A Fuzzy Cross-Classification of the Chemical Elements, Based on Their Physical, Chemical, and Structural Features

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Received May 28, 1996⊗

In this paper we discussed the classification of chemical elements and their properties using a new algorithm, namely fuzzy hierarchical cross-classification. This algorithm, described in ref 3, produces not only a fuzzy partition of the chemical elements but also a fuzzy partition of their considered properties. In this way it is possible to identify which properties (variables) are responsible for the observed similarities or dissimilarities between different elements.

1. INTRODUCTION

A paper with approximately the same title was published in this journal in 1996.[5] In the following we will refer to it as part 1. In that paper a hierarchical fuzzy clustering algorithm was described and used for the reclassification of the periodic system of elements according to their physical, chemical, and structural properties. Relevant results were obtained concerning new relationships between the chemical elements.

In order to identify which properties (variables) are responsible for the observed similarities and dissimilarities between the elements, we applied in this paper a new fuzzy algorithm, namely fuzzy hierarchical cross-classification (FHCC). This technique produces not only a fuzzy partition of chemical elements but also a fuzzy partition of the physical, chemical, and structural properties considered. Moreover, the fuzzy hierarchical characteristics clustering (FHiCC) and fuzzy horizontal characteristics clustering (FHoCC) procedures show very high similarities between chemical and structural properties of elements and also between these latter and some of the physical properties.

2. THEORETICAL CONSIDERATIONS

In certain situations the number of characteristics is very large. The design of a hierarchical classifier may be simplified if at every node is used only a small subset of the characteristics, enough for the classification decision at that node. So, at every step of the hierarchical classification process we determine a fuzzy partition of a certain class and the relevant characteristics for each of the subclasses obtained. Thus, it appears the necessity of classifying both the objects and the characteristics. This classification process will be called cross-classification (or simultaneous classification).

In what follows we will recall[3,4] a method which allows us to obtain an objects hierarchy and a characteristics hierarchy, so that the two hierarchical classifications should correspond to each other. The method we have considered is an iterative one, and the classification is done alternatively on the data set and on the characteristics set, until we will obtain two "compatible" classifications.

2.1. Simultaneously Fuzzy *n*-Means Algorithm. Let $X = \{x^1, ..., x^p\} \subset R^d$ be 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 $Y = \{y^1, ..., y^d\} \subset R^p$ 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 $y_j^k = x_k^j$.

Let P be a fuzzy partition of the fuzzy set C of objects and Q be a fuzzy partition of the fuzzy set D of characteristics. The problem of the cross-classification (or simultaneous classification) is to determine the pair (P, Q) which optimizes a certain criterion function. By starting with an initial partition P^0 of C and an initial partition Q^0 of D, we will obtain a new partition P^1. The pair (P^1, Q^0) allows us to determine a new partition Q^1 of the characteristics. The algorithm consists in producing a sequence (P^k, Q^k) of pairs of partitions, starting from the initial pair (P^0, Q^0), in the following steps:

$$\text{(i) } (P^k, Q^k) \rightarrow (P^{k+1}, Q^k)$$

$$\text{(ii) } (P^{k+1}, Q^k) \rightarrow (P^{k+1}, Q^{k+1})$$

The rationale of the hierarchical cross-classification method[3] essentially supposes the splitting of the sets X and Y in two subclasses. The obtained classes are alternatively divided in two subclasses and so on. The two hierarchies may be represented by the same tree, having in each node a pair (C, D), where C is a fuzzy set of objects and D is a fuzzy set of characteristics.

As a first step we propose ourselves to simultaneously determine the fuzzy partitions (as a particular case, the binary fuzzy partitions) of the classes C and D, so that the two partitions should be highly correlated.

With the Generalized Fuzzy n-Means algorithm, we will determine a fuzzy partition $P = \{A_1, ..., A_n\}$ of the class C, using the original characteristics.

In order to classify the characteristics, we will compute their values for the classes A_i, $i = 1, ..., n$. The value $\bar{y}_i^k$ of the characteristic k with respect to the class A_i is defined as

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⊗ Abstract published in *Advance ACS Abstracts,* October 15, 1996.

S0095-2338(96)00050-9 CCC: $12.00

$$\bar{y}_i^k = \sum_{j=1}^{p} A_i(x^j)x_k^j,\ i = 1, ..., n;\ k = 1, ..., d \qquad (1)$$

Thus, from the original d p-dimensional characteristics we computed d new n-dimensional characteristics which are conditioned by the classes A_i, $i = 1, ..., n$. We may admit that these new characteristics do not describe objects, but they characterize the classes A_i.

Let us consider now the set $\bar{Y} = \{\bar{y}^1, ..., \bar{y}^d\}$ of the modified characteristics. We define the fuzzy set $\bar{D}$ on $\bar{Y}$, given by

$$\bar{D}(\bar{y}^k) = D(y^k),\ k = 1, ..., d$$

The way the set $\bar{Y}$ has been obtained lets us conclude that if we will obtain an optimal partition of the fuzzy set D, this partition will be highly correlated to the optimal partition of the class C.

With the Generalized Fuzzy n-Means algorithm we will determine a fuzzy partition $Q = \{B_1, ..., B_n\}$ of the class D, by using the characteristics given by the relation (1).

We may now characterize the objects in X with respect to the classes of proprieties B_i, $i = 1, ..., n$. The value $\bar{x}_i^j$ of the object k with respect to the class B_i is defined as

$$\bar{x}_i^j = \sum_{k=1}^{d} B_i(\bar{y}^k)x_k^j,\ i = 1, ..., n;\ j = 1, ..., p \qquad (2)$$

Thus, from the original p d-dimensional objects we have computed p new n-dimensional objects, which correspond to the classes of characteristics B_i, $i = 1, ..., n$.

Let us now consider the set $\bar{X} = \{\bar{X}^1, ..., \bar{X}^p\}$ of the modified objects. We define the fuzzy set $\bar{C}$ on $\bar{X}$, given by

$$\bar{C}(\bar{x}^j) = C(x^j),\ j = 1, ..., p$$

With the Generalized Fuzzy n-Means algorithm we will determine a fuzzy partition $P' = \{A'_1, ..., A'_n\}$ of the class C, by using the objects given by the relation (2). The process continues until two successive partitions of objects (or of characteristics) are closed enough to each other. Thus, we have obtained **The Simultaneous Fuzzy *n*-Means Algorithm** (see ref 3).

S1. Set $l = 0$. With the Generalized Fuzzy n-Means Algorithm we determine a fuzzy n-partition $P^{(l)}$ of the class C by using the initial objects.

S2. With the Generalized Fuzzy n-Means Algorithm we determine a fuzzy n-partition $Q^{(l)}$ of the class D by using the characteristics defined in (1).

S3. With the Generalized Fuzzy n-Means Algorithm we determine a fuzzy n-partition $P^{(l+1)}$ of the class C by using the characteristics defined in (2).

S4. If the partitions $P^{(l)}$ and $P^{(l+1)}$ are close enough, that is if

$$||P^{(l+1)} - P^{(l)}|| < \epsilon$$

where ϵ is a preset value, then **Stop**, else set $l = l + 1$ and go to **S2**.

Let us denote the final partitions obtained above by $P = \{A_1, ..., A_n\}$ and $Q = \{B_1, ..., B_n\}$. If we will try to build the fuzzy partitions corresponding to the fuzzy sets A_i and B_i, $i = 1, ..., n$, with the help of this algorithm, when computing for the first time the fuzzy partition of objects, instead the original objects we may use the objects defined in the relation (2) and determined before the end of the algorithm that produced the fuzzy partitions P and Q.

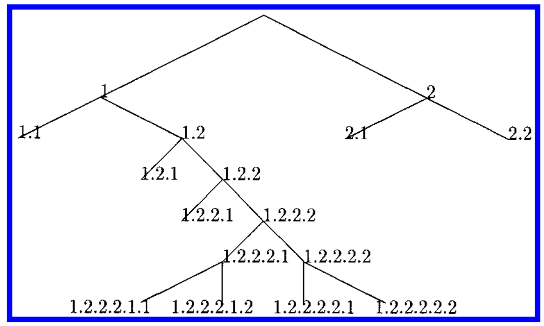

Figure 1. The classification hierarchy produced with 10 non-normalized physical characteristics.

2.2. Hierarchical Cross-Classification. Now we will present the procedure of hierarchical cross-classification. For this we will show the way of building the classification binary tree.

The nodes of the tree are labeled with a pair (C, D), where C is a fuzzy set from a fuzzy partition of objects and D is a fuzzy set from a fuzzy partition of characteristics. The root node corresponds to the pair (X, Y). In the first step the two subnodes (A_1, B_1) and respectively (A_2, B_2) will be computed by using the Simultaneous Fuzzy n-Means algorithm. Of course, these two nodes will be effectively built only if the fuzzy partitions $\{A_1, A_2\}$ and $\{B_1, B_2\}$ describe real clusters.

For each of the terminal nodes of the tree we try to determine partitions having the form $\{A_1, A_2\}$ and $\{B_1, B_2\}$, by using the Simultaneous Fuzzy n-Means algorithm, modified as we have mentioned before. In this way the binary classification tree is extended with two new nodes, (A_1, B_1) and (A_2, B_2). The process continues until for any terminal node we are not able to determine a structure of real clusters, either for the set of objects or for the set of characteristics. The final fuzzy partitions will contain the fuzzy sets corresponding to the terminal nodes of the binary classification tree.

3. CLASSIFICATION RESULTS

3.1. Fuzzy Hierarchical Cross-Clustering. We started with the same **physical properties** as in part 1 of our research on the classification of chemical elements:[5] relative atomic mass, A (1), density, ρ (2), melting point, T_f (3), boiling point T_b (4), electronegativity, χ (5), vaporization enthalpy, ΔH_v (6), fusion enthalpy, ΔH_f (7), specific heat capacity, C_s (8), ionization energy, E_i (9), covalent radius, r (10), for 84 elements, firstly **without data normalization**. The classification hierarchy produced in this way for objects (the 84 elements) and for characteristics (the 10 physical properties) is presented in Figure 1. Table 1 shows the membership degrees (MD) of the elements and of their characteristics to the fuzzy clusters of the final simultaneous fuzzy partition, and Figure 2 shows the successive partitions of elements and characteristics.

The first partitioning of elements in classes 1 and 2 is exactly the same as in the analogous classification in part 1 (ref 5, section 3.1, Figure 2) and so are the partitionings of the second level, in classes 1.1, 1.2 and 2.1, 2.2. What isnew is the partitioning of characteristics. Class 1 contains eight of the physical properties, while class 2, that includes mostly

Table 1. Membership Degrees to the Fuzzy Classes of the Simultaneous Final Fuzzy Partition Produced with 10 Non-Normalized Physical Characteristics

element		1.1	1.2.1	1.2.2.1	1.2.2.2.1	1.2.2.2.2.1	1.2.2.2.2.2.1	1.2.2.2.2.2	2.1	2.2
1	H	0.05	0.02	0.06	0.48	0.18	0.05	0.09	0.05	0.02
2	He	0.06	0.06	0.14	0.02	0.02	0.63	0.00	0.05	0.02
3	Li	0.85	0.09	0.01	0.00	0.00	0.00	0.00	0.03	0.01
4	Be	0.12	0.02	0.01	0.00	0.00	0.00	0.00	0.83	0.01
5	B	0.12	0.02	0.01	0.00	0.00	0.00	0.00	0.78	0.06
6	C	0.10	0.03	0.01	0.00	0.00	0.00	0.00	0.11	0.73
7	N	0.04	0.01	0.02	0.80	0.06	0.00	0.00	0.05	0.02
8	O	0.03	0.01	0.05	0.75	0.07	0.01	0.01	0.05	0.02
9	F	0.04	0.01	0.01	0.26	0.46	0.04	0.12	0.05	0.02
10	Ne	0.05	0.04	0.09	0.00	0.01	0.01	0.74	0.05	0.02
11	Na	0.50	0.45	0.03	0.00	0.00	0.00	0.00	0.00	0.00
12	Mg	0.86	0.08	0.01	0.00	0.00	0.00	0.00	0.03	0.01
13	Al	0.40	0.04	0.01	0.00	0.00	0.00	0.00	0.50	0.04
14	Si	0.13	0.02	0.01	0.00	0.00	0.00	0.00	0.82	0.01
15	P	0.02	0.66	0.24	0.02	0.02	0.01	0.01	0.02	0.01
16	S	0.08	0.86	0.03	0.00	0.00	0.00	0.00	0.01	0.00
17	Cl	0.01	0.04	0.79	0.04	0.05	0.01	0.02	0.04	0.01
18	Ar	0.03	0.00	0.02	0.02	0.84	0.01	0.02	0.05	0.02
19	K	0.34	0.62	0.02	0.00	0.00	0.00	0.00	0.00	0.00
20	Ca	0.85	0.02	0.00	0.00	0.00	0.00	0.00	0.11	0.02
21	Sc	0.10	0.02	0.01	0.00	0.00	0.00	0.00	0.86	0.01
22	Ti	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.97	0.02
23	V	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.91	0.09
24	Cr	0.10	0.02	0.01	0.00	0.00	0.00	0.00	0.84	0.04
25	Mn	0.39	0.04	0.01	0.00	0.00	0.00	0.00	0.51	0.04
26	Fe	0.04	0.01	0.00	0.00	0.00	0.00	0.00	0.94	0.00
27	Co	0.06	0.01	0.00	0.00	0.00	0.00	0.00	0.91	0.00
28	Ni	0.11	0.02	0.01	0.00	0.00	0.00	0.00	0.85	0.01
29	Cu	0.22	0.03	0.01	0.00	0.00	0.00	0.00	0.71	0.02
30	Zn	0.67	0.28	0.02	0.00	0.00	0.00	0.00	0.00	0.00
31	Ga	0.58	0.07	0.02	0.00	0.00	0.00	0.00	0.27	0.04
32	Ge	0.17	0.03	0.01	0.00	0.00	0.00	0.00	0.76	0.03
33	As	0.51	0.34	0.07	0.01	0.01	0.01	0.01	0.03	0.01
34	Se	0.32	0.66	0.01	0.00	0.00	0.00	0.00	0.00	0.00
35	Br	0.00	0.19	0.75	0.01	0.01	0.00	0.00	0.03	0.01
36	Kr	0.03	0.00	0.21	0.20	0.43	0.03	0.05	0.04	0.01
37	Rb	0.27	0.70	0.02	0.00	0.00	0.00	0.00	0.01	0.00
38	Sr	0.88	0.02	0.00	0.00	0.00	0.00	0.00	0.08	0.01
39	Y	0.06	0.01	0.00	0.00	0.00	0.00	0.00	0.92	0.00
40	Zr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.88	0.12
41	Nb	0.04	0.01	0.00	0.00	0.00	0.00	0.00	0.73	0.21
42	Mo	0.09	0.03	0.01	0.00	0.00	0.00	0.00	0.01	0.85
43	Tc	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.84	0.14
44	Ru	0.06	0.02	0.01	0.00	0.00	0.00	0.00	0.03	0.87
45	Rh	0.03	0.01	0.00	0.00	0.00	0.00	0.00	0.30	0.65
46	Pd	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.75	0.23
47	Ag	0.45	0.04	0.01	0.00	0.00	0.00	0.00	0.46	0.03
48	Cd	0.47	0.50	0.02	0.00	0.00	0.00	0.00	0.00	0.00
49	In	0.69	0.06	0.01	0.00	0.00	0.00	0.00	0.19	0.03
50	Sn	0.56	0.06	0.02	0.00	0.00	0.00	0.00	0.31	0.04
51	Sb	0.92	0.01	0.00	0.00	0.00	0.00	0.00	0.06	0.01
52	Te	0.77	0.19	0.02	0.00	0.00	0.00	0.00	0.01	0.00
53	I	0.02	0.53	0.35	0.02	0.02	0.01	0.02	0.02	0.01
54	Xe	0.02	0.03	0.59	0.10	0.14	0.03	0.04	0.04	0.01
55	Cs	0.27	0.70	0.02	0.00	0.00	0.00	0.00	0.01	0.00
56	Ba	0.83	0.01	0.00	0.00	0.00	0.00	0.00	0.14	0.02
57	La	0.06	0.01	0.00	0.00	0.00	0.00	0.00	0.85	0.06
58	Ce	0.08	0.02	0.01	0.00	0.00	0.00	0.00	0.82	0.07
59	Pr	0.10	0.02	0.01	0.00	0.00	0.00	0.00	0.84	0.03
60	Nd	0.10	0.02	0.01	0.00	0.00	0.00	0.00	0.85	0.02
61	Sm	0.58	0.04	0.01	0.00	0.00	0.00	0.00	0.33	0.03
62	Eu	0.86	0.02	0.00	0.00	0.00	0.00	0.00	0.10	0.02
63	Gd	0.06	0.01	0.00	0.00	0.00	0.00	0.00	0.92	0.00
64	Tb	0.10	0.02	0.01	0.00	0.00	0.00	0.00	0.86	0.01
65	Dy	0.16	0.02	0.01	0.00	0.00	0.00	0.00	0.79	0.02
66	Ho	0.15	0.02	0.01	0.00	0.00	0.00	0.00	0.80	0.02
67	Er	0.06	0.01	0.00	0.00	0.00	0.00	0.00	0.91	0.00
68	Tm	0.48	0.06	0.02	0.00	0.00	0.00	0.00	0.37	0.05
69	Yb	0.86	0.02	0.00	0.00	0.00	0.00	0.00	0.10	0.02
70	Lu	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.96	0.03
71	Hf	0.08	0.02	0.01	0.00	0.00	0.00	0.00	0.04	0.84
72	Ta	0.09	0.03	0.01	0.00	0.00	0.00	0.00	0.01	0.84
73	W	0.12	0.04	0.02	0.00	0.00	0.00	0.00	0.06	0.75

Table 1 (Continued)

element		1.1	1.2.1	1.2.2.1	1.2.2.2.1	1.2.2.2.2.1	1.2.2.2.2.2.1	1.2.2.2.2.2	2.1	2.2
74	Re	0.11	0.04	0.02	0.00	0.00	0.00	0.00	0.05	0.78
75	Os	0.10	0.03	0.01	0.00	0.00	0.00	0.00	0.02	0.83
76	Ir	0.08	0.02	0.01	0.00	0.00	0.00	0.00	0.01	0.87
77	Pt	0.04	0.01	0.00	0.00	0.00	0.00	0.00	0.35	0.59
78	Au	0.11	0.02	0.01	0.00	0.00	0.00	0.00	0.85	0.02
79	Hg	0.04	0.72	0.16	0.02	0.02	0.01	0.01	0.02	0.00
80	Tl	0.89	0.03	0.01	0.00	0.00	0.00	0.00	0.05	0.01
81	Pb	0.82	0.03	0.01	0.00	0.00	0.00	0.00	0.12	0.02
82	Bi	0.87	0.03	0.01	0.00	0.00	0.00	0.00	0.07	0.01
83	Th	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.78	0.21
84	U	0.03	0.01	0.00	0.00	0.00	0.00	0.00	0.82	0.12
					Properties					
1	A	0.21	0.78	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	ρ	0.00	0.00	0.05	0.91	0.00	0.02	0.03	0.00	0.00
3	T_f	0.28	0.10	0.03	0.01	0.01	0.01	0.01	0.56	0.00
4	T_b	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.98
5	χ	0.00	0.00	0.01	0.00	0.95	0.01	0.02	0.00	0.00
6	ΔH_o	0.01	0.04	0.95	0.00	0.00	0.00	0.00	0.00	0.00
7	ΔH_f	0.00	0.00	0.01	0.01	0.01	0.81	0.15	0.00	0.00
8	C_s	0.01	0.00	0.01	0.00	0.00	0.79	0.19	0.00	0.00
9	E_i	0.97	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	r	0.00	0.00	0.00	0.05	0.02	0.01	0.92	0.00	0.00

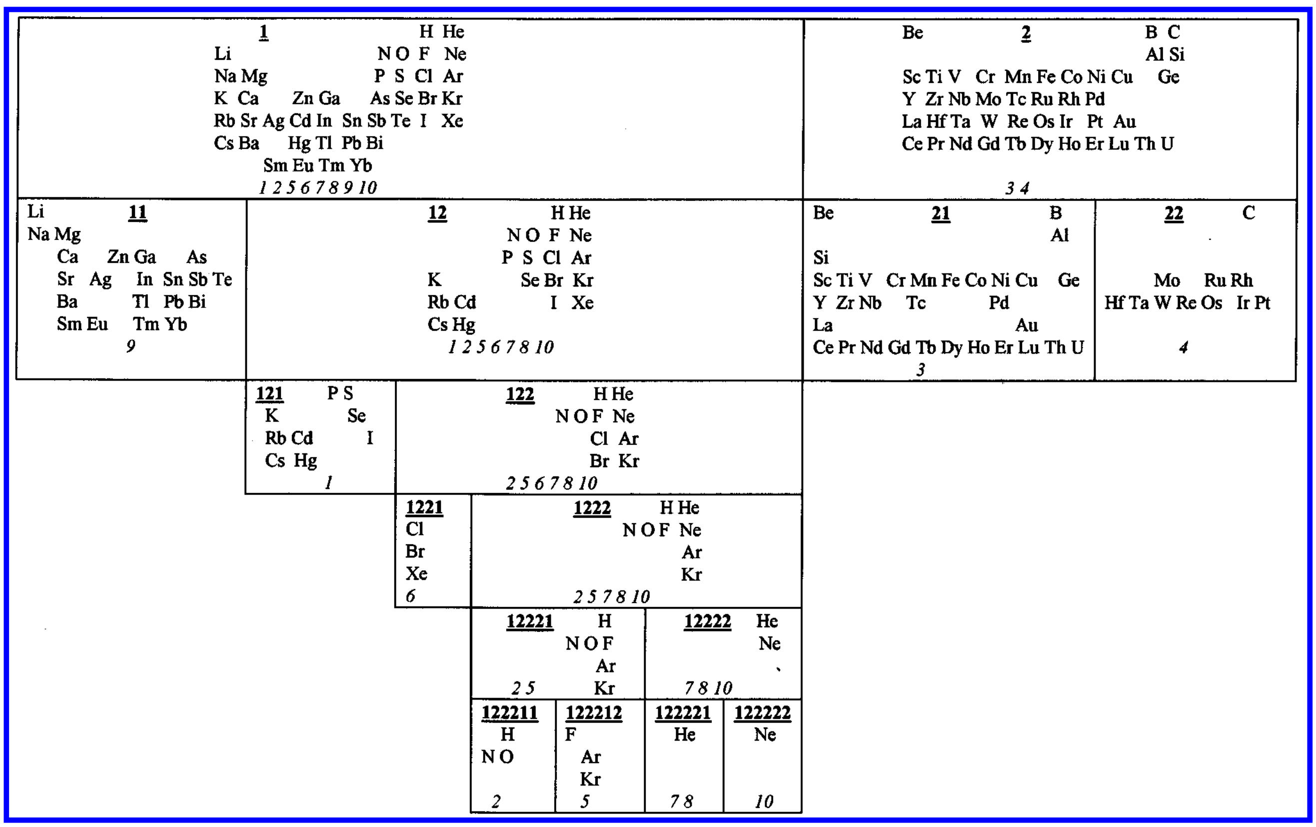

Figure 2. The classification of the elements and characteristics produced with 10 non-normalized physical properties.

elements in the secondary groups of the periodical table, is characterized mainly by the melting and boiling point. Their next division in lighter transition metals (class 2.1) and heavier ones (class 2.2) is associated with the separation of the melting point with the former class and the boiling point with the latter. There are no more subsequent divisions of the classes 2.1 and 2.2, while the analogous classification in ref 5 produced five clusters here.

The characteristic associated to the class 1.1, comprised of mostly main-group metals, is the ionization energy, but the boiling point and the atomic mass have also rather important MDs. Unlike the classification in ref 5, the cross clustering does not further divide this class, the only one deeper divided being 1.2. The classes 1.2.1 and 1.2.2 are again the same as in ref 5. The elements of the class 1.2.1, metals and nonmetals solid at room temperature, have as the main characteristic the atomic mass, but the boiling point also has some weight. They are no more divided, but so are the typical gaseous nonmetals of the class 1.2.2. As in ref 5, Cl, Br, and Xe are grouped distinctly (class 1.2.2.1), and their characteristic is the vaporization enthalpy, while from the class 1.2.2.2 the lighter noble gases He and Ne (class 1.2.2.2.1) are separated from the other elements. But these two last classes each are subject to a further division. One new class (1.2.2.2.1.1) includes N, O, and, with a smaller have significant MDs to it. Their MDs to the class to which

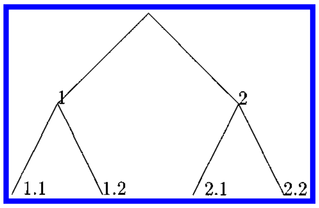

Figure 3. The classification hierarchy produced with 10 normalized characteristics.

1		2	
1, 2, 3, 4, 6, 7		5, 8, 9, 10	
1.1	**1.2**	**2.1**	**2.2**
1, 2, 7	3, 4, 6	5, 8, 9	10

Figure 4. The classification of the 10 physical normalized characteristics.

they belong (class 1.2.2.2.1.2) are much smaller than that of Ar; their characteristic is the electronegativity. On the other hand, He and Ne are separated each to a different class. For helium, the characteristics are the fusion enthalpy and the specific heat capacity; for neon, it is the covalent radius, with some contributions of the specific heat capacity and the fusion enthalpy.

The hierarchical cross-clustering using the same 10 physical properties, but with **data normalization** gives the classification hierarchy presented in Figure 3. The successive partitions of the elements are identical with those obtained in part 1, with the 10 normalized physical characteristics (ref 5: Figure 4) and so are the membership degrees of the elements to the fuzzy sets of the fuzzy partition (ref 5: Table 3). For the 10 characteristics, the successive partitions are represented in Figure 4, and their membership degrees to the four final fuzzy sets are shown in Table 2.

With the main-group elements of class 1 are classified the following properties: atomic mass, density, melting and boiling points, vaporization, and fusion enthalpy, while to the class 2 of transitional metals belong the other properties: electronegativity, specific heat capacity, ionization energy, and covalent radius. In the final cluster 1.1,

Table 2. Membership Degrees to the Fuzzy Classes of the Simultaneous Final Fuzzy Partition Produced with 10 Normalized Physical Characteristics

element		1.1	1.2	2.1	2.2	element		1.1	1.2	2.1	2.2
1	H	0.25	0.31	0.23	0.20	43	Tc	0.07	0.04	0.08	0.81
2	He	0.26	0.37	0.22	0.16	44	Ru	0.12	0.07	0.08	0.73
3	Li	0.40	0.32	0.19	0.09	45	Rh	0.09	0.05	0.05	0.80
4	Be	0.30	0.30	0.25	0.16	46	Pd	0.08	0.04	0.26	0.61
5	B	0.22	0.19	0.27	0.32	47	Ag	0.30	0.07	0.52	0.11
6	C	0.20	0.18	0.22	0.40	48	Cd	0.65	0.19	0.12	0.03
7	N	0.14	0.58	0.17	0.11	49	In	0.58	0.10	0.26	0.06
8	O	0.16	0.54	0.18	0.13	50	Sn	0.52	0.09	0.32	0.06
9	F	0.18	0.47	0.19	0.15	51	Sb	0.43	0.14	0.34	0.09
10	Ne	0.25	0.40	0.21	0.14	52	Te	0.46	0.27	0.20	0.07
11	Na	0.51	0.25	0.18	0.06	53	I	0.28	0.53	0.13	0.06
12	Mg	0.57	0.27	0.12	0.04	54	Xe	0.40	0.32	0.20	0.09
13	Al	0.46	0.20	0.25	0.09	55	Cs	0.40	0.19	0.29	0.12
14	Si	0.24	0.20	0.28	0.29	56	Ba	0.44	0.11	0.35	0.09
15	P	0.06	0.79	0.10	0.05	57	La	0.26	0.06	0.56	0.12
16	S	0.08	0.74	0.12	0.06	58	Ce	0.28	0.07	0.54	0.12
17	Cl	0.11	0.64	0.15	0.09	59	Pr	0.29	0.06	0.57	0.09
18	Ar	0.29	0.42	0.19	0.10	60	Nd	0.29	0.05	0.59	0.07
19	K	0.45	0.21	0.25	0.09	61	Sm	0.39	0.06	0.49	0.06
20	Ca	0.54	0.14	0.25	0.07	62	Eu	0.44	0.09	0.39	0.08
21	Sc	0.29	0.09	0.48	0.15	63	Gd	0.16	0.03	0.71	0.10
22	Ti	0.18	0.07	0.48	0.27	64	Tb	0.14	0.03	0.74	0.09
23	V	0.14	0.06	0.40	0.40	65	Dy	0.16	0.04	0.70	0.11
24	Cr	0.21	0.09	0.47	0.24	66	Ho	0.14	0.03	0.71	0.12
25	Mn	0.38	0.13	0.38	0.12	67	Er	0.13	0.03	0.69	0.14
26	Fe	0.17	0.08	0.45	0.30	68	Tm	0.20	0.05	0.61	0.14
27	Co	0.15	0.07	0.44	0.34	69	Yb	0.46	0.08	0.39	0.07
28	Ni	0.15	0.07	0.44	0.34	70	Lu	0.10	0.03	0.55	0.31
29	Cu	0.27	0.11	0.43	0.18	71	Hf	0.12	0.06	0.19	0.62
30	Zn	0.58	0.38	0.04	0.01	72	Ta	0.15	0.09	0.17	0.59
31	Ga	0.61	0.17	0.17	0.05	73	W	0.16	0.11	0.18	0.55
32	Ge	0.22	0.13	0.36	0.29	74	Re	0.16	0.11	0.17	0.56
33	As	0.32	0.31	0.24	0.13	75	Os	0.16	0.11	0.17	0.55
34	Se	0.15	0.72	0.09	0.04	76	Ir	0.16	0.11	0.17	0.56
35	Br	0.11	0.68	0.13	0.07	77	Pt	0.15	0.10	0.19	0.56
36	Kr	0.33	0.39	0.18	0.09	78	Au	0.19	0.12	0.31	0.38
37	Rb	0.44	0.19	0.27	0.10	79	Hg	0.37	0.27	0.25	0.12
38	Sr	0.50	0.12	0.30	0.08	80	Tl	0.38	0.15	0.35	0.12
39	Y	0.22	0.05	0.62	0.11	81	Pb	0.37	0.15	0.36	0.12
40	Zr	0.10	0.04	0.51	0.35	82	Bi	0.37	0.15	0.36	0.12
41	Nb	0.10	0.05	0.20	0.66	83	Th	0.14	0.06	0.36	0.44
42	Mo	0.12	0.07	0.12	0.69	84	U	0.18	0.09	0.33	0.40
					Properties						
1	A	0.71	0.11	0.06	0.12	6	ΔH_v	0.01	0.98	0.01	0.01
2	ρ	0.90	0.08	0.01	0.01	7	ΔH_f	0.52	0.48	0.00	0.00
3	T_f	0.05	0.94	0.01	0.01	8	C_s	0.00	0.00	0.89	0.11
4	T_b	0.05	0.94	0.01	0.01	9	E_i	0.03	0.02	0.90	0.05
5	χ	0.01	0.01	0.90	0.08	10	r	0.16	0.09	0.00	0.75

Table 3. Membership Degrees to the Fuzzy Classes of the Simultaneous Final Fuzzy Partition Produced with 10 Non-Normalized Physical, Chemical, and Structural Properties

element		1.1.1	1.1.2	1.2.1.1	1.2.1.2	1.2.2	2	element		1.1.1	1.1.2	1.2.1.1	1.2.1.2	1.2.2	2
1	H	0.08	0.03	0.60	0.08	0.09	0.11	43	Tc	0.00	0.00	0.00	0.00	0.00	0.99
2	He	0.06	0.02	0.75	0.02	0.05	0.09	44	Ru	0.01	0.04	0.00	0.00	0.02	0.92
3	Li	0.48	0.16	0.31	0.02	0.02	0.01	45	Rh	0.00	0.02	0.00	0.00	0.01	0.97
4	Be	0.27	0.03	0.01	0.01	0.04	0.64	46	Pd	0.00	0.00	0.00	0.00	0.00	1.00
5	B	0.01	0.08	0.00	0.00	0.02	0.89	47	Ag	0.61	0.03	0.02	0.01	0.03	0.30
6	C	0.03	0.06	0.01	0.01	0.03	0.87	48	Cd	0.36	0.00	0.23	0.10	0.31	0.00
7	N	0.03	0.01	0.09	0.08	0.73	0.06	49	In	0.87	0.03	0.00	0.00	0.01	0.09
8	O	0.05	0.01	0.03	0.78	0.04	0.08	50	Sn	0.09	0.60	0.00	0.00	0.03	0.27
9	F	0.04	0.00	0.01	0.68	0.21	0.07	51	Sb	0.08	0.65	0.01	0.01	0.08	0.18
10	Ne	0.05	0.00	0.02	0.31	0.57	0.05	52	Te	0.06	0.59	0.01	0.02	0.27	0.06
11	Na	0.28	0.09	0.57	0.01	0.03	0.03	53	I	0.04	0.16	0.06	0.08	0.66	0.00
12	Mg	0.79	0.03	0.10	0.03	0.04	0.00	54	Xe	0.02	0.02	0.01	0.04	0.88	0.03
13	Al	0.60	0.02	0.01	0.01	0.04	0.32	55	Cs	0.17	0.03	0.73	0.04	0.00	0.03
14	Si	0.04	0.20	0.00	0.00	0.05	0.71	56	Ba	0.73	0.17	0.00	0.00	0.00	0.09
15	P	0.00	0.00	0.04	0.04	0.89	0.02	57	La	0.01	0.08	0.00	0.00	0.02	0.89
16	S	0.01	0.11	0.02	0.02	0.84	0.00	58	Ce	0.01	0.09	0.00	0.00	0.03	0.88
17	Cl	0.01	0.09	0.04	0.05	0.80	0.01	59	Pr	0.00	0.15	0.00	0.00	0.03	0.81
18	Ar	0.04	0.00	0.02	0.26	0.63	0.05	60	Nd	0.00	0.15	0.00	0.00	0.03	0.82
19	K	0.21	0.06	0.68	0.00	0.02	0.03	61	Sm	0.01	0.61	0.00	0.00	0.04	0.34
20	Ca	0.94	0.00	0.00	0.00	0.01	0.05	62	Eu	0.15	0.74	0.00	0.00	0.01	0.11
21	Sc	0.01	0.14	0.00	0.00	0.03	0.81	63	Gd	0.00	0.09	0.00	0.00	0.02	0.88
22	Ti	0.00	0.02	0.00	0.00	0.00	0.98	64	Tb	0.01	0.11	0.00	0.00	0.03	0.85
23	V	0.00	0.00	0.00	0.00	0.00	1.00	65	Dy	0.01	0.15	0.00	0.00	0.03	0.81
24	Cr	0.01	0.04	0.00	0.00	0.01	0.95	66	Ho	0.01	0.14	0.00	0.00	0.03	0.81
25	Mn	0.04	0.26	0.00	0.00	0.04	0.66	67	Er	0.01	0.07	0.00	0.00	0.02	0.90
26	Fe	0.01	0.07	0.00	0.00	0.02	0.91	68	Tm	0.03	0.43	0.00	0.00	0.04	0.49
27	Co	0.02	0.10	0.00	0.00	0.03	0.86	69	Yb	0.13	0.75	0.00	0.00	0.01	0.11
28	Ni	0.03	0.14	0.00	0.00	0.03	0.79	70	Lu	0.00	0.01	0.00	0.00	0.00	0.98
29	Cu	0.35	0.05	0.01	0.01	0.05	0.53	71	Hf	0.02	0.05	0.00	0.00	0.03	0.89
30	Zn	0.55	0.01	0.20	0.08	0.16	0.00	72	Ta	0.03	0.07	0.01	0.01	0.04	0.85
31	Ga	0.85	0.02	0.02	0.01	0.01	0.10	73	W	0.05	0.08	0.01	0.01	0.05	0.80
32	Ge	0.07	0.25	0.00	0.00	0.05	0.62	74	Re	0.04	0.08	0.01	0.01	0.05	0.80
33	As	0.08	0.44	0.02	0.03	0.42	0.01	75	Os	0.03	0.07	0.01	0.01	0.04	0.84
34	Se	0.04	0.29	0.03	0.03	0.60	0.00	76	Ir	0.02	0.06	0.01	0.01	0.03	0.88
35	Br	0.00	0.00	0.02	0.12	0.83	0.03	77	Pt	0.00	0.02	0.00	0.00	0.01	0.97
36	Kr	0.03	0.01	0.01	0.11	0.80	0.04	78	Au	0.02	0.13	0.00	0.00	0.03	0.82
37	Rb	0.17	0.04	0.74	0.01	0.01	0.03	79	Hg	0.01	0.00	0.37	0.17	0.43	0.02
38	Sr	0.90	0.05	0.00	0.00	0.01	0.04	80	Tl	0.91	0.02	0.01	0.01	0.04	0.02
39	Y	0.00	0.09	0.00	0.00	0.02	0.89	81	Pb	0.23	0.65	0.00	0.00	0.00	0.11
40	Zr	0.00	0.00	0.00	0.00	0.00	1.00	82	Bi	0.00	0.85	0.00	0.00	0.04	0.10
41	Nb	0.00	0.00	0.00	0.00	0.00	0.99	83	Th	0.00	0.00	0.00	0.00	0.00	1.00
42	Mo	0.03	0.06	0.01	0.01	0.04	0.86	84	U	0.00	0.00	0.00	0.00	0.00	1.00
							Properties								
1	ρ	0.99	0.00	0.00	0.00	0.00	0.01	6	conf	0.03	0.02	0.00	0.00	0.93	0.01
2	T_f	0.07	0.06	0.29	0.03	0.06	0.49	7	spdf	0.03	0.02	0.05	0.59	0.29	0.02
3	T_b	0.00	0.00	0.00	0.00	0.01	0.99	8	os+	0.03	0.02	0.90	0.00	0.05	0.01
4	E_i	0.16	0.10	0.14	0.57	0.04	0.00	9	os−	0.15	0.83	0.01	0.00	0.00	0.01
5	r	0.97	0.02	0.00	0.00	0.00	0.01	10	ΔF_{Cl}	0.08	0.90	0.00	0.00	0.00	0.01

containing mostly the main-group metals, we find the properties density, atomic mass, and, with a much smaller MD, the fusion enthalpy. For the nonmetals of the class 1.2, the characteristics grouped together are the vaporization enthalpy and the melting and boiling points; an important MD to this class also has the fusion enthalpy. As for class 2.1, including the transition elements of period 4 and some of period 5 beside the lanthanides, its characteristics are the electronegativity, the ionization energy, and the specific heat capacity, all three with about the same MD. The last class, 2.2, of the transition metals from periods 6 and 5, Th, U, together with B, C, and Si, have as the only characteristic the covalent radius; MDs over 0.10 to this class also have the atomic mass and the specific heat capacity.

The same clustering method was then applied with the use of **ten physical, chemical, and structural characteristics** (see ref 5, sections 3.4, 3.5): density, ρ (1), melting point, T_f (2), boiling point, T_b (3), ionization energy, E_i (4), covalent radius, r (5), the two electron configuration

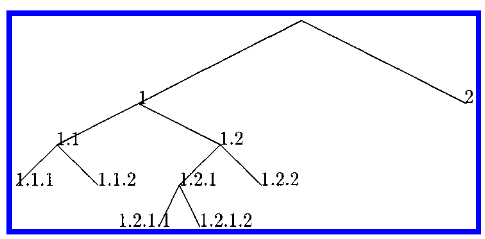

Figure 5. The classification hierarchy produced with 10 non-normalized physical, chemical, and structural characteristics.

indices: of the number of electrons in the outer shells, conf (6), and of the number of electrons in the next outer subshell, spdf (7), the index of positive oxidation states, os+ (8), and of negative ones, os− (9), and the free chloride formation energy, ΔF_{Cl} (10).

The classification hierarchy produced with these properties **without data normalization**, is presented in Figure 5, and the membership degrees of elements and characteristics to the fuzzy clusters of the simultaneous final fuzzy partition

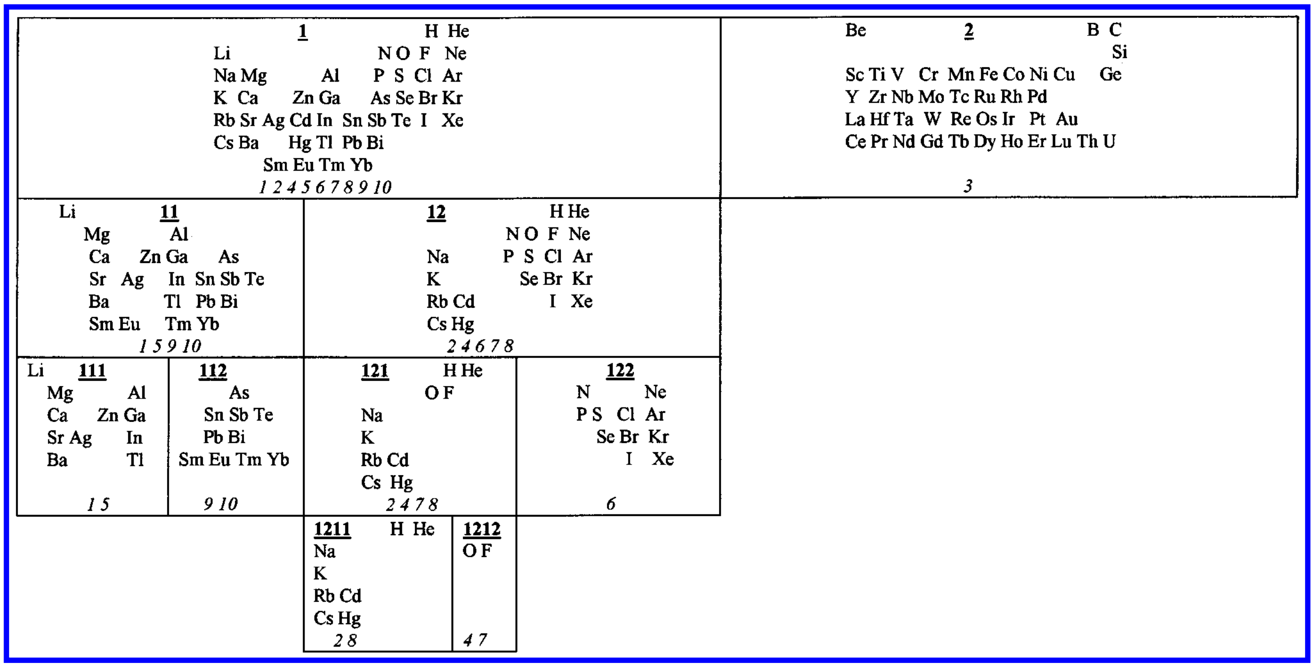

Figure 6. The classification of the elements and characteristics produced with 10 non-normalized physical, chemical, and structural properties.

are given in Table 3. Figure 6 shows the successive partitions of elements and characteristics.

The first partitioning in classes 1 and 2 is the same as in the non-normalized classification on the basis of 10 physical and chemical characteristics, except for aluminum, which is classified with the main-group elements; Tm and Cu are near the boundary between classes. All the characteristics, except the boiling point, are assigned to this class; only the melting point has a lower MD, being at the limit of the class.

The next partitioning of class 1 presents also only small differences from the previous one: Na passes in class 1.2, with the other alkaline metals, and Cd also goes to the class 1.2, while Al belongs to class 1.1; Tm is at the boundary between these classes. The characteristics attributed to the class 1.1 are the density, the covalent radius, the free chlorides formation energy, and the index of negative oxidation states. The melting point is included in class 1.2 but near the classes boundary.

The division of class 1.1 is different from that of the classification in ref 5. In class 1.1.1 are included Li, the second group elements (Mg−Ba), those of group 13 (Al−Tl), and Ag and Zn, while in class 1.1.2 we find elements of the groups 14, 15, and 16, together with the four lanthanides (Sm, Eu, Tm, Yb). The separation is rather clear-cut. Elements with significant MDs to class 1.1.1 are also Cd, Cu, Na, Pb, and K and to class 1.1.2 are Se, Mn, Ge, and Si. The characteristics of class 1.1.1 are the density and the covalent radius; smaller Md to it also have the ionization energy and the negative oxidation states. To class 1.1.2 belong the free chloride formation energy and the index of negative oxidation states.

The division of class 1.2 is also different from the previous: H, He, O, and F pass from class 1.2.2 to class 1.2.1, joining the alkaline metals (Na−Cs), Cd, and Hg, while in exchange P, S, Se, and I pass from class 1.2.1 to class 1.2.2, joining Cl, Br, and the noble gases Ne−Kr. Other elements with important MDs to this last class are Hg, As, Cd, Te, and F. The characteristics of this class is the electron configuration index for the outer shell; an important MD has also the index for the s, p, d, and f-subshells.

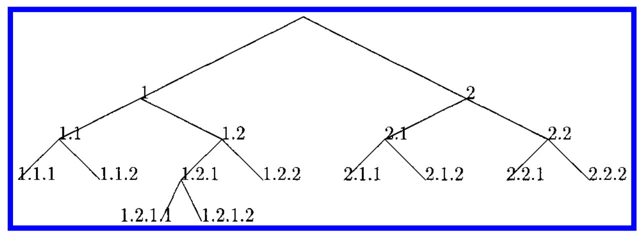

Figure 7. The classification hierarchy produced with 10 normalized physical, chemical, and structural characteristics.

Further, the former class (1.2.1) is divided by the separation of the most electronegative elements (O and F), forming the class 1.2.1.1, to which have significant MDs also Ne, Ar, and Hg. Their characteristics are the ionization energy and the number of s, p, d, and f electrons in the outer shells, both with not quite large MDs. Among the metals of the class 1.2.1.1, Cd and Hg are at the border between the two classes, this class also has important MDs Li and Zn. Here we find the characteristics: index of positive oxidation states and melting point (but with a quite smaller MD).

Unlike the classification in part 1, class 2 is not further divided; to this class are also related Tm, Sm, Al, Ag, Sn, and Sb. The characteristic here is the boiling point, but the melting point also has an MD of 0.49.

This time, the **normalized** cross-classification leads to a more profound division relatively different to the previous ones. The classification hierarchy produced is represented in Figure 7, and the membership degrees of the elements and of the characteristics to the fuzzy clusters of the simultaneous final fuzzy partition are shown in Table 4. Figure 8 shows the successive partitions of elements and characteristics.

The first partitioning brings together in class 1 particularly the main-group elements: H, He, groups 1, 2, and 13 of the periodic table (entirely), some elements of the groups 14−17, and the noble gases (except for Xe); with them are joined, as usual, Zn and Cd but also Cu and Ag (group 11) and Ni as well as three lanthanides (Sm, Eu, and Yb, i.e., without Tm). Their characteristics are density, melting and boiling points, the s, p, d, and f-configuration, and the oxidation

Table 4. Membership Degrees to the Fuzzy Classes of the Simultaneous Final Fuzzy Partition Produced with 10 Non-Normalized Physical, Chemical, and Structural Properties

element	1.1.1	1.1.2	1.2.1.1	1.2.1.2	1.2.2	2.1.1	2.1.2	2.2.1	2.2.2	element	1.1.1	1.1.2	1.2.1.1	1.2.1.2	1.2.2	2.1.1	2.1.2	2.2.1	2.2.2
1 H	0.08	0.16	0.04	0.02	0.47	0.02	0.13	0.06	0.01	43 Tc	0.05	0.02	0.00	0.01	0.01	0.00	0.01	0.05	0.84
2 He	0.01	0.03	0.02	0.01	0.92	0.01	0.00	0.00	0.00	44 Ru	0.03	0.01	0.00	0.00	0.00	0.00	0.04	0.12	0.79
3 Li	0.11	0.43	0.02	0.04	0.19	0.02	0.12	0.05	0.01	45 Rh	0.01	0.01	0.00	0.00	0.00	0.03	0.21	0.05	0.69
4 Be	0.12	0.79	0.01	0.02	0.03	0.00	0.03	0.01	0.00	46 Pd	0.03	0.01	0.00	0.00	0.00	0.08	0.63	0.06	0.20
5 B	0.46	0.52	0.00	0.00	0.00	0.00	0.01	0.00	0.00	47 Ag	0.61	0.00	0.01	0.01	0.01	0.03	0.32	0.00	0.01
6 C	0.35	0.30	0.01	0.02	0.03	0.17	0.08	0.02	0.02	48 Cd	0.33	0.44	0.00	0.01	0.01	0.03	0.16	0.01	0.01
7 N	0.01	0.02	0.67	0.01	0.22	0.05	0.00	0.01	0.01	49 In	0.50	0.15	0.00	0.01	0.01	0.02	0.29	0.01	0.01
8 O	0.02	0.04	0.15	0.02	0.64	0.08	0.01	0.02	0.02	50 Sn	0.09	0.02	0.00	0.01	0.01	0.42	0.43	0.00	0.01
9 F	0.01	0.03	0.04	0.02	0.86	0.02	0.01	0.01	0.01	51 Sb	0.00	0.00	0.00	0.00	0.00	0.89	0.04	0.03	0.04
10 Ne	0.02	0.06	0.00	0.00	0.77	0.07	0.03	0.02	0.02	52 Te	0.00	0.00	0.00	0.00	0.00	0.86	0.00	0.05	0.08
11 Na	0.09	0.53	0.02	0.05	0.14	0.01	0.11	0.04	0.01	53 I	0.00	0.00	0.00	0.00	0.00	0.73	0.06	0.08	0.12
12 Mg	0.04	0.79	0.01	0.03	0.06	0.00	0.05	0.01	0.00	54 Xe	0.00	0.04	0.03	0.05	0.12	0.46	0.09	0.09	0.12
13 Al	0.08	0.91	0.00	0.00	0.00	0.00	0.00	0.00	0.00	55 Cs	0.41	0.56	0.00	0.00	0.01	0.00	0.01	0.00	0.00
14 Si	0.12	0.52	0.06	0.12	0.13	0.01	0.03	0.01	0.00	56 Ba	0.86	0.05	0.01	0.01	0.02	0.00	0.05	0.01	0.00
15 P	0.04	0.09	0.14	0.68	0.01	0.03	0.00	0.00	0.01	57 La	0.27	0.05	0.01	0.01	0.02	0.01	0.49	0.14	0.00
16 S	0.09	0.19	0.04	0.54	0.08	0.06	0.00	0.01	0.01	58 Ce	0.18	0.03	0.01	0.01	0.01	0.01	0.59	0.15	0.01
17 Cl	0.03	0.07	0.06	0.10	0.04	0.48	0.06	0.07	0.09	59 Pr	0.26	0.05	0.01	0.01	0.02	0.01	0.49	0.15	0.00
18 Ar	0.01	0.04	0.05	0.06	0.70	0.08	0.02	0.02	0.02	60 Nd	0.20	0.04	0.01	0.01	0.02	0.01	0.55	0.17	0.00
19 K	0.07	0.70	0.01	0.03	0.07	0.01	0.08	0.02	0.00	61 Sm	0.46	0.05	0.01	0.02	0.02	0.01	0.36	0.07	0.00
20 Ca	0.28	0.69	0.00	0.00	0.01	0.00	0.01	0.00	0.00	62 Eu	0.57	0.02	0.01	0.01	0.02	0.00	0.34	0.03	0.00
21 Sc	0.83	0.05	0.01	0.01	0.02	0.00	0.08	0.01	0.00	63 Gd	0.13	0.03	0.00	0.001	0.01	0.01	0.57	0.24	0.00
22 Ti	0.26	0.03	0.01	0.01	0.01	0.00	0.63	0.04	0.01	64 Tb	0.09	0.02	0.00	0.01	0.01	0.01	0.60	0.25	0.01
23 V	0.10	0.02	0.00	0.01	0.01	0.00	0.62	0.23	0.00	65 Dy	0.07	0.01	0.00	0.00	0.01	0.00	0.65	0.24	0.01
24 Cr	0.08	0.02	0.00	0.01	0.01	0.02	0.57	0.22	0.07	66 Ho	0.09	0.02	0.00	0.01	0.01	0.01	0.65	0.21	0.01
25 Mn	0.14	0.06	0.00	0.01	0.01	0.01	0.62	0.15	0.01	67 Er	0.09	0.02	0.00	0.01	0.01	0.01	0.57	0.30	0.00
26 Fe	0.33	0.02	0.01	0.01	0.01	0.01	0.59	0.02	0.01	68 Tm	0.19	0.04	0.01	0.01	0.01	0.01	0.57	0.16	0.00
27 Co	0.45	0.01	0.01	0.01	0.01	0.01	0.48	0.01	0.01	69 Yb	0.63	0.04	0.01	0.02	0.02	0.00	0.25	0.03	0.00
28 Ni	0.51	0.01	0.01	0.01	0.01	0.01	0.43	0.01	0.01	70 Lu	0.05	0.02	0.00	0.00	0.01	0.01	0.43	0.47	0.01
29 Cu	0.75	0.01	0.00	0.01	0.01	0.01	0.19	0.01	0.01	71 Hf	0.03	0.01	0.00	0.00	0.01	0.00	0.02	0.89	0.03
30 Zn	0.09	0.88	0.00	0.01	0.01	0.00	0.00	0.00	0.00	72 Ta	0.05	0.03	0.01	0.01	0.01	0.01	0.10	0.68	0.10
31 Ga	0.28	0.66	0.00	0.00	0.00	0.00	0.04	0.00	0.00	73 W	0.11	0.06	0.02	0.02	0.04	0.04	0.11	0.02	0.59
32 Ge	0.17	0.65	0.04	0.08	0.06	0.00	0.00	0.00	0.00	74 Re	0.11	0.07	0.02	0.03	0.04	0.06	0.10	0.03	0.55
33 As	0.17	0.41	0.06	0.21	0.08	0.05	0.01	0.01	0.01	75 Os	0.10	0.06	0.02	0.02	0.03	0.05	0.08	0.05	0.58
34 Se	0.10	0.20	0.02	0.13	0.05	0.41	0.00	0.04	0.05	76 Ir	0.09	0.05	0.01	0.02	0.03	0.03	0.07	0.08	0.62
35 Br	0.01	0.04	0.06	0.20	0.62	0.05	0.00	0.01	0.01	77 Pt	0.06	0.03	0.01	0.01	0.01	0.01	0.02	0.00	0.85
36 Kr	0.01	0.05	0.06	0.10	0.34	0.26	0.06	0.06	0.07	78 Au	0.03	0.01	0.00	0.00	0.01	0.08	0.18	0.02	0.65
37 Rb	0.08	0.79	0.01	0.02	0.03	0.00	0.05	0.01	0.00	79 Hg	0.07	0.05	0.00	0.01	0.01	0.46	0.35	0.01	0.03
38 Sr	0.75	0.24	0.00	0.00	0.00	0.00	0.00	0.00	0.00	80 Tl	0.43	0.05	0.00	0.01	0.01	0.03	0.44	0.01	0.01
39 Y	0.40	0.06	0.01	0.01	0.02	0.00	0.45	0.05	0.00	81 Pb	0.05	0.01	0.00	0.00	0.00	0.51	0.42	0.00	0.01
40 Zr	0.00	0.00	0.00	0.00	0.00	0.00	0.58	0.21	0.19	82 Bi	0.00	0.00	0.00	0.00	0.00	0.87	0.06	0.02	0.04
41 Nb	0.01	0.00	0.00	0.00	0.00	0.01	0.25	0.70	0.03	83 Th	0.01	0.00	0.00	0.00	0.00	0.00	0.05	0.93	0.00
42 Mo	0.06	0.03	0.01	0.01	0.01	0.00	0.02	0.12	0.74	84 U	0.04	0.02	0.00	0.01	0.01	0.00	0.05	0.86	0.00
										Properties									
1 ρ	0.87	0.00	0.08	0.00	0.01	0.01	0.00	0.01	0.01	6 conf	0.00	0.01	0.00	0.00	0.00	0.00	0.92	0.05	0.02
2 T_f	0.01	0.01	0.95	0.00	0.02	0.00	0.00	0.00	0.00	7 spdf	0.15	0.06	0.13	0.60	0.02	0.01	0.00	0.02	0.01
3 T_b	0.01	0.01	0.06	0.92	0.00	0.00	0.00	0.00	0.00	8 os+	0.00	0.91	0.03	0.03	0.02	0.00	0.00	0.00	0.00
4 E_i	0.01	0.02	0.00	0.00	0.01	0.76	0.00	0.11	0.09	9 os−	0.06	0.08	0.00	0.00	0.75	0.01	0.01	0.09	0.01
5 r	0.05	0.07	0.14	0.13	0.00	0.05	0.03	0.53	0.00	10 ΔF_{Cl}	0.02	0.05	0.01	0.01	0.02	0.01	0.01	0.00	0.87

states (positive and negative). Class 2 includes most of the d- and f-block elements but also some p-block elements (from the groups 14−18). Near the border of the two classes lie Co, Se, Y, and Tl. The characteristics here are ionization energy, covalent radius, the first index of electron configuration, and the free chloride formation energy.

Further, similar to other classifications, are separated from class 1 the typical nonmetals and the noble gases He−Kr (class 1.2), on the one hand, and the metals, on the other hand, together with some refractory nonmetals (B, C, Si)−class 1.1. In class 1.1 the characteristics are density and positive oxidation states. From the partitioning of this latter class results a class (1.1.2) that includes the alkaline metals (Li−Cs), the first three elements of the groups 2 and 13, Si, Ge, As and also Zn and Cd, hence exclusively main-group elements and elements of the group 12. Their characteristic is the positive oxidation state. The other class (1.1.1) contains not only some elements of the main groups (Sr, Ba, In, Tl, and C) but also Sc, Ni, Cu, and Ag and the three lanthanides, with density as their characteristic. Other elements with significant MDs to class 1.1.1 are B, Co, Cs, Y, Fe, Cd, Ca, Ga, La, Ti, Pr, and Nd and to the class 1.1.2, C, Sr, Se, and S−the last four being also main group elements.

The nonmetals class 1.2 is more profoundly divided. Thus are separated N, P, and S (class 1.2.1) from which nitrogen is then classified alone as a class (1.2.1.1), having the melting point as characteristic. To this class are also related O and P, with small MDs. For the other class (1.2.1.2) of phosphorus and sulfur (the only solid nonmetals along those of class 1.2), some elements from outside it with important MDs are As, Br, Se, and S, all solid nonmetals also (except for the liquid bromine). Their characteristics are the boiling point and the configuration index for s, p, d, and f electrons in the outer shells. Class 1.2.2 contains gaseous nonmetals from the groups 16−18 and hydrogen and also Br; smaller MDs to this class have also N, Li, Na, Si, and Xe. The characteristic that belongs here is the negative oxidation state.

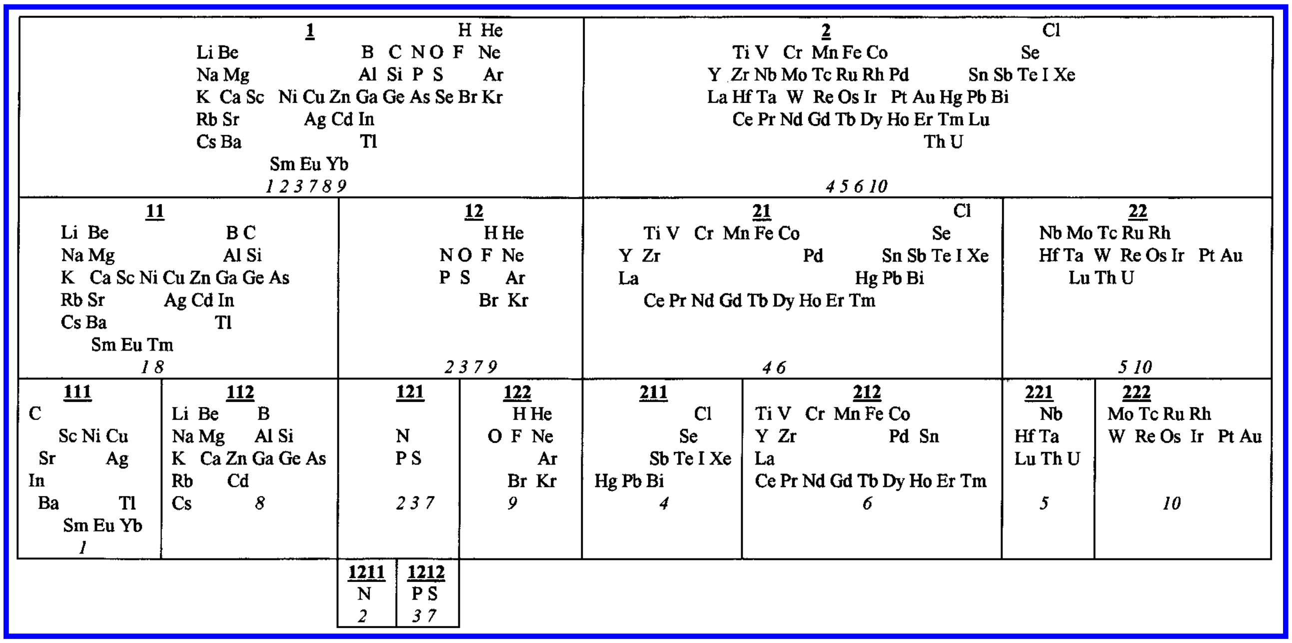

Figure 8. The classification of the elements and characteristics produced with 10 normalized physical, chemical, and structural properties.

From class 2 are grouped in class 2.1 all the p-block elements (from the main groups 14−18), the d-block elements of period 4 (Ti−Co), and some with less high melting and boiling points from the next periods as well as the lanthanides which are left, except for Lu. The properties included here are the energy of ionization and the first index of electronic configuration. In class 2.2 remain the heavy d-block elements of the periods 5 and 6: Nb−Rh and Hf−Au together with Lu, Th, and U. Lutetium lies, as a matter of fact, near the boundary between the two classes. Here the properties are the covalent radius and the free chlorides formation energy.

From class 2.1 are then separated, on the one hand, the elements of the main-groups (except for Sn, that lies however at the border of the two classes) with Hg (class 2.1.1) and the transition metals on the other hand (class 2.1.2). Elements from outside with high MDs to the class 2.1.1 are Sn, Kr, and C and to the class 2.1.2, Tl, Ni, Lu, Pb, Sm, Hg, Eu, Ag, In, Nb, Yb, and Rh. The characteristics belonging there are the ionization energy (to class 2.1.1) and the index of occupation of outer electronic shells (to class 2.1.2).

Class 2.2 is divided into two very distinct sets. The first one (class 2.2.1) comprises Nb, Hf, Ta, Lu, Th, and U; to them are related in some measure several lanthanides (Er, Tb, Gd, Dy, Ho, Nd, Tm, Ce, and Pr) and also V, Cr, and Zr. Their characteristic is the covalent radius. In class 2.2.2 are included the heavy d-block elements from periods 5 and 6: Mo−Rh and W−Au. Elements with significant MDs to this class are Pd and Zr. The characteristic of this class is the free chlorides formation energy.

It is interesting to remark that, by their form with successive ramifications, these classifications remind us of the "genealogic table" of elements proposed by Thierry William Preyer (1841−1897), who conceived a genetical system, based on a theory of elements origin,[6] but we must say that the resemblance is purely formal.

3.2. Fuzzy Hierarchical Characteristics Clustering. In order to develop the classifications presented in this section we applied the fuzzy divisive hierarchical clustering (FDHC) procedure described in refs 5 and 2 to different characteristics

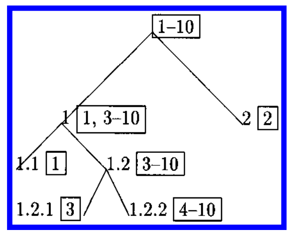

Figure 9. The classification hierarchy of the 10 physical characteristics, without normalization.

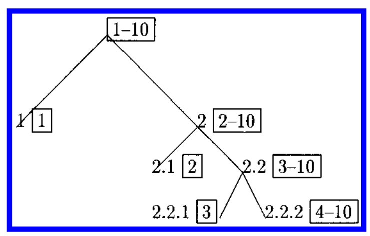

Figure 10. The classification hierarchy of the 10 physical characteristics, with data normalization.

sets considered here. The hierarchical procedure obtained in this way may be called **fuzzy hierarchical characteristics clustering** (**FHiCC**).

The characteristics clustering with the **10 physical properties** for the 84 elements, **without data normalization**, gave the hierarchy represented in Figure 9. It is interesting to note that all the divisions are clear-cut; the membership degrees to the different sets are all near 1 or 0. The first characteristic separated from the others is the **density** (2). In the next step the **atomic mass** (1) is following, and, finally, the **melting point** (3) is separated from the other characteristics. The cluster containing the seven properties left is not subjected to any more splitting.

The characteristics clustering with the same **physical properties** but **with normalization** gave the same division of the characteristics, even if the succession of the splitting is changed a little (Figure 10). It is now the **atomic mass** (1) that is separated first from the other characteristics, followed by the **density** (2), and then by the **melting point** (3). The membership degrees of the characteristics to the clusters of the final partition are given in Table 5. To cluster

Table 5. Membership Degrees of the 10 Physical Properties to the Clusters of the Final Fuzzy Partition, with Data Normalization

property		1	2.1	2.2.1	2.2.2
1	A	**0.99**	0.00	0.00	0.00
2	ρ	0.25	**0.75**	0.00	0.00
3	T_f	0.01	0.02	**0.97**	0.00
4	T_b	0.01	0.00	0.00	**0.99**
5	χ	0.01	0.00	0.00	**0.99**
6	ΔH_v	0.01	0.00	0.00	**0.99**
7	ΔH_f	0.01	0.00	0.00	**0.99**
8	C_s	0.01	0.00	0.00	**0.99**
9	E_i	0.01	0.00	0.00	**0.99**
10	r	0.01	0.00	0.00	**0.99**

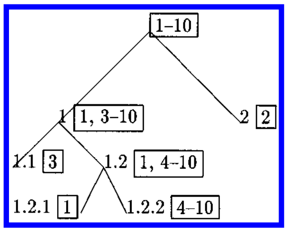

Figure 11. The classification hierarchy of the 10 physical, chemical, and structural characteristics, without normalization.

Table 6. Membership Degrees of the 10 Physical, Chemical, and Structural Properties of the Clusters of the Final Fuzzy Partition, without and with Data Normalization

property		without data normalization				with data normalization			
		1.1	1.2.1	1.2.2	2	1	2.1	2.2.1	2.2.2
1	ρ	0.22	**0.78**	0.00	0.00	**0.99**	0.00	0.00	0.00
2	T_f	0.00	0.00	0.00	**1.00**	0.28	**0.72**	0.00	0.00
3	T_b	**1.00**	0.00	0.00	0.00	0.02	0.04	**0.94**	0.00
4	E_i	0.00	0.00	**1.00**	0.00	0.00	0.00	0.00	**1.00**
5	r	0.00	0.00	**1.00**	0.00	0.00	0.00	0.00	**1.00**
6	conf	0.00	0.00	**1.00**	0.00	0.00	0.00	0.00	**1.00**
7	spdf	0.00	0.00	**1.00**	0.00	0.00	0.00	0.00	**1.00**
8	os+	0.00	0.00	**1.00**	0.00	0.00	0.00	0.00	**1.00**
9	os−	0.00	0.00	**1.00**	0.00	0.00	0.00	0.00	**1.00**
10	ΔF_{Cl}	0.00	0.00	**1.00**	0.00	0.00	0.00	0.00	**1.00**

1, of the atomic mass, the density also has a significant membership degree (MD = 0.25). For the other properties and clusters, the MDs are again near 1 or 0.

The similar clustering procedures applied for the **10 physical**, **structural**, **and chemical characteristics** gave similar results. The classification hierarchy produced with **non-normalized** data is represented in Figure 11, and the membership degrees of the characteristics to the clusters of the final fuzzy partition are shown in Table 6. In the different steps of the clustering process there are successively separated the melting point (2), the boiling point (3), and the density (1). The two other physical properties (ionization energy and covalent radius) and all the structural and chemical characteristics remain together unsplit. We are again faced with unit or zero MDs, except for the density, that has an MD of 0.22 to the class 1.1 of the boiling point.

The **data normalization** does not change the overall picture of this characteristics clustering. The classification hierarchy (Figure 12) differs only by the order of successive separations of the characteristics, the first being now the density (1), then the melting point (2), and the boiling point (3) and without any splitting for the other seven characteristics. The membership degrees of the characteristics to the final clusters, also shown in Table 6, have values near unit and zero, except for the melting point, with an MD of 0.28 to the class 1 (of the density).

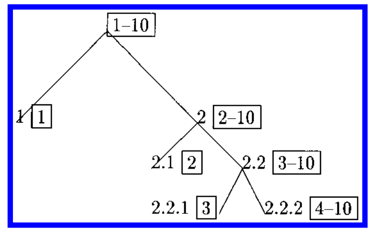

Figure 12. The classification hierarchy of the 10 physical, chemical, and structural characteristics, with data normalization.

3.3. Fuzzy Horizontal Characteristics Clustering. In order to develop the classifications presented in this section we applied the well-known Fuzzy n-Means (FNM) algorithm, described in ref 1 and discussed in ref 5 to different characteristics sets considered here. The classification procedure obtained in this way may be called **fuzzy horizontal characteristics clustering** (**FHoCC**).

The characteristics clustering for the **10 physical properties**, **without data normalization** and with a predefined number of **five classes** distribute the characteristics in three clusters only, the other two remaining empty. Cluster 1 contains the atomic mass (1), with an MD of 0.33; this characteristic appears with equal MDs (0.33) to the two empty clusters, 3 and 4. In cluster 2 we find the density (MD = 1), and cluster 5 includes all the eight other physical properties, without any separation. All the MDs, except those for the atomic mass, are either 1 or 0.

Let us remark that, even if we asked for five fuzzy classes, the clustering practically produced only three: cluster 2, cluster 5, and another cluster that was equally divided into clusters 1, 3, and 4. These last three fuzzy clusters are absolutely identical, and they were simply produced because we asked for a number of classes higher than the natural number of classes that corresponds to the cluster substructure of the considered data set. Practically, we should take into consideration the clusters 2 and 5 and the union of clusters 1, 3, and 4.

The same procedure, but **with data normalization**, produces only one empty class (class 5), with all the properties being distributed over four classes: in class 1 we find the atomic mass, in class 2—the density, and in class 3—the melting point, each of these properties having MDs equal to 1 to their own classes and 0 to the rest. Class 4 includes together all the other seven physical properties, each of them with an MD of 0.5; these properties also have MDs of 0.5 to the class 5, the vacant one.

The results are very much the same for the **10 physical**, **structural**, **and chemical characteristics**, **without data normalization**. For the five predefined number of classes, one remains vacant, the MDs of all the characteristics to this class being zero. From the other four classes, three contain again one characteristic each, while the last includes the rest of the seven properties. All the MDs are 1 or 0. The three properties separated are again the density (class 1), the melting point (class 2), and the boiling point (class 3).

The same treatment, but with a predefined number of four classes, gives absolutely the same results, except for the missing empty class. This brings us to another way in which we may find that we asked for a number of classes higher than the natural number of classes that corresponds to the cluster substructure of the considered data set. We found in the precedent case that three fuzzy classes were absolutely identical, this meaning that they were artificially split. In this case the clustering process practically produced four fuzzy classes, the fifth one, having MDs equal to 0 for all the properties, being produced only to comply with the prerequisite of five classes, that was above the natural number of four classes.

4. CONCLUSIONS

Fuzzy hierarchical cross-classification approach of chemical elements based on their physical, chemical, and structural properties allows an objective proved to be able to conserve the classification results obtained in part 1[5] by using the original fuzzy classification algorithms. Moreover, the fuzzy cross-classification procedure used in this paper allows the qualitative and quantitative identification of the properties (physical, chemical, and structural) responsible for observed similarities and dissimilarities between chemical elements.

In addition, the fuzzy hierarchical characteristics clustering (FHiCC) and fuzzy horizontal characteristics clustering (FHoCC) procedures revealed a high similarity between chemical and structural properties and also between the latter and some physical properties.

The fact that the discriminant and independent physical properties include relative mass, density, and melting point illustrates that the results obtained in this way refer especially to the elementary substances and less to the elements as a type of atoms. By contrary, the classical periodical systems of chemical elements consider first the properties (for example, valence) of the chemical elements. By the other way, electronegativity, ionization energy or covalent radius are mainly determined by electron configuration, and as a result they are grouped in the same cluster.

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CI960050G