all quantum mechanics is incorrect. Heisenberg's justified the ncertainty principle in order to save quantum mechanics. He understood that if it is possible to measure with every accuracy both the coordinate and momentum of a microparticle, then quantum mechanics will collapse, and therefore further justification was already a technical issue. It is the uncertainty principle that prohibits microparticles in quantum mechanics from having a trajectory. If the coordinates of the electron are measured at definite time intervals Δt, then their results do not lie on some smooth curve. On the contrary, the more accurately the measurements are made, the more "jumpy", chaotic the results will be. A smooth trajectory can only be obtained if the measurement accuracy is small, for example, the trajectory of an electron in a Wilson chamber (the width of the trajectory is enormous compared to the microworld, so the accuracy is small).

Heisenberg's formulated the uncertainty principle thus:

if you are studying a body and you are able to determine the x-component of a pulse with an uncertainty Δp, then you can not simultaneously determine the coordinate x of the body with an accuracy greater than $\Delta x = h / \Delta p$.

Here is a more general formulation of the principle of uncertainty: it is impossible to arrange in any way an instrument that determines which of the two mutually exclusive events has occurred, without the interference pattern being destroyed.

It should be immediately said that the Heisenberg uncertainty principle inevitably follows from the particle-wave nature of microparticles (there is a corpuscular-wave dualism is the principle of uncertainty, there is no corpuscle-wave dualism - there is no uncertainty principle, and in principle quantum mechanics, too). Therefore, there is an exact quantitative analogy between the Heisenberg uncertainty relation and the properties of waves.

Consider a time-varying signal, for example, a sound wave. It is pointless to talk about the frequency spectrum of the signal at any point in time. To accurately determine the frequency, it is necessary to observe the signal for some time, thus losing the accuracy of time determination. In other words, sound can not simultaneously have the exact value of its fixation time, as it has a very short pulse, and the exact frequency value, as it is for a continuous (and, in principle, infinitely long) pure tone (pure sine wave). The time position and frequency of the wave are mathematically completely analogous to the coordinate and (quantum-mechanical) momentum of the particle.

We also need to clearly understand that the Heisenberg's uncertainty principle practically prohibits predicting behavior (in the classical sense, since Newton was able to predict the position of the planets), for example, an electron in the future. This means that if the electron is in a state described by the most complete way possible in quantum mechanics, then its behavior at the following moments is fundamentally ambiguous [76]. Therefore, quantum mechanics can not make strict predictions (in the classical sense). The task of quantum mechanics consists only in determining the probability of obtaining a particular result in the measurement, and this is fundamental. That is why the uncertainty principle has such a fundamental meaning (there is no uncertainty principle - there is no quantum mechanics). But this does not mean that we do not know any "laws or variables that are hidden from us", etc. No. It's just the reality. This is analogous to how a particle can exhibit corpuscular and wave properties - just this is reality and nothing more. And even if we know the "hidden parameters" (compare, understand why the wave properties and corpuscular ones are manifested), this reality will not change, and the uncertainty principle will also work, but we will understand it more fully.

It must be added that not all physical quantities in quantum mechanics are measurable simultaneously, that is, they can have simultaneously definite values. If physical quantities can simultaneously have definite values, then in quantum mechanics they say that their operators commute. The sets of such physical quantities (complete sets) that have simultaneously defined values are remarkable in that no other physical quantity (not being their function) can have a definite value in this state. The fully described states (for example, the description of the electron state) in quantum mechanics arise as a result of the simultaneous measurement of a complete set of physical quantities. By results of such measurement it is possible to determine the probability of the results of subsequent measurements, regardless of what happened with the electron before the first measurement.

If physical quantities can not simultaneously have definite values, then their operators do not commute. The Heisenberg uncertainty principle establishes the limit of the accuracy of the simultaneous determination of a pair of physical quantities that are not described by commuting operators (for example, coordinates and momentum, current and voltage, electric and magnetic fields).

Let's add a little history. A. Einstein assumed that there are hidden variables in quantum mechanics that underlie the observed probabilities. He did not like the principle of uncertainty, and his discussions with N. Bohr and W. Heisenberg greatly influenced quantum mechanics and science as a whole.

In the Copenhagen interpretation of quantum mechanics (N. Bohr and followers), the uncertainty principle is adopted at the elementary level, and it is in this interpretation that it is believed that this can not be predicted at all by any method. And it was this interpretation that Einstein questioned when he wrote to Max Born: "God does not play dice." To which Niels Bohr, answered: "Einstein, do not tell to God what to do." Einstein was convinced that this interpretation was erroneous. His reasoning was based on the fact that all the already known probability distributions were the result of deterministic events. The distribution of the tossed coin or rolling bone can be described by the probability distribution (50% eagle, 50% tails). But this does not mean that their physical movements are unpredictable.

Conventional mechanics can calculate exactly how each coin will land, if the forces acting on it are known, and the eagles / tails will still be randomly distributed (with random initial forces). But it is unlikely that this experience can be extended to quantum mechanics.

The position of Bohr and Einstein must be viewed as views from different angles of view on one phenomenon (problem), and in the end it may turn out that they are right together. This can be demonstrated by lottery. Despite the fact that theoretically the results of the lottery can be predicted uniquely by the laws of classical mechanics, knowing all the initial conditions (it is necessary only to determine all the forces and perturbations, and to make the necessary calculations), in practice the lottery results are always probabilistic, and only in theory they can be predicted (try win the jackpot). Even in this simplest case, we will be "inaccessible" to all the initial data for calculations. It is logical to assume that the quantum system will be incomparably more complicated than the lottery, and therefore, if we master the "true" laws of the quantum world, the probabilistic picture will remain, since the microworld is such in essence. Moreover, if you think about it, then our world is also probabilistic. It is deterministic only in theory, and practically, in everyday life, we can only predict, for example, tomorrow (or a second, or a year, or 10 years) with a certain probability (who can guarantee the event of tomorrow with 100% probability?). And what is interesting is that only after having lived it (by making a measurement), we can say what probability was realized. Quantum mechanics in action.

Most importantly, the behavior of electrons in the atom, in the molecule, and in the chemical bond (I note that the chemical bond is the most difficult test for quantum mechanics), and here the probability picture plays a decisive role.

Consider an atom, for the description of an electron, the concept of an atomic orbital is introduced.

The atomic orbital is a one-electron wave function obtained by solving the Schrödinger equation. E. Schrödinger considered an electron in an atom as a negatively charged cloud whose density is proportional to the square of the value of the wave function at the corresponding point of the atom. In this form, the concept of an electron cloud was also perceived in theoretical chemistry. But from the physical point of view, it is true that the electron is a particle of a certain size (now we will not analyze the radius of an electron, etc. problems), that is, it is not a wave or a cloud with a negative charge. There was a contradiction between the treatment in chemistry and the fact that there is an electron in the real world (physical interpretation). Therefore, Max Born substantiated the probabilistic interpretation of the square of the wave function. E. Schrödinger did not immediately, but still agreed with the arguments of M. Born. This is a modern point of view, and note that it is not contradictory, it is true from the point of view of physics and from the point of view of chemistry.

Probabilistic interpretation of the wave function, this is a typical wave description, which corresponds to reality. And the different interpretations of Schrödinger and Bourne were the elimination of contradictions in understanding between chemists and physicists, such a "mutual agreement of the issue by physicists and chemists".

Surprisingly, in the quantum-chemical description of molecules, the chemical bond was actually "lost" [77], and the molecular orbitals were introduced to describe the behavior of an electron in a molecule (MO) completely analogous in meaning to the atomic orbitals (AO). But this contradicts the principle of quantum superposition and quantum mechanics in general. It should be noted that even with general qualitative representations it is clear that the behavior of electrons in the field of one nucleus (in an atom) and the behavior of electrons in the field of two nuclei (chemical bond) are two big differences that are qualitatively different. Therefore, to describe the chemical bond, it is proposed to introduce the concept of molecular orbital (MO) precisely for the chemical bond [77].

It is worth noting that, the measurement process in quantum mechanics has an effect on the quantum system (for example, on the electron being measured), and this effect can not be made arbitrarily small for a given measurement accuracy. If even our possibilities were unlimited (could make a "zero" perturbation on the micro object in the measurement), this would not change anything, since that is the nature of the microworld. The more accurate the measurement, the stronger the perturbation will be. This property of measurements is logically connected with the fact that the dynamic characteristics of an electron appear only as a result of the measurement itself (the electron does not have a trajectory because it does not have a coordinate without measurement, if the electron had a specific coordinate at a certain time, it would mean that it has a trajectory, but this is not so) [76]. Strictly speaking, dynamic characteristics can not be attributed to a microparticle, since a quantum object (for example, an electron) is not a corpuscle, but has a particle-wave nature. If the perturbations of measurement on a microobject could be made arbitrarily small, this would mean that the measured quantity has a definite value in itself, regardless of the measurement. But this prohibits the Heisenberg's uncertainty principle, and this is precisely the consequence of corpuscular-wave dualism (the microparticle is not a corpuscle!, and therefore has no trajectory, and therefore no dynamic characteristics without measurements).

But if we consider the measurement of the coordinates of an electron, then within the limits of the applicability of quantum mechanics, it is always possible to measure coordinates of electron with any accuracy (the electron interacts with a "classical" device when it is measured, the observer is absent).

For further analysis of chemical bond, let us consider the Compton wavelength of an electron:

$$\lambda c.e. = h/(me*c) = 2.4263*10^{\wedge}(-12)\ m$$

The Compton wavelength of an electron is equivalent to the wavelength of a photon whose energy is equal to the rest energy of the electron itself (the standard conclusion is given below):

$$\lambda = h/(m*v), \quad E = h*\gamma, \quad E = me*c^{\wedge}2, \quad c = \gamma*\lambda, \quad \gamma = c/\lambda$$

$$E = h*\gamma, \qquad E = h*(c/\lambda) = me*c^{\wedge}2, \qquad \lambda c.e. = h/(me*c)$$

where $\lambda$ is the Louis de Broglie wavelength, me is the mass of the electron, c, $\gamma$ is the speed and frequency of light, and h is the Planck constant.

It is more interesting to consider what happens to an electron in a region with linear dimensions smaller than the Compton wavelength of an electron. According to Heisenberg uncertainty in this area, we have a quantum mechanical uncertainty in the momentum of at least m*c and a quantum mechanical uncertainty in the energy of at least me*c^2 :

$$\Delta p \geq me*c \quad \text{and} \quad \Delta E \geq me*c^{\wedge}2$$

which is sufficient for the production of virtual electron-positron pairs. Therefore, in such a region the electron can no longer be regarded as a "point object", since it (an electron) spends part of its time in the state "electron + pair (positron + electron)". As a result of the above, an electron at distances smaller than the Compton length is a system with an infinite number of degrees of freedom and its interaction should be described within the framework of quantum field theory. Most importantly, the transition to the intermediate state "electron +

pair (positron + electron)" carried per time ~ λc.e./c

$$\Delta t = \lambda_{c.e.}/c = 2.4263*10^{(-12)}/(3*10^{8}) = 8.1*10^{(-20)}\ s$$

Now we will try to use all the above-mentioned to describe the chemical bond using Einstein's theory of relativity and Heisenberg's uncertainty principle. To do this, let's make one assumption: suppose that the wavelength of an electron on a Bohr orbit (the hydrogen atom) is the same Compton wavelength of an electron, but in another frame of reference, and as a result there is a 137-times greater Compton wavelength (due to the effects of relativity theory):

$$\lambda_{c.e.} = h/(m_e*c) = 2.4263*10^{(-12)}\ m$$

$$\lambda_{b.} = h/(m_e*v) = 2*\pi*R = 3.324\ Å$$

$$\lambda_{b.}/\lambda_{c.e.} = 137$$

where R = 0.529 Å, the Bohr radius.

Since the De Broglie wavelength in a hydrogen atom (according to Bohr) is 137 times larger than the Compton wavelength of an electron, it is quite logical to assume that the energy interactions will be 137 times weaker (the longer the photon wavelength, the lower the frequency, and hence the energy). We note that 1/137.036 is a fine structure constant, the fundamental physical constant characterizing the force of electromagnetic interaction was introduced into science in 1916 year by the German physicist Arnold Sommerfeld as a measure of relativistic corrections in describing atomic spectra within the framework of the model of the N. Bohr atom (therefore it is also called the constant of Sommerfeld) [78, 79].

To describe the chemical bond, we use the Heisenberg uncertainty principle:

$$\Delta x*\Delta p \geq \hbar/2$$

Given the weakening of the energy interaction 137 times, the Heisenberg uncertainty principle can be written in the form:

$$\Delta x*\Delta p \geq (\hbar*137)/2$$

According to the last equation, the quantum mechanical uncertainty in the momentum of an electron in a chemical bond must be at least me*c, and the quantum mechanical uncertainty in the energy is not less than me*c^2, which should also be sufficient for the production of virtual electron-positron pairs. Therefore, in the field of chemical bonding, in this case, an electron can not be regarded as a "point object", since it (an electron) will spend part of its time in the state "electron + pair (positron + electron)", and therefore its interaction should be described in the framework of quantum field theory.

This approach makes it possible to explain how, in the case of many-electron chemical bonds (two-electron, three-electron, etc.), repulsion between electrons is overcome: since the chemical bond is actually a "boiling mass" of electrons and positrons, virtual positrons "help" overcome the repulsion between electrons. This approach assumes that the chemical bond is in fact a closed spatial bag (a potential well in the energy sense), in which "boiling" of real electrons and also virtual positrons and electrons occurs, and the "volume" of this potential bag is actually a "volume" of chemical bond and also the spatial measure of the quantum-mechanical uncertainty in the position of the electron.

Strictly speaking, with such a consideration, the electron no longer has a certain energy, momentum, coordinates, and is no longer a "point particle", but actually takes up the "whole volume" of chemical bonding. It can be argued that in the chemical bond a single electron is depersonalized and loses its individuality, in fact it does not exist, but there is a "boiling mass" of real electrons and virtual positrons and electrons that by fluctuate change each other. That is, the chemical bond is actually a separate particle, as already mentioned, a semi-virtual particle. Moreover, this approach can be extended to the structure of elementary particles such as an electron or a positron: an elementary particle in this consideration is a fluctuating vacuum closed in a certain spatial bag, which is a potential well for these fluctuations.

It is especially worth noting that in this consideration, electrons are strongly interacting particles, and therefore the Pauli principle is not applicable to chemical bond (for more details, see the section "The Pauli Principle and the Chemical Bond") and does not prohibit the existence of the same three-electron bonds with a multiplicity of 1.5.

The above is easy to demonstrate with the example of a chemical bond of 1 Å length. Then the wavelength of Broglie is written in the form (the length of the chemical bond is $L = 2*\Delta x$):

$$\lambda = 2*\pi*\Delta x$$

and the Heisenberg uncertainty ratio takes the form:

$$\Delta x*\Delta p \geq (\hbar*137*2*\pi)/2$$

from which we get:

$$L*\Delta p \geq \hbar*137*2*\pi$$

where L is the length of the chemical bond, and Δp is the quantum mechanical uncertainty of the momentum of each electron in a given chemical bond.

Whence, we obtain a formula for determining the uncertainty of the momentum in a chemical bond:

$$\Delta p \geq (\hbar*137*2*\pi)/L$$

Having made the necessary calculations for a length of 1 Å, we obtain:

$$\Delta p \geq (\hbar*137*2*\pi)/10^{\wedge}(-10)$$

$$\Delta p \geq 9.078*10^{(-22)} \text{ kg*m/s}$$

That is, the uncertainty in the pulse is greater than me*c (me*c = 2.73*10^(-22) kg*m/s) (it is clear that the uncertainty of the electron velocity will be greater than the speed of light), which should be based on our assumptions.

## 6. 11. The Pauli exclusion principle and the chemical bond.

The Pauli exclusion principle — this is the fundamental principle of quantum mechanics, which asserts that two or more identical fermions (particles with half-integral spin) can not simultaneously be in the same quantum state. Wolfgang Pauli, a Swiss theoretical physicist, formulated this principle in 1925 [80]. In chemistry exactly Pauli exclusion principle often considered as a ban on the existence of three-electron bonds with a multiplicity of 1.5, but it can be shown that Pauli exclusion principle does not prohibit the existence of three-electron bonds. To do this, analyze the Pauli exclusion principle in more detail.

According to Pauli exclusion principle in a system consisting of identical fermions, two (or more) particles can not be in the same states [81]. The corresponding formulas of the wave functions and the determinant are given in the reference (this is a standard consideration of the fermion system), but we will concentrate our attention on the derivation: "... Of course, in this formulation, Pauli exclusion principle can only be applied to systems of weakly interacting particles, when one can speak (at least approximately on the states of individual particles)"[81]. That is, Pauli exclusion principle can only be applied to weakly interacting particles, when one can talk about the states of individual particles.

But if we recall that any classical chemical bond is formed between two nuclei (this is a fundamental difference from atomic orbitals), which somehow "pull" the electrons one upon another, it is logical to assume that in the formation of a chemical bond, the electrons can no longer be regarded as weakly interacting particles. This assumption is confirmed by the earlier introduced notion of a chemical bond as a separate semi-virtual particle (natural component of the particle "parts" can not be weakly interacting).

Representations of the chemical bond given in the chapter "The Principle of Heisenberg's Uncertainty and the Chemical Bond" categorically reject the statements about the chemical bond as a system of weakly interacting electrons. On the contrary, it follows from the above description that in the chemical bond, the electrons "lose" their individuality and "occupy" the entire chemical bond, that is, the electrons in the chemical bond "interact as much as possible", which directly indicates the inapplicability of the Pauli exclusion principle to the chemical bond. Moreover, the quantum-mechanical uncertainty in momentum and coordinate, in fact, strictly indicates that in the chemical bond, electrons are a system of "maximally" strongly interacting particles, and the whole chemical bond is a separate particle in which there is no place for the notion of an "individual" electron, its velocity, coordinate, energy, etc., description. This is fundamentally not true. The chemical bond is a separate particle, called us "semi-virtual particle", it is a composite particle that consists of individual electrons (strongly interacting), and spatially located between the nuclei.

Thus, the introduction of a three-electron bond with a multiplicity of 1.5 is justified from the chemical point of view (simply explains the structure of the benzene molecule, aromaticity, the structure of organic and inorganic substances, etc.) is confirmed by the Pauli exclusion principle and the logical assumption of a chemical bond as system of strongly interacting particles (actually a separate semi-virtual particle), and as a consequence the inapplicability of the Pauli exclusion principle to a chemical bond.

## 7. Quantum-mechanical aspects of the L. Pauling's resonance theory.

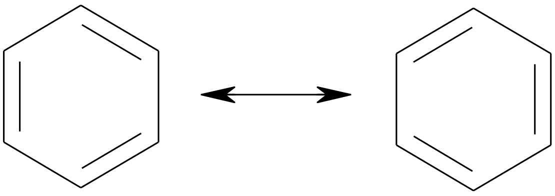
### 7.1. Results and discussion.

The basis of mathematical apparatus of quantum mechanics constitutes assertion that the state of a quantum system can be described by a certain function of the coordinates $\psi$ (q) called a wave function (the square of the modulus of this function determines the probability distribution of coordinate values) [76, pp. 19-21]. In the L. Pauling's resonance theory [73, pp. 413, 128-157, 408-416; 8, pp. 47-49], the wave function $\psi$ is used to describe the distribution of electrons in molecules and especially illustrative is example of benzene molecule. Therefore, the resonance theory (on the example of the benzene molecule) can be analyzed from the point of quantum mechanics using the principle of quantum superposition.

For example, consider two quantum states (actually existing) are described by wave functions $\psi1$ and $\psi2$. From the principle of superposition [76, p. 21] it should be clearly, that their linear combination ($\psi3 = C_1\psi1 + C_2\psi2$) will be the third quantum state (as actually existing), which will be described by a wave function $\psi3$. What does it mean? The fact that the measurement of a certain physical value d in the state $|\psi1>$ will result $d_1$, and for measure a value for of d in the state $|\psi2>$ will result $d_2$. When the third quantum state $|\psi3>$ is realized, then when measuring a physical quantity, the quantum system will take the values $d_1$ and $d_2$ with probabilities, respectively, $|C_1|$^2 and $|C_2|$^2. That is, in a quantum state $|\psi3>$ when we will have many dimensions sometimes $d_1$ value and sometimes $d_2$ (with certain known frequency). But this is in resonance theory can not be.

We describe for simplicity resonance of two Kekule structures (resonance structures) excluding structures Dewar. Then, the resonance theory it is assumed that $|\psi1>$ is a quantum state 1, which is describes a resonance structure 1 and |ψ2> is a quantum state 2, which is describes a resonance structure 2.

Wave functions ψ1 and ψ2 for the resonance structures 1 and 2 (Kekule structures):



The linear combination of the ($\psi3 = C_1\psi1 + C_2\psi2$) is normally the third quantum state |ψ3>, which is described by a wave function ψ3 and will describes the actual benzene molecule (resonance hybrid). The coefficients $C_1$ and $C_2$ will specify the contributions of resonance structures (Kekule structures, for our case $C_1/C_2 = 1$, $|C_1|^2 = |C_2|^2 = 0.5$) in a real molecule of benzene (resonance hybrid), which can not be described by separate resonance structures. And now it is important to note that the real molecule of benzene it really real and unique, and can not have a discrete description, ie the measurements we will never "see" the one Kekule molecule (resonance structure 1), then another (resonance structure 2), and this is directly contrary to the principle of quantum superposition. Moreover, adopted in theory of resonance Kekule structure, ie resonance structures are ideal structures that do not exist in reality, because they have all the bonds are equal, and this is despite the alternation of single and double C-C bonds, which in reality are different length. Therefore, the principle of quantum superposition (for resonance theory) is not executed, even for quantum states |ψ1> and |ψ2>, because as resonance structures is not reality, and any physical quantity (real) we can not measure.

If, however, as the resonance structures we take the real "curved" Kekule structures with ties that have different lengths, then the resonance theory does not make sense, since the transition from one structure to the other will vary internuclear distance. But then the principle of quantum superposition is applicable to all three quantum states (for |ψ1> and |ψ2> it is obvious, and for |ψ3> will be the one "twisted" Kekule structure, then the other, at 50 : 50). In fact, no change bond lengths have therefore chemistry is not applicable.

Especially notice, that resonance structures (Kekule structures with the same C-C bonds) is not electronic tautomers. Real benzene molecule is unique and no tautomerism exist. Incorrect represent benzene molecule as transitions between electronic tautomers (electrons in benzene does not migrate from one bond to another). There is a single benzene molecule, which has a constant electron distribution in time and which can not be represented by a discrete description. Therefore, it is accepted in resonance theory that every resonance structure contributes to the a real molecule (resonance hybrid) (usually chemists determined the contribution by the "eye"). And the third quantum state |ψ3> describes the real benzene molecule, which represents something between a resonance structures (remember the contribution of each resonance structure to the real structure (resonance hybrid)).

## 7.2. CONCLUSION.

By example of benzene molecule is shown that the principle of quantum superposition, and hence the quantum mechanics in general is in insurmountable conflict with the resonance theory. And so the assumption is that real benzene molecule (resonance hybrid) that is a cross between a resonance structures is genius chemical assumption, though not strictly from the standpoint of quantum mechanics, but that made it possible to qualitatively and quantitatively describe the benzene molecule, which could not represent a single formula.

This example clearly shows that in fundamental matters of chemistry did not reducible to physics, here there is a "chemical" highlight. And yet, the same L. Pauling's resonance theory literally changed the chemistry, had a profound influence on the minds of chemists (I'm not talking about the pedagogical impact of resonance theory), and for a long time is not a textbook on organic chemistry where there are no resonance theory. Nevertheless it should be noted that when complication of the molecule (pyridine, naphthalene, anthracene, and so on) quantitative calculations becomes difficult (for the correct calculation of naphthalene is necessary to consider of about 40 resonance structures) and therefore started to use the MO method.

# 8. Quantum-mechanical analysis of the MO method and VB method from the position of PQS.

## 8.1. Results and discussion.

The basis of mathematical apparatus of quantum mechanics constitutes assertion that the state of a quantum system can be described by a certain function of the coordinates $\psi$ (q) called a wave function (the square of the modulus of this function determines the probability distribution of coordinate values) [76, pp. 19-21]. The MO method, like the VB method [82; 8, pp. 17-18], uses the wave function $\psi$ to describe the behavior of electrons in atoms and molecules. Therefore, both the MO method and the VB method can be analyzed using the PQS. To do this, let us recall the principle of quantum superposition (PQS) [83, p. 1]: "For example, consider two quantum states (actually existing) are described by wave functions $\psi 1$ and $\psi 2$. From the principle of superposition [76, p. 21] it should be clearly, that their linear combination ($\psi 3 = C_1\psi 1 + C_2\psi 2$) will be the third quantum state (as actually existing), which will be described by a wave function $\psi 3$. What does it mean? The fact that the measurement of a certain physical value d in the state $|\psi 1>$ will result $d_1$, and for measure a value for of d in the state $|\psi 2>$ will result $d_2$. When the third quantum state $|\psi 3>$ is realized, then when measuring a physical quantity, the quantum system will take the values $d_1$ and $d_2$ with probabilities, respectively, $|C_1|$^2 and $|C_2|$^2. That is, in a quantum state $|\psi 3>$ when we will have many dimensions sometimes $d_1$ value and sometimes $d_2$ (with certain known frequency)".

It should also be noted that since L. Pauling's resonance theory is a particular case of the VB theory, the conclusion made about the insuperable conflict of resonance theory with the quantum superposition principle [83] can be transferred to the VB theory. In the VB method, the wave equations as well as in the theory of resonance are written for each of the possible electronic structures of the molecule [8, pp. 17-18] (each of them is called the canonical structure) and the total function $\psi$ is obtained by summing all conceivable functions with the corresponding weight coefficients:

$$\psi = C_1\psi1 + C_2\psi2 + C_3\psi3 + \dots$$

where $\psi1$, $\psi2$, $\psi3$ — are wave functions of canonical structures.

In calculations using the MO method, the wave function is represented by a linear combination of overlapping atomic orbitals [8, pp. 17-18] (called linear combination of atomic orbitals):

$$\psi = C_1\psi1 + C_2\psi2$$

where $\psi1$, $\psi2$ — wave functions of atomic orbitals, and $C_1$, $C_2$ — represent their weight coefficients.

But then it is obvious that both the MO method and the VB method contradict the principle of quantum superposition. Since the real molecule in the VB method will be described by a discrete set of canonical structures, which does not correspond to the existence of a single real molecule.

Similarly, in the MO method, the molecular orbital will be described by a discrete set of AO, which also does not correspond to the provisions of the MO theory. Next, we will carry out a more detailed analysis of the theory of the VB and the theory of MO.

For a more detailed analysis, it is necessary to take into account one nuance. To this end, consider a quantum system consisting of two parts. Suppose that the state of this system is given in such a way that each of the parts is described in its entirety. Then we can assert [76, p. 21], that the probabilities of the coordinates $q_1$ of the first part are independent of the probabilities of the coordinates $q_2$ of the second part, and therefore the probability distribution for the system as a whole must be equal to the product of the probabilities for its parts. This means that the wave function $\psi 12\ (q_1, q_2)$ of the system can be represented as the multiplication of the wave functions $\psi 1\ (q_1)$ and $\psi 2\ (q_2)$ of its parts:

$$\psi 12\ (q_1,\ q_2) = \psi 1\ (q_1) * \psi 2\ (q_2)$$

It should be noted that if both parts do not interact with each other, then this relationship between the wave functions of the system and its parts will continue at future times:

$$\psi 12\ (q_1,\ q_2, t) = \psi 1\ (q1, t) * \psi 2\ (q_2, t)$$

Therefore, in quantum chemistry, when considering molecules in the approximation of independent particles, the many-electron wave function must have the form of a multiplication of one-electron wave functions [82, p. 212]. But there are two ways to construct such a molecular wave function:

1. In the MO method, we choose the multiplication of members that are themselves linear combinations of one-electron wave functions:

$$\psi MO = \psi MO_1 * \psi MO_2$$

$$\psi MO_1 = C_1\psi AO\ A(1) + C_2\psi AO\ B(1)$$

$$\psi MO_2 = C_1\psi AO\ A(2) + C_2\psi AO\ B(2)$$

2. In the VB method choose a linear combination of members, each of which is a multiplication of one-electron wave functions:

$$\psi VB = C_1\psi AO\ A(1) * \psi AO\ B(2) + C_2\psi AO\ A(2) * \psi AO\ B(1)$$

Let us analyze these equations in more detail. We begin with the MO method.

$$\psi MO = \psi MO_1 * \psi MO_2$$

$$\psi MO_1 = C_1\psi AO\ A(1) + C_2\psi AO\ B(1)$$

$$\psi MO_2 = C_1\psi AO\ A(2) + C_2\psi AO\ B(2)$$

In the MO theory one basic assumption is made [8, pp. 17-18] that the wave function of the one-electron molecular orbitals is a linear combination of single-electron atomic orbitals of individual atoms (for a diatomic molecule AB, $\psi A$ (AO) and $\psi B$ (AO)):

$$\psi MO = C_1\psi A\ (AO) + C_2\psi B\ (AO)$$

for example, consider the first quantum state of an electron that represents this electron located on the atomic orbital of atom A and which is described by the wave function $\psi AO\ A(1)$. The second quantum state of the same electron will be a given electron located on the atomic orbital of atom B and described by the wave function $\psi AO\ B(1)$. From the principle of quantum superposition it follows that their linear combination

$$\psi 3 = C_1\psi AO\ A(1) + C_2\psi AO\ B(1)$$

will be the third quantum state, which will be described by the wave function $\psi 3$. According to the MO method, their linear combination will be a molecular orbital. But this directly contradicts the principle of quantum superposition. Proceeding from this equation

$$\psi 3 = C_1\psi AO\ A(1) + C_2\psi AO\ B(1)$$

and according to the principle of quantum superposition, when the third quantum state is realized $|\psi 3>$ (which is described by the wave function $\psi 3$), then when measuring a physical quantity, for example, the orbital energy, the quantum system will take the values of $E_1$ (the energy of the atomic orbital of atom A) and $E_2$ (the energy of the atomic orbital of atom B) with frequency respectively |C1|^2 and |C2|^2, that is, it will have a discrete description. When measuring the energy of a given orbital, we sometimes register the value of $E_1$, and sometimes the value of $E_2$. But this directly contradicts the idea of the MO method, since one-electron MO should be formed with an energy lower (if it is a bonding MO) than the energies of individual AO (according to the idea of linear combination of atomic orbitals, two MOs are formed from two AO, one MO with reduced energy and the other MO with increased energy). But the principle of quantum superposition prohibits this. With a linear combination of one-electron atomic orbitals, we will not be able to obtain a "new quality", that is, a one-electron molecular orbital, but we will have the spectrum of AO.

Analysis of the second equation

$$\psi MO_2 = C_1\psi AO\ A(2) + C_2\psi AO\ B(2)$$

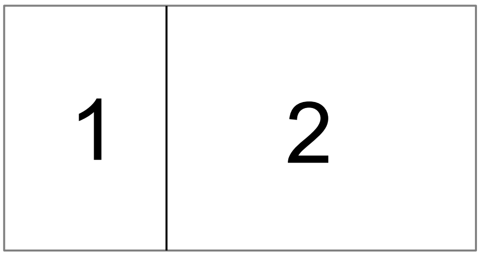
In which a linear combination of one-electron atomic orbitals of atoms A and B is considered, it is completely analogous to the foregoing. Therefore, the MO theory, like the VB theory, is insuperably contradictory to the principle of quantum superposition.

Now we will analyze the VB method.

As already mentioned above, in the VB method, choose a linear combination of members, each of which is a multiplication of one-electron wave functions. So for a diatomic molecule A-B (for example, hydrogen molecules), we get the following equation:

$$\psi VB = C_1\psi AO\ A(1) * \psi AO\ B(2) + C_2\psi AO\ A(2) * \psi AO\ B(1)$$

On the right-hand side of this equation, the first part ($C_1\psi AO\ A(1) * \psi AO\ B(2)$) describes the quantum system that consists of two parts. The first part of this system represents the atom A with the first (1) electron on the atomic orbital (atom A), the second part represents the atom B with the second (2) electron on the atomic orbital (atom B). The second part ($C_2\psi AO\ A(2) * \psi AO\ B(1)$) describes a quantum system when electrons 1 and 2 are reversed. And further in quantum chemistry is told occurrence due to these exchanges between electrons exchange interaction which leads to the formation of an appropriate molecule (in our case, hydrogen molecules). Moreover, these members are associated with canonical structures. For further consideration, it is necessary to remember how the wave function of a quantum system consisting of two parts is expressed. Consider the quantum system depicted in the figure and consisting of two parts 1 and 2.



$\psi 1\ (q_1)$ $\psi 2\ (q_2)$

In quantum mechanics [76, p. 21] it is shown that the wave function $\psi 12\ (q_1,\ q_2)$ of the system can be represented as a multiplication of the wave functions $\psi 1\ (q_1)$ and $\psi 2\ (q_2)$ and it's parts:

$$\psi 12\ (q_1,\ q_2) = \psi 1\ (q_1) * \psi 2\ (q_2)$$

And now look at the parts of the equation (from VB method):

$$\psi VB = C_1\psi AO\ A(1) * \psi AO\ B(2) + C_2\psi AO\ A(2) * \psi AO\ B(1)$$

Consider, for example, the first part:

$$C_1\psi AO\ A(1) * \psi AO\ B(2)$$

We see the multiplication of one wave function that describes the one-electron atomic orbital of atom A to another wave function that describes the one-electron atomic orbital of atom B. That is, this multiplication of two wave functions $\psi AO\ A(1) * \psi AO\ B(2)$ describes a system of two atoms A and B with the first (1) and second (2) electrons in the corresponding atomic orbitals. Especially note that it is the system of two isolated atoms, but not a molecule.

Similarly, the second part:

$$C_2\psi\text{AO A}(2) * \psi\text{AO B}(1)$$

Describes a system of two atoms A and B with the second (2) and first (1) electrons in the corresponding atomic orbitals (the electrons are reversed). Therefore, it is not entirely correct to ascribe to any member (or the sum of members) the canonical structure, since the description of two isolated atoms is not a description of the molecule that was formed from these two atoms. Permutations of electrons also do not significantly change anything, since two atoms remain two atoms in which the electrons are reversed. Two atoms are just two isolated atoms, but not a molecule. So if we mentally "place next" two hydrogen atoms, then the distance between the nuclei will be 1.06 Å (two Bohr radius), and the bond length in the hydrogen molecule is 0.74 Å, which confirms (for chemists it is obvious) that a system of two isolated atoms (the number of atoms doesn't matter) is not a canonical structure.

Therefore, when describing the molecule in the VB method, using the corresponding equations (and as a consequence of canonical structures), the chemical bond is simply "lost". Moreover, attributing to the members of the corresponding equation of canonical structures contradicts quantum mechanics, or more precisely, the description of a quantum system consisting of several parts.

The chemical bond was also "lost" in the MO description. This is easy to understand if we reduce the brackets to the corresponding equations in the corresponding equations:

$$\psi\text{MO} = \psi\text{MO}_1 * \psi\text{MO}_2$$

$$\psi\text{MO}_1 = C_1\psi\text{AO A}(1) + C_2\psi\text{AO B}(1)$$

$$\psi\text{MO}_2 = C_1\psi\text{AO A}(2) + C_2\psi\text{AO B}(2)$$

That is, we have:

$$\psi\text{MO} = \psi\text{MO}_1 * \psi\text{MO}_2 = (C_1\psi\text{AO A}(1) + C_2\psi\text{AO B}(1)) * (C_1\psi\text{AO A}(2) + C_2\psi\text{AO B}(2))$$

If we open the parentheses, we get members similar to the members of the equation from the VB method. Therefore, in order to "restore" the chemical bond in the corresponding equations and to exclude the inconsistency with the quantum superposition principle, it is necessary to not express MO in members of a linear combination of AO, but postulate the existence of MO as a new fundamental quality that describes a specific chemical bond and is not derived from simpler structural elements. Then we will "return" the chemical bond to the calculation methods and possibly significantly simplify the quantum chemical calculations. This is due to the fact that the energy of the chemical bonds is well known, and since the MO will describe the chemical bond (and the chemical bond energy is known), it will be easy to calculate the MO energy simply by substraction the chemical bond energy from the AO energy.

Since the chemical bond is the result of the interaction of fermions and they interact [84] according to the Hückel rule (4n + 2) (or 2n, n - unpaired), we can schematically depict molecular orbitals similarly to atomic orbitals. The number of electrons according to Hückel's rule will be: 2, 6, 10, 14, 18, …

Accordingly, the molecular orbitals of the chemical bond are denoted as follows:

MO (s) is a molecular s-orbital, 1 cell, can contain up to 2 electrons.

MO (p) is a molecular p-orbital, 3 cells, can contain up to 6 electrons.

MO (d) - molecular d-orbital, 5 cells, can contain 10 electrons.

MO (f) is a molecular f-orbital, 7 cells, can contain up to 14 electrons.

MO (g) is a molecular g-orbital, 9 cells, can contain up to 18 electrons.

Then the usual single bond will be described by the molecular s-orbitale (MO(s)). To describe the double bond, we need to assume that it is formed from two equivalent single bonds (as pointed out by L. Pauling [85]), and is then described by two molecular s-orbitals (2 MO(s)).

The triple bond will be described by a molecular p-orbital (MO (p)), then all six electrons of the triple bond will occupy one molecular p-orbit, which very well explains the difference between acetylene and ethylene (meaning C-H acidity).

In benzene 18 - electronic cyclic system can occupy one molecular g-orbital (MO(g)).

To describe the molecules, it is still necessary to introduce the concept of the molecular orbitals of an undivided pair, we shall designate it as MO(uns), on which the electrons of an undivided pair of atoms, unpaired electrons, and so on.

Then to describe the molecule it will be necessary to calculate the wave function which will be equal to the multiplication of all the wave functions of the chemical bonds and all the wave functions of the undivided pairs:

$$\psi MO = \psi MO(s1) * \psi MO(p) * \psi MO(s2) * \psi MO(uns) * \psi MO(uns2) \ldots$$

Wave functions that describe chemical bonds and undivided pairs are selected using mathematical expediency.

## 8.2. CONCLUSION.

Using the quantum superposition principle, the MO method and the VB method were analyzed and it is shown that they are in contradiction with quantum mechanics. Also, using the quantum-mechanical description of a system consisting of several parts, it is shown that the attribution of canonical structures to the members of the equation is incorrect. Therefore, both the MO method and the VB method did not describe molecules with chemical bonds but actually, a lot of independent atoms (of which the described molecules consisted). That is, in the quantum chemical calculations, the chemical bond was "lost". Therefore, in order to "introduce" a chemical bond into calculations and avoid conflict with quantum mechanics, it is suggested to postulate the existence of MO as a new fundamental quality that describes a specific chemical bond and is not derived from simpler structural elements.

## 9. REFERENCES.

1. Bezverkhniy V. D. Structure of the benzene molecule on the basis of the three-electron bond. http://vixra.org/pdf/1606.0152v1.pdf ; Bezverkhniy V. D. (2017) Theory of Three-Electron Bond in the Four Works with Brief Comments. Organic Chem Curr Res 6: 182. doi: 10.4172/2161-0401.1000182, https://www.omicsonline.org/open-access/theory-of-threeelectron-bond-in-the-four-works-with-brief-comments-2161-0401-1000182.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/1606.0151v2.pdf ; Bezverkhniy V. D. (2017) Theory of Three-Electron Bond in the Four Works with Brief Comments. Organic Chem Curr Res 6: 182. doi: 10.4172/2161-0401.1000182, https://www.omicsonline.org/open-access/theory-of-threeelectron-bond-in-the-four-works-with-brief-comments-2161-0401-1000182.pdf
3. Bezverkhniy V. D., Bezverkhniy V. V. Supplement to the theoretical justification of existence of the three-electron bond. http://vixra.org/pdf/1606.0150v2.pdf ; Bezverkhniy V. D. (2017) Theory of Three-Electron Bond in the Four Works with Brief Comments. Organic Chem Curr Res 6: 182. doi: 10.4172/2161-0401.1000182, https://www.omicsonline.org/open-access/theory-of-threeelectron-bond-in-the-four-works-with-brief-comments-2161-0401-1000182.pdf
4. Bezverkhniy V. D. A short analysis of chemical bonds. http://vixra.org/pdf/1606.0149v2.pdf ; Bezverkhniy V. D. (2017) Theory of Three-Electron Bond in the Four Works with Brief Comments. Organic Chem Curr Res 6: 182. doi: 10.4172/2161-0401.1000182, https://www.omicsonline.org/open-

access/theory-of-threeelectron-bond-in-the-four-works-with-brief-comments-2161-0401-1000182.pdf

5. Thomson J. J. Philosophical Magazine, 1921, 41, 510-538.
6. W.O. Kermak and R. Robinson, J. Chem. Soc. 427 (1922).
7. Ingold K. Theoretical essentials of the organic chemistry. Mir, Moscow, 1973, p. 143 (Russian translation from: Structure and mechanism in organic chemistry. Second edition, INGOLD C.K. Cornell University press Ithaca and London, 1969).
8. March J. Advanced organic chemistry. Reactions, Mechanisms, and Structure. In 4 volumes. Mir, Moscow, 1987, vol.1, p. 84 (Russian translation from Advanced organic chemistry. Reactions, Mechanisms, and Structure. Third edition. Jerry March, Professor of Chemistry Adelphi University. New York, 1985).
9. T.J. Kats, Journal of the American Society. 82, 3784, (1960).
10. Carey F., Sundberg R. Advanced Organic Chemistry. In 2 books. Chemistry, Moscow, 1981, book 1, p.335 (Russian translation from Advanced Organic Chemistry. Francis A. Carey and Richard J. Sundberg, University of Virginia, Charlottes, Virginia. Plenum Press, New York, 1977).
11. J.F.M. Oth, G. Anthoine, J.M. Gilles, Tetrahedron Lett. 6265, (1968).
12. S. Masamune, K. Hojo, Kiyoti Hojo, G. Bigam, D. L. Rabenstein, Journal of the American Society. 93, 4966, (1971).
13. Ternay. A. Contemporary organic chemistry. In 2 volumes. Mir, Moscow, 1981, vol.1, p. 583 (Russian translation Contemporary organic chemistry. Second edition. Andrew L. Ternay. University of Texas, Arlington, 1979).
14. Wells A. Structural inorganic chemistry. “Mir”, Moscow, 1988, vol.3, pp. 17-18

(Russian translation from Structural inorganic chemistry, fifth Edition, Wells A. F. Clarendon Press, Oxford, 1986).

15. Leo Gross, Fabian Mohn, Nikolaj Moll, Peter Liljeroth, Gerhard Meyer. The chemical structure of a molecule resolved by atomic force microscopy, Science, 325, 1110 (2009).
16. Dimas G. de Oteyza, Patrick Gorman, Yen-Chia Chen, Sebastian Wickenburg, Alexander Riss, Duncan J. Mowbray, Grisha Etkin, Zahra Pedramrazi, Hsin-Zon Tsai, Angel Rubio, Michael F. Crommie, Felix R. Fischer. Direct imaging of covalent bond structure in single-molecule chemical reactions. Science 2013, DOI: 10.1126/science.1238187.
17. Scheidl T. & al. (2010), "Violation of local realism with freedom of choice", arXiv:0811.3129v2 [quant-ph].
18. Herrmann L. G., et al. Carbon Nanotubes as Cooper-Pair Beam Splitters. Physical Review Letters, 2010, 04, 2.DOI: 10.1103/PhysRevLett.104.026801.
19. Lettner M., et al. Remote Entanglement between a Single Atom and a Bose-Einstein Condensate. Physical Review Letters.2011, 106, 21.DOI:10.1103/PhysRevLett.106.210503.
20. Moehring D. L., et al. Entanglement of single-atom quantum bits at a distance. Nature, 2007, 449, DOI:10.1038/nature06118.
21. Salart D., et al. Testing the speed of „spooky action at a distance“. Nature, 2008, 454, DOI:10.1038/nature07121.
22. Scott, T. C., Aubert-Frécon, M., Grotendorst, J. (2006). "New Approach for the Electronic Energies of the Hydrogen Molecular Ion".Chem. Phys. 324 (2–3):

323-338. arXiv:physics/0607081. doi:10.1016/j.chemphys.2005.10.031.

23. Burrau Ø (1927). "Berechnung des Energiewertes des Wasserstoffmolekel-Ions (H+2) imNormalzustand".DanskeVidensk. Selskab.Math.-fys. Meddel. (in German). M 7:14: 1–18.Burrau Ø (1927). "The calculation of the Energy value of Hydrogen molecule ions (H+2) in their normal position" (PDF). Naturwissenschaften(in German) 15 (1): 16–7. doi:10.1007/BF01504875.
24. Karel F. Niessen ZurQuantentheorie des Wasserstoffmolekülions, doctoral dissertation, University of Utrecht, Utrecht: I. Van Druten (1922) as cited in Mehra, Volume 5, Part 2, 2001, p. 932.
25. Pauli W (1922). "Über das Modell des Wasserstoffmolekülions". Annalen der Physik 373 (11): 177– 240. doi:10.1002/andp.19223731101. Extended doctoral dissertation; received 4 March 1922, published in issue No. 11 of 3 August 1922.
26. Urey HC (October 1925). "The Structure of the Hydrogen Molecule Ion". Proc. Natl. Acad. Sci. U.S.A. 11 (10): 618–21. doi:10.1073/pnas.11.10.618. PMC 1086173. PMID 16587051.
27. Pauling, L. (1928). "The Application of the Quantum Mechanics to the Structure of the Hydrogen Molecule and Hydrogen Molecule-Ion and to Related Problems". Chemical Reviews 5 (2): 173–213. doi:10.1021/cr60018a003.
28. Clark R. Landis; Frank Weinhold (2005). Valency and bonding: a natural bond orbital donor-acceptor perspective. Cambridge, UK: Cambridge University Press. pp. 91–92. ISBN 0-521-83128-8.
29. See (7), p. 140.
30. Krasnov K.S., Filippenko N.V., Bobkova V. A. etc. The molecular constants of

inorganic compounds:. Directory. Chemistry, Leningrad, 1979, p. 36.

31. See (7), p. 144.
32. Wells A. Structural inorganic chemistry. “Mir”, Moscow, 1988, vol. 3, p. 17 (Russian translation from Structural inorganic chemictry, fifth Edition, Wells A. F. Clarendon Press, Oxford, 1986).
33. Cottrell T.L. The Strengths of Chemical Bonds. Butterworths Scientific Publications, London, 1958.
34. See (32), p. 17-18.
35. See (7), p. 116.
36. See (30), p. 110.
37. Grey G. Electrons and Chemical Bonding. Mir, Moscow, 1967, p. 117 (Russian translation from Electrons and chemical Bonding, Harry B. Gray, New York, Amsterdam, 1965).
38. See (30), p. 416.
39. Wells A. Structural Inorganic Chemistry. “Mir”, Moscow, 1987, vol. 2, p. 566 (Russian translation from Structural Inorganic Chemictry, fifth Edition, Wells A. F. Clarendon Press, Oxford, 1986).
40. See (30), p. 365.
41. See (30), p. 198.
42. See (30), p. 106.
43. See (39), p. 543.
44. Gurvich L.V., Karachevtsev G.V., Kondratiev V. N., Lebedev Y. A., Medvedev V. A., Potapov V. K., Hodeev Y. S. Energy break chemical bonds. The ionization potentials

and electron affinities. Nauka, Moscow, 1974, p. 97.

45. See (39), p. 558.
46. See (39), p. 562.
47. Gordon A., Ford R. Sputnik chemist. Physico-chemical properties, methods, bibliography. Mir, Moscow, 1976, p. 127 (Russian translation from THE CHEMIST'S COMPANION. A HANDBOOK OF PRACTICAL DATA, TECHNIQUES, AND REFERENCES. ARNOLD J. GORDON Pfizer, Inc., RICHARD A. FORD Montgomery College, A WILEY-INTERSCIENCE PUBLICATION, JOHN WILEY AND SONS, New York – London – Sydney – Toronto, 1972).
48. See (30), p. 42.
49. See (30), p. 312.
50. See (30), p. 124.
51. See (30), p. 218.
52. Matthieu G., R. Panico course of theoretical foundations of organic chemistry. Mir, Moscow, 1975, p. 20 ( Russian translation from MÉCANISMES RÉACTIONNELS EN CHIMIE ORGANIQUE MATHIEU J., PANICO R., Hermann, 1972).
53. See (39), p. 612.
54. Kolodyazhni O. I., Chemistry phosphorus ylides. Naukova Dumka, Kiev, 1994, p. 255.
55. See (39), p. 611.
56. See (30), p. 130.
57. See (30), p. 46-47.

58. See (30), p. 236.

59. See (44), p. 106.

60. See (7), p. 116.

61. See (30), p. 200.

62. See (39), p. 564.

63. See (30), p. 122.

64. See (39), p. 577.

65. Graham L. R., Science, Philosophy, and Human Behavior in the Soviet Union, Columbia University Press, 1987.

66. Graham L. R., Wikipedia. https://en.wikipedia.org/wiki/Loren_Graham

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

68. Pauling L. Kekule and chemical bonding. Theoretical Organic Chemistry. Translation from English edition of 1959 year, Edited by R.H. Freidlin. Moscow. Foreign Literature Publishing House, 1963, p. 8.

69. Bent bond. Wikipedia. https://en.wikipedia.org/wiki/Bent_bond

70. Credit: NASA, ESA, and E. Hallman (University of Colorado), Boulder.

71. Credit: NASA, ESA and Adolf Schaller - Hubble Observes Planetoid Sedna.

72. Linnett J W, J Am Chem Soc., 1961, 83, 2643.

73. Pauling L. Nature of the chemical bond. Translated from english by M.E. Dyatkina under the guidance of professor Y.K. Sirkin. State Scientific and Technical Publishing House of Chemical Literature. Moscow, Leningrad, 1947, p. 25.

74. Matveev A. N. Electricity and magnetism. Moscow. Higher school, 1983, pp. 55-56.

75. Heisenberg W. Über den anschaulichen Inhalt der quantentheoretischen Kinematik

und Mechanik. Zeitschrift für Physik. 1927. Vol. 43. pp. 172—198. (English translation in book: Wheeler J. A., Zurek H. Quantum Theory and Measurement. Princeton Univ. Press. 1983. pp. 62-84).

76. Landau L. D., Lifshitz E. M. Theoretical physics in 10 volumes. Volume 3. Quantum mechanics. Fourth Edition. Moscow. Science, 1989, pp. 17 – 18. ISBN 5-02-014421-5 (Volume 3).
77. Bezverkhniy V. D., Bezverkhniy V. V. Quantum-mechanical analysis of the MO method and VB method from the position of PQS. http://vixra.org/pdf/1704.0068v1.pdf
78. Sommerfeld A. The structure of the atom and spectra. Moscow: Gostekhizdat, 1956. Vol. 1, p. 81.
79. Sommerfeld A. Zur Quantentheorie der Spektrallinien. Annalen der Physik. 1916. Vol. 356 (51), pp. 1—94.
80. Pauli W. Uber den Zusammenhang des Abschlusses der Elektronengruppen in Atom mit der Komplexstruktur der Spektren, Z. Phys., 1925, 31, 765-783.
81. Davydov A.S. Quantum mechanics. Second edition. Publishing house "Science". Moscow, 1973, p. 334.
82. Flurry R. Quantum Chemistry. Introduction. Translated from English. Moscow. Mir, 1985, pages 202, 212 — 217.
83. Bezverkhniy V. D., Bezverkhniy V. V. Quantum-mechanical aspects of the L. Pauling's resonance theory. http://vixra.org/pdf/1702.0333v2.pdf
84. Bezverkhniy V. D. Review. Benzene on the basis of the three-electron bond. p. 75 http://vixra.org/pdf/1612.0018v5.pdf

85. Pauling L. Kekule and chemical bonding. Theoretical Organic Chemistry. Translation from English edition of 1959 year, Edited by R.H. Freidlin. Moscow. Foreign Literature Publishing House, 1963, p. 8.