

Demystifying and Clarifying the Concept of the Resonance Rules, Valence, Chemical Structure, Chemical Reactions, and Catalysis. Gankin, Yuriy V.; Gankin, Victor Y. Institute of Theoretical Chemistry, Shrewsbury, MA, USA. Abstracts of Papers, 222nd ACS National Meeting, Chicago, IL, USA, August 26-30, 2001 (2001), CHED-407.. Publisher: American Chemical Society, Washington, D.C. CODEN: 69BUZP Conference; Meeting Abstract written in English. AN 2001: 637905 CALPUS (Copyright 2002 ACS).

MOLECULE STRUCTURE

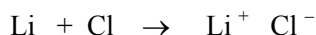
After the discovery of atom structure, scientists were confronted with the question: How do atoms bond into molecules? Other supplementary questions were: 1) How do bonds form between atoms? 2) Why is there a limit to the number of atoms that a given atom can bond?

Most welcomed by chemistry teachers, in this respect, were the Lewis Rules. According to Lewis, atoms form chemical bonds as a result of the loss, connection, or unification of such a number of electrons which can lead to the completion of the electronic configuration of inert (noble) gas atoms.

In 1916 Lewis offered a schematic description of chemical bonds in chemical compounds with the help of formulas where the valent electrons (those in the outermost shell of the atoms) are illustrated by one or two dots next to or around the symbol of the chemical element. Thus, for example, electronic atoms of the second period were shown as follows:



Bond formation at the expense of the loss or gain of an electron (as indicated in the Lewis Rules) can be described as follows:



After the shift of the electron to the chlorine, the previous electronic shell with two electrons becomes the outermost shell of the lithium. The outermost shell (the only one) of the helium atom (He) which precedes lithium in the Table of Elements, also contains two electrons.

As a result of bonding an electron to a chlorine atom, we get an electronic configuration of argon.

The formation of a chemical bond at the expense of unifying electrons, according to Lewis, can be described via the example of a chlorine molecule



The Lewis Rules allow to foretell the valence of atoms in compounds since the valence, according to the Lewis Rules, is defined

by the correlation of the atoms in the compounds where the atoms get their inert gas configuration.

The further development of the Lewis Theory presupposed the answer to the following question:

Why do atoms strive to build up their electronic shells to those of the inert gases?

Lewis's initial formulation stated: *In the course of chemical bond formation, the atoms strive to build up their shells up to the shells of the inert gases.* It is obvious that this formulation had an anthrop-physical essence.

Later on in textbooks this formulation was somewhat softened: *One gets the impression that the atoms are attempting to gain....* In other variants: *As a result of bond formation, the atoms get stable or closed electronic shells.*

From the physical viewpoint such formulations were also meaningless, but unlike Lewis's incorrect explanations, which gave rise to the question: *Why is it that the atoms strive to build up their shells to those of inert gases?* these formulations caused an illusion to the effect that somebody actually knows that these shells are stable. This somewhat lessened the tension of the question-of-the-day but indirectly slowed down the development of the theory of chemical bonding.

Besides this main shortcoming of Lewis's bonding theory, there was another one: the presence of ever so many exclusions to the Lewis Rules. For example, on the one hand, out of 16 elements of the second and third periods, 4 elements (Be, B, Mg, Al) formed stable molecules of the BCl_3 , AlCl_3 type where the outermost shells of the above shown atoms contained fewer than 8 electrons. On the other hand, 3 elements (P, S, Cl) formed stable molecules like PCl_5 , SCl_6 , ClF_3 . The number of electrons in the outermost shells of the indicated atoms (P, S, Cl) greatly exceeded 8. That is, about half of the elements (7 out of 16) actually formed stable molecules, which were exclusions from the Lewis Rules.

There were efforts made to explain the exclusions from the Lewis Rules via the Valence Bond Theory and the Theory of Molecular Orbitals.

The Valence Bond Theory (VBT) presupposes that: 1) Only non-paired electrons take part in chemical bond formation – during bond formation electrons from various atoms are paired; 2) The chemical bond is formed at the expense of closing (overlapping) the atoms' orbitals and pairing electrons with various spins.

The Theory of Molecular Orbitals (TMO) presupposed that the electrons in molecules are situated on molecular orbitals (MO) that are lineal combinations of atomic orbitals. There are bonding and antibonding MOs.

These theories did not help to understand the nature of chemical bonding and undoubtedly represented pseudo-scientific descriptions of experiments. The explanations of dependencies and ??? bonding energy values defined experimentally in the framework of these theories, as further studies have shown, were based upon the unlimited adjustment possibilities of these theories.

Thus, for example, according to calculations, the bonding energy in molecules H_2^+ and H_2 differed, as compared with the experimental

data, by less than 0.1% and comprised 260 and 432 kJ/mol respectively. It is now proven that experimentally defined bonding energy values in H_2^+ and H_2 were erroneously inflated for H_2 by two times, and for H_2^+ — by more than five times.

According to the TMO, the FIPs of metal atoms, in group I of the table of elements, should be lower than the FIPs of dual-atomic molecules, formed of the same metals. Both outermost electrons of these metals are situated, according to the TMO, on the bonding orbitals. However, the FIPs of all the metals in group I, according to the experiment, are greater than the FIPs in the molecules formed out of them. Thus, for example, the FIPs for Li, Na, K, comprise 5.39 eV, 5.138 eV, and 4.339 eV respectively while the FIPs for Li_2 , Na_2 , and K_2 comprise 5.11 eV, 4.87 eV, and 4.06 eV respectively.

These experimental data, received after the theory was approved, not only do not coincide with the theory – they actually contradict its main precepts! The dual-electronic bonding energy in molecules Li_2 , Na_2 , and K_2 comprise 1.00 eV, 0.70 eV, and 0.47 eV respectively, while the single-electronic bonding energy in molecules Li_2^+ , Na_2^+ and K_2^+ comprise 1.04 eV, 0.97 eV, and 0.70 eV respectively, which also contradicts the TMO. The disillusionment in these theories that occurred in the 1980s can be explained not only and not so much by the appearance of the above mentioned experimental material, but first of all it can be explained by the impossibility of making use of these theories for the explanation of chemical phenomena in high schools and colleges. This is because such explanations violate the golden rule of education: *New material should be introduced only on the basis of the knowledge previously gained by the student.*

In general, at the beginning of the 1980s, under the influence of such factors as the exposure of the incorrectness of the main precepts of the theory of chemical bonding (Theory of Valence Bonding and the TMO), the misinterpretations in the quantum-chemical explanations were given in detail in articles written by J. Ogilvie.

“Like the legendary emperor who displayed his newest suit of a material so fine as to be invisible, the authors and professors (teachers) who naively parrot these old mistruths succeed only in exposing their ignorance. What I have tried to undertake in this essay is to present a reason for the alteration of our thinking about the teaching of chemistry away from atoms and orbitals. In this endeavor I share similar concerns with Bent [74, 75] and others who have expressed their dissatisfaction with the traditional approach, but I have attempted to demonstrate the fallacious foundations of this approach. 'Quantum chemistry' or the quantitative and mathematical quantum-mechanical theory applied to molecular structure and properties is unnecessary and irrelevant in the general undergraduate curriculum in chemistry, at least in the compulsory component.

The qualitative explanations ('hand waving') of molecular structure and reactions based on orbitals and such ilk are not science (i. e. are nonsense) and should consequently be entirely discarded. The effort of chemists should, instead, be expended to demonstrate the myriad chemical substances and properties of real matter that makes chemistry the science of materials as well as molecules – the central science of our

present world (J.F. Ogilvie *Conceptual Trends in Quantum Chemistry*, 171-198. 1994 Kluwer Academic Publishers. Printed in the Netherlands)

THE NATURE OF THE CHEMICAL BOND 1993

There are no such things as orbitals J. F. Ogilvie

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...The important conclusion from this brief outline of a computational procedure is that, although one may start the calculation with a basic set of orbitals, the simple solutions of Schrodinger's equation for the one-electron atom, by the time that one attains the Hartree-Fock limit, or beyond, the nature of the initially chosen one-electron functions is irrelevant. Thus only at the beginning of the calculation, and even then only in a mathematical sense (within the context of a particular computational method), do the orbitals have any meaning.

A novel approach to the equations of Dirac, Hartree, and Fock with the use of a finite. basis set was claimed [21] to be suitable for both atomic and molecular calculations with no problems of spurious roots, variational collapse or continuum that h.- plagued the conventional Dirac equation for applications to systems with many electrons; this development would permit in principle the calculation of atomic and molecular properties that suffer from the (self-imposed) tyranny of Schrodinger's equation, but during the several years this claim was announced little or no further progress has been reported. **Thus the philosopher's stone for calculation of atomic and molecular structure, is, so far, as elusive as its literal precursor to make gold from base metal.**

Therefore the structure of methane ... is a regular tetrahedron"; in a later edition [29], the question "Why is CH₄ tetrahedral?" once again evokes an answer by reference to orbitals and hybridization, although the causal relationship is less succinctly stated. Gillespie [30] quoted an instance of a textbook of general chemistry in which the author wrote that the structure of methane is tetrahedral because of sp³ hybridization, and a few pages later that the hybridization is known to be sp³ because the structure is tetrahedral a completely and explicitly circular argument! Is the argument of Atkins [29] less circular because it is implicit?

We quote again from Coulson's Valence [28b]: "It would be quite wrong to say that, for example, CH₄ was tetrahedral because the carbon atom was sp³ hybridised. The equilibrium geometry of a molecule depends on energy and energy only..."

Coulson's Valence [28c], "... orbitals do not exist! They are artifacts of a particular theory, based on a model of independent particles. i. e. based on non-repelling electrons, For this reason also we refrain from interpreting photoelectron spectra as involving the ionization of electrons from (or even associated with) particular molecular orbitals, despite the widespread practice of this fallacy (for instance 5, 34). **The classification of electrons as bonding, nonbonding or antibonding is similarly erroneous because electrons are fundamentally indistinguishable**

Why has CH₄ a tetrahedral structure? Why does our solar system contain about nine planets? These are theological questions, thus extra-scientific. In the middle ages in Europe, learned philosophers (or theologians) are alleged to have debated how many angels could dance on the head of a pin; at a conference I have heard famous chemists disputing whether a certain effect in a transition-metal compound was due more to "pi donation" or to "back donation into d orbitals". In 1723 Jonathan Swift chronicled a voyage of one Lemuel Gulliver to Balnibarbi in which he observed speculative research on diverse topics; in the past sixty years, innumerable chemists have attributed chemical and physical phenomena of all kinds to [nonexistent] orbitals. Is the progress of man's thinking an illusion?

Chemistry is not only a science of molecules, but also a science of materials. Chemistry remains the only basic science to constitute the foundation of a major industry. Chemistry owes its importance in the modern community to its materials, not to its i-molecules. **All the space devoted to orbitals, the aufbau principle, hybridization, resonance, sigma and pi bonds, electro-negativity, hyper-conjugation, HOMO, LUMO, inductive and mesomeric effects and the like excess baggage that burdens the textbooks of general, inorganic, organic and (even, if to a lesser extent) physical chemistry, and the corresponding proportion of the curriculum and duration of lecture and tutorial classes, detracts from more instructive and accurate content about chemical reactions, chemical substances, and mixtures as materials.** The conspiracy interpretation' of quantum mechanics to which Condon (9b) referred has its analogue currently in the infatuation of many academic chemists with orbitals. **The authors of textbooks clearly perpetrate myths such as that the structure of methane is tetrahedral because of sp³ hybridization, and similar fallacies not because they understand quantum mechanics. The readers of these textbooks, be they professors or students, duly perpetuate the same fictions because they apparently constitute the current paradigm in chemistry.**

*"Perhaps the mood was best stunned up by Bergen Davis (1869-1958) who commented on quantum mechanics in the spring of 1928 that, 'I don't think you young [physicists] understand it any better than I do, but you all stick together and say the same thing.' This has been called the conspiracy interpretation of quantum mechanics. " [9b]

A correspondent has stated that he "prefers a universe [in which] science can attempt to answer the big question 'WHY'?" For many chemists the answer to the question "why does some phenomenon occur?" is "because of orbitals", which is equivalent to "because of Schrodinger's equation". According to this approach the further question "Why Schrodinger's equation?" although logical, is ignored because this problem lies clearly outside the province of chemical competence. If Schrodinger had devoted all his energies to his other pursuits, then the Schrodinger's equation might never have appeared. Would chemistry or physics have been the poorer? We should still have matrix mechanics that preceded the discovery of wave mechanics; because in principle the two calculation methods are entirely equivalent, algorithms to implement calculations of electronic structure would presumably have been developed in terms of matrices, in which case they might have been readily adaptable for efficient execution on current computers with vector processors. One might imagine the content of textbooks of general chemistry under these hypothetical circumstances. Whether an alternative explanation [85] of the chemical bond in terms of entropy of the electrons is useful or valid remains to be proved.

[85] Gankin, V. V. and Gankin, Y. V. (1991) "The New Theory of Chemical Bonding and Chemical Kinetics", ASTA, St. Petersburg, Russia.

Pauling wrote in *The Consequent Implications for Chemical Education*:

"The concept of the chemical bond is the most valuable concept in chemistry. Its development over the past 150 years has been one of the greatest triumphs of the human intellect. I doubt that there is a chemist in the world who does not use it in his/her thinking. Much of modern science and technology has developed because of the existence of this concept.

"The truly great discoveries about the chemical bond were made by great chemists of the 19th century: Berzelius, Butlerov, Frankland, Couper, Kekule, Van't Hoff, and LeBel. G.N Lewis and Langmuir made significant contributions during the period of 1916 to 1920...

"I agree with Ogilvie that some things, especially molecular orbitals, should be left out, but in my opinion, the chemical concept of the chemical bond, together with its recent refinements, must be included in the course, together with a good bit of descriptive chemistry... During recent years, much more information about molecules and crystals and their reactions, both experimental and theoretical, has become available, but this information has not decreased the value of the concept of the chemical bond. I am pleased and gratified that in 1992 the chemical bond is alive and well."

A NEW THEORY

Unlike the above mentioned theories (the Lewis Theory, the Valence Bond Theory, and the Theory of Molecular Orbitals) the new theory is based on the ionization potential experimental data of various elements and on the comparison of this data with that of the elements' valences.

That is, this new theory is based on the experimental data of the ionization potentials in elements of the *second and third periods* in the table of elements and on the comparison of this data with the valence of these elements in reference to hydrogen (H) and chlorine (Cl) defined on the basis of the studies of the composition of stable molecules formed of elements of the above mentioned second and third periods.

[P.S. This material effects only the *second and third periods*.]

The data on the ionization potentials allows us to define the number of electrons situated in the outermost electronic shell (OES) of atoms. According to the received data, the number of electrons in the OES of these elements increases from 1 to 8 when moving along the table lengthwise along the periods from left to right.

The valence in reference to hydrogen and chlorine (i.e., the number of hydrogen or chlorine atoms that bond to the atoms of these elements) for the first 4 groups of elements in the table increases from 1 to 4 when moving along the table lengthwise along the periods from left to right, and then decreases from 4 to zero. That is, inert gasses (Ne, Ar) do not bond to either hydrogen or to chlorine.

When comparing this data with that of the number of electrons in the outermost shells of the atoms given above, we can conclude that for the first four element groups, the valence is equal to the number of electrons enclosed in the outermost shells of the atoms. That is, on the ground of this comparison, we can conclude that when bonding atoms with hydrogen and chlorine atoms – only one electron from each of the outermost atomic shells is used.

In the case of forming a chlorine molecule (Cl_2) out of two chlorine atoms, each of the chlorine atoms is simultaneously a *bonding atom* and an *atom to be bonded*. An identical situation is obvious during the formation of other molecules like: Na_2 ; F_2 ; etc.

These examples allow us to arrive at the following conclusion: Not only does one electron of the bonding atom take part in chemical bond formation, but one electron of the atom to be bonded takes part as well. That is, 2 electrons actually take part in chemical bond formation

However, if you apply this conclusion to elements of the last four groups, we will find a contradiction. For, according to experimental data, the number of electrons in the outermost shells of these elements increases from 5 to 8 as we move lengthwise along the periods from left to right, while the valence, in regard to hydrogen and chlorine does not increase but even decreases by one unit when shifting from one element to the next.

This paradox allows understanding the data on the ionization potentials (IP) of elements. The data on the IP have shown that the maximal number of electrons that can be contained in the outermost shell of these elements is equal to 8. After 8 electrons have been accumulated in the OES (say, Ne and Ar), a new OES starts forming.

According to the data on the IPs, inert gasses do not bond electrons to the existing outermost shells even when increasing the charge by one unit, that is, for example, during the transition from Ne to Na or from Ar to K.

A comparison of this data with that of the elements' valences in the last four groups leads us to the conclusion that during the formation of one bond, the number of electrons in the outermost shells of the atoms to be bonded is increased by one unit. Relatively, the number of bonds that the atoms of these groups can form, is limited by the maximal number of electrons which the outermost shell of the atoms can carry, that is, it is limited by 8 electrons.

Now let's review the above mentioned experimental data:

1) According to the studies conducted on the stable molecules formed of elements of the second and third periods, and hydrogen and chlorine atoms, it has been found that the number of hydrogen and chlorine atoms that bond to atoms of these elements (valence) is equal to the number of electrons situated in the outermost shells of these atoms as far as the first four groups are concerned.

2) For the next four groups in the second period (atoms N, O, F, Ne) the valence in hydrogen and chlorine comprises 3, 2, 1, and 0 relatively. According to the IP, these elements contain relatively 5, 6, 7, and 8 electrons; that is, the number of hydrogen and chlorine atoms which these atoms can bond, is equal to the difference between the figure 8 and the number of electrons located in their OESs. The valence of hydrogen and chlorine via hydrogen and chlorine, is equal to 1. Molecules H_2 , HCl, and Cl_2 are stable molecules.

A comparison of the data on the FIPs has shown that the maximal number of electrons that can be contained in the outermost shell of the atoms of the second and third periods, is equal to 8.

In accordance with point 1, a conclusion was made to the effect that only one electron in the outermost shell of the atom takes part in bond formation with a hydrogen or chlorine atom. In the case of molecule formation of the H_2 and Cl_2 type, both atoms entering the bonding process are equivalent. Respectively, two electrons take part in bond formation – one from each of the atoms to be bonded.

Experimental regularities described in point 2 lead us to the conclusion that in the course of bond formation both electrons (one from each of the atoms to be bonded) enter both outermost shells of the atoms to be bonded after bond formation. That is, during chemical bond

formation, the number of electrons in the outermost shells of the atoms to be bonded increases by 1 unit.

According to point 1, the valence via hydrogen and chlorine for the first 4 groups of elements of the second and third periods is limited by the number of electrons in the outermost shells of the atoms of these elements. One electron is spent on the formation of one bond.

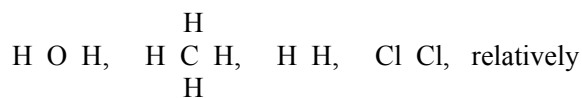
The maximal number of electrons that can enter the OESs of the atoms being bonded limits the valence via hydrogen and chlorine for elements of the last four groups. During the formation of one chemical bond, the number of electrons in the outermost shells of both atoms being bonded increases by one unit. The maximal number of electrons in the outermost shells of the atoms to be bonded of the elements of the second and third periods is never more than 8.

Negatively charged electrons in atoms rotate at a great speed around positively charged nuclei. The rapid rotation of the electrons keeps them from falling onto the positively charged nucleus.

During bond formation, the electrons partaking in such formation (further referred to as *bonding electrons*) enter the outermost shells of both atoms to be bonded. This conclusion allows us to introduce a scheme for chemical bonding according to which, in the case of a hydrogen molecule, the bonding pair of electrons rotates on a plane perpendicular to the axis connecting the hydrogen atoms' nuclei. The center of the electrons' rotation is situated at equal distances from the nuclei of the atoms to be bonded. It is only in this case that the electrons can *simultaneously* enter the OESs of both atoms to be bonded.

The given theory allows us to predict electronic formulas of compounds just as the Lewis Theory does. If, then, we make use of the Lewis designations, i.e., indicate the bonding pair with a colon (:) between the atoms, then the overwhelming majority of the stable molecules will be described by formulas built in accordance with the Lewis Rules.

Thus, for example, molecules of water (H₂O), methane (CH₄), hydrogen (H₂), and chlorine (Cl₂) are shown in the manner identical to the Lewis Rules:



Then, after all, why is the explanation of the new theory more progressive than the Lewis Rules?

Recall that the initial precept in the Lewis Rules was the *desire of the atoms to finish building up their outermost shells up to the shells of their nearest inert gas; in the case of elements of the second and third periods – up to 8 electronic shells*. This *desire* of the atoms was fulfilled in the case of covalent bonding at the expense of the unification of the electrons.

In the framework of the Lewis Rules, another problem arose: Why is it that the atoms strive to finish building their outermost shells up to the shells of the inert gases? As already indicated, all the efforts to explain this *desire* (before the new explanation came into being) were

actually reduced to the introduction of new words like *overlapping orbitals*, *bonding and antibonding orbitals* which have absolutely no experimental confirmation and are based on knowledge that neither student nor teacher ever understood (the ψ function, the Schrodinger equation and its solution).

The new approach shows, as a result of experimental data on the IPs of atoms, that the 8-electron outermost shells of the inert gases, which are characteristic for the central atoms of stable molecules of the CH_4 , H_2O , NH_3 type, are explained by the fact that the outermost shells of the elements' atoms of the second and third periods (in accordance with the experimental data on IPs) cannot contain more than 8 electrons.

That is, when there are already 8 electrons in the outermost shells, the atoms of the second and third periods cannot continue their chemical bond formation since, with the formation of each new chemical bond, the number of electrons in the outermost shells of the atoms being bonded increases by one unit. Therefore the 8-electron outermost shell of inert gasses is not at all a *desired target*, but is a condition limiting, from the top, the maximal number of bonds that the given atom can form.

A condition for limiting the number of bonds from the bottom for elements in the first 4 groups of elements is actually the number of electrons in the outermost shells of these atoms.

Thus, unlike the Lewis Rules, the formation of stable molecules of the AlCl_3 , BH_3 , BF_3 type, is no longer an exception of the rules, but is experimental data that confirms the main precepts of the theory.

The main 4 precepts of the Theory of Chemical Bonding are as follows:

I Experimental data have proven that two electrons take part in chemical bond formation – one from each of the atoms being bonded.

II After bond formation, the number of electrons in the outermost shells of the atoms being bonded increases by one unit.

III The maximal number of bonds that can be formed by atoms with elements of the second and third periods is equal to the number of electrons present in the outermost shells of these atoms – as far as the *first four groups* are concerned.

IV As far as the *last four groups* are concerned, the maximal number of bonds that can be formed by an atom with elements of the second and third periods in the table of elements is equal to the difference of 8 minus x , where x is the number of electrons situated in the outermost shell of the given atom.

Historically, chemical bonds, which were formed in accordance with these precepts, were called *covalent bonds*.

The model of a dual-atomic molecule, according to the above, is actually, in the case of a hydrogen molecule, two positively charged nuclei of hydrogen atoms (i.e., two protons) that are simultaneously attracted to the pair of bonding electrons rotating on a plane perpendicular to the axis connecting the nuclei.

If the atoms to be bonded are identical, the nuclei are at identical distances from the bonding electrons. If one of the atoms to be bonded happens to be attracted to the bonding electrons more readily than the other, then the nucleus of this atom is closer to the bonding electrons.

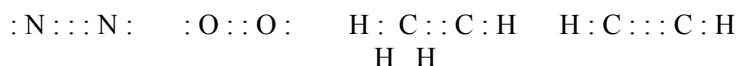
We can realize the attraction force of the nuclei to the bonding electrons by the FIPs. If the FIP of one of the atoms being bonded is greater than that of the other, then the nucleus of the atom with a higher digit is located closer to the bonding electrons than its counterpart.

Historically, in the course of the development of chemistry, chemical bonds formed of identical atoms (i.e., atoms with identical FIPs) are called *homopolar* bonds and those formed of variegated atoms (i.e., with different FIPs) are called *heteropolar* bonds.

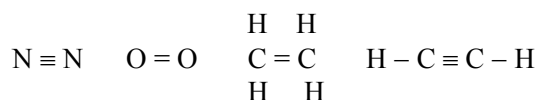
Examples of heteropolar covalent bonds are those between atoms in such molecules as NaCl and KCl. In these molecules the chlorine atoms are much closer to the bonding electrons (i.e., closer to the center of the rotating bonding electrons) than the sodium and potassium atoms.

According to the main precepts of the theory on covalent bond formation, it is possible to have 2, 3, and even 4 bonds formed between atoms with more than one electron in the OES.

It has been proven experimentally that stable molecules are widely known substances like nitrogen (N_2), oxygen (O_2), ethylene (H_2CCH_2), and acetylene (C_2H_2). The air we breathe is actually a mixture of nitrogen and oxygen. Industrial enterprises make wide use of ethylene and acetylene. The electronic formulas of these compounds can be represented thus:



The structural formulas of these molecules are illustrated as follows (each pair of bonding electrons is shown with one dash):



Each dash corresponds to a pair of electrons. The bond between nitrogen atoms (N) in a nitrogen molecule (N_2) is indicated by three dashes, i.e., by three simple bonds. Likewise, two simple bonds indicate a bond between the atom's oxygen in the oxygen molecule. The dual and triple bonds are known as *multiple covalent bonds*. A bond formed of one pair of electrons – like that between hydrogen and carbon in molecules of ethylene and acetylene – is regarded as a common covalent bond.

DONOR-ACCEPTOR BONDS (DABs)

According to the material of the previous section, bonds between atoms are formed at the expense of the attraction of the nuclei of the atoms to be bonded to the electron pair that rotates on a plane perpendicular to the axis connecting the nuclei with the said atoms.

In the case of covalent bond formation, the bonding pair of electrons is formed of electrons, which, before bond formation, used to belong to each of the atoms bonded by this bond. That is, each of the

atoms being bonded singles out one electron from its outermost shell for the formation of the bonding pair of electrons.

Since chemical bonding is conducted at the expense of the attraction of the nuclei to the bonding pair of electrons, we can suppose, in accordance with the bonding theory, that besides covalent bonding, there can also be a bond where both bonding electrons, before bond formation, used to belong to only one (not both) of the atoms being bonded.

In accordance with the bonding theory, the main regularities on covalent bond formation should be adhered to. It is worthwhile recalling once more exactly which regularities we should not violate when dealing with elements of the second and third periods.

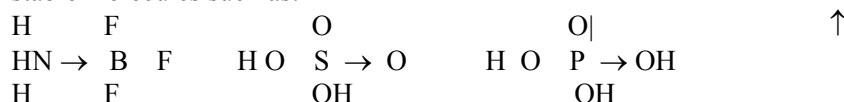
Just as in the case of covalent bonding, here we should suppose that after bond formation – both bonding electrons enter the OESs of the atoms to be bonded.

In the course of the development of chemistry, this bond received the name of *donor-acceptor bond (DAB)*.

Unlike covalent bonding, where the number of electrons in the outermost shells of the atoms to be bonded, increases during formation by one unit, during DAB formation the number of electrons in the outermost shell of one of the atoms (called *donor*) does not change, while the number of electrons in the shell of the other atom (called *acceptor*) increases by two units.

Respectively, the number of DABs that a donor atom can form is equal to the number of electron pairs present in its outermost shell. Only those atoms can be regarded as acceptors of electronic pairs whose outermost shells contain six or fewer electrons (of the second and third periods). Recall that after DAB formation, the number of electrons in the outermost shell of the acceptor atom increases by two units, while the maximal number of electrons in the outermost shell of the atoms of the second and third periods is equal to 8.

Experimentally, DAB formation is proven by the existence of stable molecules such as:



Here the dashes indicate covalent bonds; the arrows indicate DABs.



In all the indicated molecules the OESs of atoms N, B, F, Cl, and O contain 8 electrons. In sulfuric and phosphorous acids (H_2SO_4 and H_3PO_4) the bonds between hydroxyl and sulfur are covalent ones, while the bonds between sulfur and phosphor with oxygen are DABs. The number of electrons in the outermost shells of the oxygen, sulfur, and phosphor is equal to 8. Each covalent bond (—) and DAB (→) is equivalent to two electrons in the outermost shells of the atoms to be bonded with these bonds.

In compound H_3NBF_3 , the bond between nitrogen and hydrogen and between boron and fluorine are covalent bonds, while the bond between nitrogen and boron is a DAB.

This bond is made at the expense of a lone pair of nitric electrons. Analogously, in molecules formed of hydrogen, chlorine, and oxygen, the bonds between hydrogen and chlorine are covalent bonds and the bonds between chlorine and oxygen are DABs. Here both bonding electrons that cause this bonding, used to belong to the chlorine atom before bond formation.

It is of interest to generally compare the explanation concerning the physical nature of chemical bonding of the offered and the existing theories, and relatively make note of the changes in the accepted paradigms during the transition to the new explanation of the physical nature of chemical bonding.

In the framework of the Lewis Rules, the physical nature of the homoatomic covalent bond was not explained since the term *sharing of electrons* had no physical contents. The chemical nature of ionic bonding was explained as the attraction of oppositely charged ions formed as a result of the transition of an electron from one atom to another.

During the formation of a donor-acceptor bond, according to the accepted ideology, it was supposed that there was a transition of two electrons from the donor's atom to the acceptor atom, which defined the name of this type of bond.

In the case of polar bonds (say, NaCl) whose approximate calculation included the ionization energy of the first electron of atom Na , the affinity energy of atom Cl and the attraction energy of the ions Na^+ and Cl^- at a distance of the bond's length, offered an energy gain during bond formation which was equal to the experimental result. This is true because the ionization energy of two electrons, say, in sulfur atoms and those of phosphorus are 20 times greater than the energy. The affinity of the oxygen atom to the electron, the possibility of having a DAB between sulfur and phosphorus with oxygen was excluded, and it was supposed that here we have an exception to the Lewis Rules.

In the framework of the quantum-chemical explanations, it was supposed that the sulfur and phosphorus atoms were filled with **d** orbitals of sulfur and phosphorus in acids of the same elements. The same explanation was given when describing the structure of PF_5 and SF_6 .

However, these contradictory explanations are well known and included in the experimental data on the filling of the shells of the elements in the Table of Elements. When transiting from Ar to K , the next electron occurred not on the **3d** level, but on the **4s** level. The difference in the ionization potentials between Ar and K comprise about 10eV , that is, when the electron gets to the **3d** level, there is an energy gain about 10eV times greater than if it gets to the **4s** level. However, this did not happen. This is experimental proof of the absence of energetic desire in both sulfur and phosphorus to bond more than 8 electrons in the 3rd outermost shell.

In TMO bond formation was explained by the increase of the possibility of having electrons between atoms to be bonded as a result of the linear combination of atomic orbitals. Mathematically this idea was

'based' on the fact that the sum of $\psi_1^2 + \psi_2^2$ differs by $\pm 2\psi_1\psi_2$ as compared to $(\psi_1 + \psi_2)^2$. The possibility with a plus ($+2\psi_1\psi_2$) was called a *bonding orbital* while the possibility with a minus ($-2\psi_1\psi_2$) was called a *breaking orbital*.

The greatest possibility of finding electrons between atoms was explained in this theory by the fact that there was a greater energy gain.

The calculation of the molecule's energy is conducted in two stages. On the first stage the molecule's energy was calculated without considering the interaction of the bonding electrons, because the Schrodinger equation cannot be solved with this interaction. On the second stage coefficients were chosen for a simple algebraic equation, which, as expected, shows the energy of the electrons' interactions.

The criteria for choosing the coefficients was the coincidence of the molecule's energy value received in the two stages, and respectively, the bonding energy with its experimental value. This simple way of matching the calculation results with experimental results allowed to produce a calculated result that matched the experimental result first up to the 2nd digit, then up to the 4th, and finally, to the 6th digit after the comma (point), which convinced the chemists that this theory was correct. The physicists understood the methods used in calculations as possibilities for basing any suppositions. At times, in private conversations, they even referred to quantum chemistry as a "backyard theoretical chemistry."

On the other hand, the quantum chemists, who supported their idea of matching the calculated and experimental results, substantiated the participation of only the electric forces in the bonding of atoms, since they did not presuppose any other forces in the course of calculating the molecule's energy.

Thus, neither TBC nor TMO have added anything to Lewis's suppositions in reference to the above mentioned nature of chemical bonding.

All the three theories included additional suppositions (besides those, originally used when the theories were elaborated) that lacked physical sense, i.e., that lacked cause-and-effect relations. There is no bond between energies neither with sharing electrons nor with possibility (ψ^2) of their being between nuclei, because the increase of the possibility of finding them between the nuclei, on the one hand, increases their attraction to the nuclei, while on the other hand, there is an increase of interelectronic repulsion.

And besides, the physical essence of the ψ^2 function has nothing to do with the cause-and-effect connection in reference to the known essences, i.e., it is an additional, independent essence.

Unlike the cited theories, the new theory of chemical bonding, known as the *G Theory of Chemical Bonding*, does not introduce any new essences or additional suppositions that cannot be proven experimentally. All the theses that the theory includes arise out of chemical experiments, in part, from the comparison of multiply checked data on the structure of stable chemical compounds, and the data on the IP of atoms. Also, without any additional suppositions, in the framework

of the new theory, we have solved the question concerning the energy gain during bond formation.

In the course of algebraic calculations with a model, where only the widely known Coulomb interactions were considered, and the model was constructed on the basis of the data received in a chemical experiment, we got the hydrogen molecule's energy value that differed from the experimental value by less than 4%. The distances between the electrons and between the electrons and the nuclei, and the effective (active) charges of the nuclei in the molecule were defined. It turned out that the molecule had an effective nuclear charge of about 1.5 times greater than what the atoms had, while the distances between the electrons and the nuclei were smaller than those of hydrogen hydride (H^-).

These results could be received qualitatively on the basis of the Virial Theorem. The identical results of the calculation (where only the electrostatic forces were considered) and the experimental ionization results, have shown that the Virial Theorem can be applied to the molecule.

VAN DER WAALS BONDS (VWBs)

As indicated in the previous sections, chemical bonding is conditioned by the attraction of the electrons (negatively charged particles) of one atom to the nucleus (positively charged particle) of another. These forces appear even if both bonding atoms (of the second and third periods) have 8 electrons in the outermost shell, that is, in cases when the formation of neither covalent bonds nor DABs is possible.

We know that covalent bonds and DABs do not form between atoms if the outermost shells contain 8 electrons because the bonding electrons cannot enter both outermost shells of the atoms to be bonded. That is, if the outermost shells of the atoms cannot accept additional electrons, the distance between the electrons of each of the atoms to be bonded and the nuclei to be bonded by these atomic electrons is much greater.

The electrons of one atom cannot penetrate the electronic shell of another or approach another nucleus, as in the case of covalent bond formation or that of a DAB. The attraction force between positively and negatively charged particles (here – between the electrons of one atom and the nucleus of another) very strongly depends on the distance between the particles (which is proportional to the square value). That is, if the distance between the electrons and the nucleus doubles, the attraction force decreases by four times.

That is why, if we form a bond, say, between inert gas atoms, we should expect a significant increase in the length of this bond and a decrease in the bonding energy that must be spent on breaking this bond.

It has been found experimentally, that, indeed, bonds between inert gas atoms do exist, but their length (the distance between the nuclei) is about two times greater than in the case of a covalent bond and a DAB; and the bonding energy differs by more than 10 times.

As indicated above, the approach of the hydrogen atoms' nuclei in the course of the formation of molecule H_2 , as seen from the

calculation of the hydrogen molecule, leads to the increase of the effective charge (the charge of the nuclei acting upon the bonding electrons in the molecule) by 1.5 times. A ten times greater decrease in the bonding energy when increasing the distance by 2 times, is due not only to the decrease of the Coulomb interaction, but also to the decrease of the effective charge of the nuclei to be bonded, with the increase of the distance between them.

The existence of attraction between molecules was originally discovered and studied by the scientist Van der Waals. This is why these bonds were named after him.

The low bonding energy value is well observed during the temperature at which the breaking of this bond occurs. Thus, according to experimental data, in order to break a covalent bond in a hydrogen molecule (H_2), the hydrogen should be heated to a temperature over $3,000^\circ C$. In order to break a bond between neon and argon atoms (the breaking of a VWB occurs when the fluid turns into a gas) it is enough to heat fluids neon and argon to a temperature of minus 246, and minus $186^\circ C$ respectively.

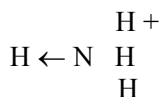
ELECTRON-NUCLEAR ISOMERIZATION

The previously given examples have shown that the atoms in molecules are often bonded to other atoms with various types of bonds. Thus, in the section devoted to the description of the covalent bond there were examples of ethylene ($H_2C = CH_2$) and of acetylene molecules ($HC \equiv CH$) in which the carbon atoms are bonded to hydrogen atoms via a single (simple) covalent bond, where the carbon atoms are bonded among themselves via multiple (double or triple) bonds.

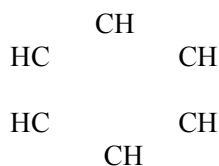
Likewise, in the chapter devoted to the description of the donor-acceptor bonds (DABs) we read about molecules H_2SO_4 and H_3PO_4 where the sulfur (S) and phosphorus (P) atoms are bonded to oxygen atoms with covalent bonds and with DABs.

Double and triple bonds are stronger and shorter than single covalent ones; covalent bonds are stronger and shorter than the DABs; DABs are stronger and shorter than the VWBs.

However, it has been found experimentally that if an atom is bonded to identical atoms but with various types of bonds, the weaker bonds become comparatively stronger and shorter, while the stronger ones become weaker and longer. Thus, for example, in ammonium cation, where, according to the bonding theory, three bonds are covalent ones and one is a DAB, all the four bonds between the hydrogen and nitrogen are equal in strength and in length:



The same is true of benzene (C_6H_6) whose structural formula, according to the bonding theory, is illustrated thus:

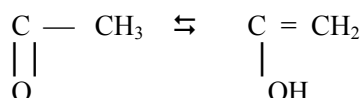


That is, benzene contains three single and three double bonds. According to experimental data, the bonding energies and lengths of all the bonds are equal among themselves. And the equalizing of the bonding energies and lengths was one of the main problems of the theory of chemical bonding.

The Lewis Rules on the structural formulas of compounds – which can be presented in the framework of rules and various structural formulas – have been a target at numerous scientific discussions for more than 20 years. The substances chosen for the discussions were mainly organic, and first of all – benzene, in which each of the carbons, according to the Lewis Rules, is bonded between themselves with three single and three double bonds. Of the inorganic substances, compounds of nitrogen and sulfur were discussed, where the atoms of nitrogen and sulfur are bonded with atoms of oxygen (dioxide of nitrogen and sulfur – NO₂ SO₂) in accordance with the Lewis Rules, via single and double bonds.

Two main interpretations were discussed. The first was offered by a group of scientists who could be conditionally called *chemists*. Their explanation was based on chemical experiments performed long before the discovery of *averaging various chemical bonds* and on the studies of isomerization reactions of chemical compounds. In the course of these reactions, the chemical composition (i.e., number of atoms of C, H, O, etc.) in the molecules did not change, though the position of the atoms did change in reference to each other. In most of the cases the chemical properties of the compounds also changed.

Some of these reactions had special names. One of the well-studied reactions was the keton-enol isomerization:



In the course of this reaction, the keton which contains the CO group turned into unsaturated alcohol. This reaction is reversible and proceeds to equilibrium. The equilibrium condition is indicated in these reactions by two arrows thus: \rightleftharpoons .

Respectively, the actual molecule in which the electron transits back and forth has different properties as compared to the expected properties of the molecules in the above described benzene formulas.

The phenomenon where the electrons move back and forth in these compounds is known as *resonance*. This kind of isomerization is indicated by one arrow with two heads thus: \leftrightarrow . That is, it was supposed that resonance greatly differed from isomerization. Indeed, it was supposed that in the case of resonance (rapid movement of the electrons

back and forth) we do not have two structures, but we do have a so-called *super-position*.

Indeed, just as in the case of benzene, all the other cases (SO₃, NO₂, NO₃, etc.) according to the analyses, there was only *one* chemical compound (not two or three) which would have been observed if isomerization took place.

Another explanation for the equalizing of the bond lengths and bonding energies was the quantum-chemical interpretation. According to Pimentel, the above-indicated cases are explained with the help of the TMO. In the framework of this theory, it was supposed that these molecules had π -orbitals whose action spread evenly along the whole molecule. That is, it limited the bond equalizing phenomenon only via coupled bonds.

According to Pimentel, quantum mechanics claimed that some resonance structures, indeed, do not exist, and the supposition that the electrons transit between two electronic configurations is pure fantasy.

The time of these discussions coincided with the period of intense introductions of chemical phenomena interpretations on the basis of quantum mechanics which was preceded by the *classical period in the development of chemistry*. The explanations of new phenomena were based on the comparison of *what was new* with the *available old experimental material*. That is, the explanations given by the chemists about the equalizing of the double and single bonds (the given compound could be described by various Lewis structures) was traditional for the classical period of the development of chemistry. This approach became known as the *phenomenological approach* when one phenomenon was explained on the basis of previously known phenomena. This approach is widely used in chemistry and was used above by us when we explained chemical bonding.

The use of the phenomenological approach for the interpretation of the resonance phenomena, at that time was closer to analogy than to phenomenological proof.

As already shown, the known cases of isomerization (including the keton-enol case) in the initial and final products were defined in mixtures. Then the speed rate of the process was defined, and the influence of the temperature and the catalyst on the speed rate. In the case of isomerization, which the chemists supposed was useful for explaining the equalization of the bonds, all the forms of analyses showed the existence of only one type of molecules. There is no doubt that the absence of data concerning the existence of isomers in the mixtures, weakened the position of the *chemists* during the discussions.

The defining factor that brought victory to quantum-mechanical interpretations in the 1960s and 1970s was nothing but euphoria in regard to the possibilities of quantum mechanics that reigned in chemistry of that period.

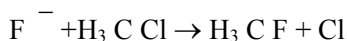
At the end of the 1970s this euphoria feeling gradually subsided. This was mainly due to the fact that the great expectations of the *chemists* of the 1960s-1970s in the development of quantum mechanical explanations was not achieved in the expected 5 or 10 year period, nor in the following 20 year period. Moreover, in the period that followed, it became obvious that the quantum chemical method of explaining

chemical phenomena was a fraudulent path in the development of chemistry.

Then in the 1970s-1980s new methods of analysis came into being (in this case — nuclear magnetic resonance) which allowed studying the conversion rate of analogous benzene compounds in themselves. It was found that the conversion of such compounds proceeded rapidly and the speed rate of the electrons was by two orders of magnitude greater than that of the nuclei. That is, the chemists' interpretation of that period received experimental confirmation.

It was proven experimentally that besides electronic isomerization, the molecules with single and double covalent bonds underwent electronic isomerization even if one atom was bonded to others with a covalent bond and a VWB or a DAB.

Thus, for example, when studying the following reaction (the nucleophyl substitution reaction):



it was found that an intermediate product ($\text{F} \dots \text{H}_3\text{C} : \text{Cl}$) was produced during this reaction, which, as a result of electronic isomerization, transited to its own electronic isomer ($\text{F} : \text{C H}_3 \dots \text{Cl}$). Here, as before, the colon (:) indicates a covalent bond; three dots (...) indicate a VWB.

On several biological objectives we have studied the electron speed rate along the chain with alternating single and double bonds (*conjugated bonds*), simple bonds, and those which alternate with simple ones and VWBs.

It was found that the rate of electron transition along the chain, composed of conjugated bonds, is by one order of magnitude higher than their electron transition speed rate along the chain that contains simple (single) covalent bonds. The speed rate of the electrons in the chain that contains VWBs (besides simple bonds) was about two times smaller than the speed of the electrons in the chain with only simple bonds (i.e., without VWBs).

Further it was found that in all the studied cases the transition rate of the electrons was by more than one order of magnitude greater than the transition rate of the nuclei.

In the 1980s-1990s when we rejected the quantum chemical interpretations, the above-mentioned experimental data on the electronic transitions were systematized. We concluded that the interpretation concerning the equalizing (aligning) of the bonds when one atom is bonded to two or three other identical atoms via single or double bonds was a correct one (offered by chemists of the 1960s-1970s). However, it was rejected because at that time there were no experimental results that could confirm the correctness of this interpretation that became available much later.

The conclusions drawn from the above mentioned experiments allow us to conclude that in all the cases there is a transition of electrons along the chain. This is because – if one atom is bonded to other identical atoms with various types of bonds, the transition of the electrons occurs in two directions: forward and back, and therefore the reaction reaches equilibrium.

Moreover, because of the electronic transition, an isomer is formed, identical to the initial one in equilibrium. The amounts of initial and final products of isomerization are the same.

If the electronic transition time is by more than 1.5 orders of magnitude greater than the transition of the nuclei from the initial isomer position to the position they occupied in the final product, as a result of isomerization, instead of two isomers (initial and final) there is only one product in the reaction compound. The distance between the nuclei has an intermediate value as compared to the distances they had occupied in the initial and final isomers.

Experimentally, on the basis of the studies of equilibrium, it was found that this intermediate state is thermally more stable than the initial state, and also the final state.

Electronic isomerization allows to realize how chemical bonding occurs between inert gases and halogens. In the above-cited cases of DAB formation between oxygen and xenon, the bonding took place at the expense of the attraction of the oxygen and xenon atoms' nuclei to the bonding pair of electrons that had belonged to the xenon prior to bond formation.

Both bonding electrons, according to the bonding theory, used to belong to the outermost shells of the atoms to be bonded by the given bond. However, besides the compounds of xenon and oxygen such as XeO and XeO₂, chemists had synthesized stable compounds of xenon with fluorine such as XeF₂ and XeF₄. In accordance with the covalent bonding theory, in this case neither covalent bonds nor DABs can be formed between xenon and fluorine.

During covalent bond formation, the number of electrons in the outermost shell of the xenon increases by one electron. According to the data on the affinity of xenon to the electron, the latter does not bond to the former. If we compare the data on the FIPs of xenon (Xe), whose FIP is equal to 13 eV, and the FIP of cesium (Cs) whose FIP is equal to 3.89 eV. [Cesium follows xenon in the Table of Elements.] The electron does not bond to the outermost xenon shell even when the nuclear charge increases by one proton unit. That is, according to the data on the affinity and the FIPs, covalent bonding cannot take place in this case.

On the other hand, when DAB formation takes place (along the scheme of DAB formation in the case of XeO) the number of electrons in the outermost shell of the fluorine after DAB formation increases to 9 (i.e., 7 former ones and 2 additional ones) which is utterly impossible since the outermost shell of the elements of the second period, according to the data on their affinity to the electrons and the FIPs – there can be not more than 8 electrons there.

It could be supposed that xenon, whose FIP is equal to 12.13 eV, gives up its only electron to the fluorine whose FIP is equal to 17.4 eV. For such a transition, the electron should spend 12.13 eV to tear the electron off the xenon atom. When bonding this electron to a fluorine atom, according to the affinity of a fluorine atom, we get an energy gain of 3.34 eV. That is, in all, as a result of this process, we have an energy loss of $(12.13 - 3.34 = 8.79 \text{ eV})$ 8.79 eV. That is, from the energetic viewpoint, this variant of chemical bond formation is illogic.

On the other hand, it can be supposed that the DAB occurs not at the expense of the xenon electronic pair, but at the expense of one of the xenon's electrons that rotates on a plane perpendicular to the axis that connects the nuclei of the xenon atoms and those of the fluorine. And finally, we can suppose that bond formation in XeF_2 between fluorine and xenon occurs as follows between the fluorine and xenon molecules. First the VWB: $\text{Xe} \dots \text{F} : \text{F} \dots \text{Xe} \dots \text{F} : \text{F}$

Electronic isomerization takes place in the formed compound along the scheme: $\text{F} : \text{F} : \dots : \text{Xe} \dots \text{F} : \text{F} \rightarrow \text{F} : \text{Xe} \dots \text{F}$ as a result of which we get: $\text{F} \text{Xe} \dots \text{F}$ where one of the fluorine atoms is bonded to a xenon via a common covalent bond, while another is bonded to a VWB. According to the above, this compound should isomerize rapidly along the scheme: $\text{F} : \text{Xe} \dots \text{F} \rightarrow \text{F} \dots \text{Xe} : \text{F}$ and, respectively, as a result of the alignment of the VWBs and covalent bonds in regard to their energies and lengths and via electronic isomerization, we will get a compound in which both bonds – xenon and fluorine – will be equal in their energies and lengths.

In order to choose between this interpretation and the previous one, we should refer to the experimental data on the composition of stable compounds of xenon with fluorine. According to the interpretation that presupposes that DABs are formed not at the expense of two, but at the expense of only one xenon electron, xenon compounds, like the following, could have been synthesized: XeF , XeF_2 , XeF_3 , etc. As far as the previous interpretation is concerned, only compounds with xenon and fluorine of the following kind can be synthesized: XeF_2 , XeF_4 , and XeF_6 , that is, compounds with an even number of fluorine atoms. All the three above-mentioned compounds were synthesized in 1962.

Compounds of xenon and fluorine with an odd number of fluorine atoms have not been received as yet (2001).

That is, the available experimental data speaks of the correctness of the interpretation that supposes that if we bond fluorine to xenon, we get a molecule where the bond length and the bonding energy between the fluorine-xenon bonds have an intermediate value in regard to covalent bonds and VWBs.

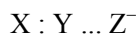
We suppose that a molecule constructed in accordance with the given interpretation, has electrons that transit from the xenon to the fluorine, just as in the first of the possible interpretations. When analyzing the first interpretation, we have shown that from an energetic viewpoint the transition of an electron from the xenon to the fluorine requires immense energetic expenditure. That is, it is hardly possible.

Unlike this interpretation, in the variant that we offer, whose correctness is confirmed experimentally, the energy expenditure used for transiting one of the xenon electrons to the fluorine atom is completely compensated by the formation of a covalent bond between the second fluorine molecule and the xenon atom. This is because in the course of covalent bond formation, according to the bonding theory, the number of electrons in the outermost shell of xenon increases by one unit, i.e., the xenon that had lost one electron, gets another one.

Making use of this interpretation, there is no use for any additional suppositions about the formation of a single-electronic

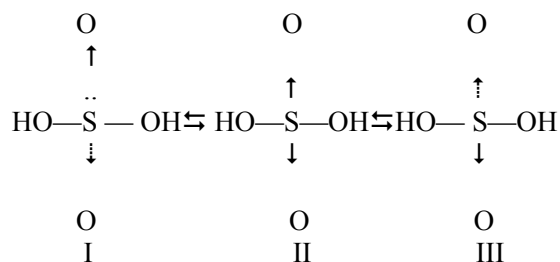
covalent bond. And finally, with this interpretation there is no violation of any of the previously installed regulations on the formation of chemical bonds. Each of the atoms in molecule $F : Xe^+ \dots F^-$ contains not more than 8 electrons in the outermost shell and all the bonds are formed in accordance with the rules of their formation introduced on the basis of the studies of a number of organic and inorganic compounds.

The understanding of the electronic structure of xenon compounds and fluorine helps to explain the formation of a great number of synthesized stable compounds of halogen molecules with halogen anions (i.e., a halogen with an attached electron). The general formula is:



Without any additional suppositions, the explanation of the bonding process between inert gases and halogens helps to explain the formation of such stable compounds as PCl_5 and SF_6 . In complete analogy with compounds of the XeF_2 type, the structural formulas like PCl_5 and SF_6 can be represented.

In the case of such compounds as H_2SO_4 and H_3PO_4 among the electronic isomers, which transit into each other, we should expect isomers as well, where one of the bonds is a covalent one and the other is an ionic VWB. Thus, for example, for sulfuric acid (H_2SO_4) the electronic transitions occur between the following isomers:



Where (—) (→) and (↔) are covalent bonds, DABs and VWBs respectively.

The experimentally defined bond length between the sulfur and the oxygen in the anion SO_4 is by 0.21\AA smaller than the sum of the covalent radiuses of the sulfur (S) and the oxygen (O). If the electronic isomerization occurred without the participation of isomers II and III, the length of bond S — O would equal the average value between the DAB and the single bond. The supposition, however, about the presence of isomerization between isomers II and III helps to explain why the bond length S — O is smaller than the length of the single bond, i.e., is situated between a double and single bond.

CONCLUSION

Chemical bonding between atoms is formed at the expense of the attraction of the nuclei of the *atoms to be bonded* to the electrons. The electrons to which the nuclei are attracted are called *bonding electrons*.

There are three main types of chemical bonds: 1) covalent bond, 2) donor-acceptor bond (DAB), and 3) Van der Waals bond (VWB).

During covalent bond formation, the nuclei being bonded are attracted to the pair of electrons each of which, before this bond formation, used to belong to the OESs of the atoms to be bonded. After bond formation, both bonding electrons enter the outermost shells of the atoms to be bonded.

The number of additional electrons that can enter the outermost shell of the atoms to be bonded is limited. Thus, for example, in the case of atoms of elements of the second and third periods, the number of electrons in the outermost atoms' shells does not exceed 8.

Respectively, the number of covalent bonds (valence) that can form an atom is defined, on the one hand, by the number of electrons situated in the outermost shell, while on the other hand – by the maximal number of electrons that the outermost shells of the atoms to be bonded can contain.

When the number of electrons in the outermost shell of the atom contains the maximal number of electrons (for elements of the 2nd and 3rd periods – 8) this shell is regarded as *saturated*. Respectively, when the outermost shell of an atom contains fewer than 8 electrons, such a shell is regarded as being *unsaturated*. Therefore, a covalent bond, according to the accepted terminology, is formed between atoms when the OESs of both atoms being bonded, are unsaturated.

Before bond formation, each of the bonding electrons rotate around the nucleus of its atom with the terrific speed of 10^8 cm/sec. After bond formation, the bonding pair of electrons simultaneously enters the outermost shells of the atoms to be bonded. The electrons rotate on a plane perpendicular to the axis connecting the nuclei.

If the nuclei's attraction force to the electrons being bonded is identical (i.e., the FIPs of the atoms being bonded are the same) the distance between the nuclei and the bonding electrons is also identical. In this case the bond is known as a *covalent-homopolar* bond. If the FIPs of the atoms differ and the center around which the bonding electrons rotate is closer to the atom with a bigger FIP, such a bond is known as a *covalent-heteroatomic* bond or a *polar bond*.

In cases when the difference in the atoms' FIPs is greater than 10 eV, such a bond has become known as an *ionic bond*.

During the formation of a heteropolar bond much more energy is discharged than during the formation of a homopolar bond.

Covalent bonds can be double and triple when the nuclei are bonded via two or three electron pairs respectively. That is, when such bonds are formed, the bonding electron pairs are formed of 4 and 6 electrons of the atoms to be bonded. Simultaneously the number of electrons in the outermost shells of each atom to be bonded increases by two and three electrons respectively during the formation of double and triple bonds.

Unlike covalent bonds, when a DAB is formed, the bonding electron pair is formed of the electronic pair that used to belong (before

bond formation) to only one of the atoms to be bonded, known as the *donor*. Respectively, after bond formation, the number of electrons in the outermost shell of the donor atom, after DAB formation, does not change. The number of electrons in the outermost shell of the second atom, known as the *acceptor*, is increased by two electrons.

The energy discharged during DAB formation is about two times smaller than the energy discharged during covalent bond formation. The DAB is formed between atoms when a covalent bond cannot be formed; that is, when the OES of the donor atom is saturated and contains 2, 4, or 6 electrons that do not take part in bond formation, and when the OES of the acceptor atom is so unsaturated, that it can accept an additional 2, 4, or 6 electrons.

Both donor-acceptor bonds and covalent bonds are formed at the expense of the attraction of the nuclei of the atoms to be bonded to the electronic pair rotating between them. Just as in the case of covalent bonds, the plane of the orbit's rotation, connecting the electrons, is perpendicular to the axis connecting the nuclei.

The VWB is formed between atoms whose OES are saturated. Just as in the case of covalent bonds and DABs, bond formation is conditioned by the attraction of certain atoms' nuclei to the electrons of the OES of other atoms.

In the case of VWB formation, an energy value of ten times smaller is discharged as compared to that of a covalent bond. That is, the bonding force (energy necessary for breaking the bond) decreases in the row: covalent ionic bond > covalent heteropolar bond > covalent homopolar bond > DAB > VWB. In the same row the bond length increases. That is, the weaker the bond, the longer it is.

If an atom is bonded to other atoms with various types of bonds (single, double, covalent, covalent and DABs, covalent and VWBs) these bonds equalize in length and energy. This effect is most obvious when an atom is bonded with various types of bonds to the same kind of atoms. In such a case we get complete equalization in length and energy. This is because electronic isomerization takes place.

Last Presentations (Extended abstracts):

New General Theory of Catalysis. Gankin, Victor Y.; Gankin Yuriy. Institute of Theoretical Chemistry, Shrewsbury, MA, USA. Abstracts of Papers, 222nd ACS National Meeting, Chicago, IL, USA, August 26-30, 2001 (2001), PETR-070. Publisher: American Chemical Society, Washington, D.C. CODEN: 69BUZP Conference; Meeting Abstract written in English.

AN 2001:641082 CAPLUS (Copyright 2002 ACS). Kinetics and

Mechanisms of Petroleum

Chicago August 26-30

A New General Theory of Catalysis

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Key Words: Reaction, Catalysis, Mechanism.

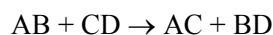
The main questions that were raised in the course of the development of the theory of chemical reactions were as follows:

1) Why don't all chemical reactions proceed if they are thermodynamically possible?

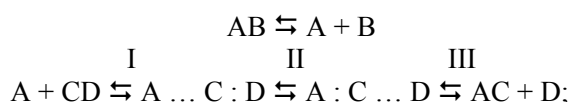
2) Why does the reaction speed increase along the exponent with the increase of temperature?

3) Why is it that in reactions proceeding with bond breaking, the activation (additional) energy is usually much smaller than that necessary to break the bond thermally? Indeed, why is it that reactions proceed with the breaking of the chemical bond in normal conditions, while we need a temperature of more than 4,000° to break such bonds thermally? Examples of such reactions are interactions of radicals and ions with molecules, catalytic and photochemical reactions.

In the course of our studies [1,2] we managed to learn that unlike the opinions accepted in 1980, the interactions between molecules take place not via the scheme:



but mainly along the chain reaction scheme:



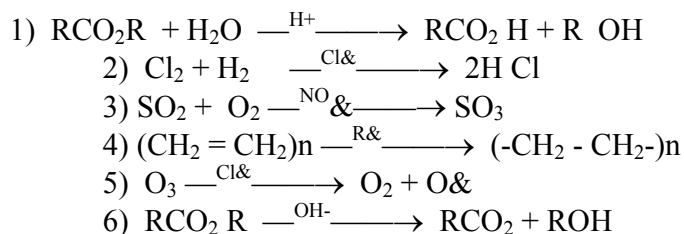
here A, B, and D are active particles (radicals, ions, conences, etc.); A : C ... D and A ... C : D are Van der Waals complexes. Stage II is the electronic isomerization stage. Stage III is the limiting stage. The given scheme for the procedure of the chemical reactions answers the main questions, which arose during the development of chemical kinetics, mentioned above.

That is, unlike the ideology accepted in 1980, the active elements in chemical reactions (i.e., species which cause chemical transformations) are not at all species or molecules with a high kinetic energy. The active elements are actually specific chemical species like radicals, ions, anions, etc.

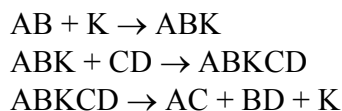
In the framework of the offered scheme, the driving forces of chemical reactions have become comprehensible.

In the light of the above, such notions as *catalysis* become understandable. A catalyst is a chemical compound which forms (produces) a greater number of active species in the system than initial molecules do at the same temperature.

The acceleration of the catalyst reaction at the expense of introducing active species into the system (radicals, ions, anions, etc.) is described in textbooks as *examples of catalyst reactions*. The reactions most commonly offered are as follows:



Another method for accelerating the interaction of molecules is by increasing the concentration of the associates in the system in the presence of catalysts. Thus, for example, a catalyst substance unites other substances that react with each other along the scheme:



where AB and CD are reacting substances.

The above scheme is a general one as far as catalysis is concerned.

The existence of all the stages for some of the reactions have been proven experimentally. Our accomplishment lies in the elucidation of the driving forces in the catalytic action of the catalysts during the reaction along this scheme.

The acceleration of the reaction (catalytic action of the substance) is explained thus: Due to the absence of the catalyst, the intermediate compound in the reaction is AB - CD; while in the presence of the catalyst it is AB - K - CD. The speed of the whole reaction in both cases is proportional to the concentration of the intermediate compound. In correlation with concentration AB - CD (without the catalyst) and AB - K - CD (with the catalyst), the concentration of these compounds in the system is defined by bonding energies AB - CD and AB - K - CD.

The bonding energies of both molecules with catalysts are much higher than the bonding energies between themselves, so the concentration of the intermediate compounds with catalysts is much greater, and correspondingly, much greater is the reaction speed. This mechanism for reaction

acceleration is, for example, typical for the metal-complex and bio catalytic systems where the catalysts are ferments (enzymes) that unite the reacting molecules in the active centers of the ferments.

Besides the above mentioned mechanisms for accelerating reactions, the catalyst can accelerate the reaction by other mechanisms. A catalyst can:

- 1) improve the role of chemically activated routes;
- 2) serve as a bridge for the transition of electrons.

As expected, the substances which accelerate the reaction in the above mentioned mechanisms, are catalysts, and the essence of catalysis, in the general approach, becomes better understood if compared with such general definitions as: a catalyst is a substance which accelerates a reaction; a catalyst carries the reaction along the route requiring less activation energy.

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Victor Y. Gankin & Yuriy V. Gankin: How Chemical Bonds Form and Chemical Reactions Proceed ITC (Institute of Theoretical Chemistry) (1998)

[See also www.lstbooks.com Gankin How Chemical Bonds (Electronic Book),

www.amazon.com www.ITChem.com

for details about these and other methods about reaction acceleration.]

Quiet Revolution in Chemistry. Gankin, Victor; Gankin Yuriy. Institute of Theoretical Chemistry, Shrewsbury, MA, USA. Abstracts of Papers, 222nd ACS National meeting, Chicago, IL, USA, August 26-30, 2001 (2001), HIST-039. Publisher: American Chemical Society, Washington, D.C. CODEN: 69BUZP Conference; Meeting Abstract written in English. AN 2001:639044 CALPUS (Copyright 2002 ACS).

The Quiet Revolution in Chemistry (Report 1)

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According to Lippard, a quiet revolution took place in Chemistry in the XX century. In part, according to Lippard, "We wish to evolve new theoretical approaches to understand chemical bonding and reactions and to test these theories against real chemical systems." Stephen Lippard MIT, C&EN, Aug. 7, 2000 p. 65

In reports 1 and 2, we offer a new interpretation of chemical bonding for high school students.

The data on the ionization potentials of elements in the first three periods of the Table of Elements have shown that the electrons in the atoms are situated in layers and that the number of electrons in the outermost shells of the elements of the 2nd and 3rd periods changes when transiting from the first group to the last, from 1 to 8.

According to the received data, after the accumulation of eight electrons in the outermost shell, a new outermost electronic shell starts to form.

A comparison of the data on the number of electrons in the outermost shell with the valence of elements according to hydrogen (H) and chlorine (Cl) have shown that the valence of elements is equal to the number of electrons in the first four groups. This proves that only one electron of the central atom actually takes part in bond formation. Relatively, the number of bonds is limited in elements of the first four groups by the number of electrons in the outermost shells of the atoms.

In dual molecular atoms, formed of identical atoms, both atoms are the same. That is, two electrons take part in bond formation — one from each of the atoms being bonded.

The valence in the last four groups of elements is equal to 8 minus X where X is the number of electrons situated in the outermost shell of the central atom.

The fact that 8 minus X, on the one hand, is equal to the valence of the element, and on the other hand, is equal to the number of additional electrons that can enter the outermost shells of the atoms of the last four groups, has shown that in the course of bond formation, both bonding electrons enter the outermost shells of the atoms to be bonded.

That is, the number of bonds that the elements in the last four groups can form, is limited by the number of electrons that can enter the outermost shells of these elements.

The simultaneous entrance of two bonding electrons into the outermost shells of the atoms to be bonded, allows us to construct a model of chemical

bonding. The simultaneous presence of electrons to be bonded in the outermost shells is possible only if the bonding electrons rotate on a plane perpendicular to the axis connecting the nuclei.

This model explains the physical essence of chemical bonding. Chemical bonding is formed at the expense of the electrostatic attraction of the atoms' cores to the pair of electrons rotating between them. (See [www. itchem](http://www.itchem) for details)

Implementation of the Historic Approach to Elaboration of New Theories. Gankin, Victor; Gankin, Yuriy. Institute of Theoretical Chemistry, Shrewsbury, MA, USA. Abstracts of Papers, 222nd ACS National Meeting, Chicago, IL, USA, August 26-30, 2001 (2001), HIST-039. Publisher: American Chemical Society, Washington, D.C. CODEN: 69BUZP Conference; Meeting Abstract written in English. AN 2001:639041 CALPUS (Copyright 2002 ACS).

About the Wave Properties of Microparticles

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The wave properties of microparticles have been worrying the physicists for over 50 years. The hypothesis about the *probability wave* is the most non-physicist hypothesis in physics. The De Broglie equation, from the very start, was regarded as quite insane. Indeed, the wave properties of particles had actually become an example of *a physical phenomenon that a human brain cannot grasp*.

In experiments with a diffraction of microparticles the beam is accompanied by electromagnetic radiation. It was found, in experiments, when obtaining electromagnetic radiation, that this energy (E_{radi}) is equal to the energy of the incident electrons:

$$E_{\text{radi}} = mV_1^2 / 2 \quad (1)$$

where m and V_1 are the mass and rate of the incident electrons.

In their experiments Davisson and Germer considered that the energy of the scattering electrons is close to that of the incident electrons:

$$mV_1^2 / 2 = mV_2^2 / 2 \quad (2)$$

where V_1 and V_2 are the rates of the *incident* and *scattering* electrons respectively.

It is known that the frequency of electromagnetic radiation is defined by the equation:

$$\nu = E/h \quad (3)$$

where E is the radiation energy; h is the Plank constant.
From equations 1 and 3 we get:

$$\nu = mV_1^2 / 2h \quad (4)$$

The wave length of the electrons vibrating with a frequency of ν and flying at a speed of V_2 is defined by the equation:

$$\lambda = V_2 / \nu \quad (5)$$

From equations 4 and 5 we get:

$$\lambda = 2hV_2 / mV_1^2 \quad (6)$$

From equation 2 it is evident that $V_1 = V_2$ and equation 6 is transformed into the following:

$$\lambda = 2h / mV_1 \quad (7)$$

Equation 7 is almost identical to the De Broglie equation, and therefore the given interpretation of *diffraction* in experiments with microparticles is regarded as more desirable if compared with the first interpretation. Equation 7 corresponds very well to the main point of the extract from an article by Davisson and Germer:

Equivalent wave-lengths of the electron beams may be calculated from the diffraction data in the usual manner. These turn out to be in acceptable agreement with the values of h/mv of the undulatory mechanics (Phys. Rev., 1927, vol. 30, No. 6, p. 705).

In all the experiments that confirm the existence of wave properties in microparticles and the inverse proportional dependence of the wave length on the speed and mass of the particle — in all these cases the beam of particles was accompanied by electromagnetic radiation whose energy is equal to the energy of the particles. That is, this explanation allows us to realize the reason for the appearance of diffraction in experiments with electrons passed through thin foil and in experiments with other microparticles.

Victor Y. Gankin & Yuriy V. Gankin: How Chemical Bonds Form and Chemical Reactions Proceed ITC (Institute of Theoretical Chemistry) (1998)

[See also [www.1st books.com](http://www.1stbooks.com) Gankin How Chemical Bonds (Electronic Book),

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Demystifying and Clarifying the Concept of the Resonance Rules, Valence, Chemical Structure, Chemical Reactions, and Catalysis. Gankin, Yuriy V.; Gankin, Victor Y. Institute of Theoretical Chemistry, Shrewsbury, MA, USA. Abstracts of Papers, 222nd ACS National Meeting, Chicago, IL, USA, August 26-30, 2001 (2001), CHED-407.. Publisher: American Chemical Society, Washington, D.C. CODEN: 69BUZP Conference; Meeting Abstract written in English. AN 2001: 637905 CALPUS (Copyright 2002 ACS).

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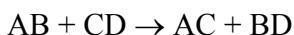
Theory of Chemical Reactions

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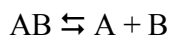
The main questions that were raised in the course of the development of the theory of chemical reactions were as follows:

- 1) Why don't all chemical reactions proceed if they are thermodynamically possible?
- 2) Why does the reaction speed increase along the exponent with the increase of temperature?
- 3) Why is it that in reactions proceeding with bond-breaking, the activation (additional) energy, as a rule, is much smaller than the energy necessary to break the bond thermally? Indeed, why is it that reactions proceed with the breaking of the chemical bond at 300 K - 600 K while we need a temperature of more than 4,000 K to break such bonds thermally?

In the course of our studies we managed to learn that unlike the opinions accepted before the 1980s, the interactions between molecules take place not via the scheme:



but mainly along the chain reaction scheme:



here A, B, and D are active particles (radicals, ions, conences, etc.); A : C ... D and A ... C : D are Van der Waals complexes. Stage II is the electronic isomerization stage. Stage III is the limiting stage. The given scheme for the procedure of the chemical reactions answers the main questions that arose during the development of chemical kinetics mentioned above.

That is, unlike the ideology accepted before the 1980s, the active elements in chemical reactions (i.e., species which cause chemical transformations) are not at all species or molecules with a high kinetic energy. The active elements are actually specific chemical species like radicals, ions, conences, etc.

The given scheme for the procedure of the chemical reactions answers the main questions arising during the development of chemical kinetics, mentioned above. Active particles are in thermodynamic equilibrium with the initial molecules. When the temperature decreases, the concentration of active particles exponentially drops, causing an abrupt decrease in the speed of the chemical reactions. This dependence answers the 1st and 2nd question.

The electronic isomerization speed is by many orders of magnitude higher than that of the dissociation stage. That is why the kinetic parameters of the electronic isomerization stage, and first of all - the activation energy, do not effect the activation energy of the whole reaction which defines the energy consumption in the course of the reaction. As a result of the electronic isomerization, the initial covalent bond, which requires about 400 kJ/mol in order to break, transforms into a Van der Waals bond (VWB) that requires less than 20 kJ/mol for its rupture. Thus it becomes comprehensible why, in order to break a chemical bond in a molecule in the presence of an active particle, we need an energy by one order of magnitude smaller than for the thermal rupture of the bond in this molecule. This answers the 3rd question. (See [www. itchem](http://www.itchem) for details.)

Demystifying and Clarifying the Concept of Chemical Bonding. Gankin, Yuriy V; Gankin, Victor Y. Institute of Theoretical Chemistry, Shrewsbury, MA, USA. Abstracts of. Papers, - American Chemical Society (2001), 221st CHED-1008. CODEN: ACSRAL ISSN: 0065-7727. Journal; Meeting Abstract written in English. AN 2001:199061 CAPLUS

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In our previous works we have worked out a new theory of chemical bonding, chemical kinetics and catalysis. In this theory we offered explanations of chemical phenomena based on the knowledge of chemistry, physics and mathematics that the students had gained at school.

THE THEORY OF CHEMICAL BONDING

The data on the ionization potentials of elements in the first three periods of the Table of Elements have shown that the electrons in the atoms are situated

in layers and that the number of electrons in the outermost shells of the elements of the 2nd and 3rd periods changes, when transiting from the first group to the last, from 1 to 8.

According to the received data, after the accumulation of eight electrons in the outermost shell, a new outermost electronic layer starts to form.

A comparison of the data on the number of electrons in the outermost shell with the valence of elements according to hydrogen (H) and chlorine (Cl) have shown that the valence of elements, according to hydrogen and chlorine, is equal to the number of electrons in the first four groups. This proves that only one electron of the central atom actually takes part in bond formation. Relatively, the number of bonds (valence) is limited for elements of the first four groups by the number of electrons in the outermost shells of the atoms.

In dual molecular atoms, formed of identical atoms, both atoms are the same. That is, two electrons take part in bond formation — one from each of the atoms being bonded.

The valence in the last four groups is equal to 8 minus X where X is the number of electrons situated in the outermost shell of the central atom.

The fact that 8 minus X, on the one hand, is equal to the valence of the element, and on the other hand, is equal to the number of additional electrons that can enter the outermost shells of the atoms of the last four groups, has shown that in the course of bond formation, both bonding electrons enter the outermost shells of the atoms to be bonded.

That is, the number of bonds that the elements of the last four groups can form (valence) is limited by the number of electrons that can enter the outermost shells of these elements.

The simultaneous entrance of two bonding electrons into the outermost shells of the atoms to be bonded, allows to construct a model of chemical bonding. The simultaneous presence of electrons to be bonded in the outermost shells is possible only if the bonding electrons are rotating on a plane perpendicular to the axis connecting the nuclei.

This model logically explains the physical essence of chemical bonding. Chemical bonding is formed at the expense of the electrostatic attraction of the atoms' cores to the pair of electrons rotating between them.

According to the model and the physical essence of chemical bonding, chemical bonding is possible even if the bonding pair of electrons belonged to one of the atoms being bonded before the bonding took place. In order to form such a bond, it is necessary that the outermost shell of the second atom to be bonded should contain fewer than seven electrons. Indeed, the formation of such bonds is well known: XeO, XeO₂, XeO₃, HClO₂, HClO₃, etc. In all these compounds the oxygen (O) bonded to xenon (Xe) and in the direction of chlorine (Cl⁻) at the expense of its free space in the outermost shell. In this case the bonding pair of electrons belonged to the xenon and chlorine before forming the chemical bond with oxygen.

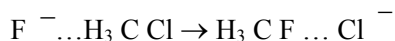
Historically, chemical bonds formed at the expense of electrons that belonged to different atoms before bond formation, became known as covalent bonds. Bonds formed at the expense of electrons that formerly belonged to one atom became known as donor-acceptor bonds (DAB).

According to the model, the attraction of the nucleus of one atom to the electrons of another should be observed also when the outermost shells of both atoms are saturated. According to experimental data, such bonds exist. The existence of such bonds is obvious during the transition of substances, like inert

gases, from the gas state to the liquid state. Such bonds became known as Van der Waals bonds (VWB)

Covalent bonds can be heteroatomic (when atoms with various IPs are bonded); and also double and triple (when there are two or three covalent bonds between two atoms). According to experimental data, the amount of energy that should be spent on breaking the bond (the strength of the bond) decreases according to the row thus: **triple > double > heteroatomic > homoatomic covalent > DAB > VWB**. The length of the bond increases in the same order.

It has been proven experimentally that if one atom is bonded to the same kind of atoms by various types of bonds, such bonds become equal in respect to energy and length. Simultaneously, the weak bonds become stronger while the strong ones become weaker. Analogously, the long bonds become shorter while the short ones become longer. The cause of this phenomenon is electronic isomerization. It has been proven experimentally (the speed of the process was even measured in some cases) that there is a balancing procedure in the following processes:



That is, the isomerization of VWB into the covalent bond and vice-versa.

Isomerization of the benzen type in single and double bonds the transition speed of the electrons was measured along the chain of carbon atoms with multiple bonds only single and various single and VWB.

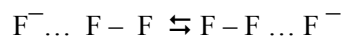
It has been defined: 1) The transition speed of the electron along the chain of conjugated bonds is by one order of magnitude higher than along the chain of single bonds. The presence of VWBs in the chain decreases the speed by only 1.5 times. 2) The transition speed of the electrons is by two orders of magnitude greater than the speed of the nuclei.

The difference between the speeds of the electrons and the nuclei leads to the fact that the distances between the atoms and the bonding energies of the atoms with a central atom are equalized. The thermal stability of the compound is determined by the stability of the weakest bond. That is why the equalizing of the bonds, in respect to energy, leads to the decrease of the thermal stability of the compound.

According to experimental data, this explanation concerning the influence of electronic isomerization on the equalization of the lengths and energies of the bonds and on the thermal stability of compounds is more vividly observed if, as a result of the isomerization, there is an identical or close to identical energy of the initial compound.

According to experimental data, complete equalization of the lengths and bonding energies, as well as the greatest possible increase of stability is observed when the electronic isomerization leads to the formation of a compound identical to the initial compound in chemical structure. Electronic isomerization explains the equalization of the lengths, bonding energies, and thermal stability of the compounds, whose stability observed in the experiment contradicted the theory of bond formation

Indeed, in the framework of the theory which considers the formation of only covalent bonds, DABs, and VWBs, the thermal stability of such compounds as XeF_2 , XeF_4 , PF_3 , SF_6 , (G_3) where G stands for halogen, contradicted the bonding theory. In the framework of simple valence schemes, F_3^- contains one VWB and, therefore, disintegrates at room temperature. The existence of equilibrium:



makes this compound much more stable thermally. Analogously, the stability of XeF_2 , XeF_4 , PF_5 , and SF_6 is explained by the reverse process of electronic isomerization.

All these compounds are constructed analogously to $(Cl_3)^-$; each of the atoms in the molecules contain 8 electrons, i.e., the number of electrons in the outermost shells does not exceed the maximal number of electrons — in accordance with the theory of chemical bonding. The stability, under normal conditions, when the temperature is equal to 20°C, the equalization of all the bonds is due to the electronic isomerization.

The existence of the stable compounds confirms the main precepts of the bonding theory, including the fact that the maximal number of electrons in the outermost shells in atoms of the second and third periods cannot exceed 8.

On the other hand, the synthesis of compounds XeF_2 , XeF_4 , and the mishaps in syntheses XeF and XeF_3 are independent confirmations of the fact that two electrons actually take part in the formation of a covalent bond (one from each of the atoms) and that both bonding electrons enter the outermost shells of both atoms to be bonded.

Thus, the theory of chemical bonding, including electronic isomerization, is based on the comparison of experimental data on ionization potentials of atoms of the second and third periods including data on the composition and structure of stable compounds, as well as experimental data received when studying electronic isomerization is very well substantiated experimentally.

The given theory does not contain any suppositions that had not been proven experimentally (like the supposition about the electrons striving to finish up 8 electronic shells, or the supposition about the increased stability of the outermost 2, 4, and 8 electronic shells). The theory describes the structure of known chemical compounds without any exceptions.

However, when considering a semi-quantitative evaluation of the theory, a number of questions arise, which, at first glance, contradict the bonding theory, and therefore require a detailed investigation.

1) According to the model, during the formation of a covalent chemical bond, there is an energy gain received at the expense of the transition of the electrons in one atom to the outermost shell of another. This energy gain can be defined by the affinity of hydrogen atoms to the electron. That is, by the value of about $0.72 \text{ eV} \times 2$, where 0.72 eV is the affinity energy of one hydrogen atom in relation to one electron.

Simultaneously, during bond formation, the electrons and the nuclei approach each other, which leads to an energy loss. According to experimental data, the distance between the nuclei in a hydrogen molecule comprises 0.74 . Relatively, the energy loss, only at the expense of the mutual repulsion of the nuclei, is equal to about 14 eV/mol . That is, according to the calculation, a hydrogen molecule cannot be stable.

2) During DAB formation we have found that the number of electrons in the outermost shell of the acceptor atom increases by two. The data on the affinity have shown that only one electron can bond to an ordinary atom.

3) According to the model, chemical bonding occurs at the expense of the attraction of the nuclei to the electrons to be bonded. Since the FIPs and the affinity of the atoms to the electrons are different, there is an increase in both the

bonding energy and the FIPs. However, experiments have shown that there is no bond between the FIPs and the bonding energies.

4) The bonding energy in NaCl (and other analogous heteroatomic molecules) is much greater than the bonding energy in Na₂ and Cl₂, though at first glance the energy of this bond should amount to something intermediate of the bonding energies of Na₂ and Cl₂

The solution of these paradoxical questions was received as a result of the analysis of the model of a hydrogen molecule based on the comparison of the data on the IP and the data on the structure of the stable molecules. As indicated above, the molecule, according to this comparison, represents two protons (in the case of H₂) between which two electrons rotate on a plane perpendicular to the axis that connects the nuclei.

The algebraic solution of this model leads to the following system of three equations with three unknowns, that is, it leads to an analytical solution. Though in rare cases (with homoatomic molecules) the system of equations can be solved without the use of a calculator or a computer. Generally, the most effective way of solving the system of equations with fractional powers is with the help of a calculator or a computer in accordance with special programs worked out for the given system.

In the course of solving the system of equations, we define all the distances between the particles (electrons and protons) and, respectively, the potential energy of the molecule, the kinetic energy of the electrons: ($mV^2/2 = q_1q_2/r$) according to the Virial Theorem. Therefore the energy of a molecule equal to the difference of the absolute values of the potential and kinetic energies, is equal to half of the potential energy. The calculated value of the energy of a hydrogen molecule differs from the experimental data by less than 3% – which indicates the correctness of the model.

According to the calculated model, the angle between the attraction forces connecting the electrons to the nuclei of the hydrogen is equal to 60°. Respectively, the projection of the attraction force bonding an electron to one of the nuclei to the attraction force of the same electron to another nucleus, force is equal to half of the electronic force attraction to the nuclei. Respectively, the attraction force of the electrons to the atoms increases by 1.5 times, as compared to the variant when only an atom is bonded to an electron and not to another atom. The increase of the attraction force of the entering electron and its own electron to the nucleus by 1.5 times is equal to the increase of the effective charge of the nuclei by 1.5 times, which, in turn, leads to an abrupt increase in the energy gain.

Thus the electronic energy of a helium-like atom with a nuclear charge of 1 and 1.5 proton units, comprises, according to the calculation: 15.3 eV and 42.5 eV. That is, when bonding only an electron to a hydrogen atom, the energy gain, according to the calculation, comprises 1.7 eV i.e., ($15.3 - 13.6 = 1.7$ eV). When an atom is bonded (electron + nucleus) during the formation of a hydrogen molecule, the energy gain becomes 28.9 eV ($42.5 - 13.6 = 28.9$ eV for each of the atoms being bonded, which fully compensates the internuclear repulsion energy. That is, the total energy gain during chemical bond formation, is conditioned, paradoxical as it may seem, to a greater extent by the mutual approach of the atoms' nuclei, than by the transition of the electrons of one atom to the outermost shell of another atom i.e., by the attraction of the nuclei of one atom to the electrons of another atom.

Experimentally, the energy of an atom with two electrons and a charge of 1.5 eV can be evaluated as an average value between the energy of a hydride ion (H) and a helium atom (He), that is, by the value of (54.4eV) i.e., close to the previous calculation, and therefore greater than the repulsion energy. The main role in energy gain and the increase of the charge allows us to solve the rest of the above mentioned paradoxes, namely, the possibility of bonding two electrons when forming DABs, a greater energy of a polar bond as compared with a covalent bond.

The description of chemical bonding cited in this work (The Theory of Chemical Bonding) differs from that of the previous works ideologically. For example, in polar molecules the electrons do not transit from one atom to another, and the cores of the atoms are closer to the bonding electrons than in the divided atoms, and the effective positive charge that acts upon the bonding electrons is much greater than in the case of divided atoms (in molecule H₂ by 1.5 times). That is, the role of the atom's positive charge in the energy gain is much greater than the role of attracting the nuclei of one atom to the electrons of another atom.

The answers to the rest of the questions, mentioned above, are given in the book *How Chemical Bonds Form and Chemical Reactions Proceed* and *General Chemistry (Part I)*. Please See www.ITChem.com

The authors would be thankful to all readers who would kindly notify them of their own viewpoints in respect to the above mentioned work. We welcome all criticism and questions. All questions and remarks are welcome via e-mail victor_gankin@hotmail.com