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Paper on Education

Analysis and Validation of Dipole Moment Calculations in Chemistry Teaching

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Abstract: In this paper, we analyze and validate of an alternative proposal for the understanding and interpretation of the dipole moment of diatomic molecules, content present in the curriculum of disciplines physical chemistry and quantum chemistry in undergraduate chemistry courses. For this, 87 students participating the degree course in chemistry at a university in Brazil, they used computational chemistry calculations and analytical calculations for the dipole moment of the considered molecules. Results show the proposed method can be an alternative for calculations involving dipole moment of diatomic molecules.

Keywords: chemistry teaching; computational chemistry; dipole moment calculation; teaching; learning

1. INTRODUCTION

The attitude of the students is generally recognized as an important factor in the success of the learning process. This is particularly true in the case of the chemistry, in which some topics are inherently difficult, and methods of traditional teaching have focused their learning process in the transmission of knowledge (teacher dictates the content and the student "learns" writing). Quantum chemistry, in general, is not commonly well appreciated by high school students, so little in higher education [1, 2] and perhaps one of the aspects that takes this discipline to be considered as one of the toughest in the practice of teaching.

Enhancing students' understanding of chemistry concepts has been a major goal of researchers in Chemistry Teaching during the last decades. One of the resources that has been used since the 1960s as a tool for learning is the computer [3]. In 1972, in the University of Lancaster, England, chemical B. J. Duke organize a course in Quantum Chemistry in order to motivate the introduction of computational techniques in chemistry teaching [4]. In their experiment, Duke used a program to calculate the properties of aromatic compounds by the quantum chemistry molecular orbital methods described in the Mulliken Theory. In 1988, in the University Chemical Laboratory Cambridge, United Kingdom, Colwell and Handy were using computers as a teaching tool for Molecular Orbital Theory [5]. Other researchers have also worked with the use of computers in Chemistry Teaching, enabling the computational chemistry definitely conquer its place among the methodologies that investigate chemical phenomena [6–8].

In an attempt to recognize limitations of the traditional form of teaching chemistry, both in high school and higher education, it has been proposed several methodological alternatives. In this sense, new teaching materials were developed. One of the main objectives of these methods and materials alternative is to promote a more participatory attitude of students in their learning process. It is crucial that students learn how to construct, decode and use structural representations early in a sequence of chemistry courses, otherwise much of what follows will simply be an exercise in memorization [9].

In this paper, we present an alternative proposal to the understanding and interpretation of the dipole moment of diatomic molecules, present content in the curriculum of physical chemistry and quantum chemistry disciplines in undergraduate chemistry

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courses.

Teaching computational chemistry

Curriculum of physical chemistry undergraduate is traditionally built around the themes of thermodynamics, quantum mechanics, molecular spectroscopy, electrochemistry and chemical kinetics. The Quantum Chemistry teaching still represents a challenge to chemistry students, due to the novelty of the abstract concepts and to the quantity calculations involved [10]. However, the use of computational quantum chemistry has been widely considered in the understanding of various issues of chemistry (Analytical, Inorganic, Organic, Physical Chemistry, Environmental Chemistry, Food Chemistry etc.) and can be attractive for students correlating their areas. Quantum computational chemistry is an inherently multidisciplinary field of study that transcends the traditional barriers separating chemistry, biology, physics and mathematics [8]. Thus, computational chemistry is a perfect tool to make the interconnections between chemistry and other sciences.

Computational chemistry is commonly presented in chemistry courses graduation in physical chemistry disciplines and focus generally on basic theory, including the wave-particle behaviour and the resolution of the Schrödinger equation for simple systems that can be evaluated analytically. As defined by IUPAC, Computational chemistry is a discipline using mathematical methods for the calculation of molecular properties or for the simulation of molecular behaviour. It also includes, e.g., synthesis planning, database searching, combinatorial library manipulation [11]. Specially as regards the molecular models, role of the computational chemical is, together with the statistical thermodynamics, language integration and chemical concepts, allowing the interpretation and rationalization of macroscopic properties for reasons at atomic-molecular level [12–16].

In this sense, computational Chemistry content graduation can be considered as complex for the understanding of the student, due to the need to comprehend abstract concepts that are largely non-intuitive, and advanced mathematical concepts, such as linear algebra and differential and Integral Calculus. Johnson and Engel published in 2011 the results of a two-year job at a major university on the integration of computational chemistry in physical chemistry curriculum of undergraduate courses [17]. Use of teaching methods in chemistry and physics has been studied at different levels of education, and research [18] shown few studies have focused on the impact of interest to teachers about their choice of teaching methods. Furthermore, the chemistry education community has paid little attention to determining discipline-specific aspects of chemistry that can lead to learning difficulties and misconceptions [19].

Dipole moment

As is known, an electric dipole (μ) is a vector which is characterized in the direction between two electrical charges, towards $+q$ to $-q$ and module given by the distance d between them [16,20]:

$$\mu = q \cdot d \qquad (1)$$

Pauling [20] describes that a molecule has electric dipole moment if its center of positive charge does not coincide with its center of negative charge. That is, the vector of the molecular dipole is given by $\delta.r$, being δ partial atomic charge and r the bond distance (Figure 1).

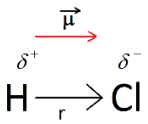

Figure 1. Vector representation of the dipole moment.

Dipole moments values can be determined with great accuracy by microwave spectroscopy and molecular resonance methods [20]. The coulombic model describes dipole moments of binary hydrides as the resultant of the dipolar contributions of the hydride ions and the electron pairs around the positively charged central atom [21]. Basically, what defines a molecule as a whole is polar or non-polar is the disposition of its bonds; for highly symmetric molecules, the resulting dipole should be null. For a molecule with more than two atoms, the dipole moment depends of the size of polarities of individual bonds as well as of the molecule geometry. The bond dipoles and the dipole moments are vector quantities. The total dipole polyatomic a molecule is the sum of their bond dipoles. When total dipole of the molecule is "zero", even if the bonds are polar, the geometry of the molecule imposes that total dipole moment is zero, makes the molecule is non-polar. Already if the molecule have a dipole moment of total nonzero, the molecule is polar. Although the international system unit of dipole moment is the coulomb meter (Cm), it is

still common to use of the *Debye* (D) unit (1 Debye = 3.336×10^{-30} C.m), in homage to Peter Debye, pioneer of experimental investigation of the dipole moments of the molecules [22].

All heteronuclear diatomic molecules are polar, single or multiple bonds are formed between the A and B atoms, the dipole moment of the AB molecule is related to the polar character of the bonding, the dipole moment of the bond itself is the molecular dipole moment. In the case of polyatomic molecules, the vector sum of the bond dipoles resulting in the total dipole [23] (figure 2).

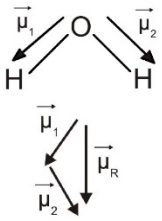

Figure 2. Vector representation of the dipole moment of the water molecule.

In first approximation, the dipole moment of a triatomic molecule may be solved by the technique of vector addition that describes the resulting dipole $\boldsymbol{\mu_{res}}$ of the sum of two dipole moments μ_1 and μ_2 that make between them an angle θ given by Equation 2.

$$\mu_{res} = \left(\mu_1^2 + \mu_2^2 + 2\mu_1\mu_2\cos\theta\right)^{1/2} \qquad (2)$$

When the two dipole moments are equal, Equation 2 is simplified:

$$\mu_{res} = \mu_1\left(1+\cos\theta\right)\sqrt{2} \qquad (3)$$

One difficulty for calculating dipole moments should the positions and magnitudes of partial charges used in the molecule [16]. In this sense, quantum chemistry arises as an ally to teaching and research in the calculation of partial charges, which are included in the output of many computer packages molecular structure calculations. Knowing the charge density *qi* on each atom and the bond distances, we can calculate the dipole moment. First, the charge density of each atom is represented as a vector of length *qi* of the some arbitrary origin in the direction of the atom *i*. If the vector is collinear with a bond and the origin is an atom, the vector represents a moment dipole bond. All vectors not need represent dipole moments of bond, because they do not need be all collinear with the bond [23]. When vectors represent all the charge densities, the vector sum is the total dipole moment. Table 1 describes some experimental values [24–26] of the dipole moment for molecules used in our survey.

Table 1. Experimental dipole moment (μ_{exp}).

Molecule	μ_{exp}	Molecule	μ_{exp}
HF	1.820 D	NaBr	9.118 D
HCl	1.080 D	NaI	-
HBr	0.827 D	KF	8.558 D
HI	0.448 D	KCl	10.239 D
LiF	6.284 D	KBr	10.603 D
LiCl	7.130 D	KI	-
LiBr	7.226 D	CsCl	10.421 D
LiI	7.43 D	HO	1.660 D
NaF	8.160 D	NO	0.153 D
NaCl	9.000 D	SO	1.550 D

A program widely used in the visualization in quantum chemistry calculations is the GaussView [27]. The dipole moment can be observed through of the menu "Results" in the option "Summary" (Figure 3) or on the output file.

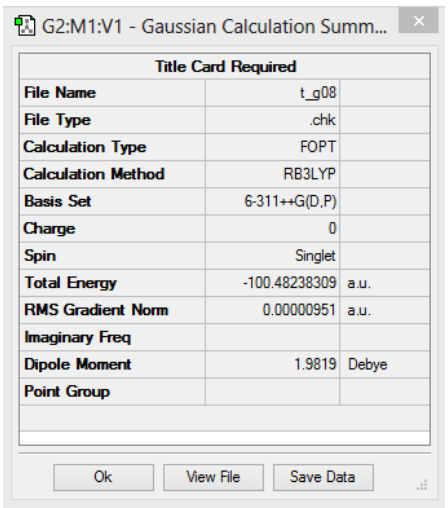

Figure 3. Summary to the HF molecule visualized in the GaussView.

Molecule dipole module used in the example has a value of 1.9819 D.

2. METHODOLOGY

Proposed method to dipole moment calculation

Partial ionic nature of chemical bonds and their relationship with the dipole moment has been understood since the 1930s in the pioneering work of Linus Pauling [28]. He supposed that a bond between two identical atoms could be considered a covalent bond; already in the bond between different atoms, one atom is more electronegative than the other, so the covalent character not is more one hundred percent, then the bond must have an ionic contribution. Thus, it sets the *ionic character* (CI) of a bond (Equation 4).

$$CI = 1 - e^{-\frac{1}{4}(\Delta\chi)^2} \qquad (4)$$

where Δχ is the Pauling electronegativity difference [20,29,30] between the bonded atoms (Δχ = χA – χB). From this, Pauling [29] proposed that the ratio of the experimental electric dipole moment and calculated dipole moment (assuming that the binding was completely ionic) would give %CI real of a polar covalent bond (Equation 5).

$$\%CI = 100\left(\frac{\mu_{\exp}}{\mu_{calc}}\right) \qquad (5)$$

With this equation, we have a kind of experimental ionic character. However, we cannot have a dipole moment calculation that is completely analytical and theoretical.

We developed a proposal for calculations of the dipole moment of form alternative to the computational methods of quantum chemistry. Initially we solved the problem of calculating the charge of the dipole from the ionic character defined by Pauling (Eq. 4). We propose that the charge of the dipole (δ) can be given by the ionic character product Pauling (Eq. 4) by the elementary charge, $(1 - e^{-0.25(\Delta\chi)^2})1.602\times10^{-19}$ C. It is usually difficult to find analytical expressions that university students use to estimate bond distances. Once again we took the opportunity to stand out also an expression developed by Pauling [31,32]. We can with this, perform the calculation of the bond distance (*r*) in a systematic form:

$$r = R_A + R_B - 0.6\log n \qquad (6)$$

where R_A and R_B are respectively the radii of the atoms A and B, *n* is the bond type (for single, double and double-resonant bond, respectively, n = 1, 2 and 1.5). We have reached an expression that uses only the atomic radii as empirical data:

$$\mu = \left(1 - e^{-0.25(\Delta\chi)^2}\right)\left(R_A + R_B - 0.6\log n\right)1.602\times10^{-19} \qquad (7)$$

We use the analytical proposal (Equation 7), results of computational quantum chemistry and experimental data to develop this work with university students, through a critical analysis of the results (which included opinion survey). We can make a comparison separately, between greatness *bond distances*, *charge* and *dipole*, for *analytical calculation*, *computational* and *experimental data*.

Context of the study and method

Main objective was to investigate and treat perceptions of students about a new proposed analytical method for dipole moment calculation in chemistry teaching. Responses are grouped into categories that reflect different perceptions of students: analytical prediction; computational prediction and; and inaccuracy in the results data.

Development of this study followed the molds of a qualitative research. Among the main features that set qualitative research, Creswell [33] identifies the following: Qualitative research uses the natural environment as a direct source of data and the researcher as its main instrument; data collected is predominantly descriptive; meaning people attribute to things and their lives are in the research focus of attention; analysis the data tend to follow an inductive process. Research was conducted by the authors of this article and has been reviewed and revised by experts for its content validity. Eighty-seven (87) students of the degree course in chemistry at a university in Brazil participated. Ages of students varies 17-30 years old and these belonged to three classes in which each consisted of 32, 30 and 25 students. Data from this study were collected in 2015 and 2016 by means of a questionnaire. For students of the second semester of 2015 (32 students), we have named as Class A. For of the first semester 2016 (30 students) as Class B and for students of the second semester of 2016 (25 students) as Class C. It stands out that the students involved in this research attended the same discipline, which is given every semester in the course.

Our pedagogical approach used computational and analytical technique to describe the dipole moment of simple molecules. To evaluate this approach the questionnaire included two questions:

1º) Calculate the dipolar molecules (HF, HCl, HBr, HI, LiF, LiCl, LiBr, LiI, NaF, NaCl, NaBr, NaI, KF, KCl, KBr, KI, CsCl, HO, NO and SO).

2º) Of the values found, what would you use in

your research? Justify.

The answers are presented as written by the participants, preserving typos, text writing errors, conceptual errors, etc. Names were removed and data that could identify subjects.

3. RESULTS AND DISCUSSION

Assessment of students' perceptions

Aiming to analyze the students' perception of the dipole moment, analytical and computational calculations were performed. Students were invited to discuss the importance of the results, comparing them with the analytical, experimental and computational results.

Experimental Data (μ_{exp})

Dipole moment of the molecules analyzed were experimentally described in Table 1, according to data presented in the literature [24–26].

Analytical Prediction (μ_a)

Using equation 7 for the calculation of what we call *analytical dipole moment* (μ_a), the values found by the students to the first question of the questionnaire are described in Table 2.

Table 2. Dipole moment values calculated analytically.

Molecule	μ_a	Molecule	μ_a
HF	3.071 D	NaBr	8.381 D
HCl	1.505 D	NaI	7.351 D
HBr	1.078 D	KF	11.743 D
HI	0.411 D	KCl	10.809 D
LiF	8.140 D	KBr	10.368 D
LiCl	7.508 D	KI	9.211 D
LiBr	7.191 D	CsCl	12.115 D
LiI	6.293 D	HO	1.822 D
NaF	9.584 D	NO	0.202 D
NaCl	8.767 D	SO	1.292 D

Students use to calculate the distance between molecules, data from the atomic radius and electronegativity found by Pauling [20,2 9–31].

Computational Prediction (μ_c)

Hoffmann, Schleyer and Schaefer [34] already warned that studies involving calculations of molecules for which no experimental evidence is yet available were growing very rapidly. The authors suggested that the computations performed be described in a circumspect way [34]. One of the electronic structure calculation methods atoms, molecules and solids, with currently most successful is the Density Functional [11]. Density Functional Theory (DFT) is a theory that deals with the quantum mechanical description of molecular systems in terms of the electronic density. Dipole moments were calculated by Kohn-Sham density functional theory. Although the calculation of the electric dipole is still a challenge, even bigger than the calculation of molecular geometries, Kohn-Sham density functional theory was well validated against experimental results for dipole moments and it is known for giving acceptably accurate dipole moments [35–38].

For the study was performed an optimization of the molecules and DFT method [39,40] was used together with the B3LYP hybrid functional [41,42] defined as:

$$B3LYP = 0{,}20Ex(HF) + 0{,}80Ex(Slater) + 0{,}72DEx(B88)^{GGA} + 0{,}19Ec(VWN)^{LDA} + 0{,}81DEc(LYP)^{GGA}$$

where *Ex* is the exchange energy *Ec* is the correlation energy, and HF, B88, VWN, LYP are the Hartree–Fock, Beck [43], Vosko-Wilk-Nusair [44], and the Lee-Yang-Parr [41] terms, respectively. The LYP term gives the local and the non-local correlations, whereas excess of the local correlation is given by the VWN term [45]. Although the extremely popular B3LYP functional is implemented in the Gaussian programs differently than Becke intended [34,46]. Basis set of Pople 6-311++g(d,p) was chosen to be used with the computational method already described [47]. Basis set is frequently used in various systems, because it includes polarization functions and diffuse, besides of dividing the valence shell improves the results when compared to the other sets minimum bases. This basis set has proved suitable to describe the molecules.

Through this method, the students found the values for which we denote by *computational dipole moment* (μ_c). This step was important to approximate the theoretical chemistry software to the reality of students, so that they themselves take ownership of this technology. We use the descriptors "accuracy" and "precision" that are well-defined in the computer-

based world of the quantum chemist, according to Hoffmann, Schleyer and Schaefer [34].

Accuracy in predicting the data

Results of analytical calculation carried out by the students are compared with the computational and experimental data (Table 3), contributing to the validation of our technique.

Data in Table 3 show analytical calculations obtained, in their majority, present accuracy of better than 90% and in the computational calculations, the results show accuracy above 75%. We also note that only one (HF) of the analytical calculations showed the percentage of precision below 60%, which indicates a degree of confidence to discussions on the dipole moment. Figure 4 shows a summary of these data.

We can say that study of the dipole moment, of diatomic molecules, beyond the experimental data found in the literature, the use of computational and analytical methods could contribute to the understanding of their properties.

Student's assessment in relation to data

As regards the second question of the questionnaire (Of the values found, what would you use in your research? Justify.) We present some answers these students.

Table 3. Values of the dipole moment (in Debye) and accuracy percentage (A%).

Molecule	μ_{exp}[a]	μ_c	A%	μ_a	A%
HF	1.820	1.981	91.11	3.071	31.25
HCl	1.080	1.403	70.09	1.505	60.64
HBr	0.827	1.082	69.06	1.078	69.53
HI	0.448	-	-	0.411	97.11
LiF	6.284	6.360	98.78	8.140	70.45
LiCl	7.130	7.087	99.39	7.508	94.70
LiBr	7.226	7.207	99.74	7.191	99.52
LiI	7.43	-	-	6.293	84.70
NaF	8.160	8.250	98.89	9.584	82.54
NaCl	9.000	9.019	99.77	8.767	97.42
NaBr	9.118	9.068	99.46	8.381	91.92
NaI	8.558	8.688	98.47	11.743	62.78
KF	10.239	10.583	96.63	10.809	94.43
KCl	10.603	10.923	96.98	10.368	97.79
KBr	10.421	-	-	12.115	83.74
KI	1.660	1.831	89.66	1.822	90.23
CsCl	0.153	0.098	64.11	0.202	67.86
HO	1.550	1.786	84.72	1.292	83.39
NO	1.820	1.981	91.11	3.071	31.25
SO	1.080	1.403	70.09	1.505	60.64

Legend: [a] [24–26]

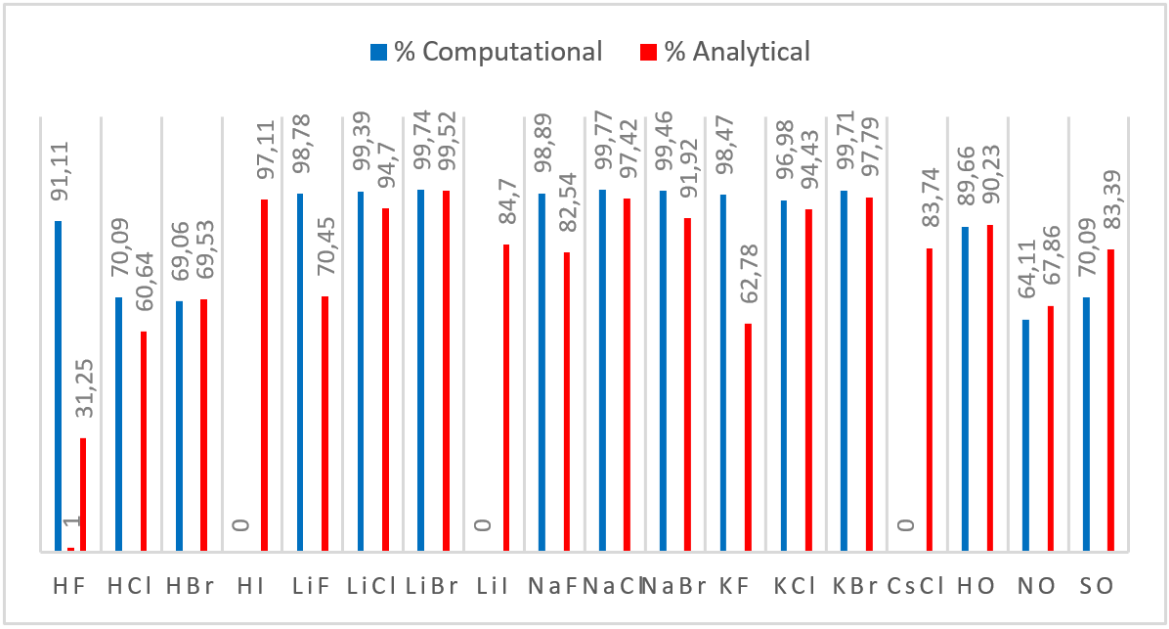

Figure 4. Computational precision x Analytical precision.

One student reports differences between the methods and suggests that the analytical dipole moment is the most suitable for their research: "*As there was a very significant difference from the real value of the molecule, the value that most closely approximates the real value, and that would bring more security in the approximation of the desired result, would be calculated by the dipole moment of the ionic character*".

This opinion is perceived in other students "*I would use the analytical because it is closer to the experimental value*" and "*the value of the GaussView gave 10.9234 D, while the analytical value done by the dipole moment gave 10.368 D. So would use in my research the analytical value that was 10.368 D.*" referring to KCl molecule.

Figure 5 summarizes the results obtained comparing the answers of students, in which it describes that the analytical method may be the most suitable for use in the calculation of the dipole moment.

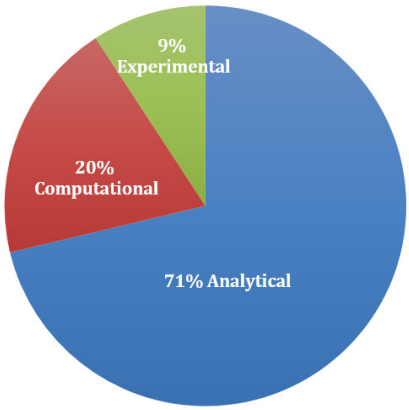

Figure 5. Choices of students regarding the method.

Choice of the analytical method (71.26% of students) possibly identifies a Cartesian feature; the value that most closely approximates the actual value should be considered the "*most effective*", as highlighted by one of the students: "*In a survey, it would use the value that had a smaller margin of error in relation to the experimental value given*".

Many of the answers found for the choice of the analytical method, present in common the described by these two students: "*I would use the analytical value, because it is closer to the experimental value*" and "*I'd use the analytical value, it is nearest the experimental value*", confirming a view that the closer to the actual value, better is the method.

As regards the answers of students considering the computational method as the most suitable for use in their research (19.54% of students), we highlight the following affirmations: "*I'd use the computer, because the computer performs calculations better*" and "*the Gaussian is a program specially created to carry out chemical calculations on the computer, so it has the best results*". In these affirmations, we see the appreciation of the use of computers as "*the machines that solve all our problems*". Nevertheless, we cannot think that is just use the computer that all our problems will be solved [11].

Already a small group of students reported they would use only the experimental value (9.19% of students), because for these the analytical and computational methods have different values of the actual value. One of those students says "*calculations by Gaussian or analytical aren't accurate in relation to the experimental because the molecules depend on several factors about experimental, therefore in some the values are different, thus in some substances uses Gaussian and others analytical*".

For this student the fact of having to use a method for a particular molecule and another method for another molecule, makes with that the use of the experimental data are more effective in their research. Such reflection is seen in another student response, in which he described that "*I would use in my research the experimental value, because the percentage of error is very small comparing the two values*". In this sense, we can consider that for these students only results obtained experimentally are correct, in their opinion no other method can be used as an approximation of the actual value.

We observed that, unfortunately, most of the students gave little importance to the experimental result. Laboratory work is an established part of courses in chemistry in higher education. Reid and Shah [48] argue that the experimental activities need to be reconsidered at higher education levels. They describe that there is a need for clarification of aims and objectives, and these need to be communicated to learners. In addition, seeing the activities in the laboratory in the context of what goes on before and after, as well as other learning, will enhance the learning potential. There is a need to prepare students for use of the laboratory as well as develop follow-up activities. These may enrich and enhance the whole laboratory experience, and enable it to contribute more effectively to the overall learning of students in chemistry [48].

Lastly, in relation the class, we obtained a positive evaluation for the use of the analytical method, being identified in all of them. Students of Class A (65.6%) consider that the analytical method is most suitable for use in their academic research. For Classes B and C the percentage is higher, 70% and 84% respectively. However, is interesting to note that some students (12.6% of class A; 10% of class B and; 4% of class C) considered the experimental value as the best to use in their calculations, without questioning how the data was obtained experimentally, this is, what the method used to obtain the values.

Table 4. Choice of methods by students

Class	Total Students	Analytical method	Computational method	Experimental Value
A	32	21 (65.6%)	7 (21.8%)	4 (12.6%)
B	30	21 (70%)	6 (20%)	3 (10%)
C	25	20 (80%)	4 (16%)	1 (4%)

Worth mentioning, that the proposed method was valid in our survey, in which students consider it more appropriate to perform in their research. Although, we cannot ignore other factors that may have led to these students opting for the analytical method, such as: difficulty in handling computer programs, distrust of computational results, little contact with lab activities, reliability in mathematical calculations – as they performed the mathematical calculations, they believe that are more accurate.

4. CONCLUSIONS

Aim of this study was to present a new approach for the calculation of the dipole moment. This new approach can help students understand how an analytical method can predict physical properties of a molecule and interpreting your accuracy in relation to the experimental data. Admitted, this work opens up a new perspective on didactic strategies for the quantum chemistry teaching and can be used as a pedagogical tool [17,49].

We have extensively tested our approach with different molecules, and it is too early to draw definitive conclusions about the real impact that this new approach can cause in teaching quantum chemistry and physical chemistry, it is evident that all its features are susceptible of application to the daily work of teachers and students. However, it is believed that the results obtained in this study highlights the educational potential of using didactic strategies for analysis and interpretation of dipole moments.

5. ACKNOWLEDGMENTS

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