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RESEARCH ARTICLE

DERIVATION OF A NEW EQUATION FOR CALCULATING THE NUMBER OF ELECTRONS CORRESPONDING TO DIFFERENT VALUES OF THE PRINCIPAL QUANTUM NUMBER

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Abstract

This paper deals with a new approach in the formation of periods in the Mendeleev's Periodic Table. Using a newly suggested formula and newly suggested quantum states for the external electron shells of atoms of chemical elements, the author proposed the reconfiguration of periods in the Mendeleev's table. The reducing of the number of periods in the table is assumed, andthe material represented in the paper proves it.The following order of formation of electron layers is suggested: the principle quantum number (n), followed by the quantum state of electrons (first and second) which constitute the electron configurations of subperiods, and only after that - the remaining quantum orbitals (s, d, f, and p).

Introduction:-

Understanding the structure of the electron shells of chemical elements'atoms is one of the most important problems of theoretical chemical science and, in particular, the methods of teaching it.This is due to a number of reasons, the main ones of which are the following. So if the existing explanations of the relationship between the structures of the outer electron shells of elements' atoms with periodicity in their chemical properties (Periodic law of D.I.Mendeleev)qualitatively somehow suit modern chemists, in quantitative terms, these explanations often cannot give, for a number of objective and subjective reasons, a clear and unambiguous interpretation. In this regard, the table of D.I. Mendeleev is the most illustrative exampleof a graphical representation of the periodic law. And first of all, this is expressed in the fact that, for more than a hundred years, there has been no proper quantitative explanation for the discrepancy between the ordinal numbers of the periods of the table and the number of outer shellelectrons of the elementsof the corresponding period, calculated according to the well-known equation.

$$N = 2n^2$$

where N - the total number of electrons in the outer electron shell of the corresponding periods of the elements' atoms

n - theprincipalquantumnumberorthecorresponding period number

This is one of the essential contradictions in the Mendeleev'speriodic table, partially depriving its explanation and application from logical harmony and order. Not to mention the purely methodological problems that arisewhen teaching this section of chemistry in educational institutions where this subject is taught.In addition, the noted quantitative discrepancies, in its turn, are reflected in the qualitative understanding of the educational material, making it difficult and complicating in mastering.That is, teaching this section of chemistry is still without significant changesfor decades.Or in other words, almost all generations of chemists living today have learned from this educational explanation. Naturally, this is a big problem that needs to be solved, since, methodologically

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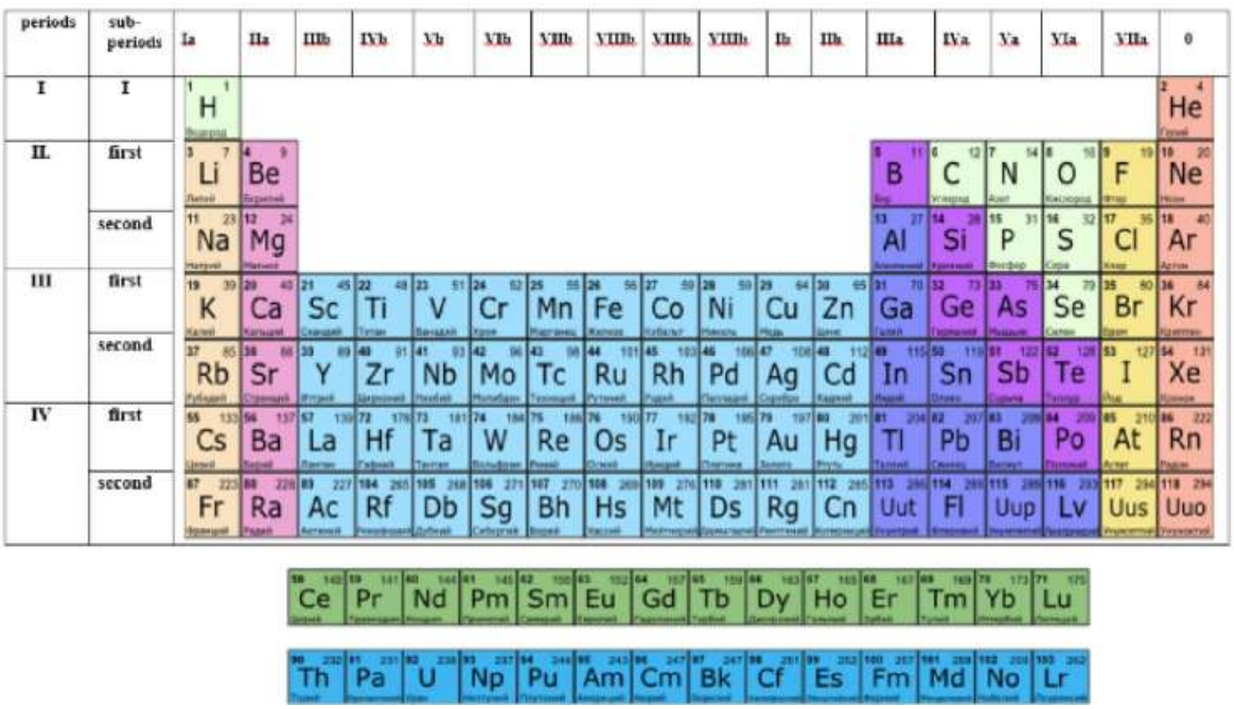
understanding the infilling of electron shells of elements' atoms with electrons, depending on the place of the element in the periodic table and itself its structureis very important.In short, the lack of correlation between the results of calculations according to formula (I) and the internal structure of the periodic table of D.I. Mendeleev was chosen as the main contradiction requiring its solution.

A similar comparison was earlier carried out in work [1], from which some especially important conclusions, which are needed to confirm the results of this article, can be highlighted.So, a long version of the Mendeleev's periodic table, which is much more convenient methodically, was taken for work and analysis in it. Such a long version of the periodic table is a much more visual that allows more clearly highlight its internal structure. In figure I this long version of the table with a modified internal structure proposed in work [1] is presented.The main and only visual difference between the proposed variant and the generally accepted is the decreasing in the total number of periods from 7 to 4. And also the introduction of a new quantum number (states "first" and "second") to designate sub-periods, which in the old table were designated as periods corresponding to that variant.

This proposed structure has its own logic of explanation and construction, clearly visible from the figure. But most importantly, it allows to regularize the understanding of the sequence of infilling the electron shells in the atoms of chemical elements.

In addition, such an internal structure of the table emphasizes the main role of the principal quantum number in the electron structure of the atom and therefore gives the table a completed view.



periods	sub-periods	Ia	IIa	IIIb	IVb	Vb	VIb	VIIb	VIIIb	VIIIb	VIIIb	Ib	IIb	IIIa	IVa	Va	VIa	VIIa	0
I	I	H																	He
II.	first	Li	Be											B	C	N	O	F	Ne
	second	Na	Mg											Al	Si	P	S	Cl	Ar
III	first	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
	second	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
IV	first	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
	second	Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Fl	Uup	Lv	Uus	Uuo

Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

Figure 1:-Reconfigured long version of the Mendeleev's table

The suggestion to introduce a new quantum number (state) for describing the number of outer electrons in atoms of chemical elements fits well with the new equation(II) capabilitieswhich is presented in that work

$$N = (2n)^2 \quad \text{(II)}$$

where N - the total number of electrons on the outer electron shell of the corresponding period of the Mendeleev periodic table

n - theprincipalquantumnumberorthecorresponding period number

2- number of subperiods

First of all, thisis confirmed by comparing the total number of electrons calculated by equation (II) with the new structure of the periods of the Mendeleev's table shown in Figure I.Indeed, the proposed equation allows, and it is important,to substantiate quantitatively the introduction of new quantum states “first” and “second” (new quantum number)andexplainqualitatively the decreasing of the number of periods in the table with the simultaneous appearance of subperiods in them.It is confirmed by the ordering of our understanding of the internal logic of the periodic table structure, which is especially important when explaining its foundations in the process of teaching students.Since the electron structure of atoms of chemical elementsprimarily determines their ability in chemical reactions. All this simultaneouslygives a special methodological value to a new equation and to new quantum states, expanding the ways of further knowledge and explanation of the chemistry problem.

At the same time, the new equation (II) proposed in [1], despite its undoubted advantages, has a kind of incompleteness. There this equation is given without derivation, and the two of square of degree is proposed empirically. Such use of equation (II) necessarily effects on its scientific and theoretical justification, leaving some points for investigation.

In order to eliminate such variants, the quite original way for solving this issue by taking into account certain assumptions is proposed.

Since the main purpose of equation (II) is to calculate the total number of electrons on the outer electron shell or on each of the two new quantum subshells, the process of our derivation should not contain sufficiently complex mathematical conditions.Naturally, this equation simultaneously confirms the existence of two sub-periods in the periods of the table and the decrease ofperiod’s total number from the previously accepted one.Directly, the derivation of equation (II) is accompanied by separate conditions that do not generally affect the overall result of the equation.First of all, they include the simplification of the mathematical apparatus by simplifying some conditions for deriving the solution of this equation.So, all the quantitative characteristics of electrons of different shells are conventionally assumed approximately equal to each other. The main characteristic of an electron, regardless of its principal quantum number, will be the moment of rotation of the electron.Taken by us,the electron’s rotation moment, according to Bohr [2], is equal to an integer multiple of the value $h/2\pi$, where h is Planck's constant.The spatial distribution of the probability of the an electron stay around the atom’snucleus of an element is taken by us equal to each other, in the common electron cloud of the corresponding electron shell, which has a predominant spherical symmetry.Electron shells for different principal quantum numbers do not intersect with each other. The electron shells of the sub-periods in the new periods are identical and differ from each other in different quantum states "first" and "second".Taking into account the accepted assumptions, it is more convenient to derive equation (II) from the primary calculation of the areas of the spherical surfaces of the electron shells related to the corresponding principal quantum numbers.This calculation is carried out according to the well-known formula $S = 4\pi r^2$, where $S -$ is the surface area of the sphere and $r -$the radius of the sphere.After the determining the estimated surface areas of the electron shells, it is necessary to determine the conditional area (or volume) corresponding to the probability of an individual electron stay in each electron sublevel, shells. The conditional area (or volume) determines the hypothetical probability of each individual electron stay in its unit for the electron shell.The total surface area is divided by the total number of electrons on the corresponding electron sublevel of the outer electron shell, i.e. the corresponding sub-period in order to find the conditional area per electron, (see Fig. I). Here the number of electrons is equal to the number of chemical elements in this sub-period. The corresponding calculations are shown in Table I.

$$S = 4\pi r^2 \left\{ \begin{array}{l} \dfrac{4\pi r^2}{2} = 2\pi, \quad (r=1) \\ \dfrac{4\pi r^2}{8} = 2\pi, \quad (r=2) \\ \dfrac{4\pi r^2}{18} = 2\pi, \quad (r=3) \\ \dfrac{4\pi r^2}{32} = 2\pi, \quad (r=4) \end{array} \right\} 2\pi$$

Table I:-Calculation of the conditional area (or volume) of the hypothetical probability ofan individual electron stay in its unit of the electron shell.

From the obtained results, it is obvious that in any case the conditional area (volume) of the hypothetical probability of an individual electron stay in its unit of the electron shell contains a value equal to 2π .But the quantity 2π is included as an important component in the first quantum Bohr condition formulated as [3]

$$P = n\frac{h}{2\pi}$$

where $P -$ electron's rotation moment, $n -$ quantumnumber (any integer value) of electron orbital.

Therefore, the value 2π , the common component for all conditional areas (or volumes) of the corresponding considered electrons in the electron shells (and subshells) of elements'atoms, can be used as a factor in the assumed selection of components for calculating the total area of the spherical surfaces of electron shells, which have different principal quantum numbers.Then the area of this surface will be mainly (qualitatively) determined by the product of two factors. The number of electrons (x) on the electron sublevel of the subperiod and a factor 2π of one of the quantitative components of the electron's rotation moment, i.e. we will have in an approximate form $S = 2\pi x$.

According to the logic of the consideredapproaches, the formulas of the spherical surfaces of the electron shells are equalized with each other in order to further solve the posed problem

$$(S = 4\pi r^2) = (S = 2\pi x)$$

or $2\pi x = 4\pi r^2$ solving for x, we obtain

$$x = \frac{4\pi r^2}{2\pi}$$

reducing we have

$$x = 2r^2$$

which is similar to equation (I).

But the number x determines the number of electrons on the outer electron subshell of the corresponding electron shell or period of the table. Therefore, to find the total number of electrons at the corresponding outer electron shell, it is necessary to multiply equation (I) by 2, since we have in each period two sub-periods with the same number of electrons.

$$2x = 2(2r^2)$$

or

$$2x = 4r^2$$

from here can be derived

$$2x = 2^2 r^2$$

and finally

$$2x = (2r)^2$$

which corresponds to equation (II), since 2 x is equal to the total number of electrons N in the outer electron shell, and r has corresponding integer values. The number of electrons on the electron shell canbe easily determined from theequation (II). By dividing by 2 (number of subshells).

Conclusion:-

Thus, equation II can be simply derived using these assumptions. It is remarkable that the generally accepted and widely used in the world equation I is a particular case of equation II. This is one more additional proof of the close relationship of these two equations and confirmation of the division of the corresponding periods of the periodic table into sub-periods characterized by new quantum states "first" and "second".

The presented derivation of equation II allows for new reviewing of thenumber of periodsin the table, and, therefore, it is better to present this new approach for explaining the main contradiction of Mendeleev's table, the discrepancy between equation (I) and the content of its internal structure.First of allthis will be useful, for a number of reasons, by the scientific and methodological view of the theory of classical chemistry in the field of teaching students studying chemistry in various educational institutions.First of all, it will be as reminder to all chemists that the solution to this issue needs to be developed. Then it will confirm that, for the required development of scientific views it is necessary to have alternative opinions of the scientific community. Thirdly, the comparison of the existing and proposed by the author changes to the structure of the Periodic Table of Mendeleev, the old and new equations and completely new quantum states "first" and "second" will give impetus to other well-reasoned explanations and analysis. Moreover, the proposed new equation (II) and new quantum states better eliminate the main contradiction in the explanation of the analyzed features of Mendeleev's table.

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