match no. 2 pp. 111-115 1976

SPIN-INFORMATION EQUATIONS OF THE GROUPS AND PERIODS IN THE PERIODIC TABLE OF CHEMICAL ELEMENTS

D. Dimov, D. Bonchev[x]

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

(received: January 1976)

Abstract

An equation of groups and periods in the Periodic Table was obtained which connects the spin information content of chemical elements with the square of their atomic number. A concept was introduced of the "defect" of information upon atomic electron shell formation.

The ways of expressing the Periodic Law in analytical form have been under study for a long time [1]. Equations have also been suggested, which connect the elements of a given period or s, p, d, f-subperiods [2]. Information Theory[3,4] was applied in the present paper in order to derive equations of groups and periods in the Periodic Table, on the basis of electron spin.

The information on electron distribution in an atom over two groups, according to their spin, we shall call "spin information". The total spin information I_s, in bits per atom, as well as the average spin information of the atom $\bar{I}_s$, in bits per electron, can be determined by the basic equations of Information Theory [3,4]:

$$I_s = z\log_2 z - z_1\log_2 z_1 - z_2\log_2 z_2; \quad \bar{I}_s = I_s/z \qquad (1)$$

[x] To whom the correspondence should be adressed

The above, z, z_1, and z_2 are the total number of electrons in the atom and the number of electrons with magnetic spin quantum number +1/2 and -1/2, respectively.

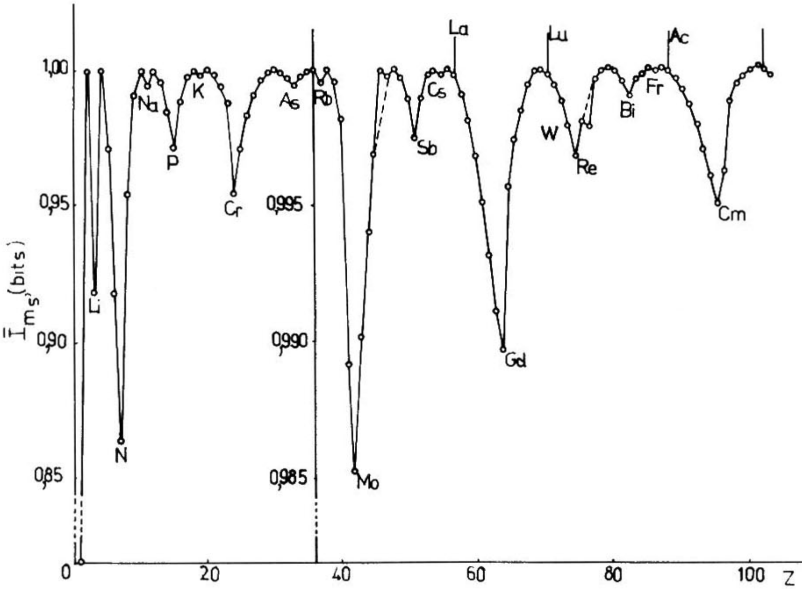

Fig.1 Average atomic spin information of chemical elements

As it can be seen in fig.1 the average spin information is a quantity reflecting the principal features of the electronic structure of atoms. The beginning of each period, as well as of s, p, d, and f-subperiods, is clearly expressed by an initial point in the descending part of the curve. These points follow directly after the value $\bar{I}_s$ = 1 bit, characterizing the elements which end the preceding periods or subperiods. This value illustrates the result important to Atomic Theory, that the spin information of the closed-shell atom, expressed in bits, is exactly equal to the atomic number of the chemical element[5]. The elements having a maximal number of single electrons in a given subshell, manifest minima in fig.1. On each of the two parts of the information well, according to Hund's rule, there are 2l + 1 elements. With the increase of the atomic number the differences in the spin information content of elements decrease and $\bar{I}_s$ tends to 1 bit.

If one connect by a common line in fig.1 the elements, belonging to a given group of the Periodic Table, curves having a parabolic character can be obtained. This indicates that it is possible to derive group equations, associating spin information with the atomic number of the element.

Let us denote by a the number of single electrons in the atom. Then the number of electrons having parallel spin will be $z_1 = (z+a)/2$ and $z_2 = (z-a)/2$ and equation (1) will be written thus:

$$\bar{I}_s = \log_2 z - \frac{z+a}{2} \log_2 \frac{z+a}{2} - \frac{z-a}{2} \log_2 \frac{z-a}{2} \qquad (2)$$

After making some transformations and developing the logarithmic function in a series one can obtain

$$\bar{I}_s = 1 - \frac{A}{z^2} \left[1 + \sum_{n=1}^{\infty} \frac{(a^2/z^2)^n}{(n+1)(2n+1)} \right] \qquad (3)$$

where $A = a^2/2\ln 2$ is a constant for a given group of elements.

Neglecting the sum in equation (3) we shall obtain a parabolic equation between the average spin information and the atomic number of the chemical element:

$$\bar{I}_s = 1 - \frac{A}{z^2} \qquad (4)$$

The error incurred by this is rather a small one. Equation (4) is quite correct for the 18 closed-shell elements. The relative error is less than 10^{-3}% for another 66 elements, it is between 10^{-3} and 10^{-2}% for another 12, it is from 10^{-2} to 10^{-1}% for four elements and only for H, N, C and Li is it more than 0,1%.

Equation (4) can be considered as an equation of groups in the Periodic Table. The elements of some groups have in their ground state an equal number of single electrons (groups II and VIII-0; groups I, III, V-1; groups IV and VI-2). For these groups the group constant will have the same value, A = 0, 0.7214 and 2.8856, respectively. The identity of group equations can be avoided taking as a basis the highest valence state of chemical elements, just as Mendeleev did in order to arrange the elements in vertical groups. Then for groups III to VII the constant A will have the following values: 6.4926, 11.5424, 18.0350, 25.9704, and 35.3486. Only a few elements with an anomalous electron structure (Cr, Cu, Nb et al.) do not obey the group equations (4), since the number of single electrons in them differs from the number typical for the group.

Equation (4) can be modified so as to be an equation of groups and periods simultaneously:

$$\bar{I}_s = 1 - \frac{A}{(z_o + n)^2} = 1 - \frac{a^2}{2\ln 2(z_o + a + b)^2} \qquad (5)$$

where z_o is a constant for every period, equal to the atomic number of the element ending the preceding period, $n = z - z_o$ can be considered as the atomic number of the element in the period, while a and b are the single and paired electrons over the closed shell of the element with atomic number z_o.

The derived spin information equations of groups and periods in the Periodic Table could be applied in analyzing the periodicity in the properties of chemical elements as well as for some other problems of the Periodic Table. Apart from this, questions arise concerning the great proximity (and in one specific case - the equality) of the spin information to the atomic number of the element. The rather small difference between two quantities (equal to A/z) can be called "defect of information", by analogy with the defect of mass in atomic nuclei. This quantity expresses the loss of spin information upon the atomic electron shell formation, since the electrons, because of the way they are distributed on the atomic orbitals, do not always carry 1 bit of information. Since deviations of I_s from the integral value of z take place only when single electrons fill the orbitals, one could expect the defect of spin information to correlate with the change in electronic energy due to Hund's first rule.

Acknowledgments

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

References

1. D.Trifonov. On the Quantitative Interpretation of Periodicity (russ.), Nauka, Moscow, 1971
2. G.Villar, J.Inorg.Nucl.Chem., 28, 25 (1966)
3. C.Shannon and W.Weaver. The Mathematical Theory of Communication, University of Illinois Press, Urbana, 1949
4. L.Brillouin. Science and Information Theory. Academic Press, New York, 1956
5. D.Bonchev and V.Kamenska (to be published).