ECLÉTICA QUÍMICA

Eclet. Quim. 49 | e-1524, 2024

Original Article, Education in Chemistry and Correlated Areas

https://doi.org/10.26850/1678-4618.eq.v49.2024.e1524

Quantum chemistry in public higher education institutions in the Brazilian state of Piauí: an analysis of the perceptions of undergraduate chemistry students

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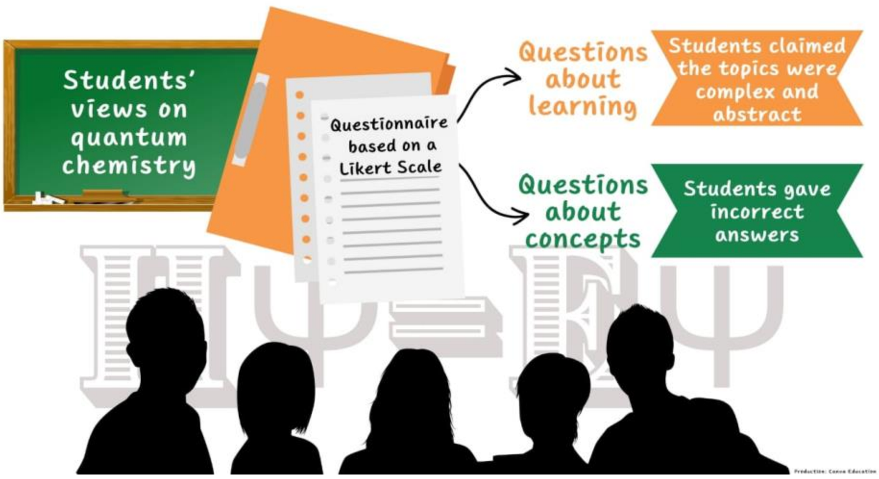
Abstract

Quantum chemistry is a challenging required course in undergraduate chemistry. Despite its unconventional concepts, it is crucial for understanding modern chemistry. This study investigated how students perceive certain topics and the learning process. Interviews were conducted using a Likert scale questionnaire and sixteen content-specific questions. Some responses differed from the existing literature, such as students' interpretations of the nature of light. In terms of learning, students acknowledged that the topic was complex due to the lack of mathematical foundations and the elevated level of abstraction. Students were primarily seeking the average grade required for admission. The data underscore the need for a deeper discussion of curriculum development and implementation. The curriculum matrix revision could provide space for more substantive thinking about content delivery and assessment processes.



Article History

Received October 05, 2023
Accepted April 02, 2024
Published June 12, 2024

Keywords

1. chemistry education;
2. higher education;
3. quantum chemistry.

Section Editor

Assis Vicente Benedetti

Highlights

- Unconventional concepts challenge students.
- Lack of math background hinders learning.
- Light-nature misconceptions exist.
- Students prioritize grades over understanding.
- Curriculum needs revision for clarity.

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1. Introduction

Quantum mechanics is one of the most important fundamental theories and one of the pillars of modern and contemporary physics. It emerged and consolidated during the great revolution that took place in physics in the first three decades of the 20th century, based on the need to explain the behavior of submicroscopic systems such as electrons, atoms, and molecules. Classical physics, which includes Newtonian mechanics and Maxwell's classical electromagnetism, proved inadequate to describe such systems. The foundations of quantum mechanics lie in the ideas of energy quantization by Max Planck (1858-1947), the quantum of electromagnetic radiation (photon) by Albert Einstein (1879-1955), the Bohr model of the atom by Niels Bohr (1855-1962), the wave-particle duality by Louis de Broglie (1892-1987), the uncertainty principle by Werner Heisenberg (1901-1976), the statistical interpretation of the wave function by Max Born (1882-1970), the spin-statistics theorem and the Pauli exclusion principle by Wolfgang Pauli (1900-1958), and many others. Currently, quantum mechanics is considered the fundamental physical theory that explains chemical phenomena at the atomic and molecular levels and is essential for discussing the behavior of matter. The application of quantum mechanics in chemistry is called quantum chemistry and is based on Erwin Schrödinger's (1887-1961) equation to determine the wave functions and energies of atoms and molecules. In this way, it becomes possible to predict atomic and molecular structures and spectra, molecular dipole moments, transition states of chemical reactions, thermodynamic properties, etc. Quantum chemistry is practiced with the help of computers using special computational programs and is called computational chemistry. People who have contributed significantly to the development of quantum and computational chemistry includes Douglas Hartree (1897-1958), Erich Hückel (1896-1980), Friedrich Hund (1896-1997), John Pople (1925-2004), Linus Pauling (1901-1994), Robert Mulliken (1896-1986), Vladimir Fock (1898-1974), and Walter Kohn (1923-2016) (Levine, 2014).

Quantum chemistry is a fundamental part of the content covered in an undergraduate or graduate chemistry course. However, most chemistry students have great difficulty understanding the concepts covered in undergraduate courses. This difficulty can be partly attributed to the technical teaching model, characterized by repetition procedures in which the teacher is the owner of the knowledge, and the student does not participate in the teaching-learning process (Libâneo and Pimenta, 1999; Saviani, 2011), and which, although it was overtaken decades ago by other pedagogical theories, is still widely used in teacher education today (Alberto *et al.*, 2020). These difficulties may also be related to deficits in the process of science education resulting from initial conceptions about the structure and understanding of scientific thinking that run throughout the educational process of students and often accompany them until postgraduate studies (Chassot, 2014). Looking specifically at the panorama of undergraduate chemistry courses, the need for a solid mathematical foundation, combined with the elevated level of abstraction of the subject and other factors such as the lack of more efficient teaching methods, leads to a high failure rate in this course, according to Belo *et al.* (2019). As noted by Gregório *et al.* (2019), these claims occur more frequently in undergraduates such as General Chemistry, Inorganic Chemistry, and Physical Chemistry, leading to a discrepancy between the number of first-year students and the number of students who drop out in the first semesters. All these cumulative factors imply a large obstacle to the understanding of topics related to quantum chemistry compared to the first theories of chemical thinking, which do not allow the construction of knowledge using the previously mentioned methods (Costa and Souza, 2017). To overcome these deficiencies, different methods can be applied to improve the relationship between teaching and learning in quantum chemistry, but it is necessary to perform a deeper analysis of the causes of this problem. In the present work, we have tried to identify learning problems related to the content of the subject quantum chemistry, based on the perceptions of students in undergraduate chemistry courses in three public universities in a state in northeastern Brazil.

2. Experimental

This work is conceived as a quantitative study, since it attempts to quantify the modalities of information gathering, and as qualitative research, which allows us to adequately interpret the nature of a social phenomenon (Beuren, 2006). To achieve the above objectives, a literature search on this topic was first conducted to obtain a solid theoretical foundation. The search initially focused on listing the topics considered fundamental to the understanding of quantum chemistry and looked for specific books in the field intended for higher education and cited in the paper. Then, the curricula for the subject of quantum chemistry from two of the three universities that participated in the study were analyzed, considering that the specific subject of quantum chemistry is not part of the compulsory curriculum at one of the universities. A sample for the interview was then conducted, consisting of students in the final phase of their undergraduate studies in chemistry at universities in a state in northeastern Brazil. The following procedure was used to select the students: the coordinators of every institution were requested to compile a roster of students currently enrolled in the 7th semester or beyond of their respective courses. From this pool, a random selection of 10 students was made. Following this selection process, each chosen student was contacted via telephone and provided with a concise overview of the research aims and methodology, subsequently extending an invitation to participate in the study.

Only 9 students were eligible to participate in the study in two of the three institutions, for a total of 28 students. Concerning the study's qualitative aspect, interviews were conducted with the participants. Both recruitment and interviews took place remotely, via the online platform Google Meet, due to the social isolation caused by the COVID-19 pandemic. In the interviews (all of which were recorded), after an appropriate introduction to the project, a Likert-scale questionnaire was used, based on a series of statements about the topic discussed, in which the respondent indicates the extent to which he or she agrees on a 5-point scale: disagree; partially disagree; undecided; partially agree; agree (Silva Júnior and Costa, 2014). At this point, the interviewer read the questions on a shared screen during an online session, and the respondent answered according to his or her point of view. After the participant indicated the extent to which he or she agreed with each statement, a brief discussion took place on the topic addressed, during which respondents were free to express themselves without interference from the interviewer. The discussions began with two questions designed to stimulate the respondents' thinking: "Do you have anything to say about this topic?" and "How would you justify your choice?"

The interview was used as a data collection method because it can more clearly capture issues of subjectivity due to the greater freedom and expressiveness of the participant (Batista *et al.*, 2017) and also because it is qualitative research. Regarding ethical procedures, the standards established by the Comitê de Ética em Pesquisa (CEP) of the Universidade Federal do Piauí (UFPI) were followed, through the Brazillian government website Plataforma Brasil (https://plataformabrasil.saude.gov.br/), whose opinion was approved for the conduct of the study. Considering the protocols established by the agency, all interviews were also approved by the respective heads of the institutions. Finally, the data were analyzed considering the division between the statements in the questionnaire, which are presented below:

- **Specific thematic topics:** The answers to the specific statements were compared with the concepts of quantum chemistry contained in the literature, which will be presented later in the paper. The questions where the answers differed the most from those expected were selected for discussion because the concepts related to quantum chemistry are predetermined and provide less room for subjectivity in the answers.
- **Pedagogically oriented topics:** The responses to the statements related to student learning were all discussed because they had a higher degree of subjectivity. They were analyzed in light of ideas from previous work that were raised in the discussion.

In both cases, the percentage of responses from each higher education institution was presented in a grouped bar graph, with each grouping represented by an alternative indicating the level of agreement and each column representing a higher education institution.

3. Results and discussion

This work is the result of interviews conducted with fourth-year chemistry students at three public higher education institutions (HEI) in the state of Piauí, northeastern Brazil. The HEI were labelled A, B, and C to avoid revealing their identities. Only B does not offer quantum chemistry as a compulsory subject in the chemistry curriculum. The analysis of the results had two foci: **(1)** the analysis of the items related to the specific topics of the subject and **(2)** the analysis of the items related to learning. To find out how HEI addresses the subject of quantum chemistry, they were characterized based on the following criteria: **(I)** subject-specific offering; **(II)** module in which it is offered; **(III)** workload; **(IV)** methodology; and **(V)** resources. Sources for this information are available the institutional website and the subject plan (UFPI, 2022).

When analyzing the two topic plans for quantum chemistry provided by the universities, it was found that both have the following contents in common: **(a)** basic concepts of quantum mechanics; **(b)** free/confined particles; **(c)** harmonic oscillator; **(d)** rigid rotor; **(e)** Schrödinger equation; **(f)** concepts of spectroscopy. All these topics appear in books on quantum chemistry and are also mentioned in the topic plans as bibliographies and supplementary materials (the data will be available upon request). When analyzing the interviews, it is interesting to mention that the questionnaire consisted of 16 statements. Generic names are used to preserve the identity of the students surveyed and their respective institutions. As for the presentation of the results, the selected items were presented in the form of grouped bar graphs, considering the individual responses of each institution, in addition to a calculation of the general percentage of respondents. The questionnaire was organized as follows: a total of 10 questions related to the specific topics of quantum chemistry, with correct and incorrect statements based on concepts of quantum mechanics, such as the nature of light, molecular orbitals and their applications; and a total of 6 questions related to the teaching and learning process of quantum chemistry, based on the main learning problems in chemistry, such as the difficulty of understanding mathematical formalisms, the high degree of abstraction, and others.

3.1. Items related to the specific topics

Considering the structure of the questionnaire based on the Likert scale (Silva Júnior and Costa, 2014), where the first ten items were related to the specific contents of quantum chemistry, the first step was to compare the participants' answers with those expected in the literature. The questionnaire was structured so that the first questions covered basic topics such as the dualistic nature of light and the photoelectric effect, while the complexity of the topics gradually increased. Five questions (3, 5, 8, 9, and 10) were selected for discussion, considering discrepancies and conflicts between respondents' answers and those expected based on the literature.

The first highlight of the respondents' answers relates to statement 3 (**Fig. 1**): "When a beam of light of a certain frequency strikes a metal, electrons are ejected from the surface with a kinetic energy proportional to the intensity of the light". This statement refers to the photoelectric effect and is false since electrons are ejected with kinetic energy regardless of the intensity of the incident light. According to the photon model presented by Albert Einstein in 1905, light consists of particles called photons whose energy E is proportional to the frequency, ν of light, according to the equation $E = h\nu$, where h is Planck's constant. Each incident photon exchanges energy with an electron, which overcomes the potential energy (work function, ω of the metal) that binds it to the surface and detaches from the surface with kinetic energy, K, following the conservation of energy, $K = E - \omega$. (Halliday and Resnick, 2014) This mechanism is fundamental to understanding the quantization of energy, which is paramount in today's discussion of chemistry. Therefore, students must be expected to understand it in quantum chemistry. However, as can be seen in **Fig. 1**, only 8% of respondents disagreed to some extent with statement 3 of the questionnaire, leaving a total of 92% (among those who agree to some extent or declare themselves undecided, like the majority) with no real idea that it is one of the most elementary principles of quantum mechanics, although it is covered at school and in undergraduate subjects such as general chemistry, quantum chemistry, and others. It is also interesting that the few students who disagree with the statement in some aspects belong to Institution C and do so with vehemence.

This difficulty in understanding the nature of light is confirmed by Coelho and Borges (2010) when they conducted a specific analysis of this topic at the beginning of high school. Even after the presentation of current concepts regarding the dualistic nature of light (wave-particle duality) and its interaction with matter, a considerable proportion of students remain with misconceptions that contain elements of errors derived from already disproven concepts or adaptations of quantum theory. This suggests that attempts are made to integrate new concepts that conflict with those already present through a process known as balancing (Piaget, 1977 cited in Mortimer, 2000), but this does not necessarily apply to the specific case. This is because on certain occasions it is necessary to abandon old ideas and make a radical paradigm shift (Mortimer, 2000).

Other problems related to the difficulty of understanding the dualistic nature of light, according to Henriksen *et al.* (2018), are the abstract nature of the concept, the lack of practical experience, and cognitive limitations. About these aspects, the author highlights that it is precisely the lack of a deterministic perspective of quantum knowledge, which is associated with uncertainty and probability, which tends to hinder the construction of new knowledge. This encounters a cognitive limitation on the part of the students, cemented by the previous study of classical physics, which much more often offers some aspects to which the students are more accustomed, such as exact values, macroscopic experimental demonstrations, and simpler mathematical applications.

One can better understand these difficulties by taking the perspective of the student who learns in elementary and high school to relate subatomic particles to spheres (which have a predictable and predictable trajectory in a macroscopic universe), and the principles of wave motion based on wavelength, frequency, intensity, amplitude, and other concepts. The difficulties become clear when one understands that quantum physics combines all these aspects and creates a new body of knowledge without necessarily invalidating earlier ideas.

Another remarkable result relates to statement 5 of the questionnaire (**Fig. 2**): "Molecular orbitals can be found using Newton's laws of mechanics". This is another deliberately false statement about the possibility of finding molecular orbitals using Newton's laws of classical mechanics. Orbitals are wavefunctions, abstract quantum entities that cannot be determined with the formalism of Newtonian mechanics, but only with the Schrödinger equation. However, as shown in **Fig. 2**, only 25% of the respondents disagreed with this statement and about 40% declared themselves undecided. This result shows that most students do not understand the quantum nature of atomic and molecular orbitals. This is one of the most important topics in chemistry, essential for understanding bonding and chemical reactions. However, it is important to highlight the fact that more than half of the Institution C students disagree with the concept in some way, indicating a greater knowledge of the topic addressed.

Although it is a subject that contains mathematical formalisms, as does much of quantum mechanics, it is well known that classical mechanics reaches its limits when trying to explain quantum phenomena, and some students show that they are not aware of this fact: "I agree, I think Newton's laws (sic) have a big impact on explaining orbitals" (Student 1, Institution A).

Several aspects can be seen in Student 1's statement that indicate that the student finds it difficult to comment on what was being discussed at the time of the interview. The first point to discuss in this context is the apparent difficulty in expressing oneself on the topic, as the speech is disjointed and not fluent, and also superficial explanations of the topic are used (Pereira *et al.* 2006). When Newton's laws are cited to justify the choice of answer, an attempt is made to support the explanation with an argumentative strategy known as the argument from authority (from the Latin *argumentum ad verecundiam*), in which a person of notable authority on a particular topic is used to lend validity to an argument (Woods and Walton, 1974). The problem is that Isaac Newton, despite his immense contribution to science, especially physics, did not publish a single paper on the subject of quantum mechanics, as he died in 1727 and the first ideas of this new branch of physics did not appear until the beginning of the 20th century.

In connection with the previous statement, we can now discuss statement 9 (**Fig. 3**): "The molecular orbitals (MO's) are obtained by linear combinations of atomic orbitals (AO's). The number of MO's is equal to half the total number of AO's." This statement has a specific error in the number of molecular orbitals formed, which must be equal to the number of atomic orbitals. Nevertheless, slightly more than 46% of the students reported being undecided and 25% agreed with the statement, as you can see in **Fig. 3**.

It can be highlighted that Institution B performs slightly better, as most respondents disagree with this statement to some extent and also have the lowest number of undecided respondents. However, the indecision of a considerable proportion of respondents on statements 5 and 9, which involve in-depth knowledge of covalent bonds, suggests a relationship with respondents' preference for more elementary concepts taught in undergraduate and introductory courses such as General Chemistry (Fernandes, 2019). This directly affects the understanding of more complex concepts because, according to Bouayad *et al.* (2014), concepts such as atomic orbitals, valence bond and molecular orbital theories, and hybridization are not fully mastered by students because a mathematical formalism and a high level of abstraction are required to understand topics that have no obvious connection to the empirical knowledge used as reference.

We continue the analysis and now focus on statement 8 (**Fig. 4**): "The harmonic oscillator model can, after appropriate adjustments, be used to explain infrared spectra". This is a true statement about the theoretical model used to explain the absorption of infrared light energy by molecular vibrational modes (bendings, stretchings, etc.). This is the process that occurs in infrared spectroscopy, a technique used (in conjunction with other techniques such as NMR spectroscopy) to elucidate molecular structure (Pavia *et al.* 2013). The harmonic oscillator, based on Hooke's law, is one of the most widely used physical models in the exact sciences and has applications in various fields such as engineering, physics, geology, and chemistry. Any oscillatory phenomenon with low amplitude can be explained with this model (Nussenzveig, 2014). In quantum mechanics, the harmonic oscillator model is obtained by solving the Schrödinger equation exactly, which gives its energy levels and the corresponding quantum states (Levine, 2014).

However, as can be seen in **Fig. 4**, about 89% of the respondents answered "undecided", revealing their ignorance of one of the most fundamental topics in undergraduate studies. The fact that Institution B does not offer quantum chemistry as a compulsory subject could serve as a justification for this statement. However, the high number of undecided students at the three universities prompts us to reflect on the influence of the subject on students' actual knowledge.

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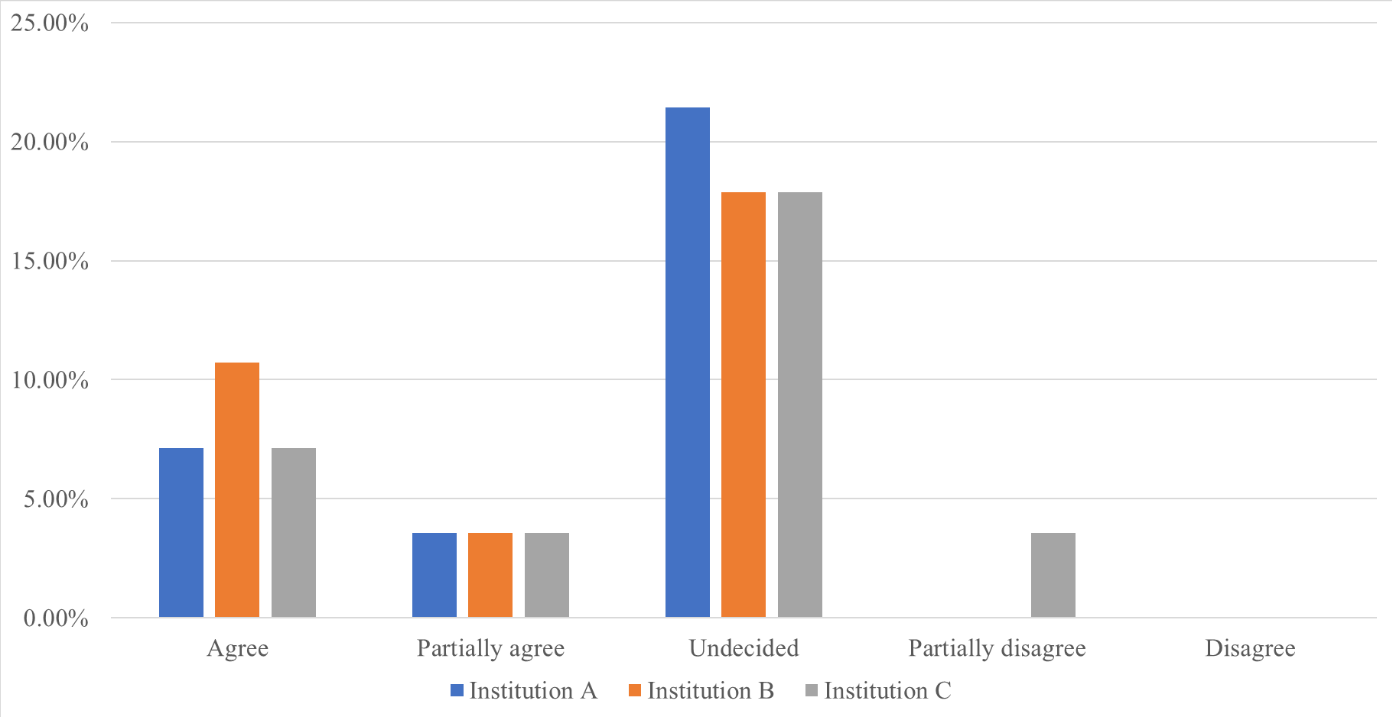

Figure 1. Answering the profile of participants in statement 3.

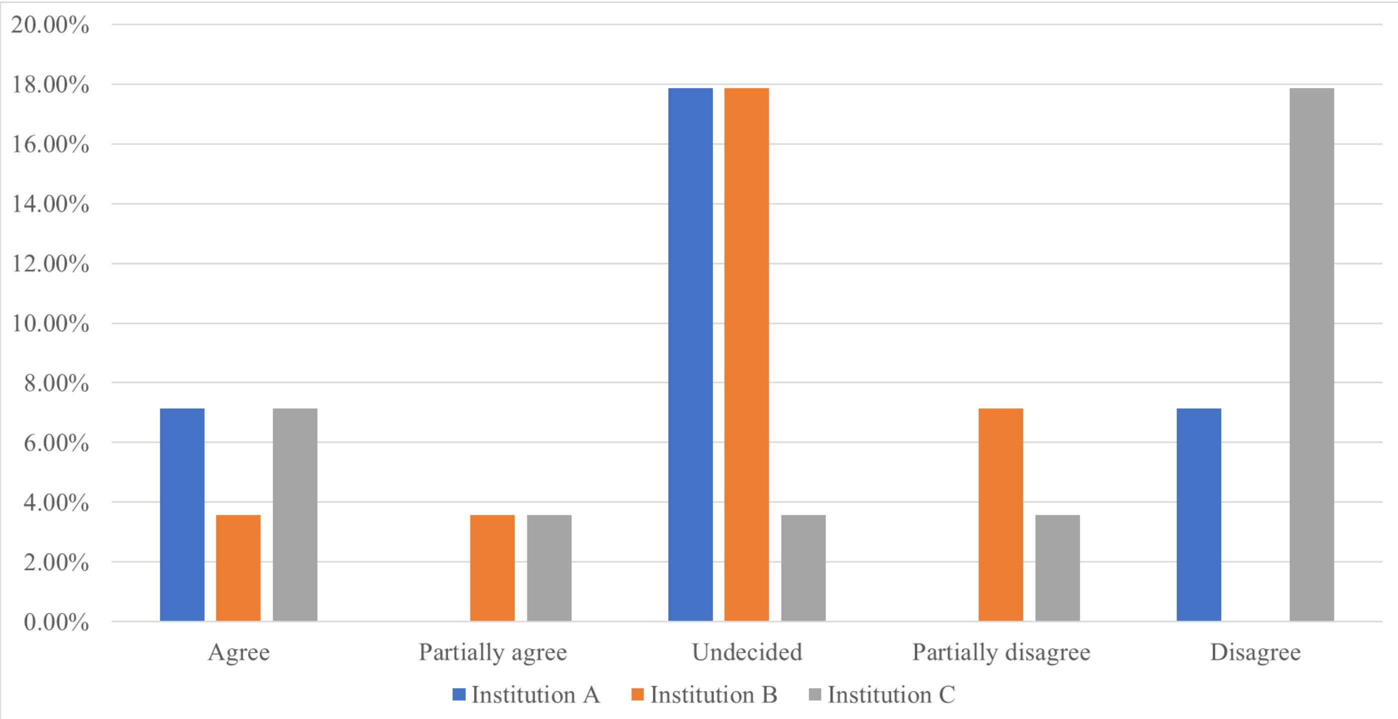

Figure 2. Answering the profile of participants in statement 5.

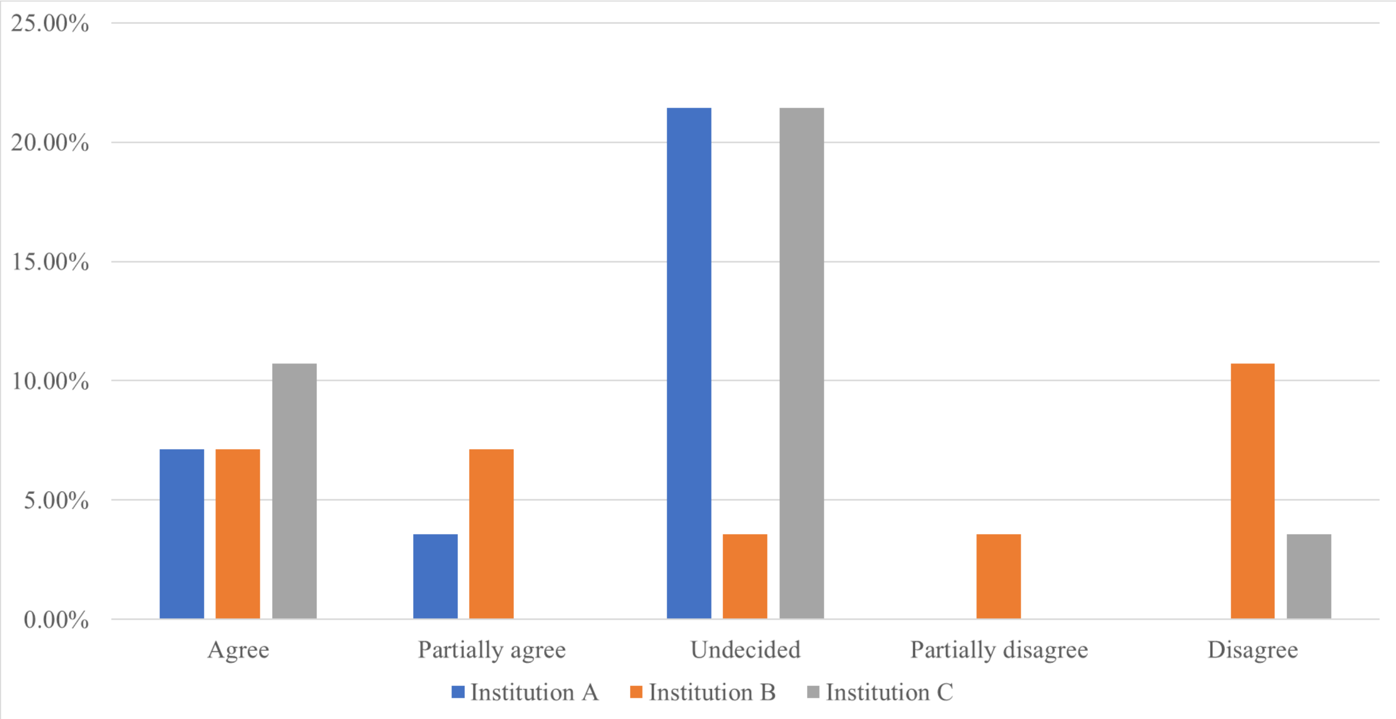

Figure 3. Answering the profile of participants in statement 9.

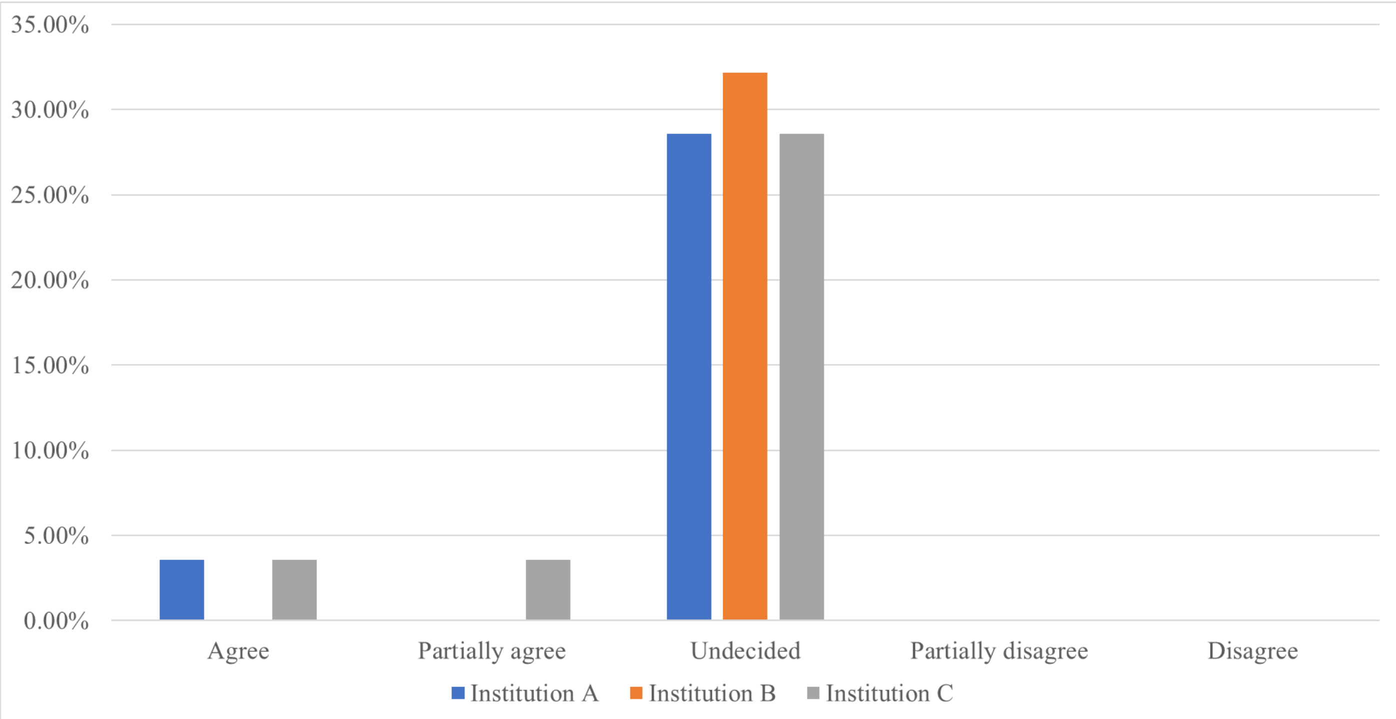

Figure 4. Answering the profile of participants in statement 8.

However, as Parnafes (2010) notes, there are several obstacles to understanding this model. These obstacles include the challenge of correlating physical behavior with mathematical idealizations, which include differential equations, differential and integral calculus, Fourier series, and other mathematical formalisms. Furthermore, there is a lack of macroscopic applicability due to an insufficient understanding of the fundamental processes of spectroscopy. It is not easy to think about harmonic motion at the level of the microscope, and without an understanding of the basic concepts of spectroscopy such as stretching, bending, oscillation and others, students have difficulty relating their knowledge to the appropriate meaning.

This difficulty regarding the relationship between mathematics and physical phenomena can be explained by the lack of meanings of mathematical symbols. Mathematics is a universal language because it has several applications in science. One of them is essential for quantum mechanics, i.e., modelling of complex systems. Differential equations, for example, are used in situations involving rates of change. They describe how physical variables change over time.

As for the second problem, there is a failure in the processes of knowledge construction and the resulting lack of meaning in the new body of knowledge that is taught to students. According to Ausubel (2003), for the assimilation of new concepts by the subject, they must be linked to the structures based on prior knowledge and experiences that serve as the foundation for the new knowledge. This means that solid knowledge of classical physics and its principles is necessary for learning concepts related to quantum mechanics to be meaningful.

The last prominent statement to analyze is number 10 (**Fig. 5**): "The consideration of the atomic nuclei at rest in relation to the electrons simplifies the solution of the electronic problem of the Schrödinger equation". This excerpt contains a true statement. The Born-Oppenheimer approximation is based on the experimental fact that atomic nuclei are much more massive than electrons and therefore must move at much slower speeds than electrons. Therefore, one can approximate that the electrons in the molecule move in an electric field generated by the set of atomic nuclei at rest. In this way, the two movements, the nuclear and the electronic, can be separated mathematically, which simplifies the problem considerably. This is a good approximation when considering the molecular electronic ground state, i.e. the one with the lower energy (Levine, 2014). This approximation is fundamental and essential to the methods used in quantum chemistry and leads to the concept of molecular geometry, which otherwise, if the approximation were not valid, would have no physical meaning (Cramer, 2004). However, about 57% of the respondents say they have no opinion on this issue and declare themselves undecided, as shown in **Fig. 5**.

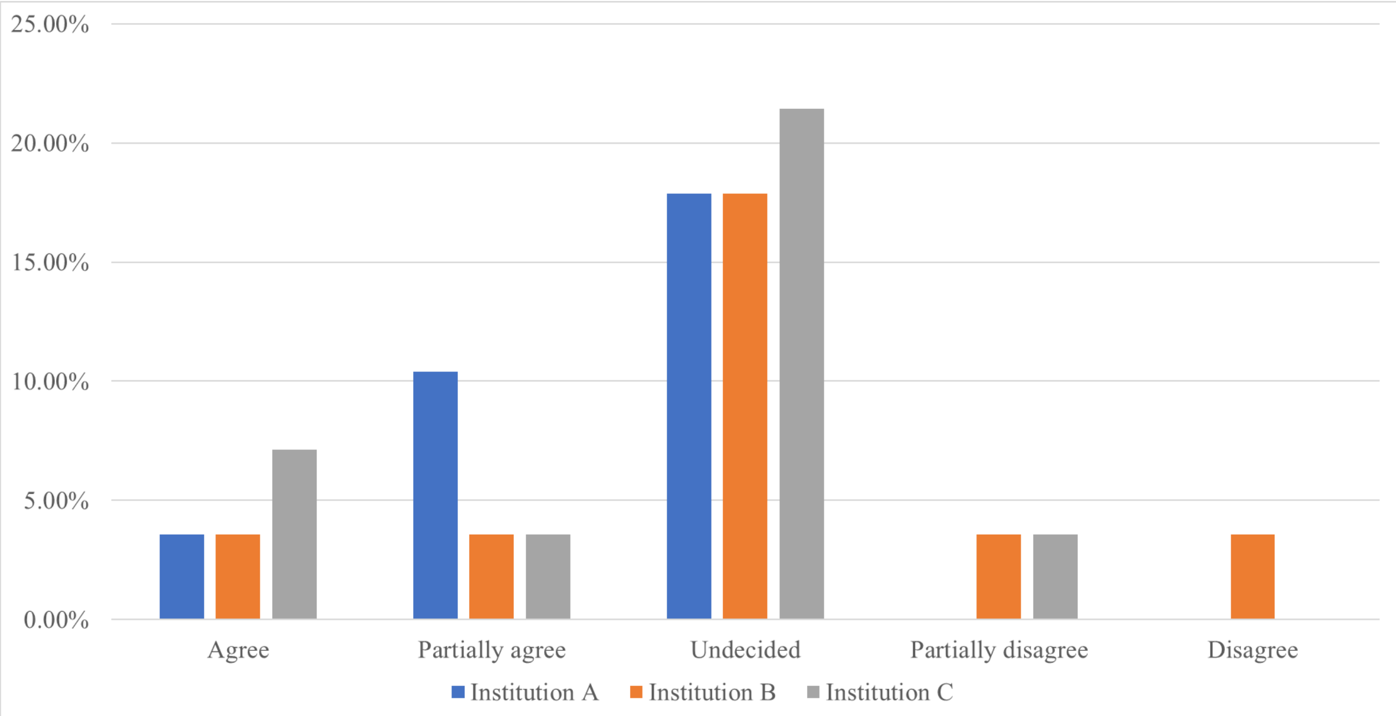

Figure 5. Answering the profile of participants in statement 10.

The last two statements (8 and 10) require a deeper understanding of the elements of quantum mechanics and are usually discussed only in the specialized discipline of quantum chemistry. According to Stefani and Tsaparlis (2009), the understanding of what really constitutes quantum chemistry is very superficial, considering that the construction of specific knowledge in this field has numerous errors, such as calling Bohr's "atomic model" the "first quantum model" even though it ignores the dualistic behavior of the electron. According to Stefani and Tsaparlis (2009), this excess of misconceptions about quantum chemistry is also due to students' insistence on basing their ideas on elementary ideas about the atom, as these are more intuitive and more plausible than what is discussed in mechanics.

An objective analysis of the data shows that most responses are inconsistent, e.g., students agree with statement 5 and then disagree with statement 6. Another example of the inconsistency of responses is the fact that only one (statement 8) of the ten questions has a higher percentage (approximately 68%) of respondents agreeing, while the remaining percentages are well distributed among the responses. Considering that the statements deal with ideas that are uniformly established in quantum mechanics and consequently in quantum chemistry, there should not be such divergences between the answers. This panorama reveals a certain weakness in the construction of knowledge about the topic under discussion, thus confirming previous works. (Bouayad *et al.*, 2014; Coelho and Borges, 2010; Cunha, 2022; Fernandes, 2019; Stefani and Tsaparlis, 2009).

At the end of the analysis of responses to specific assertions, it was also noted that many responses were partial, such as "partially agree" or "partially disagree." Although many chose these answers and claimed to partially agree or disagree with the assertions, many justified their choice as an opinion. This shows not only a certain lack of knowledge about the content under discussion but also that at least those participants who justified their answers with opinions do not appear to know the basic procedures of the scientific method, which were introduced over 400 years ago.

According to Silva and Videira (2020), discourses based on opinions and assumptions are extremely harmful, and the importance of the method and scientific knowledge should be made clear, especially for future professionals who are seen as a reference by society. And this view should not be confused with the expectation that respondents will agree or disagree with every assertion, because even if they were unfamiliar with the content, they would be expected to declare themselves undecided. No pedagogical assertions were used in this analysis as these allow for a higher degree of subjectivity.

3.2. Items related to learning

In this section, all six items (11 to 16) were selected for discussion, considering the subjective nature of the answers and the direct connection with the origin of the learning problems in the field of quantum chemistry.

The first statement that we would like to highlight in terms of the respondents' views on the teaching problems of the subject is statement 11 (**Fig. 6**): "The large number of mathematical expressions and symbols makes learning the content of quantum chemistry difficult". Despite the percentage of respondents agreeing with the statement (about 61%), as we can see in **Fig. 6**, there is an unexpected divergence between the answers, considering that historically the disciplines that have more mathematical formalisms are the "bad guys". of undergraduate courses.

This can be partly explained by the opinion of the participants themselves, who stated in the interviews that the problem is not the calculations themselves, but rather the mathematical foundations of most students, which are not solid enough to understand the topics worked on. which the students themselves confirm in statement 14 (**Fig. 7**): "I have a solid foundation in mathematics and am proficient in topics such as linear algebra and differential and integral calculus". For this topic, about 68% disagreed with the statement, as **Fig. 7** shows. The fundamentals of mathematical concepts are extremely important for understanding the content of quantum chemistry. If this part of the respondents states that they do not know this area, this question brings to light one of the main learning problems of the subject.

Below are some comments from research participants on the two topics previously addressed, which we will discuss later: "Mathematics does not make things difficult; its task is to promote understanding. The obstacle is in the teacher's explanations, forgetting that most students don't even know math from high school, let alone college" (Student 3, Institution A, re: Item 11); "I totally disagree, that was one of the most horrible subjects of the course, I haven't learned anything to this day, and not that it's the teacher's fault, but I am not able to learn these things, I don't even know how I passed Calculus 2" (Student 4, Institution B, at 14).

It is important to point out that when looking at the data presented in the previous two graphs, it is noticeable that the students of Institution C have greater difficulties in the mathematical part. We can observe that there is no unanimity among the students of this institution on the last graph (**Fig. 7**); on the contrary, there is a balance between those who agree and those who disagree with this statement. This fact must be considered considering that HEI also has in its curriculum a compulsory course in linear algebra and analytic geometry, offered in the first semester of the program and focused on developing the basic mathematical skills necessary for understanding the disciplines of differential and integral calculus.

According to Ribeiro *et al.* (2019), the subjects in which students have the greatest difficulties are related to mathematics and lead to many failures, including quantum chemistry.

Most of the students' responses agree with Macêdo and Gregor (2020), who state that one of the main obstacles to understanding and learning differential and integral calculus (essential subjects for learning quantum chemistry) is the weak mathematical foundation, much of which is taught in public education. The student's conception of the role of mathematics in quantum chemistry is a critical factor in preventing it from being an obstacle to understanding the subject's topics, because only when individuals become aware of their position in the learning process can they move through the stages of assimilation and accommodation of the new knowledge. (Mortimer, 2000).

This weakness in mathematical concepts can first be explained from the student's point of view. Often the individual does not know which concept or technique he or she should know. In addition, practicing advanced mathematics is not a general behavior, because although the use of simple operations is quite common in everyday life, other important tools such as differential calculus or linear algebra are usually not part of everyday life, i.e., to master this content, intentional and constant practice is required (Lithner, 2011).

An example of this is the application of integrals, which are usually associated with polar coordinates. To understand the application of integrals through polar coordinates, one must know the difference between Cartesian coordinates and trigonometric functions. But before you learn polar coordinates, you need to learn how integrals work, and to do that you first need to know how to use derivatives. Before derivatives, you need to know how to use limits, and before limits, you need to master the concept and use of different types of functions, such as affine, quadratic, exponential, and others. After this analysis, we come to the basic mathematical topics where students also have difficulties, such as operations with fractions, exponentiation properties, scientific notation, and others.

This is related to what was said earlier about how students relate mathematics and physical phenomena. If they have not mastered the basics, they have greater difficulty understanding more advanced topics in mathematics, and consequently, they have difficulty relating mathematical expressions to physical phenomena.

Next, we can mention statement 12 (**Fig. 8**): "Examples of the application of quantum chemistry in daily life are not uncommon". What we can highlight in this topic is the apparent inconsistency between the answers and the actual thinking of the respondents who agreed with the statement (about 67%), as can be seen in **Fig. 8**, because there was significant uncertainty in the answers and the lack of real examples. when the interviewer asked for examples.

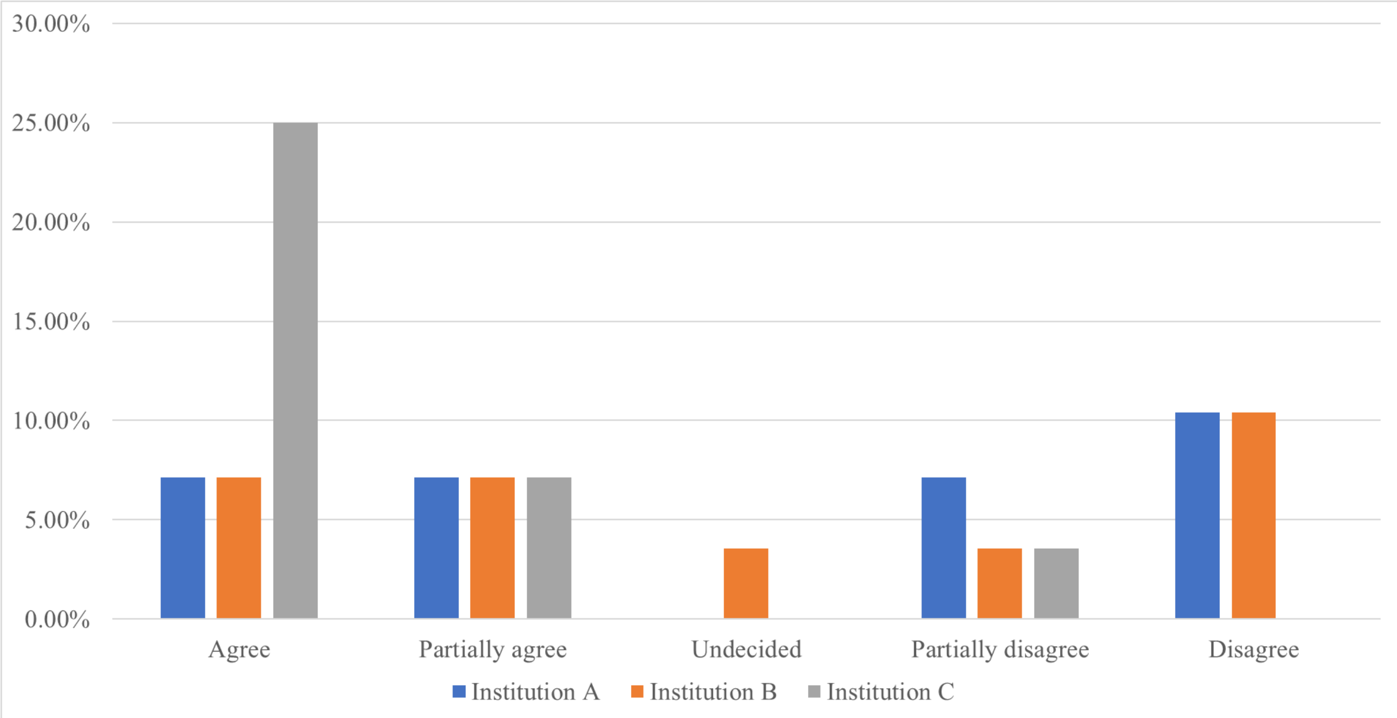

Figure 6. Answering the profile of participants in statement 11.

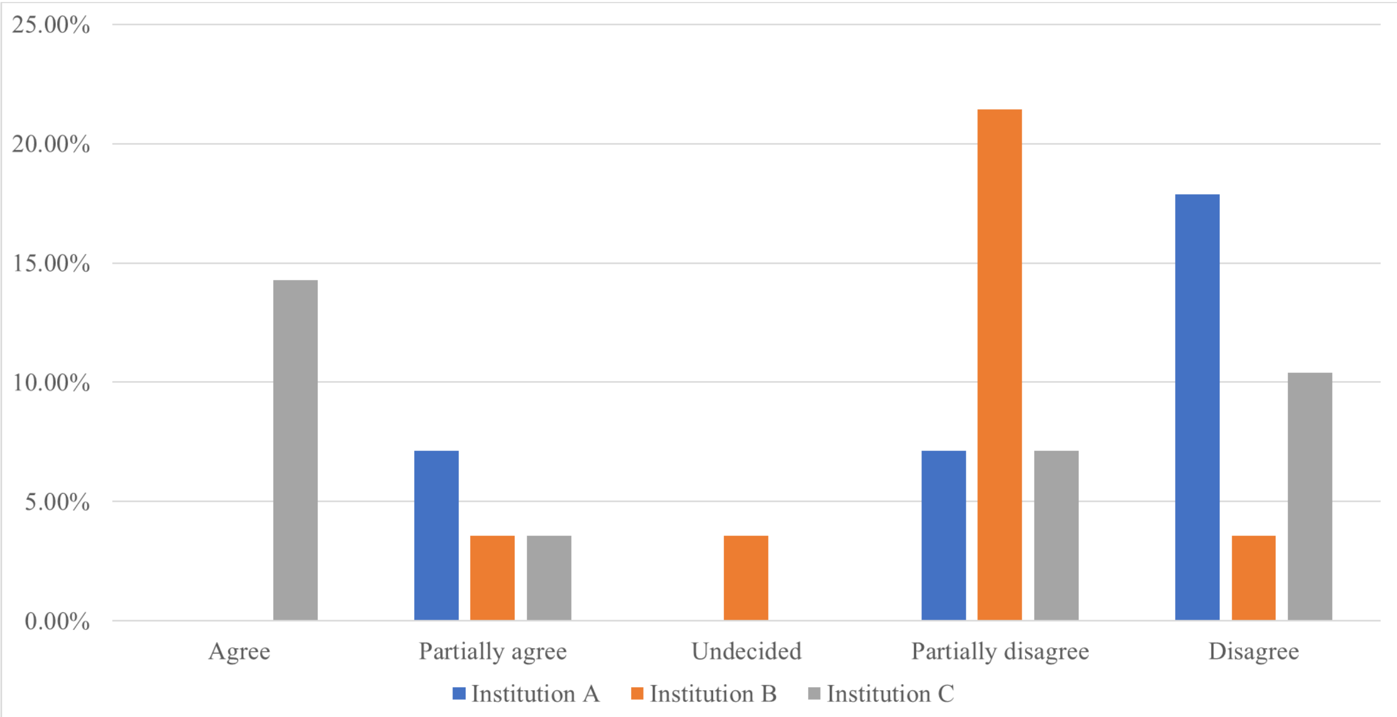

Figure 7. Answering the profile of participants in statement 14.

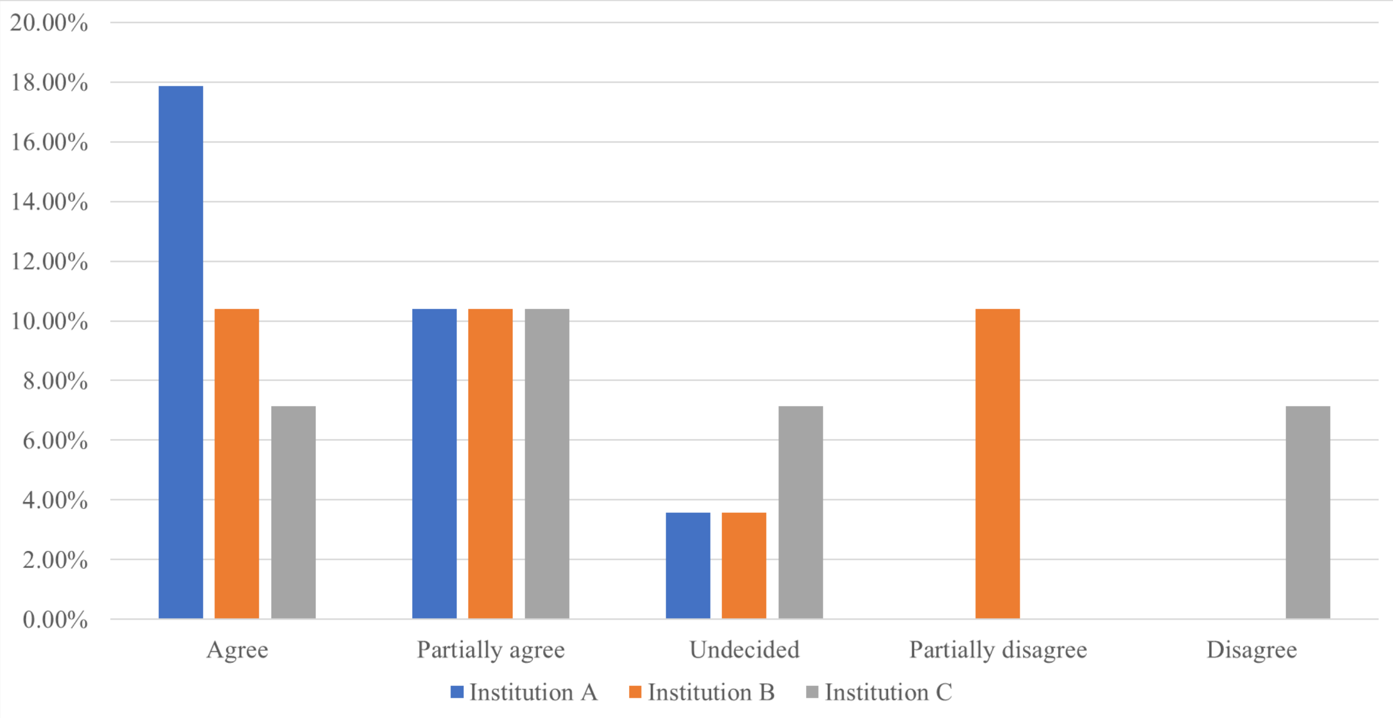

Figure 8. Answering the profile of participants in statement 12.

The difficulty that respondents have in presenting examples of applications is the high degree of abstraction that quantum mechanics, and consequently quantum chemistry, requires for their understanding. For example, automatic doors could be used as an example of a practical application if the photoelectric effect were understood in its essence, but the first statement discussed proves otherwise. In this context, Mortimer (2000) points out that common sense and science use tools such as generalization, induction, and deduction, but science tends to go beyond the limits of common sense and also produce counterintuitive findings. This new perspective acts as a rupture between science and common sense, and only the interference of culture promotes the overcoming of this barrier. Therefore, according to Sagan (1990), it is necessary for scientific knowledge to break through the boundaries of academia and reach people's daily lives, because science is more than a body of knowledge with cold formulas, but a way of thinking.

This is evident in the report of one respondent who, while acknowledging the importance of quantum chemistry, makes a remark that is far removed from what is being discussed in the discipline: "Quantum energy is energy packages that we can't live without, from our breathing to the food we eat. I believe that energy exists because otherwise we wouldn't be living here in the environment" (Student 5, Institution A).

Another respondent who showed that she knew a little more about the subject made a meaningful statement about her experience in the subject that she related to other teaching suggestions:

> I think what makes quantum chemistry difficult is the abstraction, because chemistry in itself is already abstract, and the content often needs to be connected to images or representations from everyday life in order for people to understand the phenomena. When we think of quantum chemistry, we immediately associate it with calculations, and the lack of a solid foundation in mathematics gets in the way, and there are teachers who focus only on that part. My teacher, for example, always talked about theoretical aspects, about how things work, and that helped me a lot. Computer programs make visible what you can't see with the naked eye. So, I think the association of these applications makes students' lives much easier, especially for those who have difficulty abstracting and understanding the phenomena in question (Student 7, Institution C).

Regarding statement 13, which says: "I can well understand the explanations of the teacher of the subject dealing with the contents of quantum chemistry", a look at **Fig. 9** shows a balanced result, as half of the respondents answered positively to this statement. The conclusion from this statement is that many indicated that despite the understanding, it was not a deeper knowledge that remained after the course, but rather something preliminary that served only the purpose of assessment and recognition in the course.

From this point of view, it is important that the teacher reflects on his teaching practice and tries to match the attention he pays to the technical part of his subject with the learning process of the students, which does not always happen automatically, especially in the case of quantum chemistry content. According to Quadros and Mortimer (2014), constant reflection on the teaching practice allows the development of a practice in which the strategies are diversified, and participation is favored, creating a more effective environment. We can highlight the thought of Ausubel (2003) to connect the two previous points. For students to actually learn, the added information must be linked to their prior knowledge to make sense of it. Using conceptual maps, text, pictures, and other tools, such as applying content to daily life, helps make these connections and make science instruction more meaningful, according to Tavares (2008). Another factor that contributes to meaningful learning is reflection on the assessment process. When traditional assessments consider only a numerical value of what is learned, the assessment becomes only an expression of the emotional state at the time of the assessment and ignores all the subjectivity and complexity of the assessment process (Luckesi, 2012). Thus, the student's main goal is to achieve the score required to pass the subject, not the learning itself.

Analyzing statement 15 (**Fig. 10**), which says: "It is possible to understand chemistry today without knowing the basics of quantum chemistry", we can see another problem related to learning the content of this subject, because as shown in **Fig. 10**, about 39% of the respondents agree with a statement that can be considered false. One does not have to go much further than the topics covered in school, such as Bohr's atomic model, to conclude that quantum chemistry was not essential for understanding chemistry at the beginning of the 20th century.

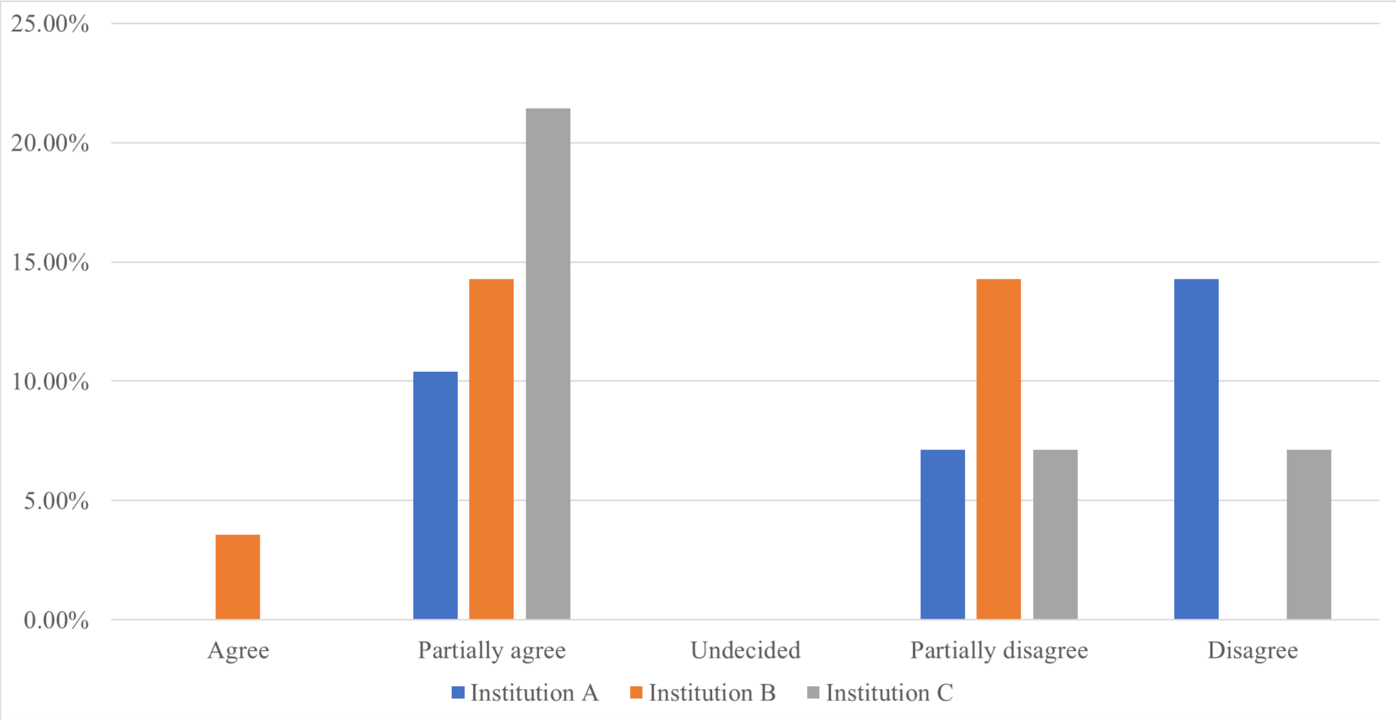

Figure 9. Answering the profile of participants in statement 13.

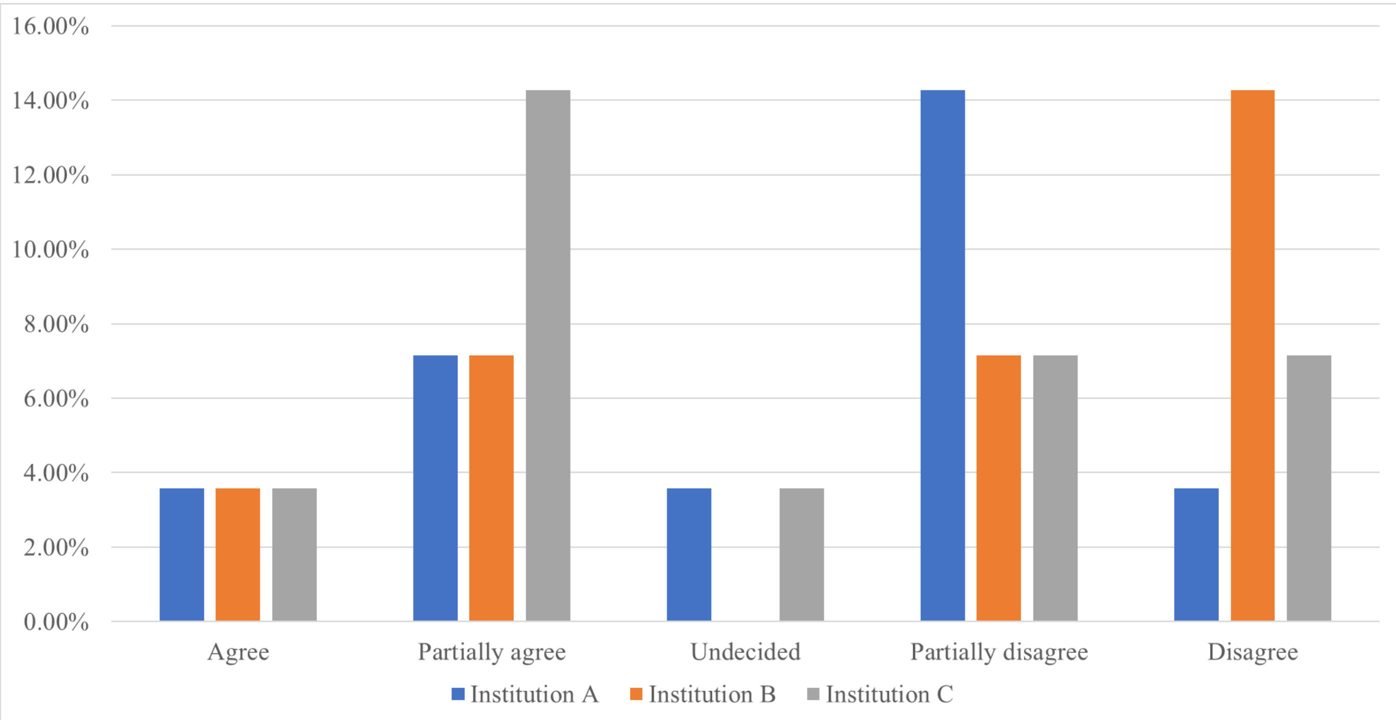

Figure 10. Answering the profile of participants in statement 15.

This perspective explains a gap in the training process of future teachers and the need to re-evaluate the curricular matrices and political-pedagogical projects of institutions, as well as a paradigm shift for higher education institution to recognize their responsibilities in the training process of these professionals (Schnetzler and Corrêa, 2017) since students do not seem to have a comprehensive idea of the scope of chemistry content, especially quantum chemistry, nor of the context in which it is embedded, as well as of its social application (Santos and Schnetzler, 1996). This problem also runs through the training of college teachers. It is important to also focus on the teacher of the teacher who needs training during his or her postgraduate studies that focuses on teaching in a different area of instruction. The teacher must view his or her educational process as a maturation of his or her previous education, rather than as a sum of specific and pedagogical disciplines. Also, there needs to be more dialogue between supervisors and students about teaching practice in addition to reflection on teaching practice (Arroio *et al.* 2006). In this way, according to Arroio (2009), something that traditionally does not appear in discussions would be discussed, namely methodological practices in higher education.

Finally, we see in statement 16: "I know many people who have mastered the basics of quantum chemistry", it is not a problem, but a reflection of learning problems related to the content of quantum chemistry when about impressive 93% of the respondents disagree with the statement, as shown in **Fig. 11**.

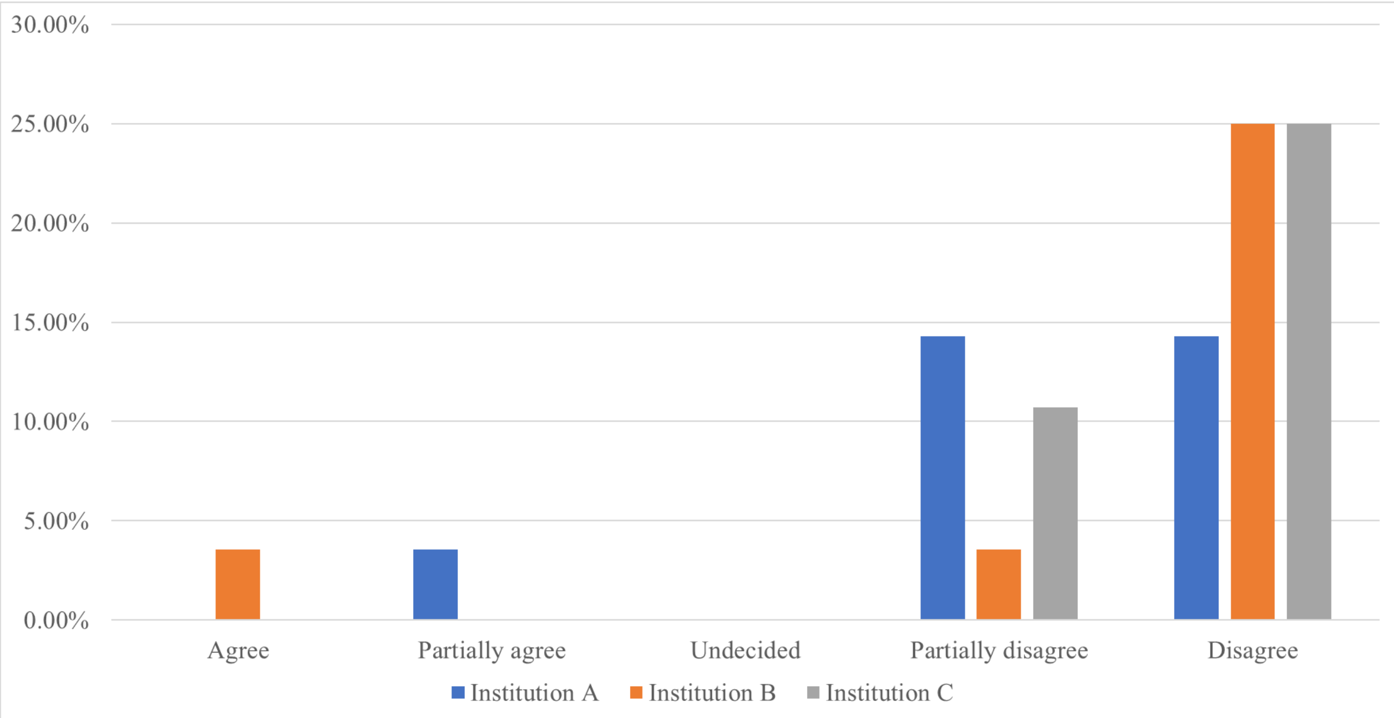

Figure 11. Answering the profile of participants in statement 16.

During their training, prospective chemistry teachers face several problems, such as the weak pedagogical base offered in chemistry curricula (Fernandez, 2018), the excessive focus on the epistemological training of the subject to the detriment of critical sense and reflection on chemistry and teaching practices (Mesquita *et al.*, 2012), and the aforementioned difficulties related to the mathematical base which is essential for the development of chemical knowledge. The answers to statement 16 reflect the result of the synthesis of the problems mentioned above and show the enormous difficulties in teaching and learning quantum chemistry, leading to a series of chain effects, such as a false understanding of the nature of matter, which is one of the most important effects observed.

Furthermore, in teaching practice, the teacher must seek the connection between mathematical theories and formalisms with observed phenomena, or at least with those that can be proven (in the case of submicroscopic phenomena), to minimize the level of abstraction of this content. This facilitates the learning of quantum chemistry as it is, and the student understands that this branch of science is more than just traces, numbers and disconnected forms.

4. Conclusions

Basic knowledge of quantum chemistry is more than necessary for a better understanding of modern chemistry, especially for chemistry students who will be responsible for teaching this field of knowledge in the future.

If we look at the specific part of the questionnaire, we first realize that the students have a misconception of the nature and interactions of matter at the atomic level, linked to the most elementary notions that could be overcome by considering the most appropriate and up-to-date theories. And with increasing difficulty of the tasks, it was found that students do not have a comprehensive idea of the application and performance of quantum chemistry.

These problems can be understood from the answers to the last 6 questions, which relate to learning the subject content. The first point refers to the mathematical basis of the students, which is not solid enough to understand the mathematical formalisms of quantum chemistry, which are essential for the interpretation of the experimentally observed physical phenomena.

The second point is related to the high degree of abstraction of the content, which is mostly counterintuitive. The fact that the observed phenomena are often in apparent contradiction with the ideas of classical physics, such as the lack of an idea of the trajectory of the electron due to its dualistic behavior, promotes a certain resistance and even cognitive blockages caused by the confrontation with these confusing situations, making it difficult for the student to become aware of the new concepts that he/she must assimilate and process.

Another aspect that can be gleaned from the students' responses is their concentration during subject lessons. Given the current assessment model, which is too quantitative, students tend to strive only to pass the subject, regardless of whether they have learned the content.

The fourth impasse is related to the design and implementation of the curricula proposed by universities, which do not make room for discussions such as these in specific disciplines within the matrix, which would be necessary to break down the barriers to learning quantum chemistry.

Discussing this scenario can help to mitigate the problems mentioned above, as universities and their faculties have the autonomy to develop projects and strategies. As Moraes and Teixeira Júnior (2014) point out, it is evident that the difficulties in the use of mathematics in undergraduate studies are inextricably linked to deficiencies in the construction of knowledge, especially in the fundamentals taught in primary and secondary education. Therefore, it is interesting to introduce specialized undergraduate courses in calculus to fill these gaps and provide a solid and reliable foundation for the study of quantum chemistry. Another important aspect, as Raupp *et al.* (2008) argue, is that the use of information and communication technologies (ICT) plays a crucial role in the teaching of quantum chemistry. Molecular modeling and computational chemistry software offer a tangible approach to overcoming the challenges posed by the inherent abstraction of the subject and compensate for the lack of macroscopically observable practical experiments.

Back to the teachers and their practice. Given the constant technological development of the last decades, we must recognize that teachers are not always able to keep up with these changes, as Pretto and Riccio (2010) and Trebien *et al.* (2020) point out. Therefore, it is important to establish professional development programs for teachers. This will ensure that they are adequately prepared to apply the aforementioned methods and adapt their pedagogical practices to today's demands. Finally, as Oliveira (2010) points out, the introduction of alternative forms of assessment such as research and group work is crucial for the development of understanding of quantum chemistry. These approaches encourage social interaction and collaboration between students, allowing for the sharing of experiences, the transmission of knowledge and the exploration of different perspectives on the topics covered, thus enriching the learning experience.

The discussion of this scenario can help to mitigate the problems mentioned above since universities have the autonomy to develop projects that improve the mathematical foundations of students; methods that deal with different ways of presenting the content of the subject; in addition to seeking reformulations of the assessment processes aimed at the meaningful learning proposed by Ausubel (2003), and thus it will be possible to envisage a more effective training of chemistry teachers, with professionals who are better prepared and aware of their social role.

Authors' contributions

Conceptualization: Ferreira, L. N. A.; Souza, A. A.; **Data curation:** Not applicable; **Formal Analysis:** Sousa, L. M. P.; Cunha, K. M. A.; **Funding acquisition:** Not applicable; **Investigation:** Sousa, L. M. P.; **Methodology:** Sousa, L. M. P.; **Project administration:** Not applicable; **Resources:** Not applicable; **Software:** Not applicable; **Supervision:** Souza, A. A.; **Validation:** Not applicable; **Visualization:** Not applicable; **Writing – original draft:** Sousa, L. M. P.; **Writing – review & editing:** Cunha, K. M. A.; Ferreira, L. N. A.; Souza, A. A.

Data availability statement

The data will be available upon request.

Funding

Not applicable.

Acknowledgments

The authors acknowledge the Federal University of Piauí (UFPI).

References

Alberto, S.; Placido, R. L.; Placido, I. T. M. A formação docente e o tecnicismo pedagógico: um desafio para a educação contemporânea. *Rev. Ibe. Est. Ed.* **2020**, *15* (2), 1652–1668. https://doi.org/10.21723/riaee.v15iesp2.13837

Arroio, A. Formação docente para o ensino superior em química. VII Enpec, Florianópolis, Santa Catarina, Brasil, 2009.

Arroio, A.; Rodrigues Filho, U. P.; Silva, A. B. F. A formação do pós-graduando em química para a docência em nível superior. *Quím. Nova.* **2006**, *229* (6), 1387–1392. https://doi.org/10.1590/S0100-40422006000600040

Ausubel, D. *Aquisição e retenção de conhecimentos*: uma perspectiva cognitiva; Plátano, 2003.

Batista, E. C.; Matos, L. A. L.; Nascimento, A. B. A entrevista como técnica de investigação na pesquisa qualitativa. *Revista Interdisciplinar Científica Aplicada.* **2017**, *11* (3), 23–38.

Belo, T. N.; Leite, L. B. P.; Meotti, P. R. M. As dificuldades de aprendizagem de química um estudo feito com alunos da Universidade Federal do Amazonas. *Scientia Naturalis.* **2019**, *1* (3), 1–9.

Beuren, I. M. *Como elaborar trabalhos monográficos*: teoria e prática; Atlas, 2006.

Bouayad, A.; Kaddari, F.; Lachkar, M.; Elachqar, A. Quantum model of chemical bonding: barriers and learning difficulties. *Procedia Soc. Behav. Sci.* **2014**, *116*, 4612–4616. https://doi.org/10.1016/j.sbspro.2014.01.994

Chassot, A. *Alfabetização científica: questões e desafios para a educação*; Unijuí, 2014.

Coelho, G. R.; Borges, O. O entendimento dos estudantes sobre a natureza da luz em um currículo recursivo. *Cad. Bras. Ens. Fís*. **2010**, *27* (1), 63–87.

Costa, H. R.; Souza, A. R. A produção de significados no modelo quântico por meio de ferramentas socioculturais: uma proposta analítica da aprendizagem. *Ensino & Multidisciplinaridade*. **2017**, *3* (1), 17–39.

Cramer, C. J. *Essentials of computational chemistry: theories and models*; Wiley, 2004.

Cunha, S. G.; Dias, D; Streit, L. A estrutura eletrônica do átomo: um estudo sobre o conhecimento de Química Quântica no ensino superior. In 41º Encontro de Debates sobre o Ensino de Química, Pelotas – RS, Brasil, October 14–15, 2022.

Fernandes, L. S. *Conceituação da ligação covalente por licenciandos em Química*; UFBA, 2019.

Fernandez, C. Formação de professores de Química no Brasil e no mundo. *Estud. Av.* **2018**, *32* (94), 205–224. https://doi.org/10.1590/s0103-40142018.3294.0015

Gregório, J. R.; Leite, C. C.; Leal, B. C.; Nitschke, W. K.; Pederzolli, F. R. S.; Nobre, K. M.; Fraga, M. V. B.; Silva, C. B. O programa de apoio à graduação em Química (PAG-Química) e sua contribuição para a democratização e permanência dos estudantes no ensino superior. Authorea. [PREPRINT] May 20, 2019. https://doi.org/10.22541/au.155836336.67356235

Halliday, D.; Resnick, R. *Fundamentals of Physics*; 10. ed. Wiley, 2014.

Henriksen, E. K.; Angell, C.; Vistnes, A. I.; Bungum, B. What is light? *Sci. Educ*. **2018**, *27* (1-2), 81–111. https://doi.org/10.1007/s11191-018-9963-1

Levine, I. N. *Quantum Chemistry*; 7. ed. Pearson Education, 2014.

Libâneo, J. C.; Pimenta, S. G. Formação de profissionais da educação: visão crítica e perspectiva de mudança. *Educ. Soc.* **1999**, *20* (68), 239–277. https://doi.org/10.1590/S0101-73301999000300013

Lithner, J. University mathematics students' learning difficulties. *Educ. Inq.* **2011**, *2* (2), 289–303. https://doi.org/10.3402/edui.v2i2.21981

Luckesi, C. C. *Educação, avaliação qualitativa e inovação*; INEP, 2012.

Macêdo, J. A.; Gregor, I. C. S. Dificuldades nos processos de ensino e de aprendizagem de cálculo diferencial e integral. *Educação Matemática Debate.* **2020**, *4* (10), 1–24. https://doi.org/10.24116/emd.e202008

Mesquita, N. A. S.; Cardoso, T. M. G.; Soares, M. H. F. B. O projeto de educação instituído a partir de 1990: caminhos percorridos na formação de professores de Química no Brasil. *Quím; Nova.* **2013**, *36* (1), 195–200. https://doi.org/10.1590/S0100-40422013000100033

Moraes, C. A.; Teixeira Júnior, J. G. Reflexões sobre o ensino de cálculo diferencial e integral em cursos de graduação em Química. *DiversaPrática.* **2014**, *2* (1), 194–217.

Mortimer, E. F. *Linguagem e formação de conceitos no ensino de ciências*; UFMG, 2000.

Nussenzveig, H. M. *Curso de Física Básica: Fluidos Oscilações e Ondas, Calor*; v. 2, 5. ed., Editora Blücher, 2014.

Oliveira, J. R. S. A perspectiva sócio-histórica de Vygotsky e suas relações com a prática da experimentação no Ensino de Química. *Revista de Educação em Ciência e Tecnologia*. **2010**, *3* (3), 25-45.

Parnafes, O. When simple harmonic motion is not that simple: managing epistemological complexity by using computer-based representations. *J. Sci. Educ. Technol.* **2010**, *19* (6), 565–579. https://doi.org/10.1007/s10956-010-9224-9

Pavia, D. L.; Lampman, G. M.; Kriz, G. S.; Vyvyan, J. R. *Introduction to spectroscopy;* Cengage Learning, 2013.

Pereira, M. E.; Brasileiro, R.; Silva J. F.; Silva, P. B.; Brachi, D.; Albuquerque, F. Esteriótipos, mentiras e videotape: estudos experimentais sobre a acurácia na identificação da mentira. *Psicologia em Estudo.* **2006**, *11* (1), 209–218.

Pretto, N. L.; Riccio, N. C. R. A formação continuada de professores universitários e as tecnologias digitais. *Educ. Rev*. **2010**, *37*, 153–169. https://doi.org/10.1590/S0104-40602010000200010

Quadros, A. L.; Mortimer, E. F. Fatores que tornam o professor de ensino superior bem-sucedido: analisando um caso. *Ciênc. Educ.* **2014**, *20* (1), 259–278. https://doi.org/10.1590/1516-731320140010016

Raupp, D.; Serrano, A.; Martins, T. L. C. A evolução da Química Computacional e sua contribuição para a educação em Química. *Revista Liberato.* **2008**, *9* (12), 13–22. https://doi.org/10.31514/rliberato.2008v9n12.p13

Ribeiro, J. C. A.; Rosa, J. V. A.; Souza, G. A. P.; Haraguchi, S. K.; Silva, A. A. Evasão e retenção na perspectiva de alunos do curso de licenciatura em Química. *South. Am. J. Bas. Edu. Tec. Technol.* **2019**, *6* (2), 609–618.

Sagan, C. Why we need to understand science. *Skeptical Inquirer.* **1990**, *14*, 263–269.

Santos, W. L. P.; Schnetzler, R. P. Função social: o que significa ensino de Química para formar o cidadão? *Química Nova na Escola.* **1996**, *4* (4), 28–34.

Saviani, D. *Pedagogia histórico-crítica*: primeiras aproximações; Autores Associados, 2011.

Schnetzler, R. P.; Corrêa, T. H. B. Da formação à atuação: obstáculos do tornar-se professor de Química. *Revista Debates em Ensino de Química*. **2017**, *3* (1), 28–46.

Silva Júnior, D. S.; Costa, F. J. Mensuração e escalas de verificação: uma análise comparativa das escalas Likert e frase completion. *XVII Seminários em Administração*, São Paulo, Brasil, 2014.

Silva, V. C.; Videira, A. A. P. Como as ciências morrem? Os ataques ao conhecimento na era da pós-verdade. *Cad. Bras. Ens. Fís.* **2020**, *37* (3), 1041–1073. https://doi.org/10.5007/2175-7941.2020v37n3p1041

Stefani, C.; Tsaparlis, G. Students' levels of explanations, models, and misconceptions in basic quantum chemistry: a phenomenographic study. *J. Res. Sci. Teach*. **2009**, *46* (5), 520–536. https://doi.org/10.1002/tea.20279

Tavares, R. Aprendizagem significativa e o ensino de ciências. *Cienc. Cogn.* **2008**, *13* (1), 94–100.

Trebien, M. M.; Souza, W. R.; Oliveira, E. R.; Silva, J. L. Formação continuada de professores: uma epistemologia da prática. *Ambiente: Gestão e Desenvolvimento.* **2020**, *13* (1), 91–102. https://doi.org/10.24979/359

Universidade Federal do Piauí (UFPI). *Sistema Integrado de Gestão de Atividades Acadêmicas – SIGAA.* 2022. https://sigaa.ufpi.br/sigaa/public/home.jsf accessed 2022-12-16).

Woods, J.; Walton, D. Argumentum ad verecundiam. *Philosophy & Rhetoric.* **1974**, *7* (3), 135–153.