INVITED THEME ISSUE: *Structural concepts*
Contributions from science, science education,
history and philosophy of science
PREFACE

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PREFACE

MOLECULES AND ATOMS AT THE CENTRE STAGE

<<ΛΕΥΚΙΠΠΟΣ ΚΑΙ … ΔΗΜΟΚΡΙΤΟΣ *ΣΤΟΙΧΕΙΑ* … ΤΟ *ΠΛΗΡΕΣ* ΚΑΙ ΤΟ *ΚΕΝΟΝ*
ΕΙΝΑΙ ΦΑΣΙ, … ΤΟ ΜΕΝ *ON* ΤΟ ΔΕ *ΜΗ ΟΝ*,… ΤΟ ΜΕΝ *ΠΛΗΡΕΣ* ΚΑΙ *ΣΤΕΡΕΟΝ*, ΤΟ
ΔΕ *ΚΑΝΟΝ* ΚΑΙ *ΜΑΝΟΝ* … *ΑΙΤΙΑ* ΔΕ ΤΩΝ *ΟΝΤΩΝ* ΤΑΥΤΑ ΩΣ *ΥΛΗ*>>

ΑΡΙΣΤΟΤΕΛΗΣ, *ΜΕΤΑ ΤΑ ΦΥΣΙΚΑ*
Α΄ 4.985β4

"Leucippus and Democritus consider as basic elements (*stoicheia*) the complete (*pleres*) and
the vacuum (*kenon*), the first one existent (*on*), the second one non-existent (*me on*), one
filled (*pleres*) and solid (*stereon*), the other empty (*kanon*) and thin (*manon*). These two are
the causes (*aitia/etia*) of what exists (*on*) as matter (*hyle*)."

Aristotle, *Metaphysica*
Α΄ 4.985β4

For many, chemistry is *the* experimental science. By this they mean that experiment
plays the leading role in the development of chemistry, while theory comes into play in order
to organise the experimental facts. It is true of course that chemistry emerged first as a
craftsmanship, the metallurgy of ancient Greek *chymeutae* (from the verb *chymeuein*,
meaning to cast molten metal into form) (Berthelot & Ruelle, 1888). A theoretical/
philosophical quest was initiated at about the same time by ancient Greek philosophers. On
the other hand, as found by Niaz in his *rational reconstructions* of a number of fundamental
experiments on the structure of matter (see the paper by Niaz and Rodriguez in this issue),
"although experimental details are important, the theoretical rationale in which the
experiment is conducted, is even more important".

Since the early days of their dedication to intellect and nature, philosophers dealt with
the explanation of worldly matters and their reduction to a common principle. However, the
ideas of Leucippus and Democritus were indeed the foundation of modern science.
Leukippos and Democritus advocated the corpuscular nature of matter through an *atomic
theory*. They declared *atoms* (from Greek *atomos,* which means indivisible) as the principle
of objects, having their own weight and moving in empty space (the void or vacuum); their
union results in the synthesis of all objects, while their breaking apart results in the

disintegration of that which exists. Atoms are so small that they are invisible; they are unborn, permanent and indestructible, of the same kind but varying in size, weight and shape, changing only their position and configuration. Presumably Greeks' concept of atoms was closer to what we consider today as molecules (IUPAC, 1993, p. 8). Note that equally revolutionary with the concepts of *atoms-molecules* was the concept of *vacuum* because one needs the vacuum if one should allow atoms-molecules to move (Nussbaum, 1997, p. 176). This first atomic theory had been neglected for centuries, only to return to the foreground in the early 1800s, and after considerable debate became a rigorous, exact, and aesthetically pleasing theory.

Chemistry deals then with a *small* (submicro) world, and at the same time a *large* world. That is both a privilege and a drawback! The positive side is the esoteric beauty of chemistry, for those who can see that beauty. However, the molecular-atomic-electronic nature of chemistry is a large pedagogic drawback; it is the most important factor in generating learning difficulties for its students.

Herron (1978) maintains that concepts such as *atom* and *molecule* which have imperceptible examples *and* imperceptible attributes should be considered formal in the Piagetian sense, hence "it is quite likely that they cannot be totally understood without some formal reasoning". On the other hand, according to Johnstone (1982, 1991, 2000), modern chemistry has three main components: the *macro* (dealing with experiments and observations of concrete substances), the *representational* (dealing with symbols, equations, and calculations), and the *submicro* (dealing with molecules, atoms, structure and bonding).[1] These three levels can be represented as the corners of a triangle. However, "it would be a mistake to imagine that all, or many, of our students follow us up the middle of the triangle ... In trying to sell the concepts of *element* and *compound* we are simultaneously having to sell the submicro concepts of *atom* and *molecule*, and representing all this by *symbols, formulas and equations*. We are in the middle of the triangle ... This new kind of concept takes a long time to grow, but once we have embedded it in long-term memory we can use it as a powerful way of looking at the world" (Johnstone, 1991).

Jensen (1998) proposed a scheme for the logical structure of chemistry, in which he distinguishes three dimensions: D1: Composition and structure; D2: energy; D3: time. Each dimension can be treated at one of three levels: L1: molar level; L2: molecular level; L3: electrical level.[2] This scheme leads to the distinction of $3 \times 3 = 9$ subdivisions, of which the simplest is the treatment of composition at the molar level, while the most complicated is the treatment of chemical kinetics at the electrical level.

This issue of *CERAPIE* deals with the structural theories and the role they play in the teaching and learning of chemistry. The treatment is at the molecular and electrical levels, with most contributions falling into the most advanced electrical level of Jensen's scheme. Contributions were invited that cover three distinct areas: science, science education, history and philosophy of science. The result is that distinguished scientists/chemical educators and science education researchers have contributed their expertise. Note that some further invited contributions (together with independently submitted work that will be peer-reviewed) are expected to be included in a second theme issue on the same theme which is planned for the May 2002 issue (see relevant CALL FOR PAPERS in this issue for deadlines and conditions). Needless to add that I thank all contributors to this theme issue.

Contributions from science

Lewis's theory of valency

G.N. Lewis's concept of valency has been a revolutionary one for chemistry and is still useful today. It is striking that quantum-chemical calculations show (Suidan, Badenhoop, Glendening, & Weinhold, 1995 - see also relevant references in Nelson's paper in this issue), in a number of common ions and molecules (e.g. the sulphate, perchlorate, and phosphate ions, sulphur trioxide, sulphur dioxide), that the original Lewis structures, which generally abide by the octet rule, represent these species *more accurately* than the leading resonance structures cited in freshman chemistry textbooks. In this issue, Lewis's theory comes up in several places.

Peter G. Nelson discusses modified Lewis theory. He first points that "although Lewis devised the theory many years before the development of quantum-mechanical calculations on molecules, it has survived these developments remarkably well. Quantum chemists have been able to obtain similar structures to his for many types of molecule by analysing wave functions or electron densities. However, Lewis's theory needs to be modified to make it consistent with the results for molecules containing polar covalent bonds (e.g. ClF) and hypervalent atoms (e.g., SF_6)." This modification is discussed in Part 1 of Nelson's paper. In this, he distinguishes between the valence shell of an atom (VS) and the Lewis shell (LS).

The VSEPR and the electron-domain models

Another powerful and very popular model is the *Valence Shell Electron Pair Repulsion* (VSEPR) that has been proposed by **Ronald J. Gillespie**. According to him, Lewis structures and the VSEPR model are all that is required for upper secondary school, while the *electron-domain model* is sufficient for general chemistry, with more emphasis placed on electron density rather than orbitals. In this issue, **Gillespie** with **Chérif F. Matta** draw attention to a number of features of the VSEPR model that are not widely appreciated. They further discuss the relationship of the VSEPR model to the electron density. It is important to take into account that the fundamental basis for the VSEPR model is provided by the Pauli principle and not by electrostatics: electrons exhibit their behaviour as a consequence of the Pauli exclusion principle of same spin electrons and not primarily as a consequence of their electrostatic repulsion. The VSEPR model "can be taught at various levels and with increasing sophistication from high school and beginning general courses to higher level inorganic chemistry and quantum chemistry courses".

It is well known that central to recent and current science-education research is the study of the alternative conceptions that students hold about many chemical concepts. Yet how often are such misconceptions generated by the instruction given by textbook and/or teachers? (Bodner, 1991). At this point, I urge readers to have a look at Figure 1 of Gillespie and Matta's paper (p. 75). I anticipate that many of them will be taken by surprise to realise that free atoms or monoatomic ions with an octet of electrons in their valence shells (such as Ne, F⁻, O^{2-}) *do not* have four electron *pairs* (as commonly depicted), but instead electrons move freely around the corresponding nucleus, giving a spherical total electron density. (A higher surprise will result by looking at Figure 3 of the paper, p. 78.) In quantum-chemical terms, this is a result of *electron correlation*.

The helium atom is the simplest atom for which the problem of electron correlation exists. In general chemistry, both electrons of helium are placed in the 1s orbital, providing

the ground-state $1s^2$ configuration. Using a corresponding trial function in a variational calculation, $\varphi_{1s}(1)\varphi_{1s}(2)$ with (1) and (2) standing for the two electrons, with a modified nuclear charge (a *scale factor*) serving as the variational parameter, leads to an energy of -2.85 a.u. for the ground state of the helium atom, about 0.05 higher than the experimental energy (Pilar, 1968, p. 243). In this way, *charge correlation*, that is, the screening effect of the other electron is taken into account. More flexibility is introduced by using different scale factors for the two 1s orbitals, that is by using *different orbitals for different spins*: $\varphi_{1s}(1)\varphi'_{1s}(2)$. The physical meaning of this is that one electron tends to be farther away from the nucleus than the other: this is termed *radial correlation effect*. In this way, an improved value of energy is calculated: -2.876 a.u.

However, because of the $1/r_{12}$ term in the Hamiltonian of the helium atom, the Schroedinger equation is not separable, and the true ground-state wave function cannot be written as a product of monoelectronic functions (orbitals) as done above. In 1930, Hylleraas investigated trial functions that diminish the probability of finding the two electrons close together, and hence better describe the tendency of the two electrons to be on opposite sides of the nucleus (*angular correlation*). One such function he used was $\varphi_{1s}(1)\varphi'_{1s}(2)(1 + br_{12})$, which includes the interelectronic distance r_{12}, and obtained an improved energy of -2.89 a.u. Using a more complicated six-term trial function containing r_{12}, Hylleraas found an energy of -2.90 a.u. for the ground state of the helium atom, which is very close to the experimental value (Levine, 1991, pp. 258-259).

Natural bond orbitals

Quantum-chemical theories of atomic and molecular structure are taught in general chemistry or introductory inorganic chemistry courses in first-year chemistry and other science departments. Atomic and molecular orbitals are also part of the upper secondary curriculum in many countries. There are, however, many educators who are against the use of the orbital and related quantum chemical concepts in basic chemistry courses: they consider these concepts highly abstract and involved, and therefore out of reach for many students. On the other hand, research reports have demonstrated confusion still exists, not only among high-school students, but also among chemistry students who have passed the quantum-chemistry course. Tsaparlis (1993, 1997a) has carried out an analysis of examination data from the compulsory, undergraduate, quantum-chemistry course. The following concepts and topics were studied: the definition of an atomic orbital (AO); the real mathematical versus the complex mathematical forms of the AOs; the representation of AOs (AO shapes); the approximate nature of AOs for many-electron atoms; Slater determinants; the definition of a molecular orbital (MO) and the nature of the chemical bond; and, finally, other related topics. The findings were attributed partly to the mathematical and abstract nature of these concepts, and partly to the elementary, imprecise and mostly pictorial coverage of these concepts in previous introductory courses.

A major source of difficulty in dealing with the quantum-chemical concepts derives from the failure of students to distinguish between *physical reality* and *mathematical manipulations*. Pauling and Wilson (1935, p. iii) stated over sixty years ago that *"quantum mechanics is essentially mathematical in character, and an understanding of the subject without a thorough knowledge of the mathematical methods involved and the results of their application cannot be obtained."* And as Coulson (1974, p. 17) has put it: *"Mathematics is now so central, so much 'inside', that without it we cannot hope to understand our chemistry ... These (quantum-chemical) concepts have their origin in the bringing together of mathematics and chemistry."* It is then quite understandable why mathematics occupies a

central part in quantum-chemistry courses, with the result that both teachers and students pay more attention to the complexities of the mathematics (the tools, the trees) and lose the physics (*the actual world,* the forest).

Despite the complicated mathematics needed to understand the concepts and methods of quantum chemistry deeply, very efficient, and user-friendly quantum-chemical programs now exist. They make the quantum-mechanical calculations on large molecules feasible, and to some extent routine, even for the non-expert experimental researcher. Realistic electron densities can be calculated for common systems, providing further powerful tools in the hands of chemistry instructors not only at a college but even at a high-school level.

Natural bond orbitals (*NBO*s) provide a method of deriving orbitals that are close to our traditional concept of bonding and valence as pioneered by Lewis. In this Issue, **Frank Weinhold** and **Clark R. Landis** discuss these *NBO*s and extensions of localised bonding concepts to transition metals. They supply information about the release of the latest version of a commercially available computer program (*NBO 5.0*) that makes feasible the computation of natural bond orbitals with related applications for systems of practical interest.

Their discussion about extending the localised bonding concepts to transition metals is of great interest. According to the authors, "Lewis's octet rule and shared electron pair concepts underlie the most broadly accepted models of localized bonding in common main-group elements. However, it is important that a quantitative wavefunction analysis should not only conform to our prejudices in these cases, but also suggest useful *extensions* of localized concepts to less well understood species". In their paper, **Weinhold** and **Landis** present empirical and *NBO*-based computational evidence for an extension of Lewis-like diagrams and bonding concepts to transition metal compounds. For d-block elements, the authors derive the so-called "Rule of 12" (*dodectet rule*), which is analogous to the famous "Rule of 8" (*octet rule*). In this way, just as the four valence orbitals ($s + 3p$) of the *p*-block underlie the usual Lewis octet rule, so may the six valence orbitals ($s + 5d$) of the *d*-block be expected to underlie the corresponding dodectet rule for transition metals.

Inorganic and organic chemistry

Sidney F. Kettle questions the division of chemistry into the traditional branches of inorganic, organic and physical. Staying however in his own field, he discusses the role that structure is called to play in future inorganic chemistry. On the other hand it was not possible to cover the special role of structure in organic chemistry, though many efforts were made towards finding an author. In particular, I wanted to cover the logic of structure in organic chemistry with special emphasis on the charge flow that is so fruitful in dealing with reaction mechanisms. It is hoped that this missing area will be dealt with in the second theme issue of *CERAPIE,* which is planned for May 2002.

Biological molecules

Everyone of us is aware, of course, of the important role that biochemistry and molecular biology play in modern science. The contribution of molecular science and theoretical chemistry to this development is decisive. Central here is biomolecular structure as related to biological function. In their contribution to this issue, **David R. Canning** and **James R. Cox** state that "understanding the three-dimensional nature of the structural elements of proteins (for instance) is essential if students are to understand how proteins fold into thermodynamically favorable structures and form biologically relevant complexes".

They further point out that "molecular models are much less effective in biochemistry, compared to organic chemistry, because it takes many atoms to demonstrate structural motifs. Large models of proteins and DNA can be purchased, but they are very costly and will only show a limited number of structures. A better and more versatile way to view the three-dimensional structure of biological molecules is through the use of molecular visualization (graphics) software". The advent of powerful computers has made it possible to use a desktop or laptop computer, and work with the complicated structures of biological molecules. **Canning** and **Cox** provide information about available tools for the molecular visualisation of biological molecules. Their approach is useful both from the scientific and the pedagogic point of view.

Science education

The contribution of studies on the structure of matter to the development of the physical sciences is without doubt the cornerstone of modern science. Not only have these studies resulted in practical applications, they also have satisfied the innate philosophical disposition of human nature. It is therefore no surprise to find that structural theories have fascinated chemistry teachers and constitute the backbone of modern chemistry curricula, even at the primary school level. As a matter of fact, the study of atomic and molecular structure - from the elementary models to the old quantum theory and later quantum mechanical concepts - is considered a *sine qua non* in chemical education. It is not then surprising that many chemistry-educators have carried out research studies about structural concepts.

With the development during the past few decades of chemistry education (and in general of science education) as a research discipline, the place of structural theories and concepts has undergone strong criticism. The main reason for this criticism is the difficulty students encounter in dealing with these concepts. An explanation of this difficulty occurs if one examines the relevant concepts from different perspectives of science education, some of which are seen as conflicting theories by many researchers. Tsaparlis (1997b) has employed the following perspectives, and arrived at the same conclusion about pupils' difficulties in learning the atomic and molecular concepts: (i) the Piagetian developmental perspective, (ii) the Ausbelian theory of meaningful learning, (iii) the information processing theory, and (iv) the alternative conceptions movement. In particular we must take into account the studies of students' alternative conceptions about structural concepts.

Recognising that the molecular-atomic-electronic nature of chemistry is a severe pedagogic drawback, and taking into account Johnstone's distinction of the three components of chemistry, we have hypothesised that the adoption of a three-cycle method which goes separately over the macro, the representational, and the sub-micro components should be considered seriously as a good method for teaching introductory chemistry at the lower-secondary level. It is true that first general-science courses treat most chemical topics from the macro point of view, although early treatments of atoms and molecules are not absent. But we are in favour of a more coherent and consistent three-cycle treatment of chemistry. We have experimentally tested the three-cycle method with promising results (Georgiadou & Tsaparlis, 2000).

In this issue, **Keith S. Taber** has compiled a review of educational research into the structural concepts of chemistry. In this he discusses not only his numerous related studies, starting with work for his Ph.D. degree, but also many other contributions. The reading of this review paper is a must for every science-education researcher as well for teachers of chemistry. Of special interest is the proposed alternative chemical ontology (see Figure 6 of Taber's paper, p. 151), in which the focus is not on atoms but on molecules and ions. This derives from the fact that most real chemistry involves molecules, or ions, or more extensive systems, while discrete atoms are seldom featured in significant chemical processes. This ontology is in contrast to the current one, in which the atom has a privileged place in the teaching and learning of chemistry.

History and philosophy of science

Although many educators are reluctant to follow the process of discovery of scientific concepts and maintain that dated ideas can cause confusion and misconceptions, we must take into consideration the view that the history of scientific discoveries shows the natural route of human thinking and matches the cognitive development of the human mind. The subject of atomic and molecular structure will thus be better understood if its historic traces are followed. Presenting, for instance, experimental evidence for the existence of atoms, including the earlier evidence, as well as the evolution of our ideas about the chemical bond, instead of a postulative approach, will not only facilitate understanding and learning, it will also show students that humans have conquered knowledge in a stepwise fashion, starting from simple and sometimes naive ideas, and proceeding to more sophisticated ones.

History and philosophy of science and its connection with science education is a relatively new area of study. Structural concepts occupy a central role in this field, so it was imperative that they should constitute an integral part of this theme issue.

Rational reconstructions of structural theories

Mansoor Niaz has used Lakatos' method of 'rational reconstructions' to study structural theories and concepts and the role which they should but actually *do not* play in chemistry education curricula and in chemistry textbooks. In this issue, **Niaz** in collaboration with **María A. Rodríguez** review Niaz's relevant contributions. The authors maintain that "various topics of the general chemistry program, at both the high school and freshman level, can be presented within a history and philosophy of science perspective. In the case of atomic structure, experimental details of the cathode ray, alpha particle and the oil drop experiments do not suffice to present to the students a glimpse of the efforts, struggles and vicissitudes in the lives of the scientists". Other topics studied were the origin of the kinetic theory and of the covalent bond, and the law of multiple proportions. "Origin shows that scientific progress does not necessarily follow the sequence: experimental details, laws and then theories", showing that although experimental details are important, the theoretical rationale in which the experiment is conducted, is even more important. The authors conclude by answering the question set in the title of their paper, stating that "history and philosophy of science is already 'inside' chemistry and this perspective can facilitate students' conceptual understanding".

Philosophy of chemistry, quantum physics and quantum chemistry

A central issue in chemistry teaching is the role of physics in chemistry. Chemistry developed as a separate discipline from physics. But as time went past, physics and physics methodology became very central in chemistry, initially through physical chemistry, chemical physics, and theoretical chemistry; eventually, physical methods became important to all chemistry fields, most notably analytical and inorganic chemistry, and further organic and biochemistry. The question then arose as to whether chemistry could be reduced to physics. This however has absolutely not been the case. **Eric Scerri** has contributed greatly to the question of reductionism in chemistry, and is considered among the founders of the new distinct field of philosophy of chemistry, being the editor of a related journal, *Foundations of Chemistry*. In this issue, Scerri discusses the new philosophy of chemistry and its relation to chemical education, with special emphasis on quantum chemistry.

POSTSCRIPT: SCIENCE EDUCATION
AND CHEMISTRY TEACHING AND LEARNING

We mentioned above that the molecular-atomic-electronic nature of chemistry, despite its esoteric beauty, is a severe pedagogic drawback, a most important factor in generating learning difficulties. Teaching and learning about atoms and molecules is a arduous task for both teachers and pupils. As the review by Taber demonstrates, research in science education has a lot to say about this!

Despite the calls from science-education researchers, chemistry textbooks continue the practice of treating too much abstract material at an elementary physical chemistry level. Fortunately, leading chemical educators such as **Ronald J. Gillespie** have put forward views and suggestions that may help surpass the above deadlock. In a commentary in the May 1997 issue of the *Journal of Chemical Education*, Gillespie pointed out that the current chemistry textbooks have not succeeded in interesting the vast majority of students or in providing them with an understanding of chemistry. As basic reasons for this, the author mentioned the difficulty students have in making the connection between the macroscopic world of observations and the microscopic world of atoms and molecules. Finally, he made a number of suggestions for textbook authors, among which central again was the need continually to emphasise the relationship between observations and atoms and molecules. Observations should be put first, thereby showing students that the theories and principles of chemistry are there not just to be learned, but to help in understanding the observations.

NOTES

[1] Ben-Zvi, *et al.* (1990, p. 183) distinguished the following three levels of functioning in chemistry (i) the macro level, (ii) the atomic molecular level, (iii) the multi-atomic level - the idea that even a small drop of water consists of many molecules with a certain organization and with their own internal structure.

[2] Current physical chemistry texts follow the logic of the three dimensions in Jensen's scheme either explicitly (e.g. Atkins, 1998) or implicitly (e.g. McQuarrie & Simon, 1997). Atkins follows the historical sequence and treats first the energy dimension, second the structure, and third chemical dynamics. McQuarrie and Simon on the other hand have put the emphasis on the molecular approach to physical chemistry (as it is featured in the title of the book), so they start with quantum chemistry.

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