Mentioning fuzzy logic in theoretical chemistry courses: motivations and extent

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Abstract

The exploration of options aiming at favouring a broad vision of theoretical chemistry since its first presentation to students may conveniently consider a variety of directions, to enhance the overall efficacy. Since, within introductory theoretical chemistry courses, the discussion of fundamental conceptual aspects has the major role, it may be convenient to complement it by mentioning mathematical instruments which, though not the most traditional or the most commonly utilised in the generation of models, overlap, by their very nature, with important aspects of the theory being presented.

The paper considers the opportunity of incorporating references to fuzzy sets and fuzzy logic, as instruments related to the uncertainty concept. It outlines the main features of a possible approach to their presentation, that can balance the various practical needs. The presentation cannot aim at reaching operational levels, because of obvious time limitations stemming from theirs not being core material for the course-content. On the other hand, acquainting students with the existence of these instruments, and with some basic information on their potentialities, contributes to a broader vision of the theoretical aspects and, simultaneously, enriches the ‘reservoir’ of instruments to which to resort in the course of more advanced stages or future work.

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1. Introduction

Investigations focusing on the approaches to the teaching of theoretical chemistry, as well as of other advanced courses, are still rather new and, therefore, both the selection of objectives and the design of the approaches need to be explored in a sort of ab initio way [1,2]. An objective that is considered particularly relevant, also in view of the continuous increase of the amount and quality of the information expected from theoretical chemistry research, is that of favouring a broad vision of theoretical chemistry since its first presentation to students, so that they can perceive it as an area open to a ample diversity of research interests, pathways and options. A parallel objective is that of avoiding that students see theoretical chemistry solely in terms of utilisation of already existing calculation software [2,3]. These objectives are more effectively pursued by utilising options of different nature, so that the diversity of the options may in itself become a contributing factor to a broader vision.

Within advanced courses, pedagogical objectives are realised through the content. The selection of the content and the mode of its presentation are the tools to maximise the acquisition of knowledge and, simultaneously, to maximise the formation of a general picture of the discipline. Therefore, the identification of the relevant information and its organisation into a pedagogically viable and effective pattern constitute a major focus in the design of options.

Within introductory theoretical chemistry courses, the discussion of conceptual aspects plays the most fundamental role. Therefore, such discussion becomes the main ground for the generation of a more complete and broader vision. The options for this purpose can focus on different features of the course content, with preference to those that play major roles. For example, the introduction of the quantization concept can offer opportunities for
2. Practical considerations for the design of options

There are easily evident practical requirements for the design of the presentation of ‘additional’ themes that can contribute to expand the conceptual vision but are not part of the mainstream course content. The presentation cannot be excessively demanding in terms of time, because it should not result in limitations to the normal development of the course and to the explanation/discussion of its core content. Moreover, it needs to take into account the background knowledge expected from the students taking the course, so as to be easily accessible, without demanding significant additional efforts that would go beyond the desired role of ‘expansion of perspectives’.

In the specific case considered, taking such requirements into account highlights the unviability of aiming at attaining levels involving operational abilities. Mastering the mathematics of fuzzy sets would require a whole course of its own, and even trying to reach a stage, where students could be able to handle it at very basic levels would be excessively demanding in terms of time. In addition, the presentation of the ‘fuzzy’ mathematical treatment of selected quantum chemistry cases (in the role of illustrative examples) would require a prior deep knowledge of the ‘traditional’ mathematical treatment of those same cases and, more in general, of the main mathematical approaches of quantum chemistry, what students are in the process of acquiring during the same theoretical chemistry course.

In view of all this, the presentation can realistically focus on acquainting students with the existence of those mathematical instruments and creating a first contact with basic information about their functions and their potentialities. The knowledge of the existence of those instruments can contribute to a broader vision of the theoretical discourse in general and, simultaneously, it enriches the ‘reservoir’ of possible instruments to which to resort when dealing with concrete problems during future activities. In other words, the presentation to students is seen from the double perspective of enlarging the theoretical picture (including also philosophical-character aspects) and enlarging the ensemble of possible operational pathways that could be explored more deeply in a more advanced stage. The next section discusses the main lines of a possible presentation to students that can simultaneously balance the various practical needs, be easily accessible conceptually, and highlight how the philosophical bases of the whole discourse are particularly significant for chemistry. The overall accessibility is evaluated with reference to the common content of introductory courses providing the foundations of theoretical chemistry. In view of the need of not adding further mathematical operational components to the course, no operational part is developed.

3. Outlines of a possible presentation

In order to be meaningful, the presentation needs to have at least a minimal degree of completeness, i.e. it needs to include some contextual and motivational aspects (the reasons or the thread-of-thought that led to the introduction of fuzzy logic), a basic description of its nature and functions, and some easily understandable examples to ensure a perception of concreteness (the latter being fundamental, in view of the fact that a diffuse abstractness perception is among the factors affecting students’ attitude towards theoretical chemistry [1,2]). A presentation responding to these criteria can conveniently develop through the following components:

- A preliminary ‘philosophical’ introduction involving considerations on the generality of uncertainty.
- Some historical information on the treatment of uncertainty. Historical information has a relevant role because it provides the motivations for the birth of new models and, in this role, it is commonly present in theoretical chemistry courses, where it provides motivations for the birth of quantum models. The ‘history of uncertainty’ can easily integrate with the historical component already present in the course, expanding its scope. An additional advantage of historical information lies in its definite capability of attracting students’ attention, thus facilitating a better focusing on the concepts considered.
- Some considerations on the differences between probability and possibility.
- The introduction of the concepts of fuzzy sets and fuzzy logic.
- Easily understandable examples of vagueness with reference to the description of molecules. (Choosing examples of this type will also contribute to underline that the main objective of theoretical chemistry is the description of molecules).
A brief overview of issues concerning the study of molecules, for which the resort to fuzzy logic has already been considered interesting and perspective.

A more detailed description of few (1–3) examples concerning the study of molecules and selected among those than can be presented in an easily accessible way.

The main types of information relevant to each of these components are outlined and discussed in some detail in the following subsections.

3.1. The generality of the presence of uncertainty

Students are already familiar with the uncertainty associated with measurements. Deeper reflections show that uncertainty does not concern only measurements, but concerns practically all the aspects of what we think about physical reality, all our forms of knowledge and its expression.

Vagueness is an intrinsic characteristic of natural language, i.e. of the tool through which we develop, express and communicate our thoughts. For example, the meaning of words denoting qualities is not sharp: it extends over a certain range. When we say that something is red, there is a range of shades that fall under the term ‘red’ [4]. Similarly, qualitative expressions may have a high degree of vagueness, and their actual meaning will depend on the context. For example, the expression ‘high temperature’ does not correspond to a single value, but to a range of values. Moreover, the range itself is different with reference to different contexts (e.g. the temperature of a patient, or the temperature of a smelting furnace, or the average temperature of a certain geographical area in a certain season) [5]. In this way, uncertainty is associated both with the experimental level (uncertainty on measurements) and with the cognitive level (through the vagueness inherent in natural languages). Therefore, uncertainty is a feature of all the interactions of human beings with the physical world [6].

All our statements, theories and laws concerning physical reality are uncertain to a degree [7].

It is easy to find illustrative examples from chemistry. Actually, there are views considering the entire chemistry as a fuzzy science [8], and the title of the first International Conference on the application of fuzzy logic in chemistry read significantly ‘Are the Concepts of Chemistry All Fuzzy?’.

An example of definition with a high degree of vagueness is the definition of ‘reaction coordinate’: both the concept itself and the words that we use to express it are abundantly vague, though we know when and how to use it and its practical usefulness is undeniable.

3.2. Brief ‘history’ of uncertainty

Scientists and philosophers have for long considered scientific information as certain, and such a belief grew stronger during the 19th century, when scientific information was considered exact, not affected by vagueness or ambiguity. The corresponding mathematical models did not take uncertainty into account, they treated the input data as exact and they expected exact output values [6].

The study of processes at molecular level caused a fundamental change—the type of change in concepts, theories, principles and methods that is termed ‘paradigm shift’ [7]. Towards the end of the 19th century, physicists realised that ‘although the precise laws of Newton mechanics were applicable to the study of these processes in principle, they were not applicable in practice, due to prohibitive computational demands resulting from the enormous number of entities involved’ [6]. The search for a different approach resulted in the development of statistical mechanics and statistical thermodynamics, which relate the macroscopic behaviour of the system to the properties of its particles through a statistical analysis considering average values of the quantities of interest.

(Although, in many cases, students have not yet encountered statistical thermodynamics when they attend a theoretical chemistry course, they already know some relationships between thermodynamics quantities and properties of molecules; e.g. they know that temperature is proportional to the average kinetic energy of molecules. Therefore, they can understand the general meaning of the discourse).

An even more radical shift from the idea of certainty in scientific information was associated with the introduction of quantum mechanics in the first decades of the 20th century. Heisenberg’s principle makes uncertainty an inherent feature to all our descriptions of the microscopic entities (elementary particles, atoms, molecules). It is impossible to have simultaneous highly precise information on couples of properties (complementary observables) that would both be necessary for a complete description of the microscopic system considered; therefore, we choose to maximise the precision of one of the two, leaving the other one highly uncertain. For example, in the description of atoms and molecules, the energy of the electrons is chosen as the property to be known with highest accuracy, and the position remains largely undetermined.

3.3. Probability and possibility

Comparatively until recent times, all the approaches to problems involving uncertainty have resorted to descriptions based on probability. Statistical mechanics and statistical thermodynamics consider the probabilistic behaviour of large ensembles of particles. In quantum mechanics, the wavefunction is related to a probability density and thus, e.g. the ‘whereabout’ of an electron is seen in terms of probability. On the other hand, the new uncertainty theories proposed in the second half of the 20th century prefer to take into account possibility.

Probability is related to the occurrence of a certain event, i.e. how many times it occurs with respect to a total number of times. Possibility is related to the extent to which
a certain event occurs. For example, in the case of a particle described by a wavefunction $\psi$, the probability of finding that particle in a volume $dV$ in space is $\psi^*\psi\ dV$. In terms of possibility, this value can be viewed as the degree (or the extent) to which the particle is present in the volume $dV$. The numerical values are the same, but the interpretation point of view changes [8]. When we consider the probability of finding the particle, we link the concept to our measurements: if we perform a very high number of determinations aiming at locating the particle, the probability of us finding it in the volume $dV$ is $\psi^*\psi\ dV$. When we consider the possibility of the particle being in the volume $dV$, the point of view is independent of our determinations of the location of the particle: $\psi^*\psi\ dV$ is the extent to which the particle is present in the volume $dV$, independently of whether we are interested in locating the particle or we are not.

3.4. Fuzzy sets and fuzzy logic

The fuzzy set concept was introduced by Lofti A. Zadeh [10]. A fuzzy set is a set whose boundaries are not sharp. For normal (crisp) sets, a certain element can either belong or not belong to the set; therefore, the only possible options with reference to its membership are 0 (i.e. the element does not belong to the set) or 1 (i.e. the element belongs to the set). In the case of a fuzzy set, a certain element may have a membership degree ($\mu$) with respect to the set, which can be expressed with any number between 0 and 1. These values constitute the membership function, which characterises the fuzzy set (just as the characteristic function characterises a crisp set). Membership functions are constructed taking into account the context of interest. The most commonly adopted shapes for the diagram of the membership functions are triangular or trapezoidal: e.g. if we consider the set of the ‘real numbers that are close to 3’ [5], a reasonable interval is $1 \leq x \leq 5$. Then the diagrams will be symmetrical, with $\mu = 0$ in correspondence to $x = 1$ and $x = 5$ (because 1 and 5 are the points with minimum correspondence to the property considered, within the selected interval) and $\mu = 1$ in correspondence to $x = 3$ (because the closest value to 3 is 3 itself). A triangular shape of the diagram will correspond to a linear decrease of the value of the membership function as the ‘distance’ from 3 of the real number considered increases on either side. Other criteria for the assignment of the values of the membership function can be selected, assigning higher importance to the real numbers that are closer to 3; then different diagrams are obtained in correspondence to the different criteria [5].

An easily understandable implication concerns classification. Classification means assignment of objects to certain categories, and these categories can be viewed like sets. If the sets are fuzzy, a certain object can simultaneously belong to two (or more) categories to a certain degree, and not fully to one of them. An easy example from chemistry can be offered by the classification of chemical bonds. There is a whole range of possibilities between the two extreme cases of a pure covalent bond (like in a homonuclear diatomic molecule) and a definitely ionic bond. If the two extreme cases are considered as the ends of a segment, then the various possibilities correspond to different positions inside the segment. If, on the other hand, the two cases are viewed as separate sets, a certain bond can be viewed as having, e.g. 0.3 membership for the ionic bond and 0.7 membership for the covalent bond. It can be added that this point of view can be more easily linked to the meaning of the coefficients $c_A$ and $c_B$ in a molecular orbital of the type $\psi = c_A\psi_A + c_B\psi_B$ for a heteronuclear diatomic molecule, than the representation on a linear segment. The example highlights the presence of a fuzzy way of reasoning in chemistry. Moreover, the issue of the bond classification cannot be reduced to probability views, because it cannot be described in terms of obtaining a certain percent of ‘ionic bond’ findings and a certain percent of ‘covalent bond’ findings on making a high number of measurements. It can only be described in terms of degree of belonging to one or the other set.

Because of their ability to express the whole range from full membership to non-membership, fuzzy sets can be associated also to expressions of natural language and, therefore, they can be utilised also with reference to qualitative concepts, e.g. the concepts very small, small, medium, large, very large. It may be useful to recall that the use of qualitative concepts in chemistry is very frequent. Adjectives like the pairs fast/slow, strong/weak, concentrated/dilute, hot/cold, etc. [11] are used commonly, and their meaning (the range of possible values that could be associated with them) is understood from the context. Even the issue of the classification of chemical bonds (as mentioned previously) is often viewed from a purely qualitative point of view.

In terms of logic, the corresponding point of view refers to the evaluation of the truth or falseness of a statement. Within classical (two-valued) logic, a statement can be either true or false. Within fuzzy logic, a certain statement can be ‘true to a certain degree’ or ‘false to a certain degree’. In its broad interpretation, ‘fuzzy logic is viewed as a system of concepts, principles and methods for dealing with modes of reasoning that are approximate rather than exact... It utilises all resources developed within fuzzy set theory for formulating various forms of sound approximate reasoning’ [5]. Fuzzy sets can be viewed as elastic constraints on the possible parameters or states that a system could assume. The membership degree can then be interpreted as a degree of possibility. On this basis, Zadeh [12] developed possibility theory, whose calculus instruments provide a way of dealing with incomplete information.

A simple example to highlight the meaning of ‘elastic constraint’ can consider a sentence like ‘the solution is hot’. If it is a water solution, we might consider that the range of temperature values to which the sentence may refer are included between a value that we perceive as ‘warm’ on
the basis of our senses (e.g. by touching the beaker) and the boiling point of the solution, which will be something higher than 100 °C. For simplicity sake, we can say that we are considering the temperature range 40–100 °C. Then this range constitutes a fuzzy restriction on the meaning of the quality ‘hot’ for the given context. The membership function μ will be 0 in correspondence to the lower temperature value (40 °C) and 1 in correspondence to the higher temperature value (100 °C). In correspondence to the other values of the interval, the membership function will have intermediate values (0 < μ < 1), which will be higher for higher temperature values, because these values correspond to a higher degree of the quality considered (being hot). The diagram has a sigmoid shape.

Fuzzy sets and fuzzy logic encountered extensive application in engineering, owing to factors like the limitations of probability-based approaches in the evaluation of structural reliability, above all for complex structures [13], or the specific needs of system control, above all for complex systems. As far as physical sciences are concerned, applications have been relatively scarce. As Kli r and Bo Yuan [14] comment, “This may be explained by the fact that classical methods based on crisp sets and additive measures have worked quite well in these areas and, consequently, there have been no pressing needs to replace them with the more realistic methods based on fuzzy sets and fuzzy measures. One exceptions is quantum mechanics, where the need for non-classical methods is acute. Based on some preliminary investigations...it is reasonable to expect that both fuzzy sets and fuzzy measures will play profound roles in quantum mechanics in the near future”. The entities of the microscopic world were viewed as those for whose description fuzzy logic might be more perspective, because of the uncertainty inherent in any approach to their description (Heisenberg’s principle).

3.5. Vagueness aspects in the description of molecules

A molecule is commonly defined as a grouping of nuclei and electrons. By taking into account the effects of the uncertainty principle on our description of the electrons, the definition can be modified to ‘A molecule is an arrangement of atomic nuclei surrounded by a fuzzy electron density cloud’ [15]. This definition immediately transmits some fundamental information—the impossibility of giving a sharp description of each point of the molecule as well as the fact that the electron cloud has no sharp boundaries. In this way, it can be utilised for a discussion leading to a more realistic image of molecules.

Nuclei are also influenced by the uncertainty principle. Therefore, the geometrical arrangement of the nuclei is not sharply defined, it has a certain degree of fuzziness. The traditional and classical assumption in chemistry is that molecules have an approximate nuclear structure, and this assumption is embedded in the Born–Oppenheimer approximation [16]. The geometrical description of molecules in terms of bond lengths and bond angles is based on this assumption. However, there are cases in which the concepts of nuclear framework and molecular structure become difficult to define. A limiting example of vagueness in the definition of the geometrical framework of the nuclei is offered by the ammonia molecule. This example is convenient also because many students are already familiar with the phenomenon in question—the ammonia-maser transition, i.e. the continuous change of the position of the nitrogen atom with respect to the plane identified by the three hydrogen atoms. Moreover, the phenomenon is often discussed in the same theoretical chemistry course as a typical example of tunnel effect, what enhances students’ familiarity with it. It is easy to highlight that the phenomenon makes it difficult to define a nuclear framework for the ammonia molecule. Though the geometry of either of the two states is commonly taken as the geometry of the molecule (in terms of bond lengths and bond angles), the definition of a nuclear structure is highly uncertain. The discussion of this example has a clear pedagogical significance, because it gives a deeper insight into the nature of one of the most common and classical concepts— the arrangement of the nuclei and the framework they form—and contributes to the awareness that such concepts might be viewed as convenient and useful simplifications, whose correspondence with physical reality is not always certain or not always complete.

The discussion on nuclear structures is conveniently expanded to stress another important feature, i.e. the fact that the molecular structure changes in response to the environment (e.g. a solvent). Stressing all these aspects since the beginning of the discussion on molecules increases students’ awareness of the complexity of the issue, what is beneficial to the development of an open-minded vision about it.

The fuzziness of the electron density distribution determines the fuzziness of the properties associated with it, like the shape of a molecule or its surface. As far as the surface is concerned, vagueness results from two factors, i.e. the approaches by which the molecular surface is ‘constructed’ (e.g. the hard sphere model, first introduced by Connolly [17]) and the flexibility of molecules. Because of its flexibility, the shape of a molecule is not ‘fixed’, it does not remain constant in time and, correspondingly, also the surface in a given portion of the molecule is not ‘fixed’, it may change with time.

3.6. Aspects of the description of molecules for which the resort to fuzzy logic has so far been considered more interesting

A list of aspects, complemented by some brief information, can be sufficient to stimulate the perception that the resort to fuzzy logic can provide additional insight for a number of questions. As highlighted in the previous section, fuzziness is associated with the two main ‘components’ of
the description of a molecule, i.e. the geometrical arrangement of the nuclei and the electron density cloud. According to the aspect under investigation, it is more relevant to take into account the fuzziness of one or the other of these two components.

The use of a fuzzy approach for the description of the nuclear structure has proved interesting in the investigation of aspects, where the geometrical arrangement of the nuclei plays either the determining role or a relevant one. Examples of such aspects are the following:

- The study of molecules whose classical description involves resonance between two or more structures (superposition of two or more states) [16].
- Aspects related to the presence or absence of symmetry: molecular symmetry and symmetry defects, chirality, and reaction mechanisms [18].

A fuzzy approach to the electron density cloud (sometimes in combination with a fuzzy approach to the nuclear structure) has proved interesting for the investigation of aspects like the following [15]:

- The electron density of macromolecules, proteins and supramolecular structures.
- The shape of molecules.
- A variety of properties associated with the shape of molecules: description of functional groups, local shape changes of a functional group caused by the molecular context (the rest of the molecule), effects of the shape, or of shape changes, on reactivity.
- The molecular surface.
- Phenomena associated with the specificities of the shape and surface of molecules in particular regions, like molecular recognition.

It is convenient to select few cases for more detailed discussion, to make the discourse more concrete. Three such examples will be briefly outlined in the next paragraphs, for illustration purposes.

### 3.7. Example: the shape of molecules

Molecules do not have a sharply defined shape, because of the nature of the electron cloud. In order to define a shape, one has to decide whether a certain point ‘belongs’ to the molecule. Within a fuzzy approach, this can be discussed in terms of ‘degree of belonging’. A point, where the electron density is high will have a higher degree of belonging, a point, where the electron density is low will have a low degree of belonging. The degrees of belonging will range from 0 to 1, thus constituting a membership function. Various criteria can be proposed to establish a correspondence between the degrees of belonging and the electron density values. The electron density values can be scaled, so as to give \( \mu = 1 \) in correspondence to the highest density values and \( \mu = 0 \) in correspondence to negligibly small density values. Alternatively, all density values higher that a certain threshold value can be associated with \( \mu = 1 \), and the smaller values can be conveniently scaled [15]. The approach is in agreement with common chemical knowledge/intuition, what makes it particularly apt for discussion with students.

### 3.8. Example: the electron density of macromolecules

Mention can be made to approaches constructing the electron density of macromolecules, proteins or supramolecular structures by assembling fuzzy electron densities of fragments, into which the molecule can ideally be subdivided. The Mulliken–Mezey additive fuzzy density fragment (AFDF) approach presented in Ref. [15] constitutes a convenient example. The fuzzy electron densities of the fragments are generated through ab initio calculations of smaller molecules, appropriately distorted so that the nuclear distribution correspond to the one of the fragment (i.e. it takes into account the modifications due to the influence of the surroundings that the fragment will have in the larger molecule). Then the fragments are assembled to ‘build’ the larger molecule. It is obvious that many distorted structures may correspond to the same ‘parent’ small molecule. Therefore, the approach was also utilised to develop a numerical electron density fragment database containing many surrounding-dependent electron density versions of the same molecule.

### 3.9. Example: the problem of molecular recognition

The issue of molecular recognition is not usually included among the themes discussed in introductory theoretical chemistry courses. On the other hand, a brief outline can be considered advantageous from several points of view. The issue has great relevance in the study of phenomena that involve specificity, like the interactions of a biologically active molecule and a receptor, or the action of catalysts. These themes are encountered also in courses perceived as more ‘concrete’ than the theoretical chemistry one. Highlighting that the molecular recognition issue can be studied from a theoretical chemistry point of view contributes to highlighting the variety of issues that are of interest to theoretical chemistry and the variety of possible interactions with the other areas of chemistry. This, in turn, is relevant to the general objective of making theoretical chemistry courses more attractive [1,2].

For presentation purposes, the interaction between an active molecule and a receptor can prove more convenient, because many students have already encountered the basic concepts concerned. The nature of the phenomenon is easily illustrated by the traditional key-and-lock model, an image that is also already familiar to a number of students. This image is particularly apt for immediate visualisation of
the meaning of molecular complementarity and also of the fact that it can be analysed in terms of complementarity of the relevant parts of the molecular surfaces. Trying to identify which molecules of a given class can be bound by a certain receptor involves an evaluation of the complementarity of the surfaces of the molecules and the receptor in the regions expected to be involved in the bonds formation.

As explained previously, there is an inherent vagueness in the identification of molecular surfaces, resulting both from the procedure utilised for its generation and from molecular flexibility. Therefore, the concept is a fuzzy concept. Fuzzy logic enables the utilisation of linguistic variables. Linguistic variables can be useful to denote the various types of shapes that can be appropriate to describe the details of the molecular surface in the region of interest: bag, cleft, saddle, ridge, knob and plateau [19]. If needed, qualifications may added (e.g. small, middle or big bag). The extent to which a given linguistic variable actually describes the molecular portion considered is expressed by the values of the membership function. Moreover, the membership function can also take into account the modifications due to molecular flexibility, by appropriate changes in its values. The approach offers the basis for an automated comparison of:

- The complementarity of the molecular surfaces in the regions of interest (e.g. the active site of an enzyme and the relevant regions of molecules expected to bind to it).
- The similarity of molecules. For illustrative purposes, it can be recalled that, e.g. comparative studies of molecules belonging to the same class—molecules with similar relevant molecular properties at the binding site—enable the identification of the pharmacophore and the evaluation of the size of the receptor binding site, since this site must have an accessible volume capable of accommodating that pharmacophore [20].

4. Discussion and conclusions

The previous outline is sufficiently simple to be presented within introductory theoretical chemistry courses of any level, including the most basic ones. It makes extensive reference to classical chemical knowledge and chemical intuition, i.e. to the information and to the form of chemical reasoning that are already familiar to students, from the other courses. In this way, it links to the ‘already known’, what contributes to a perception of concreteness.

The most important objectives of the presentation are the following:

- Stimulating reflections on major conceptual and methodological features like the complexity of physical reality, the meaning of models, the generalised presence of uncertainty in all our descriptions and interpretations, and the importance of taking it into account.
- Offering motivations for the exploration into diverse directions in general, and into options specifically taking uncertainty into account in particular.
- Avoiding the risk that students perceive our models or simulations as if they were the actual physical reality.
- Enlarging the ensemble of tools whose existence is known.

For testing purposes, the above material was presented in individual sessions to students who had shown particular interest in the course. Their response was positive and the interactions also highlighted the interdisciplinarity value of the option. In particular, students were attracted by a new aspect of the interdisciplinarity with mathematics, stemming from the resort to the set concept. They had encountered sets only in the mathematics course, but not in chemistry courses, and they showed appreciation towards the possibility that theoretical chemistry discussions involve a mathematical concept that had long remained unutilised for them.

In conclusion, it is considered that the inclusion of basic information on the existence of fuzzy sets and fuzzy logic, and of their potential roles in theoretical chemistry, can contribute to a more complete picture of theoretical chemistry, and also of the methodological and philosophical aspects that are relevant to its conceptual body. The information can be easily integrated into a theoretical chemistry course, where it will have the role of ‘expanding the boundaries’ of the ‘normal’ course content without implying additional difficulties.

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