CHALLENGES OF THE QUANTUM CHEMISTRY COURSE IN AN INADEQUATE-EPISTEMOLOGICAL-ACCESS CONTEXT AND EXPLORATION OF ADDRESSING OPTIONS

Liliana Mammino
Department of Chemistry, University of Venda, South Africa
sasdestria@yahoo.com

ABSTRACT–Courses with extensive presence of mathematics are frequently viewed as challenging by chemistry students. Quantum chemistry is considered particularly difficult, as the course involving the largest mathematics component and fairly sophisticated logical and abstract thinking abilities. The difficulties increase sharply in contexts where diffuse epistemological-access inadequacies complicate students' ability to approach conceptually demanding materials. This poses a number of pedagogical questions, from the search of the best compromise between course quality and students' accessibility on selecting the course content to the design of teaching options capable of effectively addressing students' difficulties. The paper presents an overview of diagnosed difficulties and of explored addressing approaches, based on over 27 years direct experience. The results show dominant impacts of inadequate language mastery and inadequate mathematics mastery, whose effects do not simply sum, but greatly enhance each other. It is concluded that improving language mastery and mathematics mastery should be viewed as pre-requisite for effective learning of quantum chemistry.

Keywords: Epistemological Access; Language Mastery; Mathematics Mastery; Quantum Chemistry Courses.

1. INTRODUCTION

Research into the teaching/learning of advanced chemistry courses is still scarce. The need to expand it is gaining increasing recognition in view of the changing characteristics of students' population, with the problems of underpreparedness increasingly reflecting also on the performance in advanced courses. The appearance of conferences such as *Eurovariety*, focusing specifically on tertiary level chemistry education, is a symptom of the increasing concern about educational aspects of university courses. However, the main teaching/learning focus is often on the first year courses, while the other themes relate more to issues such as streamlining curricula in view of future employment possibilities. Focus on specific advanced courses remains rare. This may be largely due to the fact that such studies would require full integration of the content perspective and the educational perspective, as the educational approaches for advanced courses are inextricably linked to the nature of the content (Mammino, 2014a). Furthermore, while communicating with other education researchers is fundamental, the specialised nature of the content of advanced courses may complicate communication with researchers who are not specialists in the same area, somewhat limiting the possibility of interchanges of opinions and experiences. It is not easy to find a univocal answer. Specific educational interchanges among specialists of a given advanced course may be useful, but there is also the need to communicate across specialisation areas, because many educational challenges are not restricted to one area: the causes behind them may affect many areas and the main criteria for the development of addressing option may have aspects common to several areas. The search for feasible and constructive ways for research and its communication is a field for novel explorations.

This paper attempts to highlight the difficulties posed by inadequate epistemological access in one of the most demanding courses of the chemistry curriculum – the quantum chemistry course. The major challenge in presenting analyses and inferences is probably the need to outline educational problems and students' difficulties in a way that goes beyond the details of the content, although diagnoses and inferences are closely linked to those details. The paper attempts both to highlight the intrinsic interconnections between content and educational perspectives and to communicate the main information to a broader range of readers than quantum chemistry lecturers/specialists. Given the novelty of the investigation, the paper constitutes a sort of new option, without existing benchmarks against which to assess its mode of presentation; it might become interesting as reference for other studies on the educational aspects of quantum chemistry courses and of other advanced chemistry courses. The paper content is based on over 27 years direct experience with the teaching of quantum chemistry courses in Sub-Saharan Africa at the University of Zambia (1988–1992), National University of Lesotho (1993–1996) and University of Venda (UNIVEN, 1997–2015). The examples reported are all from the courses at UNIVEN – an HBU in South Africa, mostly serving an underprivileged community and therefore facing the challenges of inadequate epistemological access for the vast majority of its students' population. Extensive reviews of works on epistemological access in South Africa, as well as on the impact of language-related difficulties on science learning in general, have been included in Mammino (2012, 2013a, 2014b) and will not be repeated here to avoid redundancies.

Physical chemistry courses are often considered particularly difficult by chemistry students. The reasons are related to the extensive presence of mathematics and to the dominant role of conceptual and abstract thinking (Mammino, 2009). These factors are maximal in quantum chemistry – the area which provides models to the rest of chemistry, building the models on quantum mechanics and developing them through a variety of mathematical approximation procedures. Therefore, the mathematical component and the relevance of abstract reasoning play greater roles than in any other area of chemistry. Difficulties with these aspects increase enormously in contexts where the development of students' epistemological access is constrained by historical and/or socioeconomic or environmental factors such as second-language instruction, inadequate general language-mastery, inadequate mastery of other learning and communication tools (first of all visualization) and inadequate familiarity with logical and abstract thinking. Contexts of this type pose challenging questions to educators, both in terms of selecting the course content in a meaningful way while maintaining it accessible to the students taking it and in terms of designing teaching approaches that best respond to the needs of those students.

2. METHOD AND OBJECTIVES

At UNIVEN, the quantum chemistry course is offered at honours level, where it constitutes the content of the physical chemistry course (one of the four courses that students take in the first semester). The small size of the group (not more than 10 students per year, so far) enables extensive in-class interactions.

The investigation carried out within the course is qualitative, as it aims at identifying all the details of the difficulties experienced by students, and also their probable causes, in order to tune teaching approaches to identified needs. Teaching approaches are continuously re-designed with a sort of recursion-optimisation involving continuous interplay between diagnoses of students' difficulties and responding adaptations of teaching approaches. In this way, educational research and the design of teaching approaches are fully integrated, as two sides of the same coin.

Diagnoses are based on systematic analysis of students' answers in their written works and during in-class interactions (where written answers are utilised as an interaction tool, Mammino 2013b), complemented by personal interviews when expedient. All students' answers are analysed. The answers which highlight difficulties, interpretations and perceptions calling for specific explanations within class activities are collected, to ensure that the relevant aspects will be given attention also in subsequent years and to enable comparisons through different years. The analysis of students' written answers is performed considering and integrating three points of view: content knowledge, ability to handle the relevant mathematics and relating it to the physical meaning, and language aspects (ability to understand a text on reading and ability to express information, which is tantamount to ability to express the acquired knowledge). This three-perspective approach is made possible by the fact that the author's background training included humanities training, thus enabling language-related analyses.

Besides providing information for better tuning of teaching approaches, the analysis is utilised as an explanation tool to stimulate students' active engagement during in-class interactions. Practical aspects of the latter utilisation are illustrated in Mammino (2015). The examples included in section 4 illustrate the integration of perspectives in the analysis. The comments outlined for these examples constitute the main guidelines for in-class interactions aimed at clarifying concepts though error analysis, i.e., they provide the guidelines for questions aimed at stimulating students' reflections on all the details of a given issue.

3. COURSE CONTENT AND EDUCATIONAL CHALLENGES

Selecting the material for the course content poses major educational challenges, as it implies the search for a workable compromise between the need that the course remains meaningful and the need to keep the content accessible to students. Two key features require careful consideration:

- Ensuring that the course provides adequate exposure to the nature of quantum chemistry (how the study of atoms and molecules is approached and why) and includes the information needed for other areas/courses (e.g., spectroscopy).
- Limiting the mathematical component as much as possible without jeopardising students' understanding of the role of mathematics in the study of atoms and molecules.

For the course offered at UNIVEN, it was opted to keep the content as basic as possible and to insist on clarifications of each and every detail to ensure conceptual understanding. This option somewhat limits the variety of questions that can be proposed on assessment, as they revolve around a limited number of key issues. Furthermore, problem solving is limited to problems requiring simple mathematical procedures (what is – in any case – reasonable for an introductory course). Under these circumstances, many questions are repeated in their core meaning – although with wording modifications and no regular repetition patterns – every 2-4 years. Students are also provided with a considerable number of tutorial questions closely resembling those that are asked at assessment level (an approach utilised in some universities and providing some learning-guidance to students without decreasing the need for intellectual engagement and conceptual understanding). Despite the implementation of all these aspects that would be expected to facilitate students' learning efforts, experience shows that students find it difficult to tackle those questions, even after they have been discussed extensively in the class, or even when they are proposed for the second time in the same course. The pass-rate has significantly decreased in recent year, without any increase in the course content or difficulties (actually, with some simplifications). These observations motivate the investigation of the impact of inadequate epistemological access as a probable key factor determining students' performance.

4. RESULTS: DOCUMENTATION, ANALYSES AND DIAGNOSES

The documentation collected throughout 18 years at UNIVEN is bulky, comprising several thousand answers. Representative examples to substantiate diagnoses and inferences are reported here, selecting them from contents that can be easily explained within this text and considering the recurrence of the features that they illustrate. The examples are numbered progressively to facilitate references in the text.

This section is divided into subsections – each of them referring to one of the identified major categories of difficulties – for discussion functionality and to increase readability. An actual separation of categories is impossible, because language-related difficulties are ubiquitous and often determine or enhance the others. For instance, both mathematics and conceptual understanding require logical and abstract thinking, and the level to which these abilities develop is largely determined by the level of language mastery; thus, many observed difficulties can be ultimately traced to inadequacies in language mastery. No subsection is here specifically devoted to language-related difficulties, because they appear evident from most of the examples considered for the other categories.

4.1. Passive attitudes

Passive attitudes are born from understanding difficulties and, often, also from secondary school teaching/learning approaches. They imply memorization without understanding and mechanical repetition/reproduction of memorised parts. The reproduction may be so mechanical that the parts included in a single answer may not have any relationship with the question given or with each other. For instance, answer 1 lists the values of the radius in Bohr's atom in place of the spectral series of the hydrogen atom.

1. *The hydrogen spectral lines are given by* a_o, $4a_o$, $9a_o$, $16a_o$ *and* $25a_o$.

One of the consequences is the practical inability to see and utilise connections among courses: what is memorised within one course belongs to that course alone and is not *exported* to other courses. Although a full understanding of the mechanisms of this phenomenon would require broader investigation, it occurs so frequently as to require in-class interventions. The most relevant intervention is implemented at the beginning of the course, by asking typically first-year questions concerning the structure of the atom, to be answered in writing in the class (Mammino, 2013b). Surprisingly, most students fail questions as basic as the request to write the electronic configuration of an element; in a recent experience, only one student out of nine managed to write a correct electronic configuration.

The practical component of the course comprises simple (semiempirical) calculations of assigned molecules and subsequent discussion of their geometries (bond lengths, bond angles, etc.) on the basis of information known from undergraduate courses (such as hybridisation of atomic orbitals). More than half of the students fail to utilise these concepts, e.g., to state that the planar geometry around a double bond results from sp^2 hybridisation, or that the benzene ring is planar because of the sp^2 hybridization of all its carbon atoms.

Other consequences of passive attitudes surface frequently. For instance, questions asking students to provide their own examples of something seem particularly challenging, probably because they require active mental engagement and reflection – the antonym of passivity.

4.2. Difficulties with mathematics

It is difficult to separate difficulties with mathematics from difficulties with logical reasoning, as they are often untanglably intermingled. Few illustrative examples referring to purely mathematical features or to correlated mathematical and physical features are considered in this section.

Questions such as "why f orbitals appear only from the fourth energy level", or "why there are seven f orbitals in a given energy level", only require straightforward consideration of the values taken by the quantum numbers characterising the orbitals; however, most students fail to provide answers (this issue is discussed in detail in Mammino, 2013a).

The wavefunction (ψ) is the core of quantum chemistry, as it provides the description of the system considered. It needs to comply with some conditions. Two conditions (it must be continuous and it must have continuous slope) refer to its mathematical meaning as solution of the Schrödinger equation. The logic of the reasons for these conditions is as follows:

- The wavefunction is the solution of the Schrödinger equation.
- The Schrödinger equation is a second order differential equation. Therefore, its solution must have the second derivative.
- This means that it must be continuous in order to have the first derivative, and the first derivative must be continuous to get the second derivative.

Students' explanations are often incomplete, usually very short, without an adequate logical framework and with poor mathematical terminology, or contain errors. Answers 2–6 refer to the continuity of the wavefunction and answers 7–9 to the continuity of its slope. Answer 2, 3 and 8 contain self-evident errors. Answers 4 and 5 consider the nature of the wavefunction in relation to probability, which actually relates to other conditions (see next paragraph). Answer 6 randomly ensembles parts from different unrelated themes. Answer 7 shows confusion between the *function* and *equation* concepts and answer 8 between the *solution* and *equation* concepts.

2. It must be continuous so that it cannot be meaningless. If it is not continuous it will be zero.

3. It must be continuous because it is a two-dimensional function.

4. Since its square is the probability of finding a particle in the universe, it must be continuous because the particle is somewhere in the universe.

5. It must be continuous so that it becomes smooth at the boundaries, thus enables us to find the position of the wavefunction in a certain range.

6. For the wavefunction to be acceptable according to boundary conditions it must be the same at the edges of the wall i.e. x=0 and x=l. This means that it must be continuous. The value of the wavefunction must be zero everywhere outside the walls. That is the wavelength of the electromagnetic radiation consist of discrete values.

7. Because wavefunction is a differential equation.

8. Because the solution is a second order differential equation.

9. If the slope is not continuous it means that the slope does not exist and this means the function does not exist.

The other two conditions on the wavefunction relate to its physical interpretation (the fact that $\psi^*\psi$ is a probability density). One of these conditions is that the wavefunction must be finite. The logic of its explanation is as follows:

- $\psi^*\psi$ is a probability density and, therefore, the integral $\int\psi^*\psi d\tau$ gives the probability of finding the particle in a certain volume.
- Probability cannot have an infinite value.
- Therefore ψ must be finite.

Students' explanations highlight difficulties both with mathematics and with the connections between mathematics and physical meaning. The following answers start with "the wavefunction must be finite" and proceed as follows:

10. Because an infinite wavefunction would be meaningless.

11. Because it describes the position of a particle and hence the particle has a finite position in space.

12. Because the probability density of an infinite system is meaningless.

13. So that it can reproduce itself and so it will be acceptable in the values considered.

Answer 10 is just a statement without justification. Answers 11–13 are meaningless: the wavefunction does not describe the position of a particle (11); the *finite* or *infinite* concept applies to a function, not to a system (12); answer 13 has no identifiable meaning.

Many answers show confusion between crucial aspects of mathematical procedures and their results. Only one example (14) is reported for illustration, because the confusion usually results in meaningless statements, for which the only analysis is to acknowledge the lack of identifiable meaning.

14. Quantum numbers help quantisation to take place, i.e., separation of variables will be easy.

Only few mathematical treatments (solution of the Schrödinger equation for selected systems) are included in the course, as part of reducing the content bulk without losing the course meaningfulness. The solution procedure of the Schrödinger equation for the hydrogen atom is included because of its importance in showing how quantum chemistry proceeds. The explanation focuses specifically on each step (why it is done and what is obtained) and on the overall framework (need to separate the variables in order to integrate the equation; obtainment of three differential equations, each depending only on one variable; utilisation of the solutions of these equations to write the overall wavefunction). Questions asking students to outline the logic of the mathematical procedure without actually re-writing all the equations are meant to check understanding independently of the ability to reproduce memorised pages. Although the questions specify that the answers are expected to explain what is done and why, not necessarily to reproduce all the equations, most answers reproduce memorised equations without any explanations between subsequent equations. This phenomenon is not easy to interpret. It would be expected that memorising comparatively long complex equations would be more difficult than outlining what is done and why. Since the course handout provides detailed explanations between equations, it is also difficult to understand the reasons of what is clearly a selective passive memorisation, focusing on the equations and excluding the explanations. Difficulties with logic and abstract thinking and language-related difficulties might make it more difficult to understand a logical framework and to express it (logic cannot be memorised, must be understood). It also appears that students might have being trained (in past instruction) to memorise sets of equations without paying attention to their significance and to the logic of the whole framework. This results in the perception that equations are important, but the logic connecting one equation to another is not.

4.3. Difficulties with logical and abstract thinking

The whole course requires logical and abstract thinking for conceptual understanding. The combination of language-related difficulties and difficulties with logical and abstract thinking generate difficulties with complex reasoning, even for slightly complex cases like connecting three or four pieces of information in a correct pattern. Examples 2–14 showed the effects of inadequacies in relation to mathematical components. Inadequacies also affect the understanding of individual concepts, of the interpretation of experimental information or of models and their correspondence with actual systems and their behaviours. Two topics are considered here for illustration purposes: the interpretation of the photoelectric effect and the way in which Bohr's model of the atom provided an explanation of the discrete nature of atomic spectra.

Besides the description of the phenomenon, key aspects of the discussion of the photoelectric effect refer to the features that could not be explained by classical physics and to Einstein's explanation. Answers 15–17 refer to the former issue. The answers are very short, thus failing to provide sufficient information. Answer 15 does not explain which *threshold value* is considered. Answer 16 was probably meant to be identical to answer 15, but associates *value* to *presence* instead of *threshold*, likely as a result of passive memorisation void of understanding. Answer 17 illustrates a frequent misunderstanding of what pertains to experimental information, what pertains to classical physics models and what pertains to models beyond classical physics: the quantisation of the energy of electromagnetic radiation pertains to a model beyond classical physics; it is not an experimental observation that classical physics could not explain. Answers 18–21 refer to Einstein's explanation. Answer 18 is a typical example of incorrect information resulting from lack of attention to the grammatical distinction between singular and plural (the photon gives all its energy to only one electron). Answer 19 ascribes quantization to a phenomenon, whereas quantization can refer only to physical quantities. Answer 20 shows incorrect words-combination (the electromagnetic radiation does not belong to the effect) and confusion of the meaning of photon (it is a quantum of energy, not a quantum number). The first part of answer 21 confuses photons and electrons.

15. The presence of threshold value.
16. The presence value of a threshold.
17. The fact that electromagnetic radiation is quantised.
18. When photon is sent to hit the cathode it gives all its energy to the electrons.
19. The photoelectric effect is quantized.
20. The electromagnetic radiation energy of the effect is quantized. The quantum number is called the photon.
21. Each electron gives its energy to one photon and if the energy required by photon to leave the atom is higher the electron is ejected and therefore if energy $h\nu$ is higher more electrons are ejected.

The question asking to explain how Bohr's model of the atom provided an explanation of the discrete nature of atomic spectra remains unanswered in at least 90% of the cases, as students mostly provide a reproduction (often partial) of the memorised description of Bohr's model, without relating it to the spectra, or, in fewer cases, provide a description of the spectrum of the hydrogen atom without relating it to Bohr's model. Sometimes the description of Bohr's model itself is limited to one or two lines, as in answers 22–24. Answer 23 and 24 are incorrect, as Bohr's model does not involve orbitals, the concept of *orbitals increasing* is in any case meaningless (23) and quantisation refers to the energy of the electron, not of an unspecified *hydrogen particle*. Answers that attempt to relate Bohr's model to atomic spectra may lack internal logic up to becoming absurd, as in case 25, which, besides problems with logic and language, highlights also another frequent problem: the difficulty to distinguish between what actually happens and what would be expected to happen if a certain model were true (e.g., the fact that according to classical electrodynamics the electron would end up falling on the nucleus).

22. The radius (r) of the orbit and the energy of the electron are quantised.
23. In Bohr's model, as the value of n increases, the atomic orbitals also increases.
24 The energy of the hydrogen particle is quantised. .
25. Bohr's model of the atom consists of system which are at equilibrium. As classical physics – electrons in the atomic spectra approach the nucleus, while approaching the nucleus, they will end up falling on it. As far as a circular orbit, the energy will remain the same.

4.4. Difficulties with visualization

Visualization plays important roles in quantum chemistry courses, such as:

- Use of diagrams to represent trends.
- Use of images to represent atomic and molecular orbitals.
- Use of schemes to help identify factors playing some roles.

Diagnosed difficulties with visualization include poor understanding of the meaning of diagrams representing trends, inadequate ability to describe or discuss diagrams, and lack of utilisation of visualization when it would be necessary to identify the terms of a problem. The understanding of diagrams depends on understanding their explanation, which is realised through language; thus, language-related difficulties affect the understanding of diagrams. Because of inadequate understanding, students memorise the shapes of diagrams, but often do not associate the memorised shapes with the figure captions and do not give enough attention to the corresponding explanations. When asked to draw and discuss specific diagrams (e.g., the diagrams of the radial probability densities of selected orbitals, or diagrams illustrating interesting aspects of the angular probability densities), they reproduce the diagrams without any explanation or discussion. Those who have not memorised the figures' titles may reproduce a totally different set of diagrams instead of the requested one. The problem is part of the generalised tendency to passive attitudes (section 1.4.1).

Not using visualization as a tool when studying a problem is a diffuse tendency that may seriously affect the possibility of answering certain questions, such as writing the Schrödinger equation for a given atom or a given molecule, where a scheme showing nuclei and electrons is necessary for the identification of all the attraction and repulsion terms. Although the system is always drawn during explanations or cooperative problem-solving, students tend not to draw it when answering questions individually; this results in the neglect of many (often most) energy terms in the hamiltonian operator. When reminded that it is better to draw it, they find it difficult to draw something responding to the system concerned (something having the correct number of nuclei and electrons). It proved important to insist that students make such drawings individually in the class, because this promotes reflection on their details (whereas copying a drawing from the board remains a passive exercise) and enable real-time corrections for individual students.

The drawings are also affected by the level of internalisation of relevant concepts and their implications. Basic concepts such as the fact that all electrons are identical and, therefore, have the same mass, may not be sufficiently internalised to impact on answers. So, it may happen that, when students label electrons in the scheme representing a certain system, they also consider different masses (m_1, m_2, m_3 etc.).

Poor visualisation abilities hamper the generation of mental images and this, in turn, may hamper the understanding of concepts (including basic ones) for which visualization has the power of indispensable explanation tool. For instance, the comprehension of the definitions of bond length, bond angle and dihedral angle is enormously facilitated by the use of images. However, the auxiliary role of images depends on the ability to perceive the information that an image conveys and on the ability to express it through words, with an interplay between language and visualization which has the power to enhance the advantages of both tools (Mammino 2014c). It becomes important to visualise the errors embedded in a number of students' statements, to better emphasise the meaning of definitions and concepts. Answers 26–28 illustrate the problem for the bond length and bond angle concepts. In cases of this type, the best approach is asking the student to represent the meaning of his/her statement through an image. For instance, considering answer 26 and showing its meaning utilising a model of a polyatomic molecule immediately shows that the definition is incomplete: it is possible to consider the distance of whichever pair of nuclei in a molecule, but the bond length is defined only for nuclei of consecutive atoms (atoms bonded to each other). For answer 27, it is easy to show on a model that considering *any two bonds in a molecule* is not sufficient to define a bond angle and to guide the student to the conclusion that the three atoms concerned must be consecutive, or the two bonds considered must have an atom in common. Answer 28 can be utilised to stress the importance of grammar, as it is impossible to indicate only one bond angle for molecules with 4 or more atoms.

26. *Bond length is the distance between the two nuclei.*
27. *The bond angle is an angle between any two bonds in a molecule.*
28. *Each molecule has its own bond angle that is different from any other molecule.*

4.5. Inadequate familiarity with the scientific method

The quantum chemistry course requires good familiarity with several aspects of the scientific method. A key aspect is the distinction between systems and phenomena belonging to the physical reality (or what we may agree to consider physical reality) and our models. We study the properties and behaviours of atoms and molecules by building models. Students encounter considerable difficulties in distinguishing between observed phenomena and predictions or explanations based on models. The problem surfaces whenever they are asked questions about models. For instance, the answers on early models involving quantisation highlight difficulties in realising that classical physics models failed to explain some of the experimental observations, and it was necessary to introduce a quantisation hypothesis. Many answers (e.g., 29) are consistent with the perception of two parallel (both existing) worlds, one corresponding to classical physics and one to quantum mechanics. Although an answer may convey this perception because of language-related difficulties (lack of the language sophistication necessary to convey information of the type "a certain thing would have happened if the classical physics model were true, but experiment shows that it did not happen, and it was necessary to make new hypotheses to account for it"), it appears that the core of the scientific method, where experimental information is the reference and benchmark for models, is not sufficiently internalised. Answer 30 states a term of the hypotheses beyond classical physics (the quantization of the angular momentum of the electron in the atom) in place of an experimental observation, and answer 31 mentions a mathematical tool of modern quantum mechanics (the hamiltonian operator) in place of an experimental observation. Answer 32, meant to compare the early models involving quantization with modern quantum mechanics, fails to express the main concept for the former (quantisation as a starting hypothesis in the model), and does not focus on the main issue for the latter (quantisation resulting from mathematical conditions during the solution of the Schrödinger equation); the first clause has no meaning.

29. According to classical physics no system can be at equilibrium. Quantum mechanical system is at equilibrium unless external forces acted upon it.

30. Classical physics could not explain the fact that the angular momentum of the electron is quantised.

31. Classical physics could not explain the presence of the hamiltonian operator.

32. The early models were based on only a quantum of matter whereas the modern quantum mechanics considered on Schrödinger equation is based on uncertainty.

A problem identified at undergraduate level with respect to the meaning of the values reported in physical-chemistry handbooks surfaces also in the quantum chemistry course. Values from literature are seen as "theoretical". Since it was stressed throughout the undergraduate physical chemistry course that those values respond to experimental determinations, it appears probable that equating *reported in a book* to *theoretical* must have pre-university roots. The problem appears mostly in practicals reports:

33. Most of the bond lengths between a halogen and a carbon had almost the same value as the theoretical one.

5. DISCUSSION AND CONCLUSIONS

Continuous lowering in the background preparation and acquired epistemological access of students entering university has been observed in the last 10-12 years. The impact affects the undergraduate courses and extends also to postgraduate ones. However, the impact is different on different components of chemistry learning. While several students may attain reasonable mastery of practical work and perform reasonably in areas of chemistry where experiments have dominant roles and the interpretation of experimental data does not require extensive abstract elaboration, they experience major challenges with areas where mathematics, logical reasoning and abstract reasoning play dominant roles. This, in turn, has a negative overall impact because quantum chemistry – or physical chemistry in general – are scarce skills areas in South Africa, and it would be important to train enough young persons to meet the needs of the country.

In South Africa, it is particularly important to redress past injustices. This also means ensuring the possibility of access to all areas of knowledge (including the most advanced ones) to those who were previously excluded. In order to pursue this objective, it is necessary to ensure that the epistemological access tools are sufficiently developed. Quantum chemistry is important in the preparation of highly qualified chemists, capable of handling modern chemistry. Adequate mathematical and language skills are pre-requisite for successful learning in quantum chemistry. They are also pre-requisite for understanding in general. Remodelling the course bridging secondary and university instruction by focusing on the development of epistemological access tools, as outlined in (Mammino, 2012), besides being essential to improve students' performance in the undergraduate level, would also be essential to ensure improvement in the understanding of quantum chemistry. An extension of the same criteria to mathematics (focusing on the logic of mathematical procedures and developing the ability to identify and describe the meaning of each step) would contribute to develop mathematical, logical and abstract thinking abilities. It may be further suggested that integrating the bridging interventions in the three so-called *hard sciences* (chemistry, mathematics and physics), or designing them so that they are mutually complementing, would benefit the learning success in all of them.

Students' difficulties and perceptions for each of the content topics mentioned here (photoelectric effect, Bohr's model of the atom, conditions on the wavefunction, etc.) could be (and are being) objects of individual specific studies. This paper aimed at providing an overview for the entire course, to highlight how inadequate epistemological access affects learning success in advances courses and to motivate ensuing inferences and recommendations.

As mentioned at the beginning, this study attempts to explore a largely unexplored field – the educational aspects related to advanced chemistry courses. Therefore, there are no studies that can be used as direct benchmarks for its investigation approaches or results. On the other hand, several of the obtained diagnoses and inferences are consistent with those of studies on students' difficulties in pre-university and first year chemistry course (and also courses in other sciences), showing that major inadequacies in students' background preparation and epistemological access maintain heavy impacts on specialised courses like the quantum chemistry course. This confirms the need of interventions at a sufficiently early stage, to foster successful learning.

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