PHYSICAL AND MATHEMATICAL SCIENCES

METHODOLOGY FOR CALCULATING THE ELECTRONIC CONFIGURATION OF CHEMICAL ELEMENTS

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Annotation: Five basic functions are proposed, which are sufficient to calculate the electronic configuration of an element by its atomic number and to determine the atomic number of an element by its electronic configuration. It is shown that these functions can be represented as mathematical and logical operators, as well as in the form of logical constructions, which is important for their use in software applications.

Keywords: chemical elements, atomic number, electronic configuration.

One of the basic principles of modern chemistry is the periodicity of chemical and physical properties of chemical elements, which is based on the structure of the electron shell. As a result, it becomes possible to use only its atomic number to predict the properties of any element.

For example, to calculate the value of the average molar volume of an element, a small set of simple dependences is enough [1] which use as initial parameters only the data of the electronic structure of the element, which can always be obtained from the position of the element in the periodic table using the standard writing of the outer electron shell of the atom.

The method of calculating the structure of the outer shell is considered well-known and is presented in general form in almost all books on elementary chemistry, for example [2, 3]. But in a mathematical form suitable for use in the creation of programs, such a method is absent not only in books, but also in more professional literature.

This means that when developing software products, this algorithm has to be developed almost from the beginning each time, which requires software developers to have knowledge of the chemistry as well as the programming language.

The main problem in creating an algorithm for determining the structure is the specific regularity of the periodic system. It cannot be determined by simple algebraic functions without the use of logical operations and expressions.

It should be noted that using the peculiarities of the structure of the electronic shell of the elements can greatly simplify the calculations, using only a few relatively simple functions based on the use of logical expressions and logical operations.

To display the electronic configuration, the standard notation in the chemical literature of the electronic structure of the outer shell of the atom was taken

$$N\, s^{e_0} f^{e_4} d^{e_3} p^{e_2}$$

where N – period number in the periodic system of elements;

s, f, d, p – symbol of the orbital (angular quantum number – 0,1,2,3);

e^i – is the number of electrons in the corresponding orbital.

One of the peculiarities of the structure is the actual arrangement of the elements not in accordance with the sequence of increasing orbital number - (s, p, d, f), but in a different order - (s, f, d, p). This has its own explanation from the point of view of quantum chemistry, but it is primarily necessary to take this into account for the convenience of further practical work.

That is why it is convenient to mathematically represent the electronic configuration as a vector (array of values) with the number of electrons in each orbital.

$$C = \{e_s, e_f, e_d, e_p\}$$

where C – vector of electronic configuration of the outer shell;

e_b – is the number of elements in the b-orbit of period N;

b – is angular quantum number 0,1,2,3 (respectively s, p, d, f).

The maximum number of electrons in the b-orbital for the N- period is determined by a simple formula, in which the use of logical operators results in the fact that for the first periods the number of electrons in the f and d orbitals take zero values

$$l_b = l(N,b) = 2 \cdot (2 \cdot b + 1) \cdot (N > 2 \cdot b - 1) \quad (1a)$$

where l_b – is the number of electrons in the N-period orbital.

This can also be done by using logical constructs

$$\begin{aligned} & l_b = l(N,b) \\ & l_b = 0 \qquad\qquad\qquad\qquad (1b) \\ & \textbf{\textit{if}} \quad N > 2 \cdot b - 1 \ \ \textbf{\textit{then}} \quad l_b = 2 \cdot (2 \cdot b + 1) \end{aligned}$$

The number of electrons in all completed electron shells for N periods will be equal to the sum of all electrons in each of the orbitals

$$Z_N = Z_N(N) = -2 + \sum_{b=0}^{b=3} 2 \cdot l(N,b) \cdot (N - 2 \cdot b + 1) \quad (2a)$$

where Z_N – the number of electrons in completed electron shells for N-period elements.

or by using logical constructions

$$Z_N = Z_N(N)$$

$$\begin{cases} \textbf{\textit{if}}\ N = 7\ \textbf{\textit{then}}\ Z_N = 118 \\ \textbf{\textit{if}}\ N = 6\ \textbf{\textit{then}}\ Z_N = 86 \\ \textbf{\textit{if}}\ N = 5\ \textbf{\textit{then}}\ Z_N = 54 \\ \textbf{\textit{if}}\ N = 4\ \textbf{\textit{then}}\ Z_N = 36 \\ \textbf{\textit{if}}\ N = 3\ \textbf{\textit{then}}\ Z_N = 18 \\ \textbf{\textit{if}}\ N = 2\ \textbf{\textit{then}}\ Z_N = 10 \\ \textbf{\textit{if}}\ N = 1\ \textbf{\textit{then}}\ Z_N = 2 \end{cases} \qquad (2b)$$

This makes it possible to determine the period for a given atomic number of the element (Z) or the form of the loop

$$N = N(Z)$$

$$\begin{cases} N = N + (Z_N(n) \le Z), \\ 1 \le n \le 7 \end{cases} \qquad (3a)$$

or using logical constructions

$$N = N(Z)$$

$$\begin{cases} \textbf{\textit{if}}\ Z \le 118\ \textbf{\textit{then}}\ N = 7 \\ \textbf{\textit{if}}\ Z \le 86\ \textbf{\textit{then}}\ N = 6 \\ \textbf{\textit{if}}\ Z \le 54\ \textbf{\textit{then}}\ N = 5 \\ \textbf{\textit{if}}\ Z \le 36\ \textbf{\textit{then}}\ N = 4 \\ \textbf{\textit{if}}\ Z \le 18\ \textbf{\textit{then}}\ N = 3 \\ \textbf{\textit{if}}\ Z \le 10\ \textbf{\textit{then}}\ N = 2 \\ \textbf{\textit{if}}\ Z \le 2\ \textbf{\textit{then}}\ N = 1 \end{cases} \qquad (3b)$$

where Z – the atomic number of the element.

The determined values of N and Z_N allow to finally determine the configuration of the outer shell for which the initial vector of electronic configuration values is set and the number of electrons in each orbital is calculated in the form of a loop

$$Z_O = Z - Z_N$$

$$C = \{e_1, e_2, e_3, e_4\} = \{l(N,s), l(N,f), l(N,d), l(N,p)\} \qquad (4a)$$

$$\begin{cases} e_b = Z_O - (Z_O > e_b)\cdot(Z_O - e_b) \\ Z_O = (Z_O > e_b)\cdot(Z_O - e_b) \\ 1 < b < 4 \end{cases}$$

or it can be done in through logical constructions

$$Z_O = Z - Z_N$$

$$C = \{e_1, e_2, e_3, e_4\} = \{l(N,s), l(N,f), l(N,d), 0\} \tag{4b}$$

$$\begin{cases} \textbf{\textit{if}}\ \ Z_N < e_1\ \textbf{\textit{then}}\ e_1 = Z_N,\ \ Z_N = 0 \\ \textbf{\textit{if}}\ \ Z_N > e_1 + e_2 + e_3\ \ \textbf{\textit{then}}\ e_4 = Z_N - (e_1 + e_2 + e_3),\ Z_N = 0 \\ \textbf{\textit{if}}\ \ Z_N > e_1 + e_2\ \textbf{\textit{then}}\ e_3 = Z_N - (e_1 + e_2),\ Z_N = 0\ \textbf{\textit{else}}\ \ e_3 = 0 \\ \textbf{\textit{if}}\ \ Z_N > e_1\ \textbf{\textit{then}}\ e_2 = Z_N - (e_1 + e_2)\ \ \ \textbf{\textit{else}}\ \ e_2 = 0 \end{cases}$$

where Z_O – is the number of electrons in the outer electron shell.

The reverse calculation of the ordinal number of the element at a given electronic configuration (N, e_s, e_f, e_d, e_p) is calculated by the formula using functions (1) and (2)

$$Z = Z_N + e_1 \cdot l(N,s) + e_2 \cdot l(N,f) + e_3 \cdot l(N,d) + e_4 \cdot l(N,p) \tag{5}$$

Thus as a result of the work 5 basic functions are proposed that are sufficient to calculate the electronic configuration of the element by its serial number and to determine the serial number of the element by its electronic configuration. It is shown that they can be represented as mathematical and logical operators, as well as in the form of logical constructions, which is important for their use in applications.

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