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Historical Teaching of Atomic and Molecular Structure

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Historical Teaching of Atomic and Molecular Structure

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Abstract

Besides the presentation and conclusions, the chapter is divided into two equally important sections. The first one describes the modern development of atomic and molecular structure, emphasizing some of the philosophical problems that have been taken, and those that have to be faced in its understanding. The second discusses the alternative conceptions and difficulties of students of different educational levels, and also the different approaches to its historical or philosophical teaching. Finally, we recognize the necessity for science teachers to assume a specific historical-philosophical position.

1 General Introduction

"I can safely say that nobody understands quantum mechanics"
R. Feyman (1985, p. 129)

The purpose of this paper is to argue that history and philosophy of chemistry and physics are central strategies in the teaching of atomic and molecular structure, from the Dalton model (for an earlier approach see Chalmers 1998) to modern Quantum Mechanics and Quantum Chemistry. Therefore, in addition to the presentation and conclusions, the chapter is divided into two equally important sections. The first describes the modern development of atomic and molecular structure, emphasizing some of the philosophical problems that have confronted and been addressed by scientists, and those that have to be faced in understanding the science. The second discusses the alternative conceptions and difficulties that students of different educational levels bring to this subject, and also the different approaches to the teaching of its history and/or philosophy. The conclusion is that a balance between the theoretical physico-chemical basis of this chemistry knowledge and the phenomenological-empiricist knowledge must be achieved. But this cannot be done properly if teachers do not know and/or assume a particular historical-philosophical position.

Science education practice has not been driven to any great extent by research findings or by a goal of accomplishing professional ideals. The changes that have occurred in the majority of textbooks during the past decades do not show any real recognition of the growth in scientific knowledge (Schummer 1999). This is partly because of a chemistry teaching revolution fifty years ago (in the context of a revolution in the whole of science education: one which resulted from the Soviet success in launching Sputnik 1 in 1957). Under a philosophical (but hidden) umbrella, the change placed an emphasis on the physicochemical basis of General Chemistry in

the three main projects of that decade: Chemical Bond Approach (Stern 1962), Chem Study (Campbell 1962), and Nuffield Foundation (1967).

The proposal was that the hegemony of physical chemistry would provide a basis of understanding for students' introduction to the chemical sciences through the quantum chemistry basis of the chemical bond, the kinetic model of the particulate nature of matter and the dominance of thermodynamics for explanations in several areas of chemistry. A new laboratory learning that promoted the notion of exploratory play with apparatus accompanied it. The General Chemistry course turned towards a theoretical character, losing the phenomenological approach that it had had in the preceding years. Without a deep recognition of its historical and philosophical roots, many people were led by this approach to believe that the contents of science textbooks were, in fact, science. But this is not necessarily true. The written materials employed in science education are descriptions of past science explorations (Yager 2004). Besides all this, once the majority of science teachers all over the world use textbooks as the main (sometimes the only) source of information ―and the contents of the books have to expand in an idealized attempt to cope with the increase in information, with direct references to the history of sciences disappearing― they become, paradoxically and without wanting to... history teachers! However, even if it was unconscious, it was a bad or a wrong way to teach the history of science. For example, Rodriguez and Niaz (2004) examined numerous textbooks for the History and Philosophy of Science (HPS) content in their approach to teaching atomic structure, and they found that an adequate and accurate reflection of the historical development is rarely presented. This is educationally significant because philosophers of science and science education researchers have argued that quantum mechanics is particularly difficult to understand, due to the intrinsic obscurity of the topic, and the controversial nature of its different interpretations [e.g. Copenhagen School «indeterminacy» (Bohr, Pauli, Heisenberg, Born, von Neumann and Dirac among others), Schrodinger with his cat paradox, the stochastic and the many worlds interpretations, and Bohm's «hidden variables» (Garritz, 2012 online)].

2 The Subject Matter

2.1 Introduction

In this section a brief summary of several of the most important scientific advances of atomic and molecular structure, related mainly with chemistry but with a physicochemical character, will be presented. The starting point is Dalton's model of the atom, and the whole nineteenth century atomic controversy. At the end of that century the "discovery" by J. J. Thomson of negative corpuscles initiated the appearance of models of structure within the atom, such as that of J. J. Thomson with Lord Kelvin. The nuclear model of Rutherford was followed by Bohr's model of stationary orbits, which applied the energy quantization hypothesis of M. Planck, which, in turn, started the old quantum theory in 1900. Then, A. Einstein as an explanation for the photoelectric effect recognized the wave-corpuscular duality of light. All this old quantum theory was replaced by E. Schrödinger and W. Heisenberg's wave and matrix mechanics, respectively, following on from the pilot wave hypothesis of L. de Broglie, and after that chemical bonding was interpreted in the same terms of quantum mechanics.

On this issue it is important to note that in 2008 the American Chemical Society held a symposium entitled "200 Years of Atoms in Chemistry: From Dalton's Atoms to Nanotechnology" which was followed, a couple of years later, with the publication of a book

with a similar name. For a quick view of the topic that is addressed here, some of its chapters with comments from the editor are shown in Table 1.

Table 1. Some chapters of the book by C. J. Giunta (2010).

Author	**Chapter name**	**Comments**
W. B. Jensen	Four Centuries of Atomic Theory. An Overview	A description of the dominant flavour of atomic notions over the last four centuries from the mechanical through the dynamical, gravimetric, and kinetic, to the electrical.
L. May	Atomism before Dalton	Outlines a variety of atomistic ideas from around the world. It concentrates on conceptions of matter that are more philosophical or religious than scientific.
D. E. Lewis	150 years of Organic Structures	Fifty years after Dalton, F. A. Kekulé and A. S. Couper independently published representations of organic compounds that rationalize their chemistry and even facilitated the prediction of new compounds.
W. H. Brock	The Atomic Debates Revisited	A description of episodes from the second half of the 19th century in which chemists debated the truth of atomic theory. Doubts about the physical reality of atoms led chemists to question the soundness of chemical atomism
C. J. Giunta	Atoms are Divisible. The Pieces have Pieces	Evidence for the divisibility continued and impermanence of atoms was collected even while some chemists and physicists continued to doubt their very existence
G. Patterson	Eyes to see: Physical Evidence for Atoms	By the early decades of the 20th century, through the efforts of J. Perrin and others, skepticism over the physical existence of atoms was practically eliminated

2.2 Dalton's Model. 19th Century Controversies between Physicists and Chemists

Dalton's atomic model with associated relative atomic weights was constructed in 1805 to explain results on the absorption of gases into water (Chamizo 1992; Viana & Porto 2010). Since then, in the nineteenth and early twentieth centuries several famous debates took place between atomists and anti-atomists (including some Nobel Prize winners). The early contributions of scientists from several European countries as Berzelius, Gay-Lussac, and Avogadro to the acceptance of this model were not enough to convince all chemists or physicists (Giunta 2010; Nash 1957). For example, Bensaude-Vincent indicates:

> It is well-known that French chemists were reluctant to adopt the atomic theory in the nineteenth century. Their opposition was long-standing and tenacious since the atomic hypothesis formulated in the first decade of the nineteenth century by John Dalton was

> banished from the teaching of chemistry until the early decades of the twentieth century. Instead of atomism, the French chemists preferred the Richter's language of equivalents because it avoided commitment to a speculative theory of indivisible elementary particles …[…]…There is a general agreement among historians of chemistry that this national feature was due to the overarching influence of positivism in France (Bensaude-Vincent 1998, p. 81).

Following the Karlsruhe's Congress in 1861 (Kauffman 2010) most of the chemical community accepted the distinction between atoms and molecules with their respective atomic and molecular weights, as admirably shown by S. Cannizzaro. In general, atoms were regarded by physicists as inelastic or inertial points or particles. Meanwhile chemists accepted Dalton's model:

> A group of physicists, among them Ernst Mach, John Bernhard Stallo and Pierre Duhem began to voice doubts about physical atomism because the kinetic theory did not dovetail with accurate experimentation. …The consilience between chemistry and physics had broken down. Mach, in particular, believed science to be a construct of the human mind and that it was not possible to find independent evidence for the existence of matter. Influenced by the thoughts of Georg Helm in 1887, Ostwald began to deny atomism explicitly. He opted instead for energetics –the laws of thermodynamics– rather than mechanical explanations in chemistry. He argued that energy was more fundamental than matter, which he saw only as another manifestation of energy. It followed that chemical events were best analyzed as a series of energy transactions. The difference between one substance and another, including one element and another, was due to their specific energies (Jensen 2010, p.63).

A century had to pass before the atomic model was fully accepted, which can be marked by formal recognition of J. B. Perrin's researches at the Solvay Conference of 1911 (Giunta 2010; Izquierdo 2009; 2010).

2.3 The Electron and Thomson's Atom Model

There was a controversy about the nature of cathode rays (German physicists supported the ether theory for their origin, while the British argued for their particle nature), but it was the discovery of X-rays in 1895 that triggered J. J. Thomson's interest in cathode rays. He conducted a series of experiments at the beginning of 1897, which were first presented at a Friday evening discourse of the Royal Institution on April 29, 1897, and were finally published at length in the *Philosophical Magazine* in October the same year.

Thomson points out a fundamental aspect of his experiments; namely, that cathode rays are the same whatever the gas through which the discharge passes, and concludes: "[cathode rays] are charges of negative electricity carried by particles of matter. The question that arises next is: what are these particles? Are they atoms, or molecules, or matter in a still finer state of subdivision?" (p. 302). That is why he determined the relation *m/e*. From which Thomson concluded that its value, 10^{-12} kg/C, is independent of the nature of the gas, and it's very small compared with the 10^{-8} kg/C of H^+, the hydrogen ion in electrolysis, which is the smallest value of this quantity previously known.

Thomson goes further and proposes an atomic model:

> Since corpuscles similar in all respects may be obtained from different agents and materials, and since the mass of the corpuscles is less than that of any known atom, we see that the corpuscle must be a constituent of the atom of many different substances (p. 90)… […]… The corpuscle, however, carries a definite charge of negative electricity, and since with any

> charge of negative electricity we always associate an equal charge of the opposite kind, we should expect the negative charge of the corpuscle to be associated with an equal positive charge of the other…we shall suppose that the volume over which the positive electricity is spread is very much larger than the volume of the corpuscle (Thomson 1904, p. 93).

This model would last until Geiger and Marsden's experiment of bombarding metal thin films with radioactive particles, which allowed E. Rutherford to postulate the existence of the nucleus. On this subject we should mention the book *Histories of the electron* that arose from two meetings (one in London and the other in Cambridge, Massachusetts) held to celebrate, in 1997, the centenary of the electron's discovery. The book is divided into the following four main sections that recognize the breadth of the subject being treated, and particularly the relations among the various sciences, and with technology and philosophy:

- Corpuscles and electrons
- What was the newborn electron good for?
- Electrons applied and appropriated
- Philosophical electrons.

Some of its chapters with comments from the editors are shown in Table 2.

Table 2. Some chapters of the book by Buchwald and Warwick (2001).

Author (s)	**Chapter name**	**Comments**
I. Falconer	Corpuscles to electrons	Thomson's main accomplishment at the Cavendish Laboratory in the mid-1890s was to succeed in deflecting a beam of cathode rays electrostatically; something that continental experimenters had failed to do
H. Kragh	The electron, the protyle, and the unity of matter	Identifies four different kinds of electrons before 1900: the electrochemical, the electrodynamic, the one associated with cathode-ray work, and the magneto-optical. The underlying notion of the electron as a fundamental building block of matter appealed particularly to J. J. Thomson and several others, who often thought of the electron as a sort of chemical proto-substance
W. Kaiser	Electro Gas Theory of Metals: Free Electrons in Bulk Matter	By early 1900, metallic conduction had become a central feature of a burgeoning microphysical practice, one that in this case sought to unify electrodynamics of electric sources in metals, with the model of colliding particles that underlie the kinetic theory of gases
L. Hoddeson and M. Riordan	The electron, the hole and the transistor	The use of the electron in the design of amplifiers and semiconductors not only produced the new discipline of electronics but eventually enabled the very absence of the

		electron in certain material structures to be reified as a new entity in its own right, the "hole"
M.J.Nye	Remodeling a Classic: The electron in organic chemistry	In the broader historical picture, the arrival of the electron and quantum physics in chemistry was seen as fulfilling the expectations of men like Lavoisier and Dalton who were understood to have been the driving forces of the first chemical revolution
K. Gavroglu	The physicists' electron and its appropriation by the chemist	Where physics sought a single theory that, in principle, was analytically exact in all cases, chemistry, a primarily laboratory-based science, sought one or more models that were applicable to a wide range of empirical data
P. Achinstein	Who did really discover the electron?	The historical facts about who knew what and when are complex
M. Morrison	History and metaphysics: on the reality of spin	The reality ascribed to entities is often the result of their evolution in a theoretical history. The history of belief intersects with the evolution of theoretical trajectories
N. Rasmussen and A. Chalmers	The role of theory in the use of instruments; or, how much do we need to know about electrons to do science with an electron microscope?	The effective use of an instrument does not necessarily depend in any meaningful way on theories about the way in which the device functions. The electron microscope was fruitfully used in discovering the biological cell´s endoplasmic reticulum without a theory of how it interacted with the object.

2.4 Planck, Einstein and Bohr: The Old Quantum Theory

The centennial of quantum theory has been celebrated a few years ago (Kleppner & Jackiw 2000). Quantum mechanics forced physicists and chemists to reshape their ideas of reality, to rethink the nature of things at the deepest level, and to revise their concepts of determinacy vs. indeterminacy, as well as their notions of cause and effect.

The clue that triggered the quantum revolution came not from studies of matter but from a problem in radiation. The specific challenge was to understand the spectrum of light emitted by black bodies (that absorb and emit all kinds of electromagnetic radiation). In M. Planck's seminal paper (1900) on thermal radiation, it was hypothesized that the total energy of a vibrating system cannot be changed continuously. Instead, the energy must jump from one value to another in discrete steps, or quanta, of energy. The idea of energy quanta was so radical that Planck let it lie fallow. A. Einstein (1906), then unable to obtain an academic position, wrote from the Swiss patent office in Berne: "Analyzed in classical terms Planck's black-body model could lead only to the Rayleigh-Jeans law". Kuhn (1978, p. 170) also made a contribution to this Planck-Einstein debate by saying that "Planck's radiation law could be derived instead, but only by decisively altering the concepts its author had employed for that purpose". Midway through his paper Einstein wrote:

> We must therefore recognize the following position as fundamental to the Planck theory of radiation: […]. During absorption and emission the energy of a resonator changes discontinuously by an integral multiple of $h\nu$.[1]

Delighted as every physicist must be that Planck in so fortunate a manner disregarded the need [for such justification], it would be out of place to forget that Planck's radiation law is incompatible with the theoretical foundations which provide his point of departure (Einstein 1909, p. 186).

More recently, in 1913, N. Bohr applied the quantization to the angular momentum of the hydrogen atom and obtained the whole set of J. R. Rydberg's spectral frequencies. Even then the concept was so bizarre that there was little basis for progress with this "old quantum theory". Almost fifteen more years and a fresh generation of physicists were required to create modern quantum theory. For an interesting and detailed description of the historical details of all quantum discoveries, Baggott (2011) can be consulted.

2.5 De Broglie, Heisenberg and Schrödinger. Quantum Mechanics

In 1923, L. de Broglie tried to expand Bohr's ideas, and he pushed for their application beyond the hydrogen atom. In fact he looked for an equation that could explain the wavelength characteristics of all matter. His equation, $\lambda=h/p$, in relation to the wavelength of particles was experimentally confirmed in 1927 when physicists L. Germer and C. Davisson fired electrons at a crystalline nickel target and the resulting diffraction pattern was found to match the predicted value of λ. Also G. P. Thomson ― son of Joseph John, the discoverer of the electron―, corroborated the de Broglie's wavelength of electrons going through very thin films of metals. Whereas his father had seen the electron as a corpuscle (and won the Nobel Prize in the process), he demonstrated that it could be diffracted like a wave. That is why it is said that Thomson's family contributed to the wave-particle duality of the electron by occupying the lead positions on both sides.

A second pillar of the development of quantum mechanics was W. Heisenberg, who re-invented matrix multiplication in June 1925 with his "matrix mechanics" as was confirmed by M. Born and P. Jordan after revising his work. On May 1926, Heisenberg began his appointment as a university lecturer in Göttingen and with an assistantship to Bohr in Copenhagen. Heisenberg formulated the uncertainty principle in February 1927 while employed as a lecturer in Bohr's Institute for Theoretical Physics at the University of Copenhagen. He was awarded the 1932 Nobel Prize in Physics. In Bohr's words, the wave and particle pictures, or the visual and causal representations, are "complementary" to each other. That is, they are mutually exclusive, yet jointly essential for a complete description of quantum events.

Next year the Nobel Prize was awarded to P. A. M. Dirac and E. Schrödinger. The great discovery of the latter, in January 1926, was published in *Annalen der Physik* as "Quantisierung als Eigenwertproblem" [Quantization as an Eigenvalue Problem]. It was known as "wave mechanics" and later as Schrödinger's wave equation. This paper has been universally celebrated as one of the most important achievements of the twentieth century, and created a revolution in quantum mechanics, and indeed of all physics and chemistry. On May that year Schrödinger

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[1] In German he says "Die Energie eines Resonators ändert sich durch Absorption und Emision sprungweise, und zwar ein ganzzahliges Vielfache von $(R/N)\beta\nu$" (Einstein, 1906, p.202).

published his third article, in which he showed the equivalence of his approach to that of Heisenberg's matrix formulation.

2.6 Kossel, Lewis and Langmuir; Heitler-London-Slater and Pauling; Hund and Mulliken: Quantum Chemistry and Bonding Models.

During World War I, in 1916, W. Kossel and G. N. Lewis (Lewis 1923) began independently to develop electronic models of chemical bonding, a concept fruitfully extended shortly thereafter by I. Langmuir. In the new models, the second and third periods of the periodic table each have eight members, the last of which (a noble gas) has a stable nonbonding "octet" of electrons in a shell. Beyond the octet shells are the odd electrons in the outer shell, the "valence electrons", which can be shared with adjacent atoms to form chemical bonds.

Langmuir expresses his view that the type of approach used by chemists is substantially different to that used by physicists:

> The problem of the structure of atoms has been attacked mainly by physicists who have given little consideration to the chemical properties, which must ultimately be explained by a theory of atomic structure. The vast store of knowledge of chemical properties and relationships, such as is summarized in the periodic table, should serve as a better foundation for a theory of atomic structure than the relatively meager experimental data along purely physical lines" (Langmuir 1919, p. 868).

In the late 1920s and early 1930s, W. Heitler, F. London, J. C. Slater and L. Pauling, developed the "valence-bond theory" as an application of the new quantum mechanics of E. Schrödinger and W. Heisenberg. Almost at the same time, R. Mulliken developed an alternative theory that began not from the electrons in atoms but from the molecular structure ("molecular orbital" bonding). Partly because the extensive and vitally useful role of mathematics in physics had never been transferred to chemistry, it took until 1940 for Pauling and Mulliken theories to gain wide acceptance. The Nobel committee delayed twenty and thirty years respectively to honour this revolution. Pauling became laureate in 1954 and Mulliken won it in 1966 (Feldman 2001).

P. Atkins has recently presented his latest edition of the book on Quantum Chemistry with De Paula and Friedman (2008) as co-authors, where they review the latest improvements in making calculations. For example, they write on *ab initio* methods, configuration interaction, and many body perturbation theories, that were developed with the advent of high-speed computers in the 1950s. They proceed to density functional theory and its beginnings with Hohenberg and Kohn (1964) theorems and Kohn and Sham (1965) equations. Kohn was awarded the Nobel Prize for Chemistry in 1998. They then discuss a method for approximation of exchange (proposed by Slater in 1951; a simplification that became known as the Xα method), and of correlation energies, introduced in the sixties and seventies. Their final section examines current achievements, including the impact of quantum chemistry methods on nanoscience (the structure of nanoparticles) and medicine (molecular recognition and drug design).

2.7 Molecular and Crystal Symmetry and Spectroscopy

Spectroscopy is the study of the interaction of electromagnetic radiation with matter. In 1860 the German scientists R. Bunsen and G. Kirchhoff discovered two alkali elements, rubidium and cesium, with the aid of the spectroscope they had invented the year before. Since then spectral analysis has been a central tool in chemistry, physics, and astronomy. But it is not only spherical

atoms that interact with light; molecules can also do it. Molecules may interact with the oscillating electric and magnetic fields of light and absorb the energy carried by them. The more symmetric the molecule, the fewer different energy levels it has, and the greater the degeneracy of those levels. The study of symmetry helps us to simplify problems by reducing the number of energy levels one must deal with. But more than that, symmetry helps us decide which transitions between energy levels are possible and which are not (Harris & Bertolucci 1978) through selection rules, addressing problems that were possible to pose and solve via a branch of mathematics named group theory.

The history of group theory and that of quantum mechanics can be of great assistance in understanding the applications of spectroscopy to physical problems. Nobel laureate P. W. Anderson (1972, p. 394) wrote "it is only slightly overstating the case to say that physics is the study of symmetry". While quantum theory can be traced back only as far as 1900, the origin of the theory of groups is much earlier. It was given definite form in the later part of the eighteenth and in the nineteenth centuries. F. Klein —a German mathematician, known for his work in group theory, function theory, non-Euclidean geometry, and on the connections between geometry and group theory— considered the group concept as most characteristic of nineteenth century mathematics.

The concept of a group is considered to have been introduced by E. Galois (1811-1832). Galois refashioned the whole of mathematics and founded the field of group theory only to die in a pointless duel over a woman before his work was published when he was 21 years old. J. Liouville published his ideas in 1846. Some aspects of group theory had been studied even earlier: in number theory by L. Euler, C.F. Gauss, and others, and in the theory of equations by A.L. Cauchy and J.L. Lagrange (each with a well-known group theory theorem).

At the heart of relativity theory, quantum mechanics, string theory, and much of modern cosmology lies one concept: symmetry. In *Why Beauty Is Truth*, world-famous mathematician I. Stewart (2007) narrates the history of this remarkable area of study. He presents a time line of discovery that begins in ancient Babylon and travels forward to today's cutting-edge theoretical physics.

The symmetry aspects are crucial today for the different models of chemical structure, of bonds, spectroscopic interpretations and chemical reactions. In many of these problems the crucial problem is that of the potential seen by electrons moving in the electric field of the nuclei. The relation between science and mathematics resides in the commutation of the Hamiltonian with the symmetry operators, so that the wave functions of the atoms, or molecules, are bases of some of the irreducible representations of the point group to which the system belongs. Many books have appeared devoted entirely to applications of symmetry and aspects of group theory to chemistry. Examples include two classical books (Bishop 1973; Cotton 1963), and one modern (Hargittai & Hargittai 2009).

2.8 The Problem of Reduction of Chemistry into Physics

One of the most deeply entrenched traditions, which could be seen as an orthodoxy that extends beyond the scientific community to the whole of society, is that science can be explained in terms of the logical positivist philosophical tradition. Since the nineteenth century logical positivism has sought to clearly establish a boundary between science and non-science using two additional criteria:

- An empirical-experimental approach (if something cannot be interpreted in terms of observations or measurements then it is not scientific, it is metaphysical).

- A criterion of logical-mathematical inference and scientific theory (one aspect is that if something cannot be rebuilt in a deductive way, it is not rational, it is unscientific).

Logical positivism assumes the axiomatization of theories unifying all sciences into one. In its most widely recognized version (Reish 2005), logical positivism, presenting science as a linear succession of successful discoveries and placing the emphasis on factual recall with confirmatory experiments, contributed to identify what kinds of research questions and issues were adequate. This programme of unification of science and deriving the principles of one science from another is commonly known as reductionism. The logical positivist assumes that the laws of a particular science, like chemistry, can in principle be derived from other more basic laws, in this case from physics. This position became stronger particularly with the development of relativistic quantum mechanics by P.A.M. Dirac. He indicated:

> The underlying laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that exact applications of these laws lead to quantum mechanical equations which are too complicated to be soluble (Dirac 1929, p. 714).

One of the most important philosophers of science of the time, working from a logical positivist perspective H. Reichenbach celebrated Dirac's claim, indicating that:

> The problem of physics and chemistry appears finally to have been resolved: today it is possible to say that chemistry is part of physics, just as much as thermodynamics or the theory of electricity (Reichenbach 1978, p. 129).

A few years later, Reichenbach distinguishes between contexts of discovery and justification, an issue that has occupied a prominent place in the philosophy of science. Since then, in its best-known version (Reish 2005), logical positivism has presented science as a linear succession of successful discoveries and has placed the emphasis on factual recall with confirmatory experiments. This contributed to identifying what kinds of research questions and issues were adequate for the axiomatic structure of science.

But in the 1960s, several science philosophers started to question the lack of historicity of logical positivism, which was based mainly in the context of justification (Reichenbach 1938). They proposed alternative ways of conceiving the philosophy of science based on historical ideas such as change, progress, or revolution (Kuhn 1969; Toulmin 1961; 1972). More recently several philosophers have also questioned other traditional assumptions of logical positivism such as reductionism and verificationism (Hacking 1983; Harré 2004; Laudan 1997; Popper 1969). This indicates that the philosophy of science has escaped the constraints imposed by the context of justification without losing sight of the question of rationality. New and different ways of approaching the philosophy of science have emerged, for example M. and J. Christie (2000) make a case for the diverse character of laws and theories in the sciences and particularly consider a pluralistic approach to laws and theories in chemistry. R. Giere (1999) considers that science does not need laws because: "science does not deliver to us a universal a truth underlying all natural phenomena; but it does provide models of reality possessing various degrees of scope and accuracy"(Giere 1999, p. 6).

These new and different approaches to the philosophy of science lead to reconsideration of what Dirac said. Thus the Nobel Prize in Chemistry, for his theory concerning the course of chemical reactions using quantum mechanics, R. Hoffmann indicated (1998, p. 4):

> Only the wild dreams of theoreticians of the Dirac school make nature simple.

This idea was shared by M. Gell-Man, the Physics Nobel Prize for his contributions and discoveries on the classification of elementary particles and their interactions (quarks). He said (1994):

> When Dirac remarked that his formula explained most of physics and the whole of chemistry of course he was exaggerating. In principle, a theoretical physicist using quantum electrodynamics can calculate the behaviour of any chemical system in which the detailed internal structure of atomic nuclei is not important. [But:] in order to derive chemical properties from fundamental physical theory, it is necessary, so to speak, to ask chemical questions (Gell-Man 1994, p. 109).

And some of those chemical questions, perhaps the simplest, are related to the periodic table. Much has been written about them (Jensen 2002; Scerri 2007), but it is relevant to recall what philosopher of chemistry J. van Brakel (2000) says:

> As a specific example of the reduction of chemistry to physics, it is often suggested that the periodic table can be 'derived' from quantum mechanics. Such a reduction was already ascribed to Bohr, for example, by Popper. But, contrary to his own claims (and those of Popper) 'Bohr populated the electron shells while trying to maintain agreement with the known experimental facts'. Later developments too in quantum mechanics cannot strictly predict where chemical properties recur in the periodic table. Pauli's explanation for the closing of electron shells does not explain why the periods end where they do: the closing of shells is not the same as the closing of periods in the table. Unknown electronic configurations of atoms are not derived from quantum mechanics, but obtained from spectral observations. Hund's rule states an empirical finding and cannot be derived (van Brakel 2000, p. 119).

A current periodic table shows many and various properties attached to atoms, including, for example, the size. However, the various theoretical approaches derived from quantum mechanics to calculate atomic size assume, arbitrarily, that atoms are bounded. There is no such thing as an absolute atomic size. An atom is not a rigid sphere, so "atoms differ in size depending on the type of external forces acting on them" (Cruz *et al*. 1986, p. 704). The various experimental techniques used to determine inter-nuclear distances indicate that the size of atoms depends on the surrounding environment. Therefore a periodic table can only show covalent, ionic, or metallic radii as typical outcomes from experimental measurements of many different solids.

As several researchers have discussed when addressing entanglement (Primas 1983), arising from strict quantum mechanical treatments, physical systems are never isolated nor closed. As with the size of atoms, so the geometry of molecules varies depending on their environment. Van Brakel indicated:

> According to Primas the crucial issue is not the approximations of quantum chemistry as the Born-Oppenheimer description, but the breaking of the holistic symmetry of quantum mechanics by abstracting from the Einstein-Podolsky-Rosen (EPR) correlations. It is the EPR correlations that exclude any classical concept of object, shapes or the fixed spatial structures such as presupposed in the notion of molecular structure…therefore, quantum chemistry borrows the notion of molecular structure from classical chemistry (van Brakel 2000, p.144).

R. G. Woolley (1978) defends this position in his famous and provocative article 'Must a molecule have a shape?' which indicates that the classic concept of molecule cannot be derived

from quantum mechanics. Nevertheless, since the nineteenth century chemists have determined experimentally the particular geometries of various molecules. Today we know that these geometries are relative to the time scale of measurement.

Thus, there are difficulties in interpreting even the simplest chemical phenomena, rigorously and independently, from quantum mechanics. The problems are almost intractable as can be recognized in Table 3 (Jensen 1980).

Table 3. Outline of steps which, according to our present knowledge of quantum mechanics and statistical thermodynamics, are necessary in order to predict rigorously the equilibrium or rate constant of a reaction in solution from first principles.

1	Calculation of the electronic potential energy of the static arrangement of atoms corresponding to the structures of each reactant and product.
2	Prediction of the normal modes of motion for the atoms in each structure. This amounts to setting up a mathematical description of the structure´s vibrational and rotational motions.
3	For many of these motions the lowest kinetic energy is not zero, but rather a half-quantum of the motion. This zero-point kinetic energy must be added to the potential energy.
4	From the knowledge of the normal modes of motion it is possible to compute the partition function of each species as a function of temperature, and from this is obtained the standard free energy and enthalpy of each species in the dilute gas state and at the temperature of interest.
5	The standard free energy and enthalpy of each species in solution is then computed considering the transfer from the gas phase to solution.
6	Values of ΔH^0 ΔG^0 and ΔG^* and ΔH^* are calculated for the maximum point on the surface of least energy connecting the reagents with the products. With these values it is possible to calculate the equilibrium constant and reaction rate.
7	Finally the calculated values must be recalculated to consider the actual concentration of the various species in solution using the activity coefficient of each species for the temperature and solvent under consideration.

For similar reasons there are many chemical notions that are not amenable to rigorous quantum mechanical treatment. Van Brakel (2000) mentions some of them: acidity, aromaticity, basicity, chemical bond, chemical reaction, chirality, electronic configuration, orbital, electronegativity, functional group, molecular structure, resonance, relative energy of *s* and *p* orbitals, valence.

In a similar way another philosopher of chemistry J. Schummer (1998) recognizes the differences among the various sciences when dealing with the study of material properties (which from a reductive view are those of the atomic and molecular structure):

> For sciences of materials, with chemistry at the centre, have been, from the earliest stages on, experimental science in the original meaning of studying the behaviour of objects in various and controlled artificial contexts. A material property is reproducible behaviour within certain reproducible contextual conditions. It is important to note that material properties are attributed not to isolated objects but to objects and contexts. Since everything looks red under red light, we have to specify the colour both of the object under investigation and of the light, in order to make qualified colour statements. Since everything is solid at a certain temperature and pressure, solidness always implies specification of thermodynamic conditions. Sometimes it is more the context that matters. To speak of a toxic substance does not mean that the substance itself but the context, a biological organism, falls sick or dies, if it gets in contact with the substance. Precise material predicates require precise and

> systematic details of the contexts of investigation, making contexts themselves a central subject matter of sciences of materials.

This poses a difficult problem in the teaching of atomic and molecular structure, when it ignores its historical roots and philosophical consequences, an issue that has not escaped the experts. In 1999 *Nature* published a report that orbitals had been observed (Zuo *et al*. 1999). There were philosophical objections (Scerri 2000a; 2001), which indicated a confusion of the authors of this article aforementioned between observable and unobservable (Shahbazian 2006), and between the real world and models (Pagliaro 2010). The following quotes from some of the participants in this discussion help to clarify their positions, particularly in relation to the teaching of this topic:

> …chemists have a tendency to ‘‘decompose’’ molecules arbitrarily into basic conceptual or pseudo-physical components (such as orbitals and atoms), which can cause controversy. The entities, which come from such decompositions, make a new class of mathematical objects: ‘‘non-observables’’. Using these non-observables as a tool for chemical arguments is a common practice of chemists (Shahbazian 2006, p. 39**).**

> Orbitals however are also a (quantum) chemical model of immense importance in chemistry. Their relationship to the chemical methodology is heuristic, *i.e.*, their usefulness in many branches of science justifies the use of the model (Pagliaro 2010, p. 279).

> Yes, it is important to know when approximations are made, but success in a science like chemistry is largely a matter of finding useful approximations: this is what students should be taught (Spence, O´Keeffe & Zuo 2001, p. 877).

> Chemical educators should continue to use concepts like orbitals and configurations but only while recognizing and emphasizing that these concepts are not directly connected with orbitals as understood in modern quantum mechanics, but are in fact a relic of the view of orbits in the so-called old quantum theory (Scerri 2000b, p. 412).

Finally, it is important to recognize that traditionally two types of reductionism have been considered: ontological and epistemological (Silberstein 2002). Despite the intense debates that have occurred in this area, where important issues are those related to "the kind of relations," or "the way in establishing relationships" (Lombardi 2005), recent years have witnessed a growing consensus towards a tradition that denies the possibility of reducing chemistry to physics. In particular there is a denial that such a reduction has been achieved via quantum mechanics as considered from logical positivism. Bibliography related to this subject can be found in Erduran (2005), Schummer (2008), Snooks (2006) and Velmulapalli and Byerly (1999).

3 Procedures

3.1 Introduction

This section addresses three issues. The first has to do with the way that history and philosophy of sciences are incorporated into the teaching of atomic and molecular structure. The second considers the diversity of previous ideas that students from different educational levels bring to the subject, and how these ideas hinder their learning. Finally, the third part outlines several reported experiences in teaching atomic and molecular structure. About all this M. Niaz has dedicated a book (Niaz 2009) and a full set of papers (for example Niaz 2000, and 2010) dedicated to posing the necessity of the historical teaching with episodes and experiments that

have been important in science progress. He emphasizes the validity of the following phrase of Kant and Lakatos: ”philosophy of science without history of science is empty”.

3.2 Philosophy and History in Teaching and their Importance

In present science education, history and philosophy play a fundamental role (Duschl 1994; Matthews 1994; Wandersee & Griffard 2002). But the teaching of history cannot be only the chronological narrative of past events, it requires, as indicated by Husbands (2003), “… that we, history teachers…establish a more subtle, less absolutist understanding of the way in which knowledge is created… It needs to be developed through the process of inquiry in the classroom, by teachers and learners in classrooms working to create meanings”. In a similar way Tsaparlis (1997b, p. 924) has emphasized the historical method of teaching as a way of better understanding the topic of atomic and molecular structure.

Moreover, as indicated in the previous discussion of reduction, an issue such as this requires in its teaching, the recognition of the different philosophical positions that underlie its foundation (Karakostas *et al.* 2005). About realism, and the reality of electrons, the influential philosopher I. Hacking has said (1983, p.22): “If you can spray them, then they are real…” Others, like Achinstein (2001), in discussing the discovery of the electron, puts forward the following components for a discovery:

- Ontological. Discovering something requires the existence of what is discovered.
- Epistemic. A certain state of knowledge of the discoverer is required.
- Priority. Social recognition of the discovery.

In the same book Arabatzis (2001) offers a consensus-based account of discovery, asserting that entity *x* (atom, electron, spin, and phlogiston) can be said to have been discovered just when a group *y* reaches consensus that it has been. He simply wishes to concentrate on synchronous belief, not on reality. However in another chapter of the same book Morrison addressed the reality of spin (2001). These discussions can be very technical and complicated. Nevertheless it is advisable for a teacher to adopt a position, or at least to know it.

In recent years, for example, several authors have recognized that the way chemistry is usually taught is based on a particular philosophical position, and that in general terms this position is logical positivism (Chamizo 2001; Erduran & Scerri 2002; Van Aalsvoort 2004; Van Berkel 2000). Van Berkel with researchers all around the world analyzed current and post-war textbooks and syllabi representative of secondary chemistry education in most Western countries trying to find why they are so remarkably similar. He recognizes that dominant school Chemistry is particularly isolated from everyday life and society, history and philosophy of science, technology, and chemical research. His main conclusion was:

> The structure of the currently dominant school Chemistry curriculum is accurately described as a rigid combination of a substantive structure, based on corpuscular theory, a specific philosophical structure, educational positivism, and a specific pedagogical structure, initiatory and preparatory training of future chemists (van Berkel 2005, p.67).

During the Cold War, a philosophy of science, which defended science’s superior analytical purity, was enthroned in most of the Anglo-Saxon intellectual world (Echeverria 2003). It focused on science methodology and the reduction of various scientific disciplines to physics. Since then, the best known version of logical positivism, presenting science as a linear succession of successful discoveries, and placing the emphasis on factual recall with confirmatory experiments, has contributed to identifying what kinds of research questions and

issues were adequate not only for axiomatic science (Reish 2005) but also for school syllabus, as can be seen in chemistry and physics curricula. Therefore it would be desirable, regardless of the educational level, when addressing the teaching of atomic and molecular structure, to identify the philosophical position underlying the approach.

Journals oriented to chemistry education are dedicating full sections to the history of chemistry. William B. Jensen, since 2003 until recently, had the responsibility of writing a section "Ask the historian" in the *Journal of Chemical Education*. He previously had devised a framework of three chemical revolutions from which he extended three levels of comprehension of chemistry ―Molar, Molecular, and Electrical― and three dimensions, based on whether they deal with composition/structure, energy or time (Jensen 1998). In that set of articles Jensen commented that there are a large number of histories of chemistry. In his bibliographic study, Jost Weyer (1974) listed no fewer than 71 general histories of chemistry written between 1561 and 1970, of which 29, or roughly 40%, have appeared written in English. George B. Kauffman has the responsibility of writing historical articles for the journal *The Chemical Educator*, mainly to commemorate anniversaries of outstanding achievements in chemistry (some examples are Kauffman 1999; 2004; 2006; 2010). Jaime Wisniak has played a similar role in *Educación Química*, the Ibero-American Journal of Chemistry Education, since 2001 (Wisniak 2013).

However, although there are many scholarly works on the history of chemistry, there have been few on how to incorporate them, effectively and systematically, into the teaching of chemistry. Perspectives, such as that established by Jensen (1998), in which the curriculum is built on history (in this case of atoms and molecules), or that described by Early (2004) from a new philosophical basis, are few, and therefore very important. As Talanquer recognized (2011) school chemistry needs transgression.

3.3 Introduction to Alternative Conceptions and Difficulties in Teaching and Learning Quantum Mechanics and Quantum Chemistry

Many studies have reported students' difficulties in grasping the fundamental issues of quantum mechanics and quantum chemistry in high school. We shall mention first an article by Tsaparlis and Papaphotis (2002) where findings of student difficulties with quantum numbers, atomic and molecular orbitals, are reviewed, and a case is presented against using quantum chemical concepts at this level (Bent 1984). These authors insist that the topic is highly abstract and therefore beyond the reach of many students.

Students have difficulty understanding the concepts of atomic and molecular structure (Harrison & Treagust 1996) because of the abstract nature of the sub-micro world (Bucat & Mocerino 2009). Many authors have been discussing in several studies the difficulties or misconceptions in students' learning about matter. Those related to its particulate nature[2]; to bonding in general[3]; to the covalent bonding model[4]; to the metallic bonding model[5]; and to the ionic bonding model[6].

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[2] See for example: Lee *et al.* 1993; Novick & Nussbaum 1978; 1981; Nussbaum 1985; Valanides 2000; Wightman *et al.* 1987.

[3] As can be seen in: Birk & Kurtz 1999; Boo 1998; Furió & Calatayud 1996; Griffiths & Preston 1992; Hund 1977; Kutzelnigg 1984; Magnasco 2004; Özmen 2004; Sutcliffe 1996.

[4] For example: Coll & Treagust 2002; Niaz 2001; Peterson, Treagust & Garnett 1989.

Other studies have reported students' difficulties in grasping the fundamental issues of quantum mechanics and quantum chemistry at high school[7] and college levels[8]. In particular the following concepts are indicated:

- 'Probability and energy quantization' (Park & Light 2009);
- 'Quantum numbers' or 'electron configurations of chemical elements'[9];
- 'Orbital ideas'[10];
- 'Uncertainty and complementarity' (Pospiech 2000); and
- 'The Schrödinger equation' (Tsaparlis 2001).

From the point of view of teaching, the elementary, qualitative**,** and pictorial coverage of quantum chemical concepts is approached with reservation or with strong opposition by many chemical educators (Bent 1984; Gillespie 1991; Hawkes 1992).

Physicists have also recognized the difficulties involved in understanding quantum mechanics (Einstein 1926; 1944; 1948; Feynman 1985; Laloë 2001; Styer 2000).

Taber (2001) mentions "most alternative conceptions in chemistry do not derive from the learner's unschooled experience of the world". The many problems that learners have in chemistry maybe best characterised as 'model confusion' (see subsection 3.4.4). Where there are several models for particular or closely related chemistry concepts, students become greatly confused. This is particularly so when most learners have a very limited notion of the role of models in science (Grosslight *et al.* 1991).

3.4 Experiences

3.4.1 Similarities

This subject is closely related to the previous subsection. One of the first to establish similarities between the historical development of science and the conceptual development of students was J. Piaget (Piaget & Garcia 1983) followed by Gagliardi (1988), although Matthews (1992) identifies this idea in Hegel's *The Phenomenology of Mind*. There are strong grounds for criticism of this position (Gault 1991), mainly because the equivalence between the ideas of scientists and students has not been demonstrated. Nevertheless, Scheffel *et al.* (2009) recently and carefully used the similarities in classroom teaching through the following sequence:

> 1. The teacher hands on historical, but educational purposes reduced, material to the student. This will presumably pick up students' misconceptions and their actual scientific positions.

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[5] Such as in Coll & Treagust 2003a; De Posada 1997; 1999.

[6] See, for example, Butts & Smith 1987; Coll & Treagust 2003b; Taber 1994; 1997.

[7] Such as: Dobson *et al.* 2000; Petri & Niedderer 1998; Shiland 1995; 1997; Tsaparlis & Papaphotis 2002; 2009.

[8] For example: Hadzidaki *et al.* 2000; Johnston *et al.* 1998; Kalkanis *et al.* 2003; Michelini *et al.* 2000; Paoloni 1982; Wittmann *et al.* 2002.

[9] As can be seen in: Ardac 2002; Melrose & Scerri 1996; Niaz & Fernández 2008; Scerri 1991.

[10] For example: Cervellati & Perugini 1981; Conceicao & Koscinski 2003; Ogilvie 1994; Scerri 2000a; Taber 2002a & b; Taber 2005; Tsaparlis 1997a.

2. The students discuss these ideas and propose experiments to verify or falsify one of the theories or models that has been presented. They have an opportunity to choose one of the scientists as an advocate for their preconceptions.
3. Based on experiments and if necessary on additional material, the pros and cons of each theory or model are collected and discussed. If possible, a decision should be formulated and explained.

These authors provide examples of similarities, applying this teaching methodology to: old atomism, chemical bonding, or Lewis octet model.

3.4.2 The historical narrative

Narrative can be defined as "telling someone else that something happened" (Herrestein-Smith 1981, p. 228). Norris *et al*. (2005) elaborated this approach and they identified in the narrative the roles of the narrator, the reader, and the events. Particularly important here is the responsibility of the narrator – in this situation, the teacher – because he must facilitate the interpretation of the events in context (Gilbert 2006). As Metz *et al.* (2007) recognized, the narrative approach has a spectrum of possible applications:

- Interactive vignettes (Wandersee 2002)
- Anecdotes (Shrifley & Koballa 1989)
- Curriculum unit unified by a theme (Holbrow *et al*. 1995)
- Storyline, when the thematic approach will begin with a big question (Stinner & Williams 1998)

For example, Teichmann (2008) included anecdotes from some atomic structure protagonists, Klassen (2007) has used narratives for teaching the heroic attitude of L. Slotin assembling the first atomic bomb, and for rehabilitating the story of the Photoelectric Effect (2008). In similar fashion, Nobel lectures have also been used for teaching in chemistry and in physics (Jensen *et al.* 2003; Panusch *et al.* 2008; Stinner 2008). Biographies, tributes and interviews could also be considered in this category. Some examples are: G. N. Lewis (Branch 1984); L. Pauling (Kauffman & Kauffman 1996); R. S. Mulliken (Nachtrieb 1975).

3.4.3 The historical role of rivalry, controversy, contradiction, speculation, and dispute in scientific progress, and its use in teaching strategies

In academia, conflicts in and around science have been studied for various reasons:

- to gain insight into the process of science policy making process;
- to learn more about the various roles of scientists;
- to identify the ways in which the public might participate in decision making;
- to understand how controversies arise, how they are contained within the scientific community or expand into the public domain, how they are brought to a close, or why they persist; or, among others,
- to analyze the social construction and negotiation of scientific knowledge claims by conflicted scientists (Martin & Richards 1995).

Nevertheless, dispute in scientific progress has been rarely used in the teaching and learning of science (Niaz 2009).

Teaching through the consideration of historical aspects of scientific knowledge has the potential to show the progress of scientific knowledge over time. Historical artefacts and scientific discoveries, scientists' life stories, and the details of scientific struggles in scientific

progress, could be discussed in the science classroom. Because the knowledge represented in textbooks or in any predesigned science-learning environment context is the end product of science, students and teachers do not learn and teach about those presuppositions, contradictions, controversies, and speculations existent in scientific progress (Niaz 2010; 2009; Garritz, 2012 online). Only a few teachers today believe and teach that scientific knowledge is tentative, empirically based, subjective, and parsimonious; that it includes human creativity and imagination; and that it is socially and culturally constructed (Ayar & Yalvak 2010).

3.4.4. The explicit recognition of models and modeling

The Model-Based view of Scientific Theories, and the structuring of school science (Adúriz-Bravo 2012; Develaki 2007) have recently been discussed elsewhere. As discussed earlier in this chapter, quantum mechanics forced physicists and chemists to reshape their ideas of reality, to rethink the nature of things at the deepest level, and to revise their concepts of determinacy vs. indeterminacy, as well as their notions of cause and effect. Here we adopt a realist position about molecules, atoms and electrons. In agreement with Tapio (2007), we specify that:

- Reality and its entities are ontologically independent of observers.
- Claims about the existence of entities have truth-value.
- Models of atoms and molecules are required to be empirically reliable.

Model is a polysemous word; it has been used and it is still used with several meanings. That is one of the difficulties we meet when we use it in teaching. In one usage, 'model' is exemplary; it indicates things, attitudes or people worthy of emulation. The courage of a warrior, the intelligence of a wise man, the solidarity of a doctor, and the speed of a runner are examples of 'models' in this regard. In this paper we use a previous definition of 'model' (see Chamizo 2011a for all the references) "models (m) are representations, usually based on analogies, which are built contextualizing certain portion of the world (M), with a specific goal"**.** In this definition all the words are important: the representations are essentially ideas, but not necessarily so, as they can also be material objects, phenomena or systems (all of them constitute a certain part of the world M). Representations have no meaning by themselves; they come from someone (either an individual or a group, usually the latter) that identifies them as such. An analogy is made up of those features or properties that we know are similar in (m) and (M). That 'are built contextualizing certain portion of the world M', refers to a historically defined time and place which also frames the representation. Some 'portion of the world' indicates its limited nature; models (m) are partial for the world (M). 'A specific goal', establishes its own purpose, usually (but not necessarily) to explain or teaches, and possibly also to predict. In this sense models can be understood as cognitive artefacts or mediators constructed in order to create subjective plausibility about the target. It is important to remember that explanation is one of the most significant features of science, but in some cases when models are even completely unable to offer an explanation, much of the prestige of a model may lie in its capacity to predict.

There are only two types of models: mental and material.

Mental models are reflected representations built by us to account for (explain, predict) a situation. They are forerunners of the famous "misconceptions" (see section 3.3) and can sometimes be equivalent**,** since they are unstable, generated in the moment, and then discarded when no longer needed, making them cognitively disposable.

Material models (which may be identified as prototypes) are the ones that we have empirical access to and have been built to communicate with other individuals. Material models

are expressed mental models and can be further categorized as symbolic, iconic or experimental. Here we only discuss the first two. Symbolic material models correspond to the languages of sciences, such as Mathematics or Chemistry. So mathematical equations constructed to describe precisely the portion of the world being modelled are symbolic material models. Wave mechanics is a symbolic material model. Another example of symbolic material model is the one used by chemists to represent elements, compounds, and reactions. Hence**,** when a teacher writes the molecular structure of water as H_2O using two hydrogen and one oxygen atom, the teacher uses a symbolic material model. Iconic material models correspond to images, diagrams, or scale-models, like a map or the so-called 'molecular models'. Stereochemistry was constructed with iconic material models in three dimensions. For example, in the early years of the nineteenth century Dalton constructed wooden models of atoms, after him Pasteur made his models of enantiomer tartrate crystals, Hofmann his croquet ball molecular models, and van't Hoff his cardboard tetrahedral models. In the twentieth century the stereochemical ideas of Pauling led to the most famous example of an iconic material model, the DNA structure by Watson and Crick.

Recently Seok & and Jin (2011) have reviewed the literature dealing with models and modelling and reported some important findings. Two of them related to model use in atomic and molecular structure teaching are:

- Meaning of a model. A model is understood as a representation of a target. The targets represented by models can be various entities, including objects, phenomena, processes, ideas, and their systems. A model is also considered a bridge or mediator connecting a theory and a phenomenon, for it helps in developing a theory from data and mapping a theory onto the natural world. For example; atomic models (Dalton, Bohr, Lewis); molecular models or bonding models (ionic, covalent, coordinated and metallic) or electron models (corpuscle or wave like).
- Change in Scientific Models. There are two ways of testing a model in science: the empirical and conceptual assessments. An empirical assessment is a way of evaluating a model in terms of the fit between the model and the actual phenomenon. In a conceptual assessment, a model is evaluated according to how well it fits with other accepted models as well as with other types of knowledge.

The assessment of a model is conducted differently in experimental sciences, such as physics or chemistry, from in historical sciences, or others, such as earth science. For example: Bohr's atomic model is excellent at explaining hydrogen spectra, but useless for molecular structures; Lewis' atomic model is excellent in predicting simple organic structures, but useless in (for example) infrared spectra (about Lewis model in introductory teaching of atomic and molecular structure see: Chamizo 2007; Purser 2001).

Finally because models are built in a particular historical moment for specific purposes the context should be explicitly recognized when teaching them**.** Justi and Gilbert (2000) have warned us about the frequent use of hybrid models in the textbooks, which has produced so much confusion among students. Experiences of more correct use of these models have been reported recently (Chamizo 2007; 2011; 2012).

3.4.5 Textbooks, experiments, and Information and Communication Technologies (ICTs)

There are several books that feature various aspects of the history of atoms and molecular structure[11]. One of the most influential is Kuhn's *Black-Body Theory, and the Quantum Discontinuity 1894-1912.* Another example is the history of quantum chemistry as told by E. Segrè (2007) in which a Nobel laureate offers impressions and recollections of the development of modern physics. Rather than a chronological approach, Segrè emphasizes interesting, complex personalities who often appear only in footnotes. Readers will find that this book adds considerably to their understanding of science and includes compelling topics of current interest.

However, very few of these last writers teach undergraduate chemistry. The authors of this chapter have written a book in Spanish on Quantum Chemistry, with emphasis on the development of the historical aspects of this science (Cruz, Chamizo & Garritz 1986). With hundreds of solved exercises and problems it has been used widely in Ibero-America. The historical narrative oscillates in time, from the nineteenth century chemistry until the interpretation of periodicity, as can be seen in Table 4.

Table 4.Some chapters of the book by Cruz, Chamizo, and Garritz (1986)

Chapter	**Comments**
The chemistry of the nineteenth century	From Dalton atomic hypothesis to Couper and Kekulé molecular models through Frankland and Werner's valence models and finally to the Mendeleev's work, as the empirical foundation of periodicity
Birth of quantum theory	Thomson's corpuscles discovery in cathode ray tubes, the Millikan controversial experiment of determination of the electronic charge (Niaz, 2000; Panusch *et al.* 2008; Paraskevopoulou and Koliopoulos 2011) and back to the black body radiation experiments of Stefan, Wien, Lummer and Pringsheim, Rubens and Karlbaum, that conducted M. Planck to the correct radiation formula, and a couple of months later, to the proposal of quantum theory as a brilliant solution to the ultraviolet catastrophe found theoretically by the classical analysis of Rayleigh and Jeans. This chapter closes with Einstein's light quantum hypothesis, his explanation of the photoelectric effect, and finally with the Compton experiment that confirmed the photon existence.
Atomic spectra	Bohr`s atomic model of one electron atoms as it was presented by him in 1913, and considering that Rydberg's formula is in itself a premise of his model. After the postulates of Bohr's model, the Sommerfeld and Wilson quantization rules are depicted, and the elliptic orbits with three quantum numbers are introduced, with the angular momentum modified; the Frank and Hertz experiment, the fine structure of hydrogen spectrum, and

[11] For example: Buchwald & Warwick 2001; Giunta 2010; Marinacci 1995; Nye 1993; Snow 1981; Toulmin & Goodfield 1962.

	the Moseley law show the successful application of Bohr's model.
Models of atoms and chemical bonds	The Lewis and Langmuir's model of covalent bond; Kossel's model for ionic bonding, and also Pauling's electronegativity are followed by Born-Haber's cycle and Fajans' rules.
Discovery of electronic spin	After the electron spin discovery is presented, spin dependent models of the atom and molecular structure, such as the Gillespie and Nyholm's Valence Shell Electron Pair Repulsion model, and the Linnett double quartet model, are introduced
Modern quantum mechanics (three related chapters)	The two proposals of Schrödinger and Heisenberg, later shown to be equivalent, and their application to the mono-dimensional free particle, to the particle in a box, to the hydrogen atom and to polyatomic structure, including the philosophical interpretations of quantum mechanics (Copenhagen's, stochastic, Schrödinger's cat, Einstein-Podolsky-Rosen, etc.)
The periodic behaviour of the elements	Periodicity empirically discovered by Mendeleev is now explained. A clear distinction between isolated electronic properties such as ionization energy and electron affinity, and those which come from the chemical environment, such as atomic size and electronegativity.

Experiments related to the history of atomic and molecular structure are rare. Some of them can be found in more general books like Doyle' *Historical Science Experiments on File.* However, there are some examples, ranging from the electrochemical decomposition of water (Eggen 2011) to spin through the Stern-Gerlach experiment (Didis & SakirErkoc 2009).

Information and Communication Technologies (ICTs) have so far had little impact in this area, with the exception of graphs of orbitals, electron densities and contours. The PhET project (Physics Education Technology) has branched also into chemistry and biology. Some of the designed computer simulations have been devoted to atomic and molecular structure from historical experiments. PhET conducts research on both the design and use of interactive simulations, but important as this material is, the failure to address historical context and provide historical references have made this approach so far quite weak.

4. Conclusions

Physical chemistry remains a fundamental basis for the teaching of chemistry. Mathematics, as group theory and matrix representations, are needed to understand selection rules via symmetry studies and, through them, spectroscopic transitions, an important topic since the second half of last century. Nevertheless there is a necessity for balance between the theoretical physicochemical basis of chemistry and the phenomenological and empiricist knowledge that chemistry had already produced.

The parsimonious advice of one of the reviewers of this chapter was "do not introduce needless complexity unless it is warranted to explain the necessary facts". This can be also a conclusion about the inclusion of history and philosophy of science in teaching quantum

mechanics and quantum chemistry. One has to apply Ockham's Razor rules while teaching these topics.

We can recognize in the almost two hundred works cited in this study that integration of history of science into the teaching of atomic and molecular structure has been seen as an important step, particularly since 1994. Increasing numbers and diversity of resources and studies of strategies to be used are making this incorporation more robust. Nevertheless, the way in which chemistry has been taught all around the world is based on a particular philosophical position, which comes from its acceptance as a reduced science, and can be characterized as logical positivism. This normal (in Kuhn's terminology) education practice has not been driven to any great extent by educational, historical, or philosophical research findings. A few years ago J. Moore, as editor of the influential *Journal of Chemical Education* (2005), indicated the poor impact of chemical education research on teaching and learning, in spite of the motto of the National Association of Research in Science Teaching: "Improving Science Teaching & Learning through research".

There still has not been major change regarding what the teaching of sciences requires. In general, the majority of teachers, textbooks, and science curricula still consider science teaching as a dogma or as "rhetoric of conclusions" (Schwab 1962). This situation can only change if teachers know and recognize the uniqueness of chemistry and the philosophical positions from which they approach their practice. Realism and models are some of the issues involved. Some ideas from the historian of chemistry M. J. Nye could be very helpful:

> We can say that if mechanics has always been an aim of scientific philosophy, the twentieth-century chemistry has revived its philosophical character, achieving a long-sought understanding of the dynamics of matter. But chemists more that physicists, have remained self-conscious about the fit between the phenomena taking place in the laboratory and the symbols employed in the operations of explanatory mathematics. Precision, not rigor, has been characteristic of chemical methodology. Parallel representations, not single causal principle, have been characteristic of chemical explanation.
>
> Whereas many early-twentieth-century physicists were inclined to regard conventionalism, complementarity, and indeterminacy as concessions of failure in their traditional philosophical enterprise, chemists were not surprised that a simple, "logical" account of the behaviour of electrons and atoms, like that of molecules and people, often gives way to the inconsistencies and uncertainties of empiricism (Nye 1993, p.282).

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*Response to reviewer's comments
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ANSWER TO General Copy-Editor(2):

- Almost all grammatical suggestions were accepted.
- The accuracy of the quoted passages was revised.
- Three new references were added (and the mistake of year's citation, corrected)
- The long paragraph was reduced.
- Traked changes cleaned
- New abstract added I ALREADY SENDED LAST TIME (141 WORDS)

Thanks you very much. The manuscrip was improved!

ANSWER TO General Copy-Editor(3):

title in upper/lower case
CORRECTED

abstract (70-150 words) required
I ALREADY SENT IT LAST TIME (141 WORDS)
Now in the manuscript

at least some of the book and journal titles in reference list are not italicised ...
CORRECTED