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QUANTUM vs. "CLASSICAL" CHEMISTRY IN UNIVERSITY CHEMISTRY EDUCATION: A CASE STUDY OF THE ROLE OF HISTORY IN THINKING THE CURRICULUM

ABSTRACT: In this paper we present an analysis of the situation of the discipline quantum chemistry within university chemistry curricula. In order to rationalise this situation, we have adopted a historical perspective, focusing on the work of the towering figures of G. N. Lewis and L. Pauling as the main sources of modern chemical theory. From the analysis of the contribution of these authors we have proposed three points as the most conflicting ones for the teaching of quantum foundations to chemists: the *off Physics* character of the physical vision of the microscopic realm provided by "classical" chemistry; the polysemy of several terms taken from the work of L. Pauling (e.g. "orbital"; "resonance"; etc.) when they are used in a quasi-quantum context; and finally, the divergence of the physical visions of the world provided by quantum and classical theories. [*Chem. Educ. Res. Pract.*: 2003, *4*, 131-148]

1. INTRODUCTION

It would hardly be an exaggeration to say that most chemists have nothing but a superficial knowledge of quantum mechanics, and, more precisely, of its application to chemical problems: quantum chemistry (hereafter QC). In our opinion, this situation arises from a deeply rooted conception, according to which quantum chemistry is mainly an academic subject, limited to the study of a few small systems and a fistful of very specific phenomena, all of them very far from the actual interests of chemists working in a "real world" laboratory. The reasons for such a vision of QC may be multiple, and we are not to analyse them in depth in this paper. Just to point out what we think are the most obvious ones, we have in the first place the high computational demands for solving the Schrödinger equation. For most "realistic" physical systems, reliable QC calculations have been traditionally very expensive. This is in fact the origin of a second dissuading factor: the need for a complex mathematical (numerical analysis) apparatus, intended to approximate solutions to the Schrödinger equation. This actually goes beyond the intrinsic difficulties of quantum mechanics. The "numerical technology" background of QC is the origin of the disorienting amount of methods (and, therefore, of acronyms) which litter quantum chemistry literature. But the true factor which is in our opinion behind the little interest of most

chemists towards quantum chemistry is the existence of a simple visual model of molecular structure, independent of (though related to, as we are to see below in this paper) quantum mechanics, a model which has been called by other authors "Folk Molecular Theory" (FMT) (Ramsey, 1997a).

FMT, rather than a closed physical theory, is an informal set of structural ideas and semiempirical rules. We do not know of any systematic presentation of this model (provided that such a presentation, if possible, is of any interest), but it is necessary to make clear what we refer to as FMT in this paper. FMT is the structural part of what Joachim Schummer (1998) has called *the chemical core of chemistry*. In the framework of FMT molecules are seen as tri-dimensional arrangements of atoms in a classical (Euclidean) space. Atoms are joined together by bonds which have some kind of physical entity (a bonding energy, as well as other physical properties, can be assigned to a particular bond), so that a molecule can be said to be made of atoms and bonds between them. The nature of the bonds, as well as the chemical properties resulting from this nature, can be determined by means of several models and semi-empirical rules (Lewis "forms"; atomic orbitals hybridization rules; VSEPR model; etc.) which must be regarded as the methodological nucleus of FMT. From the didactical point of view, FMT is the theoretical model used for presenting the foundations of molecular structure in every introductory text. Moreover, we think it is not exaggerated to say that FMT is the theoretical basis underlying the didactical practice of most chemistry lecturers, both at the secondary and at the higher education level.

FMT has been especially useful in guiding research in chemistry. If the quality of a theoretical model could be judged by the range of different problems it can deal with, or by the number of sound technological applications it has brought about, then it would be difficult to find, in the whole realm of the experimental sciences, a model better than FMT. And this being FMT, as we have already pointed out, an extraordinarily simple theory, lacking almost completely from any mathematical formalism, and giving a rich visualisation of chemical systems at the microscopic level. On the other hand, it is not surprising that the limited and highly complex quantum chemistry has had only a relative interest for most chemists.

The special relationship of chemistry as a whole with its physical foundations of quantum mechanics has impregnated every feature of the practice in this field, and in particular, education. Thus, the weight of quantum theory in the university chemistry curriculum (not to speak of secondary education) has been small compared with the dominant position of FMT . There is little doubt that this situation is logical, given the success of FMT. Moreover, designing the education of chemists apart from this hegemonic model would be simply destructive for university students. The relationship between QC and FMT in the framework of chemical education can therefore hardly be said to be one of *integration*. *Coexistence* is perhaps a better term to describe the epistemological isolation of the quantum mechanical approach with respect to the rest of the subjects based on FMT.

On the other hand, during the last twenty years a series of changes are challenging the position FMT must play in the formation of chemists. First is the growing interest in experimental settings in which FMT loses a great deal of its explanatory power. We mean research fields such as the chemistry of plasmas and flames, higher atmosphere, or the interstellar environment. In these fields, there is a large number of species that are difficult to model within FMT, such as multiple or ionic radicals, or reaction intermediates. Besides, different types of materials which have been shown to be difficult to study within FMT have been recently discovered or synthesised. The most obvious example is fullerenes (Kroto et al., 1985; Dresselhaus et al., 1996). Secondly, the extraordinary advance of microelectronics now allows the study of systems that only a decade ago were simply too large. In concrete,

QC calculations that required a supercomputer can now be done with a much more accessible kind of machines, usually called workstations, affordable by almost any research group or middle-size company. This means that larger chemical systems are being taken into the domain of the problems whose Schrödinger equation can be solved within what has been called *chemical accuracy*[1]. On the other hand, some of the latest generation PC's have computing performances which are at least as high as those of most workstations. And we do not think it is too optimistic to think that these performances will increase substantially within the next few years. In other words, the possibility for literally any chemist of producing high quality quantum chemistry information is now opening. This is, of course, related to what we have discussed above, but it has a feature that makes it qualitatively different: the domestic character of PC technology, which makes its potential impact in the work of chemists enormous. It could be said that quantum chemistry is getting *democratised*.

To sum up, neither can FMT now be considered a fully comprehensive model for studying any chemical problem, nor can quantum chemistry be any longer regarded as an academic, or even *useless*, subject. Of course, this situation must have some influence in chemical education. In fact, if we focus on a referential journal such as *Journal of Chemical Education*, from the 80's the number of published papers on quantum chemistry (both on basics and on applications) has steadily increased. This growing importance of quantum chemistry can also be detected in the current university chemistry curricula of most Spanish universities[2]. In concrete, besides specific courses, computational laboratories based on quantum chemistry simulations performed in PC's (the so called *dry labs*) are now a usual part of the syllabus. A *bubble* of QC education is therefore growing inside a curriculum still largely dominated by FMT. University chemistry education is now therefore facing a situation that could be said to be *critical*. Adapting (rather freely) the famous phenomenological analysis of A. Gramsci of the revolutionary times, it could be said that many old curricular conceptions are dead (or, at least –or even *at last!*- dying), while the new ones are not born yet. Of course this is a metaphor: no death is possible in the realm of ideas. Anyway, the particular situation of quantum chemistry within university chemistry curriculum cannot be seen as a *mere oddity* any longer.

Recently, we have started in our group a project to study several features of the teaching-learning of quantum chemistry in the context of tertiary chemistry education (Sánchez Gómez et al., 2001; Sánchez Gómez, 2002; Sánchez Gómez et al., 2002). In this work we have adopted an applied (or *pragmatic*) view: we have been interested in concrete features[3], rather than in trying to get a general vision of the curricular structure of university

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[1] Quantum chemistry calculations are said to be precise within the *chemical accuracy* limits when the resulting heats of formation lie close to the exact solution of Schrödinger equation within a range of 1 kcal/mol. There are several methods for estimating the accuracy of a calculation. One of the most difficult problems of computational chemistry is that energetic accuracy does not have to imply an equivalent precision for structural parameters. Anyway, the assumption that lies at the very core of the *ab-initio* philosophy is that in the limit of higher energetic accuracy, structural results have an equivalent quality. That would be true of course in the ideal limit of exact analytic solutions, but it is not clear that it has to be the case for any *chemically accurate* calculation, although this standard, though arbitrary, is really stringent (1 kcal/mol is equivalent to approximately 0.001 Hartree for a single molecule calculation). To make things more complex, we have to keep in mind that unlike energies, structural parameters are not quantum observable, and therefore they cannot be defined as eigenvalues of any operator conmuting with the hamiltonian.

[2] We of course have a first hand experience of the Spanish university system, though it is easy to see that the increasing importance of quantum chemistry in chemical tertiary education is a common trend. A extreme case in Spain is Universidad Autónoma de Madrid, where a compulsory one-term course on quantum chemistry is included during the first year.

[3] Such as the analysis of the variation of the thought of the students on atomic and molecular structure along a first year full-term course on quantum chemistry (Sánchez Gómez et al., 2002).

chemistry studies. This latter approach can perhaps be seen as a fanciful theoretical enterprise, at best useless, if not simply impossible. For is there anything *hard enough* in university chemistry curricula to be studied in such a formal way? And, if such a *hard core* of first curricular principles exists, what is the use of a formal analysis of it for chemistry educators? In fact, it is very easy to see that such a program would derive from an extreme positivistic vision of the sciences really difficult to hold nowadays. But there is another possible approach for the *conceptual* study of the curriculum, an approach based on its historical character. As Tsaparlis (2001) has shown, history can be used to illuminate the didactic context of an aspect of higher science education as complex as the teaching-learning of Schrödinger equation. In a similar way, a historical gaze can be taken on more general aspects of the chemistry curriculum. Under such perspective, the curriculum must be seen as having a twofold historical character. It is, on the one hand, the result of the particularly rich evolution of the *central* (and therefore crossed by every influence) *science*; and on the other, one of the causes of this evolution. This is, of course, an example of the well known (*paradigmatic*?) Kuhnian *normal science–normal science education* dialectics.

Such is the methodological approach we have adopted in this paper. We present an analysis from historical considerations of the situation of quantum chemistry within the university chemistry curriculum. In concrete, we have studied the historical evolution of both FMT and QC, focusing on the work of the authors that we consider to be the most influential in the development of chemical theory: G. N. Lewis and L. Pauling. As an outcome of this study, we propose three points as the most conflicting in the teaching/learning of quantum theory in the context of chemical education: the intrinsic *weirdness* of quantum mechanics; the separation of chemical and physical languages (G. N. Lewis); and the polysemy of several terms used in both quantum mechanics and FMT (L. Pauling). Finally, we present a reflection on the role of history as a tool for the curricular integration of QC and FMT.

2. THE SEPARATION BETWEEN PHYSICAL AND CHEMICAL APPROACHES: G. N. LEWIS AND THE *ELECTRONIC THEORY*

Historically, FMT stems from the microscopic model of substances developed during the last third of the 19th century, and the first years of the 20th century. This model is based, on the one hand, on the structural ideas introduced by Canizzaro, Kekulè, Van't Hoff and other pioneering chemists. On the other hand, it is based on the different evidences of the electric nature of matter, resulting from the works of Arrhenius, Ostwald, Nernst and, from a different point of view, Thompson and Rutherford. The so called *Electronic Theory*, developed by Gilbert Newton Lewis during the first two decades of the 20th century, with important contributions by I. Langmuir and W. Kossel, was the first theoretical approach that took coherently into account these two lines. Lewis' ideas were published for the first time in 1916 (Lewis 1916), and are presented in depth in a work with an explicit vocation as a textbook: *Valence and the Structure of Atoms and Molecules* (Lewis, 1923), one of the most influential books ever published in Chemistry. The transcendence of Lewis' ideas in the formation of the modern chemical thought is simply enormous. We do not think it is exaggerated to say that, from the 1930s onwards, all chemists have been initiated in the study of molecular structure through the electronic theory.

Lewis' theory brought along a model of the electronic distribution in the molecule that took into account most of the chemical experimental evidence that had been accumulated during the 19th century and the beginning of the 20th century. The electronic theory was able to justify the valence of the different chemical elements. It also provided the first satisfactory explanation of non electrostatic bonding, as well as a more satisfactory theory for the acid-

base chemistry than the previous one introduced by Arrhenius. Apart from these *accommodations* of experimental data, the electronic theory presented some predictive character, as it allowed for the first time to study theoretically the structure and properties of, in principle, any substance. The obvious corollary is that it permitted chemists to postulate (or to discard) the existence of un-synthetised compounds. We do not think the relevance of the latter in the development of synthetic and preparative chemistry has to be stressed.

Similarly important was the fact that the Lewis model admirably fitted into the wealth of theoretical speculations about mechanisms of organic reactivity that had continuously increased since the end of the 19th century. The adoption of Lewis and Langmuir's ideas of electronic pairing and covalence led to a radical clarification of the idea of *affinity*, which had dominated chemical reasoning so far. Free of the obscure semi-empirical rules of affinity, chemists, with the towering figure of C. Ingold over all of them, were able to organise mechanistic and kinetic information of the most relevant organic reactions in a coherent way (for a general overview, see Brock, 1992, pp. 521-537). It could be said that the electronic theory provided the chemists with the first *language* complete enough to coherently *speak* about chemical phenomena at the microscopic level.

Lewis' Electronic Theory was the basis on which FMT was built during the first half of the 20th century. There are two features of the Electronic Theory inherited by FMT which, in our opinion, have been particularly important in the didactic context:

1) Lewis' theory (and thus FMT) is not a model of what we now call Physics[4]. The study of a molecular system within FMT is not based on the quantitative analysis of the interactions between its components in terms of a mathematical model. Such would be the approach of quantum chemistry. But on the other hand, FMT does imply a *physics* of the microscopic world, for it is a model of the nature and interactions of nuclei and electrons which yields assertions on the structure and properties of atoms and molecules. These properties, such as composition, structure and reactivity, do have a *physically observable* character. On the other hand, this *physics* is totally different from *"Physics proper"*. Both are two distinct approaches to the same problems, of course with some contacts, but with different methods and even objectives. In the framework of the electronic theory, molecular structure and properties are derived from a set of *ad hoc* rules totally apart from the formalism of Physics. It must be pointed out that some of these rules are even difficult to justify from the point of view of Physics. The most obvious example is the postulate of electronic pairing, which is in open contradiction with the results of electrodynamics (even quantum).

2) Closely related to the previous point, FMT's arguments, the molecular data FMT is applied to (number and type of atoms; molecular charge; etc), are dimensionless. And so are their results. The information on any molecular property (polarity; ionic character; geometry) provided by FMT does not consist in a dimensional numerical output, as always happens in any model of Physics, but in a generic proposition on the presence (or absence) of such a property in the compound under study. At best, FMT yields an arrangement of a series of compounds according to the relative "amount" of a property over all of them. In other words, within FMT molecular properties are operationally treated as nominal, or, in some cases, ordinal variables. For example, it can be said that a certain compound is polar, polarity then being a nominal variable; or a set of compounds can be arranged according to their relative polarities (polarity as an ordinal variable).

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[4] We use "Physics", with capital 'P', to distinguish the discipline which is now so called, from other "physics", other models of the material world.

3. FROM CHEMISTRY TO PHYSICS, A ROUND TRIP:
L. PAULING AND THE VALENCE BOND METHOD.

L. Pauling was one of the first chemists in getting acquainted with the new ideas of quantum physics. In 1926 he had the opportunity of visiting some of the European laboratories in which the quantum theory of atomic structure was being developed. In particular, he spent some time at Copenhagen with Bohr, with Sommerfeld at Munich, and with Schrödinger at Zürich. It was in Switzerland where he met Walter Heitler and Fritz London, who were to publish in 1927 the first application of quantum mechanics to a molecular system, H_2 (Heitler & London, 1927). Back in the United States, he took the task of extending Heitler and London´s ideas to any chemical system. The method he developed (with important contributions by J. C. Slater) is usually known as *Valence Bond Method* (hereafter called VB method). The foundations of this method were published by Pauling in the early 1930's, almost always in journals of chemistry (Pauling, 1931a, 1931b, 1931c, 1932a, 1932b; Pauling & Sherman, 1933a, 1933b; Pauling & Wheland, 1933), and are the basis of an enormously transcendental book: *The Nature of The Chemical Bond* (Pauling, 1939). An indication of the importance of this work is given by the fact that during 1999, according to the *Science Citation Index* database, it was cited in 584 scientific papers[5]. This fact is still more remarkable if we keep in mind that the last revision of Pauling's masterpiece (the third one) was published in 1960.

The VB method is directly based on previous structural ideas, and in particular, on Lewis electronic theory[6]: the existence of individual atoms within the molecule is accepted in an axiomatic way; a shell model for electronic structure of the atoms is then adopted, including the idea of valence shell; and finally, "bonding" between this individual atoms is postulated as the origin of molecular frame. This approach can be thought to be almost absurdly obvious from our chemically educated perspective, but it is not from a quantum mechanical one. Within the Schrödinger equation for a molecular system, electrons are not ascribed to a particular nucleus, nor does bonding play any role, even implicit, in the formalism. It can be therefore said that VB is typically *chemical*.

Historically, the VB method has had a paradoxical fate. On the one hand, from almost the very beginning it was becoming apparent that it presented serious practical disadvantages with respect to its competitor, the Molecular Orbital (MO) method, in solving the Schrödinger equation. In fact, as early as in the 1950's it had been already almost completely discarded for applied purposes (see Brock, 1992, pp. 500-505). On the other hand, its conceptual background was adopted by many chemists, in such a productive way that it was eventually adapted into FMT, so that many terms coined by Pauling (e.g. orbital; hybridization; etc.) are now part of the vocabulary of any chemist.

There are two aspects in the VB method that seem to us particularly relevant in order to understand the didactical relationship between FMT and quantum theory. Firstly, the VB method does not provide a physical justification of FMT. In our opinion, the relationship between FMT and the VB method must be understood historically in the opposite way: FMT ideas, based on a rich tradition of research on the chemical phenomena, were used by Pauling to develop an approximate method for solving the Schrödinger equation for molecular systems. Pauling did not depart from quantum mechanics to arrive to chemistry, but rather

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[5] According to Brock (1992, p. 505), who uses the SCI database as well, the number of citations between 1955 and 1983 was over 16.000!

[6] Pauling always acknowledged this intellectual debt: *The Nature of the Chemical Bond* is actually dedicated to Lewis.

the other way around. Secondly, as we have already said, many terms coined by Pauling for the VB-method have been transposed into FMT. The important point here is that most (if not all) of these terms have experienced an essential change in their sense, to the extent that they designate completely different entities when they are used in the framework of the VB method or in that of FMT. Within the VB method, terms such as "atomic orbital", "overlap", "orbital hybridization" or "resonance" refer to either mathematical functions, or to mathematical relationships or to operations involving these functions. All these terms have a full meaning as elements of a method for solving the Schrödinger equation in molecular systems. In a somewhat crude way, it could be said that they have a *mathematical meaning*[7].

In contrast, within FMT these terms are used as if they had some type of "genuine" physical existence. Let us think, for example in the way chemical bonding properties are usually presented in textbooks (and not only in introductory ones) as resulting from the *physical* interpenetration (overlap) of *physical* entities (the atomic orbitals) belonging to the different atoms involved in the bonding. This conception is surprisingly similar to a vision of bonding common during the late 19th century, which was still frequent in the early 20th century, according to which atoms had some kind of hooks (in a number equal to its valence) so that bonding could be visualised as resulting from the union of the hooks of two different atoms. Curiously enough, this conception was never thought to be but a visual model to help to rationalise molecular structure, mainly for didactical purposes (Holton, 1952, pp 412-415). In other words, the family of "quantum" terms translated from the VB formalism into FMT did not imply a substantial change in the conceptual foundations of the latter. The process was to some extent the opposite: the terms were filled with a classical meaning, so that a polysemy with respect to the original (quantum) usage of them arose. The VB method did not turn FMT into a quantum theory, rather, the latter took some quantum look by adopting a few terms to remain proudly classical.

4. DIDACTICAL IMPLICATIONS OF THE RELATIONSHIP BETWEEN FMT AND QUANTUM APPROACHES

In the previous sections we have studied in a historical perspective two points that are crucial to understanding the didactical relationship between quantum physics and structural chemistry: on the one hand the "off Physics" character of FMT; and on the other, the usage within FMT of a series of terms taken form the quantum chemistry jargon, but with a sense typically classical. Besides, we have to study another issue that has an enormous importance in the context of chemical education: the radical divergence between the images of physical reality provided by FMT and Quantum Mechanics.

Separation between chemical and physical theories

As we have already said, FMT is a physical theory, since it deals with physical (in the ontological sense of the adjective) entities, and it postulates a set of relevant properties and interactions in order to explain molecular structure. It is curious to note the similarity of FMT approach to that of the primitive Greek scientists-philosophers: observations are explained from a limited set of basic comprehensive principles, which must be *saved* at any rate. The task of the theorist is then a *race against data*: the model must be continuously *fixed* by addition of fresh ad hoc rules to it so that is can always match experience (Sambursky, 1956,

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[7] We do not enter in the debate on the ontological status of the mathematical formalism of physical theories. We mean that those terms designate entities used within a mathematical apparatus, though of course they are part of a physical model.

pp. 1-25 & 222-244). Let us think in the paradigmatic example of the Ptolemaic astronomical model, and the continuous efforts to keep it in accordance with observation. In the case of FMT the principle to be kept would be the classical idea of structure. In simple words, the "balls-and-sticks" vision of molecules is the FMT equivalent of the celestial spheres in Ptolemaic astronomy. The adoption of terms from the VB method, and the adaptation of some quantum concepts, such as "orbital", can be seen as attempts to assimilate new experimental results.

FMT is a physical model, but it is not a model of Physics. No coherent and extensive use of the concepts and methods of Physics can be found in FMT. In particular, no mathematical apparatus is employed in the description of the microscopic world given by FMT. The formalisms of quantum chemistry and FMT are radically different. And this, of course, has deep didactic implications. The most obvious one: while mathematics and, in particular, Analysis (Calculus) and Algebra, play a crucial role in the development of physicists, the weight of mathematics is largely less important in higher chemical education. Of course mathematics, even at a very high level, is instrumental in different areas of chemistry[8], and in fact, some kind of mathematical normalisation of FMT could be possible, based on *qualitative* (in the sense on non-analytical) theories, such as Graph Theory (Hansen & Jurs, 1988a, 1988b). But anyway, it could hardly be said that chemistry is a mathematical science, and therefore that chemical education must be based on an extensive mathematical background. As a consequence, quantum mechanics, or even quantum chemistry, has a hermetic character for most chemists. And then, the system, at least at the didactical level, is fed back: chemists do not read quantum Physics because of its mathematical apparatus; thus chemistry remains apart from quantum physics; thus no extra physical education in the formation of chemists is needed; thus chemists cannot read Physics.

But the differences between the formalisms are not only restricted to the mathematical apparatus of Physics. The divergence is much deeper, and it gets to the point that "thinking" about a problem means different things in chemistry and in Physics. Let us see this in an example. If we had a substance of which we only know its empirical formula, and we were interested in its properties, we could ask a research team of molecular physicists (or quantum chemists) to study it. A priori, another sensible procedure would be to ask a team of, say, organic chemists (we'll assume this unknown substance is an organic one, which does not seem to be too stringent a restriction) to do such research. In the former case, the first step would be, no doubt, writing the Schrödinger equation for the system, and trying to get an accurate solution for it. This always requires some degree of approximation, even using a particular method, frequently implying a restricted formalism. This will "pollute" the results, in the sense that they will bear, more or less explicitly, signs of the formalism employed.

Thus, results *must always* be read as resulting from a particular method. Assuming that we eventually get a reliable enough approximation for the wave function, our team would calculate from it the different observable properties relevant to our purposes (spectra; ionisation energies; etc). Eventually we could even have a good approximation for the geometry of the molecule (though molecular geometry *is not* a physical observable).

In the second case, the team of chemists would follow a radically different way. Most likely, they would start their study by proposing Lewis structures for the compound. From these structures, a prospective evaluation of its reactivity can be given (by comparing with analogous compounds). A model of molecular geometry is also implicit in Lewis forms (Purser, 1999), and therefore qualitative physical information can be obtained (polarity,

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[8] The most obvious example is group theory. Though the utility of this theory comes from its role in quantum mechanics, group theory is now widely used in areas far from its quantum origins, such as inorganic chemistry. Perhaps it is another case of *adoption* of quantum formalism by FMT.

solubility in different solvents, etc.). Finally, a synthetic path may be proposed. Of course, our team does not have to stop at this point, but we think the previous steps are always to be taken.

It is evident that the *modus operandi* of chemists and physicists/quantum chemists is totally different. It is not just that they take different paths; not even that they arrive at different points. In fact, the results they both provide are so different that they cannot simply be reduced to each other. Quantum and "classical" results are different *in nature*. Using a linguistic simile, quantum and FMT chemists not only give different answers to the same question, they answer to it in different languages. In the terms of the jargon of modern Philosophy of Science, quantum chemistry and FMT would be incommensurable disciplines. It seems to us that such a *double discourse* situation is definitely not the ideal setting for teaching any subject. It is of course possible to *speak* both the languages of Chemistry and Physics (Lewis and Pauling are examples of such *bilingual* scientists), but that is not at all frequent. And this is true not only for students, but even for academics.

Besides the complexity of the epistemological status of quantum chemistry, it has been shown that students have a strong tendency to bear different conceptual frameworks in different contexts (Solomon, 1993; Henessy, 1993). More precisely, Taber (1998) has found that pre-university chemistry students seem to fail to use physical reasoning when asked about atomic structure. This result suggests that knowledge is not readily integrated across the border between academic disciplines. If such a strong disciplinary separation of the students' discourse were extrapolated to the dichotomy chemistry-Physics, it would superimpose to the already divergent relationship between these two models. And, therefore, we would have a double (epistemological and psychological[9]) separation between them.

These two aspects may have evolved independently, but there is another possible interpretation of this situation. Let us notice that there is a surprising symmetry between the epistemological compartmentalisation of Physics and chemistry, and the tendency of students to separate their discourses on these two subjects. In fact, the latter could be seen as a translation of the former into the students' thought realm. This coincidence is so strong that it is tempting to attribute it to a causal relationship. If such were the case, learners' ideas on atomic structure, such as those uncovered by Taber (1998), would reflect the historically consecrated divergence between Physics and chemistry. Learners think about atoms (as perhaps about any scientific subject) what they have been taught to think. This is actually a common sense vision of academic learning, and like many other common sense opinions, it is perhaps too simplistic. There is still another possibility. Let us suppose that the tendency to *contextual reasoning* is not restricted to these two particular areas, and rather it is a response to the general disciplinary structure of education (which seems sensible). If such is the case, and as this separation of the sciences into disciplines (*disciplinarization)* is not a contemporary trend, it must have played a role in the historical configuration of the different academic subjects which inform any science syllabus.

These visions are not incompatible, actually. It is very easy to see that they both describe a rather stable picture of the disciplinary configuration of Physics and chemistry. Our point is that as knowledge is *constructed* subjectively by learners, and as this *construction* is affected by the academic context in which it has been developed, then *professional* chemists' and physicists' thought must somehow show features of such a context. Therefore, a *disciplinarized* education yields a *disciplinarized* scientific thought.

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[9] Perhaps the adjective "psychological" is not accurate in this context, because it could convey an *internist* vision of learners' *ideas*. If we have used it - instead of others with different implications towards learners' ideas - it is just because "psychological" is the most common one (and therefore the least "ideologically charged").

And this further reinforces the isolation of disciplines in university science curricula, for the resulting graduated physicists and chemists eventually become lecturers, textbook authors, and so on. This is a typical *explosive loop*[10] (i.e. positive feedback cycle - or 'vicious circle'), a situation in which a given starting tendency feeds itself to get more and more intense. It is actually very easy to see that it actually does not matter much what comes first, epistemological separation, or learners' tendency to contextual thought, for once the loop is started, it keeps itself going. In other words, these two tendencies reinforce each other.

Polysemy of terms adapted from the quantum formalism

A second aspect that conditions the didactical relationship between FMT and quantum theory is, as we have already pointed out, the polysemy of terms such as orbital, resonance, etc. We do not think that the statement "Polysemy is one of the most obvious sources of didactical confusion" needs any empirical support. Neither does the fact that careful explanation of the different meanings in their respective contexts is the only way of avoiding the generation of erroneous conceptions. But, as ever happens, things are far from being that simple.

In our laboratory we have carried out field work on the evolution of the discourse on atomic and molecular structure of first year chemistry university students after a full term course on QC (Sánchez Gómez et al., 2002). Our results show a systematic deep confusion between terms before the instruction, in accordance with previous results by other authors [see, for recent revisions of the research on the teaching/learning of the foundations of chemistry, with exhaustive bibliographies, Tsaparlis and Papaphotis (2002) and Taber (2001, 2002)]. For example, words such as "orbital", "shell", "level" and "orbit" are taken by many students to be functionally indistinguishable (they are used in almost exactly the same way; many cases differ only in the usage of the particular term). In other words, within our sample, these words are taken almost as synonyms. Equivalent conclusions have been reached by Taber (1997) and by Harrison and Treagust (2000).

A particularly interesting case is that of the words "orbit" and "orbital". They tend to be systematically misunderstood, and a range of confusing relationships between them can be found in the discourse of our students. In our opinion "orbit" comes from the Bohr model, which is usually presented as an introduction to atomic structure in secondary education. The idea of "orbit" seems to be rather strong, since even students who do not use it explicitly in their discourses, are likely to employ it in pictorial descriptions of atoms, some of which evidently imitate planetary models. This fact may be related to the importance of iconic elements in the formation of misconceptions in QC pointed out by Tsaparlis (1997). The *planetary* vision of the atom has been previously reported by Cros et al. (1986). In concrete, these authors show that a mechanistic vision of the electrons in an atom as fast moving *classical* particles was dominant among first year university students. Also related to this, Shiland (1997) has focused on the way the Bohr model is treated in secondary chemistry textbooks, concluding that they do not usually provide a satisfactory treatment which could allow a transition to a quantum mechanical model.

To sum up, students' discourse on atomic and molecular structure can be defined as, at least, confusing. Polysemy, far from being an exceptional feature, seems to be the norm in the discourse of students. As expected, "quantum" terms ("shell", "level", "orbital", "orbit") form a *semantic magma* in which they play rather undifferentiated roles. This provides some empirical evidence for our theoretical analysis, pushing in fact our ideas a little bit further by

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[10] *'Explosive loop'* is a term taken from systems theory. It alludes to the cyclic structure of self feeding systems in some graphic representations (in concrete, causal or flux diagrams) used in this theory.

identifying another source of meaning for the word "orbital", Bohr's atomic model. This can be seen as a radical example of our arguments: in the case of atomic structure we do not have only two, but three competing sources of didactic meaning. To make things worse it is not only that exactly the same technical word (orbital) is used in two of them, but that the common term they are derived from (orbit) is used in the third. These three models have radically different epistemological status: one is *physically acceptable* (a quantum approach[11]); the second can be seen as a crude rationale of electronic structure within FMT [12]; and the third one has just a historical value. Students (we would say all of them, according to our results) do not have a clear idea at all of their exact role and their mutual relationships. The insidious question is, do chemical educators have it?

We would not want to adopt an *aristocratic* pose, but in our opinion many educators, especially at the secondary level, are not even aware of this complex polysemy. This is actually the implicit conclusion of almost every study of misconceptions at the university level, since we can hardly figure out any source of ideas on atomic and molecular structure other than a didactic (textbooks and/or instructors) one. The fact is of course that the usage of these terms with a "classical" meaning is so widespread, and their role at the core of FMT so instrumental, that they are deeply rooted in chemical thought. Given the essential importance of the educator in any move to challenge this kind of *polysemic (mis)conceptions*, this is a rather worrying situation.

There is a debate within the community of chemistry educators on the suitability of teaching about orbitals at an introductory level. Against is the majority of the community of the researchers on chemical education (Bent, 1984; Berry, 1986; Ogilvie, 1990; Hawkes, 1992; Shiland, 1995). Such is also the position of an author as influential as Gillespie (1991), who has proposed an alternative to the conventional valence bond approach for teaching bonding and geometry (Gillespie et al., 1996). On the other hand, and surprisingly enough, we have found only one author (Morwick, 1979) who explicitly supports the teaching of orbital theory in introductory chemistry. But this is actually a mirage: though implicitly, many (most?) textbook authors and curriculum programmers are in favour of the use of orbitals for introducing chemical theory. For they include the issue not only in college chemistry courses, but even in the (upper) secondary education in many countries. In our opinion, this acritical acceptance of the teaching of orbitals is just another consequence of the widespread ignorance of the complex status of quantum jargon within FMT. We think that for many chemistry teachers, and this is of course just a *feeling* with no empirical support, orbitals are simply necessary for the quantum description of a microscopic system. In this vision, there is no QC without orbitals.

The central role of orbitals in chemistry comes from the influence of L. Pauling in the development of chemical theory. Pauling is, no doubt, one the most towering figures in the history of chemistry, but must his shadow be so long to reach chemical education in the beginning of the 21st century? In our opinion, no. We think that "atomic orbitals" are more a problem than a help in teaching chemistry. Perhaps getting rid of all these lexical *false friends* is a good starting point for designing an integrated chemistry curriculum.

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[11] Although orbitals have no physical meaning (other than approximating functions) for atoms other than Hydrogen!

[12] We assume that the static shell distribution of electrons in an atom can be seen as the *atomic* counterpart of Lewis model for molecules.

Divergence of the visions of the physical reality provided by FMT and by quantum theory

If we adopt the criterion, common among researchers in History and Philosophy of Science, of separating contemporary physical theories as "classical" or "quantum", then there is no doubt that FMT can be labelled as classical (or semi-classical). FMT does not share the complex image of the microscopic world derived from quantum physics. Within FMT concepts such as "shape", "size" or "measurement" are fully pertinent, while in the framework of quantum mechanics they are ambiguous, if not simply meaningless (see, for an excellent recent general paper on the subject, Ramsey, 1997b). This seemingly academic issue has direct didactic implications since the intrinsic "weirdness" of quantum models has been pointed out as an explicit obstacle in the teaching/learning of atomic physics (Johnston et al. 1998) and quantum mechanics (Petri & Niedderer, 1998). Besides, some authors have noticed how students try to understand quantum ideas in term of classical ones, frequently translating macroscopic models into the quantum realm (Euler et al., 1999; Flechtner & Johnston, 1999) in a attempt to making sense of the microscopic world. It is important to insist that this problem goes beyond the intrinsic difficulties inherent to the teaching/learning of quantum mechanics (quantum chemistry) we have already studied. It is not just that the discipline quantum mechanics implies a complex mathematical formalism, but that its conception of the world is radically different from any intuitive vision.

In our opinion, these conclusions can be extrapolated to the issue we are studying in this paper. The separation of discourses and formalisms of FMT and quantum chemistry, and the polysemy of crucial terms is then worsened by the *epistemological* intrinsic difficulty of quantum mechanics.

5. CONCLUSIONS: HOW CAN A HISTORICAL APPROACH CONTRIBUTE TO THE TEACHING/LEARNING OF QUANTUM CHEMISTRY?

In this paper we have shown that the peculiar relationship between "folk" molecular theory, and the quantum approach to molecular structure implies a series of obstacles for the teaching/learning of the latter. Some of these difficulties are perhaps coming from the twofold, physical and chemical, character of quantum chemistry, and they could be traced in other border areas, such as biochemistry, geophysics or other *hyphenated* disciplines. But the bulk of the problem arises from the distinct *orientations* of Physics and chemistry as disciplinary sciences. With *orientation* we mean something that transcends their particular methods and formalisms; with *orientation* we refer to the general nature of the knowledge of the material world they look for. Chemistry's approach is inclusive: substances are studied from the point of view of their common properties, of their similarities, detail playing a secondary role. Grouping in families is a standard approach for rationalising chemical properties. In fact, these families are the true nucleus of the classic chemical description of the physical world, *since substances borrow their chemical properties from the family they belong to*. For example, given a series of, say, different alcohols, from the chemical point of view they all have equivalent properties: those of the family of alcohols. They all are essentially similar. Very few substances have some kind of chemical individual entity, some kind of epistemological independence with respect to their families. And even fewer have a *proper name* (water, ammonia, etc.). Using a thermodynamic metaphor, it could be said that chemistry is an *extensive* science. This character is perhaps due the phenomenological approach of traditional chemistry: detail at the molecular level is not that important when one is dealing with macroscopic changes in a context (the chemical lab.) where little room for

subtleties is left. Theory is often seen as a rationale for understanding phenomena, more than as an end on itself.

In contrast, Physics is an *intensive* science. Substances are studied from the point of view of their differences. The alcohols we mentioned in the previous paragraph are all, from the point of view of Physics, essentially different. Detail is precisely what modern Physics is committed to explain. It is interesting to remember here that at the birth of Physics as a modern discipline is the work of Tycho Brahe and Johannes Kepler trying to explain the "details" of Ptolemaic cosmology which did not match observation. Theory plays a role radically different from that it does in chemistry.

Quantum chemistry, located on the border of these two distinctive traditions, is a major didactic challenge. How can two such incommensurable areas as Physics and chemistry be integrated within the same curriculum? Or even, how can a marginal area, such as quantum chemistry, *survive* in a way different from being a mere *oddity*, in the framework of a curriculum dominated by a classic approach? Is not any integration possible? Some authors have approached this question in a pragmatic way: instead of trying to give an *absolute* answer to it, they propose specific classroom activities in order to facilitate learning of quantum mechanics (Hobson, 1996; Rebello & Zollman, 1999; Greca & Herskovitz, 2002). Others have focused on the teaching/learning difficulties arising in concrete academic settings, both for quantum mechanics (Petri & Niedderer 1998; Flechtner & Jonhston 1999) and for quantum chemistry education (Harrison & Treagust 2000; Taber, 2002; Tsaparlis & Papaphotis 2002). These lines are really important, and in fact much of the recent advances in science education must be credited to such pragmatic views. Nevertheless, we do not think that the attempt to answer the *big question* (or, perhaps, the *fancy question*) must be abandoned. Didactical research must of course study how to put the curriculum in practice, but the curriculum itself, its structure and evolution, is well worth studying too.

Disciplinary sciences result from a historical process which is reflected in their structures. Thus, a historical gaze can be used as a tool for studying the peculiar situation of QC. In this paper we have taken such an approach; we have employed history as a *tool for thinking* the scientific disciplines. Under such perspective, it may play a role in the specific formation of the science educator. Scerri (2001) has argued in a similar way for the interest of philosophy of chemistry for educators. We think that Scerri's arguments do reinforce ours, given the close relationship between history and philosophy of science. History can be used by the teacher and/or the curriculum programmer to get a *metadisciplinary* analysis on the scientific didactic topics. It supplies an *aerial perspective* on the curriculum, which can bring about some reflection on the Kuhnian *normal science-normal science education* loop. On the other hand, is such a historical study of any use for university chemistry students? This question is actually one of the hottest topics in science education (Hodson, 1988; Kragh, 1992; Duschl, 1994; Matthews, 1994; Moore, 1998; Niaz & Rodríguez, 2000). The general position is clearly for the introduction of history in science education, and even some consensus can be found on not including it as a distinct subject (Bevilacqua & Bordoni, 1998; Matthews, 1998; Niaz & Rodríguez 2001). The main argument of these authors, following most contemporary thinkers, is that the sciences are historical *in nature*, thus ignoring this historical skeleton leads to the teaching of an essentially incomplete model. A non historical science teaching is a mutilated one. And as history should be part of the teaching of every science, in an ideal scenario where this science education program were the norm, there would be no need of any specific subject on history of sciences.

This line of reasoning has a very solid internal logic, and we agree with it in many points, but we find it has important weaknesses. First, our *educational world* is not an ideal one, and in practice, including history as a structural part of any scientific subject is not at all

a common approach nowadays. Reforming the science syllabuses to integrate history within them is, at best, a long term project. There is no doubt that it is much more feasible, at least in the short or middle term, to include an *ad hoc* course on science history besides the traditional (non-historical) scientific subjects. If history cannot be introduced *inside* academic subjects, it can perhaps be supplied from outside them. This argument, together with our vision of history of science as a *metadisciplinary reflection* does imply a general program for the teaching of such a subject within a scientific curriculum: *the goal of a subject of history of science must not be the acquisition of some historical contents, but the development through them of a critical vision of the relations between the rest of the scientific subjects of the curriculum, in particular, between Physics and chemistry. History of science must be more a* procedural *subject than a* conceptual *one.*

A second argument for scepticism towards the teaching of history *inside* the scientific subjects is related to the origin of the science taught in academic settings. Chevallard (1985) has pointed out that the contents included in scientific education are essentially different from those resulting from scientific research. His point is that there is a process of *didactic transposition* from the "wise knowledge" (*savoir savant*) of the scientific practice to the "taught knowledge" (*savoir enseigné*) of science education. This process is seen as a natural consequence of the system of formal education, which creates its own epistemological and cultural referents (curricula, syllabuses, textbooks, classroom discourse and interaction, exams, etc.) to which scientific knowledge is reduced by the *didactic transposition.* Astolfi and Develay (1989) have elaborated this line of thought, presenting an analysis of the changes experienced by scientific knowledge when translated into the educational context. According to them, the passing from a "wise knowledge" to a "taught knowledge" is a complex process which implies the decontextualisation, depersonalisation, desyncretisation, programming (i.e. the adaptation into a didactic program), reformulation, dogmatisation, and operationalisation of the scientific discourse. In other words, school (or college) science is a processed product, with its own distinctive features, and with relations with *proper science* which are far from being obvious. Science education, if a mirror of science, is a distorting one. By including history into the scientific subjects what we get is a new didactic transposition process. The resulting subject is another idiosyncratic cultural artefact which does not have to be closer to the proper sciences than a non-historical approach. It is more correct to say that they both are related to the proper science in different ways. Under this perspective, Bevilacqua and Bordoni's (1998) statement: "[…] teaching physics and the history of physics are fellow subjects. We are not interested in adding the history of physics to teaching physics, as an optional subject: the history of physics is 'inside' physics" (p. 451) seems to us rather unsatisfactory. The amount of history 'inside' any academic subject would depend on the way it has been *transposed*. It is very much under the control of the instances in charge of designing and putting into practice the curriculum.

There is another powerful argument for our vision of history as a part of the scientific curriculum. History of science is a science itself. History of science, as any other *history*, is not a collection of past facts, but a theoretical interpretation of them. When one speaks about including history within scientific courses, is it implied that the (very complex) issue of the nature and methodology of historical inquiry must be treated?; that the historical research on the evolution of the scientific contents is to be revised? Or rather, is one usually talking of presenting historical events as well established facts to illuminate some scientific issues? This latter approach is equivalent to presenting history as a mere collection of facts. Thus to get rid of a stiff vision of science education as a mere transmission of data, such a vision is proposed for the history of the sciences. Such an approach does lend some *narrative character* to the scientific disciplines, so that their contents are presented in a rich context,

definitely more inviting than the *cold* usual presentations. This can be useful as a didactic methodology, but it is only superficially historical. On the other hand, it can be argued that it is at least theoretically possible to convey a rigorous overview of history inside a course of science. But we think there is a fundamental problem which interferes this objective. History, by definition, has an linear chronological structure, a structure which cannot be washed out without essentially damaging its foundations. Thus, a proper treatment of history *inside* the scientific subject implies the introduction of a chronological sequencing in the science course. Such a radical reformulation of science syllabuses must be based on solid grounds, and, according to our previous arguments, we do not think it is the case nowadays. From this point of view, it seems much more satisfying, at least at the university level, a specific subject on history of science (or even, on *history and philosophy of science*).

To sum up, our position is that history can be used as a *metadisciplinary* approach that could act as a bridge between FMT and quantum approaches. But to transcend the different disciplinary trends which inform chemistry university curricula, history cannot be included within a particular subject. In other words, we are for the explicit inclusion of a history of chemistry as a subject on its own within the university curriculum, as a bridge between FMT and quantum approaches.

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REFERENCES

Astolfi, J.-P. & Develay, M. (1989). *La didactique des sciences*. Paris: Seuil.

Bent, H. A. (1984). Should orbitals be X-rated in beginning chemistry courses? *Journal of Chemical Education, 61,* 421-423.

Berry, K. O. (1986). What should we teach them in high school? *Journal of Chemical Education, 63*, 697-698.

Bevilacqua, F. & Bordoni, S. (1998). New contents for new media: Pavia project physics. *Science and Education, 7*, 451-469.

Brock, W. H. (1992). *The Fontana history of chemistry*. London: Fontana Press.

Chevallard, Y. (1985). *La transposition didactique. Du savoir savant au savoir enseigné*. Grenoble: La Pensee Sauvage.

Cros, D., Amouroux, R., Chastrette, M., Fayol, M., Leber, J., & Maurin, M. (1986). Conceptions of first year university students of the constitution of matter and the notions of acids and bases. *European Journal of Science Education, 8*, 305-313.

Dresselhaus, M. S., Dresselhaus, G., & Eklund, P. C. (1996). *Science of fullerenes*. San Diego: Academic Press.

Duschl, R. A. (1994). Research on the history and philosophy of science. In D. L. Gabel (ed.), *Handbook of research on science teaching,* Macmillan, pp. 443-465. New York.

Euler, M., Hanselmann, M., MÜller, A., & Zollman, D. (1999). Student's views of models and concepts in modern physics. In *Annual Meeting National Association for Research in Science Teaching*, 1999, Boston. Collection of papers presented. [http://www.phys.ksu.edu/perg/papers/narst]

Fletchner, P. & Johnston, I. (1999). Quantum mechanics: Exploring conceptual change. In *Annual Meeting National Association for Research in Science Teaching*, 1999, Boston. Collection of papers presented. [http://www.phys.ksu.edu/perg/papers/narst]

Gillespie, R. J (1991). What is wrong with the general chemistry course? *Journal of Chemical Education, 68*, 192-194.

Gillespie, R. J., Spencer, J. N., & Moog, R. S. (1996). Bonding and molecular geometry without orbitals - The electron domain model. *Journal of Chemical Education, 73*, 622-627.

Greca, I. M. & Herscovitz, V. E. (2002). Construyendo significados en la mecánica cuántica: Fundamentación y resultados de una propuesta innovadora para su introducción en el nivel universitario. *Enseñanza de las Ciencias*, *20*, 327-338.

Hansen, P. J. & Jurs, P. C. (1988). Chemical applications of graph theory. Part I. Fundamentals and topological indices. *Journal Chemical Education, 65*, 574-580.

Hansen, P. J. & Jurs, P. C. (1988). Chemical applications of graph theory. Part II. Isomer enumeration. *Journal Chemical Education, 65*, 661-667.

Harrison, A. G. & Treagust, D. F. (2000). Learning about atoms, molecules and chemical bonds: A case study of multiple-model use in grade 11 chemistry. *Science Education*, *84*, 352-381.

Hawkes, S. J. (1992). Why should they know that? *Journal of Chemical Education*, *69*, 178-181.

Heitler, W. & London, F. (1927). Wechselwirkung neutraler Atome und homöpolare Bindung nach der Quantenmechanik. *Zeitschrift für Physik, 44*, 455-472.

Henessy, S. (1993). Situated cognition and cognitive apprenticeship: implications for classroom learning. *Studies in Science Education*, *22*, 1-41.

Hobson, A. (1996) Teaching quantum theory in the introductory course. *The Physics Teacher*, *31*, 202-210.

Hodson, D. (1988). Towards a philosophically more valid science curriculum. *Science Education, 72*, 19-40.

Holton, G. (1952). *Introduction to concepts and theories in physical sciences*. Reading (Mass): Addison-Wesley.

Johnston, I. D., Crawford, K., & Fletcher, P. R. (1998). Students difficulties in learning quantum mechanics. *International Journal of Science Education*, *20*, 427-446.

Kragh, H. (1992). A sense of history: History of science and the teaching of introductory quantum theory. *Science & Education*, *1*, 349-363.

Kroto, H. W., Heath, J. R., Obrien, S. C., Curl, R. F., & Smalley, R. E. (1985). C60: Buckminsterfullerene. *Nature, 318*, 162-163.

Lewis, G. N. (1916). The atom and the molecule. *Journal of the American Chemical Society*, *38*, 762-788.

Lewis, G. N. (1923). *Valence and the structure of atoms and molecules*. New York: The Chemical Catalogue Company.

Matthews, M. R. (1994). *Science teaching: The role of history and philosophy of science*. New York: Routledge.

Matthews, M. R. (1998). In defense of modest goals when teaching about the nature of science. *Journal of Research in Science Teaching*, *35*, 161-174.

Moore, J. W. (1998). Editorial: History, chemistry, and a longer view. *Journal of Chemical Education*, *75*, 1199.

Morwick, J. J. (1979). Should orbitals be taught in high school? *Journal of Chemical Education, 56*, 262-263.

Niaz, M. & Rodríguez, M. A. (2000). Teaching chemistry as rhetoric of conclusions or heuristic principles – A history and philosophy of science perspective. *Chemistry Education: Research and Practice in Europe, 1*, 315-322. [http://www.uoi.gr/cerp]

Niaz, M. & Rodríguez, M. A. (2001). Do we have to introduce history and philosophy of science or is it already 'inside' chemistry? *Chemistry Education: Research and Practice in Europe, 2*, 159-164. [http://www.uoi.gr/cerp]

Ogilvie, J. F. (1990). The nature of the chemical bond – 1990. *Journal of Chemical Education, 67*, 280-289.

Pauling, L. (1931b). The nature of the chemical bond. Application of results obtained from the quantum mechanics and from a theory of paramagnetic susceptibility to the structure of molecules. *Journal of the American Chemical Society, 53*, 1367-1400.

Pauling, L. (1931a). Quantum mechanics and the chemical bond. *Physical Review, 37*, 1185-1186.

Pauling, L. (1931c). The nature of the chemical bond II: The one-electron and three-electron bond. *Journal of the American Chemical Society, 53*, 3225-3237.

Pauling, L. (1932a). The nature of the chemical bond III. The transition from one extreme bond type to another. *Journal of the American Chemical Society, 54*, 988-1003.

Pauling, L. (1932b). The nature of the chemical bond IV. The energy of single bonds and the relative electronegativity of atoms. *Journal of the American Chemical Society, 54*, 3570-3582.

Pauling, L. (1939). *The nature of the chemical bond and the structure of molecules and crystals. An introduction to modern structural chemistry*. Ithaca, New York: Cornell University Press.

Pauling, L. & Sherman, J. (1933a). The nature of the chemical bond. VI. The calculation of thermochemical data of the energy of resonance of molecules among several electronic structures. *Journal of Chemical Physics, 1,* 606-617.

Pauling, L. & Sherman, J. (1933b). The nature of the chemical bond. VII. The calculation of resonance energy in conjugated systems. *Journal of Chemical Physics, 1,* 679-686.

Pauling, L. & Wheland, G.W. (1933). The nature of the chemical bond. V. The quantum-mechanical calculation of the resonance energy of benzene and naphthalene and the hydrocarbon free radicals. *Journal of Chemical Physics, 1,* 362-374. Errata: *Journal of Chemical Physics,* **1934**, *2*, 482.

Petri, J. & Niedderer, H. (1998). A learning pathway in high-school level quantum atomic physics. *International Journal of Science Education*, *20*, 1075-1088.

Primas, H. (1981). *Chemistry, quantum mechanics and reductionism.* New York: Springer Verlag.

Purser, G. H. (1999). Lewis structures are models for predicting molecular structure, *not* electronic structure. *Journal of Chemical Education*, *76*, 1013-1018.

Ramsey, J. L. (1997a) Molecular shape, reduction, explanation and approximate concepts. *Synthese, 111*, 233-251.

Ramsey, J. L. (1997b). A philosopher's perspective on the "problem" of molecular shape. In J. L. Calais & E. Kryachko (eds.), *Conceptual perspectives in quantum chemistry*, pp. 319-336. Dordrecht: Kluwer.

Rebello, N. S. *&* Zollman, D. (1999). Conceptual understanding of quantum mechanics after using hands on experiments and visualization instructional materials. Paper presented at *Annual Meeting of the National Association for Research in Science Teaching*. Boston. Collection of papers presented. [http://www.phys.ksu.edu/perg/papers/narst]

Rodríguez, M. A. & Niaz, M. (2002). How in spite of the rethoric, history of chemistry has been ignored in presenting atomic structure in textbooks. *Science & Education*, *11*, 423-441.

Sambursky, S. (1956). *The physical world of the Greeks*. London: Routledge and Kegan.

Sánchez Gómez, P. J. (2002). Un modelo pragmático de la comunicación escrita en el aula de ciencias. *Enseñanza de las Ciencias*, in press.

Sánchez Gómez, P. J., Cervelló, J., & Martín, M. (2001) Una síntesis entre los enfoques cuantitativo y cualitativo en el estudio de materiales escritos: La codificación en red, en: *Retos de la enseñanza de las ciencias en el siglo XXI. Actas del VI Congreso Internacional sobre Investigación en la Didáctica de las Ciencias, pp. 235-236.* Barcelona.

Sánchez Gómez, P. J., Morcillo, J. G., Martín, M., & Silván, E. (2002) Análisis estructural del contenido de textos de alumnos universitarios sobre estructura atómica, en: *Relación Secundaria Universidad. Actas de los XX Encuentros de Didáctica de las Ciencias Experimentales, pp. 455-463*. La Laguna.

Scerri, E. R. (2001). The new philosophy of chemistry and its relevance to chemical education. *Chemistry Education: Research and Practice in Europe*, *2*, 165-170. [http://www.uoi.gr/cerp]

Schummer, J. (1998) The conceptual core of chemistry. A conceptual approach**.** *HYLE -International Journal for Philosophy of Chemistry*, *4*, 129-162.

Shiland, T. W. (1995). What's the use of all this theory? – The role of quantum mechanics in high school chemistry textbooks. *Journal of Chemical Education, 72*, 215-219.

Shiland, T. W. (1997). Quantum mechanics and conceptual change in high schools chemistry textbooks. *Journal of Research in Science Teaching, 34*, 535-545.

Solomon, J. (1993). *Getting to know about energy in school and society.* London: Falmer Press.

Taber, K. S. (1997). Understanding chemical bonding – The development of A level students' understanding of the concept of chemical bonding (Ph.D. thesis). University of Surrey.

Taber, K. S. (1998). The sharing-out of nuclear attraction: or I can't think about Physics in Chemistry. *International Journal of Science Education*, *20*, 1001-1014.

Taber, K. S. (2001). Building the structural concepts of chemistry: Some considerations from the educational research. *Chemistry Education: Research and Practice in Europe*, *2*, 123-158. [http://www.uoi.gr/cerp]

Taber, K. S. (2002). Conceptualizing quanta: Illuminating the ground state of student understanding of atomic orbitals. *Chemistry Education: Research and Practice in Europe*, *3*, 145-158. [http://www.uoi.gr/cerp]

Tsaparlis, G. (1997). Atomic orbitals, molecular orbitals and related concepts: Conceptual difficulties among chemistry students. *Research in Science Education*, *27*, 271-287.

Tsaparlis, G. (2001). Towards a meaningful introduction to the Schrodinger equation through historical and heuristic approaches. *Chemistry Education: Research and Practice in Europe*, *2*, 203-213. [http://www.uoi.gr/cerp]

Tsaparlis, G. & Papaphotis, G. (2002). Quantum-chemical concepts: Are they suitable for secondary students? *Chemistry Education: Research and Practice in Europe*, *3*, 129-144. [http://www.uoi.gr/cerp]

Weininger, S. J. (1984). The molecular structure conundrum: Can classical chemistry be reduced to quantum chemistry? *Journal of Chemical Education*, *61*, 939-944.

Woolley, R. G. (1985). The molecular structure conundrum. *Journal of Chemical Education*, *62,* 1082-1084.