A Fuzzy Classification of the Chemical Elements[⊥]

Horia F. Pop,[§] Costel Sârbu,*[,†] Ossi Horowitz,[‡] and D. Dumitrescu[§]

Faculty of Mathematics and Computer Science and Faculty of Chemistry, "Babes-Bolyai" University, and Faculty of Mechanics, Technical University, RO-3400 Cluj-Napoca, Romania

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The fuzzy clustering algorithm is applied in order to obtain the cluster structure of the chemical elements, based on their physical, chemical, and structural properties. The results obtained with the fuzzy method are consistent with the chemical behavior of the elements and with the predictions based on their electronic structure. An IBM-PC computer has been used to run the corresponding program written in Pascal. Moreover, the results suggest some new untrivial relationships between chemical elements according to the gradual nature of their properties.

1. INTRODUCTION

It may appear that the problem of classification of the chemical elements has already been solved by the development of the periodical system of elements and that the single item to be solved is to find a certain as adequate and suggestive as possible graphic representation.[1,2] In fact, the groups of the periodic system are far from exhausting the whole wealth of relations between the properties of the elements and of their compounds. Sometimes there are unexpected similarities between remote elements in the periodic system.

It is, of course, true that most properties of the elements are eventually determined by the outer electron configurations of their atoms. These configurations are the basis for the distribution of elements in the periodic system. However, this determination is often quite indirect. Along with properties of single atoms, there are also properties collectively determined, for instance by the lattice of elementary substance.

Therefore we may raise the problem of whether the classical structure of the periodic system is really fully concordant with the physical and chemical properties of the elements. In what follows we try to resume the early procedure of Mendeleev, whose classification was not founded on electron configuration but on observable data concerning physico-chemical properties of the elements. The basic idea for our procedure is that, since the properties of elements are gradual by nature, we must acknowledge that they should be grouped in classes with no clearly-cut boundaries. So, each element should belong mainly to a single class, but this does not mean that it could not also belong with different small membership degrees to all the other classes.

If we admit that the membership degrees to a class have gradual character, we may obtain a more accurate classification of elements, able to account for some irregularities of the standard classification. On the other hand, it could suggest the occurrence of some new relationships between the elements.

This classification has to use primary physical and chemical properties of elements. Their selection is rather difficult; they have to be expressed numerically and have to be known for all the investigated elements. The method we used for the classification uses the fuzzy sets theory in order to obtain the cluster of the set of chemical elements. This method is hierarchical and does not suppose a preliminary knowledge with respect to the number of classes in the data set, nor does it suppose a certain structure of the classes. Both the number of classes and their mutual relationships will be detected by the classification algorithm used here.

2. THEORETICAL CONSIDERATIONS

The mathematics of fuzzy set theory was originated by L. A. Zadeh in 1965.[3] It deals with the uncertainty and fuzziness arising from interrelated humanistic types of phenomena such as subjectivity, thinking, reasoning, cognition, and perception. This type of uncertainty is characterized by structures that lack sharp (well defined) boundaries. This approach provides a way to translate a linguistic model of the human thinking process into a mathematical framework for developing the computer algorithms for computerized decision-making processes. The theory has grown very quickly.[4−6]

Until now the greatest part of successful application of fuzzy set theory in chemistry has been devoted to fields such as pattern recognition problems[7−12] and clustering,[13−16] calibration of analytical methods,[17−19] and recently to the design of fuzzy expert systems[20−25] and neural networks.[26]

The fuzzy divisive hierarchical clustering method proposed in ref 27 has been used for acrylonitrile selectivity,[28−30] for mineral waters classification,[31−33] for the selection and the optimal combination of solvents,[34,35] and for the classification of Roman pottery[36] and Greek muds and pelloids.[37]

Fuzzy Set and Fuzzy Partition. Let us consider a set of objects $X = \{x^1,...,x^p\}$, these objects being characterized so that it is possible to define a measure of their (di)similarity. We need to find the partition $\{A_1,...,A_n\}$ of X, with $1 \le n < p$ so that the objects members of the same class should be as similar as possible, and the objects members of different classes should be as different as possible.

† Faculty of Chemistry, "Babes-Bolyai" University.
‡ Faculty of Mechanics, Technical University.
§ Faculty of Mathematics and Computer Science, "Babes-Bolyai" University.
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One of the main difficulties of finding some classification theories is that the most classes of real objects do not have sharp boundaries. These classes may partially overlap. A certain object may have hybrid characteristics that should put it in many classes simultaneously. This difficulty is solved if we allow for each point to be a member of each class with a certain subunitary membership. In this situation a class of objects may be described as a fuzzy set. The theory of fuzzy sets was introduced in 1965 by Lotfy A. Zadeh[3] as a natural generalization of the classical set concept. The classification structure of a set X of objects may thus be represented by a fuzzy partition of X.

Let x^j be a certain point of the given set X. We suppose that x^j is characterized by the values of s characteristics, x^j_k, with $1 \leq k \leq s$, where x^j_k is the value of the kth characteristic of the jth point.

A fuzzy set on X is a mapping A: $X \rightarrow [0, 1]$. The value $A(x)$ represents the *membership degree* of the point $x \in X$ to the class A.

As usual, we denote the empty fuzzy set by $\varnothing$, that is $\varnothing(x) = 0$ for any x in X.

The fuzzy set having the membership degree equal to 1 is also denoted by X, that is $X(x) = 1$, for any x in X.

The equality of the fuzzy sets A and B is determined by the equality condition for functions:

$$A = B \leftrightarrow A(x) = B(x), \forall x \in X$$

The union and the intersection of the fuzzy sets may be defined in many ways. In this paper we consider the following definitions

$$(A \bigcup B)(x) = \min(1, A(x) + B(x)), \forall x \in X$$

and

$$(A \cap B)(x) = \max(0, A(x) + B(x) - 1), \forall x \in X$$

It may be proved (see ref 27) that the considered definitions of $\cup$ and $\cap$ are the unique ones for which the following equivalence holds:

$$\left.\begin{array}{l} A \bigcup B = X \\ A \cap B = \varnothing \end{array}\right\} \leftrightarrow A(x) + B(x) = 1, \forall x \in X$$

This means that these definitions lead to a natural definition of a fuzzy partition.

Let A, B, and C be fuzzy sets on X. $P = \{A,B\}$ is a fuzzy partition of C if the following conditions are fulfilled: 1. $A \cup B = C$ and 2. $A \cap B = \Phi$.

It is easy to note that this definition is equivalent with

$$A(x) + B(x) = C(x), \forall x \in X$$

Fuzzy Substructure of a Fuzzy Set. If the data set X is composed by two classes, then the cluster structure of the set X is described by two disjoint fuzzy sets having the union equal to X. Each fuzzy set corresponds to a class (or cluster) of points in X. The disjointness condition is a minimal separation condition of the respective classes.

We will consider a hierarchical classification scheme where the cluster structure of the data set X is given by a binary fuzzy partition. Let $\{A_1,A_2\}$ be such a fuzzy partition. It is possible for the class A_i, $i = 1, 2$, to have a cluster substructure. We may imagine this substructure as a fuzzy partition $\{A_{i,1},A_{i,2}\}$ of A_i. In this case, $A_{i,1}$ and $A_{i,2}$ represent subclusters of A_i.

So, we are entitled to search for the cluster substructure of a certain fuzzy set, and let us denote it by C. Let us suppose that the binary fuzzy partition corresponding to this substructure is $\{A_1,A_2\}$. We admit that each class A_i may be represented by a prototype L^i from the representation space, R^s. If L^i is from X we may suppose that L^i has the greatest membership degree to A_i, that is

$$A_i(L^i) = \max_{x \in X} A_i(x) \tag{1}$$

Let us denote by d a distance in the space R^s. For example, we may consider the distance induced by the norm of the space.

The dissimilarity $D_i(x^j,L^i)$ between a point x^j and the prototype L^i is defined as the square distance to the class A_i and is interpreted as a measure of the inadequacy of the representation of the point x^j by the prototype L^i.

If L^i is not a point from the data set X, then we have from ref 38 that

$$D_i(x^j,L^i) = (A_i(x^j))^2 d^2(x^j,L^i) \tag{2}$$

The inadequacy between the fuzzy partition P and its representation, $L = \{L^1,L^2\}$ is given by the following function

$$J(P,L) = \sum_{i=1}^{2}\sum_{j=1}^{p}(A_i(x^j))^2 d^2(x^j,L^i) \tag{3}$$

$J(P,L)$ may also be interpreted as the representation error of P by L.

Let us observe that J is a criteria function of the type of square errors sum. The classification problem becomes the determination of the fuzzy partition P and its representation L for which the inadequacy $J(P,L)$ is minimal. Let us note that, intuitively, to minimize J means to give small membership degress to A_i for those points in X for which the dissimilarity to the prototyle L^i is large and vice versa.

Now let us generalize the problem by considering that the fuzzy substructure of the fuzzy set C is given by a fuzzy n-partition, and let us suppose that $P = \{A_1,...,A_n\}$ is this partition. If we admit that d is a distance induced by the norm, we may write

$$J(P,L) = \sum_{i=1}^{n}\sum_{j=1}^{p}(A_i(x^j))^2 ||x^j - L^i||^2 \tag{4}$$

If the norm is induced by the inner product, we have

$$||x^j - L^i||^2 = (x^j - L^i)^T M(x^j - L^i)$$

where M is a symmetrical and positively defined matrix. The transposing operation was denoted by ^{T}.

The criteria function becomes

$$J(P,L) = \sum_{i=1}^{n}\sum_{j=1}^{p}(A_i(x^j))^2 (x^j - L^i)^T M(x^j - L^i) \tag{5}$$

Because an algorithm to obtain an exact solution of the problem (5) is not known, we will use an approximative method in order to determine a local solution. The minimum

problem will be solved using an iterative (relaxation) method, where J is successively minimized with respect to P and L.

Supposing that L is given, the minimum of the function $J(\cdot,L)$ is obtained[38] for

$$A_i(x^j) = \frac{C(x^j)}{\sum_{k=1}^{n} \frac{d^2(x^j,L^i)}{d^2(x^j,L^k)}}, \quad i = 1,2,...,n; j = 1,2,...,p \tag{6}$$

For a given P, the minimum of the function $J(P,\cdot)$ is obtained for

$$L^i = \frac{\sum_{j=1}^{p} (A_i(x^j))^2 x^j}{\sum_{j=1}^{p} (A_i(x^j))^2}, \quad i = 1,2,...,n \tag{7}$$

We observe[38] that L^i is the weighting center of the class A_i.

The iterative procedure for obtaining the cluster substructure of the fuzzy class C is called Generalized Fuzzy n-Means (GFNM).[4] Essentially, the GFNM algorithm works with Picard iterations using the relations 6 and 7. The iterative process begins with an arbitrary initialization of the partition P. The process ends when two successive partitions are close enough. To measure the distance between two partitions, we will associate to each partition P a matrix Q with the dimensions $n \times p$. Q is named the representation matrix of the fuzzy partition P and is defined as

$$Q_{ij} = A_i(x^j), \quad i = 1,2,...,n; j = 1,2,...,p \tag{8}$$

Considering that Q_1 and Q_2 are the representation matrices of the partitions P_1 and P_2, we may define

$$d(P_1,P_2) = ||Q_1 - Q_2|| \tag{9}$$

where $||Q|| = \max_{i,j}|A_i(x^j)|$.

The process ends at the rth iteration if

$$d(P_r,P_{r+1}) < \epsilon \tag{10}$$

where ϵ is an admiscible error (usually, 10^{-5}).

For $C = X$ this procedure is the well-known algorithm Fuzzy n-Means (FNM).[4]

The Problem of Inequal Size Clusters. There is one more problem. Generally, the classes have different dimensions. If we consider a small class situated near a larger one, some points from the larger class will be captured by its small neighbor. This situation may be eliminated if we use an adaptive distance (see ref 4). This distance, being influenced by the dimension of classes, will anihilate the effect of migration of peripheral points. We define the radius r_i of the fuzzy class A_i as

$$r_i = \max_{x \in X} d_i(x,L^i) = \max_{x \in X} A_i(x) d(x,L^i) \tag{11}$$

We will define the local adaptive distance, d_{ia}, as

$$d_{ia}(x,L^i) = \frac{d_i(x,L^i)}{r_i} \tag{12}$$

and the new disimilarity as

$$D_i(x^j,L^i) = d_{ia}^2(x^j,L^i) \tag{13}$$

The criteria function becomes

$$J(P,L) = \sum_{i=1}^{2}\sum_{j=1}^{p} (A_i(x^j))^2 \frac{d^2(x^j,L^i)}{r_i^2} \tag{14}$$

By using the adaptive distance, the problem of inequal clusters will not appear, because the radii of the two clusters are equal.

Polarization and Fuzziness. Because the optimal number of classes generally is not known, we will use a divisive hierachical clustering procedure. The problem that appears now is to decide whether a class may be divided or not.

Let us suppose that the fuzzy class C was divided in the two fuzzy classes C_1 and C_2. If C describes a homogenous cluster, the membership degrees tend to be uniform (the majority of points will have the membership degrees of about $C(x)/2$). On the contrary, if C contains two classes relatively well separated, this will induce a trend of polarization of the membership degrees (the majority of points will have the membership degrees polarized near the extreme values, 0 and $C(x)$).

So, the polarization of the membership degrees may be associated with the presence of a certain structure in the data set. The polarization degree of a binary fuzzy partition may be considered as measuring the partition quality. The polarization degree of P may be defined[4,38] as

$$R(P) = \frac{\sum_{x \in X} \max(C_1(x),C_2(x))}{\sum_{x \in X} C(x)} \tag{15}$$

For example, let us consider $X = \{x^1,x^2,x^3,x^4\}$ and the fuzzy partition $P = \{A_1,A_2\}$ of X is given by

	x^1	x^2	x^3	x^4
$A_1(x^j)$	0.9	0.2	0.7	0.6
$A_2(x^j)$	0.1	0.8	0.3	0.4

In this case we have $R(P) = (0.9 + 0.8 + 0.7 + 0.6)/4 = 3/4 = 0.75$.

Let us consider now the fuzzy partition $Q = \{A_{11},A_{12}\}$ of A_1 given by

	x^1	x^2	x^3	x^4
$A_{11}(x^j)$	0.2	0.1	0.6	0.4
$A_{12}(x^j)$	0.7	0.1	0.1	0.2

We have $R(P) = (0.7 + 0.1 + 0.6 + 0.4)/(0.9 + 0.2 + 0.7 + 0.6) = 1.8/2.4 = 0.75$.

If $R(P)$ is large enough ($R(P) \geq t$, where t is an appropriate threshold), we will say that the fuzzy partition P describes real clusters.

Fuzzy Divisive Hierarchical Clustering. Using the FNM algorithm we may determine a binary fuzzy partition $\{A_1,A_2\}$ of the data set X. If the partition does not describe real

clusters (that is, the polarization degree, $R(P)$ is small), the data set X does not have a substructure. If this partition describes real clusters, we denote $P^1 = \{A_1,A_2\}$. Using the GFNM algorithm of two subclasses ($n = 2$) we may determine a binary fuzzy partition for each A_i of P^1. If this partition of A_i describes real clusters, these clusters will be attached to a new fuzzy partition, P^2. Otherwise, A_i will remain undivided. The class A_i will be marked and will be allocated to the partition P^2.

The unmarked classes members of P^2 will follow the same procedure. The divisive procedure will stop when all the classes of the current partition P^l are marked, that is there are no more real clusters.

The fuzzy hierarchy obtained is richer in information (see ref 6) than a hierarchy based on classical sets, but sometimes is useful to have a classical partition also. For a complete discussion on the problem of passing from fuzzy partitions to classical partitions, see ref 6. We will only show the method used here for obtaining a classical partition.

Interpretation of the Final Fuzzy Partition. Defuzzification of the final fuzzy partition will be obtained using the maximum membership rule or a hierarchical assignment rule. This latter rule means that the classical sets corresponding to the fuzzy classes will be built simultaneously with the respective fuzzy classes, based on the following: 1. initially, $\forall x \in X$, $x \in \tilde{X}$ and 2. when we build the fuzzy partition $\{C_1,C_2\}$ of the fuzzy set C, we will say that

$$x \in \tilde{C}_1 \leftrightarrow x \in \tilde{C} \text{ and } C_1(x) \geq C_2(x)$$

and

$$x \in \tilde{C}_2 \leftrightarrow x \in \tilde{C} \text{ and } C_1(x) < C_2(x)$$

Remark. It is obvious that $\{\tilde{C}_1,\tilde{C}_2\}$ is a hard partition of the classical set $\tilde{C}$.

Finally, when obtaining the fuzzy hierarchy of the set X, we will also obtain the so-called classical hierarchy associated to the respective fuzzy hierarchy.

To conclude, the Fuzzy Divisive Hierarchical Clustering (FDHC) procedure may be used to determine the optimal cluster substructure of the data set. This method is especially useful when the number of classes is unknown.

Characteristics Clustering. In what follows we consider that in the classification processes essentially appear two sets: a set X of objects and a set Y of characteristics. As usual, we denote by $X = \{x^1,...,x^p\} \subset \mathrm{R}^d$ the set of objects to be classified. A characteristic may be specified by its values corresponding to the p objects. So, we may say that $Y = \{y^1,...,y^d\} \subset \mathrm{R}^p$ is the set of characteristics. y_j^k is the value of the characteristic k with respect to the object j, so we may write $y_j^k = x_k^j$.

Here arises the problem of characteristics clustering. This may be useful in many situations. For example, the dimensionality reduction may be considered as a characteristics classification process. The characteristics in the same class (which are, consequently, very similar to each other) will realize a reduced discrimination among the objects. On the contrary, the more distant the classes that contain two different characteristics are, the greater their discrimination power is.

If the classes of characteristics are homogenous and well separated, a class may be replaced by the most representative characteristic. This characteristic represents an average of the properties of the class. The more compact the class is, the smaller the loss of information produced by this replacement is. In this way we realize a dimensionality reduction. By choosing a unique characteristic from each class, the number of selected characteristics is equal to the number of clusters in the set Y. Alternatively, we may not only select some of the existing characteristics, but we may replace them by new characteristics, by considering that each class of characteristics is replaced by the prototype characteristic.

3. CLASSIFICATION RESULTS

3.1. Classifications Based on 10 Physical Properties. In order to use the method presented above to classify the chemical elements, the problem we are first faced with is to settle the characteristics this classification is built upon. We started with 10 physical properties: relative atomic mass, density, melting point, boiling point, electronegativity (Pauling), enthalpy of fusion and vaporization, specific heat capacity, ionization energy, and covalent radius. There values are known for 84 elements. Of course, these quantities are not independent from one another; in some cases rather strong linear correlations are found.

The most obvious correlation of this type is that between the enthalpy of vaporization (ΔH_v) and the boiling point (T_b)

$$\Delta H_v(\text{kcal}\cdot\text{mol}^{-1}) = (-8.2 \pm 2.7t) + (0.0288 \pm 0.0009t)T_b(K)$$

($s_0 = 13$; $r = 0.965$), where t is the Student parameter, r is the correlation coefficient, and s_0 is the standard deviation.

This reminds us of the well-known Trouton's rule, which states that the molar vaporization entropy ($\Delta H_v/T_b$) is approximately the same for all liquids (85 J K^{-1} mol^{-1}); this rule would give a slope of 0.021 and the intercept zero at $T_b = 0$).

Less strong is the correlation between the fusion enthalpy ΔH_f and the melting point T_f ($r = 0.836$):

$$\Delta H_v(\text{kcal}\cdot\text{mol}^{-1}) = (0.39 \pm 0.24t) + (0.00203 \pm 0.00015t)T_f(K)$$

($s_0 = 1.3$). As a matter of fact, the fusion entropy ($\Delta H_f/T_f$) is less constant than the vaporization entropy.

Even the melting and the boiling points are linearly correlated

$$T_b = (630 \pm 260t) + (1.53 \pm 0.18)T_f \quad (r = 0.888)$$

The ionization energy (E_i) may be correlated to the Pauling electronegativity (χ)

$$\chi(\text{kcal}\cdot\text{mol}^{-1}) = (-0.03 \pm 0.11t) + (0.0097 \pm 0.0006t)E_i \quad (r = 0.894)$$

On the other hand, specific heat capacities (c_s) are related to atomic masses (A) by the Dulong and Petit's Law: $A\cdot c_s$ = constant, the density is a function of the atomic mass and the covalent radius, the ionization energy is related to the atom radius, etc.

These interdependencies of the characteristics do not represent a difficulty for this classification. This analysis may order the characteristics in an importance sequence and

Table 1. Membership Degrees to the Classes of the Final Partition Produced with 10 Non-Normalized Characteristics (Part 1)

sample	1.1.1	1.1.2	1.2.1.1	1.2.1.2	1.2.2.1	1.2.2.2.1	sample	1.1.1	1.1.2	1.2.1.1	1.2.1.2	1.2.2.1	1.2.2.2.1
H	0.02	0.03	0.01	0.02	0.06	0.66	Tc	0.01	0.00	0.00	0.00	0.00	0.00
He	0.02	0.04	0.02	0.04	0.14	0.04	Ru	0.04	0.03	0.01	0.01	0.01	0.00
Li	0.17	0.68	0.07	0.02	0.01	0.00	Rh	0.02	0.01	0.01	0.00	0.00	0.00
Be	0.09	0.03	0.01	0.01	0.01	0.00	Pd	0.01	0.00	0.00	0.00	0.00	0.00
B	0.07	0.05	0.01	0.01	0.01	0.00	Ag	0.38	0.07	0.02	0.01	0.01	0.00
C	0.06	0.05	0.02	0.02	0.01	0.01	Cd	0.08	0.39	0.43	0.07	0.02	0.01
N	0.01	0.02	0.00	0.01	0.02	0.86	In	0.54	0.15	0.04	0.02	0.01	0.01
O	0.01	0.02	0.00	0.01	0.05	0.82	Sn	0.48	0.09	0.04	0.02	0.02	0.01
F	0.01	0.02	0.00	0.01	0.01	0.72	Sb	0.03	0.89	0.00	0.00	0.00	0.00
Ne	0.02	0.03	0.01	0.03	0.09	0.01	Te	0.07	0.70	0.15	0.04	0.02	0.01
Na	0.10	0.40	0.42	0.04	0.03	0.01	I	0.00	0.01	0.05	0.48	0.35	0.05
Mg	0.05	0.82	0.06	0.03	0.01	0.00	Xe	0.01	0.01	0.01	0.02	0.59	0.25
Al	0.35	0.05	0.02	0.02	0.01	0.00	Cs	0.07	0.20	0.60	0.10	0.02	0.01
Si	0.09	0.04	0.01	0.01	0.01	0.00	Ba	0.39	0.44	0.01	0.00	0.00	0.00
P	0.00	0.01	0.03	0.63	0.24	0.04	La	0.04	0.02	0.01	0.01	0.00	0.00
S	0.02	0.06	0.08	0.77	0.03	0.01	Ce	0.06	0.03	0.01	0.01	0.01	0.00
Cl	0.00	0.01	0.01	0.03	0.79	0.08	Pr	0.07	0.03	0.01	0.01	0.01	0.00
Ar	0.01	0.02	0.00	0.00	0.02	0.86	Nd	0.07	0.03	0.01	0.01	0.01	0.00
K	0.08	0.27	0.59	0.03	0.02	0.01	Sm	0.42	0.17	0.02	0.01	0.01	0.00
Ca	0.16	0.69	0.01	0.01	0.00	0.00	Eu	0.16	0.70	0.01	0.01	0.00	0.00
Sc	0.07	0.03	0.01	0.01	0.01	0.00	Gd	0.04	0.02	0.01	0.00	0.00	0.00
Ti	0.01	0.00	0.00	0.00	0.00	0.00	Tb	0.07	0.03	0.01	0.01	0.01	0.00
V	0.00	0.00	0.00	0.00	0.00	0.00	Dy	0.11	0.05	0.01	0.01	0.01	0.00
Cr	0.06	0.03	0.01	0.01	0.01	0.00	Ho	0.10	0.05	0.01	0.01	0.01	0.00
Mn	0.28	0.11	0.02	0.02	0.01	0.00	Er	0.04	0.02	0.01	0.00	0.00	0.00
Fe	0.03	0.01	0.00	0.00	0.00	0.00	Tm	0.26	0.23	0.04	0.03	0.02	0.01
Co	0.04	0.02	0.01	0.00	0.00	0.00	Yb	0.15	0.71	0.01	0.01	0.00	0.00
Ni	0.08	0.03	0.01	0.01	0.01	0.00	Lu	0.00	0.00	0.00	0.00	0.00	0.00
Cu	0.17	0.05	0.02	0.01	0.01	0.00	Hf	0.05	0.03	0.01	0.01	0.01	0.00
Zn	0.08	0.59	0.22	0.06	0.02	0.01	Ta	0.05	0.04	0.02	0.01	0.01	0.01
Ga	0.44	0.14	0.05	0.03	0.02	0.01	W	0.06	0.05	0.02	0.02	0.02	0.01
Ge	0.13	0.04	0.01	0.01	0.01	0.00	Re	0.06	0.05	0.02	0.02	0.02	0.01
As	0.11	0.41	0.19	0.15	0.07	0.02	Os	0.05	0.04	0.02	0.01	0.01	0.01
Se	0.07	0.25	0.59	0.08	0.01	0.00	Ir	0.05	0.03	0.01	0.01	0.01	0.00
Br	0.00	0.00	0.03	0.16	0.75	0.02	Pt	0.02	0.01	0.01	0.00	0.00	0.00
Kr	0.01	0.02	0.00	0.00	0.21	0.63	Au	0.08	0.03	0.01	0.01	0.01	0.00
Rb	0.06	0.20	0.62	0.08	0.02	0.00	Hg	0.01	0.03	0.08	0.64	0.16	0.03
Sr	0.08	0.80	0.01	0.01	0.00	0.00	Tl	0.19	0.70	0.02	0.01	0.01	0.00
Y	0.04	0.02	0.01	0.00	0.00	0.00	Pb	0.50	0.32	0.02	0.01	0.01	0.00
Zr	0.00	0.000	0.00	0.00	0.00	0.00	Bi	0.30	0.57	0.02	0.01	0.01	0.00
Nb	0.02	0.01	0.00	0.00	0.00	0.00	Th	0.00	0.00	0.00	0.00	0.00	0.00
Mo	0.05	0.04	0.02	0.01	0.01	0.01	U	0.02	0.01	0.00	0.00	0.00	0.00

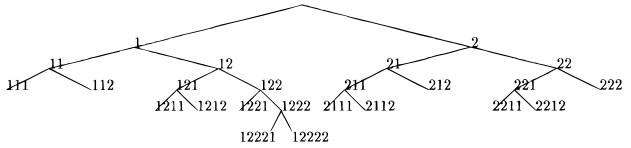

Figure 1. The classification hierarchy produced with 10 non-normalized characteristics.

reduce their number, without affecting the classification in an essential manner.

The classification hierarchy produced by using the **10 physical properties** mentioned above is presented in Figure 1. Table 1 and 2 show the membership degrees of the elements to the fuzzy sets of the final fuzzy partition, and Figure 2 shows the successive partitions of the elements produced with these properties.

The first partition separates roughly speaking the elements of the main groups of the periodic system (class 1) from those of the secondary groups (class 2). To class 1 belong as well the metals of group 12 (Zn, Cd, Hg) and also Ag; all these elements have the *d*-subshell completed and are in this way analogous to those of the main groups. Also, class 1 includes four lanthanides (Sm, Eu, Tm, Yb), all of them having the 5*d*-subshell vacant. The 4*f*-subshell is complete for Yb and half-complete ($4f^7$) for Eu, i.e., these elements have relatively stable configurations of this subshell. Tm and Sm have an electron fewer than these configurations ($4f^{13}$, $4f^6$). On the other hand, the class 2 also contains six elements of the main groups (Be, B, Al, C, Si, Ge). On the whole, the first class contains elements with lower densities and melting and boiling points (smaller fusion and vaporization enthalpies).

The next step for class 1 differentiates mainly between metals (class 1.1) and nonmetals (class 1.2), the latter class including yet the first group elements K, Rb, and Cs and the 12th group metals Cd and Hg. The elements of class 1.2 have lower densities, melting and boiling points, and as a rule, high ionization energies and electronegativities. But the dominant features here are the melting and boiling points, and this accounts for the presence of some very electropositive (K, Rb, Cs) or heavy elements (Hg). However, the metals of this class (1.2), together with the nonmetal solid at room temperature (P, S, Se, I), are separated as a class (1.2.1) from the typical nonmetal gaseous at room temperature (the class 1.2.2).

A last subdivision distinguishes a class (1.2.1.1) containing the alkali metals (membership degrees—MD—of about 0.60) and Se and Cd. The last one has a smaller MD (0.43), only a little more than its MD for the class 1.1.2. The class 1.1.2 includes, among others, Zn, which has a MD of 0.22 for the class 1.2.1. The elements of the class 1.2.1.1 are similar

Table 2. Membership Degrees to the Classes of the Final Partition Produced with 10 Non-Normalized Characteristics (Part 2)

sample	1.2.2.2.2	2.1.1.1	2.1.1.2	2.1.2	2.2.1.1	2.2.1.2	2.2.2	sample	1.2.2.2.2	2.1.1.1	2.1.1.2	2.1.2	2.2.1.1	2.2.1.2	2.2.2
H	0.14	0.02	0.02	0.02	0.00	0.01	0.01	Tc	0.00	0.05	0.08	0.71	0.03	0.07	0.04
He	0.63	0.02	0.02	0.02	0.00	0.01	0.01	Ru	0.00	0.00	0.01	0.02	0.74	0.07	0.07
Li	0.00	0.01	0.01	0.01	0.00	0.00	0.00	Rh	0.00	0.04	0.04	0.22	0.01	0.58	0.06
Be	0.00	0.24	0.58	0.02	0.00	0.01	0.00	Pd	0.00	0.07	0.06	0.63	0.02	0.16	0.05
B	0.00	0.12	0.37	0.29	0.01	0.03	0.02	Ag	0.00	0.19	0.19	0.09	0.01	0.01	0.01
C	0.01	0.02	0.02	0.07	0.15	0.07	0.50	Cd	0.01	0.00	0.00	0.00	0.00	0.00	0.00
N	0.01	0.01	0.01	0.02	0.00	0.01	0.01	In	0.01	0.08	0.06	0.06	0.01	0.01	0.01
O	0.02	0.01	0.01	0.02	0.00	0.01	0.01	Sn	0.01	0.13	0.08	0.09	0.01	0.02	0.02
F	0.16	0.01	0.01	0.02	0.00	0.01	0.01	Sb	0.00	0.02	0.02	0.02	0.00	0.00	0.00
Ne	0.75	0.02	0.02	0.02	0.00	0.01	0.01	Te	0.01	0.00	0.00	0.00	0.00	0.00	0.00
Na	0.01	0.00	0.00	0.00	0.00	0.00	0.00	I	0.03	0.01	0.01	0.01	0.00	0.00	0.00
Mg	0.00	0.01	0.01	0.01	0.00	0.00	0.00	Xe	0.07	0.01	0.01	0.02	0.00	0.00	0.01
Al	0.00	0.26	0.14	0.11	0.01	0.02	0.01	Cs	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Si	0.00	0.05	0.74	0.03	0.00	0.01	0.00	Ba	0.00	0.05	0.05	0.04	0.00	0.01	0.01
P	0.03	0.01	0.01	0.01	0.00	0.00	0.00	La	0.00	0.31	0.12	0.42	0.01	0.03	0.02
S	0.01	0.00	0.00	0.00	0.00	0.00	0.00	Ce	0.00	0.32	0.12	0.38	0.01	0.04	0.02
Cl	0.03	0.01	0.01	0.01	0.00	0.00	0.00	Pr	0.00	0.55	0.06	0.22	0.01	0.01	0.01
Ar	0.02	0.01	0.01	0.02	0.00	0.01	0.01	Nd	0.00	0.68	0.02	0.15	0.00	0.01	0.01
K	0.00	0.00	0.00	0.00	0.00	0.00	0.00	Sm	0.00	0.12	0.14	0.08	0.01	0.01	0.01
Ca	0.00	0.04	0.04	0.03	0.00	0.01	0.01	Eu	0.00	0.04	0.04	0.03	0.00	0.01	0.01
Sc	0.00	0.02	0.77	0.07	0.00	0.01	0.00	Gd	0.00	0.41	0.42	0.09	0.00	0.00	0.00
Ti	0.00	0.05	0.08	0.83	0.00	0.01	0.01	Tb	0.00	0.10	0.76	0.01	0.00	0.00	0.00
V	0.00	0.02	0.03	0.86	0.02	0.05	0.02	Dy	0.00	0.09	0.65	0.05	0.00	0.01	0.01
Cr	0.00	0.11	0.46	0.27	0.01	0.02	0.01	Ho	0.00	0.07	0.67	0.06	0.00	0.01	0.01
Mn	0.00	0.16	0.26	0.09	0.01	0.02	0.01	Er	0.00	0.09	0.74	0.09	0.00	0.00	0.00
Fe	0.00	0.14	0.58	0.23	0.00	0.00	0.00	Tm	0.01	0.10	0.16	0.11	0.01	0.02	0.02
Co	0.00	0.07	0.76	0.08	0.00	0.00	0.00	Yb	0.00	0.03	0.04	0.03	0.00	0.01	0.01
Ni	0.00	0.01	0.81	0.03	0.00	0.00	0.00	Lu	0.00	0.03	0.04	0.90	0.00	0.01	0.01
Cu	0.00	0.38	0.27	0.06	0.01	0.01	0.01	Hf	0.00	0.01	0.01	0.02	0.54	0.06	0.24
Zn	0.01	0.00	0.00	0.00	0.00	0.00	0.00	Ta	0.01	0.00	0.00	0.01	0.02	0.00	0.82
Ga	0.01	0.11	0.07	0.08	0.01	0.02	0.02	W	0.01	0.01	0.01	0.04	0.06	0.02	0.68
Ge	0.00	0.61	0.05	0.10	0.01	0.01	0.01	Re	0.01	0.01	0.01	0.03	0.04	0.01	0.72
As	0.02	0.01	0.01	0.01	0.00	0.00	0.00	Os	0.01	0.00	0.00	0.01	0.00	0.00	0.83
Se	0.00	0.00	0.00	0.00	0.00	0.00	0.00	Ir	0.00	0.00	0.00	0.01	0.55	0.02	0.31
Br	0.01	0.01	0.01	0.01	0.00	0.00	0.00	Pt	0.00	0.05	0.05	0.26	0.02	0.51	0.07
Kr	0.07	0.01	0.01	0.02	0.00	0.00	0.01	Au	0.00	0.70	0.03	0.12	0.00	0.01	0.01
Rb	0.00	0.00	0.00	0.00	0.00	0.00	0.00	Hg	0.02	0.01	0.00	0.01	0.00	0.00	0.00
Sr	0.00	0.03	0.03	0.03	0.00	0.01	0.01	Tl	0.00	0.02	0.02	0.02	0.00	0.00	0.00
Y	0.00	0.09	0.72	0.11	0.00	0.00	0.00	Pb	0.00	0.05	0.04	0.04	0.00	0.01	0.01
Zr	0.00	0.01	0.02	0.85	0.02	0.07	0.03	Bi	0.00	0.03	0.02	0.02	0.00	0.01	0.01
Nb	0.00	0.08	0.13	0.53	0.05	0.10	0.07	Th	0.00	0.04	0.04	0.70	0.02	0.14	0.05
Mo	0.01	0.00	0.00	0.01	0.19	0.02	0.63	U	0.00	0.15	0.10	0.58	0.02	0.08	0.03

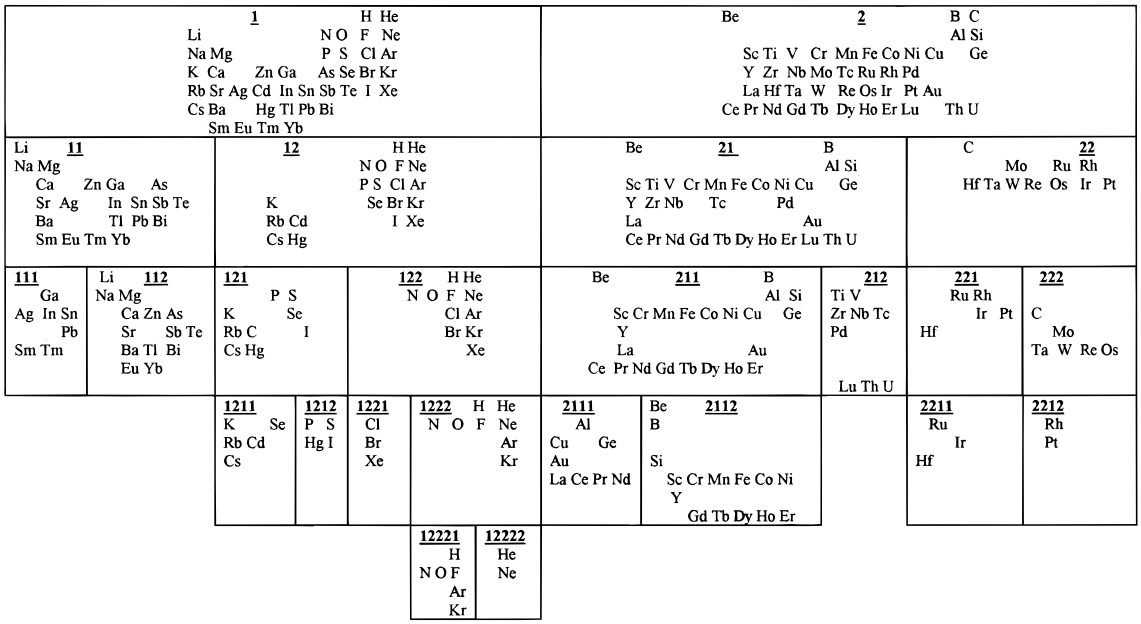

Figure 2. The classification of the elements produced with 10 non-normalized physical characteristics.

mostly with respect to their boiling points (about 700−750 °C), while the elements of the class 1.2.1.2 have lower T_b. The class 1.2.1.2 includes solid nonmetals (P, S, I) and Hg, elements with very similar ionization energies (240−250 kcal·mol^{-1}). From outside this class, As and Br have MDs of 0.15−0.16 for it. It is interesting that here are grouped

together mercury and sulfur, elements that the alchemists thought to be at the source of all the matter.

From the class 1.2.2 are first separated chlorine, bromine, and xenon (class 1.2.2.1); among them, Cl and Br have similar MDs, much higher than Xe (0.59). The last is similar to them mostly with respect to its ionization energy. The other elements having much lower densities, T_f and T_b, are grouped into two classes: one includes lighter noble gases, having the highest ionization energies, He and Ne (1.2.2.2.2), the other contains the middle noble gases (Ar, Kr) along with hydrogen and the gaseous elements of period 2 (N, O, F). These elements (class 1.2.2.2.1) have extremely low melting and boiling points and high ionization energies. To some extent, xenon also belongs to this class (MD of 0.25).

By dividing the class 1.1, a quite large class (1.1.2) is obtained. This class contains somewhat lighter elements, with lower boiling points (under 1600 °C): Li, Na (group 1), all the elements of group 2 of the periodic table, except beryllium, Tl from group 3, As, Sb, Bi from group 15, Te (group 16), Zn (group 12), and Eu and Yb (the lanthanides with relatively stable configurations of the *f*-subshell, f^7 and f^{14}). From outside this class, some elements which have significant MDs for it are Cd, Pb, Tm, Se, Rb, and Cs.

The other class (1.1.1) includes elements from group 13 (Ga, In), group 14 (Sn, Pb), silver, and the lanthanides Sm and Tm. It is a rather heterogenous class, its elements having quite different properties and relatively small MDs, from 0.54 (Ga) to 0.26 (Tm). Also, related to this class are Ba, Bi, and Mn.

Now, passing to class 2, the lighter elements of the first and second series of transition metals (class 2.1) are separated from the heavier ones, with higher melting and boiling points (class 2.2). Class 2.1 contains, besides all the transition metals of period 4, also most of those of period 5, lanthanum, and the majority of lanthanides, Th, U, and all the main-group elements of class 2, except C.

The class 2.2 includes transition metals of the periods 5 and 6 as well as carbon.

To continue, in class 2.1 is separated from the set of elements with high boiling points (3300−4000 °C) (class 2.1.2). From outside this class a few elements have substantial MDs to it: La (0.42), Ce (0.38), B (0.29), Cr (0.27), Pt (0.26), Fe, Rh, and Pr (0.22...0.24). The elements from the class 2.1.1 are further subdivided into two classes rather less differentiated: the first one (class 2.1.1.1) contains Cu, Au, and La, and the first lanthanides (Ce, Pr, Nd) as well as Al and Ge from the main groups of the periodic system. Gd has a MD for this class (0.41) almost as high as to its own class (2.1.1.2); Be and Ag also have quite large MDs (nearly 0.20). The class 2.1.1.2 contains Be, B, and Si, some transition metals of the first series, Y, and the heavier lanthanides. From outside this class, signficant MDs are Cu, Ag, Al, Tm, and Sm.

From class 2.2 is separated a class (2.2.2) that includes the elements with the highest T_f and T_b and very high densities (excepting carbon). The presence of carbon together with molybdenium reminds us that molybdenite (MoS_2) was considered for a long time as graphite. Pd and Th also have MDs for this class of about 0.15. The other class (2.2.1) is divided into two classes, their differences being again mainly the melting and boiling points; the more refractory metals (Ru, Hf, Ir) belong to the class 2.2.1.1 (Mo and C also have MDs of above 0.15), while Rh and Pt form the class 2.2.1.2 (Pd and Th have MDs for this class of about 0.14 to 0.16).

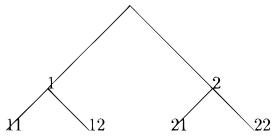

Figure 3. The classification hierarchy produced with 10 normalized characteristics.

Table 3. Membership Degrees to the Classes of the Final Partition Produced with 10 Normalized Characteristics

sample	1.1	1.2	2.1	2.2	sample	1.1	1.2	2.1	2.2
H	0.25	0.31	0.23	0.20	Tc	0.07	0.04	0.08	0.81
He	0.26	0.37	0.22	0.16	Ru	0.12	0.07	0.08	0.73
Li	0.40	0.32	0.19	0.09	Rh	0.09	0.05	0.05	0.80
Be	0.30	0.30	0.25	0.16	Pd	0.08	0.04	0.26	0.61
B	0.22	0.19	0.27	0.32	Ag	0.30	0.07	0.52	0.11
C	0.20	0.18	0.22	0.40	Cd	0.65	0.19	0.12	0.03
N	0.14	0.58	0.17	0.11	In	0.58	0.10	0.26	0.06
O	0.16	0.54	0.18	0.13	Sn	0.52	0.09	0.32	0.06
F	0.18	0.47	0.19	0.15	Sb	0.43	0.14	0.34	0.09
Ne	0.25	0.40	0.21	0.14	Te	0.46	0.27	0.20	0.07
Na	0.51	0.25	0.18	0.06	I	0.28	0.53	0.13	0.06
Mg	0.57	0.27	0.12	0.04	Xe	0.40	0.32	0.20	0.09
Al	0.46	0.20	0.25	0.09	Cs	0.40	0.19	0.29	0.12
Si	0.24	0.20	0.28	0.29	Ba	0.44	0.11	0.35	0.09
P	0.06	0.79	0.10	0.05	La	0.26	0.06	0.56	0.12
S	0.08	0.74	0.12	0.06	Ce	0.28	0.07	0.54	0.12
Cl	0.11	0.64	0.15	0.09	Pr	0.29	0.06	0.57	0.09
Ar	0.29	0.42	0.19	0.10	Nd	0.29	0.05	0.59	0.07
K	0.45	0.21	0.25	0.09	Sm	0.39	0.06	0.49	0.06
Ca	0.54	0.14	0.25	0.07	Eu	0.44	0.09	0.39	0.08
Sc	0.29	0.09	0.48	0.15	Gd	0.16	0.03	0.71	0.10
Ti	0.18	0.07	0.48	0.27	Tb	0.14	0.03	0.74	0.09
V	0.14	0.06	0.40	0.40	Dy	0.16	0.04	0.70	0.11
Cr	0.21	0.09	0.47	0.24	Ho	0.14	0.03	0.71	0.12
Mn	0.38	0.13	0.38	0.12	Er	0.13	0.03	0.69	0.14
Fe	0.17	0.08	0.45	0.30	Tm	0.20	0.05	0.61	0.14
Co	0.15	0.07	0.44	0.34	Yb	0.46	0.08	0.39	0.07
Ni	0.15	0.07	0.44	0.34	Lu	0.10	0.03	0.55	0.31
Cu	0.27	0.11	0.43	0.18	Hf	0.12	0.06	0.19	0.62
Zn	0.58	0.38	0.04	0.01	Ta	0.15	0.09	0.17	0.59
Ga	0.61	0.17	0.17	0.05	W	0.16	0.11	0.18	0.55
Ge	0.22	0.13	0.36	0.29	Re	0.16	0.11	0.17	0.56
As	0.32	0.31	0.24	0.13	Os	0.16	0.11	0.17	0.55
Se	0.15	0.72	0.09	0.04	Ir	0.16	0.11	0.17	0.56
Br	0.11	0.68	0.13	0.07	Pt	0.15	0.10	0.19	0.56
Kr	0.33	0.39	0.18	0.09	Au	0.19	0.12	0.31	0.38
Rb	0.44	0.19	0.27	0.10	Hg	0.37	0.27	0.25	0.12
Sr	0.50	0.12	0.30	0.08	Tl	0.38	0.15	0.35	0.12
Y	0.22	0.05	0.62	0.11	Pb	0.37	0.15	0.36	0.12
Zr	0.10	0.04	0.51	0.35	Bi	0.37	0.15	0.36	0.12
Nb	0.10	0.05	0.20	0.66	Th	0.14	0.06	0.36	0.44
Mo	0.12	0.07	0.12	0.69	U	0.18	0.09	0.33	0.40

It is easy to notice that the criteria of melting and boiling points are those which dominate over this classification. Nevertheless, this appears to be quite significant with respect to the chemical properties as well.

In order to ensure a more uniform participation of the various characteristics, we may use a normalization (scaling) of characteristics. The classification based on the same **10 characteristics** but **normalized**—a procedure that prevents certain properties, expressed by larger numerical values, to prevail—gives finally just four classes. The final classification hierarchy is presented in Figure 3. Table 3 shows the membership degrees of the elements to the fuzzy sets of the final fuzzy partition, and Figure 4 shows the successive partitions of the elements produced in this case.

The first separation is, as a matter of fact, the same as the one above. Only Be, Mn, and Al are moved in the class of

1	**2**
H He Li Be N O F Ne NaMg Al P S Cl Ar K Ca Mn Zn Ga As Se Br Kr Rb Sr Cd In Sn Sb Te I Xe Cs Ba Hg Tl Pb Bi Eu Yb	B C Sc Ti V Cr Fe Co Ni Cu Si Y Zr Nb Mo Tc Ru Rh Pd Ag Ge La Hf Ta W Re Os Ir Pt Au Ce Pr Nd Gd Tb Dy Ho Er Tm Lu Th U

Li Be **11**	**12**	**21**	**22** B C
NaMg Al	H He	Sc Ti V Cr Fe Co Ni Cu Ge	Si
K Ca Mn Zn Ga	N O F Ne	Y Zr Ag	Nb Mo Tc Ru Rh Pd
Rb Sr Cd In Sn Sb Te Xe	P S Cl Ar	La	Hf Ta W Re Os Ir Pt Au
Cs Ba Hg Tl Pb Bi	Se Br Kr	Ce Pr Nd Gd Tb Dy Ho Er Tm Lu	Th U
Eu Yb	I		

Figure 4. The classification of the elements produced with 10 normalized physical characteristics.

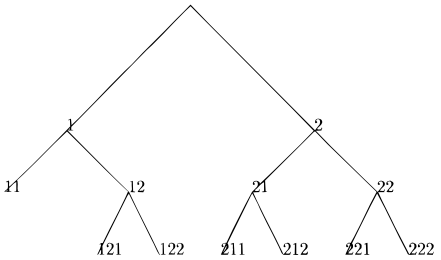

Figure 5. The classification hierarchy produced with 8 non-normalized characteristics.

main-group elements, while Ag, Sm, and Tm are passed to the class of transition elements. Thus, the separation of main-group elements and transitional metals here is more distinct. Together with the main-group elements are left Zn, Cd, and Hg (with complete *d*-subshells), Mn (d^5-configuration), and Eu and Yb (without electrons in the 5*d*-subshell and with stable configurations of the 4*f*-subshell). On the other hand, with the transition metals remain only C, Si, Ge, and B.

The elements from the main groups are divided next, as in the former classification, into metals (to which xenon joins also) and nonmetals, i.e., again a more distinct separation than that without normalization. Finally, the transition elements are divided in two classes: on the one hand, the more dense elements from the periods 5 (Nb−Pd) and 6 (Hf−Au), together with Th and U, as well as the nonmetallic refractory elements from the main groups (B, C, Si), and, on the other hand, the transition elements left and the lanthanides, together with Ge. In this way the classification is more like that given by chemical intuition but less detailed; we may say that by normalization a loss of information arises.

3.2. Classifications Based on Eight Physical Properties. Another classification was attempted, by excluding the two dominant characteristics (melting and boiling points) and therefore keeping only the **eight properties** left. The final classification hierarchy produced by using these characteristics **without normalization** is presented in Figure 5. Table 4 shows the membership degrees of the elements to the fuzzy sets of the final fuzzy partition, and Figure 6 shows the successive partitions of the elements produced in this case.

The first classes to be separated are, broadly speaking, the nonmetals and the metals. In the former class (1), boron is missing, but in exchange we find here Zn, Be, and Mg. Next, these elements are divided in a class (1.1) of elements solid and liquid at room temperature together with Xe and another class (1.2) of gaseous elements. Finally, the lighter noble gases (He and Ne) are separated from the other gaseous nonmetals.

With respect to the metals, at the first step are separated the heavy elements of period 6 (Cs−Bi), including the lanthanides, as well as Th and U (class 2.2) from the other elements (class 2.1). In this latter class are finally separated the transition elements of period 5 (Y−Ag) together with Sn and Sb (class 2.1.1) from the main-group elements Li−Rb (group 1), Ca, Sr (group 2), B−In (group 3), and Ge, beside the transition metals of period 4. Hence, it seems that in this classification the atomic mass plays a prominent role.

With the same **eight characteristics** but **normalized**, the classification is again reduced to four classes. The final classification hierarchy is presented in Figure 7. Table 5 shows the membership degrees of the elements to the fuzzy sets of the final fuzzy partition, and Figure 8 shows the successive partitions of the elements produced in this case.

The first elements to be separated are those of period 1−4, excepting Ge and V (class 1), from those of periods 5 and 6 (class 2), except for the nonmetals Te, I, Xe, and also Cd, which are included in the first class.

Class 1 is then divided into nonmetals and metals (again, with xenon joining the latter). Class 2 is separated into transition metals with high densities and melting and boiling points (V, metals of the periods 5 (Nb−Pd) and 6 (Hf−Au), U, and also Ge) and, on the other hand, the other transition metals of the period 5 and 6 (Hg, La, and lanthanides), Th, and the main-group metals of the periods 5 and 6.

3.3. Classifications Based on Seven Physical Properties. By renouncing at the atomic mass as a classification criterion (a feature that strongly affected the classification above), based on the **seven characteristics** left, **without normalization**, a rather detailed classification, that produces 13 classes, is achieved. The final classification hierarchy is presented in Figure 9. Tables 6 and 7 show the membership degrees of the elements to the fuzzy sets of the final fuzzy partition, and Figure 10 shows the successive partitions of the elements produced in this case.

The first separation groups together, on the one hand (class 1), most of the nonmetals (hydrogen and those of the groups 15−18), except for C, B, and Si (on account of their high fusion and vaporization enthalpies) but with Hg (on account of its low fusion enthalpy). As an average, the former class contains lighter and more electronegative elements. This first class is further divided by the separation of the elements having the higher ionization energy (He, Ne, F), distinguished also by lower fusion and vaporization enthalpies (class 1.2). Among them, fluorine is first separated, based on its high electronegativity (1.2.2). Next, He (1.2.1.1) and Ne (1.2.1.2) are classified apart, mainly due to the considerable difference of densities. The elements with significant MDs to the fluorine class are Ar (0.32) and N (0.12).

Table 4. Membership Degrees to the Classes of the Final Partition Produced with Eight Non-Normalized Characteristics

sample	1.1	1.2.1	1.2.2	2.1.1	2.1.2	2.2.1	2.2.2	sample	1.1	1.2.1	1.2.2	2.1.1	2.1.2	2.2.1	2.2.2
H	0.12	0.77	0.02	0.02	0.03	0.01	0.02	Tc	0.07	0.01	0.00	0.69	0.03	0.09	0.10
He	0.19	0.04	0.45	0.08	0.09	0.07	0.07	Ru	0.12	0.03	0.01	0.47	0.09	0.17	0.12
Li	0.32	0.06	0.02	0.11	0.33	0.06	0.10	Rh	0.09	0.02	0.01	0.59	0.05	0.14	0.12
Be	0.53	0.10	0.02	0.09	0.19	0.03	0.04	Pd	0.08	0.01	0.00	0.56	0.14	0.09	0.13
B	0.33	0.08	0.03	0.19	0.25	0.06	0.06	Ag	0.05	0.00	0.00	0.36	0.32	0.06	0.20
C	0.33	0.16	0.06	0.16	0.14	0.08	0.07	Cd	0.36	0.03	0.01	0.15	0.20	0.08	0.19
N	0.02	0.87	0.02	0.02	0.03	0.02	0.02	In	0.05	0.01	0.00	0.23	0.25	0.07	0.40
O	0.09	0.83	0.01	0.02	0.02	0.01	0.01	Sn	0.01	0.00	0.00	0.38	0.18	0.09	0.34
F	0.06	0.43	0.33	0.05	0.05	0.04	0.04	Sb	0.17	0.02	0.00	0.23	0.20	0.11	0.28
Ne	0.16	0.00	0.57	0.07	0.08	0.06	0.06	Te	0.35	0.04	0.01	0.13	0.16	0.09	0.22
Na	0.30	0.05	0.02	0.11	0.35	0.06	0.12	I	0.51	0.10	0.02	0.09	0.10	0.07	0.12
Mg	0.47	0.05	0.01	0.07	0.31	0.04	0.06	Xe	0.48	0.23	0.05	0.06	0.06	0.05	0.07
Al	0.26	0.04	0.01	0.10	0.48	0.04	0.07	Cs	0.14	0.03	0.01	0.15	0.18	0.10	0.39
Si	0.51	0.04	0.01	0.07	0.29	0.03	0.05	Ba	0.08	0.01	0.00	0.14	0.14	0.07	0.55
P	0.68	0.24	0.02	0.01	0.02	0.01	0.01	La	0.03	0.01	0.00	0.16	0.06	0.18	0.56
S	0.75	0.14	0.01	0.02	0.04	0.01	0.02	Ce	0.01	0.00	0.00	0.15	0.04	0.24	0.56
Cl	0.21	0.75	0.01	0.01	0.01	0.00	0.01	Pr	0.02	0.00	0.00	0.10	0.05	0.08	0.74
Ar	0.01	0.79	0.08	0.03	0.04	0.02	0.03	Nd	0.02	0.00	0.00	0.06	0.03	0.03	0.86
K	0.25	0.05	0.02	0.13	0.33	0.07	0.15	Sm	0.06	0.01	0.00	0.09	0.07	0.04	0.72
Ca	0.28	0.04	0.01	0.08	0.45	0.04	0.09	Eu	0.07	0.01	0.00	0.09	0.08	0.05	0.70
Sc	0.21	0.03	0.01	0.08	0.60	0.02	0.04	Gd	0.03	0.01	0.00	0.02	0.01	0.02	0.92
Ti	0.19	0.03	0.01	0.26	0.43	0.03	0.05	Tb	0.03	0.01	0.00	0.01	0.00	0.03	0.92
V	0.18	0.03	0.01	0.28	0.43	0.03	0.04	Dy	0.04	0.01	0.00	0.01	0.01	0.04	0.90
Cr	0.20	0.02	0.01	0.03	0.69	0.02	0.04	Ho	0.05	0.01	0.00	0.01	0.01	0.06	0.86
Mn	0.29	0.02	0.00	0.03	0.58	0.02	0.05	Er	0.05	0.01	0.00	0.02	0.01	0.03	0.89
Fe	0.25	0.03	0.01	0.15	0.52	0.02	0.03	Tm	0.06	0.01	0.00	0.03	0.02	0.03	0.85
Co	0.22	0.03	0.01	0.24	0.46	0.02	0.03	Yb	0.09	0.02	0.01	0.07	0.05	0.07	0.70
Ni	0.20	0.02	0.01	0.21	0.52	0.01	0.02	Lu	0.07	0.02	0.01	0.08	0.04	0.23	0.56
Cu	0.22	0.02	0.00	0.08	0.64	0.01	0.02	Hf	0.10	0.03	0.01	0.18	0.08	0.46	0.14
Zn	0.69	0.00	0.00	0.07	0.15	0.03	0.05	Ta	0.13	0.04	0.02	0.20	0.09	0.42	0.11
Ga	0.16	0.02	0.01	0.11	0.55	0.04	0.11	W	0.15	0.05	0.02	0.20	0.09	0.40	0.08
Ge	0.23	0.01	0.00	0.16	0.53	0.02	0.04	Re	0.12	0.04	0.02	0.18	0.07	0.54	0.04
As	0.77	0.03	0.00	0.05	0.08	0.02	0.04	Os	0.15	0.05	0.02	0.19	0.08	0.45	0.07
Se	0.72	0.03	0.01	0.06	0.10	0.03	0.06	Ir	0.16	0.05	0.02	0.18	0.08	0.44	0.07
Br	0.64	0.28	0.03	0.01	0.02	0.01	0.01	Pt	0.14	0.04	0.02	0.15	0.07	0.51	0.08
Kr	0.20	0.66	0.05	0.02	0.03	0.02	0.02	Au	0.16	0.04	0.02	0.12	0.07	0.38	0.22
Rb	0.17	0.03	0.01	0.16	0.30	0.08	0.24	Hg	0.29	0.10	0.04	0.11	0.09	0.16	0.22
Sr	0.14	0.02	0.01	0.16	0.42	0.06	0.20	Tl	0.12	0.03	0.01	0.07	0.05	0.17	0.54
Y	0.05	0.01	0.00	0.64	0.24	0.02	0.04	Pb	0.14	0.03	0.01	0.08	0.05	0.22	0.46
Zr	0.08	0.01	0.00	0.69	0.06	0.07	0.09	Bi	0.16	0.04	0.02	0.09	0.06	0.24	0.40
Nb	0.08	0.01	0.00	0.63	0.07	0.09	0.10	Th	0.13	0.04	0.02	0.12	0.07	0.45	0.18
Mo	0.09	0.02	0.01	0.62	0.06	0.11	0.11	U	0.13	0.04	0.02	0.11	0.06	0.43	0.21

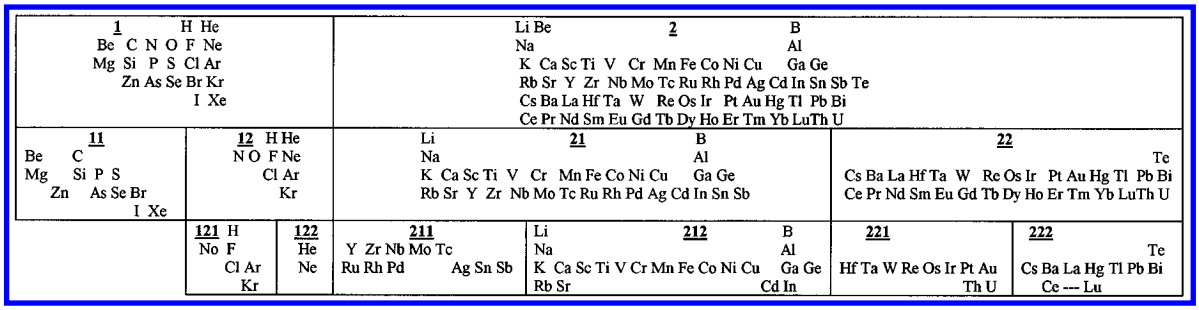

Figure 6. The classification of the elements produced with eight non-normalized characteristics.

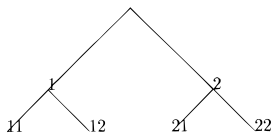

Figure 7. The classification hierarchy produced with eight normalized characteristics.

Among the other nonmetals (1.1) the gaseous elements (1.1.2) are separated from the other, having somewhat higher densities and lower ionization energies (P, As, S, Se, Br, I, and Hg)—class 1.1.1. To some extent, to this class are related Xe (with a MD of 0.41), Zr and Te (0.32), Nb (0.26), C (0.16), and Be (0.12). Among the gaseous elements, nitrogen, argon, and krypton are grouped together (1.1.2.2). These elements have high and similar ionization energies. A certain belonging to this class show O (a MD of 0.16), H (0.13), and F (0.12). The gaseous elements left are also split: on the one hand (class 1.1.2.1.1), are hydrogen and oxygen (lighter, with low fusion and vaporization enthalpies). From outside, Kr (a MD of 0.22) and Cl (0.12) are related to them. On the other hand, are chlorine and xenone (class 1.1.2.1.2). From the elements outside this class, bromine has a MD of 0.21.

For the metals, the classification is far from being so detailed. From class 2 emerges a class (2.1) that mainly includes the main-group elements (except for Be, B, and C), all the lanthanides (except for Ce) and some transition metals. The other class (2.2) contains particularly transition elements,

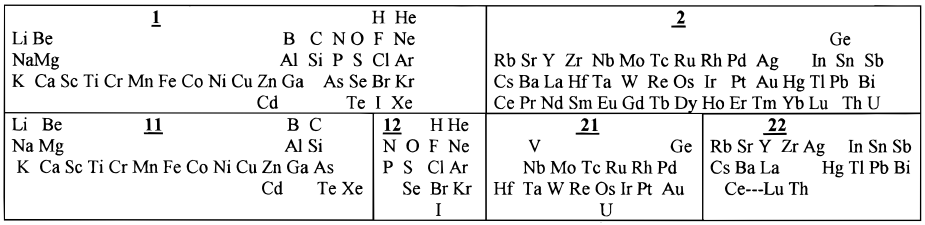

Figure 8. The classification of elements produced with eight normalized characteristics.

Table 5. Membership Degrees to the Classes of the Final Partition Produced with Eight Normalized Characteristics

sample	1.1	1.2	2.1	2.2	sample	1.1	1.2	2.1	2.2
H	0.25	0.30	0.22	0.22	Tc	0.21	0.07	0.68	0.05
He	0.25	0.34	0.19	0.21	Ru	0.23	0.10	0.57	0.09
Li	0.37	0.30	0.13	0.20	Rh	0.22	0.09	0.63	0.06
Be	0.39	0.38	0.12	0.11	Pd	0.23	0.08	0.60	0.10
B	0.36	0.25	0.24	0.15	Ag	0.23	0.05	0.34	0.38
C	0.30	0.26	0.28	0.16	Cd	0.36	0.17	0.12	0.36
N	0.14	0.56	0.15	0.15	In	0.31	0.10	0.12	0.47
O	0.17	0.51	0.17	0.16	Sn	0.26	0.06	0.17	0.52
F	0.19	0.45	0.19	0.18	Sb	0.28	0.08	0.30	0.35
Ne	0.25	0.37	0.18	0.20	Te	0.34	0.19	0.19	0.27
Na	0.40	0.23	0.12	0.26	I	0.25	0.41	0.14	0.20
Mg	0.53	0.25	0.08	0.15	Xe	0.30	0.26	0.15	0.29
Al	0.57	0.16	0.11	0.15	Cs	0.27	0.17	0.17	0.40
Si	0.31	0.22	0.27	0.20	Ba	0.26	0.12	0.12	0.50
P	0.07	0.74	0.08	0.11	La	0.19	0.06	0.12	0.63
S	0.09	0.69	0.10	0.12	Ce	0.19	0.06	0.12	0.63
Cl	0.12	0.60	0.14	0.14	Pr	0.18	0.05	0.07	0.69
Ar	0.27	0.37	0.15	0.21	Nd	0.17	0.05	0.05	0.74
K	0.32	0.19	0.15	0.34	Sm	0.18	0.06	0.05	0.72
Ca	0.39	0.16	0.12	0.32	Eu	0.22	0.09	0.09	0.60
Sc	0.47	0.08	0.18	0.28	Gd	0.10	0.03	0.09	0.79
Ti	0.44	0.07	0.25	0.24	Tb	0.08	0.02	0.10	0.80
V	0.42	0.07	0.32	0.19	Dy	0.10	0.03	0.13	0.75
Cr	0.58	0.05	0.19	0.18	Ho	0.08	0.02	0.14	0.75
Mn	0.65	0.06	0.14	0.15	Er	0.09	0.03	0.15	0.73
Fe	0.52	0.08	0.26	0.14	Tm	0.10	0.03	0.18	0.69
Co	0.44	0.08	0.33	0.14	Yb	0.20	0.08	0.08	0.64
Ni	0.42	0.08	0.36	0.14	Lu	0.11	0.03	0.31	0.55
Cu	0.52	0.09	0.24	0.15	Hf	0.16	0.07	0.53	0.24
Zn	0.58	0.30	0.04	0.08	Ta	0.20	0.10	0.50	0.20
Ga	0.56	0.13	0.10	0.21	W	0.22	0.12	0.47	0.19
Ge	0.34	0.14	0.33	0.19	Re	0.21	0.12	0.48	0.19
As	0.36	0.25	0.21	0.18	Os	0.22	0.13	0.47	0.19
Se	0.16	0.62	0.09	0.12	Ir	0.22	0.13	0.47	0.19
Br	0.13	0.61	0.12	0.14	Pt	0.20	0.12	0.48	0.20
Kr	0.29	0.33	0.15	0.23	Au	0.20	0.13	0.43	0.24
Rb	0.29	0.17	0.15	0.38	Hg	0.23	0.18	0.22	0.37
Sr	0.32	0.14	0.12	0.43	Tl	0.19	0.11	0.21	0.49
Y	0.27	0.05	0.16	0.53	Pb	0.19	0.11	0.22	0.49
Zr	0.19	0.04	0.35	0.42	Bi	0.17	0.09	0.24	0.49
Nb	0.23	0.07	0.56	0.15	Th	0.15	0.07	0.39	0.39
Mo	0.23	0.08	0.60	0.10	U	0.18	0.10	0.41	0.31

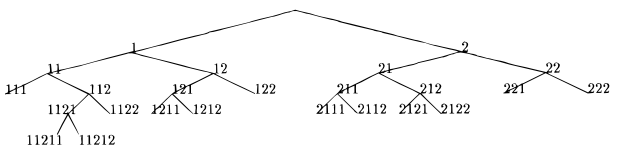

Figure 9. The classification hierarchy produced with seven non-normalized characteristics.

Ce, Th, and U, as well as Be, B, and C. The class 2.2.2, obtained by the division of the class above, gathers the elements with higher fusion and vaporization enthalpies and generally higher densities. These elements are from the period 5 (Nb−Rh) and 6 (Hf−Pt) as well as nonmetals with very high boiling points (B and C). This class has relatively large MDs: Zr (0.42), Th (0.33), U (0.22), Au (0.19), and Pd (0.16). It is interesting that the MD of carbon for this class is only 0.27.

The other class (2.2.1) contains elements with rather various properties, scattered within the periodic system; only their vaporization enthalpies are quite similar. The lowest MD here is that of Be (0.29), followed by Au (0.33). Many other elements outside this class have rather high MDs: Te (0.42), Nb (0.37), La (0.36), Cu (0.30), Ge (0.28), Lu and Sc (0.26), Hf (0.25), Pt (0.24), Ta (0.20), Pa (0.19), B and Mo (0.17), C (0.16).

In class 2.1 there is a separation between the elements of the main groups 1 and 2 (except for Mg) and 13, together with some lanthanides (Pr, Sm, Eu, Tm, Yb, Lu), forming the class 2.1.2, and, on the other hand, the transition metals of period 4, Ag, Cd, La, and other lanthanides, as well as elements of groups 14, 15 (Sb, Bi), and 16 (Te) and Mg, forming the class 2.1.1. Within this latter class, the main-group elements (excepting Sn) are assigned to the class 2.1.1.1, together with Zn, Cd, and Ag (all of them having complete *d*-subshells) and Mn (d^5-configuration). Other elements with important MDs compared to this class are Cu (0.27), Be (0.19), Sn (0.17), Au (0.15), Fe (0.13), etc. The other class (2.1.1.2) takes in Sc, Cr, La, and some lanthanides. An interesting feature of these elements is that they all have the oxidation state +3 (only chromium can also present higher oxidation states). They all have lower electronegativities than the elements of class 2.1.1.1. Elements from outside this class, with significant MDs for it, are Al (0.34), Pr (0.31), followed by Tm (0.25) (all are trivalent elements), and Ag (0.22), Lu and Mn (0.19), Fe (0.18), Ce and Ge (0.15), Ni (0.14), etc.

Within the framework of class 2.1.2, the more electropositive elements of the groups 1 and 2 (without Ca) compose a class (2.1.2.2) to which, to some extent, belong the elements Eu (MD of 0.34), Ca (0.28), Sm (0.25), Yb (0.19), and Cu (0.13). The other class (2.1.2.1) includes the elements of group 13, some lanthanides, and Ca. Elements showing significant MDs for this class are other lanthanides (Er, 0.37; Gd, 0.29; Nd, 0.28) and the elements adjacent to calcium in group 2 (Mg, 0.17; Sr, 0.15).

Using the same **seven characteristics** but **normalized**, the classification obtained is again less deep. The final classification hierarchy is presented in Figure 11. Table 8 shows the membership degrees of the elements to the fuzzy sets of the final fuzzy partition, and Figure 12 shows the successive partitions of the elements produced in this case.

First, the main-group elements are split (class 1), except for those from the middle part of the periodic system, and have just a weak nonmetallic or semimetallic character (B, C, Si, Ge, As, and Sb). Together with them are again classified the elements of group 12 and the four lanthanides Nd, Sm, Eu, and Yb, while all the other elements form the class 2.

Table 6. Membership Degrees to the Classes of the Final Partition Produced with Seven Non-Normalized Characteristics (Part 1)

sample	1.1.1	1.1.2.1.1	1.1.2.1.2	1.1.2.2	1.2.1.1	1.2.1.2	sample	1.1.1	1.1.2.1.1	1.1.2.1.2	1.1.2.2	1.2.1.1	1.2.1.2
H	0.00	0.82	0.01	0.13	0.00	0.00	Tc	0.03	0.00	0.00	0.01	0.00	0.00
He	0.03	0.01	0.01	0.03	0.62	0.00	Ru	0.06	0.01	0.01	0.01	0.00	0.00
Li	0.05	0.00	0.01	0.01	0.00	0.00	Rh	0.04	0.01	0.01	0.01	0.00	0.00
Be	0.12	0.01	0.01	0.02	0.00	0.00	Pd	0.03	0.00	0.00	0.01	0.00	0.00
Be	0.06	0.01	0.01	0.01	0.00	0.00	Ag	0.02	0.00	0.00	0.00	0.00	0.00
C	0.16	0.03	0.03	0.06	0.01	0.02	Cd	0.26	0.01	0.01	0.01	0.00	0.00
N	0.04	0.01	0.00	0.81	0.00	0.01	In	0.02	0.00	0.00	0.00	0.00	0.00
O	0.00	0.79	0.01	0.16	0.00	0.00	Sn	0.00	0.00	0.00	0.00	0.00	0.00
F	0.05	0.04	0.02	0.12	0.00	0.01	Sb	0.11	0.01	0.01	0.01	0.00	0.00
Ne	0.00	0.00	0.00	0.00	0.00	0.72	Te	0.32	0.01	0.01	0.01	0.00	0.00
Na	0.06	0.01	0.01	0.01	0.00	0.00	I	0.66	0.00	0.00	0.00	0.00	0.00
Mg	0.08	0.00	0.01	0.01	0.00	0.00	Xe	0.41	0.07	0.36	0.10	0.00	0.00
Al	0.01	0.00	0.00	0.00	0.00	0.00	Cs	0.08	0.01	0.01	0.02	0.00	0.01
Si	0.09	0.00	0.01	0.01	0.00	0.00	Ba	0.05	0.00	0.01	0.01	0.00	0.00
P	0.73	0.01	0.03	0.02	0.00	0.00	La	0.02	0.00	0.00	0.00	0.00	0.00
S	0.65	0.00	0.00	0.00	0.00	0.00	Ce	0.01	0.00	0.00	0.00	0.00	0.00
Cl	0.06	0.12	0.78	0.02	0.00	0.00	Pr	0.01	0.00	0.00	0.00	0.00	0.00
Ar	0.08	0.07	0.04	0.43	0.00	0.01	Nd	0.01	0.00	0.00	0.00	0.00	0.00
K	0.08	0.01	0.01	0.01	0.00	0.00	Sm	0.03	0.00	0.00	0.01	0.00	0.00
Ca	0.04	0.00	0.00	0.01	0.00	0.00	Eu	0.04	0.00	0.00	0.01	0.00	0.00
Sc	0.00	0.00	0.00	0.00	0.00	0.00	Gd	0.01	0.00	0.00	0.00	0.00	0.00
Ti	0.01	0.00	0.00	0.00	0.00	0.00	Tb	0.00	0.00	0.00	0.00	0.00	0.00
V	0.01	0.00	0.00	0.00	0.00	0.00	Dy	0.00	0.00	0.00	0.00	0.00	0.00
Cr	0.00	0.00	0.00	0.00	0.00	0.00	Ho	0.00	0.00	0.00	0.00	0.00	0.00
Mn	0.02	0.00	0.00	0.00	0.00	0.00	Er	0.01	0.00	0.00	0.00	0.00	0.00
Fe	0.01	0.00	0.00	0.00	0.00	0.00	Tm	0.01	0.00	0.00	0.00	0.00	0.00
Co	0.02	0.00	0.00	0.00	0.00	0.00	Yb	0.04	0.00	0.00	0.01	0.00	0.00
Ni	0.01	0.00	0.00	0.00	0.00	0.00	Lu	0.02	0.00	0.00	0.00	0.00	0.00
Cu	0.01	0.00	0.00	0.00	0.00	0.00	Hf	0.05	0.01	0.01	0.01	0.00	0.01
Zn	0.32	0.01	0.01	0.01	0.00	0.00	Ta	0.07	0.01	0.01	0.02	0.01	0.01
Ga	0.03	0.00	0.00	0.00	0.00	0.00	W	0.09	0.01	0.02	0.03	0.01	0.01
Ge	0.03	0.00	0.00	0.00	0.00	0.00	Re	0.07	0.01	0.01	0.02	0.00	0.01
As	0.56	0.00	0.00	0.00	0.00	0.00	Os	0.09	0.01	0.02	0.03	0.01	0.01
Se	0.51	0.00	0.01	0.01	0.00	0.00	Ir	0.10	0.02	0.02	0.03	0.01	0.01
Br	0.56	0.06	0.21	0.08	0.00	0.00	Pt	0.08	0.01	0.01	0.02	0.00	0.00
Kr	0.01	0.22	0.03	0.67	0.00	0.00	Au	0.10	0.01	0.01	0.01	0.00	0.00
Rb	0.08	0.01	0.01	0.01	0.00	0.01	Hg	0.63	0.00	0.00	0.00	0.00	0.00
Sr	0.05	0.00	0.01	0.01	0.00	0.00	Tl	0.04	0.00	0.00	0.01	0.00	0.00
Y	0.01	0.00	0.00	0.00	0.00	0.00	Pb	0.04	0.00	0.00	0.00	0.00	0.00
Zr	0.02	0.00	0.00	0.01	0.00	0.00	Bi	0.07	0.00	0.01	0.01	0.00	0.00
Nb	0.03	0.00	0.00	0.001	0.00	0.00	Th	0.03	0.00	0.00	0.01	0.00	0.00
Mo	0.03	0.00	0.01	0.01	0.00	0.00	U	0.02	0.00	0.00	0.00	0.00	0.00

In what follows the first class is divided into a set of nonmetals together with Be, but without Xe, and another set containing the metals and Xe. From the second class are separated: on the one hand refractary and heavy elements−transition metals of the periods 6 (Hf−Au) and 5 (Nb−Pd), Th, U, as well as Co, Ni and the nonmetals of the group 13 (B) and 14 (C−Ge). On the other hand, we have the elements of group 3 (Sc−La) and most of the lanthanides, Ti, Zr, V, As, and Sb.

From the discussion above it is obvious that our classification, even if based exclusively on physical properties, is not inconsistent with the chemical behavior of the elements and with the predictions based on electronic structure. The effects of an explicit introduction of such chemical properties and of some features of the electron configuration are dealt with in the following sections of this paper.

3.4. Introduction of Chemical and Structural Features. In order to pass beyond the limits of this "physical" classification of elements, we try here to base the classification on some chemical properties and features of the electronic structure. We have thus kept only five physical properties (density, melting point, boiling point, ionization energy, covalent radius), and, in exchange, five other chemical characteristics were added: two indices to describe the electron configuration, two others to describe the oxidation states, and the free formation energy for chlorides. For the characterization of electron configuration and oxidation states we used numbers having the same amount of digits. For the **electron configuration** the first index is built as follows: the first digit gives the number of electrons in the last (outermost) shell (1...8), the next two digits give the number of electrons in the last except for one shell (0...18), and the two decimal digits give the number of electrons in the last except for two shells (0...32). For example, for chromium this index is 113.08. The second index of electron configuration has as its first digit the number of electron shells in the atom (1...7), the next two digits give the number of *d*-electrons in the last except for one shell (1...10), and the two decimal digits give the number of *f*-electrons in the last except for two shells (1...14). For example, for Cr this index is 405.00 and for Gd is 601.07.

The index for positive **oxidation states** contains the digits which show these states, in the order of their importance, the most usual one being the most significant digit. Similarly, in order to describe the negative oxidation states a negative number was used, whose digits represent the oxidation states in the decreasing order of their importance.

In order to characterize the **chemical reactivity** of an element, the free formation energy ΔF_O of its oxide and ΔF_{Cl}

Table 7. Membership Degrees to the Classes of the Final Partition Produced with Seven Non-Normalized Characteristics (Part 2)

sample	1.2.2	2.1.1.1	2.1.1.2	2.1.2.1	2.1.2.2	2.2.1	2.2.2	sample	1.2.2	2.1.1.1	2.1.1.2	2.1.2.1	2.1.2.2	2.2.1	2.2.2
H	0.03	0.00	0.00	0.00	0.00	0.00	0.00	Tc	0.01	0.00	0.00	0.00	0.00	0.42	0.53
He	0.03	0.04	0.03	0.03	0.03	0.07	0.07	Ru	0.02	0.02	0.03	0.02	0.01	0.04	0.77
Li	0.01	0.02	0.03	0.01	0.75	0.07	0.03	Rh	0.01	0.01	0.01	0.00	0.00	0.09	0.81
Be	0.02	0.19	0.09	0.06	0.03	0.29	0.16	Pd	0.01	0.10	0.11	0.03	0.02	0.53	0.16
B	0.01	0.02	0.03	0.01	0.01	0.17	0.66	Ag	0.00	0.55	0.22	0.02	0.01	0.14	0.03
C	0.07	0.06	0.06	0.04	0.03	0.16	0.27	Cd	0.02	0.25	0.06	0.10	0.07	0.13	0.07
N	0.12	0.00	0.00	0.00	0.00	0.00	0.00	In	0.00	0.02	0.06	0.76	0.07	0.04	0.01
O	0.03	0.00	0.00	0.00	0.00	0.00	0.00	Sn	0.00	0.17	0.58	0.01	0.01	0.19	0.03
F	0.65	0.02	0.01	0.01	0.01	0.03	0.03	Sb	0.01	0.41	0.05	0.09	0.05	0.18	0.08
Ne	0.05	0.03	0.03	0.03	0.02	0.06	0.06	Te	0.02	0.20	0.07	0.10	0.08	0.12	0.06
Na	0.01	0.04	0.06	0.04	0.62	0.09	0.04	I	0.02	0.08	0.04	0.04	0.04	0.07	0.05
Mg	0.01	0.42	0.08	0.17	0.10	0.09	0.03	Xe	0.00	0.01	0.01	0.01	0.01	0.01	0.01
Al	0.00	0.05	0.34	0.41	0.10	0.07	0.02	Cs	0.02	0.07	0.09	0.13	0.36	0.13	0.07
Si	0.01	0.48	0.04	0.11	0.06	0.13	0.05	Ba	0.01	0.02	0.04	0.02	0.73	0.07	0.03
P	0.01	0.05	0.02	0.03	0.02	0.05	0.03	La	0.00	0.05	0.20	0.15	0.08	0.36	0.12
S	0.02	0.08	0.04	0.04	0.04	0.07	0.05	Ce	0.00	0.04	0.17	0.04	0.02	0.70	0.02
Cl	0.01	0.00	0.00	0.00	0.00	0.00	0.00	Pr	0.00	0.05	0.31	0.28	0.11	0.19	0.05
Ar	0.32	0.01	0.01	0.01	0.01	0.01	0.01	Nd	0.00	0.03	0.53	0.28	0.06	0.06	0.01
K	0.02	0.06	0.08	0.12	0.43	0.11	0.06	Sm	0.01	0.01	0.01	0.62	0.25	0.05	0.02
Ca	0.01	0.03	0.04	0.54	0.28	0.03	0.01	Eu	0.01	0.00	0.00	0.53	0.34	0.04	0.02
Sc	0.00	0.03	0.49	0.13	0.05	0.26	0.04	Gd	0.00	0.04	0.46	0.29	0.08	0.10	0.02
Ti	0.00	0.02	0.05	0.02	0.01	0.79	0.09	Tb	0.00	0.00	0.77	0.09	0.02	0.09	0.02
V	0.00	0.02	0.06	0.02	0.01	0.77	0.09	Dy	0.00	0.02	0.82	0.06	0.02	0.07	0.01
Cr	0.00	0.00	0.73	0.08	0.02	0.14	0.02	Ho	0.00	0.04	0.82	0.03	0.01	0.08	0.02
Mn	0.00	0.63	0.19	0.04	0.02	0.07	0.02	Er	0.00	0.04	0.43	0.37	0.07	0.06	0.01
Fe	0.00	0.13	0.18	0.04	0.02	0.53	0.08	Tm	0.00	0.05	0.25	0.69	0.06	0.02	0.01
Co	0.00	0.06	0.11	0.03	0.01	0.68	0.08	Yb	0.01	0.04	0.05	0.63	0.19	0.03	0.01
Ni	0.00	0.07	0.14	0.03	0.01	0.69	0.05	Lu	0.01	0.06	0.19	0.20	0.13	0.26	0.12
Cu	0.00	0.27	0.31	0.03	0.01	0.30	0.06	Hf	0.02	0.04	0.08	0.05	0.04	0.25	0.43
Zn	0.02	0.22	0.06	0.08	0.06	0.14	0.17	Ta	0.03	0.04	0.07	0.05	0.04	0.20	0.45
Ga	0.01	0.01	0.02	0.85	0.04	0.02	0.01	W	0.04	0.04	0.06	0.04	0.03	0.14	0.49
Ge	0.00	0.39	0.15	0.05	0.02	0.28	0.08	Re	0.02	0.03	0.04	0.02	0.02	0.06	0.70
As	0.02	0.11	0.05	0.06	0.05	0.09	0.06	Os	0.03	0.04	0.05	0.03	0.02	0.12	0.54
Se	0.02	0.12	0.05	0.07	0.06	0.09	0.06	Ir	0.03	0.04	0.05	0.03	0.02	0.15	0.50
Br	0.00	0.02	0.01	0.01	0.01	0.02	0.02	Pt	0.02	0.04	0.05	0.02	0.02	0.24	0.48
Kr	0.06	0.00	0.00	0.00	0.00	0.00	0.00	Au	0.01	0.15	0.09	0.05	0.03	0.33	0.19
Rb	0.02	0.06	0.09	0.13	0.40	0.12	0.06	Hg	0.02	0.09	0.04	0.04	0.04	0.08	0.05
Sr	0.01	0.01	0.02	0.16	0.65	0.05	0.02	Tl	0.01	0.03	0.05	0.63	0.19	0.03	0.01
Y	0.00	0.04	0.24	0.07	0.03	0.56	0.05	Pb	0.01	0.54	0.10	0.14	0.06	0.07	0.02
Zr	0.01	0.01	0.01	0.01	0.00	0.50	0.42	Bi	0.01	0.55	0.02	0.10	0.06	0.13	0.05
Nb	0.01	0.01	0.02	0.01	0.01	0.37	0.52	Th	0.01	0.04	0.09	0.06	0.04	0.38	0.33
Mo	0.01	0.01	0.01	0.00	0.00	0.17	0.74	U	0.01	0.04	0.12	0.07	0.04	0.46	0.22

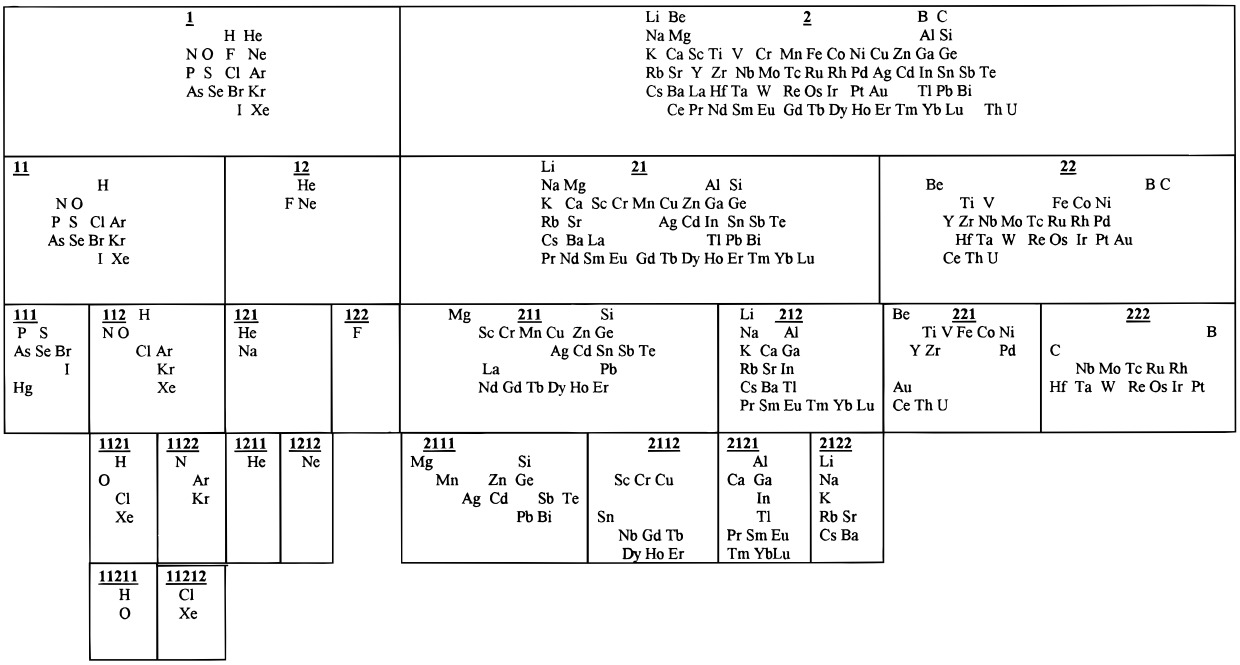

Figure 10. The classification of the elements produced with seven non-normalized characteristics.

of its chloride were taken into account. The values were computed for the standard ambient temperature and pressure (298 K, 1 bar) in kcal per mol of O, respectively, per mol of Cl. The correlation of these values is rather weak; the

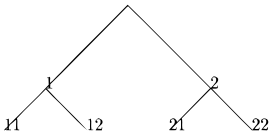

Figure 11. The classification hierarchy obtained with seven normalized characteristics.

Table 8. Membership Degrees to the Classes of the Final Partition Produced with Seven Normalized Characteristics

sample	1.1	1.2	2.1	2.2	sample	1.1	1.2	2.1	2.2
H	0.24	0.29	0.24	0.23	Tc	0.09	0.05	0.02	0.83
He	0.24	0.33	0.24	0.19	Ru	0.14	0.09	0.09	0.68
Li	0.40	0.26	0.23	0.11	Rh	0.12	0.08	0.05	0.75
Be	0.25	0.36	0.24	0.15	Pd	0.11	0.07	0.19	0.63
B	0.19	0.20	0.25	0.36	Ag	0.24	0.09	0.48	0.19
C	0.18	0.22	0.22	0.37	Cd	0.59	0.20	0.17	0.04
N	0.11	0.51	0.21	0.17	In	0.56	0.09	0.28	0.07
O	0.13	0.47	0.21	0.18	Sn	0.47	0.09	0.37	0.07
F	0.16	0.42	0.22	0.21	Sb	0.26	0.13	0.44	0.18
Ne	0.23	0.35	0.23	0.18	Te	0.31	0.30	0.26	0.12
Na	0.55	0.15	0.23	0.07	I	0.16	0.57	0.18	0.09
Mg	0.66	0.16	0.14	0.03	Xe	0.38	0.29	0.23	0.11
Al	0.45	0.16	0.30	0.09	Cs	0.40	0.16	0.29	0.15
Si	0.22	0.20	0.27	0.31	Ba	0.47	0.11	0.31	0.11
P	0.06	0.71	0.15	0.08	La	0.41	0.06	0.42	0.12
S	0.07	0.65	0.18	0.11	Ce	0.43	0.06	0.40	0.11
Cl	0.09	0.55	0.20	0.15	Pr	0.45	0.04	0.41	0.09
Ar	0.28	0.36	0.22	0.14	Nd	0.50	0.03	0.40	0.07
K	0.45	0.15	0.28	0.12	Sm	0.53	0.03	0.38	0.06
Ca	0.56	0.09	0.28	0.07	Eu	0.50	0.07	0.34	0.09
Sc	0.36	0.06	0.49	0.09	Gd	0.30	0.03	0.57	0.10
Ti	0.19	0.06	0.53	0.22	Tb	0.26	0.03	0.61	0.10
V	0.12	0.05	0.45	0.39	Dy	0.27	0.04	0.58	0.11
Cr	0.21	0.07	0.56	0.16	Ho	0.24	0.03	0.61	0.11
Mn	0.32	0.12	0.45	0.11	Er	0.24	0.04	0.60	0.13
Fe	0.11	0.06	0.47	0.37	Tm	0.25	0.04	0.57	0.14
Co	0.08	0.04	0.37	0.50	Yb	0.62	0.03	0.30	0.05
Ni	0.07	0.04	0.31	0.58	Lu	0.18	0.04	0.50	0.28
Cu	0.17	0.10	0.45	0.29	Hf	0.16	0.07	0.22	0.55
Zn	0.51	0.40	0.08	0.02	Ta	0.18	0.10	0.18	0.54
Ga	0.60	0.14	0.21	0.05	W	0.18	0.13	0.18	0.50
Ge	0.19	0.13	0.29	0.38	Re	0.18	0.13	0.18	0.51
As	0.23	0.27	0.28	0.22	Os	0.18	0.14	0.18	0.50
Se	0.10	0.65	0.16	0.09	Ir	0.18	0.14	0.18	0.50
Br	0.08	0.60	0.19	0.13	Pt	0.18	0.13	0.18	0.51
Kr	0.31	0.34	0.22	0.13	Au	0.20	0.16	0.23	0.42
Rb	0.43	0.15	0.29	0.13	Hg	0.34	0.29	0.24	0.13
Sr	0.50	0.10	0.30	0.10	Tl	0.42	0.13	0.32	0.12
Y	0.38	0.05	0.48	0.09	Pb	0.44	0.14	0.31	0.11
Zr	0.19	0.05	0.49	0.27	Bi	0.40	0.12	0.37	0.10
Nb	0.12	0.06	0.18	0.63	Th	0.17	0.05	0.34	0.43
Mo	0.23	0.07	0.10	0.71	U	0.20	0.10	0.26	0.44

equation of their linear correlation is

$$|\Delta F_O| = (22 \pm 7t) + (1.23 \pm 0.13t)|\Delta F_{Cl}|, \quad r = 0.765$$

where t is the Student parameter and r is the correlation coefficient. Finally, the free formation energy of the chlorides per mol of Cl has been kept as a characteristic for classification, due to the larger amount of available data.

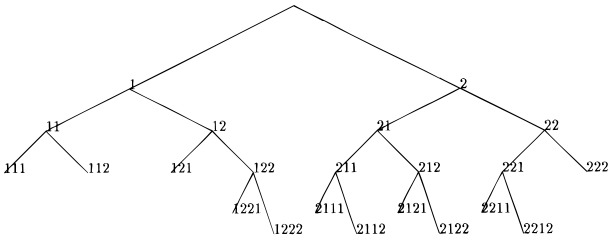

Figure 13. The classification hierarchy produced with non-normalized characteristics.

3.5. Classifications Based on 10 Physical, Chemical, and Structural Properties. The classification hierarchy produced by using the 10 properties mentioned above is presented in Figure 13. Tables 9 and 10 show the membership degrees of the elements to the fuzzy sets of the final fuzzy partition, and Figure 14 shows the successive partitions of the elements produced in this case.

It is interesting to see that the first separation in two classes is the same with that at the classification based on the 10 physical properties: class 1 contains as a whole elements of the main groups of the periodic system and class 2 elements of the secondary groups and most of the lanthanides. Silver is situated just at the boundary of the two classes (membership degree, MD of 0.50086 to class 1). The lanthanides with $4f^6$ and $4f^{13}$ configurations (Sm, Tm) also have small MDs for class 1 (0.63 and 0.57). Other elements having MDs of less than 0.7 for this class are Sn and Ga. On the other hand, the MD of Al for class 2 is small (0.534). Mn also comes near class 1 (MD of 0.44), due to its relatively stable electron configuration $4s^23d^5$. As an average, the elements of class 1 have lower densities and clearly lower melting and boiling points, more electrons in the outermost shell (the elements in class 2 generally have two such electrons), an average of four shells, against five in class 2, lower positive oxidation states and a greater trend to negative oxidation states.

The next division of class 1 is again as a matter of fact the same as for the 10 physical properties classification (class 1.1, metals; class 1.2, nonmetals plus K, Rb, Cs, and Hg). The single difference is the position of cadmium in the class 1.1 (with zinc) and not in the class 1.2 (with mercury). The alkali metals as well as selenium lie near the limit between the classes. As an average, class 1.2 contains lighter elements having high ionization energies, more electrons in the last shell, a stronger trend toward negative oxidation states, and a smaller affinity for chlorine. In class 1.1 but near the boundary of class 1.2 are situated As, Cd, and Na.

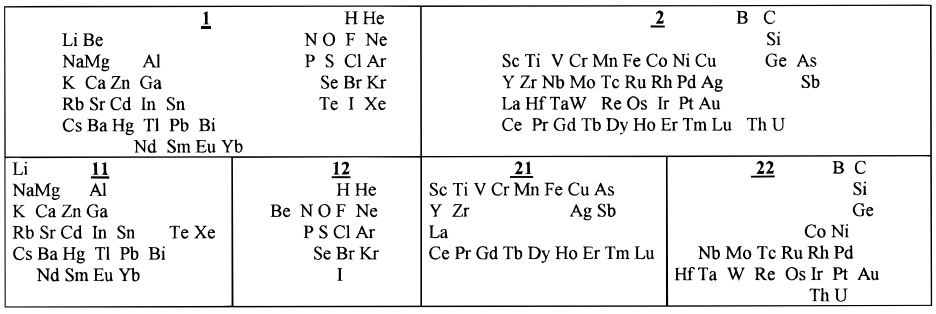

Figure 12. The classification of the elements produced with seven normalized characteristics.

Table 9. Membership Degrees to the Classes of the Final Partition Produced with Non-Normalized Characteristics (Part 1)

sample	1.1.1	1.1.2	1.2.1	1.2.2.1	1.2.2.2	2.1.1.1	sample	1.1.1	1.1.2	1.2.1	1.2.2.1	1.2.2.2	2.1.1.1
H	0.06	0.03	0.22	0.51	0.10	0.02	Tc	0.01	0.01	0.00	0.00	0.00	0.07
He	0.06	0.04	0.18	0.50	0.14	0.02	Ru	0.03	0.04	0.02	0.01	0.01	0.01
Li	0.59	0.21	0.10	0.02	0.02	0.02	Rh	0.01	0.02	0.01	0.00	0.00	0.04
Be	0.04	0.09	0.02	0.01	0.01	0.26	Pd	0.01	0.01	0.00	0.00	0.00	0.08
B	0.05	0.08	0.02	0.01	0.01	0.13	Ag	0.10	0.35	0.04	0.01	0.01	0.19
C	0.05	0.06	0.03	0.01	0.01	0.02	Cd	0.47	0.09	0.37	0.04	0.03	0.00
N	0.04	0.02	0.27	0.40	0.19	0.02	In	0.22	0.47	0.06	0.01	0.01	0.08
O	0.03	0.02	0.04	0.31	0.53	0.02	Sn	0.17	0.39	0.06	0.02	0.02	0.13
F	0.03	0.03	0.03	0.13	0.72	0.02	Sb	0.44	0.42	0.04	0.01	0.01	0.02
Ne	0.05	0.03	0.06	0.14	0.64	0.02	Te	0.57	0.16	0.20	0.02	0.03	0.01
Na	0.46	0.11	0.32	0.05	0.04	0.00	I	0.09	0.04	0.58	0.11	0.12	0.01
Mg	0.73	0.13	0.08	0.01	0.01	0.01	Xe	0.04	0.02	0.10	0.09	0.68	0.01
Al	0.10	0.30	0.04	0.01	0.01	0.23	Cs	0.30	0.10	0.45	0.07	0.06	0.01
Si	0.05	0.10	0.02	0.01	0.01	0.22	Ba	0.06	0.75	0.01	0.00	0.00	0.05
P	0.06	0.02	0.74	0.08	0.07	0.01	La	0.02	0.04	0.01	0.00	0.00	0.31
S	0.12	0.05	0.71	0.05	0.04	0.01	Ce	0.03	0.05	0.02	0.01	0.01	0.31
Cl	0.06	0.03	0.41	0.23	0.21	0.01	Pr	0.03	0.07	0.02	0.01	0.01	0.52
Ar	0.04	0.02	0.04	0.03	0.80	0.02	Nd	0.03	0.07	0.02	0.01	0.01	0.64
K	0.35	0.10	0.42	0.06	0.05	0.00	Sm	0.10	0.47	0.04	0.01	0.01	0.12
Ca	0.29	0.55	0.02	0.00	0.00	0.04	Eu	0.24	0.60	0.02	0.00	0.00	0.04
Sc	0.03	0.07	0.02	0.01	0.01	0.04	Gd	0.02	0.04	0.01	0.00	0.00	0.48
Ti	0.00	0.01	0.00	0.00	0.00	0.05	Tb	0.03	0.07	0.02	0.01	0.01	0.20
V	0.00	0.00	0.00	0.00	0.00	0.03	Dy	0.05	0.11	0.02	0.01	0.01	0.14
Cr	0.04	0.06	0.02	0.01	0.01	0.14	Ho	0.05	0.10	0.02	0.01	0.01	0.11
Mn	0.11	0.27	0.04	0.01	0.01	0.17	Er	0.02	0.04	0.01	0.00	0.00	0.13
Fe	0.02	0.03	0.01	0.00	0.00	0.15	Tm	0.16	0.32	0.06	0.02	0.02	0.11
Co	0.02	0.04	0.01	0.00	0.00	0.10	Yb	0.26	0.59	0.02	0.00	0.00	0.04
Ni	0.04	0.08	0.02	0.01	0.01	0.04	Lu	0.00	0.01	0.00	0.00	0.00	0.04
Cu	0.06	0.16	0.03	0.01	0.01	0.35	Hf	0.03	0.05	0.02	0.01	0.01	0.01
Zn	0.65	0.07	0.21	0.03	0.02	0.00	Ta	0.04	0.05	0.03	0.01	0.01	0.00
Ga	0.21	0.38	0.07	0.02	0.02	0.11	W	0.05	0.06	0.04	0.02	0.02	0.01
Ge	0.06	0.13	0.03	0.01	0.01	0.37	Re	0.05	0.06	0.04	0.01	0.02	0.01
As	0.34	0.16	0.34	0.05	0.05	0.01	Os	0.04	0.05	0.03	0.01	0.01	0.00
Se	0.26	0.10	0.55	0.03	0.03	0.01	Ir	0.03	0.04	0.02	0.01	0.01	0.00
Br	0.02	0.01	0.17	0.16	0.60	0.01	Pt	0.02	0.02	0.01	0.00	0.00	0.05
Kr	0.04	0.02	0.06	0.04	0.78	0.02	Au	0.04	0.07	0.02	0.01	0.01	0.65
Rb	0.30	0.09	0.47	0.07	0.06	0.00	Hg	0.09	0.04	0.64	0.11	0.09	0.01
Sr	0.38	0.49	0.02	0.00	0.00	0.03	Tl	0.55	0.33	0.03	0.01	0.01	0.02
Y	0.02	0.04	0.01	0.00	0.00	0.11	Pb	0.24	0.57	0.03	0.01	0.01	0.04
Zr	0.00	0.00	0.00	0.00	0.00	0.02	Bi	0.42	0.43	0.04	0.01	0.01	0.03
Nb	0.01	0.02	0.01	0.00	0.00	0.08	Th	0.00	0.00	0.00	0.00	0.00	0.05
Mo	0.04	0.05	0.03	0.01	0.01	0.00	U	0.01	0.02	0.01	0.00	0.00	0.15

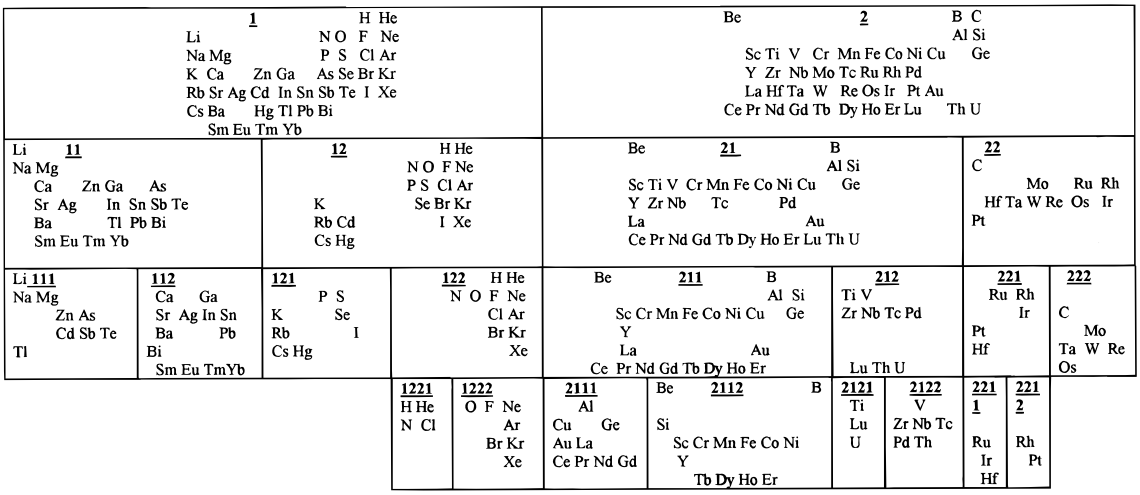

Figure 14. The classification of the elements produced with non-normalized physical, chemical, and structural characteristics.

Class 1.2 is further divided in the same way as for the 10 physical properties classification. Class 1.2.2 includes gaseous elements, with low densities, high ionization energies, smaller atomic radii, more electrons on the outermost shell, and weaker trends to positive oxidation states and to combine with chlorine. Chlorine itself is situated near the boundary of the class 1.2.1. The MD for this class is mainly determined by the physical properties. Typical elements for this class are S and Se. Significant MDs for it also have Cl, As, and Na.

While class 1.2.1 is not further divided here, class 1.2.2 is split up in a different manner than at the classification based on physical properties: on the one hand, H, He, N, and Cl (1.2.2.1) and, on the other hand, the noble gases from

Table 10. Membership Degrees to the Classes of the Final Partition Produced with Non-Normalized Characteristics (Part 2)

sample	2.1.1.2	2.1.2.1	2.1.2.2	2.2.1.1	2.2.1.2	2.2.2	sample	2.1.1.2	2.1.2.1	2.1.2.2	2.2.1.1	2.2.1.2	2.2.2
H	0.02	0.01	0.01	0.01	0.01	0.01	Tc	0.10	0.16	0.48	0.03	0.08	0.05
He	0.02	0.01	0.01	0.01	0.01	0.01	Ru	0.01	0.01	0.01	0.74	0.06	0.07
Li	0.01	0.01	0.01	0.00	0.00	0.00	Rh	0.04	0.08	0.13	0.02	0.59	0.05
Be	0.45	0.06	0.03	0.00	0.01	0.01	Pd	0.07	0.26	0.33	0.02	0.16	0.05
B	0.34	0.16	0.14	0.02	0.03	0.02	Ag	0.18	0.06	0.04	0.01	0.02	0.01
C	0.03	0.03	0.04	0.16	0.08	0.46	Cd	0.00	0.00	0.00	0.00	0.00	0.00
N	0.02	0.01	0.01	0.00	0.01	0.01	In	0.06	0.04	0.02	0.01	0.01	0.01
O	0.02	0.01	0.01	0.00	0.01	0.01	Sn	0.09	0.06	0.04	0.01	0.02	0.02
F	0.02	0.01	0.01	0.00	0.01	0.01	Sb	0.02	0.01	0.01	0.00	0.00	0.01
Ne	0.02	0.01	0.01	0.01	0.01	0.01	Te	0.00	0.00	0.00	0.00	0.00	0.00
Na	0.00	0.00	0.00	0.00	0.00	0.00	I	0.01	0.01	0.01	0.00	0.00	0.00
Mg	0.01	0.01	0.00	0.00	0.00	0.00	Xe	0.01	0.01	0.01	0.00	0.01	0.01
Al	0.15	0.07	0.04	0.01	0.02	0.01	Cs	0.00	0.00	0.00	0.00	0.00	0.00
Si	0.39	0.10	0.06	0.01	0.01	0.01	Ba	0.05	0.03	0.02	0.01	0.01	0.01
P	0.01	0.01	0.00	0.00	0.00	0.00	La	0.12	0.30	0.13	0.01	0.03	0.02
S	0.01	0.00	0.00	0.00	0.00	0.00	Ce	0.12	0.26	0.12	0.01	0.04	0.02
Cl	0.01	0.01	0.01	0.00	0.01	0.01	Pr	0.08	0.17	0.06	0.01	0.01	0.01
Ar	0.02	0.01	0.01	0.00	0.01	0.01	Nd	0.04	0.12	0.04	0.00	0.01	0.01
K	0.00	0.00	0.00	0.00	0.00	0.00	Sm	0.14	0.05	0.03	0.01	0.01	0.01
Ca	0.04	0.02	0.01	0.00	0.01	0.01	Eu	0.04	0.02	0.01	0.00	0.01	0.01
Sc	0.74	0.05	0.03	0.00	0.01	0.00	Gd	0.33	0.09	0.02	0.00	0.00	0.00
Ti	0.08	0.62	0.22	0.00	0.01	0.01	Tb	0.64	0.02	0.01	0.00	0.00	0.00
V	0.04	0.09	0.73	0.02	0.05	0.03	Dy	0.60	0.04	0.02	0.00	0.01	0.01
Cr	0.37	0.17	0.14	0.01	0.02	0.02	Ho	0.62	0.05	0.02	0.00	0.01	0.01
Mn	0.22	0.07	0.05	0.01	0.02	0.02	Er	0.67	0.08	0.03	0.00	0.00	0.00
Fe	0.55	0.18	0.05	0.00	0.00	0.00	Tm	0.16	0.06	0.05	0.01	0.02	0.02
Cu	0.71	0.07	0.03	0.00	0.00	0.00	Yb	0.04	0.02	0.01	0.00	0.01	0.01
Ni	0.76	0.03	0.01	0.00	0.01	0.00	Lu	0.05	0.71	0.16	0.01	0.02	0.01
Cu	0.28	0.05	0.02	0.01	0.01	0.01	Hf	0.01	0.01	0.01	0.50	0.07	0.27
Zn	0.00	0.00	0.00	0.00	0.00	0.00	Ta	0.00	0.00	0.01	0.02	0.00	0.82
Ga	0.07	0.05	0.03	0.01	0.02	0.02	W	0.01	0.02	0.02	0.06	0.02	0.67
Ge	0.18	0.11	0.06	0.01	0.02	0.01	Re	0.01	0.01	0.02	0.05	0.01	0.71
As	0.01	0.01	0.01	0.00	0.00	0.00	Os	0.00	0.00	0.01	0.01	0.00	0.82
Se	0.00	0.00	0.00	0.00	0.00	0.00	Ir	0.00	0.00	0.00	0.50	0.02	0.35
Br	0.01	0.01	0.01	0.00	0.00	0.00	Pt	0.05	0.10	0.15	0.02	0.51	0.07
Kr	0.02	0.01	0.01	0.00	0.01	0.01	Au	0.06	0.10	0.04	0.00	0.01	0.01
Rb	0.00	0.00	0.00	0.00	0.00	0.00	Hg	0.01	0.00	0.00	0.00	0.00	0.00
Sr	0.03	0.02	0.01	0.00	0.01	0.01	Tl	0.02	0.01	0.01	0.00	0.00	0.00
Y	0.70	0.09	0.03	0.00	0.00	0.00	Pb	0.04	0.02	0.02	0.00	0.01	0.01
Zr	0.02	0.03	0.81	0.02	0.07	0.03	Bi	0.02	0.01	0.01	0.00	0.01	0.01
Nb	0.13	0.17	0.35	0.05	0.10	0.07	Th	0.05	0.20	0.46	0.03	0.15	0.05
Mo	0.00	0.00	0.01	0.15	0.02	0.67	U	0.10	0.32	0.24	0.03	0.08	0.04

Ne to Xe, F, Br, and O (class 1.2.2.2). The former class generally contains lighter elements, with lower melting and boiling points (except for chlorine, which is placed near the limit of the class), with less electrons in the outermost shell and a marked trend for combinations in positive oxidation states (the elements in class 1.2.2.2 almost have no positive states). From class 1.2.2.2, oxygen is nearest to the class 1.2.2.1. The separation between the two classes is not a clearly cut one, except for the noble gases from Ne to Xe.

Class 1.1 is divided as for the 10 physical characteristics classification, with the difference that Ca, Sr, Ba, Bi, Eu, and Yb join to Ga, In, Sn, Pb, Ag, Sm, and Tm. Therefore, class 1.1.1 includes only main-group elements and some elements of group 12 (Zn, Cd). Bi, Sb, and Sr lie near the boundary of the two classes. Significant MDs for class 1.1.1 also have the other elements of group 1 (K, Rb) and 2 (Ca, Sr) as well as As, Os, Se, Yb, Eu, In, Ga, and Sn and for class 1.1.2 belong to some extent Tl, Al, Mn, Li, Cu, As, Ge, and Mg.

Class 2 is also divided as in the previous classification. In class 2.2 the reactivity of the elements toward chlorine is a little lower than average. Among its elements, Pt and Rh are close to the boundary of class 2.1, while Nb, Pd, and Th of this latter class have significant MDs for this class, too.

Nor does the next separation of class 2.2 bring anything new against the "physical" classification. The elements of class 2.2.2 show positive oxidation states higher on average as compared to those of the elements of class 2.2.1. Near the border of the two classes lie C and Ir, followed by Mo and Hf.

The last division of class 2.2.1 is also identical to that obtained at the "physical" classification. The elements of class 2.2.1.1 (Ru, Hf, and Ir) have a higher affinity toward chlorine than those of class 2.2.1.2 (Rh and Pt). To the former class are related to some extent Mo and C and to the latter Pd, Th, and Nb.

The division of class 2.1 is again the same as before. The elements of class 2.1.2, heavier, with higher melting and boiling points, also have a little higher positive oxidation states. Unlike in the previous classification, three elements from this class (Ti, Lu, and U) are separated (class 2.1.2.1) from the other six (Zr, V, Nb, Tc, Pd, and Th), on the basis of some lower melting and boiling points, lower ionization energies and positive oxidation states (with an average of 4 against 5 for the other class), and of the greater affinities against chlorine. Actually, U on one side and Pd on the other are near the border of the classes, while Nb, Th, and Tc are also attracted to a certain extent to class 2.1.2.1. Other elements, as well, have significant MDs for this class: La, Ce, Pr, Cr, and Fe, while elements that belong somehow to class 2.1.2.2 are Pt, Ti, Lu, Cr, La, Ce, and Rh.

Table 11. Similarity Degrees between Some Elements in the Final Partition with Non-Normalized Characteristics

class 111	class 112	class 121	class 2111	class 2121
Na−Cd 0.055	Eu−Yb 0.021	Rb−Cs 0.017	La−Ce 0.040	Ti−Lu 0.114
Zn−Te 0.117	Yb−Pb 0.023	K−Cs 0.058	Au−Nd 0.069	
Na−As 0.122	Eu−Pb 0.031	K−Rb 0.077	Cu−Ge 0.128	class 2122
Sb−Tl 0.142	Sn−Ga 0.053	I−Hg 0.081	Nd−Pr 0.136	
Li−Tl 0.147	Ca−Yb 0.060	P−S 0.101	Cu−Gd 0.190	Tc−Th 0.092
Li−Mg 0.155	K−Pb 0.061	Se−Rb 0.103	Al−Cu 0.228	V−Zr 0.105
	K−Eu 0.078	P−Hg 0.108	Cu−Au 0.411	Nb−Pd 0.130
different classes	Sr−Bi 0.079	Se−Cs 0.117		Tc−Nd 0.136
	Sn−Tm 0.105	S−Hg 0.135	class 2112	Pd−Th 0.154
Sb−Bi 0.029	Ga−In 0.106			Tb−Th 0.155
Al−Ag 0.081	Ag−Tm 0.107	class 1221	Co−Y 0.019	
Mn−Ag 0.092	Ca−Sr 0.112		Sc−Ni 0.031	class 2211
Mn−Tm 0.119	Sn−In 0.115	H−He 0.062	Dy−Ho 0.033	
Na−K 0.143	In−Pb 0.116	He−N 0.148	Y−Er 0.043	Ir−Hf 0.091
K−Cd 0.128	Ga−Tm 0.117	H−N 0.154	B−Cr 0.043	Hf−Pr 0.310
Cl−I 0.226	Sn−Sm 0.123		Co−Er 0.054	
Si−Ge 0.256	Ag−Sm 0.142	class 1222	Sc−Co 0.076	class 2212
Cu−Ag 0.269			Be−Si 0.088	
Pd−U 0.153		Ar−Kr 0.030	Co−Ni 0.092	Rh−Pt 0.096
Th−U 0.283		N−Br 0.058	Tb−Dy 0.092	
Pd−Pt 0.419		F−Ne 0.080	Sc−Y 0.093	class 222
Rh−Pd 0.498		Ne−Xe 0.087	Ho−Er 0.094	
Pt−Th 0.490		F−Xe 0.101	Tb−Er 0.101	Ta−Os 0.006
		Br−Xe 0.109	Tb−Ho 0.102	W−Re 0.040
		Kr−Xe 0.116	Ni−Y 0.110	Mo−W 0.109
			Y−Ho 0.117	Ta−Re 0.113
			B−Si 0.142	Re−Os 0.115
			Si−Cr 0.145	Mo−Re 0.126
			Fe−Er 0.159	Ta−W 0.152
				W−Os 0.155
				C−Mo 0.222

Class 2.1.1 divides as in the previous classification, with the single exception of Gd, that joins the class 2.1.1.1 (together with Ce, Pr, and Nd). The two classes are rather little differentiated as far as properties are concerned. Cu and Mn are situated at the border of the two classes, but there are many other elements having significant MDs for both classes. For instance, to class 2.1.1.1 belong in some measure Si, Tb, Fe, Cr, Dy, Sn, Er, and Sm and to class 2.1.1.2 Gd, Ge, Ag, Tm, Al, and Sm.

Consequently, the introduction of chemical properties has little influence upon classification, as their effect was indirectly contained in the physical properties taken into account at the beginning.

Le us associate to each element x^i a 12-dimensional vector defined through the membership degrees of x^i to the 12 classes, $A_k(x^i)$, $k = 1,...,12$. In order to characterize the similarity degree of two elements x^i and x^j, we can use the distance between the 12-dimensional vectors associated with these elements. Thus, we obtain the similarity degree

$$r_{ij} = \sqrt{\sum_{k=1}^{12} (A_k(x^i) - A_k(x^j))^2}$$

Some of these similarity degrees are given in Table 11 for the "closest" elements in the same class and also for some related elements from different classes. On inspection of this list some interesting features are revealed. We find such expected pairs as elements from the same group of the periodic table (Ar−Kr, Ne−Xe, Kr−Xe, Rb−Cs, K−Cs, K−Rb, Ca−Sr, Ga−In, and Mo−W), even if they are placed in different classes in the final partition (Na−K, Sb−Si, Cu−Ag); neighboring elements in a period (H−He, F−Ne, P−S, and Sn−In), especially transition metals (Co−Ni, Ta−W, W−Rb, and Re−Os), pairs of lanthanides (for instance La−Ce, Eu−Yb, Dy−Ho, and Dy−Tb), Th−U, or pairs of elements situated on the diagonal of the periodic system (Li−Mg, B−Si, Ga−Sn, In−Sb, Br−Xe, and Mo−Re). But there are also pairs of elements in the same group that have rather large r_{ij} values (F−Cl, Cl−Br, Cu−Au, and Pd−Pt). There are as well a lot of unexpected pairs of elements, some of them rather far from one another in the periodic table but near with respect to the similarity degree. For instance the "nearest" element to nitrogen is helium; remember that He replaces nitrogen in the gas "cocktail" used by divers at large depth. The similarity of Ca and Pb is supported by their chemical analogies, for instance the precipitation of Pb^{2+} and Ca^{2+} ions as oxalates. Both are also near the two lanthanides that have the oxidation state +2 (Yb and Eu). Sr is near Bi (remember that Ca, Sr, and Bi are in the composition of some superconducting oxides). Other lanthanides also present similarities to transition metals. The nearest element to silver is aluminum (although they do not belong to the same class): they have about the same atomic radius and rather similar boiling points and vaporization enthalpies. Boron is particularly near to chromium, also the resemblance seems to come essentially from the coincidence of melting and boiling points and the common oxidation state, +3. The reasons are much the same for the pairs Ni−Sc (the same boiling point) and Co−Y (melting and boiling points quite the same). As in the pairs Fe−Y and Co−Sc, the common oxidation state +3 supports the similarity. The similarity Os−Ta is rather remarkable.

As it happened in the case of the "physical" classification, the number of classes is drastically reduced by normalization. Even if only three classes have been produced, the classification agrees well with chemical intuition and is quite

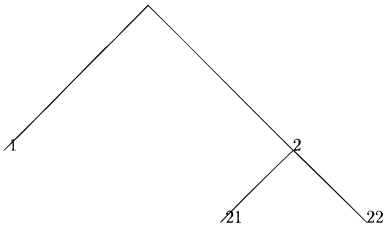

Figure 15. The classification hierarchy produced with normalized characteristics.

Table 12. Membership Degrees to the Classes of the Final Partition Produced with Normalized Characteristics

sample	1	2.1	2.2	sample	1	2.1	2.2
H	0.67	0.18	0.15	Tc	0.33	0.49	0.18
He	0.66	0.18	0.16	Ru	0.24	0.61	0.15
Li	0.46	0.22	0.31	Rh	0.22	0.66	0.12
Be	0.56	0.25	0.18	Pd	0.22	0.58	0.19
B	0.59	0.26	0.15	Ag	0.23	0.43	0.34
C	0.58	0.25	0.18	Cd	0.35	0.25	0.41
N	0.77	0.12	0.10	In	0.26	0.27	0.47
O	0.79	0.11	0.10	Sn	0.36	0.30	0.34
F	0.77	0.12	0.11	Sb	0.57	0.22	0.21
Ne	0.71	0.15	0.14	Te	0.69	0.16	0.15
Na	0.40	0.21	0.39	I	0.70	0.16	0.14
Mg	0.45	0.21	0.33	Xe	0.71	0.14	0.15
Al	0.47	0.27	0.26	Cs	0.34	0.20	0.46
Si	0.64	0.20	0.17	Ba	0.25	0.15	0.60
P	0.79	0.11	0.10	La	0.11	0.10	0.79
S	0.81	0.10	0.09	Ce	0.11	0.11	0.78
Cl	0.77	0.12	0.10	Pr	0.10	0.08	0.83
Ar	0.76	0.12	0.12	Nd	0.09	0.06	0.85
K	0.36	0.20	0.45	Sm	0.10	0.06	0.84
Ca	0.29	0.18	0.53	Eu	0.18	0.12	0.70
Sc	0.17	0.30	0.53	Gd	0.07	0.06	0.87
Ti	0.19	0.56	0.25	Tb	0.06	0.07	0.87
V	0.22	0.57	0.21	Dy	0.05	0.08	0.88
Cr	0.29	0.52	0.19	Ho	0.06	0.08	0.86
Mn	0.35	0.40	0.25	Er	0.05	0.11	0.84
Fe	0.22	0.65	0.13	Tm	0.08	0.13	0.79
Co	0.25	0.59	0.16	Yb	0.13	0.09	0.78
Ni	0.26	0.57	0.17	Lu	0.07	0.22	0.71
Cu	0.29	0.51	0.20	Hf	0.17	0.52	0.32
Zn	0.50	0.24	0.27	Ta	0.25	0.42	0.33
Ga	0.44	0.27	0.28	W	0.33	0.44	0.23
Ge	0.62	0.21	0.18	Re	0.35	0.42	0.22
As	0.74	0.14	0.12	Os	0.34	0.44	0.22
Se	0.79	0.12	0.10	Ir	0.31	0.47	0.22
Br	0.83	0.09	0.09	Pt	0.30	0.47	0.23
Kr	0.75	0.12	0.12	Au	0.30	0.47	0.23
Rb	0.34	0.19	0.47	Hg	0.43	0.27	0.30
Sr	0.26	0.16	0.58	Tl	0.26	0.26	0.48
Y	0.09	0.13	0.78	Pb	0.30	0.28	0.42
Zr	0.08	0.43	0.49	Bi	0.45	0.25	0.30
Nb	0.14	0.58	0.27	Th	0.13	0.30	0.57
Mo	0.28	0.52	0.20	U	0.24	0.41	0.36

different from that based on the 10 normalized physical properties.

The classification hierarchy produced by using the same 10 properties but normalized is presented in Figure 15. Table 12 shows the membership degrees of the elements to the fuzzy sets of the final fuzzy partition, and Figure 16 shows the successive partitions of the elements produced in this case.

The first class includes all the nonmetals as well as Be, Sb (with a MD of 0.57), and Ge; these three elements and the nonmetals B, C, Si, As, Te, and Xe add to those of the "physical" classification. From the other elements, near the boundary of the two classes are Zn (MD of 0.50) and Al (MD of 0.47).

The class 2, with the metals, is further divided, roughly speaking, in main group elements (class 2.2) and transition metals (2.1). From class 2.2 aluminum is missing but is quite near the border of the class. This set includes as well as in the other classifications elements of group 12 (Zn, Cd, and Hg), which is reasonable from the point of view of electron configuration, but also elements of group 3 (Sc, Y, La), the lanthanides and thorium. Uranium is situated in the other class but near the border. Actually, the elements of group 3 are chemically similar to the alkaline earth metals, and so are their combinations. It is also interesting the inclusion of Zr in this class (even if near the border). Indeed, its behavior show some analogies to that of the main group elements. ZrO_2 forms solid solutions with CaO (used as solid electrolyte), Zr shows some similarities to Be, and so on. The other *d*-block elements and U form the class 2.1.

The computation of the distances between the elements brings some new details concerning this classification. Some of the r_{ij} values are given in Table 13. Here are listed the closed neighbors of every element. We find here again the ordinary couples of elements from the same group in the periodic table (Ne−Xe, Ar−Kr, F−Cl, O−Se, Si−Ge, K−Rb, K−Cs, Rb−Cs, Ca−Sr, Ca−Ba, Sr−Ba, In−Tl, Ge−Si, Sn−Pb, Ti−Hf, Cr−Mo, Mn−Re, and Fe−Ru) or the pairings between lanthanides, diagonal analogies (Li−Mg, In−Pb, P−Se, S−Br, F−Ar, Ti−Nb, and Fe−Rh), and pairs of neighboring elements from the same period (H−He, Be−B, B−C, Na−Mg, Ti−V, Co−Ni, Te−I, I−Xe, Tl−Pb, W−Re, Re−Os, Os−Ir, Ir−Pt, and Pt−Au). We, however, discover some less trivial pairings and sets of elements very near to one another in a class, for instance: in class 1 the sets (O, S, Se, P, Br), (N, F, Cl, Ar, Kr, As), and (Ne, Xe, Te, I, H, He), and, rather far from the other elements, B, C, Be, and Sb (the last is relatively isolated). In class 2.1 the elements Ag, Ta, and U are similar but quite apart from the other; Al is also rather isolated, while the elements left in the class are quite near to each other. In class 2.2 we can distinguish two different sets of lanthanides: (La, Ce, Tm, Yb, and Y) and (Pr, Nd, Sm, Gd, Tb, Dy, Ho, and Er). Another set of related elements contains Ca, Sr, and Ba. Ca is also near to Rb and Cs and Sc to Th, while Zr is isolated from the other. All the

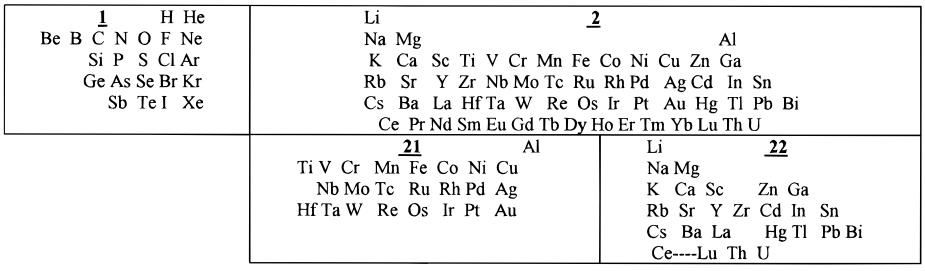

Figure 16. The classification of the elements produced with normalized physical, chemical, and structural characteristics.

Table 13. Some Similarity Degrees between Elements in the Final Partition with Normalized Characteristics

class 1	class 21	class 22	
H−He 0.019	Al−Mn 0.187	Li−Na 0.099	Y−Lu 0.111
H−Te 0.024	Ti−V 0.049	Li−Mg 0.027	Zr−Th 0.165
He−Si 0.029	Ti−Nb 0.055	Li−Bi 0.035	Cd−Sn 0.083
He−Te 0.040	Ti−Hf 0.087	Na−Mg 0.074	Cd−Pb 0.059
Be−B 0.041	V−Pd 0.026	Na−K 0.075	In−Tl 0.018
Be−C 0.016	Cr−Cu 0.017	Na−Cd 0.070	In−Pb 0.062
Be−Sb 0.037	Cr−Mo 0.011	Na−Cs 0.094	Sn−Hg 0.080
B−C 0.028	Mn−Re 0.035	Mg−Zn 0.084	Sn−Pb 0.100
C−Sb 0.040	Fe−Ru 0.047	Mg−Ga 0.082	Cs−Tl 0.093
N−F 0.006	Fe−Rh 0.013	Mg−Hg 0.070	La−Ce 0.013
N−Cl 0.001	Co−Ni 0.026	Mg−Bi 0.057	La−Yb 0.021
O−P 0.002	Co−Ru 0.027	K−Rb 0.025	Ce−Eu 0.108
O−Se 0.004	Cu−Mo 0.020	K−Cd 0.064	Ce−Tm 0.035
F−Cl 0.006	Cu−Te 0.044	K−Cs 0.021	Ce−Yb 0.029
F−Ar 0.012	Cu−Pt 0.041	Ca−Rb 0.081	Pr−Nd 0.029
Ne−I 0.020	Tc−Ir 0.043	Ca−Sr 0.065	Pr−Sm 0.025
Ne−Xe 0.017	Ag−Ta 0.013	Ca−Cd 0.069	Nd−Sm 0.020
Si−Ge 0.027	Ag−U 0.028	Ca−Cs 0.088	Nd−Gd 0.028
P−Se 0.006	Ta−U 0.031	Ca−Ba 0.086	Eu−Yb 0.105
P−Br 0.044	W−Re 0.029	Se−Th 0.049	Gd−Tb 0.010
S−Br 0.022	W−Os 0.014	Ga−Hg 0.027	Gd−Dy 0.021
Ar−Kr 0.009	Re−Os 0.025	Rb−Cs 0.011	Gd−Ho 0.022
Ar−As 0.021	Os−Ir 0.034	Rb−Tl 0.098	Tb−Dy 0.012
Te−I 0.007	Os−Au 0.043	Rb−Pb 0.079	Tb−Ho 0.019
I−Xe 0.027	Ir−Pt 0.020	Sr−Ba 0.022	Dy−Ho 0.017
	Ir−Au 0.013	Y−Ge 0.027	Ho−Er 0.035
	Pt−Au 0.010	Y−Tm 0.017	Hg−Bi 0.032
			Tl−Pb 0.070

remaining elements are strongly related to one another, especially the six elements Li, Mg, Zn, Ga, Mg, and Bi. Interesting pairs are those of Tl with elements of group 1 (Rb, Cs) and of Cd with such elements (K, Rb, and Cs) or Cd−Pb (let us note that they have similar toxicity for living organisms).

4. CONCLUSIONS

It is obvious from the discussion above that on a chemical basis as well on a physical one the same partitions are almost invariably found. These essentially agree to the traditional chemical classifications, although the details may differ. We come upon the separation in main group elements (*s*- and *p*-block elements) and transition metals (*d*- and *f*-block elements) and so on. Some elements may pass from one group to another, depending upon the type of classification, but the general frame remains unchanged. On the other hand, the classification details as the membership degrees to various classes and the distances between elements point out some less trivial similarity relationships between the elements. These could suggest some new ideas with a view to possible applications in different fields.

We may say that at every classification level there are certain physical and chemical properties that influence the separation. The problem of identifying the properties that produced a certain separation will be dealt with in the next paper of this series. We will approach then the Fuzzy Cross-Classification algorithm, discussed in ref 37.

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