# Topological Study of the Periodic System

Guillermo Restrepo,*,† Héber Mesa,† Eugenio J. Llanos,‡ and José L. Villaveces†

Grupo de Química Teórica, Universidad Industrial de Santander, Bucaramanga, Colombia, and Grupo de Química Teórica, Universidad Nacional de Colombia, Bogotá, Colombia

Received October 1, 2003

We carried out a topological study of the Space of Chemical Elements, SCE, based on a clustering analysis of 72 elements, each one defined by a vector of 31 properties. We looked for neighborhoods, boundaries, and other topological properties of the SCE. Among the results one sees the well-known patterns of the Periodic Table and relationships such as the Singularity Principle and the Diagonal Relationship, but there appears also a robustness property of some of the better-known families of elements. Alkaline metals and Noble Gases are sets whose neighborhoods have no other elements besides themselves, whereas the topological boundary of the set of metals is formed by semimetallic elements.

## INTRODUCTION

The Periodic Law shows several regularities of the properties of chemical elements.[1,2] The Periodic Table is the result of a graphic representation of the Law where it is possible to identify families of elements (groups) and periods. Since its discovery, other patterns such as the **Singularity Principle**[3,4] (the chemistry of the second period elements is often different to the later members of their respective groups), **Diagonal Relationships**[3,4] (similarity in chemical properties between an element and that to the lower right of it in the Periodic Table), **Inert Pair Effect**[3,4] (In some groups, the elements following the second and third transition periods exhibit oxidation states two below the maximum of their respective groups), and some others[3,5,6] have been found. Most attempts to explain the Law have arisen from rather crude approximations based on applications of Quantum Theory to the study of Atomic Spectra.[7−10] Yet, Klein's research[11−13] (defining the periodic system as a partial ordering set) and Kreinovich's work[8] establish the possibility to carry out a mathematical study of the periodic system.

According to Villaveces[14] a relevant aspect developed by Mendeleyev's methodology was to consider the set of chemical elements as a whole, not element by element, and, as a result, to find out several relationships among which neigborhoods are quite important. Taking this as the starting point of our work, it is possible to make a connection with Topology.[15−17]

Recently, attempts have been done to study neighborhood relationships for chemical elements as cluster analysis (CA).[18,19] Zhou[18] et al. studied a set of 50 elements ($Z = 1-50$) making use of 7 physical properties. Some of the clusters they found were as follows: {*Co*,*Ni*,*Fe*,*Rh*,*Ru*}, {*Mo*,*Tc*}, {*Sc*,*Y*,*Ti*}, {*Ga*,*In*,*Sn*}, {*N*,*O*,*F*,*H*}, {*Cl*,*Br*}, {*Zn*,*Cd*}, {*Ar*,*Kr*,*Ne*,*He*}, {*Mg*,*Ca*}, {*Li*,*Na*,*K*,*Rb*}, {*Cu*,*Ag*}, and {*B*,*C*}, where the appearance of alkaline elements and noble gases groups stands out. Sneath[19] studied 69 elements ($Z = 1-83$, omitting $Z = 58-71$) starting from 54 physical and chemical properties. Among the groups found were the following: {*He*,*Ne*,*Ar*,*Kr*,*Xe*}, {*N*,*P*}, {*S*,*Se*}, {*Cl*,*Br*}, {*O*,*F*}, {*B*,*Si*,*C*}, {*Ti*,*V*}, {*As*,*Sb*,*Te*}, {*Zn*,*Cd*,*In*}, {*Hg*,*Tl*,*Pb*,*Bi*}, {*Cr*,*Mn*,*Fe*,*Co*,*Ni*}, {*Zr*,*Hf*}, {*Nb*,*Ta*,*W*,*Mo*,*Re*}, {*Cu*,*Ag*,*Au*}, {*Tc*,*Ru*,*Os*,*Ir*}, {*Rh*,*Pd*,*Pt*}, {*Li*,*Na*,*K*,*Rb*,*Cs*}, {*Be*,*Al*}, {*Mg*,*Ca*,*Sr*,*Ba*}, and {*Sc*,*Y*,*La*}, where it is important to remark the appearance of alkaline, alkaline earth elements, and noble gases, besides fragments of other groups of the Periodic Table. In Sneath's work 25% of the values of the properties used were reported missing. In addition, out of the 54 properties used, only 14 belong to chemical elements, the rest of them being related to their compounds. Finally, taking the atomic perspective, Carbó-Dorca[20,21] et al. studied 20 nuclei of chemical elements using Quantum Similarity and found some relationships shown in the Periodic Law.

## METHODOLOGY

**Cluster Analysis.** Authors[18,19] which have developed CA on the chemical elements have used several different numbers of properties to describe each element. There is an open problem concerning how many properties are necessary to completely determine an element or the whole set of elements. It is not even clear whether the same number of properties would suffice to completely determine different elements, for example, noble gases, with their low reactivity may be determined by less chemical properties than a transition element such as iron. Besides, there are problems such as covariance, correlations, linear dependences, and so on, demanding a rigorous analysis, which, up to our knowledge, has not been answered in the current literature. Although the problem is open still, one may compare our newly proposed methodology with former works, taking at least the same number of properties. Indeed, we took a larger and more complete set of properties. We applied CA on 72 chemical elements ($Z = 1-86$, omitting $Z = 58-71$) defined by 31 physical and chemical properties (Table 1), out of which 4 are related to their chemical reactivities and 2 with

* Corresponding author phone: (577)6349069; fax: (577)6349009; e-mail: grestrep@uis.edu.co, khemeia@hotmail.com.
† Universidad Industrial de Santander.
‡ Universidad Nacional de Colombia.

10.1021/ci034217z CCC: $27.50 
Published on Web 01/08/2004

**Table 1.** Properties of Chemical Elements ($Z = 1-86$, omitting 58−71)

| j | properties | units |
|---|---|---|
| 1 | ionization potential[22] | eV/mol atm |
| 2 | polarizability[23] | $10^{-24}$cm$^3$ |
| 3 | electronegativity[23] | Pauling |
| 4 | atomic radii[24] | pm |
| 5 | ionic radii[23] | Å |
| 6 | reduction potential[3] | V |
| 7 | melting point[22] | K |
| 8 | critical temperature[23,25] | °C |
| 9 | heat of vaporization[26] | kcal/g-atom |
| 10 | heat of atomization[23,27] | kJ/mol |
| 11 | density[22] | g/cm$^3$ (25°C) |
| 12 | molar heat[23] | J/mol-K |
| 13 | electronic affinity[23] | eV |
| 14 | boiling point[22] | K |
| 15 | thermal conductivity[23,25] | W/m−K |
| 16 | atomic volume[27,28] | cm$^3$/mol |
| 17 | heat of fusion[23,27] | kJ/mol |
| 18 | electrical conductivity[27] | 1/mohm-cm |
| 19 | acid character of oxide[3,26] | $x \in \{0, 1\}$ |
| 20 | basic character of oxide[3,26] | $x \in \{0, 1\}$ |
| 21 | air reaction[27] | $x \in \{0, 1\}$ |
| 22 | reaction with HCl −6M[27] | $x \in \{0, 1\}$ |
| 23 | reaction with NaOH-6M[27] | $x \in \{0, 1\}$ |
| 24 | reaction with $HNO_3$−15M[27] | $x \in \{0, 1\}$ |
| 25 | no. of oxidation states[22] | $x \in \{0, 1, 2, 3, 4, 5\}$ |
| 26 | no. of reduction states[22] | $x \in \{0, 1, 2, 3\}$ |
| 27 | no. of *s* electrons in the valence shell[23] | $x \in \{1, 2\}$ |
| 28 | no. of *p* electrons in the valence shell[23] | $x \in \{0, 1, 2, 3, 4, 5, 6\}$ |
| 29 | no. of *d* electrons in the penultimate level[23] | $x \in \{0, 1, 2, ..., 10\}$ |
| 30 | minimum common oxidation state[23,27] | $x \in \{-4, -3, -2, -1, 0\}$ |
| 31 | maximum common oxidation state[23,27] | $x \in \{1, 2, 3, 4, 5, 6, 7\}$ |

some of their compounds. There was about 1.6% of missing experimental values which were interpolated taking the property as a function of *Z*. Second-order Lagrange polynomials were used in the cases where the missing values were bounded by known values. Two values were not bounded (electric conductivity of *H* and *He*), and they were calculated through the respective Lagrangian polynomial for *Li* and *Ne* (second period). In this way, we defined each element as a 31-tuple of physicochemical properties which was further normalized by[29]

$$\bar{x}_{jA} = \frac{x_{jA} - x_{j\min}}{x_{j\max} - x_{j\min}}$$

where $x_{jA}$ is the value of property $j$ of chemical element $A$ and $x_{jmin}$ and $x_{jmax}$ are the minimum and maximum $j$ values for all elements.

**Definition 1.** Let $Q$ be

$$Q = \{(\bar{x}_1,\bar{x}_2,\bar{x}_3,...,\bar{x}_{31}) | 0 \le \bar{x}_j \le 1\}$$

then $Q$ is called **Space of Chemical Elements** (SCE).

**Definition 2.** $X_A = (\bar{x}_{1A},\bar{x}_{2A},\bar{x}_{3A},...,\bar{x}_{31A}) \in Q$ is the vector representing the chemical element $A$, where $\bar{x}_{jA}$ is the $j$th property of element $A$.

After, we build up a data array (72 × 31) on which we applied CA[30−32] making use of 4 similarity functions *f(A,B)* and 4 grouping methodologies. The most commonly used similarity functions are those relating objects with the distance among them.[15,33] In this work we used 3 distance functions (metrics) and 1 similarity coefficient (nonmetric).

**Table 2.** Similarity Functions Employed

Hamming distance $d(A,B) = d_1(A,B) = \sum_{j=1}^{n} |x_{jA} - x_{jB}|$

Euclidean distance $d(A,B) = d_2(A,B) = [\sum_{j=1}^{n} |x_{jA} - x_{jB}|^2]^{1/2}$

Gower distance $$d(A,B) = \left[1 - \frac{\sum_{j=1}^{n} x_{jA}x_{jB}}{\sum_{j=1}^{n} x_{jA}^2 + \sum_{j=1}^{n} x_{jB}^2 - \sum_{j=1}^{n} x_{jA}x_{jB}}\right]^{1/2}$$

Cosine coefficient $$S(A,B) = \frac{\sum_{j=1}^{n} x_{jA}x_{jB}}{[\sum_{j=1}^{n} x_{jA}^2 \sum_{j=1}^{n} x_{jB}^2]^{1/2}}$$

**Table 3.** Methodologies Employed in the Cluster Analysis

| methodology | $\alpha_A$ | $\alpha_B$ | $\beta$ | $\gamma$ |
|---|---|---|---|---|
| unweighted average linkage | $n_A^*/(n_A + n_B)$ | $n_B/(n_A + n_B)$ | *0* | *0* |
| centroid linkage | $n_A/(n_A + n_B)$ | $n_B/(n_A + n_B)$ | $-n_An_B/(n_A + n_B)^2$ | *0* |
| complete linkage | *0.5* | *0.5* | *0* | *0.5* |
| single linkage | *0.5* | *0.5* | *0* | *−0.5* |

*$n_i$ is the number of elements of $i$ group.

The similarity coefficient *S(A,B)* and the metrics *d(A,B)* introduced in this work are shown in Table 2. Two of the metrics used are particular cases of Minkowski's metric families,[15,33] which are metrics over *Q*. The one not belonging to this family is Gower's distance,[19,30,33−35] amply used in CA.

We calculated a similarity array (72 × 72) for each similarity function and carried out groupings with the methodologies shown in Table 3, which are special cases of Lance and Williams' formula,[31,32]

$$f(k,i) = \alpha_A f(A,i) + \alpha_B f(B,i) + \beta f(A,B) + \gamma |f(A,i) - f(B,i)|$$

where *A,B* and *i* are objects to group, *k* is the reunion of *A* and *B*; *f(A,i)*, *f(B,i)* and *f(A,B)* are the similarity functions between *A* and *i*, *B* and *i* and *A* and *B*, respectively.

Finally, we made and visualized the 16 dendrograms (trees − graphs[36]) employing the graphic interphase TreeView[37] (Internet freeware). Due to their number they cannot be presented in this paper, but they may be requested from the authors. Together with the trees obtained with the 31 described properties we included the atomic number *Z* as a new variable and followed the same procedure. Dendrograms did not vary considerably. As there is an arbitrariness in the choice of a particular grouping or similarity function, we obtained consensus trees to search for those features common to several of the employed methods.

**Consensus Trees.** There are several methodologies to obtain consensus trees.[38,39] We applied the freeware software COMPONENT[39] to obtain 3 different consensuses:

*Majority Rule Consensus*:[40] To build a consensus tree from a set of *N* trees, we take the rule that a pair, a trio, etc. of

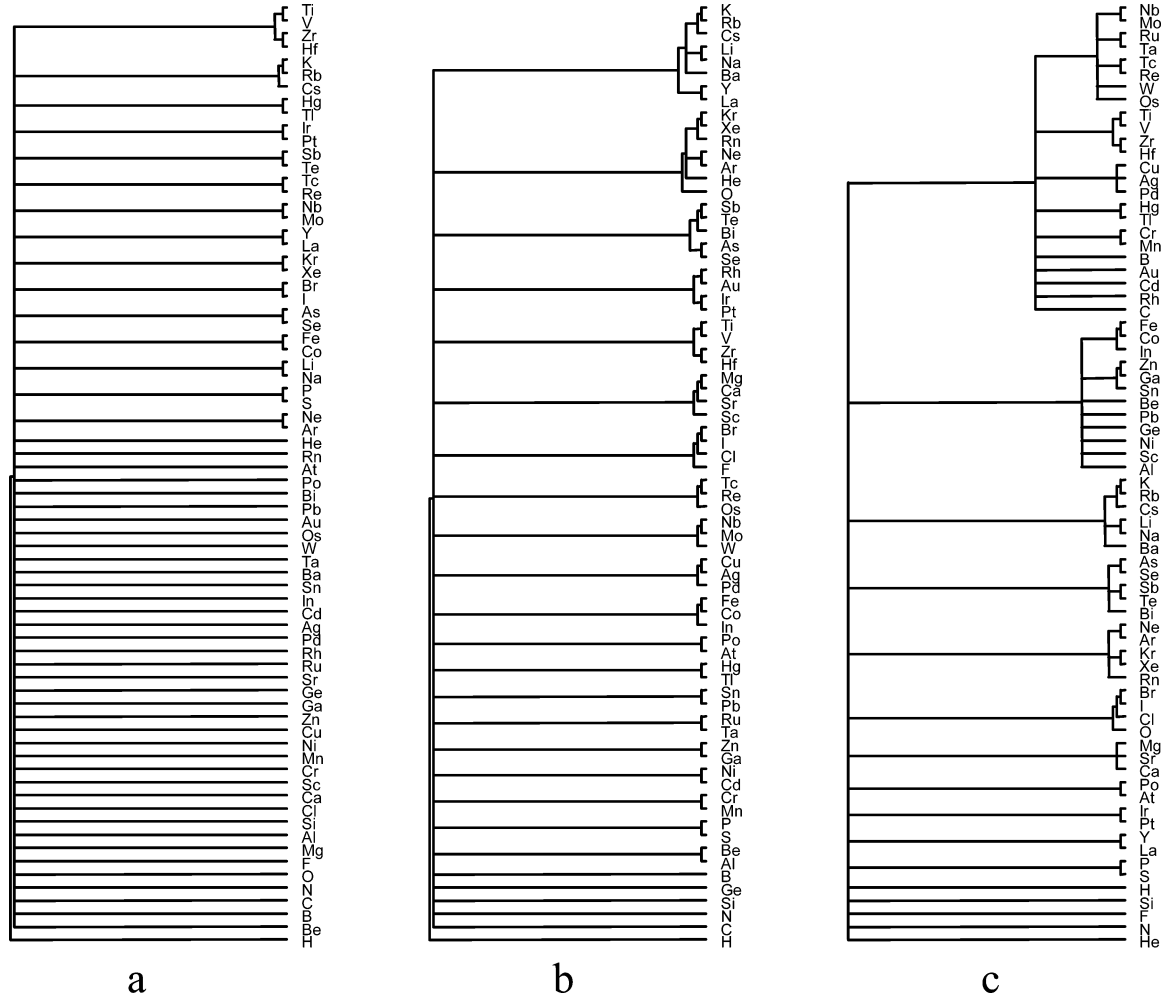


**Figure 1.** Consensus trees: a) strict, b) majority rule, and c) Adams.

elements is a pair, a trio, and so on in the consensus tree if they appear in at least $k$ out of the $N$ trees. Usually, $k > N/2$.

*Strict Consensus*:[39] A tree is called the strict consensus of a set of trees if it is built by the majority rule, taking $k = N$.

*Adams Consensus*:[39] This consensus contains the nestings common to all trees in a profile. Given two sets of elements, *A* and *B*, and a tree *T*, set *A* nests in set *B* if (1) *A* is a subset of *B*, and (2) the elements in set *A* have a more recent common ancestor in *T* than do the element in set *B*. For example, given the tree (*A*,(*B*,(*C*,*D*))), the sets {*C*,*D*}, {*B*,*C*}, and {*B*,*D*} all nest inside {*A*,*B*,*C*,*D*}, but only {*C*,*D*} nests inside {*B*,*C*,*D*}. Consensus Trees and grouping frequencies for Majority Rule Consensus are shown in Figures 1 and 2.

In these consensuses the grouping of alkaline elements and noble gases is clear. On the other hand the couple Be and *Al* appear in 93% of the trees as has been foreseen through the Diagonal Relationship.[4,6]

Some of the papers mentioned above reach this point with other choices of properties. Now, we propose to develop a topological study based on the groupings found in dendrograms.

**Topology from a Single Dendrogram.** As an example we choose the tree obtained through the cosine similarity function and the single linkage grouping methodology (Figure 3). Besides, we interpret every tree as a graph

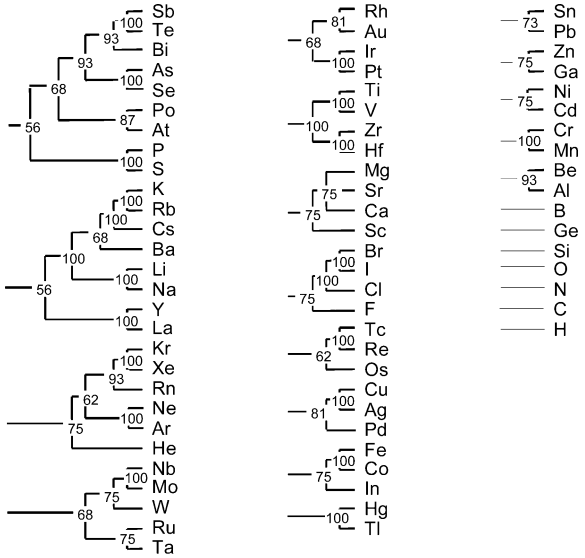

**Figure 2.** Frequencies for majority rule consensus.

acyclic and connected. In our case every graph has three different kinds of vertices: vertices of degree 1 which correspond to chemical elements, of degree greater than 3 which are called nodes and we have only one vertex of degree 2 which is called root of the tree. Aiming to build up a topology from the dendrogram we introduced the concept of subtree.

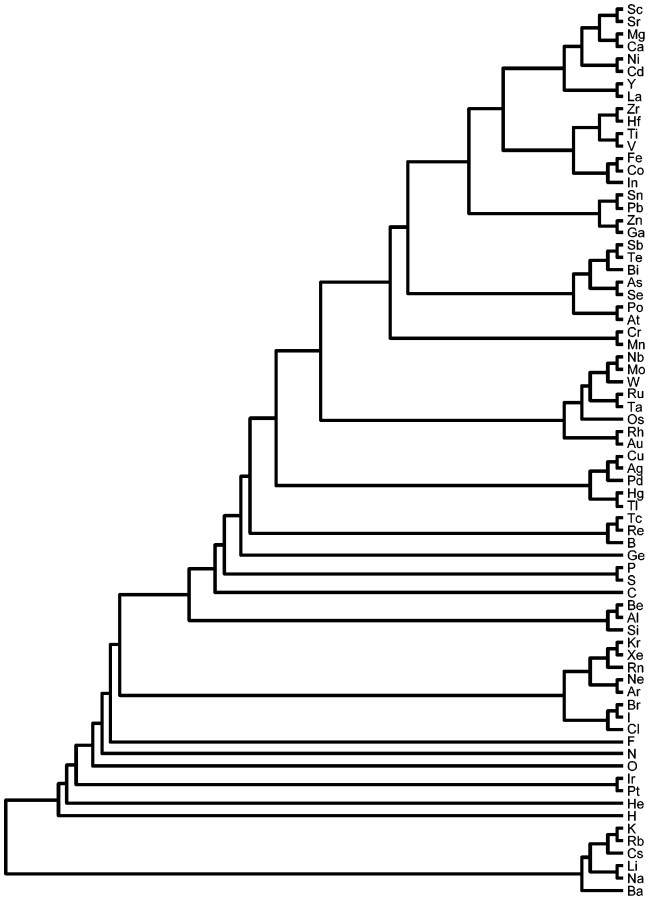


**Figure 3.** Dendrogram obtained from cosine coefficient and single linkage methodology.

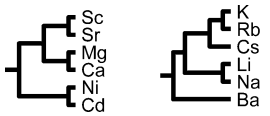


**Figure 4.** Two subtrees of dendrogram of Figure 3.

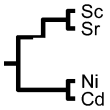


**Figure 5.** An example of a graph which is not subtree.

**Definition 3.** We define a **subtree** as any subgraph $G$ of a dendrogram $D$ such that

1. $G$ does not contain the root.

2. There is a node $p$ of $D$ whose degree is different from 1 such that $G$ correspond to one of the connected subgraphs obtained subtracting $p$ from $D$.

Some instances of subtrees for the tree in Figure 3 are shown in Figure 4.

On the other hand the graph which appears in Figure 5 arises from dendrogram in Figure 3, but it is not a subtree.

**Definition 4.** Let an ***n*-subtree** be a subtree of cardinality less than or equal to $n$.

It means that an $n$-subtree has at most $n$ elements. In this way the subtrees in Figure 4 are examples of *6*-subtrees, *7*-subtrees, ..., $m$-subtrees where $m$ cannot be lower than 6.

**Definition 5.** Let a **maximal *n*-subtree** be any $n$-subtree such that it is not possible to find another $n$-subtree containing it.

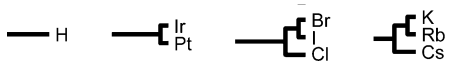


**Figure 6.** Some examples of maximal *3*-subtrees.

Thus, subtrees in Figure 6 are examples of maximal *3*-subtrees.

**Definition 6.** Let $X$ be the set of chemical elements and $\tau$ a collection of subsets of $X$ such that

(1) $X \in \tau$

(2) $\varnothing \in \tau$

(3) *If* $O_1,...,O_n \in \tau$, then $\cap_{j=1}^{n} O_j \in \tau$

(4) *If* $\alpha \in I$, $O_\alpha \in \tau$, then $\cup_{\alpha \in I} O_\alpha \in \tau$ then, $\tau$ is a **topology**, the couple $(X,\tau)$ is called a **topological space**, and the elements of $\tau$ are called **open sets**.

**Definition 7.** Let $(X,\tau)$ be a topological space. A collection $B$ of open subsets of $X$, $B \subset \tau$ is a **basis** for the topology $\tau$ iff each open set $O \in \tau$ is union of elements of $B$.

**Theorem 1.** Let B be a collection of subsets in a non empty set $X$, such that

(1) $X = \cup_{B \in \mathrm{B}} B$;

(2) *If* $B_1,B_2 \in$ B, then $B_1 \cap B_2$ is the union of elements of B; then, B is a basis for topology $\tau$, where $\tau = \{\cup_{B \in \Gamma} B | \Gamma \subseteq \mathrm{B}\}$.

Starting from each tree we search for a collection of subsets of $Q$ fulfilling the conditions in Theorem 1.

**Definition 8.** Let $\mathrm{B}_n = \{B \subseteq Q | B$ *be formed by the elements of some maximal* $n -$ *subtree*$\}$.

From the above it results that for each value of $n$ there may arise a different topology.

**Example 1.** For $n = 1$ we have $\mathrm{B}_1 = \{\{E\} | E \in Q\}$ and $\tau_1 = \mathrm{P}(Q)$, which is called the **discrete topology**.

**Example 2.** For $n \geq 72$ we have $\mathrm{B}_n = \{Q\}$ and $\tau_n = \{\varnothing, Q\}$, which is called the **indiscrete** or **coarse topology**.

As an example we develop the topology $\mathrm{B}_5$ ($n = 5$). For the dendrogram in Figure 3 the basis $\mathrm{B}_5$ is

$$\mathrm{B}_5 = \left\{ \begin{array}{l} \{Sc,Sr,Mg,Ca\},\{Ni,Cd\},\{Y,La\},\{Zr,Hf,Ti,V\},\{Fe,Co,In\}, \\ \{Sn,Pb,Zn,Ga\},\{Sb,Te,Bi,As,Se\},\{Po,At\},\{Cr,Mn\}, \\ \{Nb,Mo,W,Ru,Ta\},\{Os\},\{Rh,Au\},\{Cu,Ag,Pd,Hg,Tl\},\{Tc,Re\}, \\ \{B\},\{Ge\},\{P,S\},\{C\},\{Be,Al,Si\},\{Kr,Xe,Rn,Ne,Ar\},\{Br,I,Cl\}, \\ \{F\},\{N\},\{O\},\{Ir,Pt\},\{He\},\{H\},\{K,Rb,Cs,Li,Na\},\{Ba\} \end{array} \right\}$$

$\mathrm{B}_5$ is a basis for topology $\tau_5$ where $\tau_5 = \{\cup_{B \in \Gamma} B | \Gamma \subseteq \mathrm{B}_5\}$.

**Definition 9.** Let $A \subset Q$ and $x \in Q$, $x$ is said to be a **closure point** of $A$ iff for every $O \in \tau_5$, such that $x \in O$, then $O \cap A \neq \varnothing$.

**Definition 10.** Let $A \subset Q$; the **closure** of $A$ is defined as the following: $\bar{A} = \{x \in Q | x$ *is closure* point *of* $A\}$.

**Definition 11.** Let $A \subset Q$ and $x \in Q$, it is said that $x$ is an **accumulation point** of $A$ iff for every $O \in \tau_5$, such that $x \in O$, then $(O - \{x\}) \cap A \neq \varnothing$.

**Definition 12.** Let $A \subset Q$, the **derived set** of $A$ is defined as the following: $A' = \{x \in Q | x$ *is accumulation* point *of* $A\}$.

**Definition 13.** Let $A \subset Q$ and $x \in Q$, it is said that $x$ is a **boundary point** of $A$ iff for every $O \in \tau_5$, such that $x \in O$, then $O \cap A \neq \varnothing$ and $O \cap (Q - A) \neq \varnothing$.

**Definition 14.** Let $A \subset Q$, the **boundary** of $A$ is defined as the following: $b(A) = \{x \in Q | x$ *is boundary* point *of* $A\}$.

Now we show some application examples of these properties.

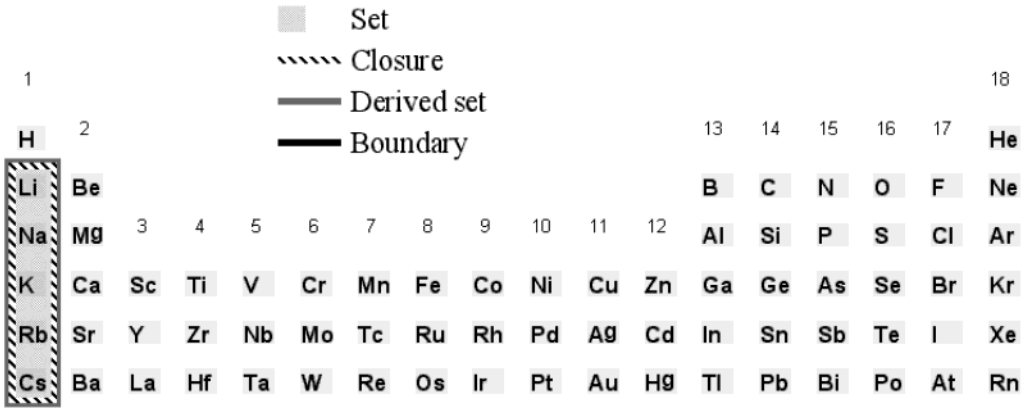


**Figure 7.** Topological properties of alkaline metals based on a single dendrogram.

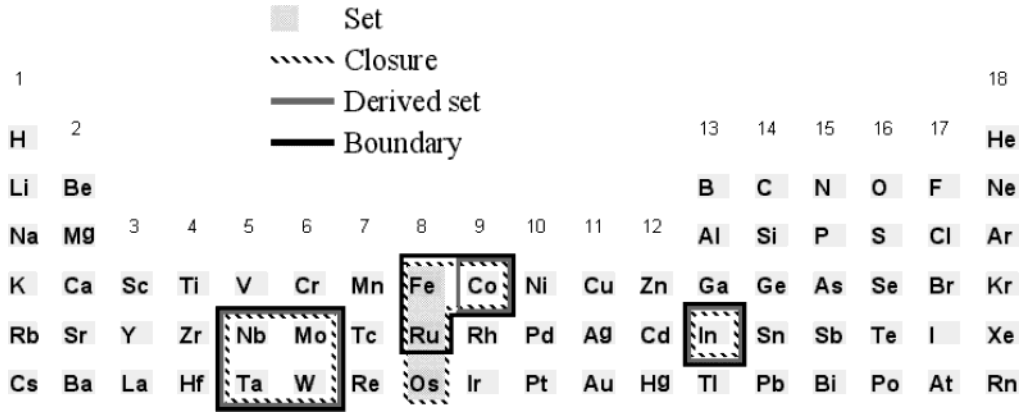


**Figure 8.** Topological properties of elements of group 8 based on a single dendrogram.

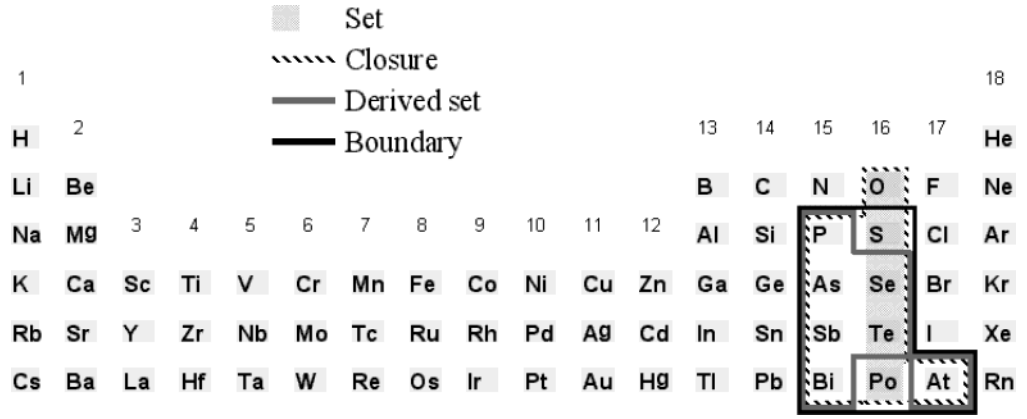


**Figure 9.** Topological properties of chalcogen elements based on a single dendrogram.

**Example 3.** Let $A = \{Li,Na,K,Rb,Cs\}$, this set is a basic open, and it is easily verified that $\bar{A} = A$, $A' = A$ and $b(A) = \varnothing$ (Figure 7).

These results indicate there are not any elements besides the alkalies whose open sets or neighborhoods contain elements strongly related to the alkalies. This, at the same time, indicates that in the space of chemical elements (provided with topology $\tau_5$) alkaline elements form a robust group with little relationship to other chemical elements.

**Example 4.** Let $D = \{Fe, Ru, Os\}$. For this subset $Fe \in \{Fe,Co,In\}$, $Ru \in \{Nb,Mo,W,Ru,Ta\}$, and $Os \in \{Os\}$ which are open sets, then $\bar{D} = \{Fe,Ru,Os,Co,In,Nb,Mo,W,Ta\}$, $D' = \{Co,In,Nb,Mo,W,Ta\}$, and $b(D) = \{Fe,Co,In,Nb,Mo,W,Ru,Ta\}$ (Figure 8).

This example suggests an existence of topological relationships between elements in group 8 and other more distant elements in the Periodic Table such as *In* which is not considered a transition element.[41] It is interesting to remark that topological properties of transition elements show, in general, a similar behavior to the elements of group 8.

**Example 5.** Let $G = \{O, S, Se, Te, Po\}$, thus $\bar{G} = \{O,S,Se,Te,Po,P,As,Sb,Bi,At\}$, $G' = \{Se,Te,P,As,Sb,Bi,At\}$, and $b(G) = \{S,Se,Te,Po,P,As,Sb,Bi,At\}$ (Figure 9).

Here we observe that chalcogen group elements (16) with the exception of oxygen are closely related to pnicogen elements (15), except nitrogen. On the other hand, it is notable that oxygen and nitrogen behave differently from

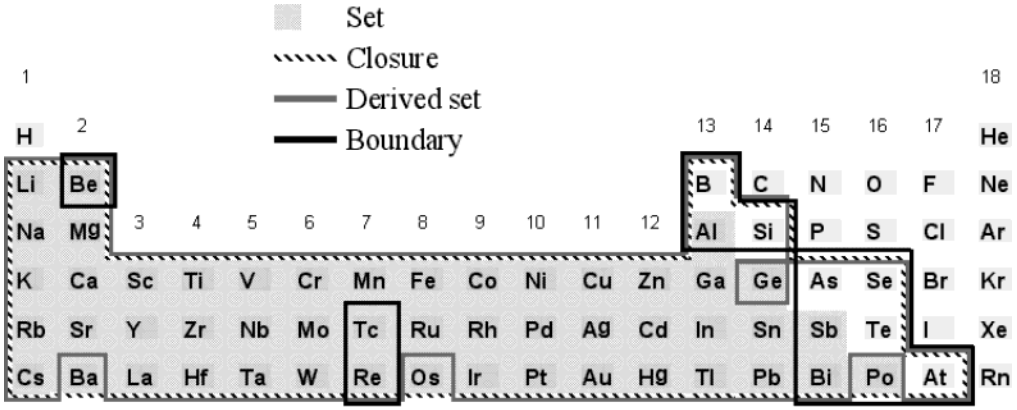


**Figure 10.** Topological properties of metals based on a single dendrogram.

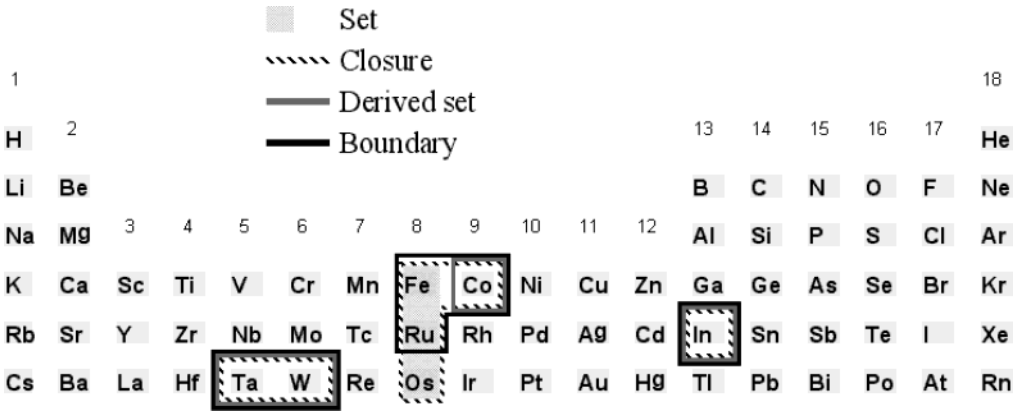


**Figure 11.** Topological properties of elements of group 8 based on a consensus tree.

the rest of the elements in their group as predicted by the Singularity Principle.[3,4]

**Example 6.** Finally, we consider the set of metallic elements.[42] The results obtained are shown in Figure 10.

$$M = \left\{ \begin{matrix} Li,Na,K,Rb,Cs,Be,Mg,Ca,Sr,Ba,Sc,Y,La,Ti,Zr,Hf,V, \\ Nb,Ta,Cr,Mo,W,Mn,Tc,Re,Fe,Ru,Os,Co,Rh,Ir,Ni,Pd, \\ Pt,Cu,Ag,Au,Zn,Cd,Hg,Al,Ga,In,Tl,Ge,Sn,Pb,Sb,Bi,Po \end{matrix} \right\}$$

$$\bar{M} = \left\{ \begin{matrix} Li,Na,K,Rb,Cs,Be,Mg,Ca,Sr,Ba,Sc,Y,La,Ti,Zr,Hf,V,Nb,Ta, \\ Cr,Mo,W,Mn,Tc,Re,Fe,Ru,Os,Co,Rh,Ir,Ni,Pd,Pt,Cu,Ag, \\ Au,Zn,Cd,Hg,Al,Ga,In,Tl,Ge,Sn,Pb,Sb,Bi,Po,At,B,Si,As,Se,Te \end{matrix} \right\}$$

$$M' = \left\{ \begin{matrix} Li,Na,K,Rb,Cs,Be,Mg,Ca,Sr,Sc,Y,La,Ti,Zr,Hf,V,Nb,Ta, \\ Cr,Mo,W,Mn,Tc,Re,Fe,Ru,Co,Rh,Ir,Ni,Pd,Pt,Cu,Ag, \\ Au,Zn,Cd,Hg,Al,Ga,In,Tl,Sn,Pb,Sb,Bi,At,B,Si,As,Se,Te \end{matrix} \right\}$$

$$b(M) = \{Be,Tc,Re,B,Al,Si,As,Sb,Bi,Se,Te,Po,At\}$$

In this example it is interesting to outline that the boundary of metals is formed by several semimetal[42] elements which chemists have considered as having intermediate properties between metals and nonmetals.

**Topology from a Consensus Tree.** Now we show an example making use of Adams Consensus. As in the case of a single tree we consider the maximal *n*-subtrees to build the subsets making up the basis of the topology $B_n$. In this example we used $B_5$.

$$B_5 = \left\{ \begin{matrix} \{Ti,V,Zr,Hf\},\{Ru,W,Ta\},\{Tc,Re\},\{Nb,Mo\},\{Os\}, \\ \{Cu,Ag,Pd\},\{Hg,Tl\},\{Rh,Au\},\{Cr,Mn\},\{B\},\{Cd\},\{Si\}, \\ \{C\},\{Zn,Ga,Sn,Pb\},\{Y,La,Sc\},\{Fe,Co,In\},\{Be,Al\},\{Ni\}, \\ \{Ge\},\{As,Se,Sb,Te,Bi\},\{P,S\},\{K,Rb,Cs\},\{Li,Na\},\{Ba\}, \\ \{Ne,Ar,Kr,Xe,Rn\},\{Br,I,Cl,O\},\{Mg,Sr,Ca\},\{Po,At\}, \\ \{Ir,Pt\},\{H\},\{F\},\{N\},\{He\} \end{matrix} \right\}$$

Here we show the same sets studied in the example above and calculate their topological properties.

**Example 7.** Let $A = \{Li,Na,K,Rb,Cs\}$, again, this set is a basic open set therefore $\bar{A} = A$, $A' = A$ and $b(A) = \varnothing$ and their representations are the same as in Figure 7.

**Example 8.** Let $D = \{Fe, Ru, Os\}$, then $\bar{D} = \{Fe,Co,In,Ru,W,Ta,Os\}$, $D' = \{Co,In,Ta,W\}$, and $b(D) = \{Fe,Co,In,Ru,Ta,W\}$ (Figure 11).

When considering consensus trees and comparing results in Figure 8 it is observed that *Nb* and *Mo* no longer share their neighborhoods or open sets with those elements in group 8. But still the relationship with *In* remains. For transition elements the open sets in the topological basis taken from different dendrograms are not always the same as occurring in a majority of cases for an element in the extremes of the Periodic Table (groups 1, 2, 15, 17 and 18). For this, it is recommendable to study transition elements with the help of consensus trees.

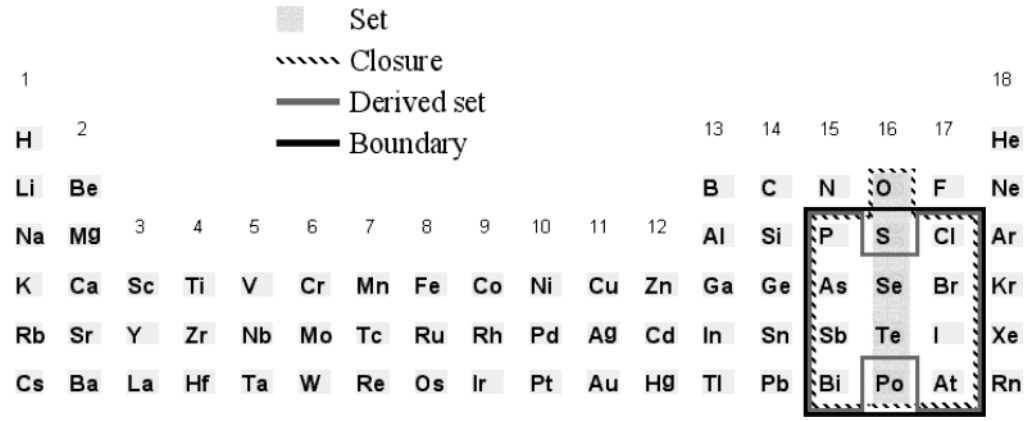


**Figure 12.** Topological properties of calcogen elements based on a consensus tree.

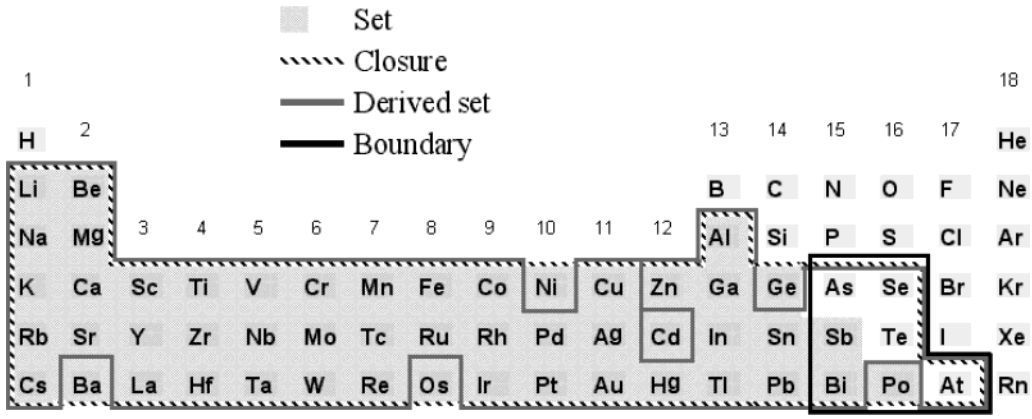


**Figure 13.** Topological properties of metals based on a consensus tree.

**Example 9.** Let $G = \{O, S, Se, Te, Po\}$, thus $\bar{G} = \{P,S,Po,At,Br,I,Cl,O,As,Se,Sb,Te,Bi\}$, $G' = \{B,I,Cl,P,As,Se,Sb,Te,Bi,At\}$, and $b(G) = \{P,S,Po,At,Br,I,Cl,O,As,Se,Sb,Te,Bi\}$ (Figure 12).

In this example the behavior is like that in example 5.

**Example 10.** Finally, we considered metallic elements (Figure 13).

$$M = \left\{ \begin{matrix} Li,Na,K,Rb,Cs,Be,Mg,Ca,Sr,Ba,Sc,Y,La,Ti,Zr,Hf,V, \\ Nb,Ta,Cr,Mo,W,Mn,Tc,Re,Fe,Ru,Os,Co,Rh,Ir,Ni,Pd, \\ Pt,Cu,Ag,Au,Zn,Cd,Hg,Al,Ga,In,Tl,Ge,Sn,Pb,Sb,Bi,Po \end{matrix} \right\}$$

$$\bar{M} = \left\{ \begin{matrix} Li,Na,K,Rb,Cs,Be,Mg,Ca,Sr,Ba,Sc,Y,La,Ti,Zr,Hf,V,Nb,Ta, \\ Cr,Mo,W,Mn,Tc,Re,Fe,Ru,Os,Co,Rh,Ir,Ni,Pd,Pt,Cu,Ag, \\ Au,Zn,Cd,Hg,Al,Ga,In,Tl,Ge,Sn,Pb,Sb,Bi,Po,At,As,Se,Te \end{matrix} \right\}$$

$$M' = \left\{ \begin{matrix} Li,Na,K,Rb,Cs,Be,Mg,Ca,Sr,Sc,Y,La,Ti,Zr,Hf,V,Nb,Ta, \\ Cr,Mo,W,Mn,Tc,Re,Fe,Ru,Co,Rh,Ir,Pd,Pt,Cu,Ag,Au, \\ Zn,Hg,Al,Ga,In,Tl,Sn,Pb,Sb,Bi,At,As,Se,Te \end{matrix} \right\}$$

$$b(M) = \{ As,Sb,Bi,Se,Te,Po,At\}$$

In this case the boundary of metal reduce to heavy metals of groups 15, 16, and 17, a fact known by chemists.

## CONCLUSIONS

There is a clear topological structure underlying the Periodic Law. Thus, a topological space of chemical elements, $(Q,\tau)$ making sense, may be defined using CA. There seem to be topologically invariant sets of elements, such as the alkali metals and the noble gases. Other sets of elements are not invariant, and their neighborhoods, boundaries, and so on seem to have interesting chemical meanings. The important fact is that we have found that the use of point set topology makes clear the origin of known regularities. Now, work must be done to apply it systematically to unravel several other possible properties of the set of Chemical Elements, but more than that, the possibility opens up to study sets of chemical compounds by their properties and move on toward the long cherished dream of periodic tables of compounds. In principle, it is the same methodology, and given that cluster analysis has been used successfully to correlate properties in several sets of elements (see for example ref 29 and references therein), there is reasonable hope that the use of topology will take us further in this direction.

## ACKNOWLEDGMENT

We thank Dr. W. Miao from the University of Texas at Austin for translating Zhou's paper, MSc. J. M. Urbina from the University of Bayreuth for helping greatly with providing bibliographic support, Dr. P. H. A. Sneath from the Uni-

versity of Leicester for his valuable explanations about his work, and finally Dr. R. Isaacs and Dr. J. B. Mayorga from the Universidad Industrial de Santander for their mathematical support and appropriate comments.

## REFERENCES AND NOTES

(1) Brooks, N. M. Developing the Periodic Law: Mendeleev's work during 1869−1871. *Found. Chem.* **2002**, *4*, 127−147.
(2) Mendeleev, D. The Periodic Law of the Chemical Elements. *J. Chem. Soc*. **1889**, *55*, 634−656. (http://webserver.lemoyne.edu/faculty/giunta/mendel.html)
(3) Rodgers, G. E. *Química Inorgánica*; Ed.; McGraw-Hill: Madrid, 1995; Chapter 9, pp 255−280.
(4) Rayner-Canham, G. Periodic Patterns. *J. Chem. Educ.* **2000**, *77*, 1053−1056.
(5) Laing, M. Melting Point, Density, and Reactivity of Metals. *J. Chem. Educ.* **2001**, *78*, 1054−1059.
(6) Laing, M. Periodic Patterns (re *J. Chem. Educ*. **2000**, *77*, 1053−1056). *J. Chem. Educ*. **2001**, *78*, 877.
(7) Scerri, E. R. Has the Periodic Table been successfully axiomatized? *Erkenntnis.* **1997**, *47*, 229−243.
(8) Scerri, E. R.; Kreinovich, V.; Wojciechowski, P.; Yager, R. R. Ordinal explanation of the periodic system of chemical elements. *Int. J. Uncertainty, Fuzziness and Knowledge-Based Systems.* **1998**, *6*, 387−400.
(9) Tonelli, R.; Meloni, F. Chua's Periodic Table. *Int. J. Bifurc. Chaos.* **2002**, *12*, 1451−1464.
(10) Négadi, T. On the Planar Periodic Table. *Int. J. Quantum Chem*. **2000**, *78*, 206−211.
(11) Klein, D. J. Similarity and dissimilarity in posets. *J. Math. Chem.* **1995**, *18*, 321−348.
(12) Klein, D. J.; Babić, D. Partial Orderings in Chemistry. *J. Chem. Inf. Comput. Sci.* **1997**, *37*, 656−671.
(13) Klein, D. J. Prolegomenon on Partial Orderings in Chemistry. *MATCH.* **2000**, *42*, 7−21.
(14) Villaveces, J. L. Química y Epistemología, una relación esquiva. *Rev. Colomb. Filosofia Cienc*. **2000**, *1*, 9−26.
(15) Mendelson, B. *Introduction to Topology*, 3rd ed.; Ed.; Dover: New York, 1990; Chapter 2, pp 29−69.
(16) Bounchev, D.; Rouvray D. H. In *Chemical Topology*; Ed.; Gordon and Breach Science Publishers: Amsterdam, 1999; Prefase, pp xiii-xiv.
(17) Daza, E. E. *Un Concepto más flexible de Estructura Química*, Ph.D. Thesis; Universidad Nacional de Colombia, Bogotá, 2001; pp 48−56.
(18) Zhou, X.-Z.; Wei, K.-H.; Chen, G.-Q.; Fan, Z.-X.; Zhan, J.-J. Fuzzy Cluster Analysis of Chemical Elements. *Jisuanji Yu Yingyong Huaxue.* **2000**, *17*, 167−168.
(19) Sneath, P. H. A. Numerical Classification of the Chemical Elements and its relation to the Periodic System. *Found. Chem.* **2000**, *2*, 237−263.
(20) Robert, D.; Carbó-Dorca, R. On the extension of quantum similarity to atomic nuclei: Nuclear quantum similarity. *J. Math. Chem.* **1998**, *23*, 327−351.
(21) Robert, D.; Carbó-Dorca, R. General Trends in Atomic and Nuclear Quantum Similarity Measures. *Int. J. Quantum Chem.* **2000**, *77*, 685−692.
(22) Firestone, R. B. *Table of Isotopes*, 8th ed.; Ed.; Wiley-Interscience: New York, 1996; pp A1−A4.
(23) Lide, D. R. *CRC Handbook of Chemistry and Physics*, 83rd ed.; Ed.; CRC Press: Cleveland, 2002. (http://www.hbcpnetbase.com/)
(24) Cruz-Garritz, D.; Chamizo, J. A.; Garritz, A. In *Estructura Atómica: Un enfoque químico*; Ed.; Addison-Wesley Iberoamericana: Wilmington, 1991; Chapter 9, pp 675−805.
(25) University of Split, Faculty of Chemical Technology, Periodic Table. (http://www.ktf-split.hr/periodni/en/index.html) Updated March 2003.
(26) Sanderson, R. T. *Chemical Periodicity*; Ed.; Reinhold Publishing Corporation: New York, 1960; p 86.
(27) http://www.chemicool.com/ (Updated November 28, 1998)
(28) Singman, C. N. Atomic Volume and Allotropy of the Elements. *J. Chem. Educ.* **1984**, *61*, 137−142.
(29) Villaveces, J. L.; Cárdenas, C.; Obregón, M.; Llanos, E. J.; Bohórquez, H.; Machado, E.; Patarroyo, M. E. Constructing a useful tool for characterizing amino acid conformers by means of quantum chemical and graph theory indices. *Comput. Chem. C* **2002**, *26*, 631−646.
(30) Sokal, R. R.; Sneath, P. H. A. *Principles of Numerical Taxonomy*; Ed.; W. H. Freeman: San Francisco, 1963; pp 143−154.
(31) Otto, M. *Chemometrics: Statistics and Computer Application in Analytical Chemistry*; Ed.; Wiley-VCH: Weinheim, 1999; pp 148−156.
(32) Brereton, R. G. *Chemometrics: Applications of Mathematics and Statistics to Laboratory Systems*; Ed.; Ellis Horwood: Chichester, 1993; pp 244−262.
(33) Willet, P. Chemical Similarity Searching. *J. Chem. Inf. Comput. Sci.* **1998**, *38*, 983−996.
(34) Lipkus, A. H. A proof of the triangle inequality for the Tanimoto distance. *J. Math. Chem.* **1999**, *26*, 263−265.
(35) Sneath, P. H. A. Private communication.
(36) Hendy, M. D.; Penny, D. Cladograms Should Be Called Trees. *Systl. Zool*. **1984**, *33*, 245−247.
(37) Page, R. D. M. TREEVIEW: An application to display phylogenetic trees an personal computers. *Comput. Appl. Biosci.* **1996**, *12*, 357−358.
(38) Rohlf, F. J. *NTSYS-pc: Numerical Taxonomy and Multivariate Analysis System*; Ed.; Exeter Software: New York, 1992; pp 8−1, 8−8.
(39) Page, R. D. M. *COMPONENT User's manual (Release 1.5) University of Auckland, Auckland;* 1989; Chapter 4, pp 4.1−4.7. (http://taxonomy.zoology.gla.ac.uk/rod/cpw.html).
(40) Margush, T.; McMorris, F. R. Consensus *n*-Trees. *Bull. Math. Biol*. **1981**, *43*, 239−244.
(41) Cotton, F. A.; Wilkinson, G. *Advanced Inorganic Chemistry*, 5th ed.; Ed.; John Wiley: New York, 1988; Cover-back.
(42) Hawkes, S. J. Semimetallicity? *J. Chem. Educ.* **2001**, *78*, 1686−1687.

CI034217Z