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Computational Chemistry Programs as a Facilitating Tool in the Teaching and learning Process

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Authors' contributions

This work was carried out in collaboration between all authors. Authors FDS, KLBS, LDS and CBRS designed the study, wrote the protocol, involved in writing the first draft, participated in experiments and data collection. Authors CCL, JSC and GACL managed the literature search, analyses of the study and manuscript preparation. Authors FDS, KLBS, LDS and CBRS performed data interpretation and were actively involved in reading the manuscript. All authors read and approved the final manuscript.

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ABSTRACT

Aims: To verify the influence of the role of ICT's (Information and Communication Technologies) as a teaching and learning process in the classes of chemistry discipline for the 3rd years high school students, and show the importance of computational chemistry programs as a methodological alternative in the comprehension of chemical concepts of macroscopic and microscopic order.

Place and Duration of Study: The research was carried out in a public high school in the city of Macapá-AP, Brazil.

Study Design: The sample population was made randomly with 3rd year high school students and the data was collected through surveys.

Methodology: The research was qualitative and initially was made the choice randomly of 54 students of the 3rd year of high school. The students were divided into two groups: Control Group (CG) and Experimental Group (EG), being each group was constituted by 27 students, where were applied traditional classes for both groups with same contents: chemistry concepts, chemical bonds, polarity of molecules, electronegativity, molecular geometry, physical and chemical properties of the molecules of ozone (O_3), water (H_2O), carbon dioxide (CO_2), methane (CH_4) and to analyze the students' comprehension about the importance and presence of these molecules in contextualization with biotic and environmental factors. The computational chemistry programs (ChemSketch and PhET Simulations) were used in the intervention classes only for students of the EG. Data collection was conducted through of a survey with open-ended and closed-ended questions. Surveys were applied for the groups after the classes (CG) and classes+intervention (EG). The responses of CG and EG were compared considering the same content studied, in order to evaluate the student's learning level and their opinions about the use of ICT's in chemistry classes.

Results: The students' responses related to the geometry of the ozone (O_3), water (H_2O) and carbon dioxide (CO_2) molecules showed superiority of GE compared to GC by differences of 40.74%, 29.63% and 37.03%, respectively. Comparing the two groups on the conception of the influence of the geometry on the behavior of molecules studied in the environment, the effect observed was a difference between the results of the groups of 18.52%, being 62.96% (CG) and 81.48% (EG). Molecular geometry is influenced by intra-molecular interactions, which may lead to polar or nonpolar structure and influences the physical properties and increases or decreases the reactivity of the molecule in the environment. The results show that, according to the students of EG, the use of ICT's in the classroom is important and ensures the computational chemistry programs as a facilitating tool, and can aid to improve the learning of concepts that were previously difficult to understand.

Conclusion: ICT's together with the contextualization of the contents have proven themselves as a very significant methodology and caused a positive influence in the teaching-learning process, due a strong relationship with the abilities and potentialities that these technological tools. This resource facilitated the formalization of ideas and consequently the understanding of content, helping students to obtain greater understanding of the concepts studied. Concerning the application of the intervention, amid different ideas, for most students the classes with the use of chemical programs have made the learning more meaningful.

Keywords: Chemistry software; information and communication technologies (ICT); chemistry teaching; chemistry teaching methodology.

1. INTRODUCTION

The appropriation of different technologies by citizens is fundamental for economical and social development of a nation. The technological advance experienced by the "information society" (21th century) provides development, and the scholar environment cannot be excluded from the benefits that technological innovation can provide. The Information and Communication Technologies (ICT's) are any kind of technology created by man that is capable to represent or convey information, from a simple pen, to something much more advanced as a computer, for example. ICTs are important because they are inserted in various ways in contemporary society, like the forms of social organization and practice, health, education, among others. The school has, among many other functions, the one to form critical citizens and professionals to enter the labor market. In this context, the ICTs are tool that can be used to aid school on this formation [1].

New proposals for education, for example chemical teaching, have been researched in order to facilitate the teaching and learning process, without prioritizing a methodology full of mathematical formulas and scripts that not always are accessible to students and that may drive them away from the main objective which is to understand the chemical science and its relations with nature, economy and society, as advocated by the National Curriculum Guidelines for High School (NCGHS) and in the Law of Guidelines and Basis of National Education (LGBNE/9394/1996) [2,3].

NCGHS are the basic reference for the development of common content for high school. NCGHS were designed to spread the principles of the curriculum reform and to guide teachers in the search for new approaches and methodologies. NCGHS establish a profile for the curriculum, based on the basic abilities to insert young, guide teachers on the significance of school knowledge, which must be contextualized in an interdisciplinary approach, and encourage logical thinking and the ability of students to learning [3].

The informatics as an educational tool can provide opportunities of improvement in learning environments, making feasible the exchange of information, experiences and knowledge, thus functioning as mediator in construction of new knowledge and potentialities. It's noteworthy that the new ICT's are not the solution to the educational problems, but a resource that must be adapted to education [4]. Distant from that, indeed, in most of schools the use of ICT's happens in disjointed and compartmentalized way, perpetuating the traditional teaching without much interactivity between subject and student [5]. Studies pointed that overloaded curriculum, lack of equipment and inappropriate training are some reasons for the absence or bad use of ICT by teachers [6].

It is notable that education now crosses a crucial moment in respect to ICTs use, and in recent years efforts have been make these resources available to schools [6,7]. But it is not simply about that such resources are available at the school, but it's a matter of to know how to use them, considering the deficiencies, and mainly, the socio-educational needing existing in the school. However, before possible applications, it must be defined how the technological resources will be applied. Science teachers need to be able to use a range of ICT related resources effectively in the science classroom [7]. The possibility of the teacher of appropriating these technologies integrating them to the chemistry teaching and learning environment can generate a more dynamic teaching of chemistry, and more closer to the constant changes that society has experienced, creating new knowledge spaces [8,9]. In previous history and current times, difficulties of this kind are proceeding from particular, abstract and non-observable nature.

ICT's can be a facilitating tool in this understanding, reducing the gap left in this learning process, where the students have difficulties in establishing relations between the learning levels in chemistry. In this way, it seems quite likely that the use of analogical models and computational graphs in structured teaching situations could be productive for students to appropriate of forms of chemical thoughts, according to what some studies have shown [10].

The use of computers is a natural practice at all levels of teaching and learning process, whether at the school or outside it, practically from the moment they were created. Computers have the capability of simulate situations and phenomenon which are not naturally observed a fundamental resource in educational environments, once it stimulates imagination about the behavior of a given phenomenon, transforming the monitor screen in a laboratory [11]. Such capability of experimentation, whether by software or in the internet, makes the students experimenters through the various possibilities that are offered and through the unexpected results, being surprised with the unpredictable, what makes them more inventive and creative. The use of the computer has to be done in cultural manner, generating a favorable environment to the meaningful learning. The teacher becomes the mediator between student and computer, organizing the knowledge in systematic way, strengthening teaching actions and also the learning processes and development of higher mental functions [12].

In virtual environments, students can perform simulations of situations that are not available in the traditional classroom. Other authors on previous research addressed the question of whether the lessons with simulations or virtual labs had the same efficiency on student learning than lessons in real laboratories, and these studies have shown that both methods resulted in improvement of students' knowledge with no significant differences in the acquisition of scientific concepts [13,14]. These virtual environments are promising in improving school performance, ensure greater involvement and development of abilities such as investigation, critical thinking, use of technology and communication [15]. The integration of ICT into teaching methods benefits not only the students, but also provides cumulative development of competencies in the teachers who use it [16]. The first reference to the use of information technology by chemistry teachers at school dates back to 1959, in the United States. Only after 1969, at Texas University, a project was developed to evaluate and perform simulation of laboratory experiments to be used in chemistry classes [17].

In context of ICTs, four concepts are relevant: media, multimedia, hypertext and hypermedia. Media is characterized by texts, images, sounds, movies, cartoons, and graphics. Multimedia corresponds to the use of different forms of media together in a specific medium, for example, the computer. Hypertext refers to the nonlinear writing, where the reader access the segments that make up a text in different sequences, from its personal interest, face of alternatives presented interactive resources of computer. Hypermedia is then the union of multimedia and hypertext [18]. Programs are classified as hypermedia, allowing the interaction with the user through links offered by hypertexts, where each element that makes it up is structured, so that there is contribution of different media [19]. Computational chemistry programs permits to access models, illustrations, equations, phenomenon, interactions of microscopic order, besides relate concepts from an interactive interface [20]. The combination of iconographic characteristics with the convergence of representation means in window ambience is also particularly attractive for education in sciences, especially when considering the transposition of the phenomenon from natural environment to the computer [10].

The development and the further use of programs in classroom help in the resolution of chemistry problems, and the versatility of computational chemistry allows not only its application in chemistry teaching, but also in research and development areas. Many programs are available on the internet for download and free access and others can be bought from their manufacturers. These tools, when properly applied, besides motivates learning, collaborate with the adaption of the student in a increasingly technological society. The advantages of the use of chemistry software are related with the modes of knowledge construction, because simulations offer an interactive environment for the student to manipulate and observe immediate results, proceeding to the modification of situations and conditions [21-23].

Computational modeling has great potential to allow students to understand the theoretical principles of the natural sciences and mathematics. It supports the student's perception to the construction of knowledge, because it can incorporate in a single moment many forms of representation of the system in study, whether they are written, visual and sound. Using just exposing class, it's almost impossible to describe the dynamics of a phenomenon, it's necessary that the students develop a certain degree of abstraction to the comprehension of the content. In this way, computational modeling in Chemistry contributes to the cognitive development in general; facilitate the construction of relations and meanings, potentiating the pedagogical possibilities of interaction between teacher and student [24,25].

This work aimed to verify the influence of the role of ICT's as a teaching and learning process in the classes of chemistry discipline for the 3rd years high school students with ChemSketch [26] and PhET Simulations [27] programs in a public high school in the city of Macapá-AP, Brazil, and show the importance of computational chemistry programs as a methodological alternative in the comprehension of chemical concepts of macroscopic and microscopic order.

2. MATERIALS AND METHODS

2.1 The Study Object of the Research

The study was conducted in a public high school in the city of Macapá-AP, Brazil. Initially 54 students randomly of the 3rd years of high school were divided into two groups, control group (CG) and experimental group (EG), being each group constituted by 27 students, where were applied traditional classes for both groups on the content of chemistry concepts, chemical bonds, polarity of molecules, electronegativity, molecular geometry, physical and chemical properties of the ozone (O_3), water (H_2O), carbon dioxide

(CO_2), methane (CH_4) molecules by the same teachers. In addition to evaluate the students' comprehension about the importance and presence of these molecules in contextualization with biotic and environmental factors, and the opinion of students about factors related to the use of the ICTs and, featured in, the use of chemical programs.

2.2 Computational Chemistry Programs Used for Intervention

The computational chemistry programs (Chem Sketch and PhET Simulations) were used in the intervention only for students of the EG as a facilitating tool in the teaching and learning process. In the EG emphasized the use of the programs with respect to three-dimensional (3D) simulations of the studied molecules (O_3, H_2O, CO_2 and CH_4), that is, the teacher helped the construction of the chemical structures attempting to lead an alternate reality with the use of the software in order to motivate students in the teaching and learning process.

2.2.1 Chemsketch program

ChemSketch is an integrated package to the Advanced Chemistry Development (ACD) program and has a module of generation and 3D visualization of molecules namely ACD/3D Viewer, which were taught to the students of EG several forms of representation of the chemical structure of the ozone (O_3), water (H_2O), carbon dioxide (CO_2), methane (CH_4) molecules, for example: wireframe (type of 3D representation that shows the molecule in form of "lines"), Sticks (type of 3D representation that shows the molecule in form of "sticks"), Ball & Sticks (type of 3D representation that shows the molecule in form of "balls and sticks"), Space fill (type of 3D representation that shows the empty spaces of the molecule as "filled" (similar to Stuart model), Dots Only (type of 3D representation that shows "only dots" representing the atoms and bonds in molecule), Disks (type of representation that show atoms in form of disks, very similar to Space fill form, however without the 3D effect), With Dots (shows the "dots" of 3D representation in any form of visualization), with Dots combined with Ball & Sticks, as well as chemistry concepts and chemical bonds.

2.2.2 PhET simulations program

PhET Interactive Simulations (Physics Education Technology) is an initiative of Colorado University, whose purpose is to offer a package of simulations that may help in the way the Sciences (physics, chemistry, mathematics and biology) are taught and learned. PhET Simulations is available on the internet through the site http://phet.colorado.edu [27] and can be freely used. The provided ambience of simulation can be executed directly in the internet or in an installation package (available for different operational systems), that can be downloaded and installed in local machines [27]. PhET Simulations program was used for investigations on chemistry teaching of the contents of polarity of molecules, electronegativity, molecular geometry, physical and chemical properties of the ozone (O_3), water (H_2O), carbon dioxide (CO_2) and methane (CH_4) molecules.

2.3 Construction of the Questionnaires

Conduction of survey in a qualitative way with the application of open-ended and closed-ended questionnaires. The questionnaires had objective of evaluate the student's concepts related to the geometry of molecules, conceptions about the influence of molecular geometry in substances' behavior in the environment, conceptions on the difference between physical states of the substances in environment, use of other methodological resources in chemistry classes, student's opinion related to the content taught in the intervention and student's opinion related to the use of chemical programs as an educational tool.

2.4 Collection and Evaluation of Data

Data collection was conducted by the application of a survey with open-ended and closed-ended questions, which were applied after the classes (CG) and classes+intervention (EG) for both the Control and Experimental groups. The teachers were present to inhibit interaction between the students during the survey. Then, the responses of CG and EG were compared considering the content studied, in order to evaluate the student's learning level and their opinions about the use of ICT's by the teacher in chemistry classes.

2.5 Ethical Aspects

Questioning of ethical aspects, where participants were instructed that there would be assurance of anonymity, because their ID's in their respective evaluation activities were treated in a respectful and confidential manner, and aimed to defend the interests of research participants in its entirety dignity to contribute to the development of research within ethical standards.

3. RESULTS AND DISCUSSION

In this section are explained the student's concepts related to the geometry of molecules, the conceptions about the influence of molecular geometry in substances' behavior in the environment, the conceptions on the difference between physical states of the substances in environment, the use of other methodological resources in chemistry classes and the student's opinion related to the content taught in the intervention

3.1 Student's Concepts Related to the Geometry of Molecules

The student's conceptions about the geometry of the ozone (O_3), water (H_2O) and carbon dioxide (CO_2) molecules were assessed through the following question: "What is the type of geometry of molecules of O_3, H_2O and CO_2?", for both the groups (CG and EG). The Results are shown in Figs 1, 2 and 3.

Fig. 1. corresponds to the understanding of the molecular geometry of the ozone (O_3) molecule, comparing both groups, CG and EG, with such question in closed nature, having just one correct answer among the following assertions: angular, linear, pyramidal, trigonal, tetrahedral. It can be seen that the yield of EG was higher than the CG, that is, students of the first group significantly assimilated the concept related to the issue, but students of CG did not have clear understanding of the geometry of O_3. Taking the difference between the yields of GC (33.33%) and EG (74.07%), 40.74% is obtained. The wrong item most repeated by the students was the one that pointed the geometry of O_3 as linear, contributing expressively to the increase of errors in CG. This did not occur with the EG due to the use of the programs, which facilitated the understanding of the concepts of geometry.

In these terms, ozone is a dark-blue atmospheric gas, which concentrates in stratosphere, in a region between 20 and 40 kilometers of altitude in the atmosphere, has a structure if form of V, due to the presence of not-bonding electron pairs present in central atom. In another words, its structure is Angular [28,29].

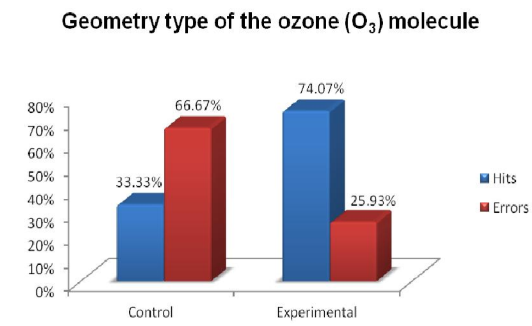

Fig. 1. Geometry of the ozone (O_3) molecule, according to CG and EG

Fig. 2. corresponds to the student's understanding about molecular geometry of water (H_2O), comparing both groups (CG and EG), where the question is of closed nature, with just one correct answer among the following assertions: angular, lineal, pyramidal, trigonal, tetrahedral. A little difference occurred among right and wrongs in CG (3.70%). Such difference can be justified by the fact that water molecule representation is one of the most showed in high school and students can easily observe this model. The difference in yields of CG (51.85%) and EG (81.48%) was of 29.63%. Water molecule presents an Angular molecular geometry, of AX_2 type, where "A" is the central atom and X are the ligands. It is noteworthy that there are quite molecules that presents Angular geometry, like OF_2 and SO_2. Water geometry is due to the presence of two non-ligands electron pairs in the central oxygen atom, that causes great repulsion in the electrons of the ligand atoms, thus acquiring a stable geometry, with angle of 104º 27’ [29,30].

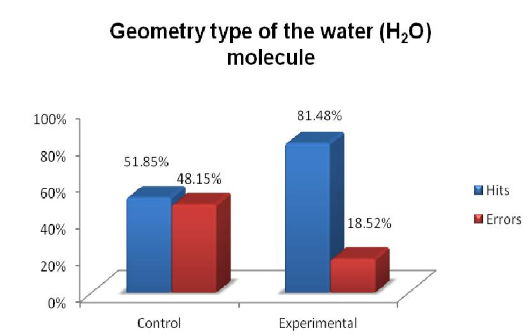

Fig. 2. Geometry of the water (H_2O) molecule, according to CG and EG

Fig. 3. Corresponds to the student's understanding about molecular geometry of Carbon Dioxide (CO_2), comparing both groups (CG and EG), being the question of closed

nature with only one correct answer among the following assertions: angular, lineal, pyramidal, trigonal, tetrahedral. Fig. 3. shows a satisfactory yield of EG relative to the CG. A comparison of the GC (37.04%) and EG (74.07%), shows a difference of 37.03%. The use of chemical programs has facilitated the understanding of the students, as seen in Figs. 1, 2 and 3, because they allowed a clear view of the spatial conformation adopted by each molecule.

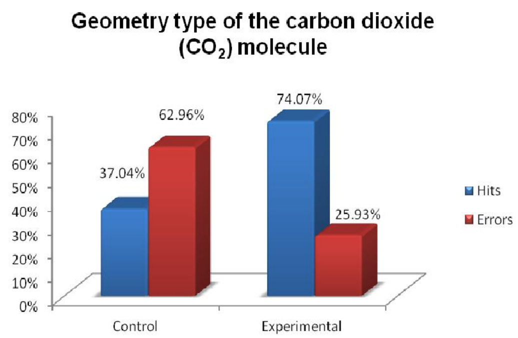

Fig. 3. Geometry of the carbon dioxide (CO_2) molecule, according to CG and EG

Structure of CO_2 has two double bonds, O=C=O. In this case, the type is AX_2, the central atom does not presents ligand electrons, thus, unlike water molecule, the repulsion between the non-ligand electrons and the shared electrons does not exist, and consequently, the geometry of the Carbon Dioxide molecule is linear [30,31].

The use of programs in the intervention exerted a fundamental paper in the comprehension of the concepts about the molecules, what is found by the discrepancy of right answers between CG and EG, proving, therefore, that a problem frequently faced by students is the conducting of activities that requires ability of tridimensional imagination as well as mental visualization of molecules that are represented in two dimensions in the books. Hence, with the use of program, it was considerable increased the capability of students to visualize the tridimensional geometry of molecules. Geometries, when represented in a more animated and dynamic form, improves the ability of tridimensional visualization of students, tending to provide a significant perception of microscopic world [10].

Similar results were found by other authors, who studied the effects of ICTs in science and mathematics teaching, and stated that students acquired a better understanding of targeted chemistry concepts during the multimedia courses [32], and also that the use of ICTs for mathematics instruction has a significantly positive effect on teaching high level concepts to students in grade eight or above [33].

3.2 Conceptions about the Influence of Molecular Geometry in Substances' Behavior in the Environment

The students' comprehension on the influence of geometry in the behavior of the molecules in the environment was assessed through the following question: "Does the geometry of the molecules influences its behavior in the environment?", which was made for both CG and EG, being this questions of closed nature and with the following assertions: Yes or No. The results are shown in Fig. 4.

In Fig. 4 there is a higher yield of EG (81.48%) compared to CG (62.96%) with a difference of 18.52%. The geometry of the molecule is influenced by intra-molecular interactions, what may lead to polar or a polar structures, that consequently can influence physical properties, and increase or decrease the reactivity of the molecule in environment. The programs greatly influenced the EG, due to simulation capability, making then possible to manipulate the variables related to a given phenomenon.

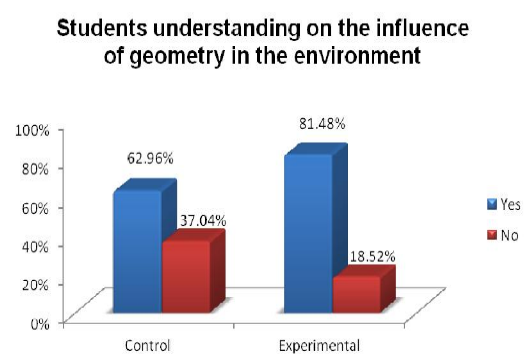

Fig. 4. Students understanding on the influence of geometry in the environment molecules, according to CG and EG

The programs requires, in a playful manner, attention and imagination of students, which expands the capacity to interfere and modify the environment in which they find themselves. This is one of the objectives proposed by the National Curriculum Guidelines for Secondary Education (PCNEM) and Transversal Themes with Environmental Education [3].

Rivers, lakes and oceans exist because its molecules strongly attract each other and form a liquid. Without liquid water there would be no life. Without the force between the molecules, our meat flesh would separate from the bones and oceans would turn into gas. Saying in a less dramatic form, the force between the molecules govern the physical properties of matter and contributes to explain the differences between the substances around us. These forces explain why the carbon dioxide is a gas which we exhale, why the wood is a solid in which we can stay on feet over it, and why ice floats in water [31,34].

3.3 Conceptions on the Difference between Physical States of the Substances in Environment

In Fig. 5 is shown the students' yields about their conceptions on the differences of physical states of water and methane. This was assessed through the following question: "Why the water (H_2O) at room temperature is a liquid and methane (CH_4) is a gas?". The question was made for both CG and EG, being of closed nature and with only one correct answer among the following assertions:

A) Because of the difference between the number of moles of the molecules
B) Because of the difference between the molecular masses
C) Because of the difference between the intermolecular interactions (H_2O = Hydrogen Bonds / CH_4 = Induced dipole)
D) Because of the nature of the chemical species (H_2O=inorganic substance/CH_4= organic substance)

The intermolecular interactions are responsible for altering the melting and boiling points of substances, thereby changing their behavior in the environment in relation to changes of physical state of matter [31]. Therefore, "C" is the correct one, because the difference is in the intermolecular interaction, which in water are hydrogen bonds, whereas in methane there are induced dipole. As seen in Fig. 5, the results for the CG (70.37%) and EG (88.89%), shows a difference of 18.52%, which is believed to be due to the simulation provided by programs, showing the difference in electronegativity and intermolecular forces in the studied molecules.

Intermolecular forces are responsible for the existence of various phases of matter. A phase is a form of matter which has both chemical composition and physical state uniform. The studied interactions are three: London forces, dipole-dipole and hydrogen bonds. London forces occur in non-polar molecules, is a very weak interaction, its compounds have low melting and boiling points, and at room temperature they are in gaseous state, for example, methane (CH_4).

Dipole-dipole interactions happens between polar molecules and are stronger than London forces. Substances which have dipole-dipole interactions usually presents intermediate melting and boiling points compared to other substances whose molecules make different intermolecular interactions. Substances presenting dipole-dipole interaction can be in solid, liquid or gaseous state at room temperature, where the main factor to determine its aggregate state will be the molecular mass. They also conduct electricity when dissolved in water, through the process known as ionization (formation of ions).

The hydrogen bond is the strongest interaction compared to London forces and dipole-dipole, and happens when hydrogen atom (H) is attracted by Fluorine (F), Oxygen (O) or Nitrogen (N) atoms. The bond arises from the great difference between the atom's electronegativity, what causes the electrostatic force to strongly approximate the atoms. That's why the melting and boiling points of substances whose molecules make hydrogen bonds are very high compared to those who have different interactions.

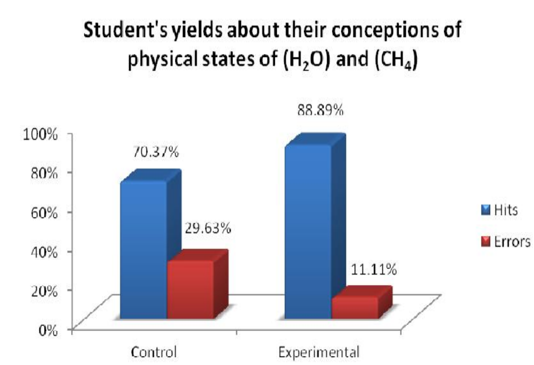

Fig. 5. Student's yields about their conceptions on the difference of physical states of water (H_2O) and methane (CH_4)

This explains the fact that water is liquid at room temperature (25°C) although it has molecular mass (18 g/mol) smaller than carbon dioxide (44 g/mol). This is because the first makes hydrogen bonds and the last does dipole-dipole interaction [31].

The consolidation of this link between technology and transversal themes, which in this case is the environmental education, offers a significant learning about environmental questions, so that there is concepts fixation, in organized, systematic and effective manner [35], what was proved from the data previously obtained (sections 3.1, 3.2 and 3.3).

3.4 Use of other Methodological Resources in Chemistry Classes

To verify the real perception of students related to other methodological resources that could be used by the teacher in chemistry classes, besides pen and magnetic board, through the following question: "Do you think the use of other instruments besides pen and magnetic board would improve the comprehension of chemistry classes? Which ones?". The question was made for both, CG and EG, and consists of a question of semi-open, thus observing the students' perception related to the use of other resources, with the assertions Yes or No, but also citing some proposals. The results are in Fig. 6 and Table 1.

It is observed in Fig. 6. that 100% of the EG students affirmed the importance of ICTs in the classroom, while in the GC only 55.56% said the same. The positive answers were more in EG in comparison with CG, since that CG have not had direct contact with resources used with EG. Then, part of CG do not know the potentialities that ICT's bring with, causing some participants to answer "no".

The number of students and the cited resources by CG and EG are in Table 1. The amount of response exceeds the number of students per group because they cite more than one didactic resource option. In EG, after contact with ICT's, students came to often cite programs, computers, multimedia projector. Interaction with these resources facilitate de settlement of problems regarding the understanding of the microscopic world, and this can increase the student's field of view, stimulating imagination and the construction of new concepts [26]. With CG the ICT's were cited but not used, what may have caused the lowest mentions of these didactic means. However, an important data is observed in CG, the experimentation, what leads one to infer that teacher may have made use of this methodology in chemistry classes.

The teacher can use in many ways the programs, being of extreme importance the knowledge and mastery of *ChemSketch* [18] and *PhET Simulations* [27]. These can be used in the preparation of tests, exercise lists, work presentations in congress or for a periodic, as well as using them in their own classes interactively to contents that require comments at the microscopic level [36].

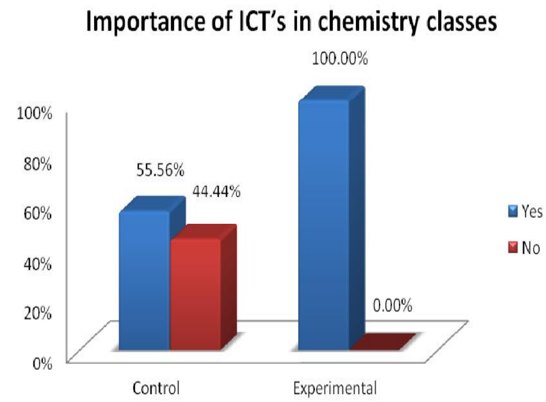

Fig. 6. The importance of ICT's in chemistry classes, according to CG and EG

Table 1. Methodological resources most mentioned by the students

Resources	GC	GE
Multimedia projector	17	18
Computers	15	23
Programs	12	24
Experimentation	15	5

3.5 Student's Opinion Related to the Content Taught in the Intervention

The following question was applied to both CG and EG to assess the student's opinion about the content taught: "In your opinion, was the class sufficient to understand the course content? Why?". This question is of closed nature, with the assertions Yes or No, and also justifying the answer. The obtained results are shown in Fig. 7.

Fig. 7. shows that the class was meaningful in the opinion of most of students of EG (81.48%), and for more than half of CG (59.26%). It's noted that the use of ICT's influences the students' answers. Below, the answers of some students from CG and from EG are exhibited.

CG:

1. "No, because need more demonstration, as experiments". (Student A)
2. "No, because the time is short and the content are long and complicated". (Student B)

EG:

1. "Yes, because the class was productive, by the use of programs." (Student C)
2. "Yes, because was used a not so common resource." (Student D)

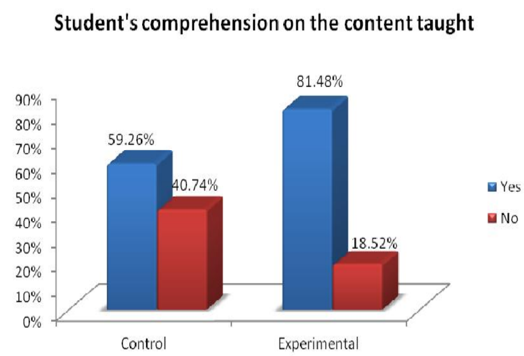

Fig. 7. Student's comprehension on the content taught, according to CG and EG

By means of the cited answers is evidenced that, in CG, students point the need of experimental classes. It's also observed that the use of programs optimized the use of class time, because students need less time to understand the content. The opposite is evidenced in CG, and student (2)' answer emphasizes this idea. It's noted that in EG the use of chemical programs profoundly improves the understanding about the content, making the class productive (answer (3).

The students' responses allow inferring that the association of theory and use of programs improves the understanding about the chemistry contents at microscopic level. It's worthy to emphasize that chemical programs must not to substitute experimentation but, instead, must be a methodological alternative, since experiments are fundamental to describe the various phenomena at macroscopic world, however programs, in other cases, are irreplaceable to explain the micro world, as exemplified in molecular geometry content.

3.6 Student's opinion related to the use of chemical programs as an educational tool

The question "What is your perspective about the use of chemical programs as educational tools in the process of teaching and learning?" was used to assess the students' opinion about the importance of the use of chemical programs, and was directed only to EG. The question is of closed nature, with the assertions listed below, with the respective numbers. The results are shown in Fig. 8.

(1) Improves the students' comprehension.
(2) As a teaching and learning object.
(3) Does not contributes to the pedagogical practice.
(4) Serves to help the practice of teaching.
(5) Does not contribute to learning, being merely illustrative

It can be inferred that the majority of students (96.00%, questions 1, 2 and 4) conceptualizes the use of chemical programs as a tool that can help to improve the learning of concepts that were difficult to understand before; the introduction of these ICT seeks to cultivate updated forms of reasoning. Previous researches about the relation of students with ICT's had achieved similar conclusions, such as that student attitudes toward computers and computer related technologies improve as a consequence of exposure to them [33,37]. The use of different resources, such as programs, can drive students to one of the actual imposed purposes for chemistry teaching, that is the ability to understand, intervene and change the medium in which it is inserted through the ability of manipulation and modification of matter [1,3].

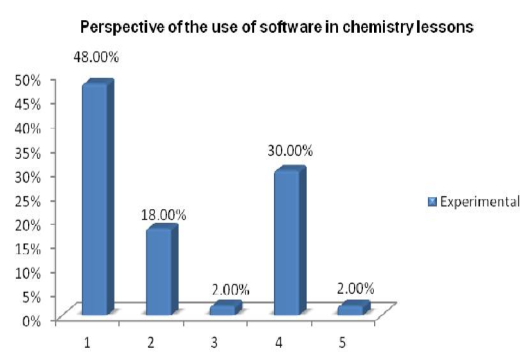

Fig. 8. EG perspective related to the use of programs in process of teaching and learning in chemistry lessons

Some difficulties encountered in chemistry teaching can be remedied through the use of chemical programs, due to the potential and feasibility that software can offer [38]. Technological culture is in exponential growth and the school does not have access to the ideal technology, so there is the need for integration between school and technology [39]. Students and their teachers need to deeply consider their own teaching and learning practice as well as the social and cultural implications for digital use for different disciplines. They also need to consider that different groups of students may be more or less able to explore and critique the programs and hardware (computer) [40].

4. CONCLUSION

The main purpose of this work was to verify the influence of the use of programs in chemistry teaching as a distinguished methodology. The development of concepts regarding ICT's showed positive results when compared GC and GE, where the EG showed that learning difficulties were reduced. This resource facilitated the formalization of ideas, and consequently, the understanding of certain content, helping students obtain greater understanding of the concepts of molecular geometry and intermolecular interactions.

The contact with ICT's enabled a more significant idealization of the importance and what these technologies represent. Concerning the application of intervention, it was found the existence of different conceptions, and for most students the classes with the use of computational chemical programs have made learning be easier and meaningful.

Given the above, with the intention of collaborating with the theme, it is suggested that ICT's must be used more often, particularly, computational chemical programs as an alternative tool in the teaching and learning process, which may enable students transpose the barriers of chemical knowledge in order to answer questions that may arise.

COMPETING INTERESTS

The authors declare no conflict of interest.

REFERENCES

1. Coll C. Psicologia da educação Virtual: Aprender e ensinar com as tecnologias da informação e comunicação. 1st ed. Artmed: Porto Alegre, Brasil; 2010. Portuguese.
2. BRASIL. Lei de Diretrizes e bases da educação nacional – LDBEN Nº 9394/96. De 20 de dezembro de. Distrito Federal. Portuguese; 1996.
3. BRASIL. Parâmetros Curriculares Nacionais do Ensino Médio (PCNEM) – Ensino Médio; Ministério da Educação,. Portuguese; 1999.
4. Ribeiro AA, Greca IM. Simulações computacionais e ferramentas de modelização em educação química: Uma revisão da literatura publicada, Química Nova; Portuguese. 2003;26(4):542-549.
5. Casanova Junior J, Weaver ER. Introduction to computer use programs for first order rate constants. Journal of Chemical Education. 1965;42(3):137-139.
6. Sorgo A, Verckovinik T, Kocijancic S. Information and Communication Technologies (ICT) in Biology Teaching in Slovenian Secondary Schools. Eurasia Journal of Mathematics, Science and Technology Education. 2010;6(1):37-46.
7. Dawson V. Use of Information Communication Technology by early career science teachers in Western Australia. International Journal of Science Education. 2008;30(2):203-219.
8. Benite AMC, Benite CRM. O Computador no ensino de Química: Impressões versus Realidade. Em foco as escolas Públicas da Baixada Fluminense. Ensaio: Pesquisa em Educação em Ciência: Belo Horizonte, Brasil. 2008;10(2):1-20. Portuguese.
9. Lambach M, Aires JA. Contextualização do ensino de química pela problematização e alfabetização científica e tecnológica: uma experiência na formação continuada de professores. In congress: VII ENPEC – Encontro Nacional de Pesquisa em Educação e Ciências, Florianópolis, SC, Brasil, March 28th. Portuguese; 2009.
10. Giordan M. Computadores e linguagens nas aulas de ciências: uma perspectiva sociocultural para compreender a construção de significados, 20th ed.; Ijuí: Unijuí, RS, Brasil. Portuguese; 2008.
11. Valente JA. A Espiral da Aprendizagem e as Tecnologias da Informação e Comunicação: Repensando Conceitos. Joly MCR, editors. A tecnologia no ensino: implicações para a aprendizagem. 1st ed. São Paulo-Brasil: Casa do Psicólogo. Portuguese; 2002.

12. Meleiro A, Giordan M. Hipermídia no ensino de modelos atômicos. Química Nova na Escola. Portuguese. 1999;10(1):17-20.
13. Baser M, Durmus S. The effectiveness of computer supported versus real laboratory inquiry learning environments on the understanding of direct current electricity among pre-service elementary school teachers. Eurasia Journal of Mathematics, Science and Technology Education. 2012; 6(1):47-61.
14. Hawkings I, Phelps AJ. Virtual laboratory vs. traditional laboratory: which is more effective for teaching electrochemistry? Chemistry Education Research and Practice. 2013;14(4):516-523.
15. Gabini WS. Informática e ensino de Química: investigando a experiência de um grupo de professores. Dissertation in teaching science and mathematics, Universidade Estadual Paulista - UNESP, Bauru. Portuguese; 2005.
16. Aksela M, Meisalo V. A professional development project for improving the use of Information and Communication Technologies in science teaching. Technology, Pedagogy and Education. 2006;15(2):159-174.
17. Smith TK. Elementary Science Instruction: Examining a Virtual Environment for Evidence of Learning, Engagement, and 21st Century Competencies. Educ. Sci. 2014;4(1):122-138.
18. Hood JB. Research on computers in chemistry education, Journal of Chemistry Education. 1994;71(3):196-200.
19. Machado DI, Nardi R. A hipermídia no ensino de física moderna e contemporânea. In congresso: Simpósio Nacional de Ensino de Física, São Paulo, SP, Brasil, Portuguese; 2011.
20. Ramos CS, Sousa MAC. TIC's no ensino médio: utilização do ambiente virtual moodle e hipermídias educacionais nas aulas de química. Monography. Macapá-AP: State University of Amapá, Brasil. Portuguese; 2011.
21. Raupp D, Serrano A, Martins TLC. A evolução da química computacional e sua contribuição para a educação em química. Revista Liberato, Portuguese. 2008;12(9): 13-22.
22. Francisco Junior WE, Francisco W, Morais MA, Manochio CVA, Ruiz M. Implementação e Avaliação de um curso introdutório ao software ACD Labs ChemSketch® a graduandos em Química. In congress: XIV Encontro Nacional de Ensino de Química, Portuguese; (Congresso). 2008;.
23. Franco Neto JR, Silva RMG. Tecnologias no ensino de geometria molecular. Dissertation in Chemistry, Universidade Federal de Uberlândia - UFU, Uberlândia, 2007;
24. Zara RA. Reflexão sobre a eficácia do uso de um ambiente virtual no ensino de Física. In congress: II ENINED - Encontro Nacional de Informática e Educação, Cascavel, PR, Brasil, Portuguese. 2011;
25. Greca IM, Moreira MA. Mental, physical, and mathematical models in the teaching and learning of physics. Science Education 2002;86(1):106-121.
26. Software ACD/Chemsketch Freeware, version 12.00. Advanced Chemistry Development, Inc., Toronto, ON, Canada, 2010;
27. Software PhET Interactive Simulations, version 06/2014. University of Colorado, Inc., Boulder, CO, United States of America; 2012.
28. Rocha JC, Rosa AH, Cardoso AA. Introdução à Química Ambiental. 2nd ed. Porto Alegre: Bookman, Portuguese; 2009.
29. Lee JD. Química Inorgânica não tão concisa, tradução da 5th ed. São Paulo: Edgard Blücher, Portuguese; 2001.
30. Mahan BH, Myers RJ. Química: Um Curso Universitário. 4th ed. São Paulo: Edgard Blücher, Portuguese; 1995.
31. Atkins P, Jones L. Princípios de Química: questionando a vida moderna e o meio ambiente. 5th ed. Porto Alegre: Bookman, Portuguese; 2012.
32. Su, KD. The effect of a Chemistry course with integrated Information Communication Technologies on university students' learning and attitudes. International Journal of Science and Mathematics Education. 2008;6(2):225-249.
33. Ungerleider CS, Burns TC. Information and Communication Technologies in Elementary and Secondary Education: a State of the Art Review. In congress: Pan-Canadian Education Research Agenda Symposium; 2002.
34. Brown T, Lemay HE, Bursten BE. Química: a ciência central. 9th ed. São Paulo: Prentice Hall, Portuguese; 2012.
35. Moreira MA. Aprendizagem significativa em David Ausubel: Contributos para uma adequada visão da sua teoria e incidência

no ensino. Faculdade de Ciências da Universidade do Porto: Peniche, Portugal, Portuguese. 2000;5(1):121-134.
36. Moraes UC. Tecnologia educacional e aprendizagem: O uso dos recursos digitais. 1st ed. São Paulo: Livro Pronto, Portuguese; 2008.
37. Juuti K, Lavonen J, Aksela M, Meisalo V. Adoption of ICT in Science Education: a case study of communication channels in a teachers' professional development project. Eurasia Journal of Mathematics, Science and Technology Education. 2009;5(2):103-118.
38. BRASIL. Secretaria de Educação Básica. Orientações Curriculares para o Ensino Médio. Ciências da Natureza, Matemática e suas tecnologias. Ministério da Educação: Brasília, Brasil, Portuguese; 2006.
39. Cowie B, Khoo E. Digital Tools Disrupting Tertiary Students' Notions of Disciplinary Knowledge: Cases in History and Tourism. Education Science. 2014;4(1):87-107.
40. Ketelhut DJ, Nelson B, Schifter C, Kim Y. Improving Science Assessments by Situating Them in a Virtual Environment. Education Science. 2013; 3(2):172-92.

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