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Predicting the Properties of the 113-120 Transactinide Elements

Danail Bonchev* and Verginia Kamenska

Department of Physical Chemistry, The Higher School of Chemical Technology, 8010 Burgas, Bulgaria (Received: May 9, 1980; In Final Form: November 11, 1980)

The information indices, recently introduced for the description of the electronic structure of atoms, are used as a more convenient basis than atomic number (or period number) for correlations with the properties of the chemical elements within the main groups of the periodic table. When the derived equations are extrapolated, the expected values for a number of properties or characteristics of the 113-120 transactinide elements are obtained: entropies in the gas and solid state, heats of melting and sublimation, melting and boiling points, first and second ionization potentials, atomic volumes, densities, covalent radii, and orbital exponents. Some corrections to the predictions were made by proceeding from the similarity in the trend of the expected values for elements 113-120 and the known data on elements 81-88. Some properties of elements 85-88, missing from the literature, were also calculated.

Introduction

During the last 35 years the periodic table of chemical elements was considerably extended when the 15 transuranium elements up to element 106 were synthesized.¹⁻⁴ The prediction of islands of nuclear stability⁵⁻⁷ around elements 114 and 164 has prompted greatly the efforts to synthesize new superheavy elements as well as to search for some of them in nature.⁸⁻¹⁰ Relativistic Hartree-Fock-Slater (or Dirac-Slater) calculations¹¹⁻¹³ have been carried out for chemical elements up to 172 providing estimates of their most stable electron configurations. The prospect of further evolution of the periodic table has been a subject of considerable interest.¹⁴⁻¹⁹ All this has encouraged attempts to predict the physical and chemical properties of superheavy elements by extrapolating the properties of the known elements in Mendeleev's style, as well as by using various approximate methods.²⁰⁻²⁵

A question may arise whether the method of predicting the properties of superheavy elements by continuation of the trends in chemical groups has not lost its meaning since relativistic quantum mechanical calculations allow us, in principle, to do this in a more rigorous way. Only a few quantities, however, like ionization potentials, atomic and ionic radii, etc., can be directly calculated. Even in these cases theoretical calculations do not seem to be entirely satisfactory. As shown by Keller et al.²³ a systematic correction, determined from experiment, improves the theoretical values of the ionization potential. The quantum mechanical calculations of atomic and ionic radii for most of the 7p elements, as pointed out by Fricke et al.,^{12,13,17} are inaccurate since it is not possible to define the atomic radius as the radius of the principal maximum of the outermost electron shells. "If one continues, however, the trends in the behavior of metallic or ionic radii, as it done by Grosse,²⁰ Keller et al.,²³ and Cunningham,²¹ one gets results which will be quite accurate" (ref 17). In light of these comments, attempts to improve the extrapolation technique for predicting the properties of the superheavy elements seem justified.

Recently, we have applied the information theory^{26,27} to the characterization of the electronic structure of atoms.^{28,29} In general, the proposed concept of atomic information indices is a suitable mathematic model which is likely to be homomorphic to the periodic table. The information approach was used in the analysis of the quantitative aspects of periodicity, by deriving information equations for

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groups and periods in the periodic table, as well as revealing correlations between information indices and properties of chemical elements. By reflecting adequately on the details of the electronic structure of atoms, the information indices seem to be much more promising than the atomic number (which equals only the total number of electrons) in the search for structure-property correlations.^{29d}

In the present paper we shall use the atomic information indices for predicting various properties of elements 113–120 which belong to the main groups III–VIII of period VII, and main groups I and II of period VIII. The correlations between the properties and information indices, which have been derived for each of these groups, are extrapolated to the superheavy elements of interest.

The properties of element 116 have not, up to now, been a subject of a detailed study. Some of the examined properties of the other seven elements (boiling and melting points, ionization potentials, density, etc.) have already been treated by Grosse²⁰ ($z = 118$), Cunningham²¹ ($z = 117$ –120), and Keller et al. ($z = 113, 114,^{23} 115^{25}$), making use mainly of correlations (within a chemical group) with the row number or atomic number. These works are excellent examples of predictions on the basis of extrapolation of known properties of lower homologues in the periodic table. Still, a reexamination of the predicted properties of these elements might be of interest since atomic information indices are supposed to be a more appropriate basis for correlations and extrapolations. In addition to the expected more reliable "vertical" correlations, such a systematic study of the superheavy elements of the eight main groups of the periodic table makes it possible to use a "horizontal" correlation by comparing the trend in the period formed with that of the preceding period. It is hoped, in compliance with Mendeleev's ideas, that in such a way the predictive power of the periodic table could be used more effectively.

Method

An atom having z electrons will be considered. If certain criterion are used, the set of electrons can be partitioned into k subsets, having z_1, z_2, \dots, z_k electrons, respectively. A finite-probability scheme for the set can be constructed so that it specifies a definite probability $p_i = z_i/z$ for a randomly chosen electron to be in the i th subset:

subset	$1, 2, 3, \dots, k$
cardinality	$z_1, z_2, z_3, \dots, z_k$
probability	$p_1, p_2, p_3, \dots, p_k$

Using the Shannon equation,²⁶ we can define the average entropy for the probability distribution of electrons over subsets in bits per electron as

$$\bar{I} = -\sum_{i=1}^k p_i \log_2 p_i = -\sum_{i=1}^k \frac{z_i}{z} \log_2 \frac{z_i}{z} \quad (1)$$

The total entropy of the probability distribution of electrons in the atom can also be specified by using an equation derived¹⁶ from (1):

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

There is no general agreement in the literature about how to name the quantities defined by eq 1 and 2. Some authors prefer to call them the mean and total information content of the system under consideration, respectively. For instance, according to Mowshovitz³⁰ the quantity \bar{I} is

not a measure of entropy since it does not express the average uncertainty per structure having z elements of a given ensemble of all possible structures having the same number of elements. \bar{I} is rather the information content of the structure under consideration in relation to a system of transformations leaving the structure invariant. In this paper we shall term the quantities \bar{I} and I as information indices. More details concerning the terminology can be found in ref 31.

Various information indices can be introduced for the atoms of chemical elements depending on the criterion used for grouping electrons into different subsets. Within the one-electron approximation the different atomic quantum numbers and some of their combinations can be taken as criteria. It is possible in principle to define an atomic information index in such a way that the valence electrons are given a larger weight than the innermost electrons. Such an index might be of interest in chemistry since the outermost electrons are those which determine the chemical properties of the atoms. The different weights of the valence and inner electrons can, however, be introduced only empirically. Therefore, it seems logical to develop first the information approach to the description of the atomic electron shells without any additional assumptions. The essential role of the valence electrons could be more effectively taken into account in a future development of the approach.

Related to the above, atomic information indices were defined in our preceding publications^{28,29} by taking each electron with an equal weight. The following electron subsets in the atom were used: (1) electron shells, (2) subshells, (3) atomic orbitals, (4) spin orbitals, (5) (nlj) subshells, as well as groups of electrons having the same quantum number, (6) angular momentum (l), (7) magnetic (m), (8) magnetic spin (m_s), (9) inner (j), and (10) total magnetic (m_j). In this paper we use the first two criteria only, i.e., the mean information indices \bar{I}_n and \bar{I}_{nl} are used in parallel with the total information indices I_n and I_{nl} . These indices are readily calculated from the known electron configurations of the chemical elements. As for the superheavy elements of interest, their electronic structure is also regarded as well established on the basis of quantum mechanical calculations.^{11–13} Thus, the 7p subshell should become populated in elements 113–118 by 1–6 electrons, respectively, while the valence electronic configuration of elements 119 and 120 is expected to be $8s^1$ and $8s^2$, respectively.

The procedure developed for the prediction of the properties of elements 113–120 includes deduction by comparison of equations correlating a certain property of the elements of the corresponding main group in the periodic table with one of their four information indices \bar{I}_n , \bar{I}_{nl} , I_n , and I_{nl} (denoted in what follows by I_1, I_2, I_3 , and I_4 , respectively), as well as with their atomic number z . The latter was considered not only for the purpose of comparing results with those obtained by means of the information indices, but the information indices are expected to be, in general, more reliable for structure-property correlations than the atomic number. The limited variety of such indices used in the present paper (only two out of 10 indices specified above) in some cases may, however, result in a worse correlation as compared with the atomic number and, hence, in a less precise prediction of the properties of the superheavy elements.

Each of the above five correlations was obtained by least-squares fitting to eight different versions of trial equations. The latter are expected to be mainly different

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power or exponential type of functions (eq 5–8), due to the logarithmic dependence between the atomic information indices and the number of electrons in the atom and its electron subsets:

$$y = A + Bx \quad (3)$$

$$y = A + Bx + Cx^2 \quad (4)$$

$$y = Ax^B \quad (5)$$

$$y = Ax^B + C \quad (6)$$

$$y = 10^{Bx} A \quad (7)$$

$$y = 10^{Bx} A + C \quad (8)$$

$$y = \frac{x}{A + Bx} \quad (9)$$

$$y = \frac{x - x_1}{A + Bx} + y_1 \quad (10)$$

Using a computer program we have selected out of the 40 equations the best correlation for a given property the one which displays the lowest mean relative error.

The predictions of the properties of elements 113–120, made on the basis of the best-group correlation, if necessary can be corrected in the second stage of our procedure. The similarity in the trend at the end of periods VI and VII, and the beginning of periods VII and VIII, is regarded here as another criterion for the reliability of the predictions. This assumption originates from Mendeleev's ideas for the properties of a certain element being an arithmetic mean of the properties of its neighbors both in the vertical (group) and horizontal (row) directions. An additional justification of this assumption is the similarity in the trend of the properties of elements along the eight main groups. With few exceptions, which will be discussed in the next section, the properties examined have the same (increasing or decreasing) trend along each of the main groups examined in the periodic table.

Results and Discussion

After selecting the properties to be dealt with, we have proceeded from the available experimental or theoretical data taking into account that some of the properties of the superheavy elements of interest have already been satisfactorily predicted by other authors.^{11–13,20,21,23,25} This holds in particular for the chemical properties like oxidation states,³² ionic and metallic radii, etc.

Though failing so far, there is still some hope of finding in nature small amounts of some superheavy elements that are within the predicted regions of nuclear stability. Related to this, some macroscopic properties, already treated or not by other authors, were also taken into consideration. Thus, the following properties of chemical elements were studied: entropy in the gas and solid state,^{33,34} heats of melting^{33–35} and sublimation,³⁴ melting and boiling points,^{33,34} first and second ionization potentials,³³ atomic volumes,³⁴ (X-ray) densities,³⁴ Pauling's covalent radii,³⁴ and orbital exponents.^{36,37}

The best-group correlations found for each of the 12 properties under study are given in Table I. Every entry contains the type of equation (eq 3–10 are marked as 1–8,

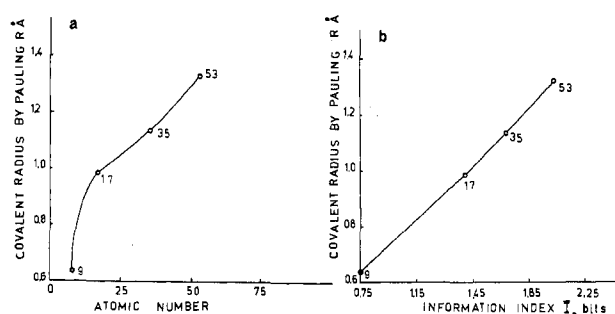


Figure 1. The covalent radius of elements of group VII vs. (a) atomic number and (b) information index I_n .

respectively), then the variable used (the type of information index I_1 to I_4 , or the atomic number z), followed by the mean relative error in percent. Coefficients A , B , and C from eq 3–10 are presented in the next three lines. Four different symbols a, b, c, and d may also appear there as superscripts to I or z . The first three refer to cases where the number of data used in the correlation is not the maximum one; c indicates cases where no data are available for the heaviest known element in the group; a and b refer to cases (27 and 8 in number, respectively), where the first, or first and second elements, respectively, in the group is excluded from the correlation. The latter was made in order to improve the correlations since the first and second elements in the group often behave differently from the other elements. Thus, a certain property could have a minimum or maximum in the second or third element of the group, the elements after the extremum being of importance only for the extrapolation of the function to higher z . 15 other cases are denoted by the superscript d . They refer to cases in which the function changes its slope from negative to positive, or vice versa, for the element which is forelast in the group. It is hard to judge in such cases if this change will continue in the next superheavy element or, contrary to it, if the extremum is a starting point for a zig-zag like trend for the curve. All these cases are discussed later in detail.

Seven places in Table I are empty. In five cases (groups VII and VIII) this is due to lack of data for some of the properties. The heats of melting and the elements from group IV do not display a common regularity because of the different crystal modifications of these elements. The boiling points of elements from group V are of type d , described above, which makes their prediction unreliable.

Analysis of Table I reveals that the correlations with the information indices substantially prevail on those made with the atomic number of chemical elements (66 against 23 cases). The decrease in the mean relative error achieved when replacing the correlations with the atomic number by those with the information indices is in some cases very impressive: S_{solid}° (group IV), 0.9% instead of 6.5%; R_{kov} (group VII), 0.14% instead of 3.2%; V_A (group I), 2.4% instead of 10.6%; ΔH_M (group VIII), 3.7% instead of 17.9%, etc. Still greater prevalence of the information indices was found in a preceding study (36 against 1 cases) where polynomial-type functions were solely examined in the correlations.^{29d} The atomic number proved to be of greater importance only for the density and entropy in the gas phase (5 out of 8 group correlations). One could, however, expect the systematic examination of the other eight information indices, mentioned in the previous section, to demonstrate also in the remaining cases the advantage of the information indices for group correlations in the periodic table. Being detailed and flexible characteristics of the electronic structure of atoms, the information indices are capable of describing more adequately

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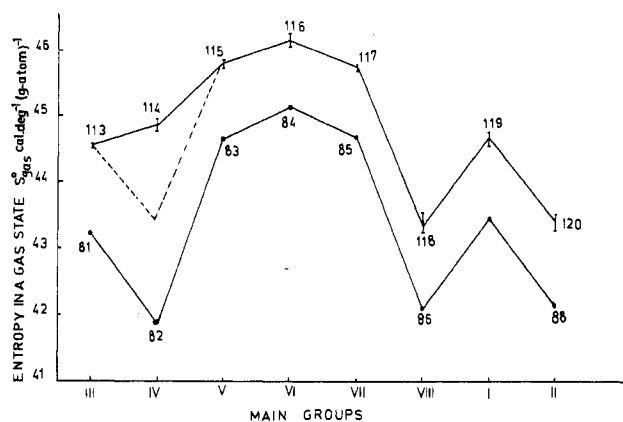


Figure 2. Entropy in the gas state of elements 81-88 (experimental) and 113-120 (predicted). The dashed line shows the correction for element 114 according to the horizontal correlation (the similarity in the trends of the two neighboring periods).

Chart I

group IV	S° , cal deg $^{-1}$ (g-atom) $^{-1}$
Si	40.12
Ge	40.10 $\Delta_1 = -0.02$
Sn	40.24 $\Delta_2 = +0.14$
Pb	41.89 $\Delta_3 = +1.65$

than the atomic number or row number the structure-dependent properties of the chemical elements. As an illustration we show the change in the trend of the covalent radius of the elements from group VII from irregular, when expressed vs. atomic number, to a linear one for the information index I_n (Figure 1a,b).

It should be taken into account that, in several cases, Table I does not present the best correlations defined on the basis of the lowest mean relative error. Using the horizontal correlation as a second criterion we gave preference to cases where the correlation with an information index had a larger mean relative error than that for the corresponding correlations with atomic number (ρ_R , group V, $\epsilon_I = 10.11 > \epsilon_z = 7.23$; ζ , group VI, $\epsilon_I = 1.28 > \epsilon_z = 0.94$). The opposite correction was made in two other cases (r_{cov} , group I, $\epsilon_z = 3.30 > \epsilon_I = 1.24$; I_2 , group VII, $\epsilon_z = 3.47 > \epsilon_I = 2.45$).

The accuracy attained in the correlation, presented in Table I, is as follows: in 30 cases the mean relative error is less than 1%, in 50 cases it is within the 1-5% range, and only in 9 cases it is larger than 5%. The large mean relative error in the later cases is a result of the irregular trend of some properties. Some of them will be discussed later.

In Table II we present the values for 13 macroscopic properties or atomic characteristics of elements 113-120, as predicted according to our extrapolation scheme. The corresponding values of the same properties, which were found in the literature as calculated by other authors, are given for the sake of comparison in Table III.

Entropy in the Gas State. A fairly good coincidence in the entropy trend is manifested in Figure 2 for the two last periods in the periodic system of chemical elements. The only exception is element 114 for which the extrapolated value of 44.8-45.0 cal deg $^{-1}$ (g-atom) $^{-1}$ seems too high. The analysis made for the entropies of the elements of group IV reveals the reason for the unsatisfactory prediction for element 114. The change in entropy on going from Si to Ge and from Ge to Sn is very small (Chart I), while on going from Sn to Pb it is (in cal deg $^{-1}$ (g-atom) $^{-1}$) considerable ($\Delta_3 \gg \Delta_2 \approx \Delta_1$). The mathematical functions used in the correlation provide for a further fast increase of S°_{gas}

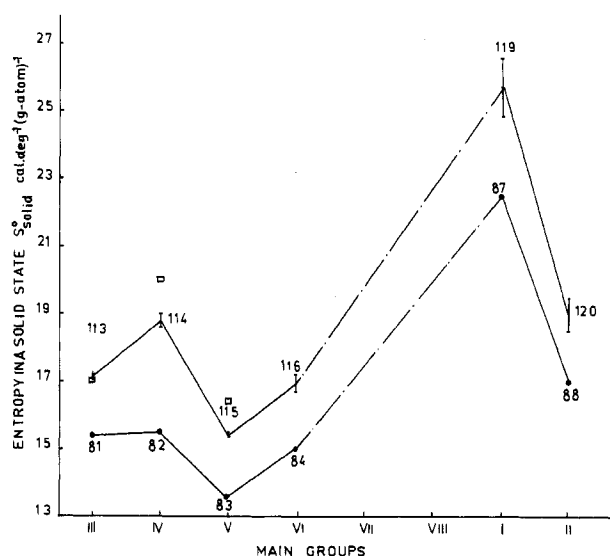


Figure 3. Entropy in a solid state of elements 81-88 (experimental) and 113-120 (predicted); (□) values predicted by Keller et al.^{23,25} No data for groups VII and VIII.

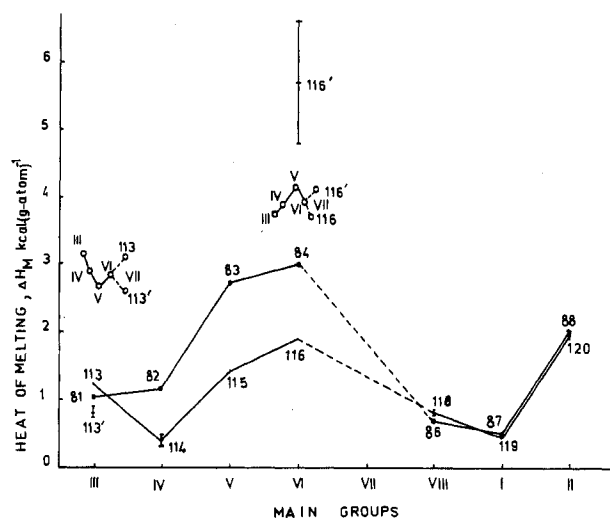


Figure 4. Heats of melting of elements 81-88 (experimental) and 113-120 (predicted). The points 113' and 116' are predicted by using the correlations for groups III and VI, respectively (illustrated in the upper part of the figure). Points 113 and 116 are obtained by assuming $\Delta H_m(\text{period VII-VI}) \approx \Delta H_m(\text{period VI-V})$. No data for group VII.

($\Delta_4 = S^\circ_{114} - S^\circ_{Pb} \gg \Delta_3$). If we assume, however, that the increase in entropy is approximately the same for a pair of neighboring periods ($\Delta_1 \approx \Delta_2$, $\Delta_3 \approx \Delta_4$) a value of $41.89 + 1.65 = 43.52$ cal deg $^{-1}$ (g-atom) $^{-1}$ is obtained for element 114. The same value can be determined directly from Figure 2 by assuming a parallel trend of the two curves also in the region of element 114 (the dashed line in Figure 2). Thus, the horizontal correlation between the elements of periods VI and VII also manifests good predicting power.

Entropy in the Solid State (Figure 3). The lack of experimental data for groups VII and VIII makes it difficult to compare fully the last two periods. Nevertheless, the curves have similar trends with the exception of group IV where both predicted values, ours and that of Keller²³ (18.6-19.0 and 20 cal deg $^{-1}$ (g-atom) $^{-1}$, respectively) are overestimates. The horizontal correlation results in a lower value for the entropy of element 114 within the range 17.4-17.5 cal deg $^{-1}$ (g-atom) $^{-1}$. On the other hand, the entropy of elements 113 and 115 is nearly the same in our calculations and those by Keller^{23,25} ($z = 113$: 17.1 and 17.0 cal deg $^{-1}$ (g-atom) $^{-1}$, respectively; $z = 115$: 15.4-15.5 and

TABLE I: Equations Used in the Prediction of the Properties of Elements 113-120

properties	group I	group II	group III	group IV	group V	group VI	group VII	group VIII
$S^\circ_{\text{gas}}, \text{ cal deg}^{-1} (\text{g-atom})^{-1}$	3, z; 0.17 30.17 0.08218	3, z; 0.29 28.68 0.08649	8, I_1^a ; 0.05 44.32 0.07817	2, I_1^a ; 0.18 40.18 -0.002948 0.00003021	3, I_2 ; 0.09 31.67 0.0604	3, z; 0.22 33.06 0.07027	8, z; 0.09 3.731 0.08612	3, z; 0.29 28.52 0.08805
$S^\circ_{\text{solid}}, \text{ cal deg}^{-1} (\text{g-atom})^{-1}$	4, I_1^a ; 3.15 0.1773 3.181 11.56	4, z; 2.35 353.5 0.01339 -357.8	8, I_1^a ; 0.31 3.574 0.05394	2, I_1^a ; 0.91 -14.20 13.42 0.1192	8, I_2 ; 0.33 13.86 0.06230	4, z; 0.99 1.196 0.5245 2.518		
$\Delta H_{\text{melt}}, \text{ kcal (g-atom)}^{-1}$	8, z; 0.76 -0.9169 -1.900	7, I_2 ; 3.33 -0.8885 0.5055	8, I_1^d ; 11.3 -1.120 -0.2110	5, I_2^b ; 0.11 9.685 -0.001847	4, I_3^d ; 16.5 0.9283 2.328 -1.715			2, I_1 ; 3.71 0.0500 -0.05426 0.1495
$\Delta H_{\text{subl}}, \text{ kcal (g-atom)}^{-1}$	5, I_1^a ; 2.27 38.55 -0.1577	8, I_1 ; 5.61 0.03207 -0.02819	5, I_1^a ; 0.81 86.70 -0.003781	2, z; 1.52 121.8 -0.9945 0.0006961	8, I_1 ; 0.63 0.01247 0.01003	8, I_1 ; 0.14 -0.02752 -0.003751		4, I_1^b ; 1.24 0.01913 3.892 1.205
$T_M, \text{ K}$	8, I_1 ; 0.35 -0.07876 -0.006144	8, I_1 ; 5.94 0.006198 -0.001403	3, I_1^b ; 0.39 42.83 0.5060	5, I_1^d ; 12.3 18520 -0.7416	5, I_2^b ; 2.64 1444 -0.001367	4, I_3^d ; 10.61 116380 0.004872 -116180	8, I_1^a ; 0.33 0.3548 0.0003092	6, I_1 ; 2.14 35.16 0.3723 -311.0
$T_B, \text{ K}$	8, I_2 ; 0.71 -0.007112 -0.001447	8, I_1 ; 3.28 0.01264 -0.001159	5, I_1^a ; 2.04 2875 -0.0007150	5, I_1^a ; 3.43 3925 -0.003189		4, I_3^d ; 3.04 3488 0.3208 -3172	4, I_1^a ; 1.98 2.435 0.9154 173.6	6, I_1 ; 2.50 39.72 0.2221 -312.8
$I_1, \text{ eV}$	3, I_1 ; 1.42 5.232 -0.3611	7, z; 2.11 -0.4734 0.1877	8, I_1 ; 1.33 1.957 -0.4367	8, I_1^d ; 0.91 0.1527 -0.2180	3, z; 4.31 22.73 -0.2520	3, I_1 ; 2.95 17.95 -0.1361	5, I_1 ; 1.67 23.43 -0.1774	8, I_1 ; 1.91 -4.046 -0.05752
$I_2, \text{ eV}$	3, I_1 ; 2.66 70.39 -0.8829	8, I_1^d ; 1.25 0.01503 -0.07501	8, I_1^a ; 2.77 -23.88 15.58	8, I_1^d ; 1.48 0.07159 -0.09348	8, I_2^d ; 3.70 0.7276 -0.8914	8, I_3^d ; 2.38 0.05662 -0.05215	7, z; 3.47 -0.2186 0.05387	3, I_1^a ; 1.32 33.74 -0.6040
$V_A, \text{ cm}^3 (\text{g-atom})^{-1}$	4, I_1^c ; 2.37 13.47 2.009 8.181	4, I_1^c ; 1.92 261.1 0.1529 -256.3	8, I_1 ; 1.79 0.02242 0.03434	5, I_1^a ; 0.66 5.953 0.2242	6, I_1 ; 6.04 357.3 0.00004479 -344.0	1, I_1^c ; 2.33 13.75 0.05760	6, I_1^a ; 0.97 0.02377 1.299 15.81	2, I_1^c ; 4.75 19.43 -17.08 13.24
$\rho_R, \text{ g cm}^{-3}$	1, z; 3.6 0.3769 0.02945	7, I_1^b ; 0.02 17.94 0.1326	4, z; 8.06 0.1532 0.9625 1.349	4, z; 2.11 1.157 0.5599 -2.734	7, I_1 ; 10.1 6.115 0.0723	8, z; 1.95 6.670 0.03832	4, z; 1.87 134.4 0.01855 -139.6	4, I_1^b ; 1.88 89.91 0.01390 -92.92
$R_{\text{cov}}, \text{ \AA}$	3, z; 3.30 0.9944 0.2147	8, I_1^c ; 1.06 -0.2080 0.5939	4, I_1^a ; 2.37 0.06938 2.644 1.070	4, I_1^a ; 1.85 0.0170 0.6667 1.024	8, I_1 ; 0.89 0.7119 0.4495	3, I_1 ; 1.16 0.7791 0.8305	1, I_1^c ; 0.14 0.2258 0.5436	
ξ	3, I_1^c ; 1.34 0.5704 0.1197	3, z; 1.22 0.8230 0.1066	6, I_1 ; 1.45 0.3538 0.1688 0.5714	3, z; 0.87 0.8482 0.1988	5, I_1 ; 3.78 1.735 0.0005945	8, I_1^a ; 1.28 2.947 -0.08222	4, z; 0.99 0.009916 0.7144 1.935	4, I_1^b ; 1.06 0.002824 0.9714 2.212

^{a, b} The first, or first and second element, respectively, in the group is excluded from the correlation.^c No data are available on the heaviest known element in the group.^d The function changes sign of its slope in the element which is penultimate in the group.

TABLE II: Predicted Properties of Elements 113-120 and 84-88 According to the Equations of Table I^{b,c}

prop- erties ^a	113	114	115	116	117	118	119	120
S°_{gas}	44.5-44.6	43.4-43.5 ^b	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°_{solid}	17.1-17.2	18.6-19.0	15.4-15.5	16.8-17.2			24.9-26.6	18.5-19.5
ΔH°_M	1.26 ^c		1.41-1.43	1.82 ^c		0.80-0.86	0.48-0.49	1.92-2.05
ΔH°_S	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
T_M	724-730	265-340	340-358	637-780	765-769	250-260	295-297	900-1020
T_B	1370-1420	1640-1760		1035-1135 ^c	825-860	252-266	928-942	1770-1890
I_1	5.92-6.08	7.8-8.0 ^c	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	18.4-19.4	16.4 ^c	21.3 ^c	18.3-19.2	18.5-19.9	19.2-19.8	20.3-21.4	9.28-9.52
V_A	17.9-18.6	20.6-20.8	22.4-25.2	29.4-30.8	44.4-44.5 ^b	55.5-61.1	92.5-96.9	44.3-46.1
ρ	14.5-17.1	13.4-14.0	12.5-13.0 ^b	11.0-11.4	7.1-7.3	4.9-5.1	3.7-4.0	5.2
R_{cov}	1.72-1.80	1.71-1.77	1.56-1.58	1.62-1.66	1.56-1.57		2.63-2.81	2.06-2.10
ξ	2.15-2.21	2.15-2.19	2.32-2.36 ^b	2.48-2.54	2.69-2.75	2.88-2.94	1.18-1.22	1.35-1.39

$V_A^{84} = 23.9-25.0$; $V_A^{85} = 33.9-34.5$; $V_A^{86} = 45.4-49.8$; $V_A^{87} = 78.3-82.1$; $V_A^{88} = 40.3-41.9$; $\rho^{85} = 6.2-6.5$; $\rho^{86} = 4.4-4.5$; $\rho^{87} = 2.8-3.0$; $\rho^{88} = 4.4$; $R_{\text{cov}}^{85} = 1.43$; $R_{\text{cov}}^{87} = 2.58$; $R_{\text{cov}}^{88} = 2.05$; $\xi^{87} = 1.13-1.17$; $\xi^{88} = 1.23-1.27$

^a Same dimensions as in Table I. ^b Values found by horizontal correlation in Figure 2-13. ^c Values found by the condition $X_{\text{VII}} - X_{\text{VI}} \approx X_{\text{VI}} - X_{\text{V}}$ or similar considerations.

TABLE III: Some Properties of Transactinide Elements 113-120, as Predicted by Grosse,²⁰ Cunningham,²¹ Keller et al.,^{23,25} and Fricke et al.^{12,13,17}

properties ^{a, b}	113 ²³	114 ²³	115 ²⁵	116	117 ²¹	118 ²⁰	119 ²¹	120 ²¹
S°_{solid}	17	20	16					
ΔH°_S	34	10	34			5.6		
T_M	700	340	~700		620-820	258	273-303	950
T_B	1400	420	~1400		880	263	900	1970
I_1	7.4	8.5	5.2		9.3	9.8	3.4-3.8	5.4
I_1^{12}	7.5	8.5	5.9	6.8	8.2	9.0	4.1	5.3
I_2		16.8	18.1		16	15	23	10
V_A	18	21			45	50	80-90	45
ρ	16	14	13.5 ¹⁷	12.9 ¹⁷		5.7	3	7
ρ^{12}	14.7	15.1	14.7	13.6			4.6	7.2
R_{cov}^{17}		1.7			1.8	2.3	2.6 ^c	2.0 ^c
						2.2 ¹²		
R_{at}^{13}	1.13	1.21	1.77	1.51	1.38	1.31	2.55	2.16

^a Same dimensions as in Table I. ^b The references cited in the columns should be taken into account only when there is no citation in the rows. ^c Atomic radius.

16 cal deg⁻¹ (g-atom)⁻¹, respectively.

Heats of Melting (Figure 4). The coincidence between the two periods is not very good. The heats of melting of elements 118, 119, and 120 are nearly the same as those of the corresponding elements 86, 87, and 88 of the preceding period. On the other hand, the situation denoted in Table I by superscript d occurs in groups III and VI. It is illustrated in Figure 4 above points 113 and 84. The correlations given in Table I provide the values of 0.73-0.87 and 4.8-6.6 kcal (g-atom)⁻¹ for elements 113 and 116, respectively (denoted as 113' and 116' in Figure 4). Alternatively, we can suppose, however, that the extrema in the curves of groups III and VI are the initial points of an increasing, or decreasing, branch of these curves, respectively. Assuming the same change on going from period VI to VII as on going from period V to VI we obtain for elements 113 and 116 that the heats of melting are 1.26 and 1.82 kcal (g-atom)⁻¹, respectively. The choice between the two estimates for elements 113 and 116 needs additional argumentation. For this reason we present in Figure 4 both estimates for each element although chemical intuition may point to the values calculated in analogy with the preceding periods.

Heats of Sublimation (Figure 5). Similar to heats of melting, the heats of sublimation of elements 118-120 are very much the same as those of elements 86-88. A very good coincidence was found between our result and that of Grosse²⁰ for element 118 (5.2 and 5.6 kcal (g-atom)⁻¹, respectively).

One should not expect the curve for elements 113-116 to be parallel with that for elements 81-84 since the heats of sublimation in group V tend to increase with atomic

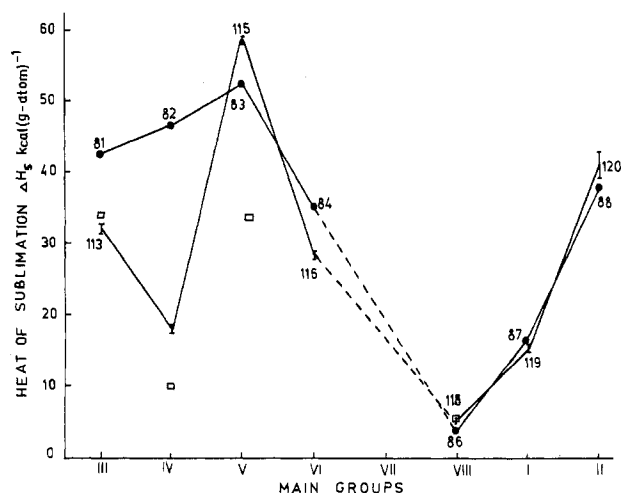


Figure 5. Heats of sublimation of elements 81-88 (experimental) and 113-120 (predicted): (□) values calculated in ref 23 ($z = 113, 114$), ref 25 ($z = 115$), and ref 20 ($z = 118$). No data for group VII.

number while the opposite tendency occurs in groups III, IV, and VI. Our estimate for element 113 is close to that of Keller²³ (32.2-32.7 vs. 34 kcal (g-atom)⁻¹, respectively), while for elements 114 and 115 our values are considerably higher than his:^{23,25} $z = 114$, 17.5 vs. 10 kcal (g-atom)⁻¹; $z = 115$, 58.1-58.9 vs. 34 kcal (g-atom)⁻¹.

The heat of sublimation of element 114 has also been discussed by taking into account relativistic effects.^{38,39}

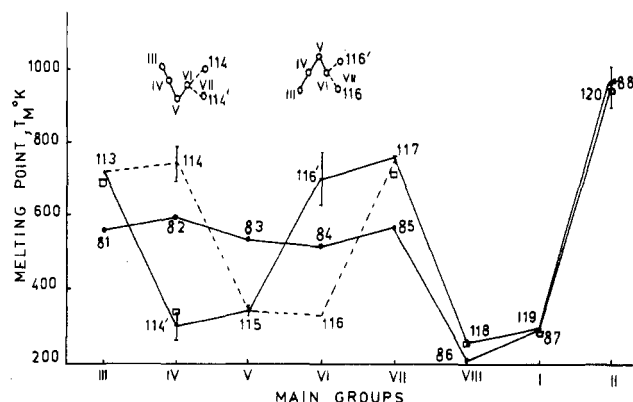


Figure 6. Melting points of elements 81–88 (experimental) and 113–120 (predicted): (□) values predicted in ref 20 ($z = 118$), ref 21 ($z = 117, 119, 120$), and ref 23 ($z = 113, 114$). Two predictions are made for elements 114 and 116 following the two possible extrapolations of the melting points of the elements of groups IV and VI shown in the upper part of the figure. Points 114' and 116' are obtained by the corresponding equations in Table I while points 114 and 116 are obtained by the conditions: $\Delta T_M(\text{period VII-VI}) > \Delta T_M(\text{period VI-V})$, and $\Delta T_M(\text{period VII-VI}) = \Delta T_M(\text{period VI-V})$, respectively.

Chart II

group IV	mp, K	group VI	mp, K
Si	1688	S	392
Ge	1110	Se	490
Sn	505	Te	723
Pb	600	Po	527
114	?	116	?

Since this element is believed to have a closed $p_{1/2}^2$ shell it is expected to be a gas or a very volatile liquid. A similarity in the properties of elements 113 and 115 is also expected due to their similar electronic structure ($z = 113, p_{1/2}^1; z = 115, p_{3/2}^1$). Hence, one could conclude that the heats of sublimation of elements 114 and 115 predicted by Keller^{23,25} seem consistent with the real electronic structure of these elements.

Melting Points (Figure 6). Again, the values obtained for elements 118–120 are close to those of elements 86–88. A good coincidence is manifested with the values predicted by Keller et al.²³ for elements 113 and 114, by Cunningham²¹ for elements 117, 119, and 120 (here we have taken the mean value of 720 K from the range of 350–550 °C reported²¹ for element 117), by Grosse²⁰ for element 118.

By considering the horizontal correlation, one can see from Figure 6 that the trend of melting points on going from elements 81 through 85 cannot be reproduced for elements 113 to 117. This is due to two different reasons. Primarily, the trend in melting points with increasing atomic number is not the same for all groups. Thus, it increases for groups III and VII, whereas it decreases for the heavy elements of group V. As a result, points 113 and 117 lie above the curve of period VI, while the point 115 lies below. Another complication occurs in groups IV and VI: the trend in melting points changes in the last known element of each of these groups (this is illustrated by the corresponding curves above elements 114 and 116 in Figure 6) (Chart II).

The correlations reported in Table I yield, with a mean relative error of 10–12%, the melting points of elements 114 and 116 (points 114' and 116' in Figure 6) in the range 265–340 and 637–780 K, respectively. If one assumes, however, that the extrema, appearing in period V both in

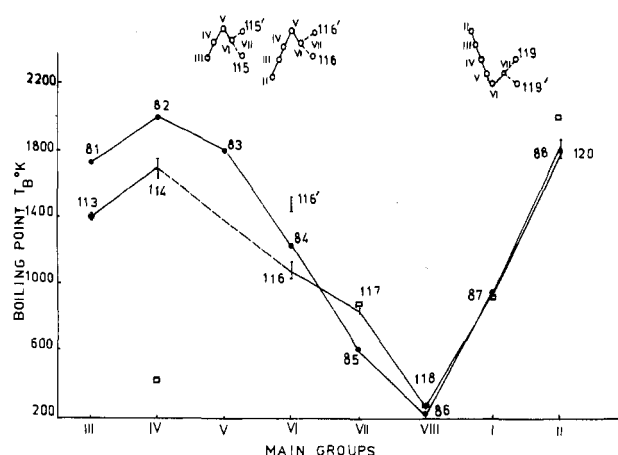


Figure 7. Boiling points of elements 81–88 (experimental) and 113–120 (predicted): (□) values predicted in ref 20 ($z = 118$), ref 21 ($z = 117, 119, 120$), and ref 23 ($z = 113, 114$). The trend in groups V, VI, and I is shown in the upper part of the figure. No estimate for element 115 is given. Points 115', 116', and 119' are obtained by the corresponding equations in Table I, point 116 is obtained by assuming $\Delta T_B(\text{period VII-VI}) < \Delta T_B(\text{period VI-V})$, while for point 119 the condition $\Delta T_B(\text{period VII-VI}) = \Delta T_B(\text{period VI-V})$ is used.

groups IV and VI, were the initial points for a new branch of a parabolic type of curve, the opposite predictions can be made. Assuming also that the change from periods VI to VII is the same as that for periods V to VI, one obtains for element 116 $T_m \approx 330$ K, while for element 114 $T_m \approx 695$ K. It seems reasonable, however, to take a higher value for element 114 since $\Delta_3 \ll \Delta_2$, assuming $\Delta_4 > \Delta_3$. For this reason we propose the second possible value for the melting point of element 114 to be regarded as being within the range 695–800 K. Evidently, one should go beyond the criteria used in this paper to make a choice between the two alternatives for elements 114 and 116. The Lindeman formula used by Keller et al.,²³ for element 114, can be regarded as such an additional criterion. Since the melting point obtained on this basis (340 K) coincides with our value obtained from the equations in Table I we present these values for elements 114 and 116 in Table II.

Boiling Points (Figure 7). The tendency in elements 118–120 to have their heats of melting and sublimation, as well as their melting points near to the respective values of elements 86–88 seems to hold also for the boiling points. On the other hand, the curves of periods VI and VII (groups III to VIII) intersect due to the tendency of the boiling points to diminish with atomic number along groups III and IV, and to rise along groups VII and VIII. As can be seen from Figure 7 our predictions practically coincide with those of Keller et al.²³ for element 113, and Cunningham²¹ for elements 117 and 119. The boiling and melting points of element 118 found in our study (-14 ± 7 and -18 ± 5 °C) agree quite well with those previously calculated by Grosse²⁰ ($T_B = -10$ °C and $T_M = -15$ °C). The boiling point of element 114 (420 K) reported in ref 23, however, seems more reliable than ours, due to relativistic effects. In groups V, VI, and I there is once again the situation where the trend in the group alters for the last known element (superscript d in Table I) (Chart III). The change in boiling point around the minimum of group I is very small. This makes the estimate based on the respective correlation of Table I ($T_B = 928$ – 942 K) close to the second estimate denoted in Figure 7 as point 119 ($T_B = 957$ K) in the increasing part of the curve for group I on going from period VI to VIII.

The estimates for elements 115 and 116 are not straightforward. The correlation given in Table I yields for element 116 the value of 1430–1520 K. This seems

(39) O. L. Keller in "Predictions in the Study of Periodicity", B. M. Kedrov and D. N. Trifonov, Ed., Academy of Sciences, USSR, Institute of Science and Technology, Moscow, 1976, pp 202–203 (in Russian).

Chart III

group V	bp, K	group VI	bp, K	group I	bp, K
N	77.3	O	90	Li	1615
P	548	S	718	Na	1151
As	885	Se	930	K	1032
Sb	1898	Te	1285	Rb	959.2
Bi	1830	Po	1235	Cs	943
115	?	116	?	Fr	950
				119	?

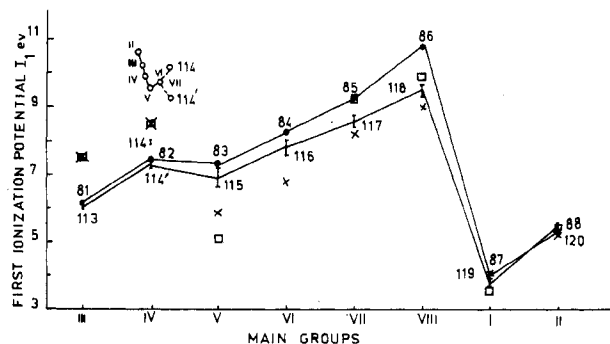


Figure 8. First ionization potentials of elements 81–88 (experimental) and 113–120 (predicted): (\square , \times) values obtained in ref 21, 23, 25 and in ref 12, respectively. The two possible extrapolations for group IV are given in the upper part of the figure. Point 114' is obtained by the corresponding equations of Table I while point 114 is obtained by assuming $\Delta I_1(\text{period VII-VI}) < \Delta I_1(\text{period V-IV})$.

unrealistic especially when compared with the boiling points of Po and Te (1235 and 1285 K, respectively). On the other hand, analysis of the boiling points in group VI indicates a characteristic behavior: the change is larger on going from one period to another of the same size ($\Delta_{\text{II-III}} = 628^\circ$, $\Delta_{\text{IV-V}} = 355^\circ$) than on going from a smaller to a larger period ($\Delta_{\text{III-IV}} = 212^\circ$, $\Delta_{\text{V-VI}} = 50^\circ$), both effects decreasing with the atomic number. Then, if this trend still holds for period VII, one should expect $\Delta_{\text{VI-VII}}$ to be within the 100–200° range. This leads to $T_B = 1035\text{--}1135$ K for element 116. The prognosis for element 115 was quite uncertain since no clear regularity was found for the boiling points of group V.

Ionization Potentials. The trend for the first ionization potentials of element 113–120 was found to parallel that of elements 81–88 (Figure 8). Two expected values can be given for element 114 due to the change in the behavior of group IV in Pb (see below). The correlation presented in Table I yields a value for element 114 that is lower than that of Pb by 0.1–0.2 eV. Treating the minimum point for Sn as the onset of an ascending part of the curve, however, we predict a value higher than that for Pb ($I_1 = 7.8\text{--}8.0$ eV, point 114, connected with a dashed line in Figure 8). Although the horizontal correlation shown in Figure 8 looks very attractive, the agreement with the data predicted by other authors (Table III) is not quite satisfactory. Our results are close to those of Cunningham²¹ for elements 119 and 120, Fricke, Greiner, and Waber¹² for elements 117, 118, 119, and 120, and Grosse²⁰ for element 118. The point 114 in Figure 8 also approaches the value predicted in both ref 23 and 12. The largest disagreement occurs for element 113 (Chart IV).

Analysis of the data for group III reveals a tendency for I_1 to decrease when no new type of electron subshell appears in the next period ($\Delta I_1 > 0$ on going from period II to III, and from IV to V) and to increase in the opposite case ($\Delta I_1 < 0$ on going from period III to IV (d subshell), and from V to VI (f subshell)). Then, it is logical to expect that a small decrease will occur again in element 113 as compared with Tl. The quantum mechanical calculations,^{12,14} however, provided the value of 7.4–7.5 eV which

Chart IV

group III	IP, eV	group IV	IP, eV
B	8.30	C	11.26
Al	5.98	Si	8.15
Ga	6.00	Ge	7.88
In	5.79	Sn	7.33
Tl	6.11	Pb	7.42
113	?	114	?

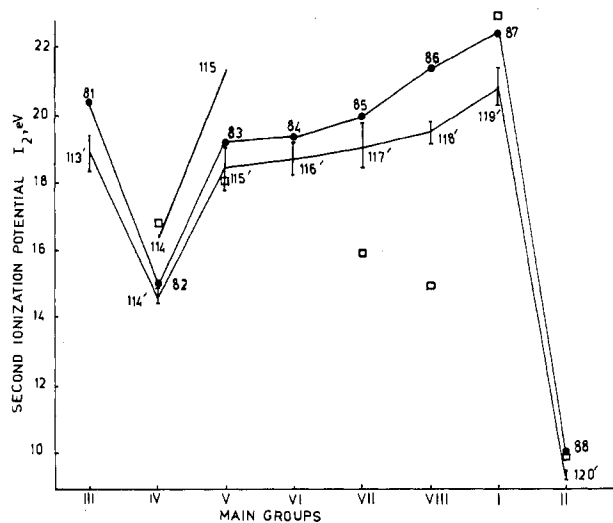


Figure 9. Second ionization potentials of elements 81–88 (experimental) and 113–120 (predicted): (\square) values obtained in ref 23, 25, and 21 for elements 113, 114; 115; and 117–120, respectively. The points denoted as 114' to 120' are obtained by the corresponding equations in Table I while points 114 and 115 are obtained by assuming $\Delta I_2(\text{period VII-VI}) \approx \Delta I_2(\text{period V-IV})$.

is much larger than that of Tl (6.1 eV). This increase in the first ionization potential of element 113 is due to the strong spin-orbit coupling occurring in the superheavy elements. Such new physical effects appearing at higher atomic numbers obviously reduce the predictive power of the periodic table related to some properties of the superheavy elements such as ionization potentials and atomic radii. Still, periodicity could be of use for the improvement of such quantum mechanical calculations by a systematic empirical correction within a chemical group or period as demonstrated by Keller et al.^{23,25} and Fricke et al.,¹² respectively.

The prediction of the second ionization potentials is not straightforward. In six out of eight cases two prognoses can be made, due to the minimum that appears in the penultimate known element in main groups II, IV–VIII. We present in Figure 9 the values obtained by extrapolating the corresponding equations from Table I. All these values are lower than the values of their lower homologues in the groups. Our prognoses for elements 117–119 seem more plausible than those of Cunningham²¹ and are close to them for element 120. Due to the spin-orbit coupling between $7p_{1/2}$ and $7p_{3/2}$ levels,^{12,17} however, our estimates for elements 114 and 115 seem underestimated and will be changed below.

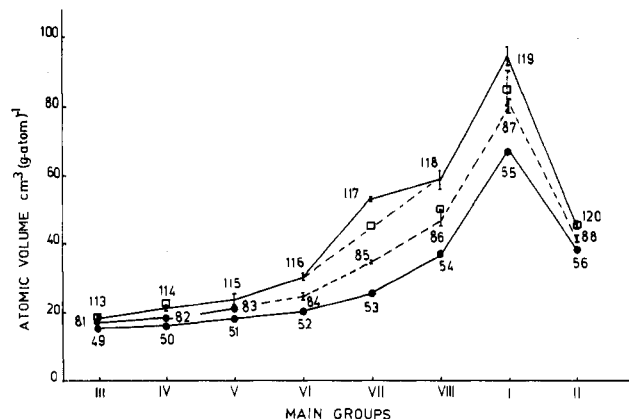


Figure 10. Atomic volumes of elements 49–56, 81–83 (experimental), 84–88 (dashed line), and 113–120 (expected): (□) values predicted in ref 23 for $z = 113, 114$, ref 20 for $z = 118$, and ref 21 for $z = 117, 119$, and 120.

An alternative prognosis could be made in dealing with the minimum in the second ionization potential of group II, IV–VIII as an initial point of the group correlation curve. An analysis similar to that presented above for I_1 for the elements of group IV, and specifically the condition $\Delta I_2(\text{VII–VI}) \approx \Delta I_2(\text{V–IV})$, could result in another series of I_2 values for elements 114–118 and 120. The uncertainty in such a prediction is, however, too high. Moreover, in view of the quantum mechanical calculations¹² revealing a tendency for the first ionization potentials to increase for $7p_{1/2}$ and to decrease for $7p_{3/2}$ levels, the values thus predicted for elements 116–118 would be strongly overestimated. For this reason we present in Figure 9 two more plausible predictions of this kind made for element 114 ($I_2 \approx 16.4$ eV), which is close to the estimate of Keller et al.²³ ($I_2 = 16.8$ eV), and element 115 ($I_2 \approx 21.3$ eV). The prediction made by Keller et al.²⁵ for the second ionization potential of element 115 is, however, closer to our initial estimate (18.1 vs. 18.4 eV).

Atomic Volumes (Figure 10). Elements 49–56 have been taken here as analogues of the transactinide elements 113–120 since data on the next homologues within the eight main groups have been found in the literature only for elements 81–83. The coincidence in the trends of the two periods is satisfactory. The results obtained are very much the same as those of Keller et al.²³ for elements 113 and 114, and Cunningham²¹ for element 120, and are somewhat higher than those reported by Cunningham²¹ (elements 17 and 119) and Grosse²⁰ (element 118). Using the similarity in the trends of the neighboring periods we have corrected the value $V_A^{117} = 53\text{--}54 \text{ cm}^3 (\text{g-atom})^{-1}$, obtained by the best group correlation, to $V_A = 44\text{--}45 \text{ cm}^3 (\text{g-atom})^{-1}$ which also coincides with the Cunningham value.²¹ We also present in Figure 10 and Table II the atomic volumes of elements 84–88 calculated by us according to the corresponding equations of Table I. Our value of $47.6 \pm 2.2 \text{ cm}^3 (\text{g-atom})^{-1}$ for emanation (element 86) is close to the estimate presented by Grosse²⁰ ($42.3 \text{ cm}^3 (\text{g-atom})^{-1}$).

Densities (Figure 11). A horizontal correlation is shown with the data available for four elements of the preceding period (81–84) and the elements 49–56. On this basis, the expected value of $\rho_{115} = 9.5\text{--}11.7 \text{ g cm}^{-3}$, obtained by group correlation (Table I), is corrected to a higher one ($12.5\text{--}13.0 \text{ g cm}^{-3}$). Accord with the results of other authors^{17,20,21,23} using the continuation of trends of the known elements (see Tables II and III) is good for elements 113, 114, 115, 118, and 119. For elements 116 and 120 our values are lower by 1.7 and 1.8 g cm^{-3} , respectively. A systematic deviation from the results of Fricke et al.¹³ was, however,

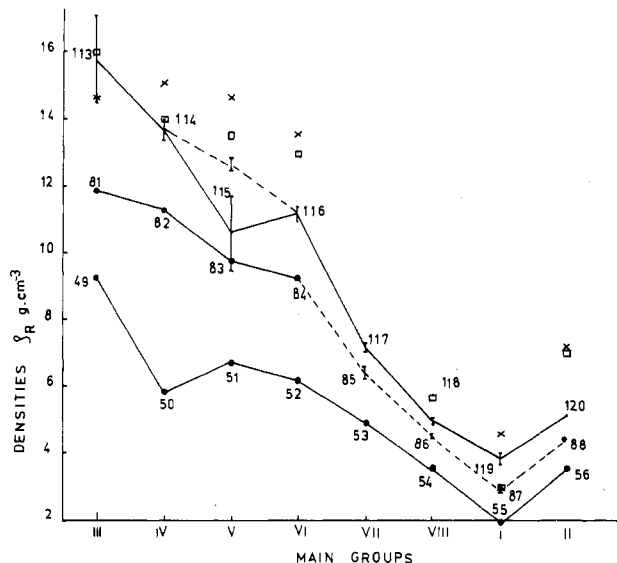


Figure 11. Densities of elements 113–120 and 85–88 obtained in this work, as well as those obtained by Fricke et al.¹³ (X); Keller et al.²³ ($z = 113, 114$), ref 16 ($z = 115, 116$), Grosse²⁰ ($z = 118$), and Cunningham²¹ ($z = 119, 120$): (□) comparison with the experimental densities of elements 81–84 and 49–56.

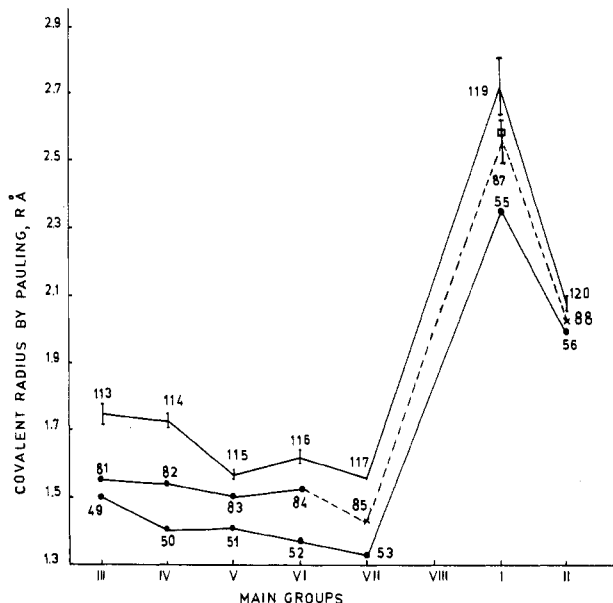


Figure 12. Pauling's covalent radii for elements 49–56 and 81–84 (experimental); elements 85, 87, 88 (X and the dashed line) and 113–120 (expected): (□) covalent radii reported by Fricke and Waber¹⁷ ($z = 114, 119$, and 120), Cunningham²¹ ($z = 117$), and Grosse²⁰ ($z = 118$).

found within the range of $1\text{--}2 \text{ g cm}^{-3}$. The densities of elements 85–88, calculated by extrapolations of the corresponding equations of Table I, are also presented in Figure 11 and Table II. Again, our estimate for emanation (element 86) and that of Grosse,²⁰ taken at 0 K, are relatively close (4.45 ± 0.05 and 5.25 g cm^{-3} , respectively).

Pauling's Covalent Radii (Figure 12). The extrapolated values for elements 113–120 are compared with those of elements 49–56 and 81–84. The radii of elements 85, 87, and 88, calculated in this work, are also shown in Figure 12 and Table II. (The van der Waals' radii of group VIII elements are not presented there.) Our results coincide very well with those of Keller et al.²³ for element 114, and those of Fricke et al.¹⁷ for elements 119 and 120. In the light of the recent quantum mechanical calculations^{12,13,17} showing that the relativistic effects increase the contraction

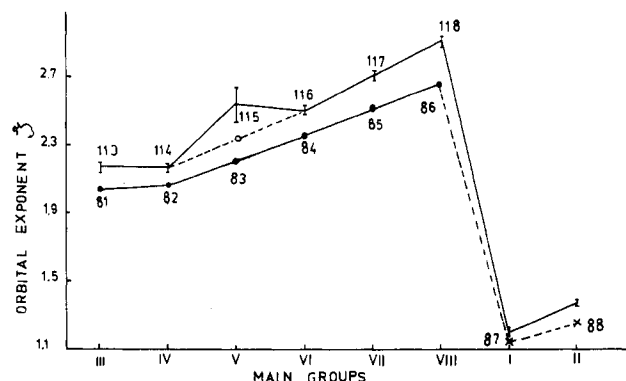


Figure 13. Orbital exponents by Clementi et al.^{36,37} for elements 81–86, as well as the expected values for elements 87, 88, and 113–120. A correction is made for element 115 on the basis of the similarity in the two curves ($\xi = 2.32$ – 2.36).

of the outermost shells, some of our estimates, particularly those for elements 113 and 114 ($7p_{1/2}$ subshell), seem, however, overestimated.

Orbital Exponents (Figure 13). As an addition to the various properties of transactinide elements 113–120 we have also extrapolated the orbital exponents of the atomic wave functions used by Clementi et al.^{36,37} for elements 1–86. The horizontal correlation presented in Figure 13 shows that the values expected for elements 113–118 manifest in general the same trend as the exponents of elements 81–86. The only exception is element 115 where the correlation within group V leads to a higher value ($\xi_{115} = 2.44$ – 2.64). Making use of the similarity in trends of the two curves, we have corrected the value expected for element 115 to 2.32–2.36. Predictions for elements 87 and 88 are also presented in Figure 13 ($\xi_{87} = 1.13$ – 1.17 , $\xi_{88} = 1.23$ – 1.27).

Concluding Remarks

The great capability of the periodic table to predict properties of chemical elements is known since the time of Mendeleev. Numerous correlations have been obtained in which a certain property of the chemical elements in a group or period is expressed as a function of the atomic number or the period number. The latter two numbers, however, are equal to the total number of electrons in the atom, and the number of electron shells, respectively. Thus, extrapolations made for the properties of the superheavy elements are not based on a *detailed* description of the electronic structure of atoms. The information indices proposed recently for the description of atoms seem to provide a better basis for the prediction of structure-dependent properties of chemical elements since they reflect the electronic structure of atoms in details. Hence, it is logical to expect that more precise extrapolations can be made within the group of the periodic table making use of atomic information indices. These expectations are additionally supported by the greater precision reached

in the correlations with these indices than in the correlations with atomic numbers.

On the other hand, the great flexibility to reflect the atomic electronic structure that is the principal advantage of information approach may or may not be entirely realized in a certain correlation depending on the type of the mathematical function used. Taking into account the fact that the functions used in the present paper cannot always express in the best way the trend of a certain property in a group of elements, we have completed our procedure by examining also the trend within the periods (vertical and horizontal correlations, respectively). We suppose that the combined use of the atomic information indices for correlations within groups and periods is *the most promising way* for the prediction of properties of the superheavy elements by means of extrapolations. Naturally, making use of a greater variety of indices and functions for the correlations, some of the expected values, reported in this paper, could be further improved. An additional refinement of the extrapolation procedure may come from modification of the atomic information indices so as to take into account the major role of the outermost electrons in the chemistry and including them with larger weights in the information functions.

The reliability of the extrapolation methods will, however, in some cases be insufficient. Two reasons should be taken into account. Primarily, the trend of a certain property can drastically change in the last known element of the group in the periodic table (14 out of 96 cases examined above). Two opposite extrapolations result in these cases and additional criteria (some rules or approximate formulas) are needed to choose between them. What prediction could, however, be done if such a drastic change did occur in the superheavy element of a chemical group? The method of extrapolations based on the periodicity of the chemical elements is in principle incapable of predicting neither the appearance of new effects nor their magnitude. As shown by quantum mechanical calculations, such important effects are the strong spin-orbit coupling in the superheavy elements and the large relativistic contraction of their orbitals with a low angular momentum. They cause a considerable change in the ionization potentials and a decrease in the size of atoms which cannot be obtained by extrapolations. Still, the periodicity could be of use in the prediction of such atomic properties, providing empirical corrections to the calculated magnitudes as shown in the most convincing way in the studies of Keller et al.,^{23,28} Fricke et al.,¹⁷ and other authors.

One can conclude that, although limited to some extent, the periodicity of the chemical elements has not lost its importance for the prediction of the properties of superheavy elements up to $z = 120$.

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