

# On the Nature of Conductors and Dielectrics

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## **Abstract**

In this article, the theory of chemical bonding, developed based on the author's theory of compressible oscillating ether, is applied to the analysis of the interaction of valence electrons of atoms in the metallic crystal lattices of Group I metals and the molecular crystal lattices of Group VII halogens. It is demonstrated that the valence electrons of metals are weakly bound by their intersecting parts, which ensures the stability of the metals' crystal structure and proves the existence of a current in a conductor in the form of a directed wave of disturbances of interacting valence electrons, traveling at the speed of light along the conductor's metallic lattice. This refutes the conclusions of modern quantum band theory of solids regarding the causes of metal electrical conductivity. It is also demonstrated that the valence electrons of diatomic halogen molecules (except iodine) located at adjacent sites of molecular crystal lattices do not intersect, which excludes the possibility of an electric current wave passing through such a molecular crystal lattice. The causes of the electrical conductivity of solid crystalline iodine are elucidated.

**Key Words:** Compressible Ether, Chemical Bond, Metallic and Molecular Lattices, Electric Current, Conductors and Dielectrics.

## **1. Introduction**

As is well known, the modern quantum theory of conductivity is based on the electron band theory, which is a theory of electron motion in materials depending on the type of electron energy spectrum [1-4]. According to this theory, the conduction and valence bands of metals, which are good conductors of electric current, overlap, which explains the electrical conductivity of metals by the presence of a large number of free valence electrons (electron gas) and their ability to move freely within the metal. It is known that only a quarter of all chemical elements are non-metals, and half of these can exhibit semiconductor properties. The remaining elements are dielectrics, and it is believed that dielectrics, unlike conductors, contain very few or no free electrons, which determines their inability to conduct electric current.

In [5], a theory of the chemical bonding of atoms in the metallic crystal lattice of lithium is constructed based on the author's theory of compressible oscillating ether [6-7]. It is demonstrated that the valence electrons of lithium are weakly bound by their intersecting parts, which ensures the stability of the lithium crystal structure and excludes the presence of free electrons in the conductor. This result refutes the conclusions of modern quantum band theory regarding the causes of the electrical conductivity of metals. A solution to the system of ether equations is found in which the compression and expansion of the ether density in the sphere of the valence electron occurs exclusively in the direction of the electron spin (the axis of rotation of the azimuthal wave within the electron). This proves the existence of a directed oscillation wave with a specific frequency of interacting valence electrons of lithium atoms. Based on the evidence, it was concluded that electric current is not the movement of free electrons within the crystal lattice of a conductor, as postulated by the modern band theory of conductivity, but a directed wave of disturbances of interacting valence electrons, running at the speed of light along a metallic crystal lattice.

In the present paper, the results of [5] are generalized to the metals of the first group and the halogens of the first subgroup of the seventh group of the periodic table of chemical elements. Data on the radii of atoms of chemical elements, their covalent and van der Waals radii and bond lengths of atoms in molecules are taken from the website WebElements.com [8], data on the values of the dissociation energies of molecules and ionization energies of atoms are taken from works [9-11]. It is proven that the valence electrons of atoms of any metal of the first group have intersecting interacting parts, which ensures the passage of an electric current wave through the crystal lattice of the metal. In contrast, the valence electrons of halogen atoms located in different nodes of their molecular crystal lattices do not intersect and do not interact (except for the valence electrons of atoms of the crystal lattice of solid iodine), which explains the lack of conductivity in halogens and the nature of dielectrics in general as the impossibility of the passage of a directed electric current wave.

## 2. Chemical Bonding of Atoms by Only Outer Valence Electrons

The simplest example of such a bond is the bond between two hydrogen atoms to form a hydrogen molecule. A detailed description of such a bond is given by the author in [5, 12]. The diatomic molecule  $A_2$  consists of two atoms  $A$  of some element. Any atom  $A$  of a metal of the first group of the periodic table, as well as any halogen atom of the first subgroup of the seventh group, can be represented as a positive cation of the atom  $A^+$ , bound to the outer valence electron  $e$ . Let the values of the dissociation energy of a diatomic molecule of element  $D_{A_2}(A_2 \rightarrow A + A)$  and the ionization energy  $E_A(A \rightarrow A^+ + e)$  of atom  $A$  be experimentally known. Let the bond length  $d$  of the molecule, that is, the distance between the nuclei of two atoms of the molecule, also be measured experimentally. The energy expended on the dissociation of a diatomic molecule is equal to the energy released when two atoms  $A$  bind into a molecule. And since the binding energy of an electron with a cation in atom  $A$ , which is its ionization energy, is equal to  $E_A$ , then the total binding energy of two electrons with two cations of the atom during the formation of a diatomic molecule from two free cations and two free electrons is equal to  $(E_A + E_A + D_{A_2})$ . On the other hand, the binding energy of a diatomic molecule consists of two binding energies of two electrons with two cations located at distances  $s = d$  and  $s = 0$  from the nuclei, minus the energy required to bring two cations  $A^+$  closer to the distance  $d$  between their nuclei. Consequently, the equation holds

$$2E_{ek}(d, r_b) + 2E_{ek}(0, r_b) - E_{kk}(d) = E_A + E_A + D_{A_2}, \quad (1)$$

where  $E_{ek}(s, r_b)$  is the binding energy (in electron volts) of an electron of radius  $r_b$  with one cation located at a distance  $s$  from the center of the electron, and  $E_{kk}(s)$  is the energy that must be expended to bring two cations closer to a distance  $s$  between them. In [12], it was shown that the energy  $E_{pp}(s)$  of bringing two protons together in a hydrogen molecule is a fraction of the Coulomb energy

$$E_{pp}(s) = 0.34(E_H r_H)/s, \quad (2)$$

where  $E_H=13.598$  eV is the ionization energy of the hydrogen atom,  $r_H = 0.528\text{\AA}$  is the radius of the hydrogen atom, which is the radius of the electron in the state bound to the proton. Since any cation  $A^+$  has a proton charge, we will assume that formula (2) is valid for all diatomic molecules, the bond between the atoms of which is realized by two outer valence electrons. Then  $E_{kk}(d) = E_{pp}(d)$ . The binding energy  $E_{ep}(s, r_b)$  for the hydrogen molecule is calculated in [5,12]:

$$E_{ep}(s, r_b) = \frac{E_H}{(2a + \frac{\pi}{2})} \int_0^\pi \frac{(a + \sin\theta)\sin\theta d\theta}{\left(\left(\frac{s}{r_H}\right)^2 + \left(\frac{r_b}{r_H}\right)^2 - 2\left(\frac{s}{r_H}\right)\left(\frac{r_b}{r_H}\right)\cos\theta\right)^{1/2}}, \quad (3)$$

where  $a = 1/7$ , and  $E_{ep}(s, r_b) = E_H$  for  $s = 0$ ,  $r_b = r_H$ . Generalizing formula (3) to the bond of an electron with a cation of an arbitrary atom, we find that

$$E_{ek}(s, r_b) = \frac{E_A}{(2a + \frac{\pi}{2})} \int_0^\pi \frac{(a + \sin\theta)\sin\theta d\theta}{\left(\left(\frac{s}{r_A}\right)^2 + \left(\frac{r_b}{r_A}\right)^2 - 2\left(\frac{s}{r_A}\right)\left(\frac{r_b}{r_A}\right)\cos\theta\right)^{1/2}}, \quad (4).$$

Then, assuming  $x = r_b/r_A$ ,  $b = d/r_A$ , we rewrite equation (1) in the form

$$\frac{2E_A}{(2a + \frac{\pi}{2})} \int_0^\pi \frac{(\sin\theta/7 + \sin^2\theta)d\theta}{(b^2 + x^2 - 2 \cdot bx\cos\theta)^{1/2}} + \frac{2E_A}{x} = 2E_A + D_{A_2} + E_{pp}(d). \quad (5)$$

By numerically solving integral equation (5) for the parameter  $x = r_b/r_A$ , we find  $x$  and then the radius  $r_b$  of the electrons in a diatomic molecule. If an outer valence electron with radius  $r_b$ , located at a crystal lattice site, intersects with other valence electrons located at other crystal lattice sites, an electric current wave can flow through the lattice. In this case, the chemical element is a conductor. Otherwise, when valence electrons located at different crystal lattice sites do not intersect, an electric current wave cannot exist, and the chemical element is an insulator.

### 3. Chemical Bonding of Atoms in The Crystal Lattices of Metals of The First Group

It is known that the elements of the first group of the periodic table are metals that conduct electricity well. We will construct a theory of the chemical bonding of atoms in the crystal lattices of metals of the first group by analogy with the above-discussed theory of the chemical bonding of atoms by two outer valence electrons to form diatomic molecules. Since all initial data regarding the atomic radii of the metals under consideration are now taken from a single source, WebElements.com, the results obtained previously in [5] for lithium have been recalculated. This ultimately led to a slight increase in the size of the valence electrons in the metallic crystal lattice of lithium compared to [5], further confirming the nature of metallic lithium's electrical conductivity.

#### 3.1 Chemical Bonding of Atoms in The Metallic Lattice of Lithium

Metallic lithium has a body-centered cubic metallic lattice structure with a lattice parameter of  $a = 3.49\text{\AA}$  and the shortest possible distance between lattice sites of  $3.03\text{\AA}$ . A lithium atom has only three electrons, two of which are in the first energy level, close to the nucleus, and the third valence electron is in the third energy level. Therefore, although the radius of a lithium atom is  $1.45\text{\AA}$ , the radius of its  $\text{Li}^+$  cation is only  $0.60\text{\AA}$ . The inner, tightly bound electrons will have little effect from other lithium atoms, so we conclude that one and only one valence electron of each atom imparts metallic properties to the lithium crystal. All bonds of the atom with its nearest eight neighbors are due to this single electron (per atom), the binding force of which is thus "smeared out." This also follows from a comparison of the bond length ( $2.67\text{\AA}$ ) in the diatomic molecule  $\text{Li}_2$  with the shortest possible distance ( $3.03\text{\AA}$ ) between atoms in the metal. The increased bond length in the metal means that the bond is weakened; at the same time, the number of bonds in the metal is greater, as a result of which the total bond energy per atom increases from  $0.56\text{ eV}$  in the molecule to  $1.692\text{ eV}$  in the metal. However, the bond energy between two individual atoms is  $1.12\text{ eV}$  in the molecule and  $0.212\text{ eV}$  in the metal. Consequently, valence electrons are bound more strongly in the metal than in the molecule, but their binding force is distributed among a larger number of objects. Thus, the energy expended on the bond between two lithium atoms in the metal is  $0.212\text{ eV}$ .

The values of the dissociation energy of a gaseous lithium molecule and the ionization energy of a lithium atom are known experimentally

$$D_{\text{Li}_2}(\text{Li}_2 \rightarrow \text{Li} + \text{Li}) = 1.128\text{eV}, \quad E_{\text{Li}}(\text{Li} \rightarrow \text{Li}^+ + e) = 5.39\text{eV}.$$

The bond length of a gaseous lithium molecule, i.e. the distance between the two nuclei of the molecule's atoms, was also measured experimentally:  $d = 2.67\text{\AA} = 5.057r_{\text{H}}$ , where  $r_{\text{H}} = 0.528\text{\AA}$  is the radius of a hydrogen atom. By analogy with the hydrogen atom, we will assume that the bond between two lithium atoms in the metal is realized by binding two positive lithium ions  $\text{Li}^+$  with two electrons. On the one hand, the total binding energy of two electrons with two lithium cations during the formation of a metallic bond of two lithium atoms from two free lithium cations and two free electrons is equal to the sum of the formation energies of two lithium atoms (the sum of two ionization energies  $5.39\text{eV} + 5.39\text{eV}$ ) and the binding energy of two adjacent lithium atoms in the metal ( $0.212\text{eV}$ ). On the other hand, this binding energy consists of the energy required to bring two positive lithium ions closer to a distance of  $a = 3.49\text{\AA} = 6.61r_{\text{H}} = 2.4r_{\text{Li}}$  and two binding energies of two electrons with two positive lithium ions located at distances of  $s = 2.4r_{\text{Li}}$  and  $s = 0$ . That is, the equation

$$2E_{\text{ek}}(2.4r_{\text{Li}}, r_{\text{b}}) + 2E_{\text{ek}}(0, r_{\text{b}}) - E_{\text{kk}}(2.4r_{\text{Li}}) = 10.99\text{eV},$$

where  $E_{\text{ek}}(s, r_{\text{b}})$  is the binding energy (in electron volts) of an electron of radius  $r_{\text{b}}$  with one cation located at a distance  $s$  from the center of the electron, and  $E_{\text{kk}}(s)$  is the energy that must be expended to bring two cations closer to a distance  $s$  between them.

Since the positive lithium ion has a proton charge, we can assume that  $E_{\text{kk}}(s, r_{\text{b}}) = E_{\text{pp}}(s, r_{\text{b}})$ . And since  $s = a = 6.61r_{\text{H}}$ , then under the assumptions made,  $E_{\text{kk}}(s) = 0.7\text{eV}$ , and, following (5), we have an equation for determining the radius  $r_{\text{b}}$  of valence electrons in the lithium metal lattice.

$$\frac{2E_{\text{Li}}}{(2a + \frac{\pi}{2})} \int_0^{\pi} \frac{(\sin\theta/7 + \sin^2\theta)d\theta}{(2.4^2 + x^2 - 2 \cdot 2.4x\cos\theta)^{1/2}} + \frac{2E_{\text{Li}}}{x} = 11.69\text{eV}. \quad (6)$$

By numerically solving the integral equation (6) for the parameter  $x = r_{\text{b}}/r_{\text{Li}}$ , we find that  $x = 1.46$ , that is, the radii of the valence electrons in the metallic lattice of lithium are  $r_{\text{b}} = 1.46r_{\text{Li}} = 2.12\text{\AA}$ , which is more than three times greater than the radius of the lithium cation  $\text{Li}^+$  (Fig. 1). And, since the size of the metallic crystal lattice of lithium is  $a = 3.49\text{\AA}$ , and the radii of the valence electrons binding the atoms in the crystal lattice are  $r_{\text{b}} = 2.12\text{\AA}$ , we obtain as a result that the valence electrons are bound by their intersecting parts, which ensures the stability of the crystalline structure of metallic lithium and ensures the passage of an electric current wave through it.

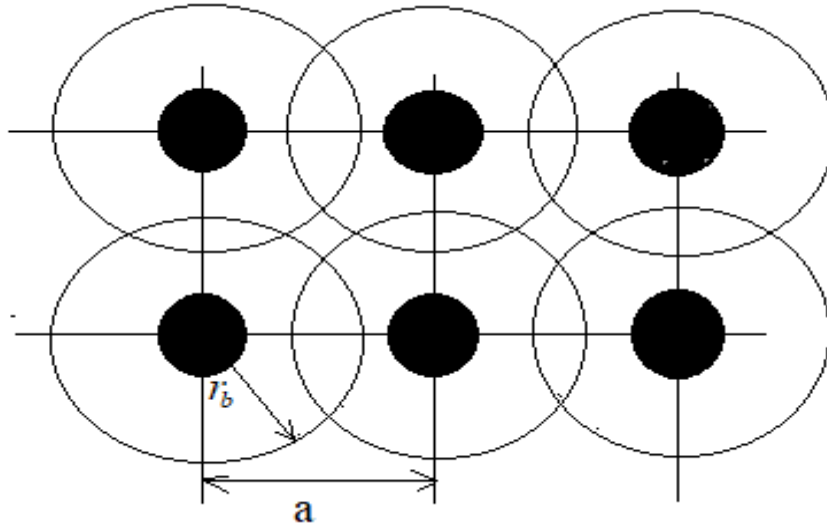


Fig. 1. Approximate diagram of the crystal lattice of metals of the first group.

### 3.2. Chemical Bonding of Atoms in The Metallic Lattice of Sodium

We will construct a theory of the chemical bonding of atoms in the sodium metallic crystal lattice by analogy with the theory of chemical bonding of atoms in the lithium metallic crystal lattice discussed above. Metallic sodium has a body-centered cubic crystalline structure with a lattice parameter of  $a = 4.29\text{\AA}$  and the shortest possible distance between lattice sites of  $3.72\text{\AA}$ . The sodium atom has eleven electrons, two of which are in the first energy level, close to the nucleus, eight electrons are in the second energy level, and one eleventh valence electron is in the third energy level. Therefore, although the radius of the sodium atom is  $1.8\text{\AA}$ , the radius of its cation  $\text{Na}^+$  is only  $0.95\text{\AA}$ . The inner, tightly bound electrons will be almost unaffected by other sodium atoms, so we conclude that the one and only one valence electron of each atom imparts metallic properties to the sodium crystal. All bonds of the atom with its nearest eight neighbors are due to this single electron (per atom), the binding force of which is thus "smeared out." This also follows from comparing the bond length ( $3.08\text{\AA}$ ) in the diatomic molecule  $\text{Na}_2$  with the shortest possible distance ( $3.72\text{\AA}$ ) between atoms in a metal. The increased bond length in a metal means that the bond is weakened; at the same time, the number of bonds in a metal is greater, as a result of which the total bond energy per atom increases from  $0.4\text{ eV}$  in a molecule to  $1.13\text{ eV}$  in a metal. But the bond energy between two individual atoms is  $0.793\text{ eV}$  in a molecule and  $0.141\text{ eV}$  in a metal. Consequently, valence electrons are bound more strongly in a metal than in a molecule, but their binding force is distributed among a larger number of objects. Thus, the energy expended in bonding two sodium atoms in the metal is  $0.141\text{ eV}$ .

The values of the dissociation energy of a gaseous sodium molecule and the ionization energy of a sodium atom are known experimentally

$$D_{\text{Na}_2}(\text{Na}_2 \rightarrow \text{Na} + \text{Na}) = 0.793\text{eV}, \quad E_{\text{Na}}(\text{Na} \rightarrow \text{Na}^+ + e) = 5.14\text{eV}.$$

The bond length of a gaseous sodium molecule, i.e. the distance between the two nuclei of the molecule's atoms, was also measured experimentally:  $d = 3.08\text{\AA} = 5.83r_{\text{H}}$ . By analogy with hydrogen and lithium atoms, we will assume that the bond between two sodium atoms in the metal is realized by the binding of two positive sodium ions  $\text{Na}^+$  with two valence electrons. On the one hand, the total binding energy of two electrons with two sodium cations during the formation of a metallic bond of two sodium atoms from two free sodium cations and two free electrons is equal to the sum of the formation energies of two sodium atoms (the sum of two ionization energies  $5.14\text{eV} + 5.14\text{eV}$ ) and the binding energy of two adjacent sodium atoms in the metal ( $0.141\text{eV}$ ). On the other hand, this binding energy consists of the energy required to bring two positive sodium ions located at the nodes of the crystal lattice closer to a distance of  $a = 4.29\text{\AA} = 2.383r_{\text{Na}} = 8.125r_{\text{H}}$  and two binding energies of two electrons with two positive sodium ions located at distances of  $s = 2.383r_{\text{Na}}$  and  $s = 0$ . That is, the equation

$$2E_{\text{ek}}(2.383r_{\text{Na}}, r_{\text{b}}) + 2E_{\text{ek}}(0, r_{\text{b}}) - E_{\text{kk}}(2.383r_{\text{Na}}) = 10.421\text{eV}, \quad (7)$$

where  $E_{\text{ek}}(s, r_{\text{b}})$  is the binding energy (in electron volts) of an electron of radius  $r_{\text{b}}$  with one cation located at a distance  $s$  from the center of the electron, and  $E_{\text{kk}}(s)$  is the energy that must be expended to bring two cations closer to a distance  $s$  between them. Since the positive sodium ion has a proton charge, we will assume that  $E_{\text{kk}}(s, r_{\text{b}}) = E_{\text{pp}}(s, r_{\text{b}})$ . Under these assumptions,  $E_{\text{kk}}(s) = 0.57\text{eV}$ . Then, from (5), it follows that the equation for determining the radius  $r_{\text{b}}$  of valence electrons in the sodium metallic lattice holds

$$\frac{2E_{Na}}{(2/7 + \frac{\pi}{2})} \int_0^{\pi} \frac{(\sin\theta/7 + \sin^2\theta)d\theta}{(2.383^2 + x^2 - 2 \cdot 2.383x\cos\theta)^{1/2}} + \frac{2E_{Na}}{x} = 10.991\text{eV}. \quad (8)$$

By solving numerically the integral equation (8) with respect to the parameter  $x = r_b/r_{Na}$ , we find that  $x = 1.495$  that is, the radii of the valence electrons in the metallic sodium lattice are equal to  $r_b = 1.495r_{Na} = 2.69\text{\AA}$  which is approximately 2.5 times greater than the radius of the sodium cation  $\text{Na}^+$ , and, since the size of the metallic sodium crystal lattice is  $a = 4.29\text{\AA}$ , and the radii of the valence electrons that bind the atoms in the metallic crystal lattice are equal to  $r_b = 2.69\text{\AA}$ , we obtain as a result that the valence electrons are bound by their intersecting parts, which ensures the stability of the crystalline structure of metallic sodium and ensures the passage of an electric current wave through it.

### 3.3. Chemical Bonding of Atoms in The Metallic Lattice of Potassium

We will construct a theory of the chemical bonding of atoms in the potassium metallic crystal lattice by analogy with the theory of chemical bonding of atoms in the lithium and sodium metallic crystal lattice discussed above. Metallic potassium has a body-centered cubic crystalline structure with a lattice parameter of  $a = 5.32\text{\AA}$  and the shortest possible distance between lattice sites of  $4.54\text{\AA}$ . The potassium atom has nineteen electrons, two of which are in the first energy level, close to the nucleus, eight electrons are at the second energy level and belong to the second electron layer, eight electrons are at the third energy level and belong to the third electron layer, and one, the nineteenth valence electron is at the fourth energy level and belongs to the fourth electron layer. Therefore, although the radius of the potassium atom is  $r_K = 2.2\text{\AA}$ , the radius of its cation  $\text{K}^+$  is only  $1.33\text{\AA}$ . The inner, tightly bound electrons will be almost unaffected by other potassium atoms, so we conclude that the one and only one valence electron of each atom imparts metallic properties to the kalium crystal. All bonds of the atom with its nearest eight neighbors are due to this single electron (per atom), the binding force of which is thus "smeared out." This also follows from comparing the bond length ( $3.92\text{\AA}$ ) in the diatomic molecule  $\text{K}_2$  with the shortest possible distance ( $4.54\text{\AA}$ ) between atoms in a metal. The increased bond length in a metal means that the bond is weakened; at the same time, the number of bonds in a metal is greater, as a result of which the total bond energy per atom increases from  $0.275\text{ eV}$  in a molecule to  $0.941\text{ eV}$  in a metal. But the bond energy between two individual atoms is  $0.55\text{ eV}$  in a molecule and  $0.117\text{ eV}$  in a metal. Consequently, valence electrons are bound more strongly in a metal than in a molecule, but their binding force is distributed among a larger number of objects. Thus, the energy expended in bonding two potassium atoms in the metal is  $0.117\text{ eV}$ .

The values of the dissociation energy of a molecule of potassium gas and the ionization energy of a potassium atom are known experimentally

$$D_{K_2}(\text{K}_2 \rightarrow \text{K} + \text{K}) = 0.55\text{eV}, \quad E_K(\text{K} \rightarrow \text{K}^+ + e) = 4.341\text{eV}.$$

The bond length of the potassium gas molecule, that is, the distance between the nuclei of two atoms of the molecule, was also measured experimentally:  $d = 3.92\text{\AA} = 7.424r_H$ . By analogy with the atoms of hydrogen, lithium and sodium, we will assume that the bond between two potassium atoms in a metal is carried out by the bonding of two positive potassium ions  $\text{K}^+$  with two valence electrons. On the one hand, the total binding energy of two electrons with two potassium cations during the formation of a metal bond of two potassium atoms from two free potassium cations and two free electrons is equal to the sum of the formation energies of two potassium atoms (the sum of two ionization energies  $4.341\text{eV} + 4.341\text{ eV}$ ) and the binding energy of two neighboring potassium atoms in the metal ( $0.117\text{ eV}$ ). On the other hand, this binding energy consists of the energy required to bring two positive potassium ions closer to a distance  $a = 5.32\text{\AA} = 2.418r_K = 10.076r_H$  and two binding energies of two electrons with two positive potassium ions located at distances  $s = 2.418r_K$  and  $s = 0$ . That is, the equation holds

$$2E_{ek}(2.418r_K, r_b) + 2E_{ek}(0, r_b) - E_{kk}(2.418r_K) = 8.8\text{ eV}, \quad (9)$$

where  $E_{ek}(s, r_b)$  is the binding energy (in electron volts) of a valence electron of radius  $r_b$  with a potassium cation, the center of which is located at a distance  $s$  from the center of the electron, and  $E_{kk}(s)$  is the energy that must be spent on bringing two potassium cations closer to a distance  $s$  between them. Since the positive potassium ion has the charge of a proton, we will assume that  $E_{kk}(s, r_b) = E_{pp}(s, r_b)$ . And since  $s = a = 10.076r_H$ , then with the assumptions made  $E_{kk}(s) = 0.459\text{eV}$ . Then from (5) it follows that there is an equation for determining the radius  $r_b$  of valence electrons in the potassium metal lattice.

$$\frac{2E_K}{(2/7 + \frac{\pi}{2})} \int_0^{\pi} \frac{(\sin\theta/7 + \sin^2\theta)d\theta}{(2.418^2 + x^2 - 2 \cdot 2.418x\cos\theta)^{1/2}} + \frac{2E_K}{x} = 9.259\text{ eV}. \quad (10)$$

Solving numerically the integral equation (10) with respect to the parameter  $x = r_b/r_K$ , we find that  $x = 1.492$ , that is, the radii of valence electrons in the potassium metal lattice are equal to  $r_b = 1.492r_K = 3.282\text{\AA}$ , which

is more than twice the radius of the potassium cation  $K^+$ . And, since the size of the potassium metal crystal lattice is  $a = 5.32\text{\AA}$ , and the radii of the valence electrons connecting atoms in the potassium crystal lattice are equal to  $r_b = 3.282\text{\AA}$ , the result is that the valence electrons are connected by their intersecting parts, which ensures the stability of the crystal structure of potassium metal and ensures the passage of an electric current wave through it.

### 3.4. Chemical Bonding of Atoms in The Metal Lattice of Rubidium

We will construct the theory of the chemical bond of atoms in the crystalline metal lattice of rubidium by analogy with the theory of the chemical bond of atoms in the crystalline metal lattices of lithium, sodium and potassium discussed above. Metallic rubidium has a crystalline body-centered cubic structure with a metal lattice parameter  $a = 5.7\text{\AA}$  and the shortest possible distance between lattice points equal to  $4.96\text{\AA}$ . The rubidium atom has thirty-seven electrons, two of which are in the first energy level close to the nucleus, eight electrons are in the second energy level and belong to the second electron layer, eight electrons are in the third energy level and belong to the third electron layer, ten and eight electrons belong to the fourth electron layer, and one thirty-seventh valence electron belongs to the fifth electron layer. Therefore, although the radius of the rubidium atom is  $r_{Rb} = 2.35\text{\AA}$ , the radius of its cation  $Rb^+$  is only  $1.48\text{\AA}$ . The internal strongly bonded electrons will be largely unaffected by other rubidium atoms, so we conclude that one and only one valence electron of each atom imparts metallic properties to the rubidium crystal. All bonds of an atom with its nearest eight neighbors owe their existence to this single (per atom) electron, the binding force of which is thus "smeared out". This also follows from a comparison of the bond length ( $4.20\text{\AA}$ ) in the diatomic  $Rb_2$  molecule with the shortest possible distance ( $4.96\text{\AA}$ ) between atoms in the metal. An increased length of the bond in the metal means that the latter is weakened; at the same time, the number of bonds in the metal is greater, as a result of which the total binding energy per atom increases from  $0.215\text{ eV}$  in a molecule to  $0.858\text{ eV}$  in a metal. But the binding energy between two individual atoms is  $0.429\text{ eV}$  in a molecule and  $0.107\text{ eV}$  in a metal. Consequently, valence electrons are bound more strongly in a metal than in a molecule, but their binding force is distributed among a larger number of objects. Thus, the energy spent on the bond of two rubidium atoms in the metal is  $0.107\text{ eV}$ .

The values of the dissociation energy of a molecule of gaseous rubidium and the ionization energy of a rubidium atom are known experimentally

$$D_{Rb_2}(Rb_2 \rightarrow Rb + Rb) = 0.429\text{ eV}, \quad E_{Rb}(Rb \rightarrow Rb^+ + e) = 4.18\text{ eV}.$$

The bond length of a gaseous rubidium molecule, that is, the distance between the nuclei of two atoms of the molecule, was also measured experimentally:  $d = 4.2\text{\AA} = 1.787r_{Rb} = 7.955r_H$ . By analogy with the atoms of lithium, sodium and potassium, we will assume that the bond between two rubidium atoms in a metal is carried out by the bonding of two positive rubidium ions  $Rb^+$  with two valence electrons. On the one hand, the total binding energy of two electrons with two rubidium cations during the formation of a metallic bond of two rubidium atoms from two free rubidium cations and two free electrons is equal to the sum of the formation energies of two rubidium atoms (the sum of two ionization energies  $4.18\text{ eV} + 4.18\text{ eV}$ ) and the binding energy of two neighboring rubidium atoms in the metal ( $0.107\text{ eV}$ ). On the other hand, this binding energy consists of the energy required to bring two positive rubidium ions closer to a distance  $a = 5.7\text{\AA} = 2.425r_{Rb} = 10.795r_H$  and two binding energies of two electrons with two positive rubidium ions located at distances  $s = 2.425r_{Rb}$  and  $s = 0$ . That is, the equation holds

$$2E_{ek}(2.425r_{Rb}, r_b) + 2E_{ek}(0, r_b) - E_{kk}(2.425r_{Rb}) = 8.467\text{ eV}, \quad (11)$$

where  $E_{ek}(s, r_b)$  is the binding energy (in electron volts) of a valence electron of radius  $r_b$  with a rubidium cation, the center of which is located at a distance  $s$  from the electron center, and  $E_{kk}(s)$  is the energy that must be spent on bringing two rubidium cations closer to a distance  $s$  between them. Since the positive rubidium ion has the charge of a proton, we will assume that  $E_{kk}(s, r_b) = E_{pp}(s, r_b)$ . And since  $s = a = 10.795r_H$ , then with the assumptions made  $E_{kk}(s) = 0.428\text{ eV}$ . Then from (5) it follows that there is an equation for determining the radius  $r_b$  of valence electrons in the rubidium metal lattice.

$$\frac{2E_{Rb}}{(2/7 + \frac{\pi}{2})} \int_0^\pi \frac{(\sin\theta/7 + \sin^2\theta)d\theta}{(2.425^2 + x^2 - 2 \cdot 2.425x\cos\theta)^{1/2}} + \frac{2E_{Rb}}{x} = 8.895\text{ eV}. \quad (12)$$

Solving numerically the integral equation (12) with respect to the parameter  $x = r_b/r_{Rb}$ , we find that  $x = 1.495$ , that is, the radii of valence electrons in the rubidium metal lattice are equal to  $r_b = 1.495r_{Rb} = 3.513\text{\AA}$ , which is approximately 2.5 times greater than the radius of the rubidium cation  $Rb^+$ . And, since the size of the metal crystal lattice of rubidium is  $a = 5.7\text{\AA}$ , and the radii of the valence electrons connecting atoms in the crystal lattice of rubidium are equal to  $r_b = 3.513\text{\AA}$ , the result is that the valence electrons are connected by their intersecting parts, which ensures the stability of the crystal structure of metal rubidium and ensures the passage of an electric current wave through it.

### 3.5. Chemical Bonding of Atoms in The Metallic Lattice of Cesium

We will construct a theory of the chemical bonding of atoms in the cesium metallic crystal lattice by analogy with the theory of chemical bonding of atoms in the metallic crystal lattices of lithium, sodium, potassium, and rubidium discussed above. Metallic cesium has a body-centered cubic crystalline structure with a lattice parameter of  $a = 6.14\text{\AA}$  and the shortest possible distance between lattice sites equal to  $5.3\text{\AA}$ . The cesium atom has fifty-five electrons, two of which are in the first energy level, close to the nucleus, eight electrons are in the second energy level and belong to the second electron shell, eight electrons are in the third energy level and belong to the third electron shell, eighteen electrons belong to the fourth electron shell, eighteen electrons belong to the fifth electron shell, and one fifty-fifth valence electron belongs to the sixth electron shell. Therefore, although the radius of the cesium atom is  $r_{Cs} = 2.6\text{\AA}$ , the radius of its cation  $Cs^+$  is only  $1.69\text{\AA}$ . The inner, tightly bound electrons will be almost unaffected by other cesium atoms, so we conclude that one and only one valence electron of each atom imparts metallic properties to the cesium crystal. All bonds between an atom and its eight nearest neighbors are due to this single electron (per atom), whose binding force is thus "smeared." This also follows from a comparison of the bond length ( $4.64\text{\AA}$ ) in the diatomic molecule  $Cs_2$  with the shortest possible distance ( $5.3\text{\AA}$ ) between atoms in a metal. The increased "bond" length in a metal means that the bond is weakened; at the same time, the number of bonds in a metal is greater, as a result of which the total binding energy per atom increases from  $0.245\text{ eV}$  in a molecule to  $0.827\text{ eV}$  in a metal. However, the binding energy between two individual atoms is  $0.49\text{ eV}$  in a molecule and  $0.103\text{ eV}$  in a metal. Consequently, valence electrons are bound more strongly in a metal than in a molecule, but their binding force is distributed among a larger number of objects. Thus, the energy spent on the bond between two cesium atoms in the metal is  $0.103\text{ eV}$

The values of the dissociation energy of a gaseous cesium molecule and the ionization energy of a cesium atom are known experimentally

$$D_{Cs_2}(Cs_2 \rightarrow Cs + Cs) = 0.49\text{eV}, \quad E_{Cs}(Cs \rightarrow Cs^+ + e) = 3.89\text{eV}.$$

The bond length of a gaseous cesium molecule, i.e. the distance between the nuclei of two atoms of the molecule, was also measured experimentally:  $d = 4.3\text{\AA} = 8.144r_H$ . By analogy with the atoms of lithium, sodium, potassium and rubidium, we will assume that the bond between two cesium atoms in the metal is realized by binding two positive cesium ions  $Cs^+$  with two valence electrons. On the one hand, the total binding energy of two electrons with two cesium cations during the formation of a metallic bond of two cesium atoms from two free cesium cations and two free electrons is equal to the sum of the energies of formation of two cesium atoms (the sum of two ionization energies  $3.89\text{eV}+3.89\text{eV}$ ) and the binding energy of two adjacent cesium atoms in the metal ( $0.103\text{eV}$ ). On the other hand, this binding energy consists of the energy required to bring two positive cesium ions closer to a distance of  $a = 6.14\text{\AA} = 2.361r_{Cs} = 11.629r_H$  and two binding energies of two electrons with two positive cesium ions located at distances of  $s = 2.361r_{Cs}$  and  $s = 0$ . That is, the equation holds

$$2E_{ek}(2.361r_{Cs}, r_b) + 2E_{ek}(0, r_b) - E_{kk}(2.361r_{Cs}) = 7.883\text{ eV}, \quad (13)$$

where  $E_{ek}(s, r_b)$  is the binding energy (in electron volts) of a valence electron of radius  $r_b$  with a cesium cation centered at distance  $s$  from the electron center, and  $E_{kk}(s)$  is the energy required to bring two cesium cations closer together to a distance of  $s$  between them. Since the positive cesium ion has a proton charge, we assume that  $E_{kk}(s, r_b) = E_{pp}(s, r_b)$ . And since  $s = a = 11.629r_H$ , under the assumptions made,  $E_{kk}(s) = 0.398\text{ eV}$ . Then it follows from (5) the equation for determining the radius  $r_b$  of valence electrons in the metallic cesium lattice

$$\frac{2E_{Cs}}{(2/7 + \frac{\pi}{2})} \int_0^\pi \frac{(\sin\theta/7 + \sin^2\theta)d\theta}{(2.361^2 + x^2 - 2 \cdot 2.361x\cos\theta)^{1/2}} + \frac{2E_{Cs}}{x} = 8.281\text{ eV}. \quad (14)$$

By numerically solving the integral equation (14) for the parameter  $x = r_b/r_{Cs}$  we find that  $x = 1.514$ , that is, the radii of the valence electrons in the metallic lattice of cesium are  $r_b = 1.514r_{Cs} = 3.936\text{\AA}$  which is approximately 2.5 times greater than the radius of the cesium cation  $Cs^+$ . And, since the size of the metallic crystal lattice of cesium is  $a = 6.1\text{\AA}$  and the radii of the valence electrons binding the atoms in the crystal lattice of cesium are  $r_b = 3.936\text{\AA}$ , we obtain as a result that the valence electrons are bound by their intersecting parts, which ensures the stability of the crystal structure of metallic cesium and ensures the passage of an electric current wave through it.

### 4. Chemical Bonding of Atoms in Molecular Crystal Lattices of Halogens

It is well known that halogens, elements of the first subgroup of Group VII of the Periodic Table of Chemical Elements, are dielectrics that conduct electricity poorly. In liquid and gaseous states, halogens exist as diatomic molecules, forming molecular crystalline structures in the solid state. We will construct a theory of the covalent chemical bonding of atoms in the molecular crystal lattices of halogens by analogy with the theory discussed above of the chemical bonding of two atoms by their two outer valence electrons, forming diatomic molecules. Using

fluorine, chlorine, and bromine as examples, we will demonstrate that the diameters of diatomic halogen molecules, even in their crystalline solid state, are small compared to the dimensions of their crystal lattices. That is, the valence electrons of different diatomic halogen molecules do not intersect, and therefore, electric current waves cannot propagate through their crystal lattices. This result is also true for the liquid and gaseous states of the halogens under consideration: fluorine, chlorine, and bromine. We will also show that an electric current wave can propagate through the molecular crystal lattice of solid iodine.

#### 4.1 Chemical Bonding of Atoms in The Fluorine Molecule

The fluorine molecule  $F_2$  in the solid, liquid, and gaseous states consists of two fluorine atoms F linked by a covalent non-polar bond. The covalent bond length of the fluorine molecule, that is, the distance between the nuclei of the atoms in the molecule, has been measured experimentally:  $d = 1.42\text{\AA} = 1.42 \cdot 10^{-8}\text{cm} = 2.689r_H$ . The radius of the free fluorine atom  $r_F = 0.50\text{\AA}$  and the van der Waals radius of the fluorine atom  $r_v = 1.46\text{\AA}$ , that is, the bond radius of an atom in a diatomic fluorine molecule  $F_2$ , defined as half the minimum distance between non-valently bonded atoms of adjacent molecules in crystals or condensed phases, have also been experimentally determined. Experimental values of the molecular crystal lattice parameters of fluorine in the solid state are also known.

Let us consider the formation of a fluorine molecule  $F_2$ , from two fluorine atoms linked by a covalent bond. Applying the concept of binding energy to explain the formation of a diatomic molecule yields the following results. Each fluorine atom contains nine electrons, seven of which are valence electrons, and only one of them is in the ninth energy level, the furthest from the nucleus. Therefore, since the radius of a fluorine atom is  $r_F = 0.5\text{\AA}$ , and the radius of its cation,  $F^+$  is 20-30% smaller, it can be assumed that the covalent bond between two fluorine atoms is realized exclusively by the two outer valence electrons, which are least bound to the nuclei. The inner electrons, which are strongly bound to the nuclei, should not participate in the formation of the covalent bond between the atoms in a fluorine molecule. Therefore, the bond between two fluorine atoms in a molecule can be represented as the bond between two positive fluorine ions  $F^+$  with two electrons. The values of the dissociation energy of the fluorine molecule and

$$D_{F_2}(F_2 \rightarrow F + F) = 1.562\text{eV}, \quad E_F(F \rightarrow F^+ + e) = 17.423\text{eV}.$$

On the one hand, the total binding energy of two electrons with two positive fluorine ions during the formation of a fluorine molecule from two free fluorine cations and two free electrons is equal to the sum of the energies of formation of two fluorine atoms (the sum of two ionization energies  $17.423\text{ eV} + 17.423\text{ eV}$ ) and the binding energy of two adjacent fluorine atoms in the molecule, equal to its dissociation energy ( $1.562\text{ eV}$ ). On the other hand, this binding energy consists of the energy required to bring two positive fluorine ions closer to a distance of  $d = 1.42\text{\AA} = 2.84r_F = 2.689r_H$  and two binding energies of two electrons with two positive fluorine ions located at distances  $s = 0$  and  $s = d = 2.84r_F$ . That is, the following equation holds:

$$2E_{ek}(2.84r_F, r_b) + 2E_{ek}(0, r_b) - E_{kk}(2.84r_F) = 36.408\text{eV}, \quad (15)$$

where  $E_{ek}(s, r_b)$  is the binding energy (in electron volts) of an electron of radius  $r_b$  with a fluorine cation whose center is at a distance  $s$  from the electron's center, and  $E_{kk}(s)$  is the energy required to bring two fluorine cations closer together to a distance  $s$  between them. Since the positive fluorine ion has a proton charge, we will assume that  $E_{kk}(s, r_b) = E_{pp}(s, r_b)$ . And since  $d = 2.689r_H$ , then under the assumptions made,  $E_{kk}(s) = 1.719\text{ eV}$ . Then it follows from (15) the equation for determining the radius  $r_b$  of the outer valence electrons in a fluorine molecule

$$2E_{ek}(2.84r_F, r_b) + 2E_{ek}(0, r_b) = 38.127\text{eV}.$$

Then, denoting  $x = r_b/r_F$ , we obtain the equation

$$\frac{2E_F}{(2/7 + \frac{\pi}{2})} \int_0^\pi \frac{(1/7 + \sin\theta)\sin\theta d\theta}{(2.84^2 + x^2 - 2 \cdot 2.84x \cos\theta)^{1/2}} + \frac{2E_F}{x} = 38.127\text{eV}.$$

Numerically solving the resulting integral equation, we find that  $x = 1.332$ , that is, the radii of the outer valence electrons in the fluorine molecule are  $r_b = 1.332r_F = 0.67\text{\AA}$ , which is much smaller than the van der Waals radius of the fluorine molecule  $r_v = 1.46\text{\AA}$  (Fig. 2).

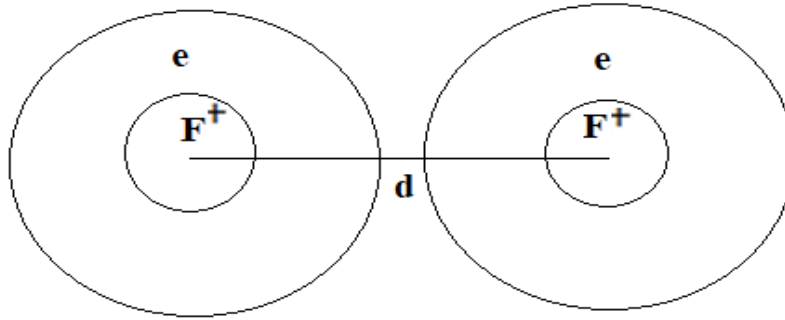


Fig. 2. Diagram of a diatomic fluorine molecule.

Thus, the electrons of different fluorine molecules located at different sites in the crystal lattice do not intersect. Consequently, an electric current wave cannot propagate through the fluorine crystal lattice. Furthermore, fluorine is not a conductor in its liquid or gaseous state under normal conditions

#### 4.2. Chemical Bonding of Atoms in The Chlorine Molecule

The chlorine molecule  $Cl_2$  in the solid, liquid, and gaseous states consists of two chlorine atoms Cl, linked by a covalent non-polar bond. The covalent bond length of the chlorine molecule, that is, the distance between the nuclei of the atoms in the molecule, has been measured experimentally:  $d = 1.98\text{\AA} = 1.98 \cdot 10^{-8}cm = 3.75r_H$ . The radius of the free chlorine atom  $r_{Cl} = 1.00\text{\AA}$  and the van der Waals radius of the chlorine atom  $r_c = 1.82\text{\AA}$ , that is, the bond radius of an atom in a diatomic chlorine molecule  $Cl_2$ , defined as half the minimum distance between non-valently bonded atoms of adjacent molecules in crystals or condensed phases, have also been found experimentally. The experimental values of the parameters of the molecular crystal orthorhombic lattice of chlorine in the solid state are also known  $a = 6.29\text{\AA}$ ,  $b = 4.5\text{\AA}$ ,  $c = 8.21\text{\AA}$ .

Let's consider the formation of the chlorine molecule  $Cl_2$  from two chlorine atoms linked by a covalent bond. Applying the concept of bond energy to explain the formation of a diatomic molecule yields the following results. Each chlorine atom contains 17 electrons, seven of which are valence electrons, and only one of them is in the ninth energy level, the furthest from the nucleus. Therefore, since the radius of the chlorine atom is  $r_{Cl} = 1.00\text{\AA}$ , and the radius of its cation  $Cl^+$  is 20-30% smaller, it can be assumed that the covalent bond between the two chlorine atoms is realized exclusively by the two outer valence electrons, which are least bound to the nuclei. The inner electrons, which are strongly bound to the nuclei, should not participate in the formation of the covalent bond between the atoms in the chlorine molecule. Therefore, the bond between two chlorine atoms in a molecule can be represented as the bond between two positive chlorine ions  $Cl^+$  with two electrons. The dissociation energy of a chlorine molecule and the ionization energy of a chlorine atom  $Cl$  are experimentally known.

$$D_{Cl_2}(Cl_2 \rightarrow Cl + Cl) = 2.476eV, \quad E_{Cl}(Cl \rightarrow Cl^+ + e) = 12.97eV.$$

On the one hand, the total binding energy of two electrons with two positive chlorine ions during the formation of a chlorine molecule from two free chlorine cations and two free electrons is equal to the sum of the energies of formation of two chlorine atoms (the sum of two ionization energies  $12.97\text{ eV} + 12.97\text{ eV}$ ) and the binding energy of two adjacent chlorine atoms in the molecule, equal to its dissociation energy ( $2.476\text{ eV}$ ). On the other hand, this binding energy consists of the energy required to bring two positive chlorine ions closer to a distance of  $d = 1.98\text{\AA} = 1.98r_{Cl} = 3.75r_H$  and two binding energies of two electrons with two positive chlorine ions located at distances  $s = 0$  and  $s = d = 1.98r_{Cl}$ . That is, the following equation holds:

$$2E_{ek}(1.98r_{Cl}, r_b) + 2E_{ek}(0, r_b) - E_{kk}(1.98r_{Cl}) = 28.416eV, \quad (16)$$

where  $E_{ek}(s, r_b)$  is the binding energy (in electron volts) of an electron of radius  $r_b$  with a chlorine cation whose center is at a distance  $s$  from the electron's center, and  $E_{kk}(s)$  is the energy required to bring two chlorine cations closer together to a distance of  $s$  between them. Since the positive chlorine ion has a proton charge, we assume that  $E_{kk}(s, r_b) = E_{pp}(s, r_b)$ . And since  $d = 3.75r_H$ , under the assumptions made,  $E_{kk}(s) = 1.2339B$ . And, as follows from (16), there is an equation for determining the radius  $r_b$  of the outer valence electrons in the chlorine molecule:

$$2E_{ek}(1.98r_{Cl}, r_b) + 2E_{ek}(0, r_b) = 29.649eV.$$

Then, denoting  $x = r_b/r_{Cl}$ , we obtain the equation

$$\frac{2E_{Cl}}{(2/7 + \frac{\pi}{2})} \int_0^{\pi} \frac{(1/7 + \sin\theta)\sin\theta d\theta}{(1.98^2 + x^2 - 2 \cdot 1.98x \cos\theta)^{1/2}} + \frac{2E_{Cl}}{x} = 29.649eV.$$

Solving the resulting integral equation numerically, we find that  $x = 1.491$ , meaning the radii of the outer valence electrons in the chlorine molecule are  $r_b = 1.491r_{Cl} = 1.491\text{\AA}$ , which is much smaller than the van der Waals radius of the chlorine molecule,  $r_v = 1.82\text{\AA}$ . Thus, the electrons of different chlorine molecules, located at different sites in the molecular crystal lattice, do not intersect. Consequently, an electric current wave cannot propagate through the crystalline chlorine lattice. Furthermore, chlorine is not a conductor in its liquid or gaseous state under normal conditions.

### 4.3. Chemical Bonding of Atoms in The Bromine Molecule

The bromine molecule  $Br_2$  consists of two bromine atoms Br, linked by a covalent non-polar bond. The covalent bond length of the bromine molecule, that is, the distance between the nuclei of the atoms in the molecule, has been measured experimentally:  $d = 2.28\text{\AA} = 2.28 \cdot 10^{-8}cm = 4.318r_H$ . The radius of the free bromine atom  $r_{Br} = 1.15\text{\AA}$  and the van der Waals radius of the bromine atom, that is, the bond radius  $r_v = 1.86\text{\AA}$  of the atom in the diatomic bromine molecule  $Br_2$ , defined as half the minimum distance between non-valently bonded atoms of adjacent molecules in crystals or condensed phases, have also been found experimentally. The experimental values of the parameters of the molecular crystal lattice of bromine in the solid state are also known:  $a = 4.48\text{\AA}$ ,  $b = 6.67\text{\AA}$ ,  $c = 8.72\text{\AA}$ .

Let's consider the formation of a bromine molecule  $Br_2$  from two bromine atoms linked by a covalent bond. Applying the concept of binding energy to explain the formation of a diatomic molecule yields the following results. Each bromine atom contains 35 electrons, seven of which are valence electrons, and only one of them is in the eighteenth energy level, the furthest from the nucleus. Therefore, since the radius of a bromine atom is  $r_{Br} = 1.15\text{\AA}$ , and the radius of its cation,  $Br^+$ , is 20-30% smaller, it can be assumed that the covalent bond between the two bromine atoms is realized exclusively by the two outer valence electrons, the ones least bound to the nuclei. The inner electrons, strongly bound to the nuclei, should not participate in the formation of the covalent bond between the atoms in the bromine molecule. Therefore, the bond between two bromine atoms in a molecule can be represented as the bond between two positive bromine ions  $Br^+$  with two electrons. The values of the dissociation energy of a bromine molecule and the ionization energy of a bromine atom are experimentally known.

$$D_{Br_2}(Br_2 \rightarrow Br + Br) = 1.973eV, \quad E_{Br}(Br \rightarrow Br^+ + e) = 11.814eV.$$

On the one hand, the total binding energy of two electrons with two positive bromine ions during the formation of a bromine molecule from two free bromine cations and two free electrons is equal to the sum of the energies of formation of two bromine atoms (the sum of two ionization energies  $11.814\text{ eV} + 11.814\text{ eV}$ ) and the binding energy of two adjacent bromine atoms in the molecule, equal to its dissociation energy ( $1.973\text{ eV}$ ). On the other hand, this binding energy consists of the energy required to bring two positive bromine ions closer to a distance of  $d = 2.28\text{\AA} = 1.983r_{Br} = 4.318r_H$  and two binding energies of two electrons with two positive bromine ions located at distances  $s = 0$  and  $s = d = 1.983r_{Br}$ . That is, the following equation holds:

$$2E_{ek}(1.983r_{Br}, r_b) + 2E_{ek}(0, r_b) - E_{kk}(1.983r_{Br}) = 25.601eV, \quad (17)$$

where  $E_{ek}(s, r_b)$  is the binding energy (in electron volts) of an electron of radius  $r_c$  with a bromine cation whose center is at a distance  $s$  from the electron's center, and  $E_{kk}(s)$  is the energy required to bring two bromine cations closer to a distance  $s$  between them. Since the positive bromine ion has a proton charge, we will assume that  $E_{kk}(s, r_b) = E_{pp}(s, r_b)$ . And since  $d = 4.318r_H$ , then under the assumptions made,  $E_{kk}(s) = 1.07eV$ . It follows from (17) there is an equation for determining the radius  $r_b$  of the outer valence electrons in the bromine molecule

$$2E_{ei}(1.983r_{Br}, r_c) + 2E_{ei}(0, r_c) = 26.671eV.$$

Then, denoting  $x = r_b/r_{Br}$ , we obtain the equation

$$\frac{2E_{Br}}{(2/7 + \frac{\pi}{2})} \int_0^\pi \frac{(1/7 + \sin\theta)\sin\theta d\theta}{(1.983^2 + x^2 - 2 \cdot 1.983x \cos\theta)^{1/2}} + \frac{2E_{Br}}{x} = 26.67eV.$$

Solving the resulting integral equation numerically, we find that  $x = 1.518$ , that is, the radii of the outer valence electrons in the bromine molecule are  $r_b = 1.518r_{Br} = 1.746\text{\AA}$  (Fig. 3), which is less than the van der Waals radius of the bromine molecule  $r_v = 1.86\text{\AA}$ .

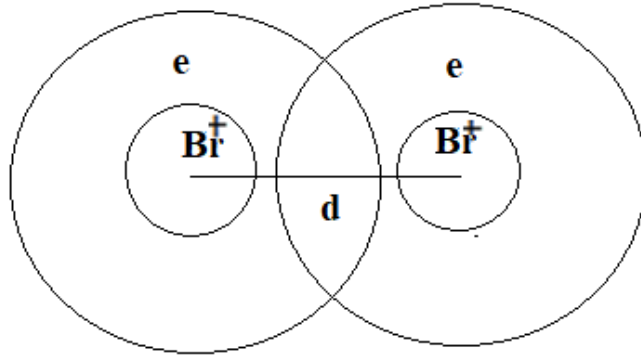


Fig. 3. Diagram of a diatomic bromine molecule.

Thus, the electrons of different solid bromine molecules located at different sites in the molecular crystal lattice do not intersect. Consequently, an electric current wave cannot propagate through the bromine lattice. Furthermore, bromine is not a conductor in its liquid or gaseous state under normal conditions.

#### 4.4 Chemical Bonding of Atoms in The Iodine Molecule

The iodine molecule  $I_2$  in the solid, liquid, and gaseous states consists of two iodine atoms I linked by a covalent nonpolar bond. The experimentally found radius of a free iodine atom  $r_I = 1.4 \text{ \AA}$ , the covalent radius of the iodine atom  $d/2 = 1.33 \text{ \AA}$  and the van der Waals radius of the iodine atom  $r_v = 2.04 \text{ \AA}$ , that is, the bond radius of an atom in a diatomic iodine molecule  $I_2$ , defined as half the minimum distance between non-valently bonded atoms of adjacent molecules in crystals or condensed phases. Thus, the covalent bond length of the iodine molecule, that is, the distance between the nuclei of atoms in the molecule is equal to  $d = 2.66 \text{ \AA} = 2.66 \cdot 10^{-8} \text{ cm} = 5.038 r_H$ . The experimental values of the parameters of the molecular orthorhombic crystal lattice of iodine in the solid state are also known:  $a = 7.18 \text{ \AA}$ ,  $b = 4.71 \text{ \AA}$ ,  $c = 9.81 \text{ \AA}$ .

Let us consider the formation of the iodine molecule  $I_2$  from two iodine atoms linked by a covalent bond. Applying the concept of binding energy to explain the formation of a diatomic molecule yields the following results. Each iodine atom contains 53 electrons, seven of which are valence electrons, and only one of them is in the twenty-seventh energy level, the furthest from the nucleus. Therefore, since the radius of the iodine atom is  $r_I = 1.4 \text{ \AA}$ , and the radius of its cation  $I^+$  is 20-30% smaller, it can be assumed that the covalent bond between two iodine atoms is realized exclusively by the two outer valence electrons, which are least bound to the nuclei. The inner electrons, strongly bound to the nuclei, should not participate in the formation of the covalent bond between the atoms in the iodine molecule. Therefore, the bonding of two iodine atoms into a molecule can be represented as the bonding of two positive iodine ions  $I^+$  with two electrons. The values of the dissociation energy of the iodine molecule and the ionization energy of the iodine atom are known experimentally

$$D_{I_2}(I_2 \rightarrow I + I) = 1.542 \text{ eV}, \quad E_I(I \rightarrow I^+ + e) = 10.45 \text{ eV}.$$

On the one hand, the total binding energy of two electrons with two positive iodine ions during the formation of an iodine molecule from two free iodine cations and two free electrons is equal to the sum of the energies of formation of two iodine atoms (the sum of two ionization energies  $10.45 \text{ eV} + 10.45 \text{ eV}$ ) and the binding energy of two adjacent iodine atoms in the molecule, equal to its dissociation energy ( $1.542 \text{ eV}$ ). On the other hand, this binding energy consists of the energy required to bring two positive iodine ions closer to a distance of  $d = 2.66 \text{ \AA} = 1.9 r_I = 5.038 r_H$  and two binding energies of two electrons with two positive iodine ions located at distances  $s = 0$  and  $s = d = 1.9 r_I$ . That is, the following equation holds true

$$2E_{ek}(1.9r_I, r_b) + 2E_{ek}(0, r_b) - E_{kk}(1.9r_I) = 22.442 \text{ eV}, \quad (18)$$

where  $E_{ek}(s, r_b)$  is the binding energy (in electron volts) of an electron of radius  $r_c$  with an iodine cation whose center is at a distance  $s$  from the electron's center, and  $E_{kk}(s)$  is the energy required to bring two iodine cations closer together to a distance  $s$  between them. Since the positive iodine ion has a proton charge, we will assume that  $E_{kk}(s, r_b) = E_{pp}(s, r_b)$ . And since  $d = 5.038 r_H$ , then under the assumptions made,  $E_{kk}(s) = 0.918 \text{ eV}$ . It follows from (18) there is an equation for determining the radius  $r_b$  of the outer valence electrons in the iodine molecule

$$2E_{ek}(1.9r_I, r_b) + 2E_{ek}(0, r_b) = 23.36 \text{ eV}.$$

Then, denoting  $x = r_b/r_I$ , we obtain the equation

$$\frac{2E_I}{(2/7 + \frac{\pi}{2})} \int_0^{\pi} \frac{(1/7 + \sin\theta)\sin\theta d\theta}{(1.9^2 + x^2 - 2 \cdot 1.9x \cos\theta)^{1/2}} + \frac{2E_I}{x} = 23.36\text{eV}.$$

Solving the resulting integral equation numerically, we find that  $x = 1.577$ , meaning the radii of the outer valence electrons in the iodine molecule are  $r_b = 1.577r_1 = 2.2\text{\AA}$ , which is slightly greater than the van der Waals radius of the iodine molecule,  $r_v = 2.04\text{\AA}$ . Thus, the electrons of different molecules of solid crystalline iodine, located at different sites in the crystal lattice, may have a slight intersection. Consequently, an electric current wave can propagate through the lattice of crystalline solid iodine. However, iodine is not a conductor in either the liquid or gaseous state.

## 5. Results and Discussion

The reasons for the good electrical conductivity of metals, which are elements of the first group of the periodic table of chemical elements, and the poor electrical conductivity of halogens, which are elements of the first subgroup of the seventh group, are examined. It is shown that the reason for the good electrical conductivity of metals is the intersection of their outer valence electrons of atoms belonging to adjacent sites of their metallic crystal lattices. In this case, an electric current can propagate through the metal's crystal lattice in the form of a directed wave of oscillations of interacting valence electrons. In contrast, the valence electrons of halogen atoms (except iodine), located at different sites of their molecular crystal lattices, do not intersect, which precludes the passage of an electric current wave through such a crystal lattice. An exception is the crystal lattice of solid iodine, through which an electric current wave can propagate, since the valence electrons of the atoms located at its sites intersect.

Research plans include constructing other models of multivalent chemical bonds of atoms in the crystal lattices of metals, semiconductors, and dielectrics.

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