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АКАДЕМИЯСИ МИНТАҚАВИЙ БЎЛИМИ
ХОРАЗМ МАЪМУН АКАДЕМИЯСИ

ХОРАЗМ МАЪМУН АКАДЕМИЯСИ АХБОРОТНОМАСИ

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МУНДАРИЖА

КИМЁ ФАНЛАРИ

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A NEW LOOK AT CHEMICAL BONDING AND THE THEORY OF TRANSFORMATION OF ELECTRONIC CLOUDS

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Аннотация. *Мақолада орбиталлар гибридизацияси ҳақидаги мавжуд назариялар кўриб чиқилган, ушбу назарияларнинг камчиликлари кўрсатилган ва атомларда электрон орбиталларни трансформация назарияси ҳақида кимёвий боғлар ҳосил бўлишини янги механизмлари таклиф қилинади.*

Калит сўзлар: *электронлар шакли, орбиталь, қўзғалган холат, электронларни тортилиши ва итарилиши, электрон орбиталларни трансформация назарияси, кимёвий боғ*

Аннотация. *В статье исследуются существующие теории гибридизации орбиталей, указываются некоторые недостатки этих теорий и предлагаются новые механизмы для объяснения образования химических связей с преобразованием электронных орбиталей в атомах.*

Ключевые слова: *форма электронов; орбитальный; возбужденное состояние; притяжение и отталкивание электронов; теория превращения электронных орбиталей в химические связи*

Abstract. *The article examines the existing theories on hybridization of orbitals, points out some of the shortcomings of these theories and proposes new mechanisms for explaining the formation of chemical bonds with the transformation of electron orbitals in atoms.*

Keywords: *shape of electrons; orbital; excited state; attraction and repulsion of electrons; theory of transformation of electron orbitals into chemical bonds*

A chemical bond is a force that holds two or more atoms, ions, molecules, or any combination of these together. According to its nature, the chemical bond is an electrostatic force of attraction between negatively charged electrons and positively charged nuclei. The magnitude of this attractive force depends mainly on the electronic configuration of the outer shell of the atoms [1].

The ability of an atom to form chemical bonds is called its valence. However, this concept is considered very outdated, since nowadays it is much more common to consider a chemical bond not in general, but taking into account its specific type. The electrons involved in the formation of chemical bonds are called valence electrons. These electrons are in the highest energy orbitals of the atom. The outer shell of an atom that contains these orbitals is called the valence shell.

Currently, the electronic theory of valence is used to explain the formation of a chemical bond between atoms of one or different elements,

Electronic theory of valence. Modern ideas about the nature of chemical bonds are based on the electronic theory of valence. This theory was developed independently by G.N. Lewis and W. Kossel in 1916. According to the electronic theory of valence, atoms, forming bonds, approach the achievement of the most stable (i.e., having the lowest energy) electronic configuration. Atoms can achieve this in two ways:

1. They can lose or gain electrons, forming ions. If atoms acquire electrons, they turn into anions. If they lose electrons, they turn into cations. Anions and cations with a filled outer electron shell have a stable electronic configuration. A chemical bond arises between the anion and the cation, which is an electrostatic force of attraction. A chemical bond of this type was previously called an electrovalent bond; the modern name is an ionic bond.
2. Atoms can also acquire stable external electronic configurations through the sharing of electrons. The resulting chemical bond is called a covalent bond. A covalent bond is formed by the

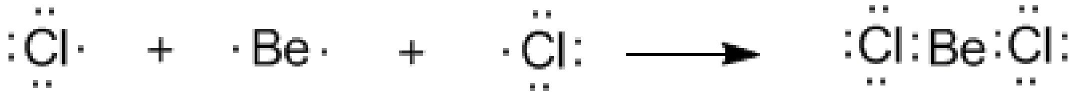
socialization of a pair of electrons supplied one from each atom. However, in some molecules or polyatomic ions, both of these electrons can be supplied by only one atom. This type of covalent bond is called coordination, donor-acceptor, or dative covalent bond.

Octet rule. When an atom of any element forms a chemical bond, acquiring, losing, or socializing valence electrons, its electronic configuration becomes the same as that of a noble gas atom located at the end of the same period as this element or the end of the previous period. The atoms of all noble gases, except helium, have a stable octet (so called "eight-shaped") of electrons in the outer shell. Therefore, the formation of chemical bonds by achieving stable electronic configurations, as in atoms of noble gases, is the essence of the so-called octet rule. This rule applies to both ionic and covalent bonds.

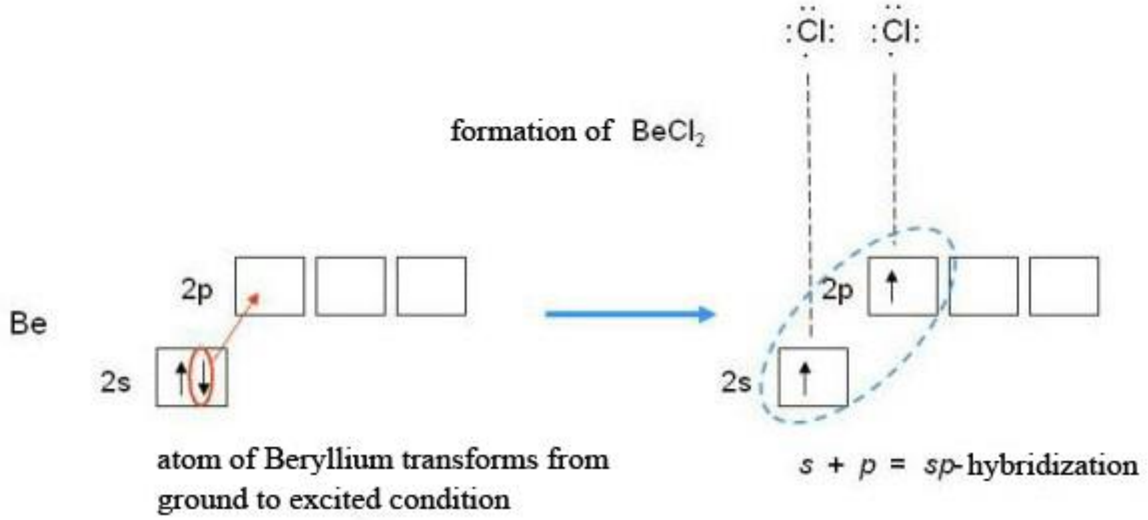
As can be seen from the provisions of the electronic theory of valence, the pairing of the valence electrons of the outer shell of the elements occurs when a chemical bond is formed between atoms. In this case, states are possible in which two electrons of one element have different shapes and states and form two chemical bonds with two electrons of the second atom, which, logically, should have different natures based on the difference between the electrons forming the bond. However, as practice shows, all bonds between the atoms of two elements are usually identical.

How is this possible, and how to explain it? The formation of identical bonds from atomic orbitals of different types required introducing such a concept as hybridization (that is, "crossing") of atomic orbitals.

Let us consider the formation of the $BeCl_2$ molecule. Its formation is quite understandable from the electronic structure of beryllium and chlorine atoms, which is depicted by the Lewis formulas:

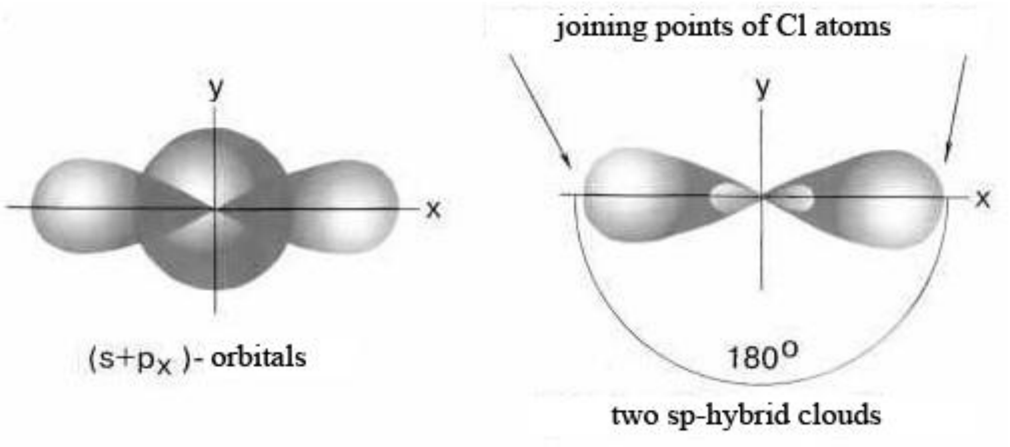


The electronic configuration of the valence shell of beryllium is $2s^2$. For a reaction with two chlorine atoms, a transition of beryllium electrons to an excited state is required:



If one chlorine atom were bound to beryllium due to the 2s-electron of beryllium and the other - due to the 2p-electron of beryllium, then the Be – Cl bonds would not be equivalent. However, in reality, both bonds have the same length, strength and are located at an angle of 180°.

To explain the equivalence of the Be – Cl bonds, one speaks of sp-hybridization of the valence atomic orbitals of beryllium, in which one s-orbital and one p-orbital (they are enclosed by an oval in the orbital diagram) seem to mix and align in shape and energy, giving two identical sp-hybrid orbitals.

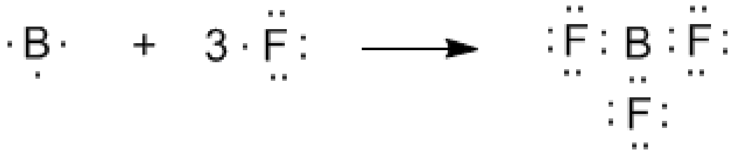


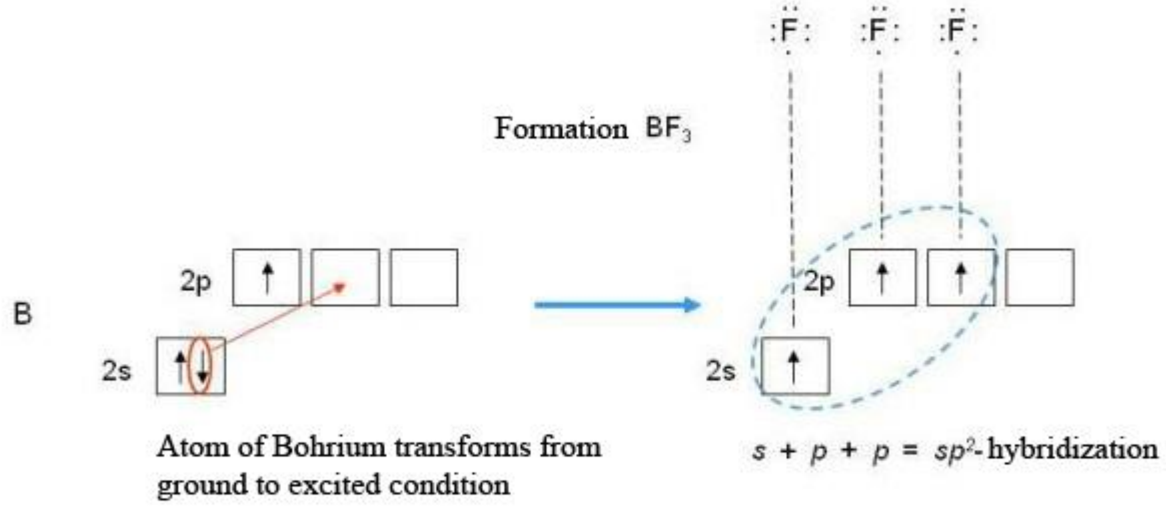
Each hybrid orbital is asymmetric (stretched out from the core). Both hybrid beryllium orbitals lie on the same straight line.

It is believed that due to sp-hybridization, the $BeCl_2$ molecule has a linear shape and all three of its atoms are on the same straight line, and both Be – Cl bonds are identical. It is the geometry of all other sp-hybridized molecules, regardless of the elements that are included in these molecules [2].

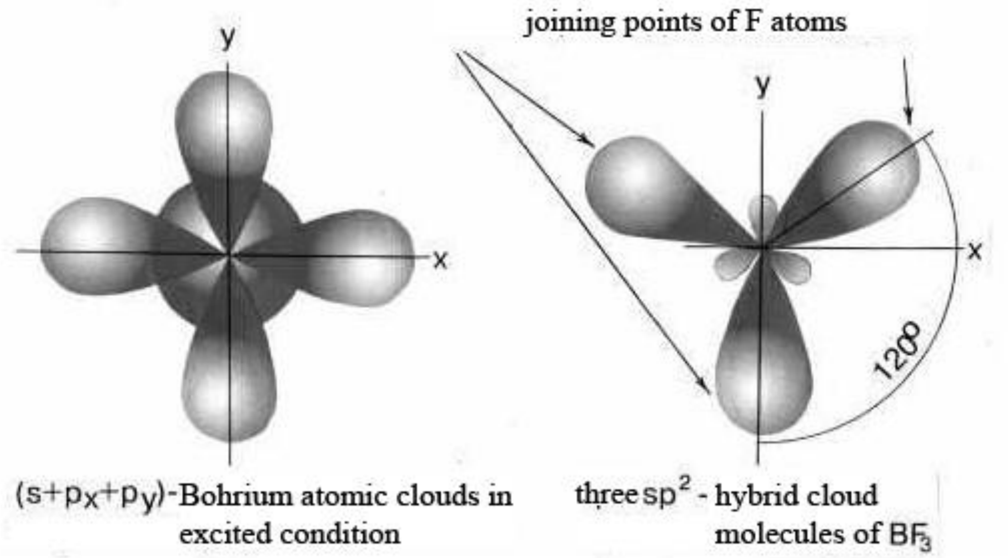
Furthermore, there is a misunderstanding: how can one s-electron and one p-electron form two independent units (hybrids)? Is it possible that the dumbbell-shaped electrons are divided into two parts, and the s electron merges with two half-electrons to form one hybrid? Is it possible for half an electron to exist, as well as an asymmetric hybrid form of an electron? Indeed, in this form of hybridization, a small part of the dumbbell is located closer to the nucleus, which once again proves the inconsistency of the theory of hybridization of electron shells and the existence of a dumbbell-shaped form of electron clouds.

If the valence shell of an atom includes electrons in one s-orbital and two p-orbitals, then sp2-hybridization of the orbitals takes place. An example is the sp2 hybridization of boron during the formation of the BF_3 molecule.





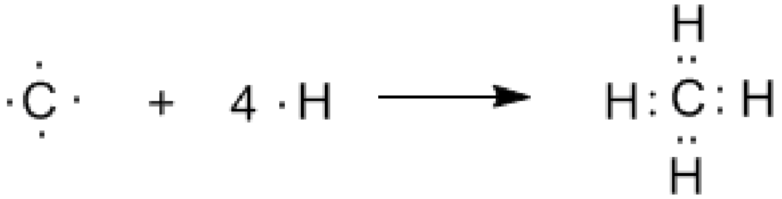
On the orbital diagram, one s- and two p-orbitals are circled, which "mix"; that is, they hybridize.

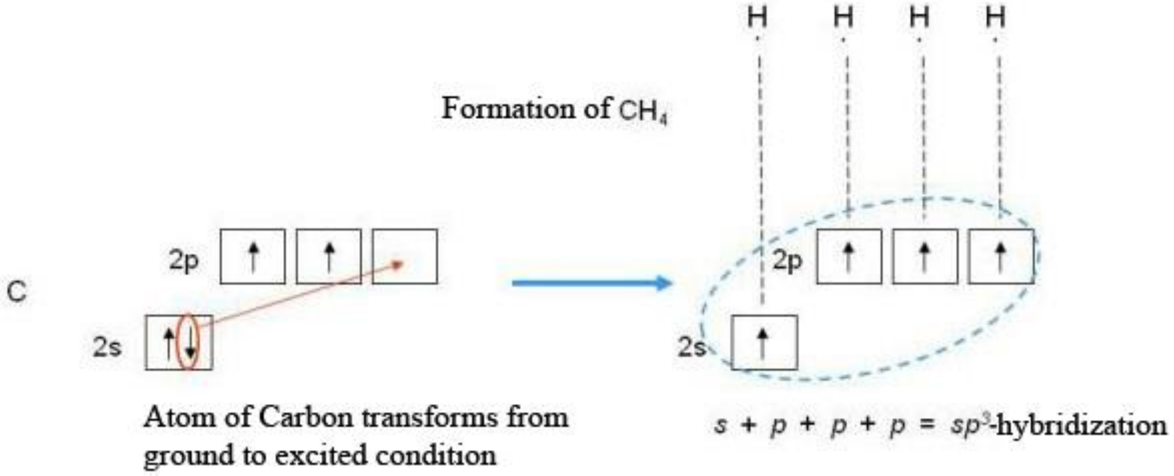


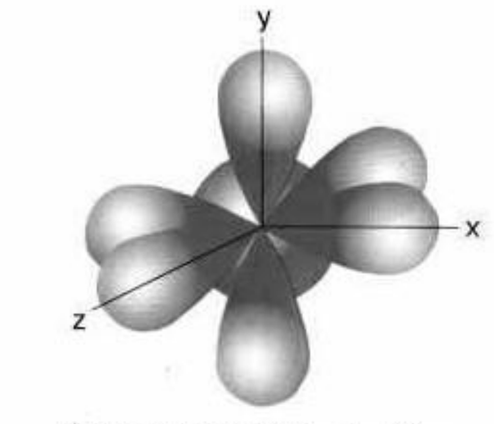
Three sp^2-hybrid boron orbitals lie in the same plane at an angle of 120° [2].

Here we see that one s-electron splits into three parts to bind (hybridize) with two p-electrons. Again, the formation of a semi-electronic intermediate form occurs, which contradicts the existing canons. In this case, the formation of elongated shapes occurs in the resulting hybrid orbitals, which in turn leads to the formation of two ends of different energies. One of these ends is closer to the nucleus, and the other is farther away. It is not consistent with the claim that all hybrid clouds are equal.

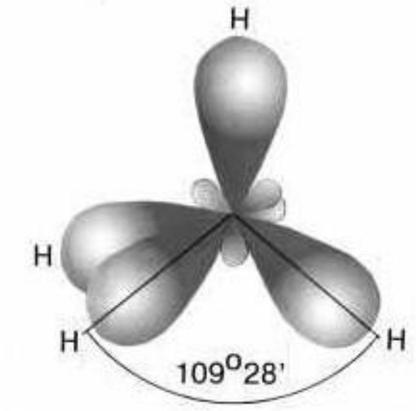
Finally, when one s- and three p-orbitals are mixed, sp^3-hybridized molecules with a tetrahedral geometry appear. An example is the CH4 methane molecule.







$(s+p_x+p_y+p_z)$-Clouds of the Carbon atom in excited condition



four sp^3-hybrid cloud of CH_4 molecules

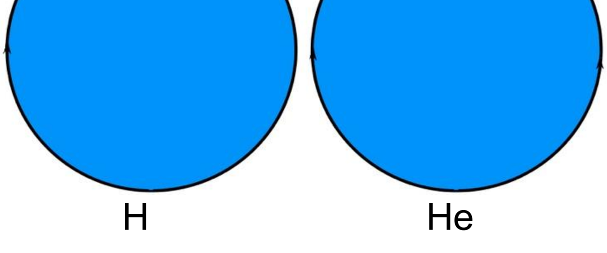
Four sp^3-hybrid carbon orbitals point to the vertices of a regular tetrahedron. The carbon atom is at the center of the tetrahedron. The angles between all bonds are equal and amount to 109°28' [2].

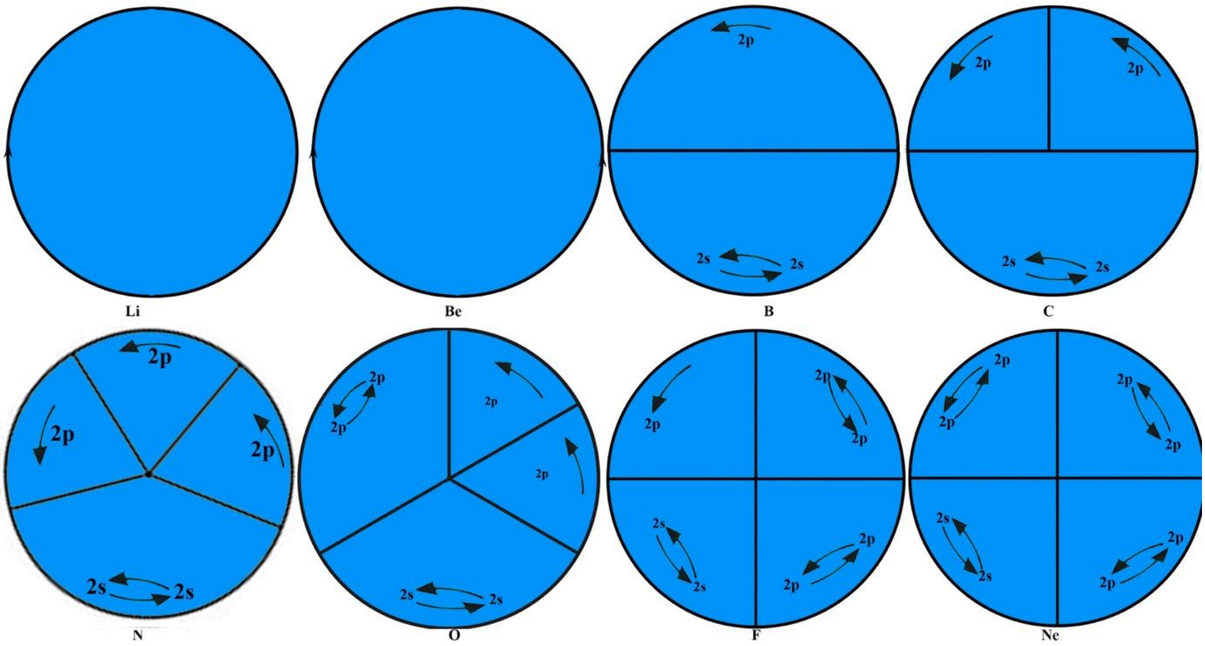
And again, the division of the s-electron, but already into four parts. Again, the location of the beginning and end of hybrid clouds at a different distance from the core. All this leads to the fact that the statement of the equivalence of hybrid clouds is controversial.

Based on the above data, we see that there are still ambiguities in explaining the nature of the chemical bond. The hybridization theory operates with most relativity when explaining the formation of a chemical bond, which includes such concepts as π-bond, hybridization, separation of electrons into species. Therefore, the following **theory of the transformation of electron clouds (TEC)** is proposed. The theory consists of five postulates:

1. An electron has a single charge, the momentum of which has a wave function of an electromagnetic cloud moving in free space of atom (spherical, hemispherical, or multisectorial spherical shape), electrons are located in the orbital singly or in pairs in the cells into which the orbital is divided, but on one orbit of the cell is not can be arranged throughout the layers, have various shapes (for example, dumbbell-shaped).
2. The electron orbitals are filled according to the Pauli principle, while the maximum number of cells in the orbital to fill is equal to half the maximum number of electrons according to the Pauli principle.
3. Electrons of one orbital tend to fill the entire orbital, uniformly distributing the space of the spherical orbital according to the principle of minimum total energy.
4. During the formation of a chemical bond of elements with variable valencies, the transformation of electron clouds occurs. All valence spherical electron clouds participating in the chemical reaction are transformed by forming a shape and quantity corresponding to the valence value.
5. The chemical bond has a single character and is not divided into σ - and π - bonds.

According to the proposed theory, the electronic structure of the last layer of elements of the first and second periods will look as follows.





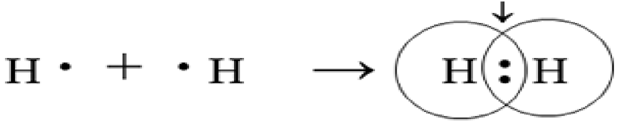
As can be seen from the above diagrams of the structure of the valence layer of the elements of the first and second periods, the electrons in the orbital occupy the entire space of the orbital. In hydrogen, the orbital is filled with one electron cloud, and in the helium atom, the orbital is filled with an electron cloud of a pair of electrons.

During the transition to the second period, for lithium and beryllium, the electronic structure of hydrogen and helium is repeated, but it must be kept in mind that for these atoms during this period, the possibility of forming cells for the arrangement of electrons is up to four. We can observe such a division of the cells for the boron valence layer, and here two cells are formed, each occupying half of the sphere. One cell contains an electron pair of s electrons, and the other half contains an unpaired p electron. In a carbon atom, two unpaired p electrons are located on two cells and a paired s electron pair on half of the sphere; as a result, the orbital in the carbon atom is divided into three parts. In the nitrogen atom, the orbital and the carbon atom are divided into four parts, but unlike carbon, the nitrogen atom has an unallocated electron pair of s-electrons. This pair leads to a greater repulsion of the remaining p-electrons, as a result of which the orbital is not divided into equal four parts. The bond angle between electrons is about 107°. Furthermore, in the oxygen atom, the orbital is also divided into four cells, but unlike the previous atoms, there is an unallocated electron pair of s- and p-electrons, the mutual repulsion of which decreases the bond angle. In the case of water, it is equal to 104.3°.

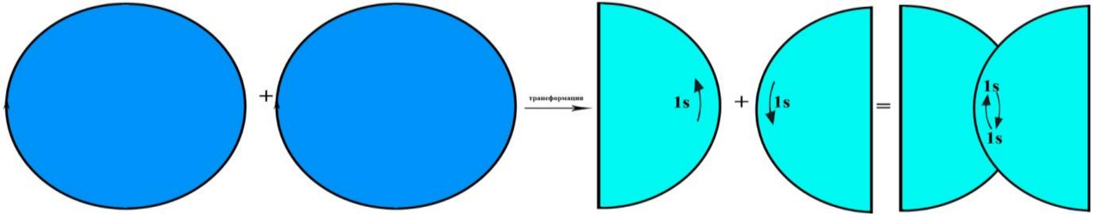
Let us consider the formation of various molecules based on the theory of the transformation of electron clouds.

Let us start with the simplest hydrogen molecule:

In the classical style, the formation of a hydrogen molecule is as follows:



We propose the following scheme for the formation of a hydrogen molecule:



When a chemical bond is formed, two spherical electron clouds of hydrogen atoms transform and forming a hemisphere and, under this condition, form an electron pair. According to experimental data, the radius of the electron cloud of the hydrogen atom is 0.53 Å, and the radius of the electron cloud of the hydrogen molecule is 0.74 Å. It was necessary to introduce correction coefficients into the equations of quantum chemical calculations to explain these values under the classical method since if there is an overlap of two-electron clouds of a spherical shape, the radius value would be close to 0.106 Å (the sum of the radii of two-electron clouds) [3]. However, as we can see, a decrease of 0.32 Å is observed here, and this is in good agreement with the proposed theory, where the radius of the electron cloud of molecular hydrogen is no longer the sum of the electron clouds of two hydrogen atoms but has the value of the sum of the radii of the two hemispheres plus the intercloud distance.

As we can see from the above facts, the proposed theory better reflects the formation of a hydrogen molecule and even helps to explain some phenomena that classical theories have not explained.

Now let us talk about the hybridization of electron clouds in the formation of connections. As shown above, during hybridization, electrons of various forms and orbitals are displaced, and a single cloud of a transitional form is formed, which will react with the second element as a whole.

Furthermore, now we will try to explain the formation of compounds based on the proposed theory without using hybridization.

Let us start with beryllium chloride. Here, in the reaction of beryllium with chlorine, a transition of the beryllium atom to an excited state occurs, in which one s-electron of beryllium is transferred to the 2p-orbital and is transformed into two hemispherical orbitals, i.e., the 2s2 spherical orbital transforms into 2s1 and 2p1 hemispherical orbitals and completely separates the space between themselves, being located at an angle of 180 ° to each other and form two valence electron clouds.

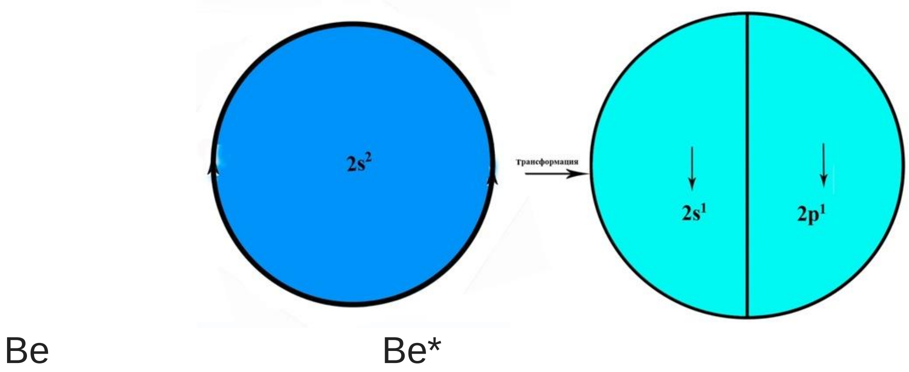


Fig. 1. Transformation of 2s2 electrons of beryllium into $2s^1$ and $2p^1$

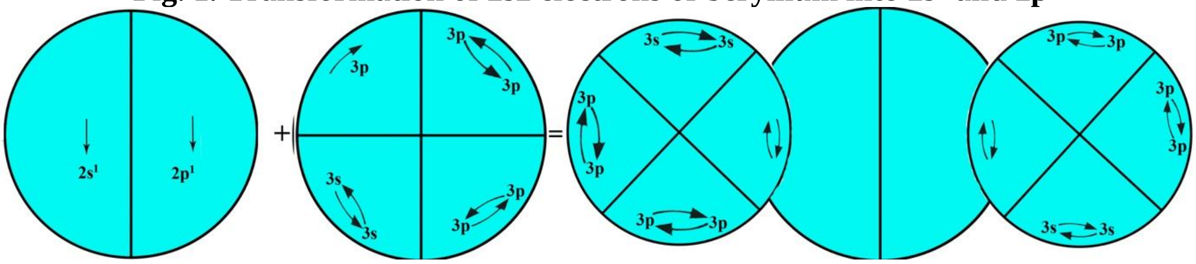


Fig. 2. Formation of a beryllium chloride molecule

Thus, a beryllium chloride molecule with two identical bonds is formed.

When boron salts are formed, two electrons form an electron pair, and one electron is in an unpaired state; under the action of the electrons of another atom, electrons are transformed, with each electron occupying 1/3 of the sphere and located at an angle of 120°, which ensures the equidistance of electrons from each other and the formation of a bond between the electrons of the reacting atom:

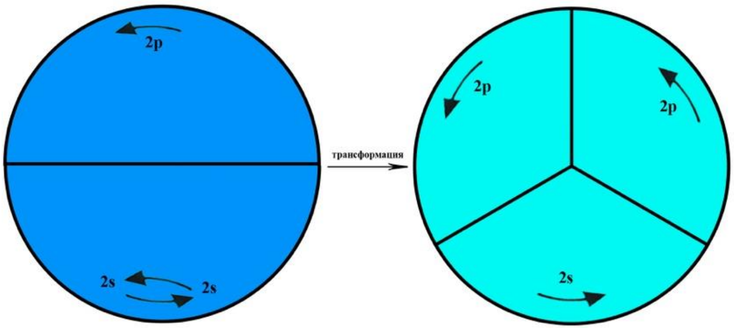


Fig. 3. Transformation of electrons in a boron atom

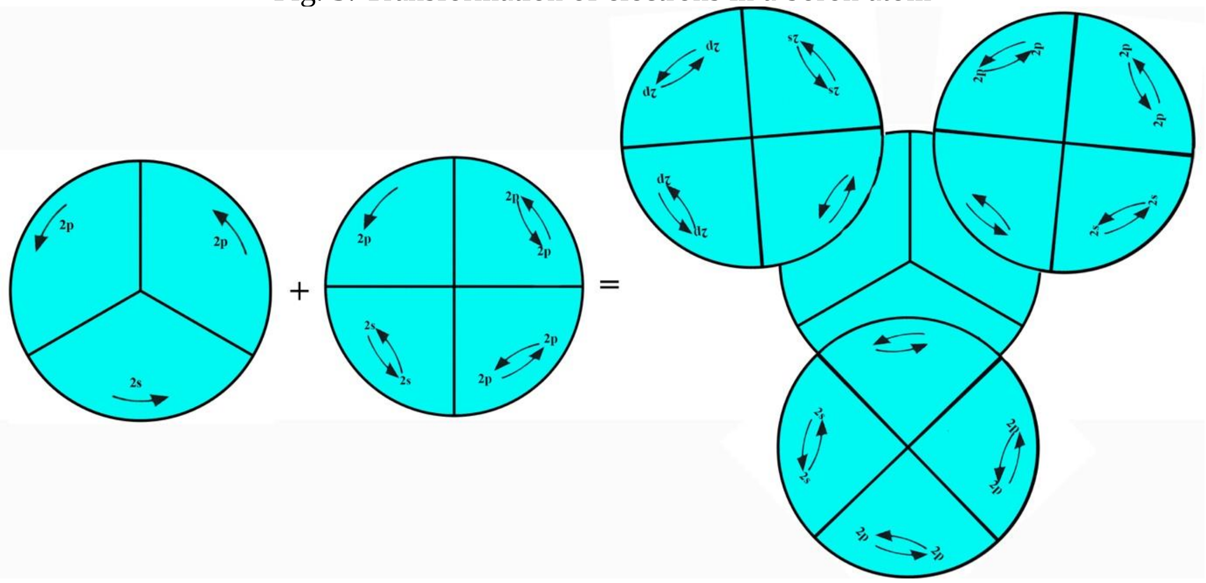
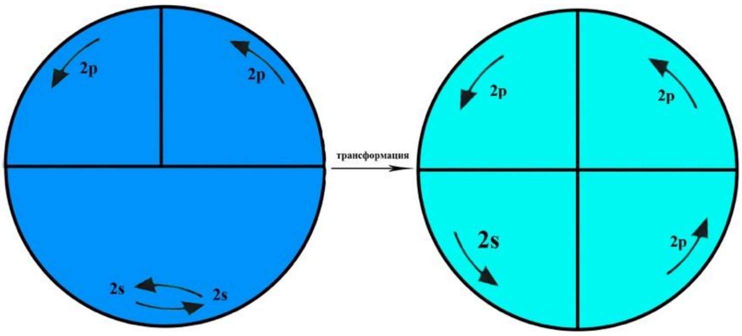


Fig. 4. Formation of a boron fluoride molecule

All four electrons of the second orbital participate in carbon compounds, while the orbital sphere is divided into three parts; in one part, which occupies half of the sphere, two paired s electrons are located, the remaining half of the sphere, in turn, is also divided into two parts, in which one is located p electron.

The impact on a carbon atom of some energy during the interaction of another atom leads to the transformation of electron clouds. In this case, as a result of the transformation, the orbital sphere is divided into four parts, which are located in relation to each other in space at an angle of 109o28 '. On these parts of the sphere, one s and three p electrons are located and form a tetrahedral structure, in which the electrons will be equidistant from each other.



Tetrahedron

Fig. 5. Transformation of electrons in a carbon atom

A reasonable question arises how to explain the formation of a π-bond in molecules of unsaturated hydrocarbons. In fact, according to the proposed theory, there is no π-bond. Two electrons form a bond between carbon atoms; since the bond is equivalent, the excess energy of the double bond arises, which leads to the breaking of the double bond. It should be said here that the two bonds formed by carbon atoms are the same, i.e., there is no concept of σ- and π-bond.

Therefore, any of the two bonds can participate in the addition reactions. Why did the idea of the inequality of bonds in a double bond arise? The point is that the researcher sees only the initial and final state. When interacting with other substances, any of the two bonds can enter into a reaction, but after the formation of a new bond, the energy of the remaining bond between the carbon atoms increases, and the researcher has the feeling that one of the bonds has always been stronger than the second. Both bonds are equivalent and have the same energy.

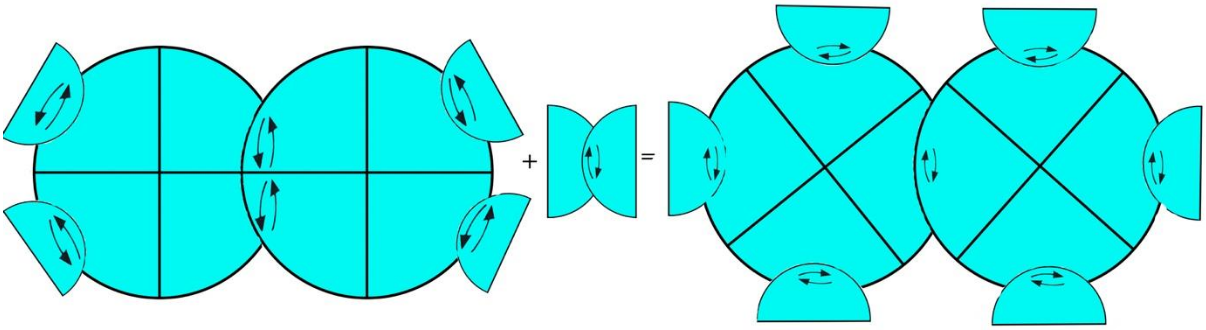


Fig. 6. The reaction of ethylene with hydrogen to form ethane

The use of the proposed theory of transformation of electron clouds easily explains the structure of the benzene molecule and the equivalence of carbon atoms without the use of a migrating double bond:

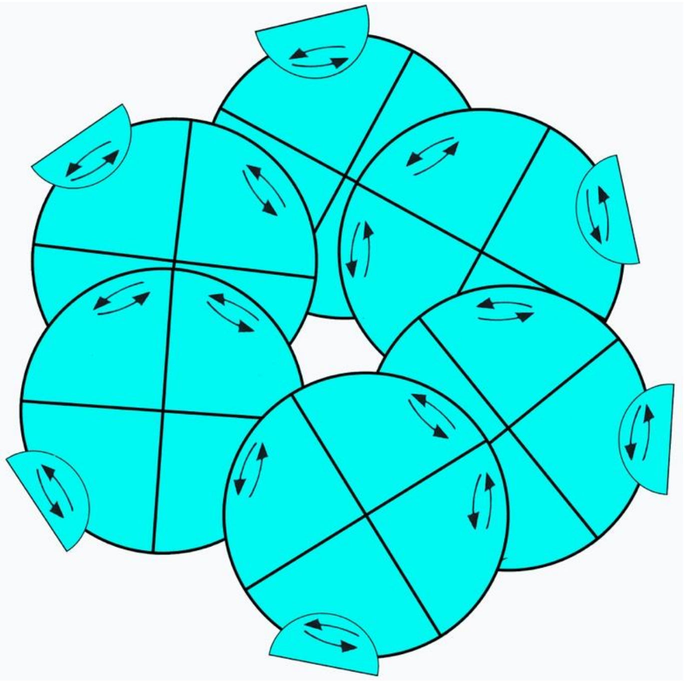


Fig. 7. The structure of the benzene molecule according to the theory of the TEC

As we can see from the proposed structure, each carbon atom has a pair bond with another carbon atom, and as in the case of ethylene, excess energy accumulates, which leads to an increase in the reactivity of such a bond. As a result, all carbon atoms can undergo an addition reaction.

As can be seen from the above examples, the proposed theory of the transformation of electron clouds thoroughly explains even some problematic issues, such as a local minimum in the formation of a hydrogen molecule, the equivalence of all carbon atoms in a benzene molecule.

Now consider the molecules, which have been used to explain the hybridization of the additive "type."

For example, the structure of ammonia was explained by the fact that the unallocated nitrogen pair in ammonia would be considered one bond, and thus a hybridization compound of the type - sp3 would be formed. However, based on the proposed theory, one can forget ***about terms like hybridization and, in general, about hybridization.*** When an ammonia molecule is formed, the unallocated electron pair of nitrogen repels p-electrons from itself, and, as a result, the bond angle will not be 90 °, but a little more, 107.3°.

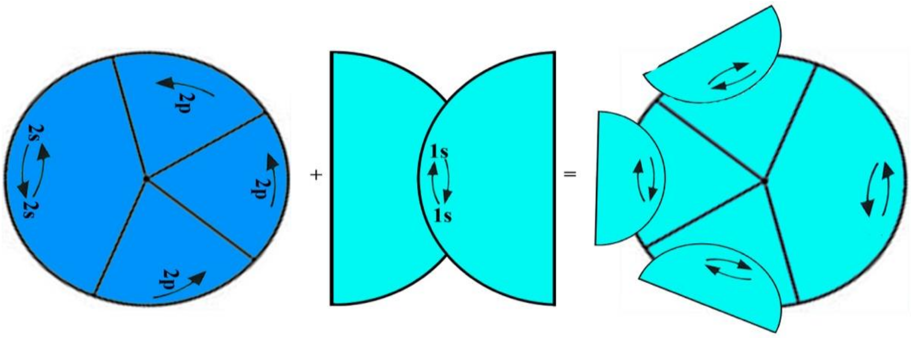


Fig. 8. The electronic circuit of ammonia molecule formation

Also, in a water molecule, one should not assume that two unallocated oxygen pairs will act as a pseudosigma bond, thereby forming sp3 hybridization. Indeed, if we assume that in all compounds where the central atom forms four sigma bonds or sp3-hybridization, the bond angle will have a different value each time.

Therefore, proceeding from the theory of transformation of electron clouds, we will talk about the bond angle without hybridization (there is no need for hybridization). In the oxygen atom, the unallocated electron pair of s-electrons and p-electrons mutually repel, but unlike the nitrogen atom, here two s-electrons are opposed by four p-electrons, and 2 of them form a pair, as a result of repulsion by s-electrons of p-electrons leads to less expansion of the bond angle. Furthermore, as the experimental results show, the bond angle of water is 104.27° and less than the bond angle of ammonia.

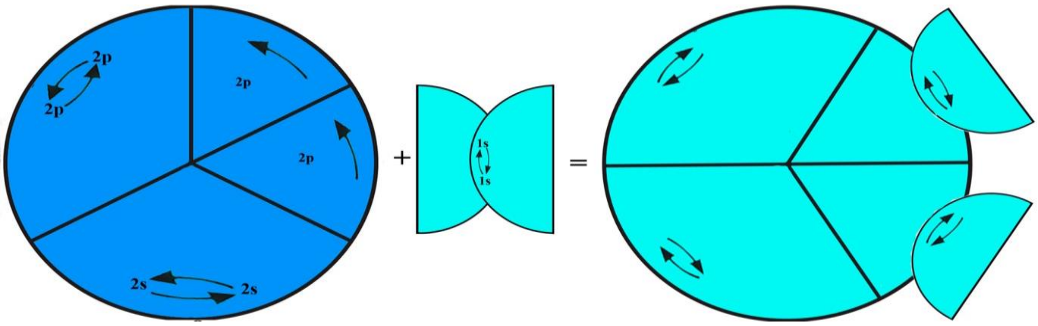
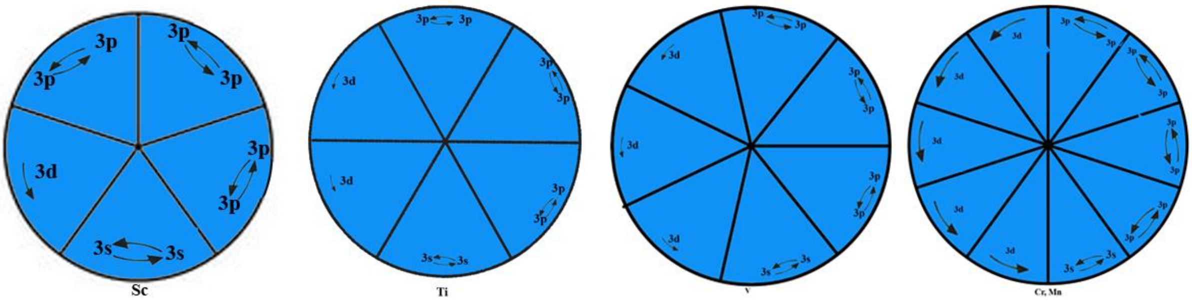


Fig. 9. The electronic circuit of water formation

As can be seen from the above data, the proposed theory of the transformation of electron clouds makes it much easier to describe the process of the formation of a chemical bond, while there is no need for crossing electrons of different types. At the same time, within the framework of the theory of the transformation of electron clouds, we have explained some points that the existing theories could not explain and attributed to special cases.

We examined the structure of the valence shells of the elements of the first and second periods. What happens when the so-called d-electrons appear? Absolutely nothing. Additional cells appear on the shell, on which these electrons begin to be located, like s and p electrons.



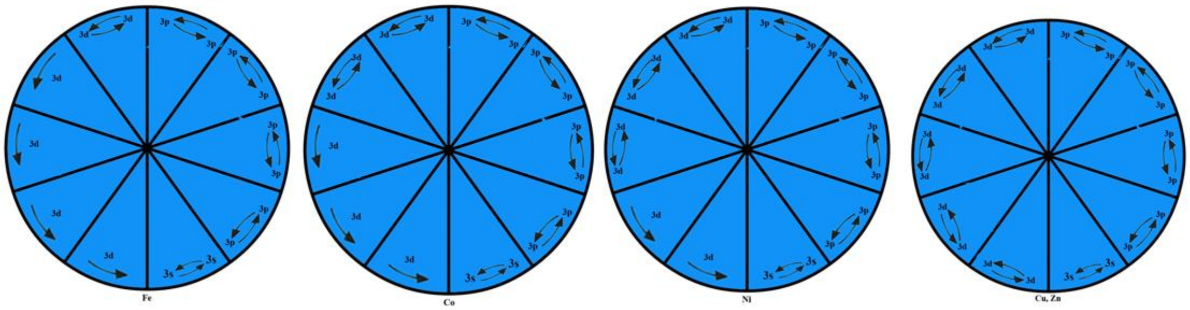
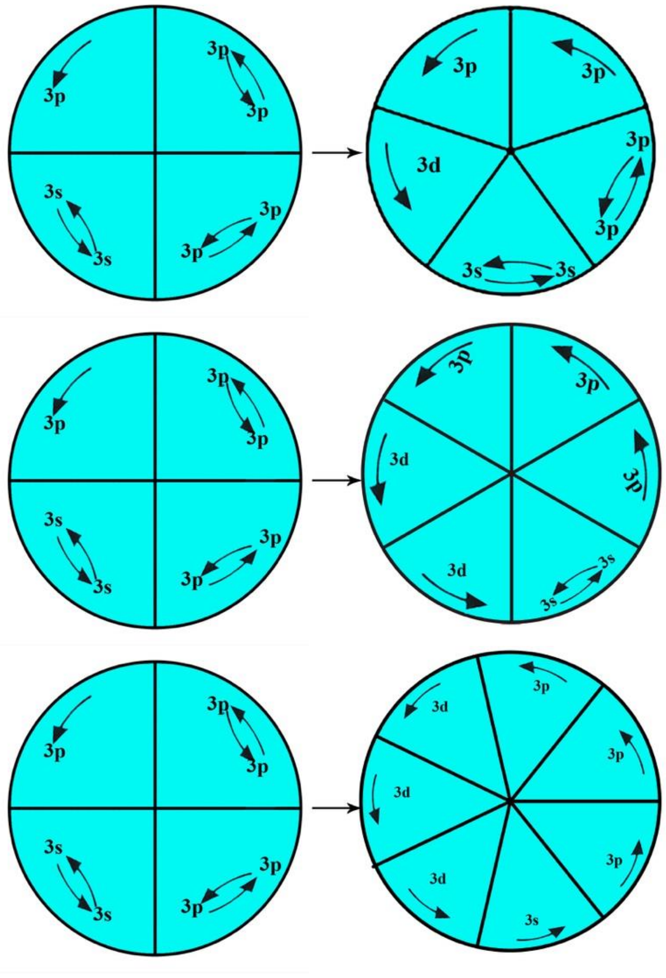


Fig. 10. The structure of the valence layer of 4-period elements

Thus, according to the second postulate of the **theory of the TEC**, the number of cells in the third orbital is, at most, equal to half of the maximum number of electrons according to the Pauli principle, and electrons uniformly occupy it as they appear in the atom of the element.

As we know, some elements exhibit variable valence, which is associated with the transition of the element to an excited state. Let us consider, using the example of a chlorine atom, its transition to an excited state. Chlorine is in the third period of the periodic system of chemical elements of D.I. Mendeleev and has three orbitals that can be filled with electrons. According to the Pauli principle, the maximum number of electrons in the third orbital can be equal to $2x3^2 = 18$, according to the second postulate of the theory of TEC, the maximum number of cells in the third orbital is equal to half of the maximum number of electrons, i.e., $18/2 = 9$. At rest (normal state), the third orbital of chlorine is divided into four cells in which there are three pairs and one unpaired electron.



During the transition to the excited state, the electron pairs are depairing, and the transition of unpaired electrons with the formation of new cells in the third orbital. As a result of the gradual evaporation of electron pairs, chlorine can exhibit valencies equal to 1, 3, 5, and 7.

Conclusion. Based on the above data, the following conclusions can be drawn:

1. The currently existing theories about the structure of electron orbitals and the nature of the formation of a chemical bond do not fully describe all cases, and with the development of chemistry, more and more special cases and exceptions from these theories appear.

2. The proposed theory of transformation of electronic orbitals fully describes the structure of electronic orbitals of chemical elements and reveals the nature of chemical bonds. At the same time, it brings clarity to many phenomena for which there was no explanation in existing theories.

3. On the basis of the proposed theory, the theory of hybridization is completely refuted, and the possibility of explaining the equivalence of chemical bonds formed by two atoms without the formation of hybrid clouds is proved.

4. On the example of the structure of ethylene and benzene molecules, the same nature of all bonds between carbon atoms and the illogicality of separation of chemical bonds into σ- and π-bonds have been proved.

5. Explained the transition of elements into an excited state with the manifestation of variable valence using the theory of transformation of electron orbitals.

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ЎЗБЕКИСТОН РЕСПУБЛИКАСИ ФАНЛАР АКАДЕМИЯСИ МИНТАҚАВИЙ БЎЛИМИ
ХОРАЗМ МАЪМУН АКАДЕМИЯСИ

ХОРАЗМ МАЪМУН АКАДЕМИЯСИ АХБОРОТНОМАСИ

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