

# Chemical bond as the main problem of modern chemistry and physics.

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**Abstract:** The formation of the chemical bond is considered from the general theoretical standpoint as the interaction of different fermions. It is shown that using the modern classical concepts of chemical bond, it is impossible to obtain (strictly theoretically) a physical justification of the cause of the formation of a chemical bond. The shows the inapplicability of the Pauli principle to chemical bond and a new theoretical model of the chemical bond is proposed based on the Heisenberg uncertainty principle.

**Keywords:** fermion, three-electron bond, chemical bond and A. Einstein's special theory of relativity, Heisenberg's uncertainty principle and chemical bond, the Pauli exclusion principle and the chemical bond, the L. Poling's theory of resonance and chemical bond.

## INTRODUCTION.

Chemistry in the theoretical aspect can be considered as a science of chemical bond (the chemical reaction is in fact a breakdown of "old" chemical bonds and the formation of "new" chemical bonds) and therefore the theoretical basis for the formation of a chemical bond is fundamental for both theoretical chemistry and synthetic chemistry as it is the basis for their further development. As was shown earlier [1], a chemical bond can be considered as an interaction of fermions, and since fermions are particles with half-integer spin, it follows logically that the interaction of two electrons (electron spin  $\frac{1}{2}$ ) with the formation of

a two-electron bond, and the interaction of two three-electron bonds (through the circle) in benzene (three-electron bond is typical fermion with spin  $\frac{1}{2}$ ) with the formation of aromatic system, and in the general case the interaction of one fermion with another fermion (one fermion can be an unpaired electron and another fermion, for example, three-electron bond, etc.).

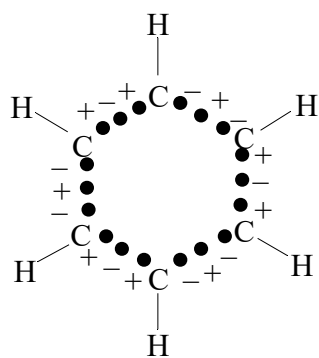


figure 1

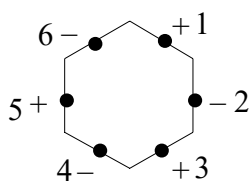


figure 2

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

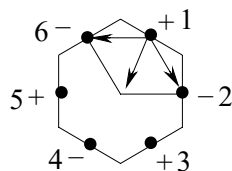
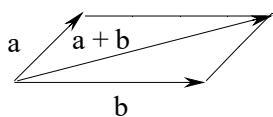


figure 3

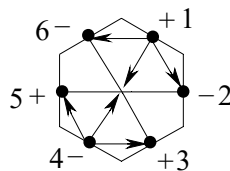
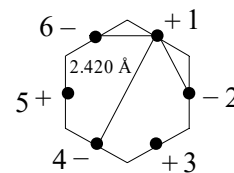
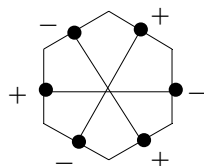
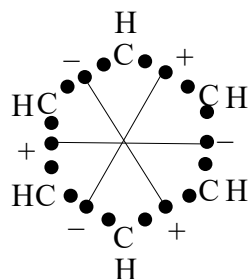


figure 4



$$L_{1-2} = L_{1-6} = 1.210 \text{ \AA}$$

$$L_{1-4} = 2.420 \text{ \AA}$$



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

In the study of chemical bond, the transition from electrons to fermions was very successful, since he make theory of the chemical bond to more general theoretical positions and showed that the chemical bond is a semi-virtual particle [1].

## RESULTS AND DISCUSSION.

### Hückel rule, fermions and Linett's theory.

Let us consider the Hückel rule (which actually regulates the interaction of fermions in aromatic systems) and Linett's theory from the position of fermion interaction.

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 [2]. 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, p. 2] 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 [3, 4]. 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.

### **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 [5, 6] 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 [7], the bond in  $H_2^+$  is formed (if we consider the system as two protons and one electron), and no one particularly doubts this, since  $H_2^+$  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 its 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" [5]:

in which

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

and

$$I_2 = \int \frac{\psi^2}{r_A} d\Omega = \frac{Z}{a_0} e^{-\rho} (1 + \rho). \quad (19c)$$

The total energy, including the internuclear term, is then

$$W_{\text{Total}} = W_{\text{H}} - e^2 \frac{I_1 + I_2}{1 + S} + \frac{e^2}{r_{AB}} \quad (22)$$

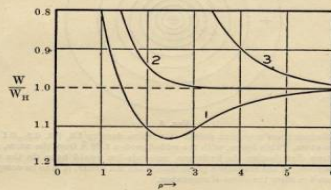


FIG. 7.

Curve 1 represents the total energy of the hydrogen molecule-ion as calculated by the first-order perturbation theory; curve 2, the naive 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  $r_e = 1.32 \text{ \AA}$  (correct value,  $1.06 \text{ \AA}$ ), and the energy of the ion is then  $-15.30 \text{ v.e.}$  (correct value,  $-16.30 \text{ v.e.}$ ).

## 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 [8]:

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

$$F = k (q_1 * q_2) / r^2$$

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:

$$dp^2/dt^2 = F^2 \quad (2)$$

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 fundamental 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 ...

## 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 [9]. If the uncertainty principle is incorrect, then all quantum mechanics is incorrect. Heisenberg's justified the uncertainty 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  $\Delta t$ , 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  $\Delta p$ , then you can not simultaneously determine the coordinate x of the body with an accuracy greater than  $\Delta x = \hbar/\Delta p$ .

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 [10]. 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" [11], 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 [11].

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) [10]. 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:

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

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):

$$\lambda = h/(m*\nu), \quad E = h*\gamma, \quad E = m_e*c^2, \quad c = \gamma*\lambda, \quad \gamma = c/\lambda$$

$$E = h*\gamma, \quad E = h*(c/\lambda) = m_e*c^2, \quad \lambda_{c.e.} = h/(m_e*c)$$

where  $\lambda$  is the Louis de Broglie wavelength,  $m_e$  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  $me*c^2$  :

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

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  $\sim \lambda_{c.e.}/c$

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

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):

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

$$\lambda_b. = h/(me*v) = 2*\pi*R = 3.324 \text{ \AA}$$

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

where  $R = 0.529 \text{ \AA}$ , 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) [12, 13].

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

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

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

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

According to the last equation, the quantum mechanical uncertainty in the momentum of an electron in a chemical bond must be at least  $m_e \cdot c$ , and the quantum mechanical uncertainty in the energy is not less than  $m_e \cdot c^2$ , 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  $L = 2 \cdot \Delta x$ ):

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

and the Heisenberg uncertainty ratio takes the form:

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

from which we get:

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

where L is the length of the chemical bond, and  $\Delta p$  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:

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

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

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

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

That is, the uncertainty in the pulse is greater than  $m_e \cdot c$  ( $m_e \cdot c = 2.73 \cdot 10^{-22} \text{ kg} \cdot \text{m/s}$ ) (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.

### **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 [14]. 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 [15]. 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)"[15]. 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.

### **Notes on the chemical bond.**

If we analyze the formation of the chemical bond (one-electron, many-electron) strictly theoretically, then it is difficult to understand the cause of the formation of the chemical bond. There are several problems here:

1. When a chemical bond is formed, when the domain of "existence" of electrons actually decreases (the "volume" of the chemical bond (MO) is much smaller than the "volume" of the corresponding AO, this was emphasized by L. Pauling) in comparison with the original AO ((in other words, that the electron distribution function in a diatomic molecule is much more concentrated than in the case of atoms), the repulsion between electrons inevitably must increase significantly. And then according to Coulomb's law ( $F=f(1/r^2)$ ) this repulsion can not be compensated in any way. This is also noted by L. Pauling, and we assume [16, pp. 88 — 90] that he therefore analyzed the interaction of the hydrogen atom and the proton in the entire range of lengths (admitted that the hydrogen

atom and  $H^+$  are retained when approaching) and showed that the connection is not formed in this case (since there is no exchange interaction or Pauling resonance). This actually showed that even a one-electron bond can not be explained only by the electro-magnetic interaction (that is, the classical approach), and if we go to many-electron bond (two-electron bond, three-electron bond, etc.) and take into account the repulsion between the bonding electrons, it becomes evident that the classical explanation (the electromagnetic approach) can not even provide a qualitative explanation of the cause of the formation of a chemical bond. It inevitably follows that the cause of the formation of a chemical bond can only be explained by quantum mechanics. Moreover, the chemical bond is a "pure" quantum-mechanical effect, in principle this is strictly indicated by the exchange interaction introduced by quantum mechanics, but not having the physical justification, that is, the exchange interaction is a purely formal, mathematical approach, which makes it possible at least some results. The fact that the exchange interaction has no physical meaning can be confirmed by the fact that the exchange integral essentially depends on the choice of the basis wave functions (more precisely, the overlap integral of the basis functions), and therefore, when choosing a certain basis, it can be less modulo, and even change sign on the reverse, which means that two atoms can not be attracted but repelled. In addition, the exchange interaction by definition can not be applied to the one-electron coupling, since there is no overlap integral since we have one electron (but Pauling's resonance can be applied to explain the one-electron bond).

2. In addition, using A. Einstein's theory of relativity, it can be shown that, in the motion of electrons, the field in a molecule can not by definition be a conservative field [16, pp. 90 — 93]. When describing the behavior of electrons in atoms or molecules, it is

often (more precisely, almost always) assumed that the motion of electrons is in the average conservative field. But this is fundamentally not true (based on the theory of relativity), and therefore further assumptions are not theoretically rigorous. Moreover, this case (application of the theory of relativity to a chemical bond) directly indicates that it is only possible to explain the cause of the formation of a chemical bond by using jointly quantum mechanics and the theory of relativity of A. Einstein, which we will try to do [16, pp. 93 - 103].

3. It is also especially worth noting that when analyzing the Pauli principle [16, pp. 104 - 105] it turned out that it can not be applied to chemical bonds, since the Pauli principle can be applied only to systems of weakly interacting particles (fermions), when one can speak (at least approximately on the states of individual particles). Hence it inevitably follows that the Pauli principle does not forbid the existence of three-electron bonds with a multiplicity of 1.5, which has a very important theoretical and practical significance for chemistry. In chemistry, a three-electron bond with a multiplicity of 1.5 is introduced, on the basis of which it is easy to explain the structure of the benzene molecule and many organic and inorganic substances [1].

4. It is shown [11, 17] that the main assumption of the molecular orbitals method (namely, that the molecular orbital can be represented like a linear combination of overlapping atomic orbitals) enters into an insurmountable contradiction with the principle of quantum superposition. It is also shown that the description of a quantum system consisting of several parts (adopted in quantum mechanics) actually prohibits ascribe in VB method to members of equation corresponding canonical structures.

5. See pp. 7 – 8 [11].

«...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 subtraction the chemical bond energy from the AO energy.

Since the chemical bond is the result of the interaction of fermions and they interact [5] 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 [6]), 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))...».

Taking into account the above reasoning about the chemical bond, we can say that modern concepts of the chemical bond can not be strictly theoretically fair, but rather qualitative with empirical quantitative calculations. Using quantum mechanics, namely the Heisenberg uncertainty principle and A. Einstein's theory of relativity, one can explain the reason for the formation of a chemical bond [16, pp. 93 — 103] and understand how electrons form a chemical bond, and how the binding process itself in the molecule. It should be noted that the chemical bond is in fact a separate particle (a fermion or a boson depending on the number of electrons), which we called a semi-virtual particle [1, pp. 12 – 13], which exists indefinitely long in a particular molecule.

Now let us consider the L. Poling's theory of resonance and chemical bond from the position of the theory of resonance.

It is important to understand that there are no resonance structures in reality, and the resonance theory is simply a very convenient and intuitive model for describing benzene. The concept of "resonance" (in L. Pauling's theory of resonance) does not imply a really occurring resonance between the Kekule structures, it is just a good name for the theory. Successful, because it clearly indicates that at the resonance of the Kekule structures a real molecule of benzene is formed, which has an electronic structure intermediate between them (Kekule structures). And most importantly, I especially note that the real structure of benzene

will have energy below the energy of the Kekule structures (that is why the "resonance theory" is a decrease in the energy of the system, and as it is known at real resonance (as a physical process), one can say "ejection" of energy). This also applies to chemical bonds.

L. Pauling, the theory of resonance extended not only to benzene, but also to chemical bonds [6, pp. 13 – 33, 43 – 45, 50 – 60, 78 – 82, 128 – 161, 194 – 225, 232 – 247, 255 – 278], in fact it was the only systematic approach to describing the chemical bond. And despite the fact that in a strictly theoretical analysis (within the framework of quantum mechanics) the resonance theory contradicts the principle of quantum superposition, the idea of resonance (that is, the idea of a real physical process) as an approach for studying the chemical bond is very successful and fruitful. Since it is precisely the idea of resonance that clearly indicates that in the formation of a chemical bond there must be a "zest", that is, a real physical process that leads to the release of energy (bond energy). The classical, modern representation of the chemical bond, in fact, ignores the physical justification of the chemical bond. From modern ideas, there is no reason why energy should be released when a chemical bond is formed. Conversely, with the concentration of electrons in the inter-nuclear region, that is, when a chemical bond is formed, it is logical to expect an increase in the energy of the system (the Coulomb repulsion between electrons increases). Moreover, some physicists (or quantum chemists) generally deny the existence of a chemical bond between two atoms and believe that the chemical bond is a successful concept for non-physicists on the binding of atoms. Naturally, chemists categorically disagree with this, although they understand the reasons for such a perception of the chemical bond.

It is worth noting that Heisenberg first used the concept of resonance in quantum mechanics to study the quantum states of helium [18].

L. Pauling spent one year (1926 - 1927) spent in Europe, in the alma of the mother of quantum mechanics. He actually studied quantum mechanics at A. Sommerfeld (Munich) and at the seminars of E. Schrödinger (Zurich), and the great physicists who stood at the origins of quantum mechanics had a profound influence on him. After this brief (only 1 year) business trip, L. Pauling understood that only quantum mechanics could be the theoretical basis for understanding the chemical bond. Moreover, now it is obvious, the physical essence, the physical substantiation of various processes for it became vital, therefore in the future the theory of resonance was born. Here some explanations are needed.

In the 20-30s of the 20th century, after the birth of quantum mechanics, many great physicists tried to solve the problem of chemical bonding. But all their attempts were unsuccessful, or rather not very successful. But this should not be taken as a failure, on the contrary, they clearly indicated the problem: if the reason for the formation of a chemical bond is explained by a real physical process (obviously, it should be so), then an acceptable solution could not be found. Moreover, the creation of MO and VB methods, and in fact the introduction of exchange interaction in chemistry to explain the chemical bond, did not solve this problem, since the exchange interaction has no physical meaning, it is a "purely" formal approach, and this is well known in quantum mechanics. In addition, both the MO method and the VB method, and, naturally, the exchange interaction contradict the principle of quantum superposition, that is, quantum mechanics itself [11, pp. 3 — 7]. And most importantly, these formal methods do not contain conceptual ideas for solving the problem of chemical bonding.

The resonance theory is a "pure" chemical theory, the idea of which implies that there must be a physical process (real), which is the reason for the formation of a chemical bond,

we assume that therefore Pauling called the theory "resonance theory". And there is no doubt that only this approach will lead to a full understanding of the chemical bond. For this, it is necessary to simultaneously apply quantum mechanics and the theory of relativity of A. Einstein [16, pp. 93 - 103]. Probably this is the only way (the combination of quantum mechanics and the theory of relativity), not very simple, but perhaps the only one that will lead to an understanding of both chemical and many physical processes.

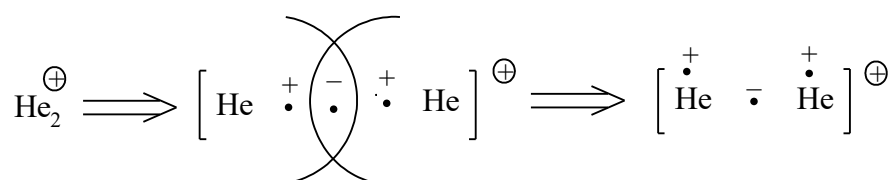
How successful is the application of the concept of a real physical process can be demonstrated by the following example. In 1935, in an article by Linus Pauling, L. O. Brockway and J. Y. Beach entitled "The Dependence of interatomic distance on single bond-double bond resonance" [19], the multiplicity of the bond in benzene was found to be 1.5 (based on two Kekule structures). But this way of calculating Pauling within the framework of the theory of resonance in 1937 was criticized by William Penney (English mathematician and professor of mathematical physics at the Imperial College London) [20]. The essence of the objections is the following: if the multiplicity of the bond in benzene is 1.5, then it follows logically that the heats of formation of benzene and cyclohexatriene (or one of the "resonant" Kekule structures) also coincide, which contradicts the resonance theory (the real benzene molecule should have a lower energy). From this it follows logically that the multiplicity in benzene should be greater than 1.5 and W. G. Penney received the number 1.62 [20].

As we can see, the concept of a real physical process (since it is a decrease in the energy of a real benzene molecule) led to the understanding that the multiplicity of the bond in benzene should be greater than 1.5, which was shown by quantum chemical calculations (1.67) [21]. The concept of three-electron coupling explains why there is an increase in the

multiplicity: this is a consequence of the interaction of two three-electron bonds on opposite sides of benzene (with different spins), benzene just "shrinks, decreases" a little. Calculations give a multiplicity of 1.66 [1, p. 5]. If we logically think, then the concept of three-electron coupling follows from the theory of resonance: the resonance of two Kekule structures "creates" a real molecule of benzene with the distribution of electrons averaged between the Kekule structures, that is, we actually get benzene with three-electron bonds.

### One-electron bond in He<sub>2</sub><sup>+</sup>.

Let us consider the chemical bond in the molecular ion of helium He<sub>2</sub><sup>+</sup>. The helium atom has 2 electrons and one energy level (1S). Therefore in He<sub>2</sub><sup>+</sup> there are 3 electrons. The assumption that the bond in He<sub>2</sub><sup>+</sup> is three-electron is incorrect. The multiplicity of the bond is still determined by the fundamental rule of the octet. Therefore, it is easy to show that the bond in He<sub>2</sub><sup>+</sup> is one-electron (hence its multiplicity is 0.5). For this it is sufficient to apply the octet rule to He<sub>2</sub><sup>+</sup>, see scheme.



From the scheme it is obvious that in order for the octet rule to be fulfilled in He<sub>2</sub><sup>+</sup>, the bond must be one-electron (only one electron can belong to both atoms simultaneously). Moreover, it can be concluded that the octet rule in a "condensed" form reflects the balance of the Coulomb repulsive-attraction forces between the electrons and the nuclei. Since, with the example of He<sub>2</sub><sup>+</sup>, it is obvious that, for a three-electron bond, the nuclei would remain without electrons, which led to a strong increase in the repulsion between the helium nuclei.

The one-electron bond in He<sub>2</sub><sup>+</sup> explains why He<sub>2</sub><sup>+</sup> and H<sub>2</sub><sup>+</sup> are equally stable,

because they are connected by a one-electron bond: compare the bond energies and the bond length [6, p. 23 - 26, p. 262]:

$$E(\text{He}_2^+) = 58 \text{ kcal/mole}$$

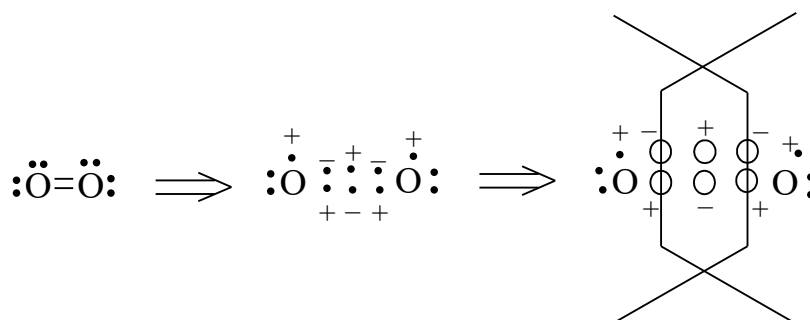
$$L(\text{He}_2^+) = 1.09 \text{ \AA}$$

$$E(\text{H}_2^+) = 61 \text{ kcal/mole}$$

$$L(\text{H}_2^+) = 1.06 \text{ \AA}$$

The fact that using the MO method in  $\text{He}_2^+$  yields a three-electron bond (with a multiplicity of 0.5) should not be misleading, since the MO method contradicts quantum mechanics [11].

If we do a similar procedure with oxygen in which there are two three-electron bonds (we calculate the octet of the electrons of each atom), then it becomes immediately clear why the oxygen multiplicity is 2 (in spite of two three-electron bonds, see scheme).



### Conclusion.

In conclusion, we add that the development of the theory of the three-electron bond and chemical bond by Heisenberg will lead not only to the quantitative calculation of the chemical bond (complete) but also the application of these calculations to the synthesis of substances (use in the laboratory) and the prediction of biological activity of chemicals. It means that it will be possible to easily calculate the basic properties of a molecule (substance) by the structural formula, and the accuracy must be such that synthesis of substances is not needed. Similarly, with biological activity: the development of the theory

(for example, the development of electronegativity in organic compounds, etc.) chemical bond should lead to a deeper understanding of the dependence of biological activity on the chemical structure, which undoubtedly will have an explosive effect on the appearance of new drugs (and new classes) and significantly simplify the task of searching for new substances in the structure. To calculate the chemical bond by Heisenberg, we will have to resort to the introduction of new concepts and postulates in quantum mechanics, which will also favorably affect its development.

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