Topological space of the chemical elements and its properties

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We carried out a mathematical study of 72 chemical elements taking advantage of the chemotopological method. We selected 128 properties to define the elements (physico-chemical, geochemical and chemical properties). Then, we looked for correlated properties and we reduced the number of them to 90. In this way we defined each element as a 90-tuple. Afterwards, we applied principal component analysis and cluster analysis (4 similarity functions and 5 grouping methodologies). Then, we calculated a consensus tree for the 20 dendrograms generated by the CA. Afterwards, we extracted the similarity relationships from the consensus tree and built up a basis for a topology on the set of chemical elements. Finally, we calculated some topological properties (closures, derived sets, boundaries, interiors and exteriors) of several subsets of chemical elements. We found that alkali metals, alkaline earth metals and noble gases appear not related to the rest of the elements. Also, we found that the boundary of non-metals are the semimetals with a stair-shape on the periodic table.

KEY WORDS: chemical elements, periodic table, topology, cluster analysis, chemotopology

AMS subject classification: 54A10, 05C05, 80A50

1. Introduction

At this moment we have more than 700 [1] periodic tables where the most common is the "short form" [2]. The reason for having so many periodic tables is to show in several ways the patterns or relationships among the chemical

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elements [2]. However, the important fact of the periodic table is not the best representation of the periodic law but the relationships in themselves.

The first periodic table was done considering the physico-chemical and chemical properties of the chemical elements [3]. However, the majority of the studies on the chemical elements developed after 1926 have been done from the quantum theory [4,5]. These studies try to explain the patterns among the elements studying the quantum behaviour of isolated atoms abandoning the study of sets of elements from their properties. However, recent studies [6–12] have shown that it is possible to retake the Mendeleevian methodology of considering sets of elements defined through their properties [3]. The examples of this sort of researching are the works of Zhou et al. [6], Sneath [7] and Restrepo et al. [8–12]. These authors consider each chemical element as a set of properties, the majority of them physico-chemical. These studies follow Mendeleev's methodology considering mathematical tools (chemometric methodologies [13,14]). The common technique applied in these studies is the cluster analysis (CA) [15,16]. Zhou et al. [6] considered 50 elements ($Z=1-50$) making use of 7 physico-chemical properties and some of the clusters found were: {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}. On the other hand, Sneath [7] studied 69 elements ($Z=1-83$, omitting $Z=58-71$) by means of 54 physico-chemical and chemical properties. Some groups found were: {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}. Finally, we developed a study of 72 chemical elements ($Z=1-86$, omitting $Z=58-71$) by means of 31 physico-chemical and chemical properties [8–11]. Some of the clusters found were: {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} and {He}. In the development of that study of the chemical elements we built up a mathematical method for studying the results of the cluster analysis. This method was called "chemotopology" because it combines chemometrics and topology [17]. The chemotopological procedure is a tool that can be applied to whatever set of objects defined through their properties. It extracts neighbourhoods from the results of CA and builds up a topology from those neighbourhoods. A profound discussion on chemotopoly appears in Ref. [17]. Using this method we found that the mathematical boundary of the subset of metals is made from some elements considered as semimetals [8–11]. This result and some others [11] show the importance of the properties in the searching for similarities among the chemical objects (elements and compounds).

Regarding the semimetals, there is not a consensus of opinion in the chemical society on the number and nature of semimetals [18] but it is possible to say, according to the chemical knowledge [2] that they are in-between metals and non-metals in a stair-shaped region of the periodic table. One of our aims in this paper is to show how we can obtain some results on the semimetalicity of the chemical elements using the chemotopological approach and the properties of the elements.

2. Methodology

The chemotopological method can be summarised in two main steps: (1) Study of the similarity relationships among chemical objets by means of CA. (2) Application of general topology to the clusters shown by the results of CA (dendrograms or consensus trees). We applied these steps to the study of 72 chemical elements ($Z = 1$–86, omitting $Z = 58$–71) using 128 properties (57 chemical, 50 geochemical and 21 physico-chemical). Thus, in the present study we used 97 more properties than in the former research [8,9]. The lists of the chemical, geochemical and physico-chemical properties considered in this study appear in table 1–3, respectively.

We can define our set of work in mathematical terms in the following way:

Definition 1. Let $Q = \{q_z | Z$ is the atomic number, $1 \leqslant Z \leqslant 57 \cup 72 \leqslant Z \leqslant 86\}$, then Q is called the *set of chemical elements*.

Then, we normalised each property by means of the following function [8,9]:

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

where x_{jA} is the value of the property j of the chemical element A and $x_{j\min}$ and $x_{j\max}$ are the minimum and maximum j values for all the elements, respectively. In this way we assured that all the values of the properties were in between 0 and 1. Next, we calculated the correlations among the 128 properties and we gathered those with $r \geqslant 0.7$. Thus, we found 38 correlated properties that were not considered for the clustering (CA) of the elements. In this way we reduced the number of properties from 128 to 90. The properties ignored appear in the tables 1–3 with an asterisk (*). Thus, the number of the chemical, geochemical and physico-chemical properties that we used for the next steps of the chemotopological method was 37 chemical, 48 geochemical and 5 physico-chemical properties. On the other hand, the application of principal component analysis (PCA) [27] to this new set of variables showed that the variability of the properties was not concentrated in few components (the first 31 components showed 90% of the accumulated variability). For this reason we did not reduce the dimension of the space of properties by linear combination of the 90 properties.

Table 1
Chemical properties of the chemical elements ($Z = 1$–86, omitting 58–71).

No. of oxidation states [19]	Acid character of oxide [20,21]	Basic character of oxide [20,21]
Minimum common oxidation state [22,23]	Maximum common oxidation state [22,23]	*Reduction potential [20]
*No. of reduction states [19]	Air reaction [23]	Reaction with HCl-6M [23]
Reaction with NaOH-6M [23]	Reaction with HNO_3-15M [23]	E that occur as native minerals [24]
E^a that form hard cations, coordinate	E with intermediate cations	E that make natural mineral alloys with Fe [24]
$F^{1-} > O^{2-} > N^{3-} = Cl^{1-} > Br^{1-} > I^{1-} > S^{2-}$ [24]	(soft cations) that coordinate with O^{2-} [24]	E that make natural mineral alloys with Fe [24]
E that make natural mineral alloys with Os [24]	E that make natural mineral alloys with Cu [24]	E that make natural mineral alloys with Au [24]
E that make natural mineral alloys with Pt [24]	E that form anions [24]	E that form E^{1-} [24]
E that form E^{2-} [24]	E that form E^{3-} [24]	*E that form E^{4-} [24]
*E that appear in nature too without charge [24]	A with which hard cations preferentially coordinate [24]	*A with which soft cations preferentially coordinate [24]
A^b that form minerals with K^{1+} and Na^{1+} [24]	A that form minerals with Au^{1+} [24]	A that form minerals with Ag^{1+} [24]
A that form minerals with Mg^{2+} [24]	*A that form minerals with Al^{3+}, Ti^{4+}, Zr^{4+} [24]	*A that form minerals with Si^{4+} [24]
E^{1+} that form simple oxide minerals [24]	*E^{1+} that form simple fluoride minerals [24]	E^{1+} that form simple sulphide minerals [24]
E^{1+} that form simple bromide or iodide minerals [24]	E^{1+} that coordinate with H_2O or OH^- [24]	E^{2+} that form simple oxide minerals [24]
E^{2+} that form simple fluoride minerals [24]	E^{2+} that form simple sulphide minerals [24]	*E^{2+} that coordinate with H_2O [24]
E^{2+} that coordinate with OH^- [24]	E^{3+} that form simple oxide minerals [24]	E^{3+} that form simple sulphide minerals [24]
E^{3+} that form oxysalt minerals [24]	E^{3+} that coordinate with OH^- [24]	E^{4+} that form simple oxide minerals [24]
E^{4+} that form simple sulphide minerals [24]	E^{4+} that form oxysalt minerals [24]	E^{4+} that coordinate with OH^- [24]
*E^{5+} that form simple oxide minerals [24]	*E^{5+} that form oxysalt minerals [24]	E^{5+} that coordinate with OH^- or O^{2-} [24]
E^{6+} that form simple oxide minerals [24]	E^{6+} that form oxysalt minerals [24]	*E^{6+} that coordinate with O^{2-} [24]

[a] E means elements.
[b] A means anions.

Table 2
Geochemical properties of the chemical elements ($Z = 1$–86, omitting 58–71).

E^a of the Earth's core	E^{1+} lithophiles
E^{1+} commonly content in residual soils and sediments	E^{1+} 2nd–8th most abundant solutes in river water
E^{1+} 8th most abundant solutes dissolved in seawater	*E^{1+} essential to the nutrition of at least some vertebrates
E^{1+} 9th–16th most abundant	*E^{1+} macronutrients solutes on land
E^{2+} lithophiles	E^{2+} commonly concentrated in residual soils and residual sediments
E^{2+} that enter early forming phases in igneous rocks	*E^{2+} concentrated in deep-sea ferromanganese nodules
*E^{2+} least depleted from mantle in formation of crust	*E^{2+} 2nd–8th most abundant solutes in average river water
*E^{2+} most abundant solutes dissolved in seawater	E^{2+} 9th–16th most abundant
*E^{2+} 17th–22nd most abundant	*E^{2+} macronutrients solutes an land
E^{2+} micronutrient solutes on land	E^{2+} that can be limiting nutrients in the oceans
*E^{2+} essential to the nutrition of at least some vertebrates	E^{3+} that enter early forming phases in igneous rocks
E^{3+} concentrated in deep-sea ferromanganese nodules	E^{3+} commonly concentrated in residual soils and sediments
E^{3+} least depleted from mantle in formation of crust	*E^{3+} 9th–16th most abundant
*E^{3+} micronutrient solutes on land	E^{3+} essential to the nutrition of at least some vertebrates
E^{4+} least depleted from mantle in formation of crust	E^{4+} concentrated in deep-sea ferromanganese nodules
E^{4+} commonly concentrated in residual soils and residual sediments	E^{4+} that enter early forming phases in igneous rocks
*E^{4+} most abundant solute in average river water	*E^{4+} most abundant constituents in atmosphere
*E^{4+} 2nd–8th most abundant solutes in average river water	E^{4+} 8th most abundant solutes dissolved in seawater
*E^{4+} 9th–16th most abundant	E^{4+} essential to the nutrition of at least some vertebrates
*E^{5+} commonly concentrated in residual soils and sediments	E^{5+} 17th–22nd most abundant
E^{5+} macronutrient solutes on land	E^{5+} essential to the nutrition of at least some vertebrates
E^{5+} that can be limiting nutrients in the oceans	E^{5+} 9th–16th most abundant
E^{6+} 2nd–8th most abundant solutes in average river water	E^{6+} 8th most abundant solutes dissolved in seawater
E^{6+} 17th–22nd most abundant	E^{6+} macronutrients solutes on land
E^{6+} micronutrient solutes on land	E^{6+} essential to the nutrition of at least some vertebrates

[a] E means elements.
All the geochemical properties of this table were extracted from Ref. [24].

Table 3
Physico-chemical properties of the chemical elements ($Z = 1$–86, omitting 58–71).

Atomic number [20]	*Atomic radii [25]	Atomic volume [23]
Boiling point [19]	*Critical temperature [22,26]	*Density [19]
Electrical conductivity [23]	Electronegativity [22]	Electronic affinity [22]
No. of s e$^-$ in the valence shell [22]	*Heat of atomisation [22,23]	*Heat of fusion [22,23]
*Heat of vaporisation [21]	*Ionic radii [22]	Ionisation potential [19]
*Melting point [19]	Molar heat [22]	*No. of d e$^-$ in the penultimate level [22]
No. of p e$^-$ in the valence shell [22]	Polarisability [22]	*Thermal conductivity [22,26]

According to the above-mentioned, we propose a mathematical definition (Definition 2) for a chemical element and an alternative definition for the set of chemical elements Q (Definition 3).

Definition 2. Let x_{jk} be the j property for k and $q_k = \{\overline{x}_{1k}, \overline{x}_{2k}, \overline{x}_{3k}, \ldots, \overline{x}_{90k} \mid 0 \leqslant \overline{x}_{jk} \leqslant 1\}$. Then q_k is called the k *chemical element*.

Definition 3. Let $Q = \{q_k \mid 1 \leqslant k \leqslant 72\}$, then Q is called the *set of chemical elements*.

We have, at this point, two definitions for the set Q of chemical elements; the former (Definition 1) is related to the protons of the atoms that compound each element and the latter to the properties of the elements. We call the atomic definition *nuclear definition of the set of chemical elements* (Definition 1) and the second one *phenomenological definition of the set of chemical elements*.

Definition 2 allows imagining a chemical element as a point in the space of properties of 90 dimensions where it is possible to calculate the similarity among the points considering their "nearness". We calculated such similarities using the similarity functions (SF) that appear in table 4. Afterwards, we built up clusters of elements using the 5 grouping methodologies (GM) that appear in table 5. These GMs can be obtained from Lance and Williams' formula [13,14,28]:

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

where L is formed by merging clusters A and B and $f(L, i)$, $f(A, i)$, $f(B, i)$ and $f(A, B)$ are the nearness between clusters L and i, A and i, B and i and A and B, respectively.

The Hamming and Euclidean SFs are special cases of the family of Minkowski's metrics [29,30]. The Gower metric is a very used SF when the properties of the objects are defined by continuous and discrete variables, which is our case in this study [7,8]. The Cosine coefficient is not a metric but is used to measure the similarity between objects [30,31] due to the fact that its value refers

Table 4
Similarity functions.

Hamming distance	$d(A, B) = \sum_{j=1}^{n} \lvert x_{jA} - x_{jB} \rvert$
Euclidean distance	$d(A, B) = \left[\sum_{j=1}^{n} \lvert x_{jA} - x_{jB} \rvert^2 \right]^{1/2}$
Gower distance	$d(A, B) = \left[1 - \dfrac{\sum_{j=1}^{n} x_{jA} x_{jB}}{\sum_{j=1}^{n} x_{jA}^2 + \sum_{j=1}^{n} x_{jB}^2 - \sum_{j=1}^{n} x_{jA} x_{jB}} \right]^{1/2}$
Cosine coefficient	$s(A, B) = \dfrac{\sum_{j=1}^{n} x_{jA} x_{jB}}{\left[\sum_{j=1}^{n} x_{jA}^2 \sum_{j=1}^{n} x_{jB}^2 \right]^{1/2}}$

Table 5
Grouping methodologies.

Methodology	α_A	α_B	β	γ
Single linkage	0.5	0.5	0	−0.5
Complete linkage	0.5	0.5	0	0.5
Unweighted average linkage	$\dfrac{n_A{}^*}{(n_A + n_B)}$	$\dfrac{n_B}{(n_A + n_B)}$	0	0
Centroid linkage	$\dfrac{n_A}{(n_A + n_B)}$	$\dfrac{n_B}{(n_A + n_B)}$	$\dfrac{-n_A n_B}{(n_A + n_B)^2}$	0
Ward's method	$\dfrac{n_A + n_i}{n_A + n_B + n_i}$	$\dfrac{(n_B + n_i)}{(n_A + n_B + n_i)}$	$\dfrac{-n_i}{(n_A + n_B + n_i)}$	0

$^*n_j$ is the number of elements of the j group.

to the angle between the two vectors that can be defined for each object under study.

We obtained by means of this clustering procedure a hierarchical classification of the 72 chemical elements. We visualised such a hierarchy using the Internet freeware software TreeView [32] that builds up a dendrogram or complete binary tree for each combination of SF and GM. In this way we built up 20 dendrograms but due to their sizes they cannot be presented in this paper. However, they may be requested from the authors. Now, the question is which of the 20 dendrograms should we select to keep applying the chemotopological method? The answer, as we discussed recently [8,9], is none of them, because it is possible to calculate a consensus tree to search for those features common to several of the dendrograms [33]. We calculated the Adams consensus for the 20 dendrograms through the freeware software COMPONENT [34] (figure 1).

In order to apply the chemotopological approach based on the consensus tree, we extracted the similarity neighbourhoods for the chemical elements from the branches of the consensus tree. These neighbourhoods correspond to the elements that share a hyper-region of the space of properties of 90 dimensions; it means the similarity region in that hyper-space.

The second and final step of the chemotopological method takes advantage of the branches of the consensus tree. In recent works [8–12] we showed
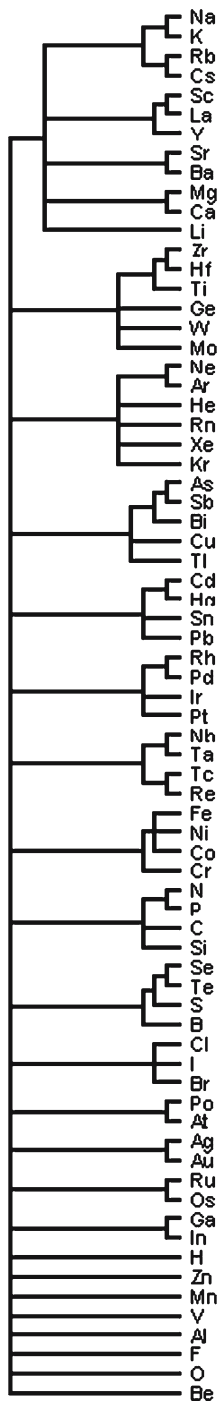
Figure 1. Adams consensus.

the mathematical background of this approach defining subtree, n-subtree and maximal n-subtree as the way to introduce the concept of basis for a topology. We show these definitions in the Appendix A1–A6 of this paper. We made cuts in the tree by means of the chemotopological approach; in this way we obtained the branches of the tree. Using those branches we built up the basis for a topology and taking advantage of that basis we calculated several topological properties that appear in the Appendix A7. We explained, recently [17], the chemical meaning of these topological properties. We show the basis that we built up and the topological properties of some subsets of the chemical elements in the next section.

3. Topological properties of some subsets of chemical elements

We show the basis B_5 that we built up for the set of 72 chemical elements according to the Adams consensus of figure 1, in the following:

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

Taking advantage of this topological basis we studied some subsets of chemical elements and their topological properties.

3.1. Alkali metals

Let $A = \{Li,Na,K,Rb,Cs\}$. For calculating the topological properties (A7) of this set we looked for the neighbourhoods of each element of A in B_5. We have, in this way, that $\{Na,K,Rb,Cs\}$ and $\{Li\}$ appear as open sets of the basis. The topological properties of A are $\overline{A} = A$, $A' = \{Na,K,Rb,Cs\}$, $b(A) = \emptyset$, Int $(A) = A$ and $Ext(A) = Q - A$ (figure 2). These results mean that the alkali metals have no relationships with other elements different from themselves in the hyperspace of 90 properties. On the other hand, the fact of having a derived set where *Li* does not appear means that this element is the one that is less related to the other alkali metals. This is a fact that has been observed through the singularity principle [2,20–36] establishing that the chemistry of the second period elements is often different to the one of later members of their respective groups. It is important to note from B_5 that H appears not related to any other chemical element. This result shows that the classification of the alkali metals without the consideration of H as member of the class is correct and also it supports the idea of not considering H as a member of the first group of the periodic table due to its dissimilarity regarding the alkali metals [2].
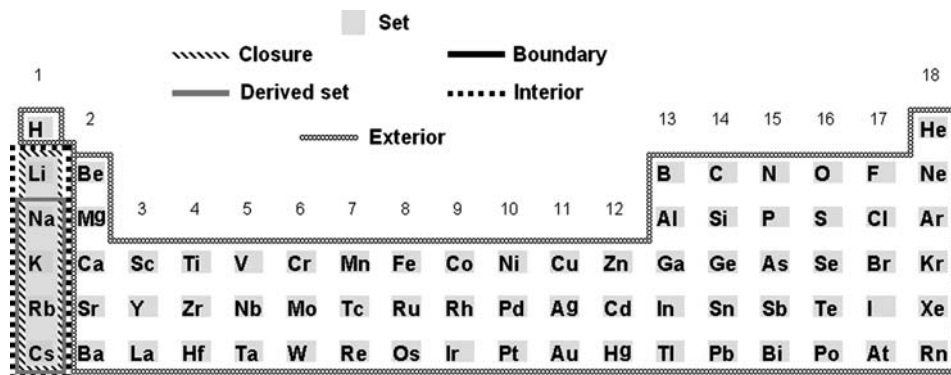
Figure 2. Topological properties of the set of alkali metals.

3.2. Noble gases

Let NG = {He,Ne,Ar,Kr,Xe,Rn}. The topological properties (A7) of NG are $\overline{NG}$ = NG, NG' = {Ne,Ar}, $b(NG) = \emptyset$, Int(NG) = NG and Ext(NG) = $Q - NG$ (figure 3). These results are similar to those showed by the alkali metals, except in the case of the derived set. It is important to note that the groups that are in the extremes of the periodic table (1 and 18 in the short form [2]) have very similar topological behaviour. This means that in the hyper-space of 90 properties the alkali metals and noble gases appear as very dense clusters that do not have any other near element different from alkali metals in the first case and noble gases in the last case.
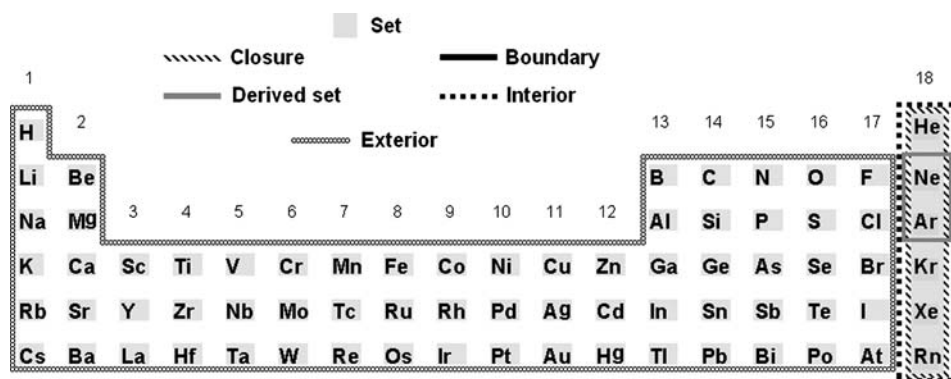
Figure 3. Topological properties of the set of noble gases.
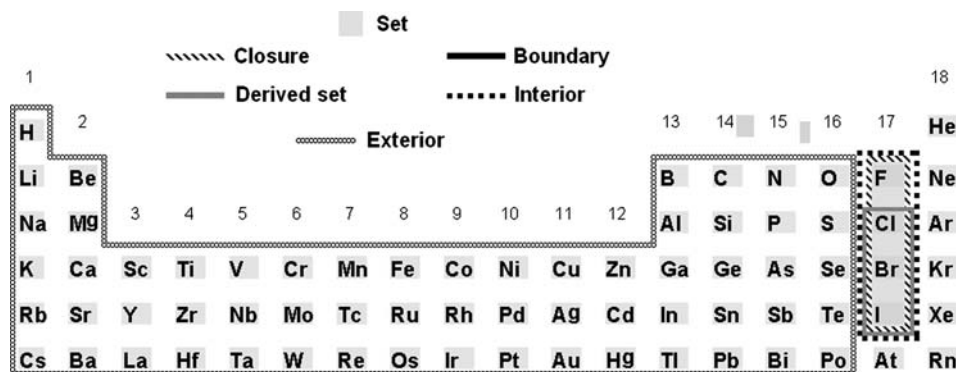
Figure 4. Topological properties of the set of halogens.

3.3. Halogens and the fluorine group

Let HA = {F,Cl,Br,I}. The topological properties of HA are $\overline{HA}$ = HA, HA′ = {Cl,Br,I}, b(HA) = Ø, Int(HA) = HA and Ext(HA) = Q − HA (figure 4). Here we have another evidence of the singularity principle due to the derived set of the halogens does not include the F. On the other hand it is notorious that the topological properties of this set are similar to those of the alkali metals and noble gases. However, an important question is, what is the topological behaviour of the complete group 17 (fluorine group)? The topological properties for this group FG = {F,Cl,Br,I,At} are the following: $\overline{FG}$ = HA ∪ {Po,At}, FG′ = {Cl,Br,I,Po}, b(FG) = {Po,At}, Int(FG) = HA and Ext(FG) = Q − (HA ∪ {Po,At}). Then, when we consider At within the set of halogens, we found that new relationships appear with a different element from themselves (Po). Then, we can say that the At should not be considered as a halogen, as has been correctly classified by the chemists [2].

3.4. Non-metals

Let NM be the set of non-metals and those listed below its topological properties.

NM = {H,He,C,N,O,F,Ne,P,S,Cl,Ar,Se,Br,Kr,I,Xe,At,Rn}

$\overline{NM}$ = NM ∪ {B,Si,Te,Po}

NM′ = {N,P,C,Si,Ne,Ar,B,S,Se,Te,Cl,Br,I,Po}

b(NM) = {B,S,Se,Te,Po,At,N,P,C,Si}

Int(NM) = {H,He,O,F,Ne,Ar,Cl,Br,I,Kr,Xe,Rn}

Ext(NM)=Q–{H,He,N,P,C,Si,O,F,Ne,Ar,B,S,Se,Te,Cl,Br,I,Kr,Xe,Po,At,Rn}.
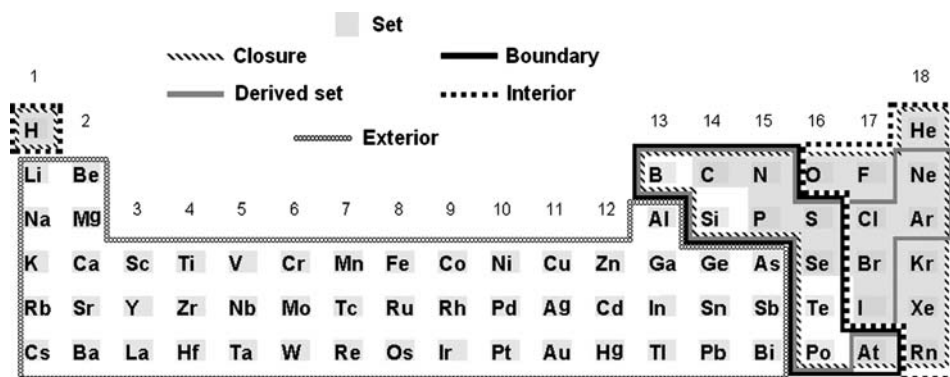
Figure 5. Topological properties of the set of non-metals.

It is important to note that the boundary of NM is made from elements known as semimetals [2]. The most important fact of this result is the stair-shape of this boundary region on the periodic table (figure 5). On the other hand, we found in a previous study [8–11] that the boundary of the set of metals was made from some semimetals of the lower part of the well-known stair-shape division of the metals and non-metals. Furthermore, we showed that the same boundary is the boundary of the set of non-metals of Klemm's classification [37], recently discussed by King [38]. However, in that previous study appeared no element in the upper region of the stair-shaped division of metals and non-metals. Now, in this study we found such a result and also that there is a border between metals and non-metals built up with semimetals. Finally, it is important to state that this new result was possible by the consideration of a large number of chemical and geochemical properties of the chemical elements compared with the physico-chemical properties considered in the previous study [8–11].

4.   Conclusions

We started this study with 128 properties (57 chemical, 50 geochemical and 21 physico-chemical) and we found correlated variables allowing the reduction of the number of them to 90 (37 chemical, 48 geochemical and 5 physico-chemical). In this way we showed that it is possible to define mathematically the chemical elements as 90-tuples of phenomenological properties. Then, we applied the chemotopological procedure and we described a mathematical structure for the set of chemical elements. That structure is the topological space (Q, τ_5), where τ_5 can be generated from the topological basis B_5 that we built up according to the similarities among the elements. Regarding the topological properties of the subsets considered in this study we found that the alkali metals, noble gases

and halogens are groups that do not have any relationship with other elements different from themselves. This means that we can imagine every one of these subsets as isolated groups in the hyper-space of 90 properties used to define each element. We found that hydrogen is a chemical element not related to any other element, where the most important fact is the dissimilarity among the alkali metals and hydrogen. However, hydrogen is commonly placed in the first group of the periodic table, joined to the alkali metals. This result shows that the similarity among the electronic configuration of the valence electrons of an atom is not enough to classify the chemical elements according to their properties. On the other hand, we found evidence of the singularity principle as was in the case of the fluorine (halogens). Also we found that the astatine has different properties from those of the halogens in such a way that, like hydrogen, it cannot be considered as a member of the group of similar elements called halogens. Another result was the fact of finding that the mathematical boundary of the set of non-metals is a set of elements made from semimetals. The stair-shaped region of that boundary in the periodic table was evident, which is in the region between metals and non-metals. Finally it is important to note that these results were the product of taking into account 37 chemical, 48 geochemical and 5 physico-chemical properties.

Appendix

A1. 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 corresponds to one of the connected subgraphs obtained subtracting p from D.

A2. Let an *n-subtree* be a subtree of cardinality less than or equal to n.

A3. Let a *maximal n-subtree* be any *n-subtree* such that it is not possible to find another *n-subtree* containing it.

A4. Let X be a non-empty set and τ a collection of subsets of X such that:

1. $X \in \tau$.

2. $\varnothing \in \tau$.

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

4. If $\alpha \in I$, $O_\alpha \in \tau$, then $\cup_{\alpha \in I} O_\alpha \in \tau$.

Thus, τ is a *topology*, the couple (X, τ) is called a *topological space* and the elements of τ are called *open sets*.

A5. Let B be a collection of subsets of a non-empty set X, such that:

1. $X = \cup_{B \in \mathbf{B}} B$.

2. If B_1, $B_2 \in$ B, then $B_1 \cap B_2$ is the union of elements of B, then B is called a *basis for the topology* τ, where $\tau = \{\cup_{B \in F} B | F \subseteq \mathbf{B}\}$.

A6. Let $\mathbf{B}_n = \{B \subseteq Q | B$ be formed by the elements of some maximal $n -$ subtree$\}$, then $\mathbf{B}_n$ is a basis for the topology τ_n. The proof of this theorem appears in Ref. [16].

A7. Some topological properties are the following:

Let $A \subset X$ and $x \in X$; x is said to be a *closure point* of A iff for every $O \in \tau$, such that $x \in O$, then $O \cap A \neq \emptyset$.

Let $A \subset X$; the *closure* of A is defined as: $\overline{A} = \{x \in X | x$ is closure point of $A\}$.

Let $A \subset X$ and $x \in X$; it is said that x is an *accumulation point* of A iff for every $O \in \tau$, such that $x \in O$, then $(O - \{x\}) \cap A \neq \emptyset$.

Let $A \subset X$; the *derived set* of A is defined as:

$$A' = \{x \in X | x \text{ is accumulation point of } A\}.$$

Let $A \subset X$ and $x \in X$; it is said that x is a *boundary point* of A iff for every $O \in \tau$, such that $x \in O$, then $O \cap A \neq \emptyset$ and $O \cap (X - A) \neq \emptyset$.

Let $A \subset X$; the *boundary* of A is defined as: $b(A) = \{x \in X | x$ is boundary point of $A\}$.

Let $A \subset X$ and $x \in X$; it is said that x is an *interior point* of A iff for every $O \in \tau$, such that $x \in O$, then $O \cap (X - A) = \emptyset$.

Let $A \subset X$; the *interior* of A is defined as: $\text{Int}(A) = \{x \in X | x$ is interior point of A$\}$.

Let $A \subset X$ and $x \in X$; it is said that x is an *exterior point* of A iff for every $O \in \tau$, such that $x \in O$, then $O \cap A = \emptyset$.

Let $A \subset X$; the *exterior* of A is defined as: $\text{Ext}(A) = \{x \in X | x$ is exterior point of $A\}$.

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