

Reflections on the Nature of the Periodic Table of the Elements: Implications in Chemical Education

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Periodic table of the elements (PTE) results essential to understand our nature and place in whole of beings. The same happens with our food, drugs, materials, *etc.* Ideas in PTE should be valued by the number of questions that generate. A series of questions is risen to introduce PTE helping creative thinking. A need exists to develop PTE and its education theoretical and experimental research to understand PTE properties and law. Objective of this report is to present a teaching module based on inquiry-based learning: rising questions, answers and working guide for PTE subject study. Work is performed from viewpoint of empirical didactics and uses experiential methodology based on inquiry-based learning. It accomplishes PTE experimental introduction and its application to chemistry, physics and education *via* atipic examples. Open problem remains in PTE: situating H (in group I but having nothing to do with alkalines). Risk is observed in PTE use. Future trends are analyzed: towards a periodic table of molecules? It is still to be explored methodological application of the approach enriching present teaching techniques: implementing new methods in learning situations is technically simple but checking usefulness in practice of teaching is extraordinarily complex requiring research that hardly began. The PTE represents an opportunity for integrating teaching and research into European Space for Higher Education (ESHE).

Keywords: Periodic system, Periodic law, Periodicity, Valence, Atomic number, Atomic volume, Empirical chemometrics, Qualitative chemistry, Empirical definition, Ordering concept, *Doubly connected* arrangement, Core–valence gap, Scientific achievement, Empirical fact, Empirical didactics, Inquiry-based learning, Preconcept, Philosophical discussion, Culture.

INTRODUCTION

In chemistry, the first systematic correlations come from Lavoisier's law of conservation of mass and energy followed by Dalton conception of structural matter. Nevertheless, Meyer and Mendeleev were the first ones to place the quantitative structure–activity/property relationships (QSARs/QSPRs) in the centre of chemistry with their vision of the empirical periodic table of the elements (PTE); *e.g.*, atomic volume was the first PTE property (*cf.* Fig. 1) measured by Meyer in an attempt to systematize chemical-elements ordering: alkaline-element volume results the greatest from the elements in the corresponding period. However, with the advent of quantum theory (QT) the relations among elements of periods and down groups of PTE acquired in-depth quantitative, meaning relating the elementary electronic structure with the observed atomic reactivity, which in every aspect results a certain manifestation of QSPR pair, which is quantified since the derivation of the associated equation. When two atoms come into contact with each other they perturb the electron distribution within one another, which interplay between the electrostatic potentials of the two atoms in many instances is rather subtle but in some cases it leads to unexpected effects when the two atoms are allowed to bind to each other. Problems (*e.g.*, reactivity, mutual polarizability) that occur when two atoms come into intimate contact are, however, able to be tackled *via* QT.

- a Helium
- b Potassium
- c Rubidium
- d Caesium
- e Radon

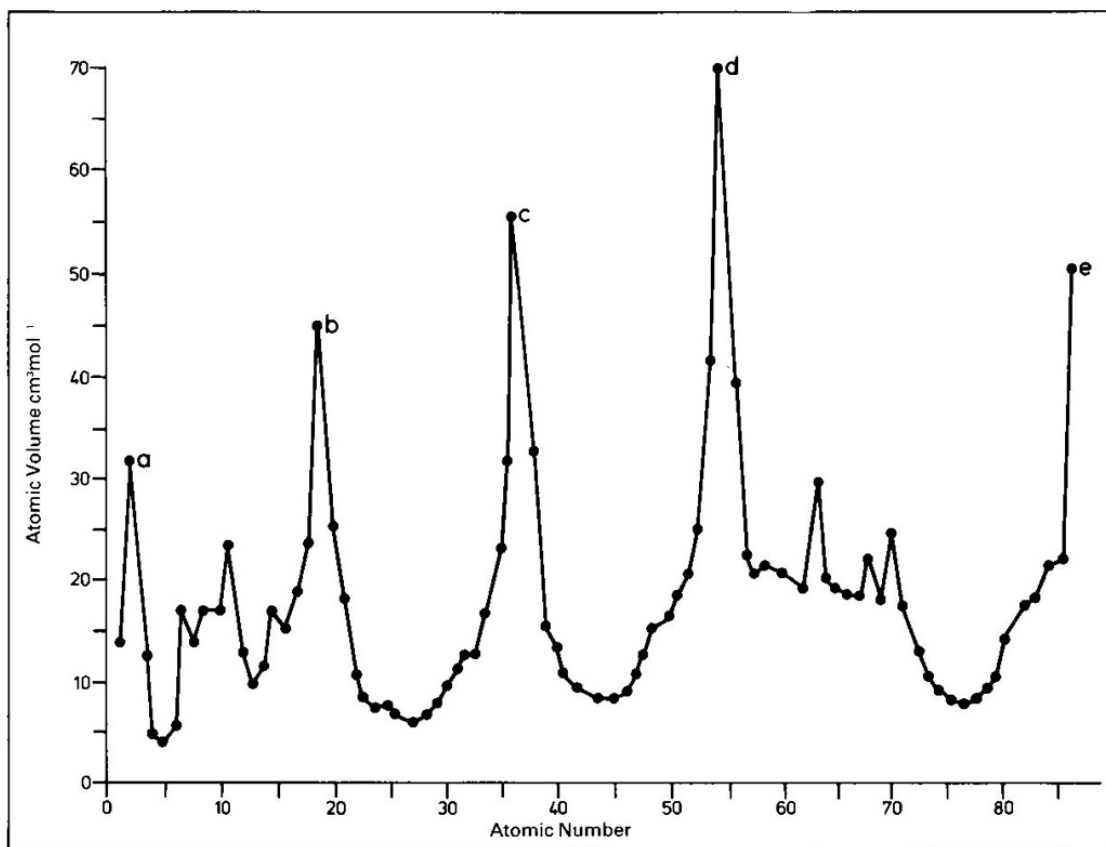


Fig. 1. Variation of atomic volumes with atomic number.

The PTE (*cf.* Fig. 2) illustrates the ability of chemists to summarize a lot of information in a two-dimensional (2D) representation; *e.g.*, alkalines with the greatest volume in the corresponding period lie in group 1A. The PTE was related to electron configurations [1–16]. The PTE results essential to understand our nature and place in the whole of beings. The same happens with food, drugs, materials, *etc.* Elements emergence (nucleosynthesis) in physics was explained [17–19].

	1A	2A											3A	4A	5A	6A	7A	8A
1	H																	He
2	Li	Be											B	C	N	O	F	Ne
3	Na	Mg	3B	4B	5B	6B	7B	8B		1B	2B	Al	Si	P	S	Cl	Ar	
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
6	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
7	Fr	Ra	ACT															
Lanthanide	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu			
Actinide	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lw			

Fig. 2. PTE: American Standard Code for Information Interchange (ASCII)-art representation.

Studies reported students' alternative conceptions that associate the formation of chemical bonds with obtaining a complete shell (octet rule, OR) [20]. This view forces to introduce differentiated teaching strategies facing that thematic [21]. In this group Valero Molina reported PTE and its relationship with daily life [22]. Earlier publications presented empirical didactics [23–25], resonance in interacting induced-dipole polarizing force fields [26], its implementation in chemical education [27] and tool for macromolecular-structure interrogation/retrieval [28]. The objective of the present report is to present a teaching module based on inquiry-based learning for a methodological approximation to PTE study. The goal is to facilitate and implement an *authentic* and question-based approach for science students. The activity is based on empirical didactics. In the last years, the interest for interdisciplinarity in education rose and showed in many didactic renewal projects, which is because of the fact that in the present reality one finds many problems that cannot be solved in one only subject. The multidisciplinary focus moves closer the university to the realism as it allows the study of the problems as they are, extends the curiosity, and increases the observation and research capacities that are restricted *via* partial studies. New didactical techniques are based on empirical fields, *e.g.*, problem solving, planned learning and computer-code implementation. This methodology allowed the Institute to develop a research line in the application

of the Empirical Didactics of Chemistry, Physics and Biology, and Computer-Aided Design (CAD) and Development. The following section exposes open questions in PTE educational introduction. The next section presents the working guide. Following that, two sections state an open question and risk observed in PTE use. Next, a future prospect of a periodic table of molecules is communicated. The following section illustrates the results and divulges the discussion made on its findings. Finally, the last section wraps up the discussion with concluding remarks.

OPEN QUESTIONS IN THE EDUCATIONAL INTRODUCTION OF THE PERIODIC TABLE

The ideas on PTE should be valued by the number of questions that they generate. Schwarz and Rich rose a series of questions (Qs) to introduce PTE and provided answers (As) [29].

Q1. Why are the halogens and alkali metals among the first groups treated in chemistry courses?

A1. A few groups before and after the *inert* gases form PTE empirical *and* theoretical *backbone*.

Q2. What is the physical origin of the periods' lengths?

A2. A large *energy gap* exists among the atomic outer-core shells $1s/2-6p$ and the following valence shells, which causes the exceptional position of the *inert* gases and adjacent groups just before and after them. The sequence of orbital-energy distances forms the quantum-chemical origin of the *periodic law* (PL) periodicity of 2, 8, 8, 18, 18 and 32.

Q3. Why are the closed p^6 shells of the *inert* gases more stable than other closed shells, *viz.* s^2 and d^{10} of chemically *active* metals (of groups 2, 12 and 10) [30]?

A3. A little above ns^2 , np shell exists and a little above $(n-1)d^{10}$, ns shell exists; *no* pronounced energy gaps exist. The near-degenerate $(s-p)^2$ and $(d-s)^{10}$ shells are not really closed.

Q4. Textbooks give the electron configuration of the transition elements as $ns^2(n-1)d^{G-2}$ with a few exceptions (G is the number of valence electrons or group number in PTE and n , the main quantum number or period number). Why is transition-metal chemistry practically pure d-atomic orbital (AO) chemistry [31]?

A4. For all chemically *bonded* transition-metal atoms, $(n - 1)d < ns$, energetically and spatially $(n - 1)d$ is *always* occupied first in the transition-metal cations M^{q+} . The leading configuration of M^{q+} of charges q from G to 0 is $(n - 1)d^{G-q}ns^0$. Only the chemically less important *free* neutral atoms in vacuum present an exceptional ns occupation.

Q5. He, Be–Ra and Zn–Hg present an outer ns^2 configuration. Should one count them as s-block elements? Should the first and last elements of the lanthanoid and actinoid series, *viz.* La, Ac and Lu, Lr, be counted as d- or f-elements [32]?

A5. More important than nomenclature are the facts of chemical behaviour depending on the outer-core shells and frontier orbitals (FOs). Groups-2–12 metals differ in their outer-core and valence FO shells; *e.g.*, the alkaline-earth elements Mg–Ra present outer $(n - 1)p^6$ cores, while the group-12 elements Zn, Cd and Hg show outer $(n - 1)d^{10}$ cores. Helium (He) differs more because it exhibits an inactive $1s^2$ shell without valence FOs nearby. In period n , bonded Y, La and Ac atoms from group 3.0 to the last elements of the f-series, Lu and Lr from group 3.14, present $(n - 2)d^{10}(n - 1)p^6$ to $(n - 2)f^{14}(n - 1)p^6$ core shells with somewhat different atomic and ionic radii (lanthanoid and actinoid contractions) [33,34].

Q6. Are the $(n + l, n)$ Madelung and triad rules basic chemical principles?

A6. The Madelung rule was constructed for neutral, free, chemically unbound atoms. Its statement that ns is occupied before $(n - 1)d$ applies *only to the first two groups* of PTE. The sequence of atomic nl shells changes from the core to valence region and changes in the valence shell from the first two to the later groups. The triad concept is a PL *corollary*, which follows quantum-chemically from the above-mentioned core–valence gaps above $1s$ and np , $n \leq 6$.

Q7. Can one extrapolate the trends of the chemical properties of the elements in PTE with the help of Madelung rule up to nuclear charges of $Z = 120, 200$ or 1000 ?

A7. Of course one *cannot*. The common vertical and horizontal trends begin to change significantly already below period 6. Owing to the short nuclear lifetimes, only little condensed-phase chemistry and gas-phase spectroscopy will exist from period-7 end onward.

Q8. Why does a large energy gap appear above the outer np shells?

A8. The following relation holds for outer shells:

$$(n-1)p \ll (n-2)f < (n-1)d < ns < np \ll \dots \quad (1)$$

Q9. Do valence configurations alone determine the chemistry?

A9. The occupied-orbitals valence configuration of an element is important determining its chemical behaviour; however, its properties also depend on the *lowest virtual* orbitals, *energies and spatial extensions* of FOs and, in the case of heavy elements, on the *spin-orbit splittings*. In addition, the extension and softness of the *outer-core shells* is important.

Q10. If the orbital energy of 4s is always above that of 3d, how does one account for the fact that a 4s orbital must be used before 3d in order to obtain electron configurations in accord with PTE [35–38]?

A10. The explanation follows quite simply from the variational basis of the *self-consistent field* [SCF] model: since it is the total energy and not the sum of the orbital energies which is minimized, no *a priori* reason exists to expect that using the lowest energy orbitals necessary leads to the lowest total energy.

Q11. Why is Ti^{2+} not isoelectronic with Ca [Ar]4s²?

A11. Cation Ti^{2+} is [Ar]3d² rather than [Ar]4s².

WORKING GUIDE

Casanova Freixas and del Barrio Estévez rose questions providing answers. We plan activities, neither objectives nor contents to help teachers stimulate inquiry-based learning. We propose thinking and answering individually the following questions. Pending problems can be worked in groups.

Q12. (a) What does it mean that for H, $Z = 1$? (b) In addition, for U, $Z = 92$?

A12. (a) For H, $Z = 1$ indicates that it presents one proton in the nucleus and one electron in the shell. (b) For U, $Z = 92$ points to it contains 92 protons and 92 electrons.

Q13. What does it mean that a neutral atom of an element presents atomic number $Z = 7$ and mass number $A = 15$?

A13. These mean that it contains seven protons, seven electrons and eight neutrons ($A - Z =$ neutron number).

Q14. What does it mean that an electron is designed by $2, 1, 0, 1/2$?

A14. It means that it is found in the second shell, in subshell p and orbital p_y , and positive spin $1/2$.
Electron configuration: $2p_y^1$.

Q15. Do observe Pauli exclusion principle the following pairs of electrons? (a) $(2, 1, 1, 1/2)$ and $(2, 1, 1, -1/2)$. (b) $(1, 0, 0, 1/2)$ and $(2, 0, 0, 1/2)$. (c) $(2, 0, 0, 1/2)$ and $(2, 1, 0, 1/2)$.

A15. Yes. (a) Two electrons with the same level ($n = 2$), sublevel (2p) and orbital ($2p_x$), and different spin. (b) Two electrons with different level ($n = 1$ and $n = 2$), the same sublevel (s) and the same spin. (c) Two electrons with the same level ($n = 2$), different sublevel (s, p) and the same spin.

Q16. (a) What does the hydrogen ion (H^+) mean? (b) How does the HCl molecule separate in ions?

A16. (a) The H^+ is an H atom that lost the unique electron that it presented. It is, so, a cation and its positive charge is symbolized as superindex. (b) The HCl is a gas that on dissolving in water is separated into two ions, the H^+ cation and Cl^- anion, according to the reaction $HCl \rightarrow H^+ + Cl^-$.

Q17. What does the sodium cation (Na^+) mean?

A17. The Na^+ is a Na atom that lost one electron; *i.e.*, it presents 11 protons and 10 electrons, that is why the positive sign in the formulation.

Q18. Sodium (Na), $Z = 11$, presents electron configuration $1s^2 2s^2 2p^6 3s^1$ or abbreviated $[Ne] 3s^1$; which will be its configuration on losing the electron of the last shell?

A18. On losing the electron of the last shell, Na becomes Na^+ , of configuration $1s^2 2s^2 2p^6$, *i.e.*, the configuration of Ne.

Q19. (a) In which group and period of PTE is found an element which has atomic number $Z = 17$?

(b) Which properties can be deduced according to its position in PTE?

A19. (a) First, one should obtain the electron configuration: $1s^2 2s^2 2p^6 3s^2 3p^5$. It is seen that the last electron level is 3, so it must be found in period 3. The sum of the electrons: $2 + 5 = 7$ indicates that it lies in the group of the halogens. (b) It is a nonmetal that will present high electronegativity, it will tend to form ionic compounds with valence -1 with metals, acquiring OR, and will form molecular acidic oxides.

Q20. What does the chloride anion (Cl^-) mean?

A20. The Cl^- is a Cl atom that gained one electron; *i.e.*, it presents 17 protons and 18 electrons, that is why the negative sign in the formulation.

Q21. Chlorine (Cl), $Z = 17$, presents configuration $1s^2 2s^2 2p^6 3s^2 3p^5$ or abbreviated [Ne] $3s^2 3p^5$; it tends to gain an electron. Which will be its electron configuration on gaining this electron?

A21. The Cl^- acquires the electron configuration of the following inert gas, $1s^2 2s^2 2p^6 3s^2 3p^6$, Ar.

Q22. An element that have a configuration in its last shell of $5s^2 5p^2$, in which group and period of PTE is found and which is its atomic number?

A22. Given that the quantum level is 5, it is deduced that it corresponds to period 5; the sum of the electrons gives 4. Its atomic number is obtained adding the previous levels, taking into account that the configurations of the d and f sublevels are filled in the penultimate and antepenultimate levels: $Z = 2$ (level 1:2) + 8 (level 2:2 + 6) + 8 (level 3:2 + 6) + 18 (level 4:2 + 6 + 10 of the 3d) + 14 (level 5:2 + 10 of the 4d + 2 of the 5p) = 50. It is Sn.

Q23. The following electron configurations, in ground state, are incorrect: (a) $1s^2 2s^2 2p^4 3s^1$; (b) $1s^2 2s^2 2p^6 3s^2 3p^6 3d^3$; (c) $1s^3 2s^2 2p^4$. Indicate the reason.

A23. (a) It is incorrect because before filling the 3s orbital, the 2p orbitals must be completed with six electrons. (b) It is incorrect because before filling the 3d orbitals, the electrons must be placed in the 4s orbital, which presents lesser energy than 3d. (c) It is incorrect because the 1s orbital presents more electrons than is due (maximum 2).

Q24. Which elements are monovalent?

A24. Alkaline metals are monovalent (they present only an electron in the last shell).

Q25. Which elements can form bivalent cations?

A25. Oxygen (O), Ca, Mg, Cd, Zn, *etc.* can develop bivalent cations: O^{2+} , Ca^{2+} , Mg^{2+} , Cd^{2+} , Zn^{2+} , *etc.*

Q26. Which elements can form trivalent cations?

A26. Aluminum (Al), Ni, Fe, Co, *etc.* can develop trivalent cations: Al^{3+} , Ni^{3+} , Fe^{3+} , Co^{3+} , *etc.*

Q27. In addition to inert gases, which species present OR configuration?

A27. As well as inert gases, cation Na^+ ($1s^2 2s^2 2p^6$), anion Cl^- ($1s^2 2s^2 2p^6 3s^2 3p^6$) and cation Fe^{2+} ($1s^2 2s^2 2p^6 3s^2 3p^6 3d^6$) show OR configuration.

OPEN QUESTION IN THE PERIODIC TABLE OF THE ELEMENTS

Q28. A problem remains in PTE: the situation of H. It lies in group I (it presents a unique electron) but it has nothing to do with alkaline metals. In which group of PTE should one place H?

A28. Chemically, H is an element more similar to halogens than to alkalines.

RISK OBSERVED IN THE USE OF THE PERIODIC TABLE OF THE ELEMENTS

Q29. While geologists and mining engineers measure the abundance of an element in the Earth's crust in terms of mass as a proportion of total mass, does it make more sense for chemists to quote abundance in terms of the number of atoms per n atoms, *i.e.*, molar abundance [39]?

A29. This may be suitable for geologists and mining engineers but for chemists it would make more sense to reckon abundance in terms of the number of atoms per n atoms, *i.e.*, molar abundance.

TOWARDS A PERIODIC TABLE OF MOLECULES?

Molecules whether natural or synthetic are made from atoms, which are created in turn from three components: protons, neutrons and electrons. The protons, which are positively charged, and neutrons, which are electrically neutral, form a dense nucleus within the heart of each atom, which is surrounded by a swarm of negatively charged electrons. However, when one puts atoms together to

build molecules certain atoms attract more of the electron density towards themselves on average than others, which leads to the surface of typical molecules being electron rich or electrostatically negative in some areas, and electron deficient or electrostatically positive in others. These facts have implications in rational drug design, QSAR/QSPR, pharmacophore model, *etc.*

RESULTS AND DISCUSSION

Students learn most effectively about science when the material is interesting and relevant. To begin again the interest in the students that want to study PTE, chemistry, physics and beyond is by far to offer interesting courses and practical sessions, which allow scholars to use modern methodology that put text-book theory in their hands in an easy-to-use and direct way. A series of questions was risen to introduce PTE and provide creative thinking. The peer groups had to discuss and explain these questions based on their respective experience and expertise. The discussion was open to questions and answers. As a matter of fact, it was not a must to reach to a consensus. The challenge is for teachers and those that work in developing relevant didactic tools that excite the chemists of tomorrow. It is unknown if the training model experienced with our didactics is going to be exerted or not by our future teachers in its professional life but it is thought that a first step was taken in that direction. The outcome of this teaching module will be changes in classroom practice, reflecting improved concepts of science teaching.

The PTE is empirical: more important than nomenclature are the facts of chemical behaviour depending on the outer-core shells and frontier orbitals. The PTE illustrated the ability of chemists to summarize information in a 2D representation. However, an open problem remains in PTE and it is the situation of H: it lies in group I but it has nothing to do with alkalines. A risk was observed in PTE use. Future trends were analyzed: towards a periodic table of molecules?

Diversification is the word of the day: we should use the technologies that best fit our needs in order to solve the problem. New paradigms should be tested. Research and development task is essential. Challenge is needed for the digital society.

CONCLUDING REMARKS

From the present teaching module of inquiry-based learning the following remarks can be drawn.

1. The general objectives of this work were accomplished: the familiarization of students with interdisciplinarity and use of empirical didactic methodology based on inquiry-based learning. An introduction *via* an empirical way for subjects, *e.g.*, chemistry, physics, *etc.* was solved. In the treatment of the periodic table, topics were avoided and our methodology allowed using new examples. Naturally, in an empirical didactics of chemistry, the knowledge of the answer to a question is not precisely the final objective but learning the techniques that lead to its discovery. A need exists to develop theoretical and experimental research on the periodic table and its didactics to understand periodic properties and periodic law. Our series of questions and answers was written for the analysis of information from the periodic table. This effort allows a better didactic strategy and methodological adaptation for study of periodic table, *etc.* in chemical education. Teachers will find the approach useful for demonstrations. In addition, questions can be used by students to explore periodic table, *etc.* and their implications in chemistry and its education.

2. The study of the periodic table of the elements was included in different phases of the Grade of Chemistry. Our procedure helped understanding the concepts of the periodic table, periodic properties and periodic law. It is still to be explored the methodological application of this approach enriching the present teaching techniques: implementing new methods in learning situations is technically simple but checking their usefulness in the practice of teaching is extraordinarily complex and requires a research that hardly began. The subject of the periodic table represents an opportunity for the integration of teaching and research into the European Space for Higher Education. A work in progress will adapt the study of the periodic table to a learning strategy based on the statement of a situation, case-based learning and problem-based learning. It is interesting to study the possible generalization of the conclusions above to the periodic properties and periodic law, chemistry, physics and beyond.

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