

Chapter

Periodicity of the Chemical Elements and Nuclides: An Information Theoretic Analysis

Danail Bonchev

Program for the Study of Complex Natural Systems, Texas A&M University, Galveston, Texas 77551, and Center for the Study of Biological Complexity, Virginia Commonwealth University, Richmond, Virginia 23284

1. INTRODUCTION

For over a century, millions of children have started out every year on their journey into the fascinating world of chemistry with the Periodic Table of the Chemical Elements. Periodicity of the chemical elements has also been a magnet that has attracted scientists to studies on the foundations of chemistry. Hundreds of versions of the Periodic Table have been proposed, and a variety of methods have been applied to its analysis. Where is the hidden magic of The Table? What is it that so strongly attracts its supporters even in the twenty-first century? Some authors consider the Periodic Table of the Chemical Elements to be the most comprehensive generalization in science, encoding a huge amount of information about chemistry. Others emphasize the potential of the Periodic Table as a tool for making predictions, a tool that singled out Dmitrii Mendeleev as perhaps the most important of the discoverers of the table among the many scientists who contributed greatly to the study of chemical periodicity.

The fascination of the Periodic Table inspired the present author in the 1970s–1980s, then based at the Higher Institute of Chemical Technology in Burgas, Bulgaria, to start with his coworkers a series of studies on the periodicity of the chemical elements and nuclides [1–18]. The mathematical tool selected was Shannon’s information theory [19], which the author first met through Brillouin’s *Science and Information Theory* [20]. The studies of the Burgas group were the first to use information theory to characterize the structure of atoms and atomic nuclei. The culmination of the work during that period was the generalization that the electron distribution in atoms obeys a certain principle of maximum information content [18]. In addition, some predictions were made for a number of the properties of the transactinide chemical elements 113–120 [17] and for the nuclear binding energies of the nuclides of the elements 101 to 108 [16].

The first prediction cannot yet be verified because only a few atoms of the elements 113–116 have presently been synthesized. However, many isotopes of the elements 101–108 have now been synthesized and their binding energies measured, which has made it possible to verify our predictions. The excellent agreement between the predicted and measured values (a standard deviation of only 0.1%) added considerably to the motivation to summarize and update some of our previous results, providing one more example for the great predictive power of the Periodic Table of the Chemical Elements. It is also our hope that the present chapter will demonstrate the possibilities offered by information theory as a tool for quantifying periodicity, for identifying common patterns in the periodicity of the chemical elements and nuclides, and for investigating the possible connections between the laws controlling the distribution of electrons, protons and neutrons and a conjectured general trend toward a maximum information content for atoms and molecules.

2. SHANNON'S INFORMATION THEORY APPLIED TO FINITE DISCRETE SETS

Although Shannon's theory [19] was introduced as a theory of communications, its validity was soon extended to other areas of science [20–22]. Mowshowitz developed a scheme for applying information theory to finite discrete sets [23] which established a sound basis for applications to atoms and molecules.

Consider a system of N elements, which are distributed according to a certain equivalence criterion () into k classes, with the i th class having N_i elements. A finite probability, p_i , can be defined for a randomly chosen element to belong to the class i :

Groups of elements:	1, 2, ... , k
Number of elements:	N_1, N_2, \dots, N_k
Probability distribution	p_1, p_2, \dots, p_k

with $p_i = N_i / N$, $\sum N_i = N$, and $\sum p_i = 1$. The mean entropy $H(\)$ and the total entropy $H(\)$ of the probability distribution are then defined as:

$$H(\) = - \sum_{i=1}^k p_i \log p_i = \sum_{i=1}^k \frac{N_i}{N} \log \frac{N_i}{N} \quad (\text{bits/element}) \quad (1)$$

$$H(\) = N \log_2 N - \sum_{i=1}^k N_i \log_2 N_i \quad (\text{bits}) \quad (2)$$

Shannon called his H -function the *entropy of information* and regarded information as a measure for the reduced uncertainty in an experiment in which a certain outcome i results from k possible outcomes. Mowshowitz [23] argued that in the case of a graph having N vertices, distributed among the k orbits of the automorphism group of the graph, the H -function is rather the graph's *information content* with respect to the symmetry transformations included in the corresponding automorphism group which leaves the graph unchanged. Since graphs are used to represent molecules, the same arguments are then valid for a molecule having N atoms of k different symmetry classes, because the molecule remains invariant with respect to the respective symmetry transformations. Bonchev presented additional arguments in favor of Mowshowitz' interpretation. He suggested [14, 18] that, in the case of molecules and atoms, the "experiment" reducing the uncertainty of possible outcomes is the very process of their formation from atoms, and protons, neutrons, and electrons, respectively. This is the information content that is stored in the structure formed and dissipated when the structure is destroyed.

There are many ways to partition atoms in a molecule as well as to partition electrons in an atom. For this reason, the term "information content" is frequently replaced here by the more general term "information index(es)". We will alternatively use both terms in our discussion.

3. DEFINING THE INFORMATION CONTENT OF CHEMICAL ELEMENTS AND NUCLIDES

In defining the information content of atoms one proceeds first by considering the distribution of the protons, neutrons and electrons into two substructures: the atomic nucleus and the electron shell. The information content of a nuclide having z protons, z electrons, and n neutrons (i.e., with atomic mass $A = z + n$), can then be defined as [1]:

$$I_{nuclide} = (A + z) \log_2 (A + z) - A \log_2 A - z \log_2 z \quad (3)$$

With few exceptions, chemical elements have more than one stable nuclide, that differs in terms of the number of neutrons (and, therefore, the total atomic mass they contain). One may define [1] the information content of a chemical element i as the

average information content of its naturally occurring nuclides, allowing for their abundance c_i :

$$I_{chem.element} = \sum_i I_{nuclide,i} \quad (4)$$

Although some correlations of this information index with atomic properties have been reported [1], its properties have remained largely unexplored. Instead, the focus of our studies shifted toward the distributions of the electrons in electronic shells and to the distribution of the protons and neutrons in the atomic nuclei. Proceeding from the quantum-mechanical description of an atom, the following information indices were defined: the information on the distribution of electrons over the atomic shells, I_n , the subshells, I_{nl} , the atomic orbitals, I_{nlm} , and the spin-orbitals, I_{nlmms} , as well as the information on the electron distribution according to the values of the orbital, magnetic, and spin quantum numbers, I_l , I_m , and I_{ms} . In all of these cases, one is dealing with the distribution of z electrons into k groups, having z_1, z_2, \dots, z_k electrons, respectively. Denoting by x the combination of quantum numbers, which determine the type of distribution, one may define the total information content, I_x , and the mean information content, \bar{I}_x , as

$$I_x = z \log_2 z - \sum_i z_i \log_2 z_i \quad (5)$$

and

$$\bar{I}_x = - \sum_i \frac{z_i}{z} \log_2 \frac{z_i}{z} \quad (6)$$

respectively.

A third information function termed the *differential information*, $I_x(z)$, was also defined as the increase in the atomic information content $I_x(z)$ in a chemical element with atomic number z and a combination of atomic quantum numbers x , compared to that for an element having atomic number $z - 1$ [8, 11]:

$$I_x = I_x(z) - I_x(z-1) \quad (7)$$

The filling of a given electron subset (shell, subshell, etc.) $k+1$ begins and ends most frequently at a constant population of the preceding k subsets. Then, Equation (7) becomes transformed into:

$$I_x = z \log_2 z - (z-1) \log_2 (z-1) - z_{k+1} \log_2 z_{k+1} - (z_{k+1}-1) \log_2 (z_{k+1}-1) \quad (8)$$

In describing the information content of an atomic nucleus one may similarly proceed with the distribution of protons and neutrons into nuclear shells, subshells, etc., as well as according to the nuclear quantum numbers [2, 7]. The information-theoretic analysis of the nuclear shell model will be reviewed in a forthcoming publication [24]. Here, we will limit our analysis to the information index on the proton-neutron composition of atomic nuclei, $I_{p,n}$,

$$I_{p,n} = A \log_2 A - p \log_2 p - n \log_2 n \quad (9)$$

which will be shown to possess a number of interesting properties [4, 9].

4. INFORMATION-THEORETIC ANALYSIS OF THE ELECTRON DISTRIBUTIONS IN THE ATOMS OF CHEMICAL ELEMENTS

4.1. Electron Distribution over Shells (n-Subsets)

This is a distribution of electrons over the values of the principal quantum number n . For the elements in the Periodic Table these are the values $n = 1, 2, 3, 4, 5, 6,$ and 7 , determining the periods of the chemical elements. The differential information index, I_n characterizing this distribution is a sensitive descriptor of the periodicity displayed by the chemical elements (Figure 1).

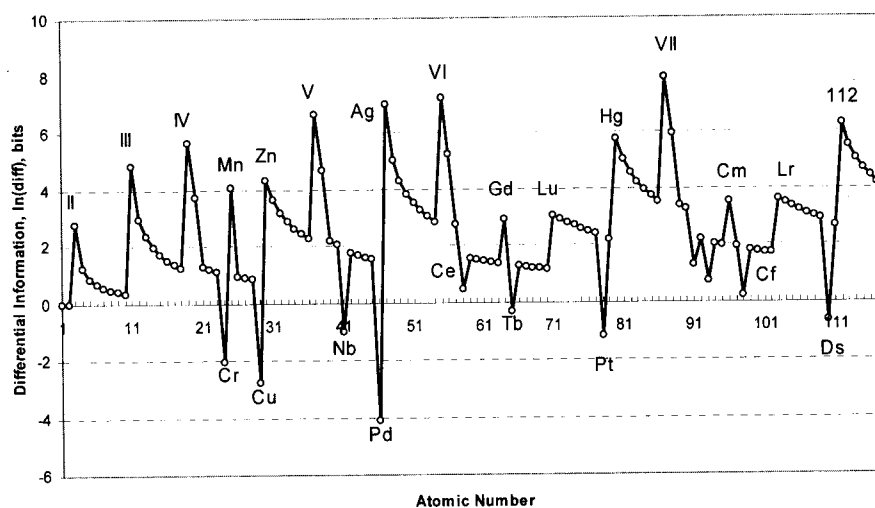


Figure 1. Differential information on the distribution of electrons over electron shells.

It follows from Equation (8) that the information index I_n increases maximally in the first element in each period, for which $z_{k+1} = 1$, and $z_{k+1} - 1 = 0$. I_n gradually goes down with the filling of the period and ends with a minimum value for the last element in the period. This regular trend is best demonstrated for the periods II and III. In the periods IV to VII, a second trend, caused by the delayed filling of the d and f subshells, is superimposed on the basic one. This delay makes the increase in the I_n index when adding d electrons less than that for adding p electrons, and the corresponding increase for the f electrons is less than that for the d electrons. Thus, although the orbital quantum number ℓ is not taken into account in this type of electron distribution, the differential index I_n describes the variations in periodicity caused by the delay in the filling of the d and f subshells, as well as, by the ratio:

$$\Delta I_n((n-2)f) < I_n((n-1)d) < I_n(np) < I_n(ns) \quad (10)$$

In addition, this information index also indicates clearly the violations in the “ideal order” of filling the electron f and d subshells caused by an accelerated adding of $(n-1)d$ or $(n-2)f$ electrons to reach d^5 and d^{10} , as well as f^7 configurations, at the cost of the decreased population of the ns subshell. In Figure 1 this is demonstrated by sharp minima for the extra d electron in Cr, Cu, Nb, Pd, etc., and by maxima for restoring the “normal” trend in Mn, Zn, Ag, etc. The minima in the f elements, however, appear in the element returning the extra f electron from the preceding element(s) back to the s subshell: Tb after Gd; Np after Pa and U; Cf after Cm and Bk. Conversely, adding a *single* d electron in Gd and Cm leads to a maximum in I_n because the $(1 \ln 1)$ s term within the sum of Equation (8) is indeed smaller than the competing term for the f subshell $(8 \ln 8 - 7 \ln 7)$ for Gd and Cm having seven instead of eight electrons in their 4f and 5f subshells, respectively. The minima and maxima for the “anomalous” f elements are lower than those for the corresponding d elements, following the ordering given above in the inequalities in Expression (10).

The regularity at the beginning and end of the electron shells and subshells of the maximum and minimum values of I_n provides new insights on the controversial question where the 4f and 5f elements begin and end [11]. In the literature, the view prevails that the lanthanides begin at element 58, Ce, and end with element 71, Lu. Similarly, the actinides are assumed to begin with element 90, Th, and end at element 103, Lr. Our data indicate a maximum value of I_n in Lu and Lr. Therefore, they should be regarded as the initial elements in a new subshell (5d or 6d) rather than as the last elements in another subshell (4f or 5f). Also, the lanthanides and actinides should end in Yb and No (elements 70 and 102), respectively, because it is in these elements that I_n reaches a minimum. The presence of a d^1 instead of an f^1 electron configuration in La and Ac may be interpreted as resulting from an $(n-2)f \rightarrow (n-1)d$ electron transition by analogy with other elements in these series (Gd, Cm, etc.). This view is additionally supported by the minimum of I_n at Ce and Pa, indicating the return of the

normal electron configuration, violated by the $f \rightarrow d$ electron transition in La, Ac and Th.

4.2. Electron Distribution over (n, ℓ) -Subshells

Figure 2 shows the differential information for the electron distribution over all (n, ℓ) -subshells from 1s in H and He to 7p in the elements 113–118. The subshell periodicity trend, which was secondary to the shell periodicity as described by I_n , is a dominant trend when I_{nl} is used as a criterion. As follows from Equation (8), each subshell starts with a I_{nl} maximum and ends with a minimum in the last element of the subshell. The violations of this trend, discussed in Figure 1, are expressed in Figure 2 by sharper minima and maxima. For d subshells, the minima include the elements with an extra d electron: Cr, Cu, Pd, Pt, Ds (darmstadtium, element 110), and the maxima correspond to those with a restored “normal” number of d electrons. In fact, these maxima are clearly expressed only at Mn and Zn in period IV. In period V all elements from Nb, element 41 to Rh, element 45, have an extra d electron at the cost of the 5s subshell. This causes the small minimum for Nb, and the lack of a maximum at element 42, Mo. At the end of the series of 4d elements one finds two extra d electrons in Pt (valence electron configuration $5s^0 4d^{10}$), and one such electron in Ag ($5s^1 4d^{10}$). This is the reason why the I_{nl} maximum appears in Ag but not in Cd, in which the 5s subshell restores its normal filling of two electrons. The analysis of the subshell trend violations in the 4f and 5f elements is similar to that in the preceding subsection.

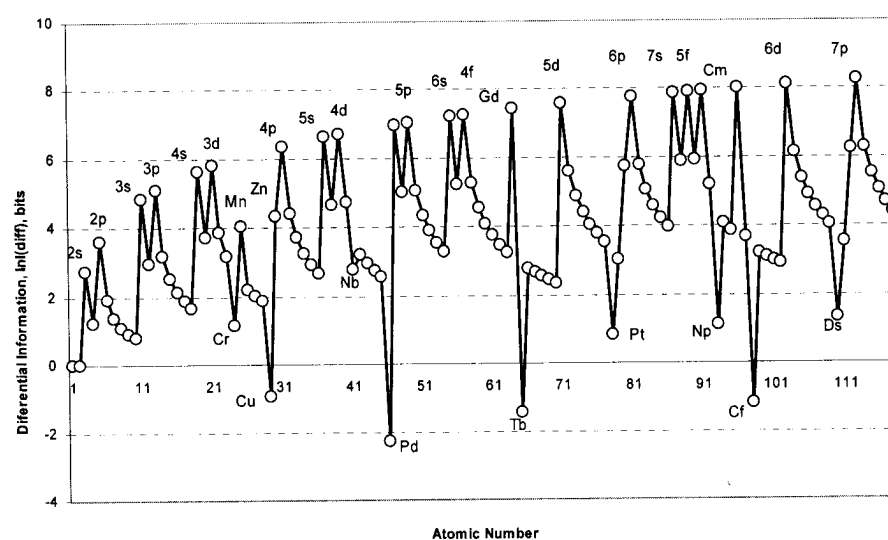


Figure 2. Differential information on the distribution of electrons in the chemical elements over electron subshells.

The elements from each main group of the Periodic Table can be connected in Figures 1 and 2 by a common curve described by a group differential information equation. These group equations are specific instances of Equation (8) with the group constant $z_{k+1} = 1$ to 8 for the I_n equations, whereas for the I_{nl} equations $z_{k+1} = 1$ and 2 for Groups 1 and 2, and $z_{k+1} = 1$ to 6 for Groups 13 to 18. One may also introduce group equations for d-elements (Groups 3–12) with $z_{k+1} = 1$ to 10 although the validity of these equations is limited by the frequent violations of the normal order of filling d subshells.

4.3. Electron Distribution over Atomic Orbitals (n, ℓ, m -States)

The Pauli Exclusion Principle limits the population of an atomic orbital to either one electron or two electrons with opposite spin. This reduces greatly the possible values of the I_{nlm} index. Figure 3 shows a rather regular variation of this information descriptor. The overall curve contains two parallel branches. The upper branch includes the elements in which, in accordance with Hund's first rule, every AO in a given subshell is populated by single electrons only. They correspond to one s, three p, five d, and seven f elements. The lower branch of the curve includes the same number of elements in which the atomic orbitals of the corresponding subshell are filled with a second electron. The two branches can be described by Equation (8), with $z_{k+1} = 1$ and 2, respectively. It immediately follows that the difference between the two curve branches is constant and equals two bits. One may conclude that the data shown in Figure 3 are an illustration of Hund's rule, which may be interpreted as demanding a maximum value of the information index I_{nlm} .

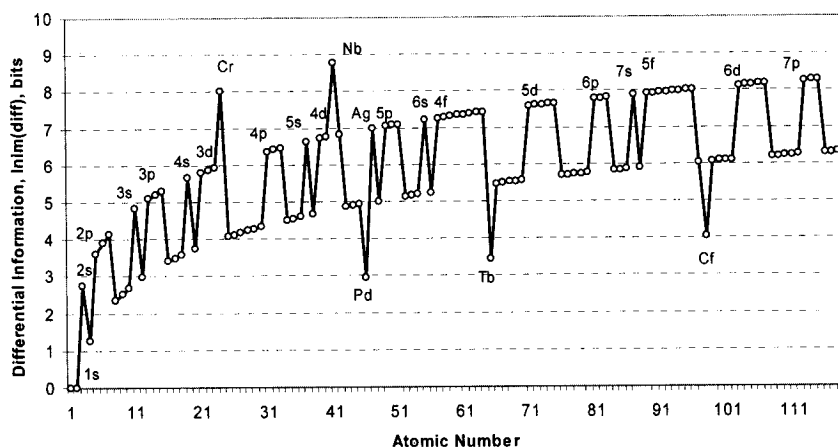


Figure 3. Differential information on the distribution of electrons in the chemical elements over atomic orbitals.

4.4. Electron Distribution over the Values of the Orbital Quantum Number ℓ

Pronounced maxima indicate in Figure 4 the elements in which the first p, d, and f electron appears: element 5, B, element 21, Sc, and element 58, Ce. Each of these elements begins a new section of the overall curve characterized by a higher value of the I_ℓ information index than in the previous curved section. It can be seen that s and p elements can again be connected by a common line and described by common group equations. The minima and maxima appearing in some of the d and f elements are those observed in Figures 1 and 2 (Cr, Cu, Nb, Pd, Gd, Tb, etc.).

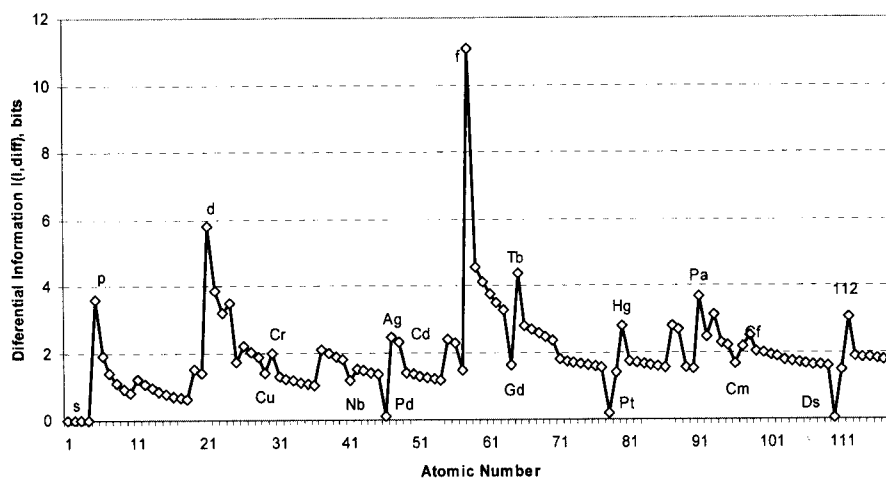


Figure 4. Differential information on the distribution of atomic electrons over the values of the orbital quantum number.

4.5. Electron Distribution over the Values of the Magnetic Spin Quantum Number

The values of the differential spin information, I_{ms} , fluctuate around the mean value of 1 bit (see Figure 5). The deviations from the latter are considerable in lighter elements but they decrease gradually with the increase in the atomic number. The minima are associated with the elements having half-filled p, d, or f subshells. The only exception is Nb, which displaces Mo from the minimum for the 4d subshell because of the 5s → 4d electron transition. The latter increases the number of unpaired electrons in Nb by two as compared to the preceding chemical element, whereas Mo has only one unpaired electron more than the preceding Nb.

$$I_{n\ell} = z \log_2 z - \sum_{n\ell} z_{n\ell} \log_2 z_{n\ell} \quad (11)$$

Denote the sum of the constant terms in Equation (11) by A , that is:

$$A = \sum_{\ell=0}^{n-1} [(n - 2\ell - \delta) \cdot 2(2\ell + 1) \log_2 2(2\ell + 1)] \quad (12)$$

where n is the period sequential number, $\delta = 1$ for $l = 0$ and $\delta = 0$ for $l > 0$. Equation (11) can now be rewritten as:

$$I_{n\ell} = z \log_2 z - A - \sum_{\ell} k_{n\ell} \log_2 k_{n\ell} \quad (13)$$

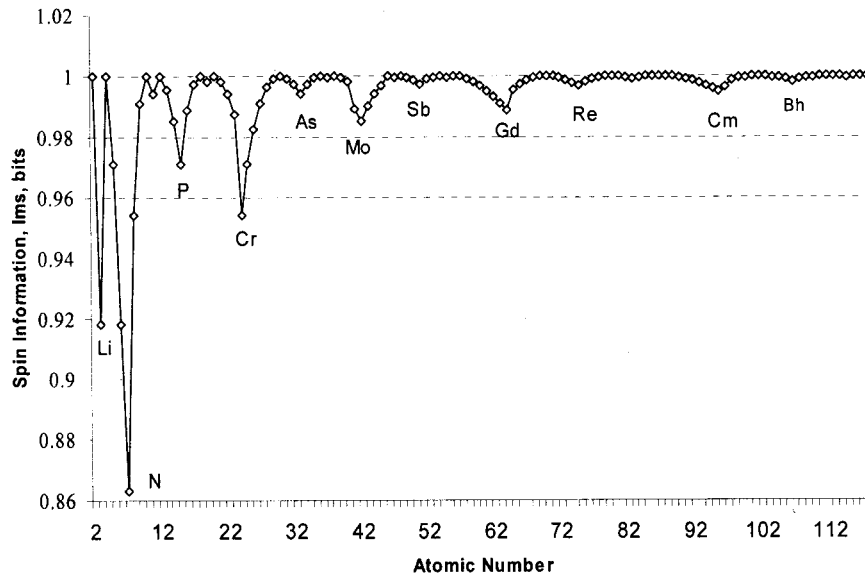


Figure 6. Average information on the distribution of atomic electrons over the values of the magnetic spin quantum number (atomic spin information).

Equation (13) is an equation for the periods and groups in the Periodic Table. The periods are characterized by the constant A , which for periods I through VII is equal to 0, 2, 19.51, 37.02, 87.75, 138.48, and 242.51 bits, respectively. The group constants $k_{nl} = 1$ or 2 for the Groups 1 and 2, $k_{nl} = 1$ to 10 for the Groups 3 to 12, and $k_{nl} = 1$ to 6 for the Groups 13 to 18, respectively.

5.2. Information on Electron Distribution over Atomic Orbitals, $I_{n/m}$

Let the number of single electrons in an atom be denoted by a . Since every atomic orbital can be occupied by only one or two electrons, the number of electron pairs in the atom will be $(z - a)/2$. Then, the total information on the electron distribution over an AO, expressed in bits per atom, will be:

$$I_{n/m} = z \log_2 z - \frac{z-a}{2} \times 2 \log_2 2 - a \times 1 \log_2 1 = z \log_2 z - z + a \quad (14)$$

Equation (14) may also be interpreted as an information equation of the groups and periods in the Periodic Table. In the ground valence state of the atom, the group constant a is equal for Groups 1, 2, and 13 to 18 to the lowest valence of the element (1, 0, 1, 2, 3, 2, 1, 0), whereas in the highest valent state it equals the old numbering of the eight main groups (1 to 8). To turn it into an equation for the periods of the chemical elements one needs to introduce a period constant z_0 as the atomic number of the noble gas that ends the preceding period ($z_0 = 2, 10, 18, 36, 54, 86$). Since $z = z_0 + a + b$, where b is the number of paired electrons in the atomic orbitals of the elements of the period of interest, one can write Equation (14) in its final form as:

$$I_{n/m} = (z_0 + a + b) \log_2 (z_0 + a + b) - z_0 - b \quad (15)$$

5.3. Information on the Electron Distribution over the Values of the Magnetic Spin Quantum Number m_s

Using the notations introduced in the preceding section, denote the number of electrons with $m_s = +1/2$ and $m_s = -1/2$ by $z_1 = z_0/2 + a + b/2 = (z + a)/2$, and $z_2 = z_0/2 + b/2 = (z - a)/2$, respectively. The information on the electron distribution into these two groups is:

$$\bar{I}_{ms} = - \frac{z+a}{2z} \log_2 \frac{z+a}{2z} - \frac{z-a}{2z} \log_2 \frac{z-a}{2z} \quad (16)$$

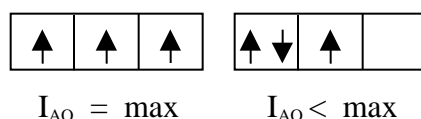
After some elementary transformations, expanding the logarithmic function into a McLaurin series, and neglecting the higher terms in the series, one obtains:

$$\bar{I}_{ms} = 1 - \frac{1}{2 \ln 2} \times \frac{a^2}{z^2} = 1 - \frac{k}{(z_0 + a + b)^2} \quad (17)$$

Here, as in Subsection 5.1, the period constant $z_0 = 2, 10, 18, 36, 54,$ and 86 for periods II through VII. The group constant $k = a^2/(2 \ln 2)$ includes the number of unpaired electrons a , as given above in subsection 5.2. The error produced by the approximation used decreases with the fourth degree of z , and even for Li, element 3, is only 0.0015.

6. INFORMATION-THEORETIC INTERPRETATION OF THE PAULI EXCLUSION PRINCIPLE AND HUND'S FIRST RULE

The information equations for the electron distributions in atoms permit some interesting interpretations of the physical principles and rules controlling the building up of atomic electronic structure. Hund's first rule, which requires the atomic orbitals (AOs) in s, p, d, and f subshells (as well as those in all degenerate molecular orbitals, MO) to fill maximally with unpaired electrons, may be interpreted as a rule demanding maximum information on atomic orbitals, I_{nlm} . This can be illustrated by comparing the values of the information index resulting from filling AOs with unpaired and paired electrons, respectively. If the added electron is paired with one of the available unpaired electrons, the parameter a in Equation (14) will be diminished by one, thus reducing the information content. The maximum information content is reached when all AOs in the subshells are occupied by unpaired electrons, which maximizes a .



It follows from the basic Equations (5) and (6) that the atomic information content reaches its absolute maximum when all $z_i = 1$. This case corresponds to electron distribution over spin orbitals, SO , defined by the four quantum numbers $n, \ell, m,$ and m_s , and controlled by the Pauli Exclusion Principle.

$$I_{SO} = z \log_2 z = \max \quad \bar{I}_{SO} = \log_2 z = \max \quad (18)$$

A similar result has been obtained by Watanabe [25] for the Neumann entropy of a particle in an atomic nucleus. Neumann's entropy of a particle in an ensemble of fermions is defined as:

$$S = -\text{Tr}(G \log G) = -\sum_i \gamma_i \log \gamma_i \quad (19)$$

where G is a quantum-mechanical operator, defined on the normalized determinantal Hartree-Fock wave function; γ_i is the statistical weight of state i in the mixture of states described by G . Since γ_i meets the requirements for a probability function, the Neumann entropy of a particle in an ensemble of fermions is equal to (up to a coefficient) the Shannon entropy in Equation (1). When the Hartree-Fock wave function obeys the Pauli Exclusion Principle, again the entropy of the particle is maximal: $\gamma_i = 1/z$, and $S = \log z = \max$, thus yielding Equation (18).

In our earlier work [18], the above ideas were generalized by information-theoretic analysis of the irreducible representations of the S_N symmetry group of the particles. It was concluded that the Pauli Exclusion Principle indicates a trend toward acquiring a maximum information content for atoms and molecules, and more generally, any system of fermions. In contrast, systems of bosons are always associated with a minimum (zero) information content. Another study [12] has shown that light emissions from atoms are associated with a decrease, and light absorption is accompanied by an increase, in the atomic information content, determined from the electron distribution over the atomic orbitals.

7. PREDICTING THE PROPERTIES OF THE TRANSACTINIDE ELEMENTS 113–120

The information indices introduced in the preceding sections describe adequately the atomic electronic structure and reproduce the structure of the Periodic Table [8, 10, 11]. On the other hand, the electronic structure of atoms essentially determines the properties of the chemical elements. One might therefore expect the structural information indices to correlate well with the diverse elemental properties. It was conjectured that the information indices will correlate considerably better than the atomic charge, which presents the total number of electrons, but not their detailed distribution over the energy states. It was also of interest to verify to what extent the potency of the Periodic Table to predict elemental properties, brilliantly used by Mendeleev, could still be of help for characterizing the unsynthesized elements at its upper end.

To test these ideas we first performed a systematic comparative study [15] of the correlations of atomic charge and the information indices with eight properties of

elements from Group 1, five properties of Group 13, and three properties of Groups 16 and 17. The properties included the entropy in the gaseous and solid state, the melting and boiling points, the heats of melting and sublimation, the first and second ionization potential [26–28]. The Slater orbital exponent, $\xi_{nl} = (z - k)/n$, was also examined because the screening constant k it includes depends essentially on the details of the electron distribution in an atom. The information indices tested were those of the total and mean information on the electron distribution over shells and subshells ($I_n, I_{nl}, \bar{I}_n, \bar{I}_{nl}$). Eight correlation functions have been used: $a + bx$, $a + bx + cx^2$, ax^b , $ax^b + c$, $a10^{bx}$, $a10^{bx} + c$, $x/(a + bx)$, and $y_1 + (x - x_1)/(a + bx)$. The best correlation for each property was selected based on the lowest standard deviation.

From the nineteen cases tested for the elements of Groups 1, 13, 16 and 17, only in one case (the absolute entropy of the elements of Group 1 in the gaseous state) was the correlation with the atomic number higher than the best of the four information indices. In most cases, the improvement of the result by the information indices was considerable. Using a polynomial function for the atomic number and the information indices, we performed additional tests with nine properties of the elements from Group 1, seven from Group 2, eight from Group 13, six from Group 16, and six from Group 17. Again, with the exception of only one case out of thirty-seven studied, the information indices provided a much higher correlation, and a five- to ten-fold smaller standard deviation, than the atomic number. Particularly good results were obtained for the boiling and melting points, which correlated rather poorly with the atomic number. It was found that the examined properties of Group 1 and 2 elements correlated better with the information on the electron distribution over the subshells, I_{nl} , whereas those of Group 13, 16 and 17 elements with the information on the distribution over the shells, I_n .

The structure-property analysis described in the previous paragraph was performed during 1979–1980. The data used for the properties of chemical elements were published even earlier [26–28]. It seemed worthwhile in preparing our chapter to update this part of the study with a wider number of properties and the most recent data. The purpose of the study being to demonstrate the advantage of information indices over the atomic number in modeling the properties of the chemical elements, we did not search for the best possible correlation for each atomic property. Rather, we limited ourselves to all of the properties known for a single group of chemical elements. These included 23 properties of the Group 1 elements [29], shown in Table 1, which represent five atomic, twelve thermodynamic, and six physical properties and parameters. The correlation functions used were limited to those included in the Excel Chart program: the linear, polynomial, power, exponential, and logarithmic ones, with the polynomials of degree two usually providing the best statistics. The comparison of the correlations produced by the atomic number and the four information indices $I_n, I_{nl}, \bar{I}_n, \bar{I}_{nl}$, was done with both the correlation coefficients and the standard deviations.

Table 1. Correlation coefficients and standard deviations for the best models of alkali metal properties produced by atomic information indices and atomic charges

Property*	Units	$r^2(I)$	$r^2(z)$	$s(I)$	$s(z)$
Melting Point	K	0.9994	0.9991	8.6	117.9
Boiling Point	K	0.9939	0.9476	0.04	2.24
Critical Temperature	K	0.9972	0.9868	10.7	21
Enthalpy of Fusion	kJ/mol	0.9983	0.9878	0.0002	0.0155
Enthalpy of Vaporization	kJ/mol	0.9915	0.9716	1.03	4.17
Enthalpy of Atomization	kJ/mol	0.9974	0.9667	0.69	2.18
Molar Volume	cm ³	0.9983	0.9703	0.39	1.75
Specific Heat (s)	J/g.K	0.9983	0.9964	0.048	0.07
Heat of Formation (g)	kJ/mol	0.9971	0.9730	0.73	1.97
Absolute Entropy (s)	J/K.mol	0.9998	0.9852	0.12	1.33
Absolute Entropy (g)	J/K.mol	0.9998	0.9994	0.08	0.15
Free Energy of Formation (g)	kJ/mol	0.9989	0.9752	0.41	1.73
Density	kg/m ³	0.9707	0.9497	49.6	48.6
Resistivity	10 ⁻⁸ ohm.m	0.9973	0.9437	0.12	3.33
Thermal Conductivity	W/cm.K	0.9328	0.7555	0.042	0.112
Linear Expansion Coefficient	cm/cm/°C	0.9982	0.9904	0.25	0.58
Elastic Modulus (bulk)	100/Gpa	0.9935	0.9624	0.12	0.33
Hardness (Mohs)		0.9999	0.9943	0.0007	0.0054
Effective Nuclear Charge		0.9996	0.9991	0.019	0.028
First Ionization Energy	kJ/mol	0.9979	0.9333	1.14	6.42
Atomic Radius	pm	0.9902	0.9792	1.99	2.76
Covalent Radius	pm	0.9958	0.9400	0.51	6.55
Ionic Radius	pm	0.9946	0.9713	1.1	2.67

*Property values from <http://webelement.com>

In all twenty-three cases examined, the correlation coefficients of the models derived with the information indices were higher than those produced by the atomic number. More considerable improvements were found for the boiling point (0.948 0.994), covalent radius (0.940 0.996), first ionization potential (0.933 0.998) and, particularly, the thermal conductivity (0.756 0.933). Yet, in half of the models, the increase in the correlation coefficient was within the 0.02–0.03 range, and in the remaining nine models it was less than that because the atomic number also produced some high correlations. The information indices produced much more significant

improvement for the standard deviation of the models. In the majority of cases the standard deviation of the information models was two- to five-fold smaller than that of their atomic number counterparts. It was 10- to 15-fold smaller for the absolute entropy in the solid state (from 1.33 to 0.12 kJ/mol), covalent radius (from 6.55 to 0.51 pm), and melting point (from 117.9° to 8.6°), 28-fold for the resistivity (from 3.33 to 0.12×10^{-8} ohm.m), 56-fold for the boiling point (from 2.24° to 0.04°!), and even 77-fold for the enthalpy of fusion (from 0.0155 to 0.0002 kJ/mol). The only property for which the atomic model produced a slightly better standard deviation was the density (48.6 vs. 49.6 kg/m³).

The models of the properties of the chemical elements obtained from the atomic information indices provided a basis for predicting some properties of the unsynthesized elements at the upper end of the Periodic Table [17]. Some predictions were already made at the time by Grosse [30], Fricke et al. [31–33], and Keller et al. [34, 35] for the properties of the individual transactinide elements 113–120 (except element 116, which was almost unstudied). The methods used were basically extrapolations from group trends in the Periodic Table with allowance for possible relativistic corrections because of the high nuclear charge of these elements. We have also considered relativistic effects and additionally adjusted our information models to match better the periodicity trends not only in groups but also in periods in line with the Mendeleev tradition. These corrections were needed for better predictions as there was no warranty that the models derived were based on the best mathematical function for each property. The elemental properties were those predicted in Refs. [30–35]: the absolute entropy in the solid state, $S^\circ(s)$, enthalpy of sublimation, H_s , boiling point, T_B , melting point, T_M , first and second ionization potential, I_1 and I_2 , molar volume, V_M , density, ρ , Pauling's covalent radius, R_{cov} , to which we added absolute entropy in gaseous state, $S^\circ(g)$, enthalpy of melting, H_M , and the Slater orbital exponent, ξ .

The predicted ranges of the elemental property values are given in Table 2. It is not yet possible to verify these predictions with experimental values. However, the continuing progress in moving the upper end of the Periodic Table, culminating in the recent syntheses of several atoms of elements 113 to 116, has brought us closer to this goal.

8.1. Information on Proton-Neutron Composition

The information-theoretic analysis of the structure of atomic nuclei was an essential part of our series of studies on atomic structure. We started this part of the project with the proton-neutron composition of the atomic nuclei [4], proceeded with the study of the nuclear shell structure [2, 7], proposed a new systematics of nuclides [9], and made predictions of the nuclear binding energies of the unsynthesized isotopes

of the chemical elements 101–108 [16] based on extrapolations from derived information-theoretic models for isodifferent groups of nuclides [13].

Table 2. Predicted Properties of the Transactinide Elements 113–120

Properties	113	114	115	116	117	118	119	120
$S_o(g)$, kcal/mol	44.5–44.6	43.4–43.5	45.7–45.9	46.1–46.3	45.7–45.9	43.3–43.5	44.6–44.8	43.3–43.5
$S_o(s)$, kcal/mol	17.1–17.2	18.6–19.0	15.4–15.5	16.8–17.2			24.9–26.6	18.5–19.5
H_M , kcal/mol	1.26		1.41–1.43	1.82		0.80–0.86	0.48–0.49	1.92–2.05
H_S , kcal/mol	32.2–32.7	17.2–17.7	58.1–58.9	28.5–28.6		5.14–5.26	15.1–15.8	39.2–42.8
TM , K	724–730	325–340	340–358	637–680	765–769	250–260	195–297	900–1020
TB , K	1370–1420	1740–1760		1035–1135	825–860	252–266	928–942	1770–1890
I_1 , eV	5.92–6.08	7.8–8.0	6.6–7.2	7.60–8.00	8.43–8.71	9.30–9.66	3.69–3.80	5.33–5.55
I_2 , eV	18.4–19.4	16.4	21.3	18.3–19.2	18.5–19.9	19.2–19.8	20.3–21.4	9.28–9.52
V_M , cm ³ /mol	17.9–18.6	20.6–20.8	22.4–25.2	29.4–30.8	44.4–44.5	55.5–61.1	92.5–96.9	44.3–46.1
$d(R)$, g/cm ³	14.5–17.1	13.4–14.0	12.5–13.0	11.0–11.4	7.1–7.3	4.9–5.1	3.7–4.0	5.2
R_{cov} , Å	1.72–1.80	1.71–1.77	1.56–1.58	1.62–1.66	1.56–1.66		2.63–2.81	2.06–2.10
–	2.15–2.21	2.15–2.19	2.32–2.36	2.48–2.54	2.69–2.75	2.88–2.94	1.18–1.22	1.35–1.3

8. PERIODICITY PATTERNS IN ATOMIC NUCLEI

The composition of the atomic nucleus is characterized by the number of protons, z , and neutrons, n , and their sum, the atomic mass, $A = z + n$. Introducing these quantities into Equations (1) and (2) we defined the total and mean information indices for the proton-neutron composition of the nucleus, I_{np} :

$$I_{np} = A \log_2 A - z \log_2 z - n \log_2 n \quad \text{bits/nucleus} \quad (20)$$

$$\bar{I}_{np} = -\frac{z}{A} \log_2 \frac{z}{A} - \frac{n}{A} \log_2 \frac{n}{A} \quad \text{bits/nucleon} \quad (21)$$

From Equations (20) and (21) one finds that the maximum information on the proton-neutron composition of the atomic nuclei is reached in symmetric nuclei having equal number of protons and neutrons, i. e., for $z = n$. In these nuclei the total

information on the proton-neutron composition is equal to the mass number A , and the mean information is exactly 1 bit:

$$I_{np}(\text{max}) = A \text{ bits/nucleus} \quad (20a)$$

$$\bar{I}_{np}(\text{max}) = 1 \text{ bit/nucleon} \quad (21a)$$

The symmetric stable nuclei of the elements from the beginning of the Periodic systems are: ${}^2\text{H}$, ${}^4\text{He}$, ${}^6\text{Li}$, etc., up to ${}^{40}\text{Ca}$. With the increase in the atomic number of an element, the filling of the proton energy levels in the nucleus is retarded as compared to the filling of the neutron energy levels. The difference in the number of neutrons and protons is termed the *isotopic number*:

$$\beta = n - z = A - 2z. \quad (22)$$

Figure 7 illustrates the basic features of the I_{np} index for all of the stable nuclides up to ${}^{204}\text{Hg}$, the term “stable” meaning a half-life too long to be measured. The upper bound of the information index is presented by the line of nuclei with a maximum mean information content of 1 bit. The deviation from this line increases with increasing atomic mass. The minima in the figure correspond to the largest excess of neutrons for the series of several isotopes of the same chemical element. Conversely, the maxima after ${}^{40}\text{Ca}$ refer to the least excess of neutrons. The largest series of stable nuclides shown is that of Sn, which begins with a maximum at ${}^{112}\text{Sn}$ ($n - z = 62$) and ends with a minimum at ${}^{124}\text{Sn}$ ($n - z = 74$).

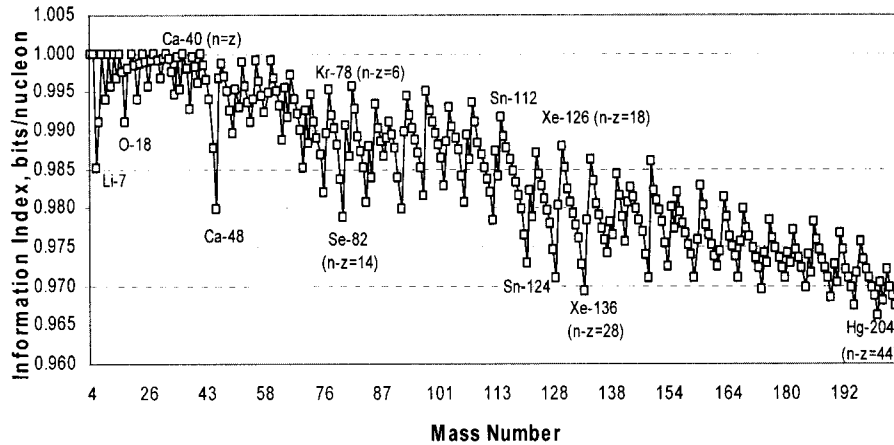


Figure 7. Average information on the proton-neutron composition for naturally occurring atomic nuclei.

Proceeding from Equation (21) and taking into account that $A = n + z$ and $n = n - z$, we substitute $n = (A + \beta)/2$ and $z = (A - \beta)/2$ into that equation to give:

$$\bar{I}_{np} = -\frac{A+}{2A} \log_2 \frac{A+}{2A} - \frac{A-}{2A} \log_2 \frac{A-}{2A} \quad (23)$$

After some elementary transformations, expanding the logarithmic function into a McLaurin series, and neglecting the higher terms in the series, one obtains:

$$\bar{I}_{np} = 1 - \frac{1}{2 \ln 2} \times \frac{1}{A^2} = 1 - \frac{1}{2 \ln 2} \times \frac{(A - 2z)^2}{A^2} \quad (24)$$

The error introduced by neglecting the second and higher terms in the McLaurin series is a small one, the largest error occurring for ${}^3\text{He}$ (0.15%). For the remaining stable nuclei the error does not exceed 0.02%; it is 0.02% in 43 cases, 0.01% in 28 cases, and less than 0.01% for the remaining 137 stable nuclei.

Equation (24) shows that the information index on the proton-neutron composition of atomic nuclei generally increases with an increase in the mass number and atomic number, and decreases with an increase in the isotopic number and the number of neutrons. These trends are however reversed for nuclei having a negative isotopic number.

8.2. The Information “Defect”

The total information on the proton-neutron composition of a nucleus, I_{np} , expressed in bits according to Equation (20), is very close to the mass number A . The difference between the two quantities was introduced in our studies [4] as the “defect” in the information by analogy with the defect of mass upon atomic nuclei formation:

$$I_{np}^* = A - I_{np} = \frac{1}{2 \ln 2} \times \frac{1}{A^2} = 1 - \frac{1}{2 \ln 2} \times \frac{(A - 2z)^2}{A} \text{ bits/nucleus} \quad (25)$$

The values of the “defect” in the information are for all stable nuclei within the 0 – 3.2% range of the I_{np} values and in most cases are smaller than 1%. The only exception is ${}^3\text{He}$ with an 8.1% defect.

The mean defect of information per nucleon, i , can also be defined:

$$I = \frac{I_{np}^*}{A} = \frac{1}{2 \ln 2} \times \frac{1}{A} = \frac{1}{2 \ln 2} \times \left(1 - 2 \frac{z}{A}\right)^2 \text{ bits/nucleon} \quad (26)$$

It can be seen from Equation (26) that i depends on the isotopic number β , as well as on the relative charge z/A . This means that nuclei having the same relative charge z/A also have the same mean defect of information. The mean defect of information is zero for $z/A = 0.5$ and increases with z/A when it is larger than 0.5, and decreases for $z/A < 0.5$.

Besides the relative charge, the i -index is also connected with the projection of the total isotopic spin of the nucleus, $T_z = z - (A/2) = (z - n)/2 = -\beta/2$, by the relation:

$$I = \frac{1}{2 \ln 2} \times \frac{T_z^2}{A} \quad (27)$$

When the number of protons and neutrons in a given atomic nucleus is equal, each of these particles carries exactly 1 bit of information (Equation 21). One may then interpret I_{nl}^* as the loss of information upon atomic nucleus formation caused by deviation of the nucleus from the symmetrical state $n = z$. Since this deviation also results in a decrease of the binding energy, we have conjectured an inverse proportional dependence between the “defect” of information and the “defect” of mass. Specific expressions of this dependence will be presented in Section 10. Here, we emphasize the idea that the defect of information can be regarded as a negative component of the binding energy, E_b . In fact, I_{nl}^* coincides (with a transition coefficient $k = 25.1$ MeV/bit) with the parameter of the relative symmetry of the nucleus, δ , in Weizsäcker’s equation for the nuclear binding energy:

$$= -18.1 \times \frac{(A - 2z)^2}{A} \text{ MeV} \quad (28a)$$

$$= -k I_{nl}^* \quad (28b)$$

The remarkable equivalence of Equations (25) and (28a) affords evidence for the usefulness of information theory in the study of atomic nuclei.

We proceeded with more analysis on the possible link between our information indices on proton-neutron composition and nuclear binding energy [2, 13]. It was found that for isodifferent series of nuclides ($\beta = n - z = \text{const}$; id series) the nuclear binding energy E_b increases with a decrease in the defect of information:

$$E_b(id) = a + \frac{k}{I_{np}^*(id)} \quad (29)$$

and increases with the total information on the proton-neutron composition:

$$E_b(id) = bI_{np}(id) + c \quad (30)$$

where the coefficient k varies with the isotopic number beta according to the empirical equation:

$$k = 8539 \times \beta^{1.819} \quad (31)$$

The accuracy of Equations (29–31) increases with the excess of neutrons and for $\beta \geq 15$ the standard deviation is less than 1%. Equations (29) and (30) may be considered as supporting Baker's ideas [37, 38] that the nuclear binding energy depends primarily on the isotopic number beta.

8.3. Information Equations for the Four Main Classes of Nuclides

The existing systematics of the nuclides groups them into four main classes: isobars, having a constant atomic mass; isotopes, having a constant number of protons; isotones, having a constant number of neutrons; and isodifferents, having a constant difference in the number of neutrons and protons. We derived information equations for these classes of nuclides (Table 3), characterizing each class by the mean information, the defect of information, and the differential information on the proton-neutron distribution. These equations may be regarded as an information-theoretic interpretation of nuclear periodicity and the systematics of nuclides. In the next section, we show that the information equations derived can also provide a basis for extending nuclide systematics.

9. INFORMATION-THEORETIC VERSION OF THE SYSTEMATICS OF NUCLIDES

9.1. The New Series of Isodefactive Nuclides

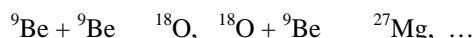
The introduction of the mean defect of information via Equation (26) has led to some unexpected consequences. If the ratios β/A and z/A in that equation are multiplied by $k = 1, 2, 3, \dots$, the mean defect of information does not change. Thus, a new class of nuclide series is formed by starting with a different nuclide and including in the series those nuclides whose atomic masses, number of protons and neutrons, and isotopic

number are multiples of the atomic mass of the first nuclide: $A = kA_1$, $z = kz_1$, $n = kn_1$, and $\beta = k\beta_1$, with $k = 1, 2, 3, \dots$. This implies a possible common generation mechanism: each member of a series of isodefect nuclides can be synthesized from two of the preceding members of the series.

Table 3. Information Equations for the Four Main Classes of Nuclides

#	Equations	Constants
I. Isobars ($A = \text{const}$)		
8.1	$\bar{I}_{np}(\text{isobars}) = 1 - c^2 = 1 - c(A - 2z)^2$	$c = (2 \ln 2A^2)^{-1}$
8.2	$I_{np}(\text{isobars}) = a - bz$	$a = \frac{2(A+1)}{A \ln 2}, b = \frac{4}{A \ln 2}$
8.3	$I_{np}^*(\text{isobars}) = cA(A - 2z)^2$	
II. Isodifferents ($\Delta = n - z = \text{const}$)		
8.4	$\bar{I}_{np}(\text{isodifferents}) = 1 - \frac{d}{A^2}$	$d = \frac{2}{2 \ln 2}$
8.5	$I_{np}(\text{isodifferents}) = 2 \left[1 + \frac{d}{A(A-2)} \right]$	
8.6	$I_{np}^*(\text{isodifferents}) = \frac{d}{A}$	
III. Isotopes ($z = \text{const}$)		
8.7	$\bar{I}_{np}(\text{isotopes}) = 1 - \frac{1}{2 \ln 2} \left[1 - \frac{e}{A} \right]^2$	$e = 2z$
8.8	$I_{np}(\text{isotopes}) = f + \frac{g}{A(A-1)}$	$f = 0.2786, g = \frac{4z^2}{2 \ln 2}$
8.9	$I_{np}^*(\text{isotopes}) = \frac{A}{2 \ln 2} \left[1 - \frac{e}{A} \right]^2$	
IV. Isotones ($n = \text{const}$)		
8.10	$\bar{I}_{np}(\text{isotones}) = 1 - \frac{1}{2 \ln 2} \left[\frac{e}{A} - 1 \right]^2$	$e = 2n$
8.11	$I_{np}(\text{isotones}) = f + \frac{g}{A(A-1)}$	$g = \frac{4n^2}{2 \ln 2}$
8.12	$I_{np}^*(\text{isotones}) = \frac{A}{2 \ln 2} \left[\frac{e}{A} - 1 \right]^2$	

As an example, consider the nuclear fusion reactions in the series starting with ${}^9\text{Be}$:



The same proportionality holds for the total isotopic spin of the isodeficient nuclides: $T_z = kT_{z,1}$. In Table 4 some of the largest series of isodeficient nuclides are shown with their first member, the serial numbers of the first and the last [40] series member, and the constant defect of information of the series.

Table 4. The first nuclide and the constant defect of information for the first twenty series of the isodeficient nuclides

#	1	2	3	4	5	6	7	8	9	10
First Nuclide	${}^2\text{H}$	${}^3\text{H}$	${}^5\text{He}$	${}^7\text{Li}$	${}^9\text{Be}$	${}^{11}\text{B}$	${}^{12}\text{B}$	${}^{13}\text{C}$	${}^{15}\text{N}$	${}^{16}\text{N}$
k	1–30	1–17	1–53	1–30	1–20	1–11	1–18	1–10	1–11	1–12
$i \times 10^2$	0	8.17	2.91	1.48	0.89	0.60	2.01	0.43	0.32	1.13
#	11	12	13	14	15	16	17	18	19	20
First Nuclide	${}^{17}\text{N}$	${}^{17}\text{O}$	${}^{19}\text{O}$	${}^{19}\text{F}$	${}^{20}\text{F}$	${}^{22}\text{F}$	${}^{23}\text{Ne}$	${}^{25}\text{Na}$	${}^{26}\text{Na}$	${}^{27}\text{Na}$
k	1–15	1–8	1–11	1–7	1–9	1–12	1–8	1–7	1–8	1–9
$i \times 10^2$	0.26	0.25	1.81	0.20	0.72	2.40	1.23	1.04	1.71	2.49

9.2. Representation of the Chart of the Nuclides with Five Classes of Nuclides

The new class of nuclides formulated above extends the Chart of the Nuclides with a fifth dimension. Figure 9 shows a portion of the new chart that we propose to be built with defect of information/mass number coordinates (i/A diagram). The illustration includes nuclides having mass numbers between 100 and 120, and atomic numbers between 39 (Y) and 56 (Ba). The coordinate system selected allows manifesting all five classes of nuclides in a single two-dimensional graph. Besides *isobars* along the vertical direction (e.g., ${}^{100}\text{Rd}$ to ${}^{100}\text{Y}$), and *isodeficientants* along the horizontal direction (e.g., ${}^{102}\text{Nb}$ to ${}^{120}\text{Ag}$), one can also find in Figure 8 *isodifferent series* descending slowly from left to right, e.g. the $n = 18$ series, descending from ${}^{100}\text{Nb}$ to ${}^{120}\text{Sb}$. The *isotone series* descend steeply in the same left to right direction, as shown with the series from ${}^{105}\text{Nb}$ to ${}^{120}\text{Ba}$. The *isotope series* ascend steeply from left to right; the example selected is the Rh series from ${}^{100}\text{Rh}$ to ${}^{114}\text{Rh}$. The direction and magnitude of change for these

three series are respectively described by Equations (8.6), (8.12), and (8.9) (Table 3). Equations (8.9) and (8.12) show a more complex behavior of the isotopic and isotonic series curves than that shown in Figure 8. These curves are actually parabolas with a zero point at $n = z$. The isotopic curve at $n < z$ has a short left branch showing a decreasing information defect with increase in the atomic mass. Conversely, the isotonic curve under the same conditions ($n < z$) has a short right branch increasing with atomic number. These short branches do not appear for the stable nuclei having $A > 49$ as the $n < z$ condition cannot be satisfied.

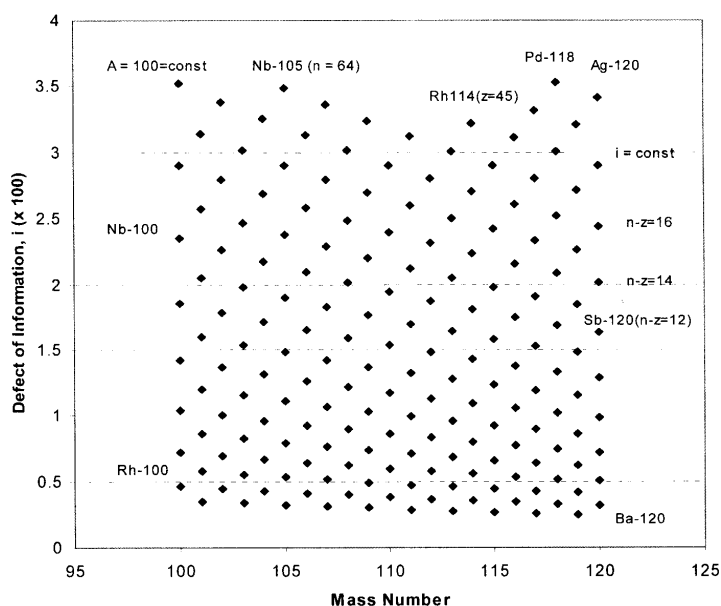


Figure 8. A fragment from the proposed extended systematics of the nuclides which includes five nuclide classes: isobars (e.g., Rh-100 to Nb-100), isotopes (e.g., Rh-100 to Rh-114), isotones (e.g., Nb-105 to Ba-120, isodifferents (e.g., Nb-100 to Sb-120), and isodeflectants (e.g., the line with $i = 3$).

9.3. Nuclide Periods as Analogues of the Periods of the Chemical Elements

The i/A chart enables the formation of nuclide periods either in the traditional manner proceeding from the proton magic number or in a novel way using analogies with the Periodic Table of the chemical elements. In both versions, the nuclide periods are formed by isodifferent series of nuclides, but differ at the beginning and end of each

period. When the periods are limited by the values of the proton magic numbers, one arrives at the systematics proposed by Selinov [39]. In the second case, the seven periods formed have respectively 2, 8, 8, 18, 18, 32, and 32 nuclides in a given isodifferent series (Period VII remaining incomplete), each series beginning with an alkali metal nuclide and ending with an inert gas one. Each nuclide period of this type is represented by a large number of isodifferent series and this number increases with the period number (Table 5). The nuclide period multiplicity represents the major difference with the structural organization of the chemical elements.

Table 5. Periods for the nuclides as analogues of the periods of the chemical elements.

Period	First and Last Nuclide	?-range	?-series
I	$^1\text{H} - ^{10}\text{He}$	-1 to +6	7
II	$^4\text{Li} - ^{32}\text{Ne}$	-5 to +12	17
III	$^{17}\text{Na} - ^{53}\text{Ar}$	-6 to +17	23
IV	$^{32}\text{K} - ^{97}\text{Kr}$	-7 to +25	32
V	$^{71}\text{Rb} - ^{147}\text{Xe}$	-3 to +39	42
VI	$^{112}\text{Cs} - ^{228}\text{Rn}$	+2 to +56	54
VI	$^{200}\text{Fr} - ^{289}\text{Uuh}$	+26 to +60	38*

*The number of isodifferent series according to July 2003 data [29].

10. FROM SIMILARITY OF INFORMATION EQUATIONS TO SIMILARITY OF PERIODICITY IN CHEMICAL ELEMENTS AND NUCLIDES

10.1. Correspondence Between the Classes of Nuclides and Classes of Chemical Elements

The information equations derived in Section 8 provide the basis for a comparative analysis of the periodicity trends in chemical elements and nuclides. Of particular interest is the similarity of Equation (17) for the average spin information per electron in a chemical element to Equation (24) for the average information for proton-neutron composition per nucleon in a nuclide:

$$\bar{I}_{np} = 1 - \frac{1}{2 \ln 2} \times \frac{1}{A}^2 \quad \bar{I}_{ms} = 1 - \frac{1}{2 \ln 2} \times \frac{a}{z}^2 \quad (32)$$

It is seen from comparison of the two equations that the atomic number z of the element corresponds to the mass number A of the nuclide, and the number of single electrons ($a = e_{-1/2} - e_{+1/2}$) in the electron shell is an analogue of the number of “single” neutrons that remain unpaired with protons ($= n - z$). The analogy of the information equations can be extended to a more general correspondence between the classification of the chemical elements and nuclides (Table 6).

Table 6. Information correspondence between the classes of chemical elements and nuclides

NUCLIDES				CHEMICAL ELEMENTS				
Parameters		Classes		Parameters		Classes		
1.	$\beta = \text{const}, A$	const	Isodifferents	$a = \text{const}, z$	const	Groups		
2.	A	$A + 1, \beta$	$\beta + 1$	Isotones	z	$z + 1, a$	$a + 1$	Periods (first half) ($s^1, p^1-p^3, d^1-d^5, f^1-f^7$)
3.	A	$A + 1, \beta$	$\beta - 1$	Isotopes	z	$z + 1, a$	$a - 1$	Periods (second half) ($s^2, p^4-p^6, d^6-d^{10}, f^8-f^{14}$)
4.	$A = \text{const}, \beta$	const	Isobars	$z = \text{const}, a$	const	Electronic states with different spin multiplicity		
	β	$\beta + 2$		a	$a + 2$			

As seen in Table 6, the isodifferent and isobar series of nuclides have individual analogues in the classes of the chemical elements — the groups of elements and, respectively, the different spin states of a single element (e.g., $Cl_{1/2}$, $Cl_{3/2}$, $Cl_{5/2}$, and $Cl_{7/2}$). The isotope and isotone series of nuclides, however, are a common analogue of the elements of a given period. The first half of the elements of a period, characterized by a filling of atomic orbitals with unpaired electrons according to Hund’s first rule, are analogues of the nuclides in the isotone series. The second half of the elements in a period, in which the atomic orbitals are sequentially filled by a second electron, are analogues of isotopes. The similarity in the periodicity patterns of the chemical elements and nuclides provides not only a basis for their common systematics. As shown in the next subsection, this similarity opens the way to correlation of the properties of elements and nuclides.

10.2. Empirical Correlations Between Electronic Energy and Nuclear Binding Energy and Prediction of Nuclear Binding Energies of the Nuclides of Elements 101–108

The correlations found between the information on the proton-neutron composition or the defect of this information, and the nuclear binding energy (Equations 30 and 29, respectively), along with the similarities found in the periodicity of the nuclides and chemical elements, prompted us to search for direct relationships between the nuclear and electronic energies. Examining a variety of functions, we found two of them to relate fairly well the ground state electronic energy E_e of the chemical elements to the nuclear binding energy $E_b(id)$ of isodifferent series of nuclides:

$$E_e = a \times E_b(id)^b \quad (33)$$

and

$$E_e = \frac{E_b(id) - E_{b,0}(id)}{c + d \times E_b} + E_{e,0} \quad (34)$$

Here a , b , c , and d are empirical coefficients characterizing a given isodifferent series, whereas $E_{b,0}$ and $E_{e,0}$ are the nuclear binding energy and the electron energy of the first nuclide and the first element in the series, respectively. The electronic energies were taken from Fricke, Greiner and Waber [32], and the nuclear binding energies from Kravtsov [41]. The accuracy of the models systematically increased from lower to higher periods, and the standard deviation of the models for Periods V and VI was between 0.2% and 0.9%.

We were thus encouraged to use our models to predict in 1980 the nuclear binding energies of unsynthesized nuclides of the elements from the upper end of the Periodic Table [16]. Nine isodifferent series with $\beta = 49$ to 57, atomic charges within the 87–103 range, and mass numbers between 224 and 257, were used to obtain predictive models. The average standard deviation of the models was 0.13%. Forty-five extrapolations from our models were made for nuclides of the elements 101–108. We found that forty-four of these forty-five nuclides have now been synthesized and the nuclear binding energies of 41 of them have been measured [29]. The excellent agreement of the predicted and measured values is shown in Table 7. The standard deviation is only 1.9 MeV for a binding energy range of 1890–1950 MeV, i.e. the relative standard deviation is approximately 0.1%.

Table 7. Comparison of the predicted and measured values of the nuclear binding energies of some nuclides of chemical elements 101 to 108

z	A	$E_b(\text{pred.})$	$E_b(\text{exper.})$	z	A	$E_b(\text{pred.})$	$E_b(\text{exper.})$		
49	103	255	1889.235	1887.465	53	106	265	1945.166	1943.199
	104	257	1899.300	1896.954		107	267	1954.800	1952.342
	105	259	1909.259	1906.121	54	102	258	1913.639	1911.128
	106	261	1919.112	1915.447		103	260	1924.599	1919.621
	107	263	1928.862	1924.336		104	262	1935.477	1930.934
50	104	258	1903.592	1904.563		105	264	1946.285	1939.257
	105	260	1912.916	1912.603		106	266	1957.026	1950.468
	106	262	1922.085	1923.259	55	102	259	1916.513	1916.569
	107	264	1931.101	1930.932		103	261	1926.384	1926.418
	108	266	1939.969	1941.345		104	263	1936.086	1936.563
51	104	259	1912.138	1910.716		105	265	1945.581	1946.224
	105	261	1921.943	1920.042		106	267	1954.913	not synth.
	106	263	1931.617	1929.620	56	101	258	1910.768	1911.701
	107	265	1941.163	1938.568		102	260	1920.146	1923.139
	108	267	1950.582	1947.803		103	262	1929.240	1931.927
52	103	258	1911.461	1906.916		104	264	1938.056	1943.295
	104	260	1922.186	1918.037		105	266	1946.616	unknown
	105	262	1932.856	1926.206	57	101	259	1918.088	1917.837
	106	264	1943.456	1937.123		102	261	1928.501	1928.317
	107	266	1953.973	1944.952		103	263	1938.762	1938.413
53	103	259	1915.474	1913.955		104	265	1948.874	unknown
	104	261	1925.505	1923.949		105	267	1958.840	unknown
	105	263	1935.472	1933.417					

11. CONCLUDING REMARKS

The change of a century always offers the opportunity to look back, summarize what has been achieved, and to try to predict future developments. Where stands the theory of Periodic Table at the beginning of the twenty-first century? Is this theory completed? Are the properties of all of the chemical elements entirely described by contemporary quantum chemical calculations [42, 43]? One must not mistakenly take the very

accurate calculations for *explanation*. The latter were achieved by using models and approximations rather than precise calculations [44, 45]. This explains why the periodicity of the chemical elements has been studied by powerful methods alternative to quantum mechanics, such as group theory beginning with the seminal work of Fock [46] and ending with the elementary particle approach [47, 48].

Information theory is another alternative way to describe the periodicity of the chemical elements. Our studies summarized in this chapter have introduced a number of information indices for characterizing the electronic and nuclear structure of atoms of the chemical elements. These descriptors of atomic structure express in different ways the information content of the atom encoded in the distributions of the atomic particles, namely electrons, protons and neutrons. The information indices were shown here to be sensitive mathematical models of the periodic patterns in electron distributions. The beginning and end of electron shells and subshells are marked in these information models by maxima and, respectively, minima. The trends of regular change of the information content of atoms within the periods of the chemical elements and the s, p, d, and f blocks is mirrored adequately by the information equations derived. Included also are the subtle effects of the delay in filling the d and f atomic orbitals, as well as the “anomalies” of accelerated filling up of the d^5 , d^{10} and f^7 subshells. The periodicity trends identified provided the basis for interpretation of the controversial problem of the first and last 4f and 5f elements. The trends were used to model a variety of chemical element properties with considerably better statistics than the respective atomic charge/property correlations. All this enabled a detailed prediction of the properties of the transactinide elements 113–120. It was also shown that essential parts of the Aufbau Principle, such as the Pauli Exclusion Principle and Hund’s first rule are associated with a trend toward a maximum information content in atoms and molecules. More generally treated with group theory methods, this trend was shown to extend to all fermionic systems, and to require a minimum information content for bosonic systems.

An important part of our study was related to the periodicity trends in atomic nuclei. Using information equations derived for the proton-neutron composition of the nuclei, we found a similarity in the periodicity patterns of electronic shells and atomic nuclei. This similarity was used to specify nuclide periods by a strict analogy with the periods of the chemical elements. Another concept introduced was that of the “defect” of information on proton-neutron composition in nuclides whose nuclei deviate from the symmetric proton/neutron composition. The new nuclear descriptor was used as the basis of a new version of nuclide systematics which included a fifth type of nuclide series incorporating nuclides having the same information defect. The similarity of the information equations derived for nuclei and electron shells also produced a direct correspondence between the nuclide classes of isobars, isotopes, isotones, and isodifferents, with the groups and periods of chemical elements. It was shown that the

defect of information, with an accuracy up to a numerical coefficient, coincides with the symmetry term in the Weizsäcker equation for the nuclear binding energy. This finding provided the basis for a direct successful search for defect of information/nuclear binding energy correlations.

Making use again of the similarity in periodicity trends in electronic shells and atomic nuclei, we found in 1979–1980 the first correlations between electronic and nuclear properties. The models relating electronic ground state energy and nuclear binding energy within series of nuclides with a constant isotopic number were used in that work to predict the binding energies of 45 unsynthesized isotopes of the elements 101 to 108. Twenty-three years later, we found data for 41 synthesized nuclides, and our predictions were confirmed with a standard deviation of only 0.1% from the measured values. Even more intriguing than the high prediction accuracy was the fact that the models used were based on correlating electronic with nuclear properties, which has never been done before.

Recently, other manifestations of such relations between the seemingly incomparable electronic and nuclear properties have been reported; these are nuclear excitations caused by electronic transitions (NEET) [49]. We are also encouraged by the recent interest in applying information theory to atomic nuclei and atoms, which has resulted in finding a direct link between Shannon's entropy and the kinetic energy for quantum many-body systems [50–52], as well as in applying the Shannon entropy as a measure for the quality of the nuclear density distribution [53]. It is our belief that the twenty-first century will make further essential contributions to the theory of the Periodic Table, particularly in relation to the recent progress in the topological theory of discrete space-time [54].

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