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INFORMATION-THEORETIC VARIANT OF THE SYSTEMATICS OF NUCLIDES

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Abstract

The concept of the defect of information of nuclides on atomic nuclei formation is used as a foundation for a new version of the nuclide systematics, which is graphically represented in a diagram of the information defect versus the mass number of nuclides (i/A diagram). The new systematics introduces a new genetic line of nuclides (i-lines), besides those of isotopes, isotones, isobars, and isodifferents. It emphasizes the unity that exists between the nuclear and electronic structure, and makes possible the grouping of nuclides in periods both by the magic numbers of protons, and by analogy with the Periodic Table of chemical elements. A correlation is demonstrated to exist between nuclear binding energy and electron energy for the nuclides of the periods thus formed.

Introduction

The attempt to compose a rational systematics of nuclides** and atomic nuclei, has a long history. All attempts have been essentially based on systematized empirical data for the atomic nuclei (nuclear masses[1,2], spins, etc.), as well as on

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** According to the definition of IUPAP (1956), the nuclide is a certain type of atom, or the atom of an isotope of a certain element.

the theoretical concepts for atomic nuclei. On the other hand the systematics of nuclides should express visually, and in a practically convenient form, their grouping in these four kinds of lines: isotopes, with a constant number of protons, Z; isotones, with a constant number of neutrons, N; isobars, with a constant mass number, $A = N + Z$; isodifferents, with a constant difference in the number of neutrons and protons, $\beta = N - Z = A - 2Z$.

As a result of this, different diagrammatic versions of the systematics exist, like the so-called Chart of the Nuclides[3], as well as the version of systematics[4,5] similar to it but based on the relative nuclear charge, Z/A. Another version of systematics is suggested[6] in tabular form grouping the nuclides within vertical groups, identical to those of the Periodic Table of chemical elements, but within periods of different size. In another attempt to tabulate nuclear systematics[7] the nuclides having even and odd numbers of protons are grouped separately.

The solution of the problem of the Periodic Table of isotopes is hindered by the lesser degree in which the periodic properties of nuclei are manifested in comparison with those of the chemical elements. The nuclear shell model[8-12] appears as the most natural basis for such a systematization of nuclides. The magic numbers[13-15], used in this model to denote the number of protons or neutrons, in the different nucleon shells of the nucleus, determine the different nuclear periods. Several variants of this kind are suggested for nuclide systematics, proceeding from the periodicity of such nuclear properties as binding energy[16-18], nuclear spin and magnetic momentum[19], isotope distribution in the Universe[20], etc.

Although best substantiated theoretically, such attempts also have some disadvantages. First of all, the principle chosen for systematization mostly does not cover all nuclides. The periodicity is manifested in only one "major" nuclide of the different groupings of nuclides which is a 2 - stable one with either the greatest stability[16-18] or with the greatest distribution[20]. Following this, a different number of isotopes of different chemical elements are included in a nuclide period. This violates the unity which is supposed to exist between the systematics of nuclides and the Periodic Table of chemical elements. Difficulties in the selection of the "major" isotope arise in some cases. Additional problems arise when one defines the nuclear periods. The latter may end in a magic number of protons, or neutrons, or a double magic number. It is also not completely clear whether the numbers 14 and 28 should be handled as magic ones. Thus the number of variants possible for the Periodic System of nuclides is growing. This number is also large when dealing with the systematics not directly constructed on the basis of the nucleon shell concept. The lack of a unique solution to the problem of the bounds of nuclear periods is again the main difficulty here[4,6,21].

In the present paper we proceed from the point of view that a general systematics should include all the nuclides, not only their selected representatives, and should also conserve the greatest possible proximity to the Chart of the Nuclides and Periodic Table of chemical elements. Alternatively, the systematics of nuclides ought to be constructed on the basis of such nuclear properties which adequately reflect the regularities of nucleus structure. As such properties, we studied the information characteristics of the atomic nuclei, recently introduced[22-25]. These are the information on proton-neutron composition of nuclei, on nucleon distribution over shells and subshells, as well as their derived quantities like the differential information characteristics, and the so-called defect of information. One of the quantities under study was found to be a suitable criterion for nuclide systematization.

Defect of Information of Nucleons on Atomic Nuclei Formation

Introduced on the basis of Information Theory[26-28], the structural information contained in nuclei, atoms or molecules[22-25,29-33] represents their statistical characteristics depending on the degree of complexity or organization. This makes this quantity worthwhile from a classificational point of view.

The division of A nucleons in a nucleus into two groups, Z protons, and N neutrons, can be used for defining the so-called information for proton-neutron composition of a nucleus[22,25]:

$$I_{np} = A.\log_2 A - Z.\log_2 Z - N.\log_2 N \quad , \text{bits} \qquad (1)$$

When $Z = N = A/2$, $I_{np} = A$ bits, i.e. every nucleon in symmetrical nuclei, having an equal number of protons and neutrons, carries exactly 1 bit information for the proton-neutron composition of the nucleus. The same quantity of this information is carried by a free nucleon, since the probability of the latter being proton or neutron is 1/2. When $Z \neq N$, $I_{np} < A$. The difference:

$$\Delta I^{*}_{np} = A - I_{np} \quad , \text{bits} \qquad (2)$$

is viewed here as a measure of the information for proton-neutron composition, lost on formation of a nucleus, because of the deviation from the symmetric nucleus with an equal number of protons and neutrons. It can be called "defect of information". This quantity has an analogy with the mass defect in nuclei and correlates with it for isodifferent groups of nuclides[25]. The mean defect of information per nucleon, i, shows by how many bits the information on proton-neutron composition, carried by every nucleon in symmetric nuclei, is less than the information of a free nucleon (1 bit). It can be calculated by the equation:

$$i = \frac{\Delta I^{*}_{np}}{A} = \frac{1}{2 \ln 2}\left(\frac{\beta}{A}\right)^2 = \frac{1}{2 \ln 2}\left(1 - 2\,\frac{Z}{A}\right)^2, \text{ bits/nucleon} \qquad (3)$$

It can be seen from eqn.(3) that i depends on the isotopic number β, as well as on the relative nuclear charge Z/A, i.e. the nuclei having the same relative charge Z/A also have the same mean defect of information. By increasing the relative charge, the mean defect of information increases, when $Z/A > 0,5$, and decreases when $Z/A < 0,5$. When $Z/A = 0,5$, i obtains its minimum value, equal to zero.

Besides the relative charge, the i-quantity is also connected with the projection of the total isotopic spin of the nucleus, T_Z:

$$T_Z = Z - \frac{A}{2} = \frac{Z - N}{2} = -\frac{\beta}{2} \qquad (4)$$

From (3) and (4) one obtains:

$$i = \frac{2}{\ln 2}\left(\frac{T_Z}{A}\right)^2 \qquad (5)$$

Information-Theoretic Variant of the Nuclide Systematics. A Diagrammatic Expression.

The diagrammatic expression of the dependence of the information defect of a nucleon i on the mass number A is suggested in the present paper as a new variant of nuclide systematics. In FIG. 1 a fragment of the new systematics is shown, which includes all known isotopes of the chemical elements of period IV. It can be seen that the four lines of nuclides: isotopes, isotones, isobars, and isodifferents, appearing in the Chart of Nuclides and the existing systematics, are conserved in the new one. Each of these four lines of nuclides forms a curve described by an equation[25] of the kind $i = f(A)$, for Z = const, N = const, A = const, and β = const, respectively. The curves of isotopes represent parabolas with a left and right branch, and a minimum at $A = 2Z$. There are no nuclei with a negative isotopic number after $^{49}_{25}Mn$. Thus, only the right branch of each parabola remains for $A > 49$, and the dependence tends to a linear one for large mass numbers. The same holds for isotones - the lines of constant number of neutrons. The isobar lines are vertical ones in which the larger the excess of neutrons in the nuclides, the larger is the defect of information in them. The nuclides having the same value of the isotopic number β form curves, with the exception of the case $\beta = 0$,

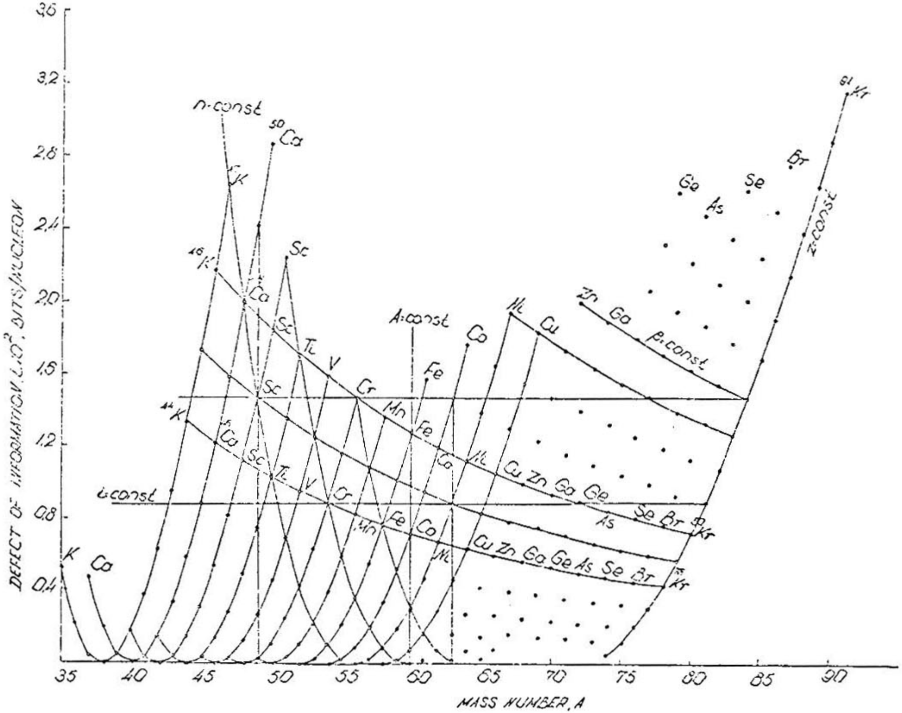

FIG.1.Dependence of the defect of information per nucleon on the mass number of nuclides of period V .

in which a line is formed lying along the abscissa. In FIG. 1 the lines of the mirror nuclei, having isotopic numbers of the same value but different sign, coincide.

Series of Nuclides with the Same Defect of Information (i-lines).

The diferentiation of the lines of a constant defect of information for proton-neutron composition, i = const, as independent grouping of nuclides, is a new element in the systematics of nuclides. The first line, having i = 0, originates from the nuclide ${}^{2}_{1}H$, with a mass number $A_1 = 2Z$, total isotopic spin projection $T_{z,1} = 0$, and an isotopic number $\beta = 0$. It comprises 30 symmetric nuclei having an equal number of protons and neutrons. The remaining lines of nuclides originate from nuclei, having mass number $A_1 = 2Z + \beta$, where $\beta = -1$ to 10 for the most populated series. If the nuclides incorporated in a certain series with i = const, are ordered according to the increase of their mass number, and enumerated with a serial number k = 1,2,3,..., the following equations hold:

$$A = kA_1 \qquad ; \qquad T_z = kT_{z,1} \qquad (6),$$

i.e. the numbers of each of the series of isodefective nuclides have a mass number and total isotopic spin projection multiple to the relevant value of the first nuclide in the series.

The most populated twenty-four lines of isodefective nuclei are shown in Table 1. It can be seen from the table that the line starting from ${}^{5}_{2}He$ (isotope with a magic number of protons) has the largest number of nuclides. The series starting from isotopes having more protons than ${}^{5}_{2}He$ becomes smaller and smaller, being only two-membered for $Z > 30$. Since the heaviest known nuclide has an atomic number $Z < 107$ all nuclei having $Z \leq 53$ can be treated as first members of i-lines, with the exception of those with the largest excess or deficiency of neutrons.

The atomic nuclei in the systematics suggested are located on the intersection of five lines: Z = const, N = const,

TABLE 1

Series of nuclides having the same defect of information on proton-neutron composition per nucleon (i-series of nuclides)

No. of the series	First nuclide in the series	Defect of information, i.10²	Serial number of nuclides, k	No. of the series	First nuclide in the series	Defect of information, i.10²	Serial number of nuclides, k
1	$^{2}_{1}H$	0	1-30	13	$^{19}_{8}O$	1,81	1-2,4-11
2	$^{3}_{1}H$	8,17	1-5	14	$^{19}_{9}F$	0,20	1-5
3	$^{5}_{2}He$	2,91	1-4,10,18-20, 25-51	15	$^{20}_{9}F$	0,72	1-6,8
4	$^{7}_{3}Li$	1,48	1-4,6-29	16	$^{22}_{9}F$	2,40	1,4-10
5	$^{9}_{4}Be$	0,89	1-20	17	$^{23}_{10}Ne$	1,23	1-8
6	$^{11}_{5}B$	0,60	1-10	18	$^{25}_{11}Na$	1,04	1-7
7	$^{12}_{5}B$	2,01	1-2,4,6-18	19	$^{26}_{11}Na$	1,71	1-8
8	$^{13}_{6}C$	0,43	1-9	20	$^{27}_{11}Na$	2,49	1,3-8
9	$^{15}_{7}N$	0,32	1-7	21	$^{30}_{13}Al$	1,29	1-6
10	$^{16}_{7}N$	1,13	1-11	22	$^{34}_{15}P$	1,00	1-5
11	$^{17}_{7}N$	2,26	1,3,5-12	23	$^{37}_{16}S$	1,32	1-5
12	$^{17}_{8}O$	0,25	1-6	24	$^{40}_{17}Cl$	1,63	1-5

β = N - Z = const, A = const, and i = const. The nuclei genesis can be traced from each of these lines. Each nucleus in the first four lines can be obtained from the preceding nucleus by the addition of neutron, proton, deutron, respectively; and for isobars - by an electron or positron radiation. A new genetic line is forming in the series of isodefective nuclei, in which each nucleus is obtained from the preceding one by the addition of the first nucleus in this series, as in the following reactions occurring in the stars:

$$^{4}_{2}He + ^{4}_{2}He = ^{8}_{4}Be \quad ,$$

$$3\ ^{4}_{2}He = ^{12}_{6}C \quad ,$$

$$^{12}_{6}C + ^{12}_{6}C = ^{24}_{12}Mg \quad , \text{etc.}$$

Differing from the remaining four lines, the new genetic line allows considerably heavier nuclei to be used in nuclear genesis.

The known restrictions for the exothermal reactions of nuclear fusion in generating nuclei far from the maximum of the binding energy curve at Z = 26, elucidates the lack of more than two-membered i-lines within the range of Z = 30-53, as well as the lack of i-lines for Z > 53.

Information Defect in the Radioactive Series of Nuclei and Nuclear Fission Reactions

It is of interest to study not only the lines of a constant information defect in FIG. 1, but also those of the change in the information defect on emission of alpha and beta particles of isotopes of the natural radioactive series. The actinium series is shown in FIG. 2 where the number given for each isotope represents its mean information defect.

In the case of an alpha emission:

$$^{A}_{Z}X \longrightarrow ^{4}_{2}He + ^{A-4}_{Z-2}Y$$

the nuclei X and Y are isodifferent ones, i.e. $\beta = N - Z =$ $= const$. Then following eqn. (3):

$$i = const/A^2 \qquad (3),$$

one should conclude that <u>α- emission is accompanied by an increase in the mean information defect of nuclei.</u>

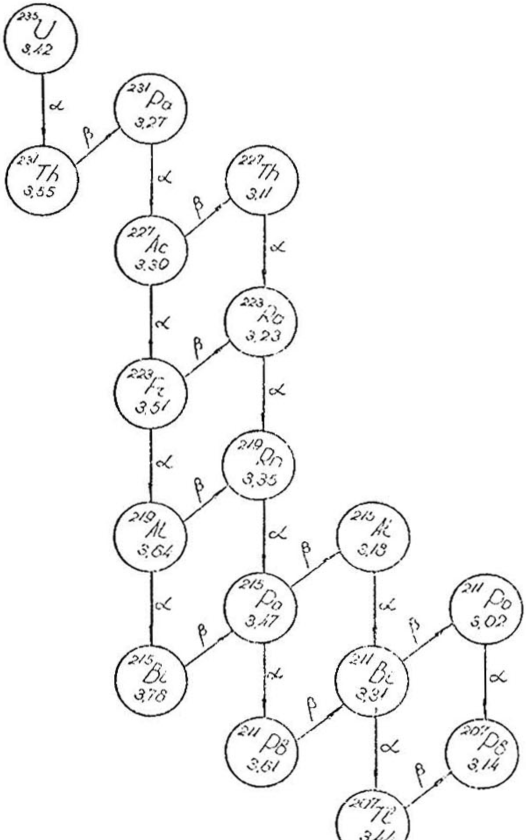

FIG. 2. Change in the mean information defect of nuclides of actinium series on emission of α- and β-particles

Let beta- emission be considered:

$$ {}^{A}_{Z}X \longrightarrow {}^{0}_{-1}\beta + {}^{A}_{Z+1}Y $$

The difference in the information defect of the nuclei X and Y:

$$ i_X - i_Y = (A^2 \ln 2)^{-1}.(A - 2Z - 1) \quad (7), $$

is positive for $\beta = A - 2Z > 1$, which holds for all natural radioactive series. Hence, the conclusion can be made that <u>beta-emission is accompanied by a decrease in the mean information defect of nuclei.</u>

It can be easily proved that the decrease in the information defect on beta-emission is greater than the corresponding defect on alpha-emission of the same isotope. As a result the last isotope in each of the natural radioactive series has always a smaller mean information defect than the initial one.

The fission of heavy nuclei into two parts of comparable atomic mases, discovered by Hann and Strassmann[39] in 1939, can be handled in a similar way. The two nuclear fragments can have smaller, as well as greater information defect than the initial nucleus:

$$ {}^{235}_{92}U \xrightarrow{\ {}^{1}_{0}n\ } {}^{236}_{92}U \longrightarrow {}^{140}_{55}Cs + {}^{94}_{37}Rb + 2.{}^{1}_{0}n $$

$$ i.10^2 = 3,42 \qquad 3,53 \qquad 3,34 \qquad 3,29 $$

$$ {}^{236}_{92}U \longrightarrow {}^{140}_{54}Xe + {}^{94}_{38}Sr + 2.{}^{1}_{0}n $$

$$ 3,53 \qquad 3,80 \qquad 2,66 $$

Diagrams of Defect of Information vs. Mass Number (i/A - diagrams)

In FIGS. 3 and 4 the dependence is shown of the defect of information per nucleon, i, on the mass number A of the 1725 known nuclides (cited by Kravtsov[2]). The lines of a minimum and maximum value of i for every series are outlined in Fig. 3, limiting the region of the known nuclei. The curve of i_{min}

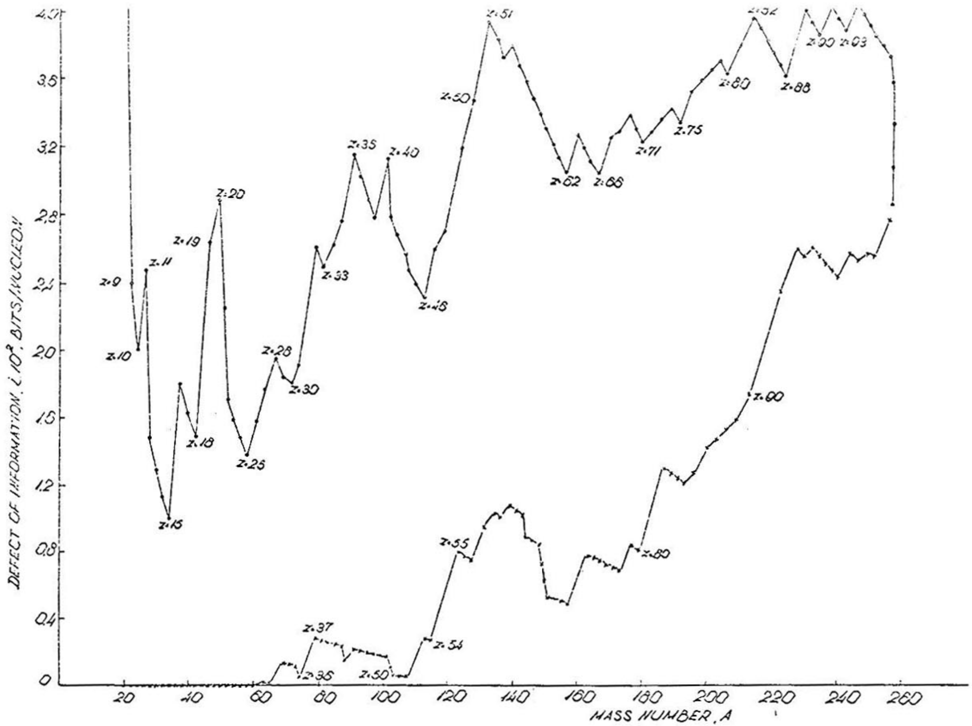

FIG.3.Dependence of the maximum and minimum defect of information (o - i_{max} and × - i_{min} ,respectively) .

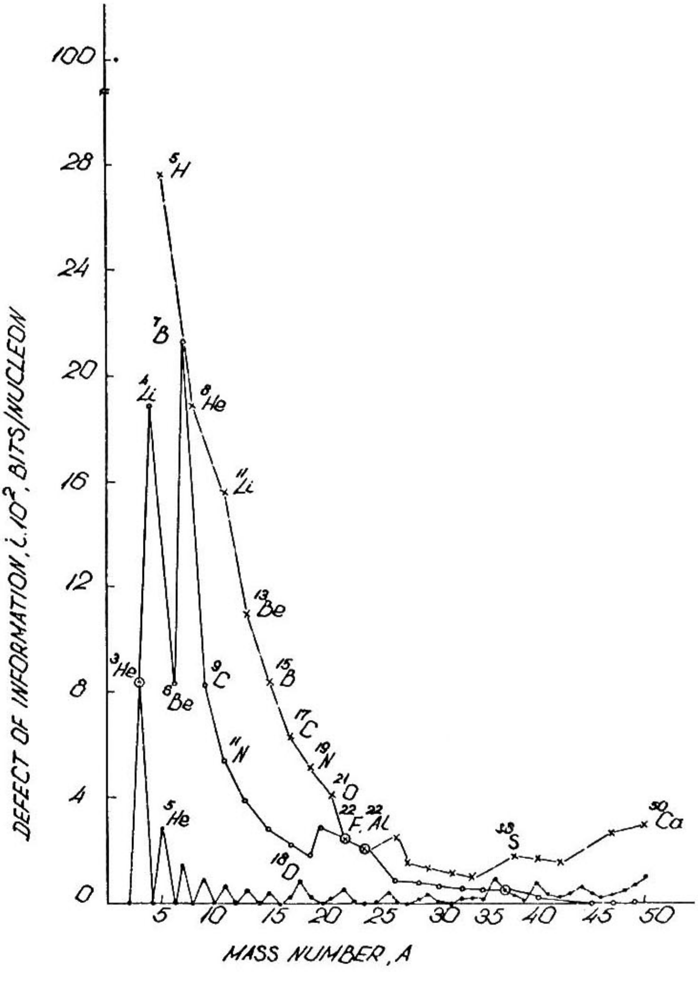

FIG. 4. Dependence of the maximum and minimum defect of information on the mass number A for nuclides with $A \leq 50$ (o and full line-i_{max}; × and dashed line-i_{min}; • and dotted line-2β-stable nuclides, respectively).

after $^{49}_{25}Mn$ corresponds to the lightest isotope, whilst that of i_{max}, after $^{24}_{14}Si$, corresponds to the heaviest one.

The first part of the i/A diagram, which comprises the nuclides up to A = 50, is given separately in FIG. 4. The lines of the defect of information of the heaviest and lightest isotopes are given separately in this figure due to the presence of a large number of nuclei with a great excess of neutrons. The line of the lightest isotopes differs from i_{min} which coincides with the abscissa. The line of i_{max} is not shown, because of its anomalous character. When the mass numbers are small ones, the nuclides with a greater number of protons often appear in this line before those with a smaller number of protons. The line of 2β -stable nuclei is also given in this figure.

The i/A diagram is rather interesting with its ability to express the major regularities of both nuclear and electronic periodicity of nuclides. The proton magic numbers Z = 20, and Z = 82 correspond to maxima in the curve of the greatest defect of information, whilst a point next to a sharp maximum in this curve relates to the magic number Z = 50. One might expect that the last maximum would be displaced from Z = 51 towards the magic number Z = 50, after the discovery of still unknown isotopes of $_{50}Sn$. The defect of information on the proton-neutron composition of each nucleon is defined by eqn. (3) as a relative quantity, and for small values of Z and A the relative changes are great. As a result the i_{max} curve descends steeply and the maxima possible at the proton magic numbers Z = 2, and Z = 8, do not appear.

Other features of the i_{max} and i_{min} curves can be associated with the features of the electronic structure. Most of the minima in the curve of the maximum information defect correspond to the chemical elements whose electron shells are completely or half populated: p^6(Z = 10, 18), d^{10}(Z = 30, 46, 80), f^{14}(Z = 71); p^3(Z =15, 33), d^5(Z = 25, 75). This remarkable link between nuclear and electronic properties recalls the similar result of Asunmaa and Lepsius[35] obtained in a Z/β - diagram, as well as to some extent the results of Znoiko[4] for the major nuclides in the diagram: relative charge vs. mass number.

In addition, a substantial increase in i_{min} occurs in the cases Z = 36 → 37 (Kr → Rb), and Z = 54 → 55 (Xe → Cs). The same holds for the increase in i_{max} for Z = 18 → 19 (Ar → K), and, though less expressed, for Z = 10 → 11 (Ne → Na), i.e. again for two chemical elements one at the end and the other at the beginning of the next period in the Periodic Table. The lack of such sharp increase for Z = 86 → 87, i.e. upon the transition from period VI to period VII, can be explained by the large number of still unknown isotopes of the heavy chemical elements. The transition from period I to period II (Z = 2 → 3) also does not appear on i_{max}-curve for the reasons mentioned above for the proton magic numbers Z = 2, and Z = 8.

One should take into account the circumstance that the zone between the curves of a maximum and minimum defect of information on proton-neutron composition of nuclei will extend with the discovery of new isotopes of chemical elements, One ought to expect, however, this extension in i/A-diagram to reflect even better the main regularities in the nuclear and electronic structure of the atoms.

Formation of Periods of the Nuclides (Nuclear Periods)

The systematics of the nuclides proposed in the present paper can be further developed by forming periods of the nuclides. The i/A diagram, whose features were analysed above, allows the nuclear periods to be formed either on the basis of the proton magic number or by analogy with the periods in Periodic Table of the chemical elements. In both cases they are formed by the lines of isodifferent nuclei, differing only in the beginning and end of each period. When the periods are limited by the values of the proton magic numbers one achieves the systematics of Selinov[16-18]. In the second case seven periods are formed having respectively 2, 8, 8, 18, 18, and 32 nuclides in a given isodifferent series (period VII is not completed) between the isotopes of an alkali metal and a noble gas. The difference between these nuclear periods and those of the chemical elements is in the ability of the nuclear period to be realised simultaneously by a large number of isodifferent nuclei, completed or not (Table 2).

TABLE 2

Nuclide periods, analogues of the periods of chemical elements

No. of the period	First and last nuclei	β from	till	Total number of isodifferents	Number of the complete series of isodifferents	Complete series of isodifferents
I	$_1H$ - $_2He$	-1	4	6	5	-1,0,1,2,3
II	$_3Li$-$_{10}Ne$	-3	5	9	7	-2,-1,0,1,2,3,4
III	$_{11}Na$-$_{18}Ar$	-4	6	11	8	-3,-2,-1,0,1, 2,3,4
IV	$_{19}K$- $_{36}Kr$	-3	19	23	6	3,4,5,6,7,8
V	$_{37}Rb$-$_{54}Xe$	3	32	30	13	7,8,9,10,11,12, 13,14,15,16,17, 18,19
VI	$_{55}Cs$-$_{86}Rn$	13	50	38	5	28,29,30,31,32
VII	$_{87}Fr$-	29	58	30	1	50

It is seen from the table that the number of isodifferent series of nuclides increases with the increase in the period number. The same holds for the isotopic number $\beta = N - Z$.

The formation of periods in the systematics of the nuclides in a way analogous to the periods in the Periodic

Table of chemical elements is not a formal procedure. It expresses the fundamental unity that exists between the nuclear and electronic structure. It was already shown above that the defect of information of the nuclides, a quantity related to some basic characteristics of the nuclear structure like the number of protons and neutrons, isotopic number β , relative charge Z/A, total isotopic spin projection T_z, etc. reflects also some important features of the electronic structure of the atoms. In support of this point of view four isodifferent series of nuclides were found to demonstrate a high correlation between the binding energy of atomic nuclei[2] and the total electron energy of the chemical elements of period V, the latter calculated by the Hartree-Fock method[36,37] (FIG. 5). A detailed study

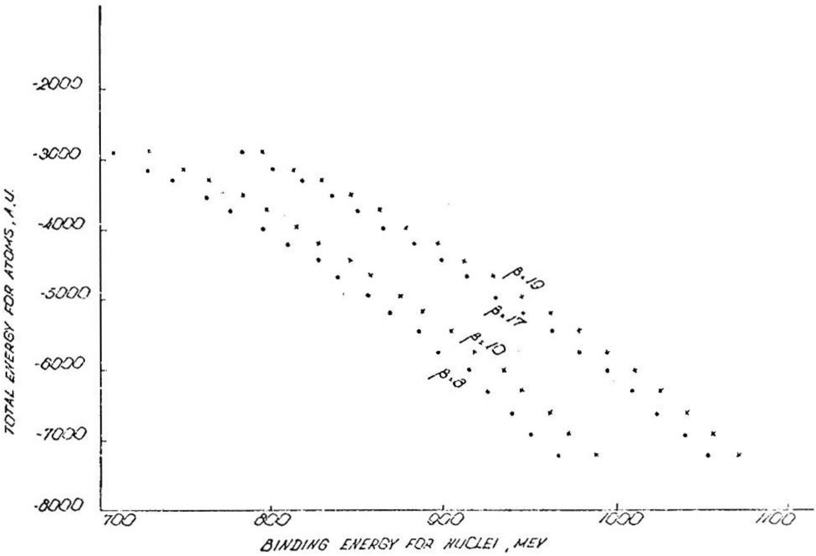

FIG. 5. Binding energy of the isodifferent nuclei and total electron energy of the atoms of chemical elements of period V.

on this correlation for the isodifferent series of the periods I-VII will be published elsewhere[38].

In conclusion one should emphasize that the systematics of the nuclides proposed in the present paper on the basis of the diagram of the defect of information on proton-neutron composition vs. the mass number of the nuclides conserves the main advantages of the existing systematics permitting the prediction of still unknown isotopes, nuclear properties, types of radiation etc. In addition, this systematics introduces a new genetic line of nuclides, and combines the basic notions and structural elements of the Chart of the Nuclides and the Periodic Table of the chemical elements. It makes more obvious the relation between nuclear and electronic structure, and indicates some possibilities for correlation between nuclear and electronic properties.

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