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THE BINDING ENERGY OF THE ELEMENTS OF THE BIOLOGICAL TISSUE IN MOLECULES

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Abstract

The following was noticed in this study. The bond length in the molecules H-F, H-Cl, H-Br, H-I is 0.092; 0.128; 0.142; 0.162 nm, i.e. with an increase in the atomic number and size of the halogen atom, the length of its chemical bond with hydrogen increases accordingly. There are three main types of chemical bonds: metallic, covalent and ionic. The binding of metals occurs in metal crystals. The binding energy is determined for different molecules. It is known that with PDT, a photosensitizer is first injected into the tumor. The photosensitizer consists of organic elements.

Keywords: Photodynamic therapy (PDT), biological tissue, chemical bond length, electronegativity, effective charge, electron clouds, photosensitizer.

Introduction

With PDT, processes occur with the destruction of chemical bonds between the atoms of molecules in the biological tissue (BT). Therefore, it is interesting to see these parameters in the main elements of BT. Table 1 shows the main elements of BT as a percentage.

Table 1. Basic elements of BT in percentages

Elements	Quantity (in %)	Elements	Quantity (in %)
Oxygen	65-75	Calcium	0,04-2,00
Carbon	15-18	Magnesium	0,02-0,03
Hydrogen	8-10	Sodium	0,02-0,03
Nitrogen	1,5-3,0	Iron	0,01-0,015
Phosphorus	0,20-1,0	Zinc	0,0003
Potassium	0,15-0,4	Copper	0,0002
Sulfur	0,15-0,2	Iodine	0,0001
Chlorine	0,05-0,10	Fluorine	0,0001

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It is known from atomic physics that a chemical bond arises only if the total energy of the interacting atoms decreases, therefore, when a chemical bond is formed, energy is always released. The amount of energy released during the formation of a chemical bond is called the energy of a chemical bond.

This value is the most important characteristic of the bond strength, it is expressed in kilojoules per 1 mol of the formed substance. The bond energy is determined by comparing it with the state that preceded the formation of the bond. For example, the binding energy of hydrogen chloride, equal to 431.8 kJ / mol, shows that, compared with the ground state of hydrogen 1s1 and the ground state of chlorine ls22s22p63s23p5, the sum of the energies of which is taken as the initial level, the formation of HC1 released energy in the amount of 432 kJ /mol. The electron shell of the atoms of the BT elements is shown in Table 2.

Table 2. The structure of the electron shells of atoms of the first 20 elements of the D.I. Mendeleev

Period	**Element**	**The structure of the electron shell**	**Period**	**Element**	**The structure of the electron shell**
1	$_{1}H$	$1s^1$	3	$_{11}Na$	$1s^22s^22p^63s^1$
1	$_{2}He$	$1s^2$	3	$_{12}Mg$	$1s^22s^22p^63s^2$
2	$_{3}Li$	$1s^22s^1$	3	$_{13}Al$	$1s^22s^22p^63s^23p^1$
2	$_{4}Be$	$1s^22s^2$	3	$_{14}Si$	$1s^22s^22p^63s^23p^2$
2	$_{5}B$	$1s^22s^22p^1$	3	$_{15}P$	$1s^22s^22p^63s^23p^3$
2	$_{6}C$	$1s^22s^22p^2$	3	$_{16}S$	$1s^22s^22p^63s^23p^4$
2	$_{7}N$	$1s^22s^22p^3$	3	$_{17}Cl$	$1s^22s^22p^63s^23p^5$
2	$_{8}O$	$1s^22s^22p^4$	3	$_{18}Ar$	$1s^22s^22p^63s^23p^6$
2	$_{9}F$	$1s^22s^22p^5$	3	$_{19}K$	$1s^22s^22p^63s^23p^64s^1$
2	$_{10}Ne$	$1s^22s^22p^6$	3	$_{20}Ca$	$1s^22s^22p^63s^23p^64s^2$

For three and polyatomic molecules with the same type of bond, the average bond energy is calculated. The average bond energy is determined by dividing the energy of formation of a molecule from atoms by the number of bonds. For example, the energy of formation of an ammonia molecule NH3 at 298 K is 1170 kJ/mol. Accordingly, the average N—H bond energy is 1170/3=390 kJ/mol. The greater the bond energy, the stronger the bond. For example, the H-C1 bond is stronger than the H-Br bond, but less strong than the H-F bond (Table 3).

The most important geometric characteristics of a chemical bond are the length, the angles between bonds in molecules, crystals, etc. The length of a chemical bond is the distance between the nuclei of atoms in a molecule. It is determined experimentally using molecular spectroscopy, X-ray diffraction, etc. The bond lengths are determined by the size of the reacting atoms and the degree of overlap of their electron clouds. For example, the bond lengths in HX molecules are:

In H-F, H-Cl, H-Br, H-I molecules, the bond length is 0.092; 0.128; 0.142; 0.162 nm, respectively, i.e., as the atomic number and, accordingly, the size of the halogen atom increase, the length of its chemical bond with hydrogen increases. There are three main types of chemical bonds: metallic, covalent and ionic. A metallic bond occurs in metal crystals.

Table 3. Binding energy for hydrogen molecules

Connection	E, kJ/mol	Connection	E, kJ/mol	Connection	E, kJ/mol
H—H	436	H—F	536	F—F	159
H—C	415	H—CI	432	Cl—C1	243
H—N	390	H—Br	360	Br—Br	193
H—O	468	H—I	299	1—1	151

A covalent bond between atoms exists both in molecules and in crystals. It arises both between identical atoms (for example, in H2, C2 molecules, in a diamond crystal) and between different atoms (for example, in H2O and NH3 molecules, in SiC crystals). Almost all bonds in the molecules of organic compounds are covalent (C-C, C-H, C-N, etc.). Characteristic features of a covalent bond are its saturation and direction. The saturation of covalent bonds is due to the fact that only electrons of external energy levels participate in the chemical interaction, i.e. limited number of electrons.

According to Pauling, the force of attraction of an electron to an atom in a covalent bond is characterized by electronegativity (EO). If the interacting atoms are characterized by different electronegativity, then the socialized pair of electrons is shifted to the nucleus of a more electronegative atom. For example, the electronegativity of fluorine (4.0) is greater than the electronegativity of hydrogen (2.1), so the shared electron pair in the HF molecule is shifted towards fluorine. If a pair of electrons forming a chemical bond is shifted to one of the nuclei of atoms, then the bond is called a polar covalent bond.

Due to the displacement of a pair of electrons from one nucleus to another, the average negative charge density of one of the atoms will be higher than that of the other. Therefore, one of the atoms acquires an excess negative charge, the other an excess positive charge. These charges are called the effective charges of the atoms in the molecule. For example, the effective charges of atoms in the HC1 molecule are +0.17 and -0.17, i.e.
H + 0.17 - Cl-0.17, and in the LiF compound + 0.9 and -0.9, i.e. Li + 0.9 - F-0.9. A quantitative measure of the polarity of a chemical bond is the electric moment of the bond dipole rsv. The electric moment of the coupling dipole is the product of the effective charge δ and the distance between the centers of gravity of positive and negative charges l:

$$p_{\text{св}} = \delta l$$

Ionic bonding is carried out as a result of the formation and electrostatic interaction of oppositely charged ions. An ionic bond can only arise when there are large differences in the electronegativity values of the atoms. For example, an ionic bond occurs between cesium and fluorine, the difference in EO for which is more than three units. Typical compounds with ionic bonds include alkali metal halides, such as CsF, CsCl, NaCl.
An ionic bond can be considered as a limiting polar chemical bond, for which the effective charge of an atom is close to unity. At the same time, for a nonpolar covalent bond, the effective charge of the atoms is zero. The chemical bond of most compounds is polar, that is, it has an intermediate character between non-polar covalent and ionic bonds. We can say that such a covalent bond has a partially ionic character. The proportion of the ionic nature of the bond is called the degree of ionicity, which is quantitatively characterized by the effective charges of atoms in the molecule. For example, the degree of ionicity of HC1 and LiF molecules is 0.17 and 0.9, respectively. Therefore, these compounds have both covalent and ionic bonds. The degree of ionicity of a bond increases with an increase in the difference in the electronegativity of its constituent atoms (Pic. 1).
Thus, the nature of the chemical bond is one and the existing difference between the types of bonds has a quantitative character.

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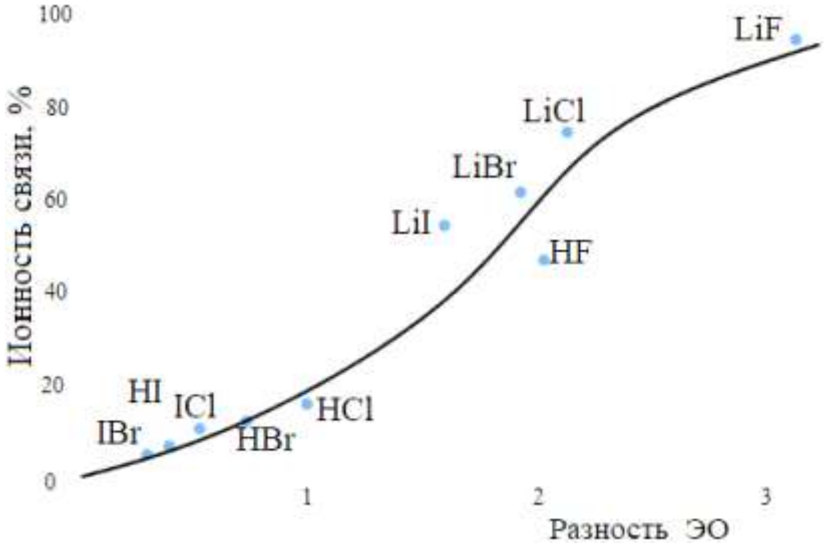
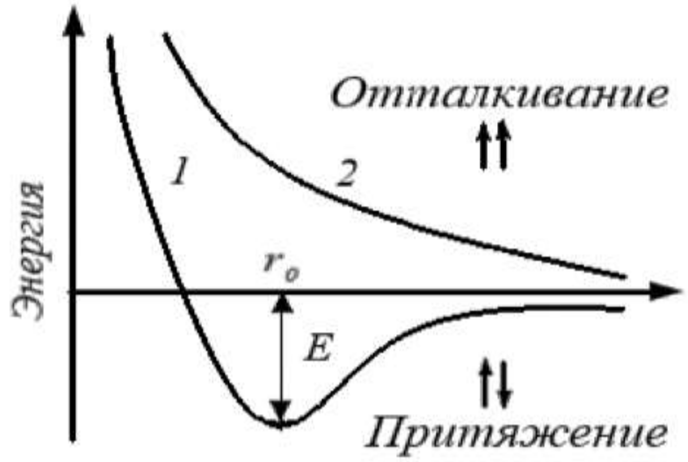


Pic. 1. Dependence of the bond ionicity on the EO of two atoms.

The method of valence bonds. The VS method assumes that a chemical bond is formed by two unpaired electrons with antiparallel spins. In this case, the socialization of electrons occurs, i.e., an electron pair is formed, belonging to two atoms.

In 1927, German scientists W. Geitler and F. London carried out a quantum mechanical calculation of the interaction of hydrogen atoms during the formation of the H2 molecule. As a result of an approximate solution of the Schrodinger equation, they deduced the dependence of the potential energy of the system on the distance between the nuclei of hydrogen atoms (Fig. 2). When two atoms approach, electrons with antiparallel spins are attracted simultaneously by two protons, so the potential energy of the system decreases (curve 1). When two atoms come together, not only the forces of attraction, but also the forces of repulsion act. Two electrons repel each other, the same is observed for two protons. The repulsive forces begin to prevail at very small distances between atoms. At a certain distance between the cores r0, the energy of the system is minimal. The system becomes the most stable, a chemical bond occurs and a hydrogen molecule is formed. For example, in a hydrogen molecule r0 = 0.074 nm. When atoms whose electrons have parallel spins approach, only their repulsion is observed, and the energy of the system increases (curve 2). Quantum mechanical calculations show that the electron density in the system during the interaction of two hydrogen atoms having antiparallel electron spins is maximal in the region lying between the nuclei.

At the same time, the electron density in the region between the nuclei of two atoms with parallel electron spins is minimal.



Pic. 2. Dependence of the potential energy of a system of two hydrogen atoms on the distance between the nuclei: 1 — antiparallel electron spins; 2 — parallel electron spins

Binding energies have been determined for various molecules. As is known, with PDT, a photosensitizer is first injected into the tumor. The photosensitizer consists of organic elements.

Table 4. Binding energies for various organic molecules are given.

Organic molecules	Bond energy, kJ/mol
$CH_3O–H\cdots O(C_2H_5)_2$	10,47
$CH_3O–H\cdots N(C_2H_5)_3$	12,56
$C_6H_5O–H\cdots O(C_2H_5)_2$	15,49
$C_6H_5O–H\cdots N(C_2H_5)_3$	24,28
$Cl_3C–H\cdots N(C_2H_5)_3$	16,74
$Cl_3C–H\cdots OC(CH_3)_2$	10,47
$HO–H\cdots OH_2$	20,93
F–H···F–H	29,31

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