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THE MECHANISM OF COMPOUND OF CHEMICAL ELEMENTS FOR THE TABLE OF D.I. MENDELEYEV AND THE VIRTUAL INTERAKTIVIZATION IN THE PROGRAM ENVIRONMENT FLASH-CC, JAVA SCRIPT

Abstract. It is asked creations of the virtual interactive laboratories with obviousness of deep mechanisms of chemical reactions at the atomic level in inorganic chemistry.

On the basis of a research practical use of results of the virtual laboratory operated (interactive) with visualization and animation of mechanisms course of processes, on inorganic and organic chemistry are planned. Will be applied to upgrading of tutoring, big saving of time (about 60% for assimilation of a subject), to self-contained carrying out research works, to development of creativity of students. The product will be used all system of secondary education (schools, lyceums, gymnasiums), all system of the higher education where study chemistry, research institutes and laboratories and also food, chemical, pharmaceutical, other technological industries.

Keywords: periodic system of elements, atom, electron, proton, neutron, atomic weight, Pauli's exclusion principle, rule Hunda, orbital, energy levels, valence.

Introduction. The periodic law – the greatest achievement for chemical science, fundamentals of all modern chemistry. With its opening the chemistry stopped being descriptive science, in it scientific anticipation became possible.

The periodic law is opened by D.I. Mendeleyev in 1869. The scientist formulated this law so: "Properties of simple bodies, also forms and properties of connections of elements are in periodic dependence on the size of atomic weights of elements" [1, 2].

More detailed studying of a structure of substance showed that frequency of properties of elements is caused not by atomic weight, but an electronic structure of atoms.

Nuclear charge is the characteristic defining an electronic structure of atoms and consequently, and properties of elements. Therefore in the modern formulation the Periodic law sounds: properties of simple substances and also forms and properties of connections of elements are in periodic dependence on ordinal value (from the size of nuclear charge of their atoms). Expression of the Periodic law is the periodic system of elements.

Periodic system of D.I. Mendeleyev

The periodic system of elements of D.I. Mendeleyev consists of seven periods which represent the horizontal sequences of elements located on increase of a charge of their atomic nucleus. The periods 1, 2, 3, 4, 5, 6 contain respectively 2, 8, 8, 18, 18, 32 elements. The seventh period is not complete. The periods 1, 2 and 3 call small, the others - larger.

Every period (except for the first) begins atoms of alkali metals (Li, Na, To, Rb, Cs, Fr) and comes to an end with a rare gas (Ne, Ar, Kr, Xe, Rn) to which typical nonmetal precedes. In the periods from left to right metal gradually weaken and nonmetallic properties as with body height of positive charge of atomic nuclei the number of electrons at the external level increases amplify [2].

In the first period, except helium, there is only one element - Hydrogenous. It is conditionally placed in IA or VIIA to subgroup as he shows similarity and to alkali metals, and to halogens. The similarity of Hydrogenous to alkali metals is shown that Hydrogenous, as well as alkali metals is reducer and, giving one electron, forms singly charged caution. It is more than common at Hydrogenous with halogens: Hydrogenous, as well as halogens nonmetal, its molecule it is biatomic, it can show oxidizing properties, forming with the fissile metals similar salts hydrides, for example, of NaH, CaH_2.

In the fourth period after Sa 10 transition elements (decade of Sc - Zn) are located behind which there are other 6 basic elements of the period (Ga - Kg). The fifth period is similarly constructed. The concept a transitional element is usually used for designation of any element with valence d– or f-electrons.

The sixth and seventh periods have double inserts of elements. Behind Ba element plug-in decade of d-elements (La - Hg), and after the first transition element of La follow 14 f-elements - lanthanides is located (Ce - Lu). After Hg other 6 main r-elements of the sixth period settle down (Tl - Rn).

In the seventh (incomplete) period for the Expert 14 f-elements-actinides follow (Th - Lr). Recently La and the Expert began to rank respectively as lanthanides and actinides. Lanthanides and actinides are placed separately in the bottom of the table.

Thus, each element in a periodic system holds strictly particular position which is noted serial, or atomic, by number [3].

In a periodic system eight groups are divided into subgroups (I-VIII) which in turn - main, or subgroups A and the secondary's, or B. Subgroups the VIII B-special are down located, it contains triads of the elements making families of iron (Fe, With, Ni) and platinum metals (Ru, Rh, Pd, Os, Ir, Pt).

Similarity of elements in each subgroup - the most noticeable and important regularity in a periodical system. In the main subgroups metallic from top to down amplify and nonmetallic weaken. At the same time there is an increase in stability of connections of elements in the lowest rate of oxidation for this subgroup. In the secondary subgroups – on the contrary – from top to down metallic weaken and stability of connections with the highest rate of oxidation increases.

Periodic system and electronic configurations of atoms

As at chemical reactions of a core of the reacting atoms do not change, chemical properties of atoms depend on a structure of their electronic shells.

Filling of electron layers and electronic shells of atoms happens according to a Pauli's exclusion principle and the rule Hunda.

Exclusion principle Pauli's (will lock Paulie)

Two electrons in atom can't have four identical quantum numbers (on each atomic orbital there can be no more than two electrons).

The Pauli's exclusion principle defines the maximal number of the electrons possessing this main quantum number of n (i.e. being on this electron layer): $N_n = 2n^2$. On the first electron layer (energy level) there can be no more than 2 electrons, on the second – 8, on the third – 18 etc.

In Hydrogenium atom, for example, there is one electron which is on the first energy level in 1s – a state. The spin of this electron can be directed randomly ($m_s = +1/2$ or $m_s = -1/2$). It is necessary to emphasize once again that the first energy level consists of one subtotal – 1s, the second energy level – of two subtotals – 2s and 2r, the third – of three subtotals – 3s, 3p, 3d etc. The subtotal, in turn, contains orbitals which number is defined by the secondariest quantum number l or equal $(2l + 1)$. Each orbital is conditionally designated by a cage, the electron which is on it – an arrow which direction indicates orientation of a spin of this electron. The arrangement of spins is defined by the rule Hunda which says: filling of energy levels happens so that the cooperative spin was maximal.

In atom each electron occupies the free orbital with the lowest energy answering to its greatest communication with a core. In 1961 M. Klechkovsky formulated the general provision according to which energy of electronic orbitals increases in an order of increase in the sum of the main and secondariest quantum numbers (n + l), and in case of equality of these sums, smaller energy has the orbital with smaller value of the main quantum number of n [5, 7].

Determination of valency

It agrees according to polarity formulas, all elements VI A and VI B group have the electronic configurations finished on p^4 and d^{4-5}. Within the electronic theory the valency of atom is defined on the basis of number of unpaired electrons which participate in formation of electronic couples with electrons

of other atoms. Only the electrons which are on an external envelope of atom participate in formation of chemical bonds. Therefore the maximum valence of chemical element is a number of electrons in the external electronic shell of its atom. Proceeding from it, all elements VI A and VI B group show different valencies: II, III, IV, V, VI.

And in cases of these three elements their valence is defined by the phenomenon of "breakthrough". The phenomenon of "breakthrough" represents symbolical transferring of one of two valence s-electrons on a d-subtotal that reflects no uniformity of deduction by a core of outer-shell electrons.

Determination of ability to react an element with other elements, the reason of limitation of reaction of chemical elements VI A and VI B group

External level of atom is called the level, farthest from a core, at which still there are electrons. This envelope adjoins at collision with external levels of other atoms in chemical reactions. At interaction with other atoms oxygen is capable to accept the 2nd padding electron on the external level. At the same time atom oxygen will receive complete, that is as much as possible the filled external electronic level on which 6 electrons will settle down. And the reason of limitation of reaction of chemical elements is explained by it. Proceeding from it, the rule Gunda is similar and for all elements of this group.

Characteristics of chemical elements naturally change in groups and the periods [13].

As the chemical bond, an atom structure, electronic shells of atom influence properties of an element, ability to react an element depend on these factors too. For example, the molecule of oxygen consists of two atoms. The chemical bond is the covalent non-polar.

Oxygen is distinguished by high reactivity, it oxidizes many substances already at ambient temperature. Oxygen forms connections with all chemical elements, except helium, neon and argon. It interacts with the majority of elements immediately, except halogens, except for fluorine, gold and platinum.

Determination of ability to react an element with other elements, the reason of limitation of reaction of chemical elements of lantanoyd's

Лантаноиды – это 14 элементов, следующих за лантаном, у которых к электронной конфигурации лантана последовательно добавляются 14 4f-электронов.

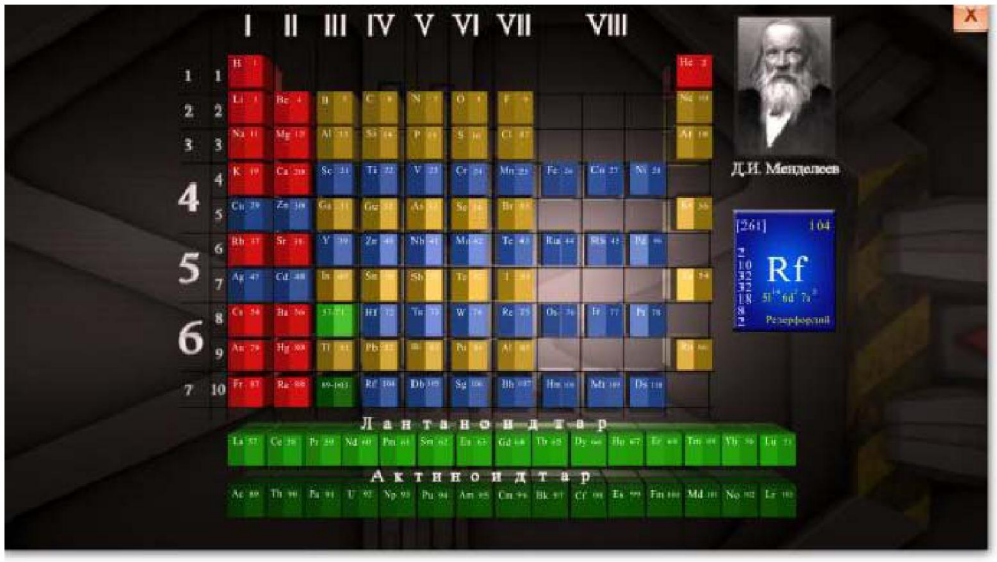
Animation images of movements and work with them demands the large volume of memory. And for reduction of memory size, there is use of the virtual – interaktivization of processes, Flash is very efficient [14-17]. From the basic vektorno – the graphic Flash format of technologies Shorewave Flash (SWF) – a branch was created. But, it is not the first vector format, it is the Web broadcast mechanism – pages to SWF as finding of the graphic representation, the coordinating link of an instrumental inventory and the graphic representation. Advantage of SWF-of the application it is easily an acceptability on other Wednesday, i.e. this format is used in different is information – the program platform (in the Mac OS Macintosh operating system, in OS - Windows OS). One more feature of SWF – the constructed main images not only accept animation but also is padding, an opportunity to create interactive elements and audio of installation, and to form interactive virtual laboratory, very conveniently the formats SWF, CC of them – the program Flash environment. One more reason of popularity of SWF – a format this very mild and convenient application instruments for other platforms development of Macromedia. For example: creations of the multimedia presentations use the program device – Macromedia Director Shockwave Studio, - and are applied the program device to creation of graphic images – Macromedia Authorwave, Macromedia Course Builder. Therefore among Web – the publication the most recognizable and easily applied publication is Macromedia Flash Web – gives the chance to decorate each website with animation and to collect the complete page. Action Script Tools - allows to collect Web addition efficiently and its modern languages similarly probably on the scenario Java Script, Action Script and by means of the editor of Devigger is the solution of often applied elements. For virtualization and an interactivity of electronic orbitals, electronic configurations on each element of the table of Mendeleyev Wednesday in a format CC – the program Flash and Web environment addition the scenario Java Script, Action Script and by means of the editor of Devigger is chosen computer program. On each element of the table of Mendeleyev it was created an electronic configuration according to the law Gunda. By the rule Gunda when filling with electrons of orbitals, identical on energy, electrons settle down first of all on the single on each orbital, and a population of these orbitals begins only then the second electrons.

For example the polarity formula of oxygen bears very important information: the external electronic level of oxygen is filled with electrons not till the end (on it 4+ 2 = 6 electrons) and before the complete filling there are not enough two electrons. The general view of the virtual and interactive table in the called program environment is given in the drawing-1. When pressing any button are automatically represented in movements - dynamics electronic configurations of any chemical element in flat-2D and volume - a 3D format and also the sequence of energy levels in ascending order of energy according to the following scheme:

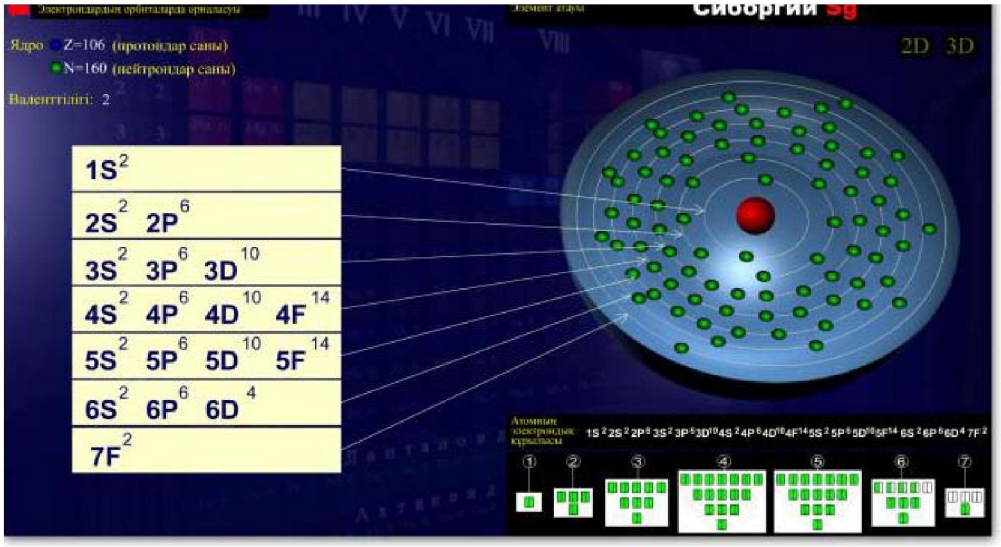
1s < 2s < 2p < 3s < 3p< 4s ≈ 3d < 4p < 5s ≈ 4d < 5p < 6s ≈ 5d ≈ 4f < 6p.

We see atomic weight, valencies, quantity of neutrons, the Russian and English name and polarity formulas for I (A, B) groups of elements. And also for each chemical element I (A, B) groups are brought ordinal values and polarity formulas in the form of drawings. As it is specified in the drawing-1, the ordinal value of chemical element is atomic number. It is equal to quantity of protons. A symbol of a proton is Z. For definition of a neutron the formula is used:

N = Ar-Z [9]. Preceding from a formula of energy levels the ability of chemical elements to chemical reactions or connections is also defined.



Picture 1 - Virtual and interactive periodic table chemical elements of D.I. Mendeleyev



Picture 2 - Flat picture of electronic orbital's the Seaborgium element in driving, atomic weight, valence, quantity of neutrons and protons, polarity formula of energy levels of orbital's