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CORRELATION BETWEEN INFORMATION INDICES AND PROPERTIES OF CHEMICAL ELEMENTS

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Abstract

Information Theory was recently applied to the characterization of atomic electron shells[1-7]. The structural indices of the chemical elements thus introduced were found to correlate much better than atomic number with a number of properties, such as thermodynamic entropy, boiling and melting point, screening constant, ionization potential, etc. The possibility of prediction the properties of hypothetical elements having z=113 - 120 is discussed on this basis.

Introduction

Recently an information-theoretic approach to the description of the electronic structure of chemical elements was developed [1-7]. It is essentially based on the concept of information content, introduced by means of the Shannon eguation in Information Theory[8]. This equation could be written out for an atom of a chemical element in the form:

$$\bar{I} = - \sum_{i=1}^{k} \frac{z_i}{z} \log_2 \frac{z_i}{z} \text{ , bits per electron} \qquad (1),$$

where the z electrons in the electron shell of the atom are regarded as being distributed in k different groups: z_1, z_2, ...z_k, and z_i/z is the probability of an electron of this atom being in the group i. I is the mean per electron information on electron distribution of the atom, or otherwise, the mean information content of the atom. The total information content of the atom may also be specified by an equation derived from (1):

$$I = z.\bar{I} = z \log_2 z - \sum_{i=1}^{k} z_i \log_2 z_i \qquad (2).$$

Depending on the criterion of electron grouping k various atomic information indices can be defined by egns. (1) and (2): information on electron distribution over shells (I_n), subshells (I_{nl}), nlj- subshells (I_{nlj}), atomic orbitals (I_{nlm}), spin- orbitals (I_{nlmm}), (n+1)- electron groups (I_{n+1}), as well as over groups of the same values of the atomic quantum numbers: angular momentum (I_l), magnetic (I_m), magnetic spin (I_m), inner (I_j), and total magnetic (I_{m_j}).

Results and Discussion

These indices reflect adequately the atomic electronic structure and reproduce the structure of the Periodic Table[2-4]. Their importance for various aspect of the quantitative analysis of periodicity is reviewed in another report of this conference[1]. The present work stresses on another field of application of atomic information indices. The physical and chemical properties of chemical elements essentially depend on their electronic structure. Therefore, one might expect the structural information indices to correlate well with the diverse properties of chemical elements.

Evidencing this point of view a fairly good correlation was found to exist between the informations (total, as well as mean one) on electron distributions on shells (I_n) and subshells (I_{nl}) from the one hand, and such properties of the

elements of groups I, III, VI, and VII, as entropy in gaseous and solid state[9], melting and boiling point[9], heats of melting[9] and sublimation[10], and the first ionization potential[10] (Fig. 1-7), on the other hand. The data for S^{o}_{gas} of Fr and Po, as well as S^{o}_{solid} for Fr were taken from reference[10], whilst T_b, T_M, and ΔH_M of Fr- from reference[11].

Naturally, due to the periodicity in the electronic structure, the properties of chemical elements are expected to correlate with any quantity that reflects correctly this periodicity. The correlation between information indices and properties would be of importance only if they were higher than the respective correlations with the atomic number of chemical elements. It is logically supposed that they are actually such, since the atomic number represents only the total number of electrons, whilst information indices reflect all features of the electronic structure of atoms.

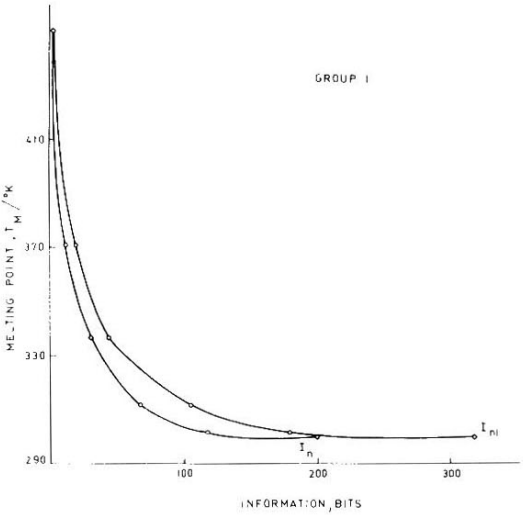

FIG. 1. Melting point of the chemical elements of group 1 vs. total information indices on electron distribution over shells (I_n), and subshells (I_{nl})

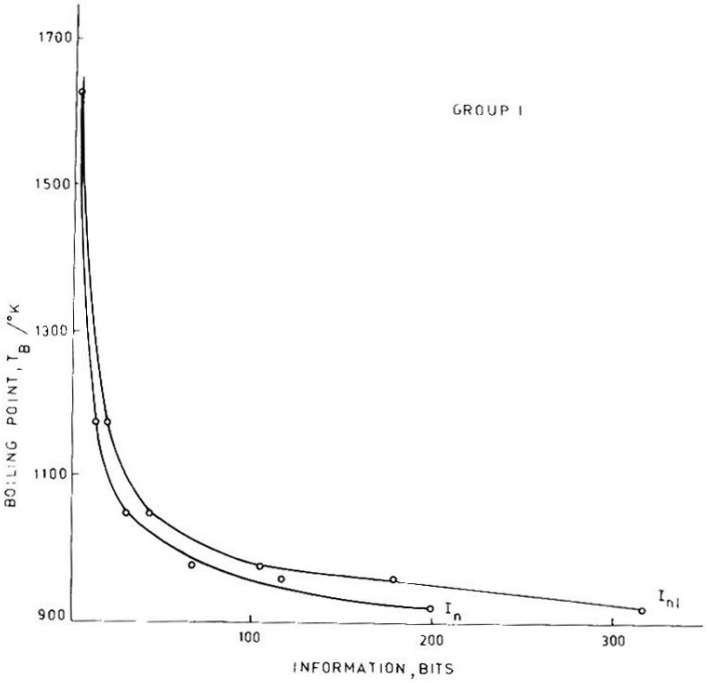

FIG. 2. Boiling point of the chemical elements of group I vs. total information indices on electron distribution over shells (I_n), and subshells (I_{nl})

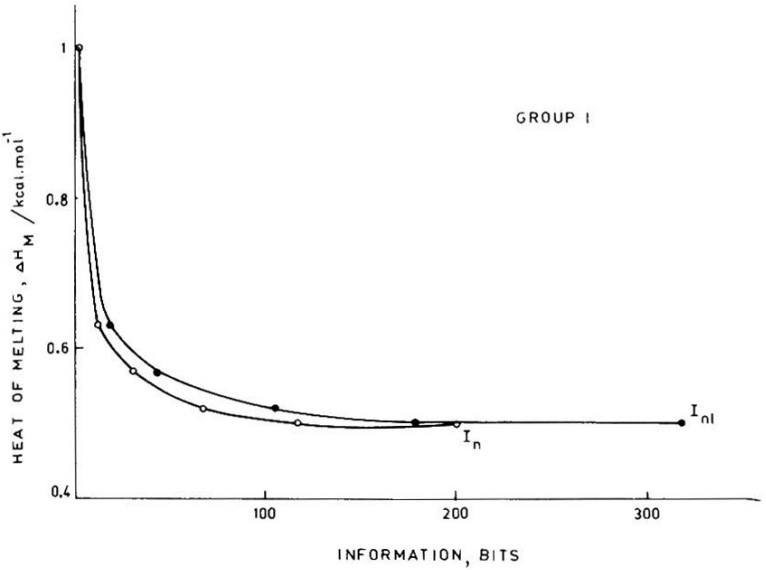

FIG. 3. Heat of melting of the chemical elements of group I vs. total information indices on electron distribution over shells (I_n), and subshells (I_{nl})

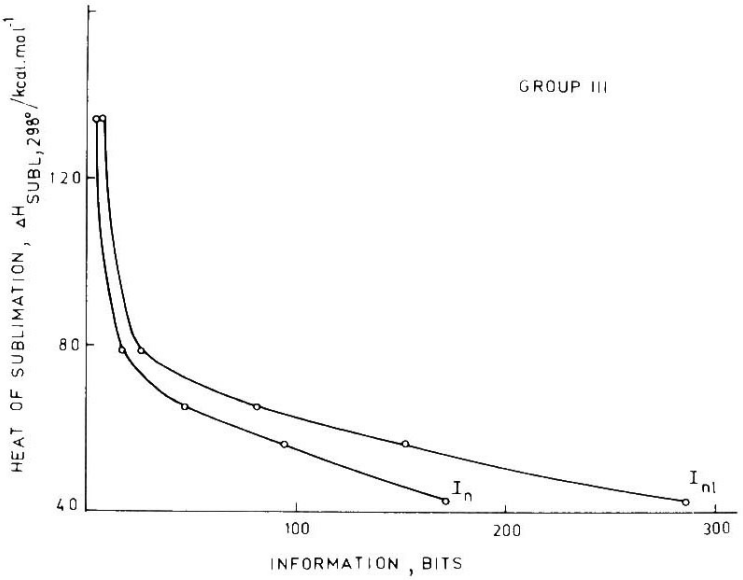

FIG. 4. Heat of sublimation of the chemical elements of group III vs. total information indices on electron distribution over shells (I_n), and subshells (I_{nl})

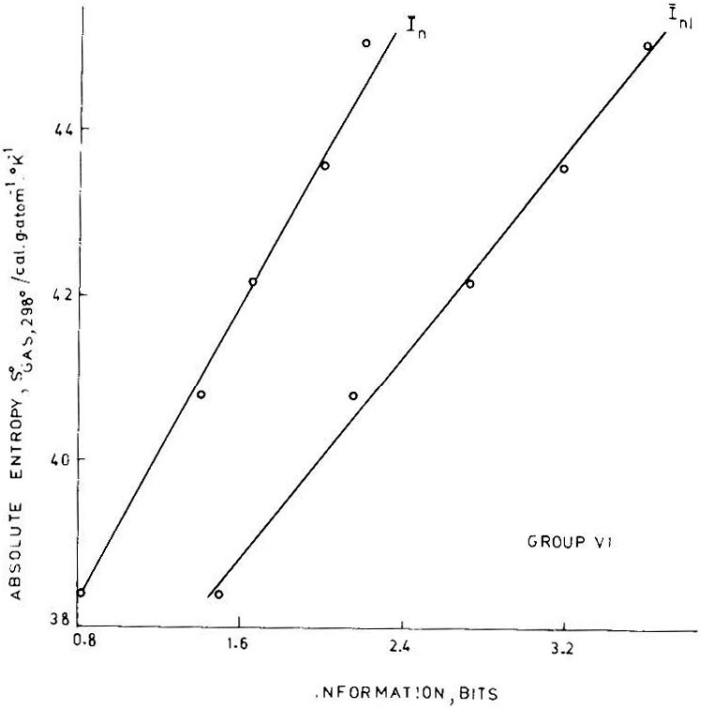

FIG. 5. Absolute entropy of the chemical elements of group VI vs. total information indices on electron distribution over shells (I_n), and subshells (I_{nl})

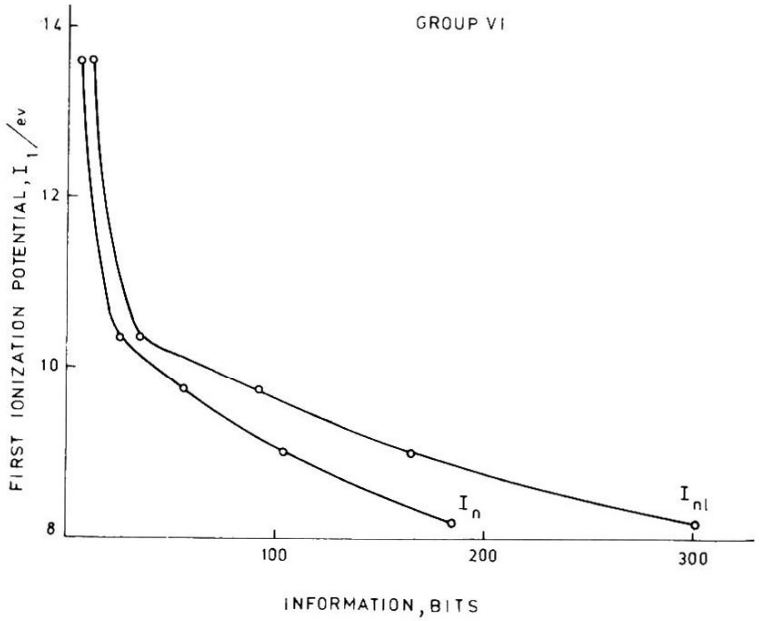

FIG. 6. First ionization potential of the chemical elements of group VI vs. total information indices on electron distribution over shells (I_n), and subshells (I_{nl})

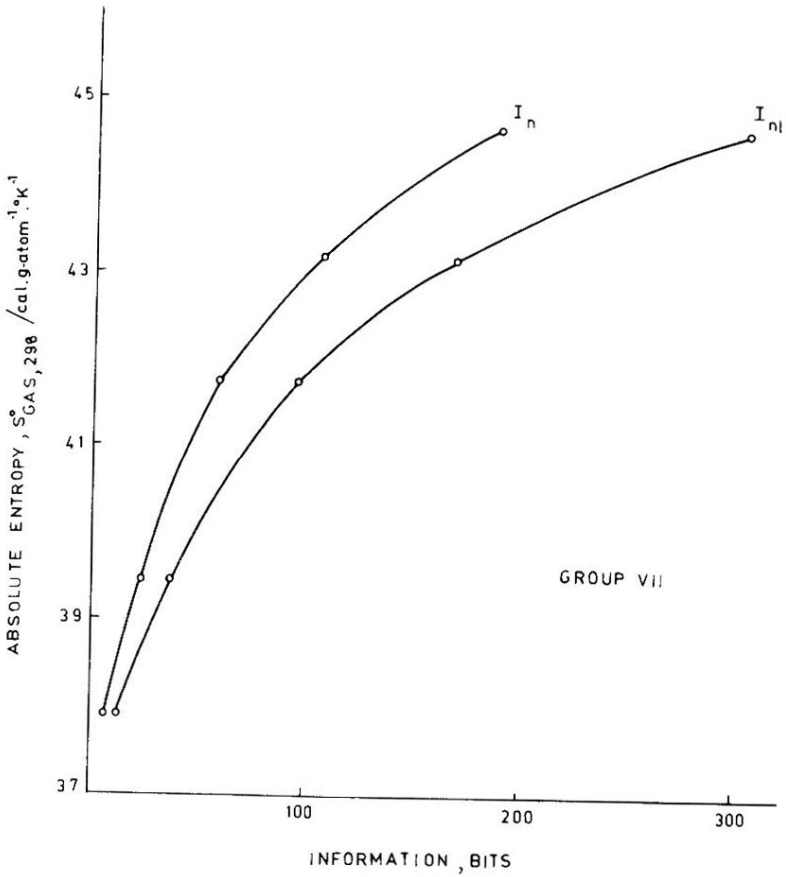

FIG. 7. Absolute entropy of the chemical elements of group VII vs. total information indices on electron distribution over shells (I_n), and subshells (I_{nl}).

In order to check this assumption each of the properties under study was correlated with the atomic number of the chemical element, and alternatively, with the abovementioned four information indices (I_n, $\bar{I}_n$, I_{nl}, and $\bar{I}_{nl}$). The correlations were derived by a computer program which selects that equation out of eight which provides the best least sqare fit[12]. The Slater orbital exponent[13,14], ζ_{nl}, was also examined since it includes the screening constant k ($\zeta_{nl}=(z-k)/n$) which essentially depends on electron distribution on shells and subshells. The results thus obtained are summarized in Table 1 where for every property under examination the correlation is given with the atomic number and that of the four information indices which provides the leas error. The dimensions of the quantities in use are given in Table 2.

The date from table 1 are a convincing evidence in support of the assumption that atomic information indices are better structural indices than the atomic number of chemical elements. From 19 examined cases (8 for group I, 5 for group III, 3 for groups VI and VII) only in one (Nos. 1, 2) the information indices do not manifest such a better correlation. In the other 18 cases they provide the decrease in the relative error, the latter often being considerable (Nos. 5,6; 9,10; 13,14; 29,30; 35,36). Some selectivity exists for the indices in these correlations, that is, entropy and first ionization potential correlate best with the information on electron distribution over shells, whilst orbital exponent, heat and point of melting- with that over subshells.

TABLE 1

Correlations Between Properties and Information Indices (or Atomic Number) of the Chemical Elements of Groups I, III, VI and VII

№	Y_i / X_i	Type of equation	Mean relative error, %
	Groups I		
1.	S^o_{gas}/z	$y = Ax^B$	0,17
2.	S^o_{gas}/I_n	$y = Ax^B$	0,35
3.	S^o_{solid}/z	$y = Ax^B + C$	2,99
4.	S^o_{solid}/I_{nl}	$y = Ax^B + C$	2,57
5.	T_M/z	$y = \frac{x - x_1}{A + Bx} + y_1$	7,62
6.	T_M/I_{nl}	$y = \frac{x - x_1}{A + Bx} + y_1$	3,59
7.	T_B/z	$y = \frac{x - x_1}{A + Bx} + y_1$	0,96
8.	$T_B/\bar{I}_{nl}$	$y = \frac{x - x_1}{A + Bx} + y_1$	0,66
9.	$\Delta H_M/z$	$y = \frac{x - x_1}{A + Bx} + y_1$	0,76
10.	$\Delta H_M/\bar{I}_{nl}$	$y = \frac{x - x_1}{A + Bx} + y_1$	0,35

TABLE 1 (Continuation)

№	Y_i / X_i	Type of equation	Mean relative error, %
11.	$\Delta H_s/z$	$y = \frac{x - x_1}{A + Bx} + y_1$	2,32
12.	$\Delta H_s/\bar{I}_{nl}$	$y = \frac{x - x_1}{A + Bx} + y_1$	1,90
13.	I_1/z	$y = A + Bx + Cx^2$	3,33
14.	$I_1/\bar{I}_n$	$y = Ax^B$	1,42
15.	ζ_{ns}/z	$y = Ax^B$	1,38
16.	ζ_{ns}/I_{nl}	$y = Ax^B$	1,34
	Group III		
17.	S^o_{gas}/z	$y = Ax^B$	0,76
18.	$S^o_{gas}/\bar{I}_n$	$y = \frac{x}{A + Bx}$	0,63
19.	S^o_{solid}/z	$y = \frac{x - x_1}{A + Bx} + y_1$	4,85
20.	S^o_{solid}/I_n	$y = \frac{x - x_1}{A + Bx} + y_1$	2,95
21.	T_B/z	$y = Ax^B$	9,41
22.	$T_B/\bar{I}_n$	$y = \frac{x}{A + Bx}$	7,49

TABLE 1 (Continuation)

№	Y_i / X_i	Type of equation	Mean relative error, %
23.	$\Delta H_s/z$	$y = Ax^B$	6,05
24.	$\Delta H_s/\bar{I}_n$	$y = \frac{x - x_1}{A + Bx} + y_1$	4,72
25.	$\mathfrak{Z}_{np}/z$	$y = 10^{A+Bx} + C$	1,74
26.	$\mathfrak{Z}_{np}/\bar{I}_{nl}$	$y = 10^{A+Bx} + C$	1,45
	Group VI		
27.	S^o_{gas}/z	$y = \frac{x - x_1}{A + Bx} + y_1$	0,15
28.	S^o_{gas}/I_n	$y = \frac{x - x_1}{A + Bx} + y_1$	0,12
29.	I_1/z	$y = \frac{x}{A + Bx}$	2,60
30.	$I_1/\bar{I}_n$	$y = Ax^B$	1,42
31.	$\mathfrak{Z}_{np}/z$	$y = 10^{A+Bx} + C$	4,40
32.	$\mathfrak{Z}_{np}/I_{nl}$	$y = 10^{A+Bx} + C$	4,29
	Group VII		
33.	S^o_{gas}/z	$y = A + Bx + Cx^2$	0,61
34.	S^o_{gas}/I_n	$y = A + Bx + Cx^2$	0,31

TABLE 1 (Continuation)

№	Y_i / X_i	Type of equation	Mean relative error, %
35.	I_1/z	$y = Ax^B$	2,94
36.	$I_1/\bar{I}_n$	$y = A.10^{Bx}$	1,67
37.	ζ_{np}/z	$y = \frac{x - x_1}{A + Bx} + y_1$	4,45
38.	$\zeta_{np}/\bar{I}_{nl}$	$y = \frac{x - x_1}{A + Bx} + y_1$	2,79

We compared once again the correlations derived for atomic numbers and the competing four information indices with a number of properties of chemical elements of groups I (9 properties), II (7), III (8), VI (6), and VII (6 properties). Polynomials of degree four were taken as a basis of this comparison[12].

As can be seen from Table 2 again, with the exception of only one out of 37 properties under study, the information indices provide much higher correlations than atomic number does. The standard deviation is often 5-10 times smaller. One should especially stress on the fairly good correlations obtained for boiling and melting points which correlate poorly with the atomic number.

TABLE 2

Comparison Between the Mean Square Deviation of the Correlation Polynomical Functions for Some Properties of the Chemical Elements and Their Atomic Number Z or Informations Indices I

Properties	Mean square deviation					
	Group I		Group II		Group III	
	Z	I	Z	I	Z	I
S^{o}_{gas}, cal.g-atom^{-1}.^{o}K^{-1}	0,086	0,071[a]	0,050	0,064[a]	0,970	0,250[b]
S^{o}_{solid}, cal.g-atom^{-1}.^{o}K^{-1}	0,397	0,126[a]	0,298	0,189[a]	0,854	0,262[a]
T_M, ^{o}C	4,77	0,97[a]	65,54	35,80[a]	219,5	50,91[b]
T_B, ^{o}C	31,19	4,69[a]	127,8	61,33[a]	194,5	119,1[b]
ζ	0,043	0,017[a]	0,037	0,017[a]	0,044	0,019[a]
I_1, eV	0,062	0,014[b]	0,100	0,090[a]	0,266	0,111[b]
I_2, eV	1,872	0,302[a]	0,258	0,068[b]	0,768	0,496[b]
H_M, cal.g-atom^{-1}	0,028	0,008[a]	-	-	-	-
H_{SUBL}, kcal.g-atom^{-1}	0,806	0,109[a]	-	-	7,150	2,996

	Group VI		Group VII	
	Z	I	Z	I
S^{o}_{gas}, cal.g-atom^{-1}.^{o}K^{-1}	0,733	0,079[a]	0,694	0,145[b]
T_M, ^{o}C	43,73	30,02[a]	15,44	11,34[b]
T_B, ^{o}C	84,87	20,80[b]	20,72	8,27[b]
ζ	0,050	0,034[b]	0,062	0,033[b]
I_1, eV	0,348	0,088[b]	0,467	0,082[b]
I_2, eV	1,372	0,179[b]	1,280	0,183[b]

a- $\bar{I}_{nl}$, b- $\bar{I}_{n}$.

Some differences however appear between the data of Table 1 and 2. Thus, for the polynomical type of correlation only the mean information indices $\bar{I}_n$ and $\bar{I}_{nl}$ are of importance while both total and mean information indices provide a good correlation for the equations from Table 1. The association of a certain atomic property to a specific kind of information index, occuring in Table 1 on al large basis of different functions, is not confirmed in Table 2 for the polynomial type function. Instead, another regularity appears: the properties of elements of groups I and II correlate best with the information on electron distribution over subshells, whilst for groups III, VI and especially VII- with that on electron distribution over shells.

The correlation with the information indices might be applied for a better prediction of the properties of the hypothetical superheavy elements from the end of period VIII that are potential members of the main groups I to VIII. Recently such prognoses have attained a special significance in connection with the predicted stability regions[15,16] at atomic numbers z=114 and z=126.

Illustrating the possibilities offered by the information approach in use we obtained for the absolute entropy in gaseous state of elements 113, 116, 117, 119, and 120, respectively:

S^o_{gas}=41,83±0,45; 45,22± 0,14; 44,84± 0,26; 44,60± 0,14; and 43,11± 0,12 cal.g-atom^{-1} $^oK^{-1}$.

A detailed predictions on a large number of properties of all the superactinides having atomic numbers within the range z=113 to 120 will be published elsewhere[17].

One should not view the results presented above as the best possible correlations between information indices and properties of chemical elements, as well as the most accurate possible predictions if the entropies (and other properties) of elements 113, 116, 117, 119, and 120. The correlation equations examinde are among those most often used in chemistry. It may well be that the usage of other functions will further improve these correlations making the values of predicted properties more reliable. The main result of the present work is then regarded rather as being in demonstration of the importance

of atomic information indices if chemical elements, especially in comparison with the atomic number - the only such index so far used.

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