match no. 2 pp. 117-122 1976

EQUATIONS FOR THE ELEMENTS IN THE PERIODIC TABLE, BASED ON INFORMATION THEORY

D. Bonchev, V. Kamenska, C. Tashkova

Department of Physical Chemistry, Higher School of Chemical Technology, 8005 Burgas, Bulgaria

(received: January 1976)

Abstract

Information equations were obtained on the distribution of electrons in the atoms over electron subshells, atomic orbitals and over the values of the azimuthal quantum number. The equations were modified to describe the groups and periods in the Periodic Table.

Information Theory[1,2] can be applied to an investigation of every system possessing distinct elements or a definite structure. Recently the information on electron distribution in atomic electron shells was defined and calculated for all known chemical elements[3-6]. The information characteristics introduced there are of use in the analysis of periodicity in the properties of chemical elements, and especially in the attempts at its quantitative description. Information equations of the groups and periods in the Periodic Table were also suggested[7] on the basis of electron spin. In the present paper some new information equations are derived.

I. Information on Electron Distribution over Subshells, I_{nl}

Let us denote the total number of electrons in an atom by z, and their number in a given electron subshell - by z_{nl}. The total quantity of information on electron distribution over subshells, expressed in bits per atom, will be[2] :

$$I_{nl} = z\log_2 z - \sum_{nl} z_{nl}\log_2 z_{nl} \qquad (1)$$

The sum in equation (1) can be divided into two parts. The first of them is constant and it includes summation over all completed subshells, which are the same as in the noble gas ending the preceding (n-1)-th period of elements. It can be shown that this quantity is

$$A = \sum_{l=0}^{n-1} (n-2l-\delta).2(2l+1)\log_2 2(2l+1) \qquad (2)$$

where = 1 for l = 0, and = 0 for l ≠ 0. The variable part of the sum is over those subshells which are to be filled in the final, n-th period. Then equation (1) will be transformed to

$$I_{nl} = z\log_2 z - A - \sum_{l} k_{nl}\log_2 k_{nl} \qquad (3)$$

Equation (3) can be treated as an <u>equation of periods</u> in the Periodic Table. The constant A, characterizing the individual periods, is equal to : 0, 2, 19.51, 37.02, 87.75, 138.48 and 242.51 bits, for the periods I to VII, respectively. Equation (3) is simultaneously an <u>equation of the groups</u> in the Periodic Table having the following group constants : k_{ns} = 1 or 2 for the main groups I and II; k_{np} = 1÷6 for the main groups III-VIII; and k_{nd} = 1÷10 for the secondary groups I-X.

II. Information on Electron Distribution over Atomic Orbitals, I_{nlm}

Let us denote the number of single electrons in an atom by a. Since every atomic orbital can be occupied by only 1 or 2 electrons, the number of electron pairs in the atom will be $\frac{z-a}{2}$. Then the total information on electron distribution over AO, expressed in bits per atom, will be[2] :

$$I_{nlm} = z\log_2 z - \frac{z-a}{2}.\ 2\log_2 2 - a.1\log_2 1$$

$$I_{nlm} = z\log_2 z - z + a \qquad (4)$$

and the average information, carried by every electron in the atom :

$$I_{nlm} = \log_2 z - 1 + a/z \qquad (5)$$

From equation (4) the difference in information content of the chemical elements having atomic numbers z and z+1 can also be determined. There are only two possibilities : when the new electron is single, and when it forms an electron pair :

$$I'_{nlm} = (z+1)\log_2(z+1) - z\log_2 z \qquad (6')$$

$$I''_{nlm} = (z+1)\log_2(z+1) - z\log_2 z - 2 \qquad (6'')$$

The comparison of the two equation shows that in the first case I_{nlm} increases more strongly. This leads to the conclusion that Hund's first rule (allowing the atomic orbitals to be initially occupied by single electrons only) is connected with the tendency of atoms towards maximal information content.

Equations (4) and (5) can be considered as information <u>equations of the groups</u> in the Periodic Table. In the ground state of an atom the group constant <u>a</u> is equal to the lowest valency of the element (1,0,1,2,3,2,1,0) as in the highest valence state it equals the number of the group. These equations can also be considered as <u>equations of the periods,</u> if a constant be introduced in them, which is equal to the atomic number of the noble gas, ending the preceding period (z_o = 2,10,18,36,54,86). Since $z = z_o + a + b$, where <u>b</u> is the number of paired electrons in the subshells populated in the last period, one can finally write equation (4) in the form :

$$I_{nlm} = (z_o + a + b)\log_2(z_o + a + b) - z_o - b \qquad (7)$$

<u>III. Information on Electron Distribution over the Values of the Azimuthal Quantum Number, I_l</u>

The atoms of chemical elements contain s, p, d and f-electrons. The information on electron distribution over these four "l - groups" will be :

$$I_l = z\log_2 z - z_s\log_2 z_s - z_p\log_2 z_p - z_d\log_2 z_d - z_f\log_2 z_f \quad (8)$$

Let us consider an element of the n-th period having atomic number z. Let us denote by k_l (l = s, p, d, f) the number of electrons in the valence subshells of this period. The total number of these electrons will be $k = \sum k_l = z - z_o$. The following equalities are in force:

$$\begin{aligned} z_s &= 2(n-1) + k_s \\ z_p &= 6(n-2) + k_p \\ z_d &= 10(n-4) + k_d \\ z_f &= 14(n-6) + k_f \end{aligned}$$

$$\text{total} \qquad z_l = 2(2l+1)\,(n-2l-\delta) + k_l \quad (9)$$

By introducing z_o, k and z_l in equation (8), the information on electron distribution over the values of azimuthal quantum number can be obtained as a function of n and l:

$$I_l = (z_o+k)\log_2(z_o+k) - \sum_l \Big\{\big[2(2l+1)(n-2l-\delta) + k_l\big] \cdot \log_2\big[2(2l+1)(n-2l-\delta) + k_l\big]\Big\} \quad (10)$$

The information equation (10) is valid for all the elements in the Periodic Table. The presence of some characteristic constants makes it a suitable equation for the elements in a given period or group. The constant z_o specifying a given period is the same as in the previous two sections. The groups are characterized by k_l which is equal to 1, 2 and 1, 2, 3, 4, 5, 6 for s- and p-elements of the main groups I, II and III ÷ VIII, respectively. In the case of the d-elements of the secondary group k_l = 1 ÷ 10.

Equation (10) can be expressed as a function of the azimuthal quantum number l only. Let us consider electron distribution over the "l-periods", i.e. the groupings including all the elements from the first one with a given azimuthal quantum number l to the first one with l+1. These first l-elements are known to be H, B, Sc and Ce for l = 0, 1, 2 and 3, respectively. If La is taken as the first f-element instead of Ce (La having $(n-2)f \to (n-1)d$ electron transition[8]), a simple dependence can be derived between l and the number of electrons in the "l-periods":

Number of electrons with l =		0	1	2
l-period I	($z = 1 \div 4$)	4	-	-
l-period II	($z = 5 \div 20$)	8	12	-
l-period III	($z = 21 \div 56$)	12	24	20

The total number of electrons having a given l will be equal to

$$z_l = 4(2l+1)(l_{max}-l) + k_l \tag{11}$$

where l_{max} is the highest value of l, realized in the chemical element. k_l is the number of electrons with a given l which belong to the "l-period" of the element. By introducing (11) into (8) the final result is obtained:

$$I_l = \left\{\sum_l \left[4(2l+1)(l_{max}-l) + k_l\right] + k_{l_{max}}\right\} \log_2 \left\{\sum_l \left[4(2l+1)(l_{max}-l) + k_l\right] + k_{l_{max}}\right\} - \sum_l \left\{\left[4(2l+1)(l_{max}-l) + k_l\right] \log_2 \left[4(2l+1)(l_{max}-l) + k_l\right]\right\} \tag{12}$$

The information equations derived in the present paper may be useful in the analysis of the quantitative aspects of periodicy, as well as in the search for correlations between the information content and properties of chemical elements.

Acknowledgements

Financial support from the Science Department of the Committee of Science, Technical Progress and Higher Education in Bulgaria is gratefully acknowledged.

References

1. C.Shannon and W.Weaver. The Mathematical Theory of Communication, University of Illinois Press, Urbana, 1949
2. L.Brillouin. Science and Information Theory. Academic Press, New York, 1956
3. D.Bonchev, D.Kamenski, V.Kamenska (to be published)
4. D.Bonchev, V.Kamenska (to be published)
5. D.Bonchev, V.Kamenska (to be published)
6. D.Bonchev, V.Kamenska (to be published)
7. D.Dimov, D.Bonchev, this MATCH
8. G.Villar, J.Inorg.Nucl.Chem., 28, 25 (1966).