The Philosophy of Chemistry as a New Resource for Chemistry Education

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The philosophy of chemistry is a new subdiscipline of the philosophy of science. Only a decade ago this philosophical field branched off from the traditional philosophy of science and acquired autonomy with respect to the philosophy of physics. This late development was mainly due to an assumption about the relationship between chemistry and physics: the impressive predictive power of quantum mechanics led most chemists, physicists, and philosophers of science to consider that chemistry can be completely reduced to physics. Dirac's famous dictum, according to which chemistry can be explained in principle by quantum mechanics *(1),* expresses a position that counts against the autonomy of chemistry and its status as a scientific discipline: whereas physics is conceived as a "fundamental" science that describes reality in its deepest aspects, chemistry is viewed as a "phenomenological" science, which merely describes phenomena as they appear to us.

From this perspective, since chemistry is only a branch of physics, it does not have specific problems in need of philosophical analysis: when considered in depth, the philosophical problems of chemistry are problems belonging to the philosophy of physics. Consequently, philosophical issues concerning quantum mechanics and relativity in physics engaged the attention of the philosophers of science during most of the last century. However, in the mid-1990s there was an upsurge of interest in the philosophy of chemistry. In this context, traditional assumptions about the relationship between chemistry and physics begun to be questioned: at present many authors deny that chemistry can be reduced to physics *(2)*. Although the philosophers of chemistry repeatedly emphasize this point, the preconceptions of the scientific community are still tied to a reductionistic position *(3)*.

This reductionistic standpoint has had a great impact on chemical education: there is an increasing tendency to explain some topics of chemistry, such as atomic structure and the periodic system, by means of physical principles *(4)*. Chemistry is indeed considered as a branch of physics because it deals with complex systems or particular processes that, nevertheless, could in principle be described and explained by means of quantum theory. This supposed difference between fundamental and phenomenological disciplines justifies the traditional hierarchy of the natural sciences, rooted in the positivistic thought of the end of the 19th century. Physics is at the top of the hierarchy because of its fundamental character, whereas chemistry is relegated to an inferior position to the extent that it can be derived from fundamental laws.

How can chemistry educators face the problem of reduction from this perspective? And, consequently, how can they argue for the autonomy of chemistry as a natural science? Is it possible to redress the traditional idea of the "superiority" of physics with respect to chemistry? These questions pose an interesting challenge: they show the need to introduce philosophical arguments as a new pedagogical resource in teaching chemistry. Of course this is not an easy task, yet the philosophy of chemistry offers the necessary tools. In fact, it not only allows teachers to answer the above questions: the philosophy of chemistry also leads them to a deeper understanding of the nature of chemistry. In this paper we shall address these issues by facing the traditional and subtle problem of the reduction of chemistry to physics.

Chemistry as a Scientific Discipline: The Usual Defense

When the problem at issue is reduction, the first step is to distinguish between ontological reduction and epistemological reduction. *Ontology* is the branch of philosophy (metaphysics, in particular) that studies reality, its structure, and the entities existing in it. *Epistemology* is the branch of philosophy dealing with human knowledge, its scope, and its limits. *Ontological reduction* refers to the ontological dependence of the *entities, properties, and regularities* of a stratum of reality upon the entities, properties, and regularities of another stratum considered as ontologically fundamental. Therefore, ontological reductionism is a metaphysical thesis that postulates the ontological priority of a certain level of reality to which all the other levels directly or indirectly reduce. *Epistemological reduction* is concerned with the relationship between *scientific theories:* a theory can be reduced to another when it can be deduced from the latter. Thus, epistemological reductionism is an epistemological thesis according to which science can be—or should be—unified by deducing all scientific theories from a privileged one.

Only during the last decades have some authors begun to argue for the liberation of chemistry from the constraints imposed by physical thought. In some cases, the autonomy of chemistry as a scientific discipline is defended on historical grounds, emphasizing the different historical traditions that marked the evolution of chemistry and physics *(5)*. However, the usual line of argumentation proposed by the philosophers of chemistry to defend the autonomy of chemistry points out the impossibility of reducing some chemical concepts (such as composition, bonding, or molecular structure) and properties (such as chirality) to fundamental physics. In other words, it is argued that the epistemological reduction

of the whole of chemistry to physics is impossible. For instance, Vemulapalli and Byerly *(6)* claim that epistemological reduction fails even in relatively simple cases: in general, the properties of a chemical system cannot be explained in terms of the properties of the physical micro-components; and even when the properties of a chemical macro-system can be derived from those micro-components, this requires additional assumptions related with macroscopic phenomena.

Equilibrium in nonideal multicomponent systems is one of the topics we have investigated: although there exists a method for relating the properties of a system to the activities of its components, the numerical values of the individual activities must be derived empirically from experiments on the system or theoretically from postulated intermolecular forces or from other ad hoc hypotheses coming from outside of the main body of the theory; in either case, they cannot be deduced from theories involving only the micro-components of the system.

van Brakel addresses the traditionally alleged reduction of thermodynamics to statistical mechanics from a similar perspective *(7)*. He correctly points out that, in general, temperature cannot be defined as mean molecular kinetic energy: this is true for perfect gases composed of idealized "billiard-ball" molecules in random motion, but not for solids, plasmas, or a vacuum. According to van Brakel, all the problems for reduction seem to be related to the macroscopic notion of equilibrium, the central notion of thermodynamics. For instance, the macroscopic concept of temperature only makes sense for systems in equilibrium—yet microscopically there is no such thing as equilibrium.

In a similar line of thought, Scerri and McIntyre *(8)* distinguish between "quantitative reduction" and "conceptual reduction". Quantitative reduction refers to the calculation of chemical properties from physical theories, in particular, quantum mechanics. This kind of reduction requires approximation techniques that can only be justified on a post hoc basis, that is, on the basis of the experimentally observed data that one is trying to calculate. On the other hand, conceptual reduction refers to the definition of chemical concepts in terms of physical concepts. According to the authors, this form of reduction is not possible due to the very nature of the chemical concepts themselves: the concepts of composition, bonding, or molecular structure cannot be expressed except at the chemical level. As the result of the failure of both kinds of reduction, we should "eschew the epistemological reduction of chemistry to physics" *(8)*.

Widespread agreement exists among philosophers of chemistry with respect to the impossibility of epistemologically reducing chemistry to physics. Nevertheless, nobody casts doubts on ontological reduction: chemical entities are, when analyzed in depth, no more than physical entities. For instance, Vemulapalli and Byerly *(6)* adopt the physicalist position that although the properties of a chemical system cannot be effectively derived from physical properties, chemistry remains ontologically dependent on fundamental physics: "Ontological reduction, in the sense of showing the dependence of all phenomena on constituent physical processes, has been a highly successful research program". From a similar perspective, Scerri and McIntyre *(8)* believe "the ontological dependence of chemistry on physics to be almost a foregone conclusion"; for them, the problem of reduction—which must be solved to preserve the autonomy of chemistry—is an epistemological and not an ontological question.

Of course, the impossibility of epistemological reduction safeguards the autonomy of chemistry as a scientific activity. However, the ontological dependence of chemistry on physics places chemistry in an inferior position with respect to physics in the hierarchy of natural sciences: whereas physics turns out to be a "fundamental" science that describes reality as it is in itself, chemistry is conceived as a "phenomenological" science that only describes phenomena, that is, "apparent" facts. The question is why we have to accept this conclusion. Here we have a philosophical problem and, consequently, we need philosophical arguments to address it. In the next sections we shall argue that the direct reference of a scientific theory is not the independent reality, but a scientific model. We have no access to reality independently of a model: it is the model, built in terms of the concepts of the theory, that cuts an ontology out of the reality in itself. When this point is recognized, the traditional assumption of the ontological reduction of chemistry to physics can be reassessed from a new philosophical perspective.

The Notion of "Model" in Science

The word "model" is widely used in everyday language and in all scientific disciplines. Here we shall focus on the use of the notion of model in factual sciences, where theories supposedly describe the features and regularities of reality. It is usually assumed that reality always involves a huge number of factors, in such a way that it is too complex for an exhaustive description; moreover, in many cases the precise specification of certain properties is an impossible task because of the unobservable character of the properties themselves. For these reasons, scientists always work with idealized systems, abstract entities in which only the relevant variables are considered and some properties of the unobservable elements are assumed. Such abstract entities are the *models* of a real system; for instance, a model of a real pendulum is constructed by disregarding friction, or a real gas is modeled as a collection of hard spheres interacting according to the laws of elastic collision.

A scientific model must have certain features in order to be a good model: simplicity, self-consistency, power, and flexibility *(9)*. The construction of a model is not an easy task, since it involves different operations that require scientific skills and creativity; for instance, ignoring external or internal factors, postulating certain ideal entities, or even assuming the unobservable structure of the system. These different operations—which are always combined in the construction of a particular model—show that the relationship between model and reality is not as simple as usually supposed: usually, it is not a "pictorial" relationship that assigns one element of the model to any element of reality. It is a complex relationship in which many variables of the model may not be directly accessible, for instance, in the case of unobservable properties. The strict correspondence between model and reality must be preserved only in the case of directly measurable variables: it is precisely the measurement of the values of such variables that allows us to assess not only the empirical value of the theory but also the adequacy of the

model for representing the real system. As Mary Hesse says in her classic account of models in science *(10):*

> I would say, for example, that a three-dimensional space curved in a fourth dimension is a perfectly good *model* in relativity theory, but it is certainly not picturable. A model, for me, is any system, whether buildable, picturable, imaginable, or none of these, which has the characteristic of making a theory *predictive.*

Model construction is well known as a central activity in the scientific practice of chemistry: the use of models pervades chemistry education from chemical kinetics *(11)* to organic chemistry *(12)*. Erduran *(13)* points out, however, that the role of models in chemistry is being gradually replaced by the application of quantum mechanics because it is conceived as the fundamental theory of nature. But this teaching approach ignores a central point: in chemistry education it is necessary to emphasize the qualitative aspects of chemical processes. Although a quantum description may offer a different and fruitful perspective, it does not explain the vast diversity of the observable chemical phenomena. These two approaches have been extensively discussed in contemporary literature *(14)*.

Distinguishing between "Model" and "Models"

Although science is usually thought to describe reality, the elucidation of the notion of scientific model shows that the direct reference of a scientific theory is not a real system, but a model of the system. In other words, the links between theory and reality are *always mediated by a model.* But there is not a single model for a system: reality may be modeled in many different ways, according to the particular viewpoint of the scientist in each case. Therefore, a given model cannot be considered as "better" than another in an absolute sense, but only with respect to the specific perspective of the research. Of course, some models are more complex than others, yet this fact does not mean that a complex model has to be preferred over a simpler one: in many cases, general properties of a system may not be accounted for by the most detailed and complex model. For instance, to model a gas in terms of thermodynamic variables such as temperature, pressure, and volume supplies information that is not available in a detailed model designed in terms of mechanical variables like the positions and velocities of the component molecules.

The fact that many different models may be good models for a single system has been recognized in the literature on the philosophy of science *(10);* however, the deep implications of this fact are usually passed over. In general, the coexistence of equally acceptable models is conceived in pragmatic terms: the decision about the proper model depends on the particular interest of the scientist or the specific goals of the research. At the same time, it is generally assumed that certain models—usually, microscopic models—are "closer" to describing reality than others. For instance, a mechanical model describes the real and intrinsic nature of a gas better than a thermodynamic model. Based on this assumption (in spite of the failure of epistemological reduction), many authors still claim that, from an ontological point of view, temperature is no more than the mean value of the kinetic energy of the molecules of a gas *(15)*.

When it is accepted that reality can be modeled in many different yet equally adequate ways, why are the microscopic models endowed with that "closeness" to reality? Why is it usually assumed that a quantum model of a chemical system is "superior" to a model in terms of chemical variables? The reason is again rooted in the philosophical premise of ontological reductionism: even though the full epistemological reduction of chemistry to physics is not possible, the reduction of the chemical world to the world of physics cannot be denied. As a consequence, when the construction of a quantum model is possible, it is preferred since it is "closer" to describing the "true" fundamental reality. Once again, although the methodological role of models in chemistry is accepted, ontological reduction is still present to determine the way in which the relationship between models and reality is conceived.

In recent years, some authors have begun to challenge the traditional assumption of ontological reduction by appealing to symmetrical relations between the discourses of chemistry and physics or to autonomous though related levels of reality. This new perspective recognizes the fact that we have no access to reality in itself independently of a model built in terms of the discourse and the conceptual scheme of a particular theory. As we shall see, such a philosophical viewpoint places chemistry in the same hierarchical position as physics within the context of natural sciences by justifying the ontological autonomy of the chemical world.

The Autonomy of the Chemical Ontology

Somebody could ask about the need of addressing ontological issues in the context of the relationship between chemistry and physics: if the failure of epistemological reduction is sufficient to guarantee the methodological autonomy of chemistry with respect to physics, ontological questions do not need to be discussed. However, when we ignore ontological issues, we miss an important philosophical question: why is chemistry a "secondary" science? The answer to this question strongly depends on the assumption of ontological reduction: if the physical reducing realm has ontological priority on the chemical reduced world, the chemical concepts that are non-reducible to quantum mechanics refer to apparent or secondary entities endowed with a derived ontological status. For instance, molecular shape turns out to be only a *"powerful and illuminating metaphor" (16).* Under this assumption, whereas physics describes the deepest and fundamental structure of reality, chemistry is a secondary science that studies "metaphorical" entities not really existent.

In recent years, some authors have addressed ontological questions related to the referring character of chemical descriptions. One of them is van Brakel *(17–18)*, who discusses the reference of the physical and the chemical discourses under the paradigm of the mirror of nature *(18):*

> Each mirror gives a different autonomous picture of (part of) the world, but one mirror—the ideal physical one—mirrors reality as it *is* (ontologically speaking). All other mirrors…picture mere appearances, without cosmic significance.

According to the author, this paradigm should be abandoned by denying the asymmetric relationship between chem-

istry and physics: "The same event can have a chemical and a physical description,…but no privileged description exists" *(18)*. In fact, if quantum mechanics would turn out to be wrong, it would not affect the chemical knowledge about molecular shape, bonding or chirality. As a consequence, the relationships between chemistry and quantum mechanics "are best seen as symmetrical relations" *(18)*. On this basis, van Brakel concludes that *(18):*

> [W]e could be tolerant enough to leave equal *ontological* room for manifest water, water in terms of the thermodynamic theory of substances, the molecular structure of water ("constructed" out of spectroscopic measurements), the "proper" quantum mechanical equations for an isolated water molecule, and experiments with isolated water molecules which, depending on the measurement technique, show more of less of the "classical" molecular structure.

An even more interesting case of this new interest in ontological issues is the position of Scerri about the interpretation of the concept of orbital. Scerri admits that, under the assumption of ontological reduction, terms such as "orbital" or "molecular shape" "philosophically speaking, are nonreferring terms" *(19)*. But chemists are often realists in the sense that they believe in orbitals as though they were real and concrete entities; chemists and chemical educators show a great reluctance to abandon that realistic interpretation in spite of the theoretical assumption that orbitals do not correspond to anything in the real world. In this sense, Scerri *(19–20)* proposes an intermediate position between realism and ontological reductionism, which leads to the autonomy of chemistry as the result of a form of liberation from "physics imperialism". According to this new view, the interpretation of scientific terms is theory-contextual *(20):*

> Not only is the question of the realistic as opposed to the antirealistic interpretation of the orbital concept contextual with regards to whether one considers chemistry or theoretical physics, but even within chemistry it emerges that practitioners in different subfields generally adopt opposite interpretations.

In other words, there is no single ontology to which all the scientific knowledge refers. On the contrary, each science, and even each theory, operates on its own ontological level, in which the entities and regularities referred to by the theory may be legitimately considered as real: there is no contradiction in conceiving of orbitals as existent entities at the chemical level but not real in the quantum mechanical world. For this reason Scerri argues for the view of "*autonomous though related levels of reality*" *(20),* in terms of which the autonomy of the secondary sciences can be consistently defended.

Even more recently, and following the way opened by van Brakel and Scerri, we have defended the ontological autonomy of the chemical world on the basis of a philosophically founded ontological pluralism *(21)*. In particular we show that, from a position rooted in Kantian philosophy, the ontology of science always results from the synthesis between a conceptual scheme, provided by the scientific theory, and the noumenal, independent reality. Any scientific model is built in terms of the contextual scheme of a theory; as a consequence, the model is the vehicle to cut the corresponding ontology out of the independent reality. On the other hand, since different theories describe reality successfully, there are different legitimate conceptual schemes, each one of which constitutes its corresponding ontology through its models. If we had access to the noumenal reality independently of a model, we could decide which model is "closer" to the "real" ontology. But since we always describe reality from the perspective of a model and its associated conceptual scheme, the privileged viewpoint of "God's eye" does not exist: there is not a single "true" ontology with respect to which some models are closer than others. In other words, all ontologies have the same metaphysical status because all of them are constituted by equally objective descriptions.

From this philosophical position, it is not yet possible to conceive the description of reality in itself: even quantum theory and quantum models correspond to a particular conceptual scheme that constitutes the quantum ontology. On the other hand, chemistry involves its own conceptual framework and, as a consequence, refers to its own ontology. As a consequence, chemical concepts like composition, chemical bonding, molecular shape, and orbital refer to entities and properties belonging to the chemical ontology, which only depends on the theory that constitutes it and does not derive from an ontologically more fundamental level of reality. In this way, chemistry begins to be conceived not as a secondary field devoted to study of secondary and derived entities, but as a scientific discipline referring to an ontologically autonomous realm. The ontological autonomy of the chemical world places chemistry in the same hierarchical position as physics within the context of natural sciences.

The Case of the Concept of "Orbital"

The case of the concept of orbital is an interesting example for illustrating how philosophical questions have relevant repercussions not only on the foundations of chemistry but also on the way in which chemistry is taught and learned.

In 1999, the prestigious journal *Nature* spectacularly announced that the d-orbitals of Cu_2O had been observed *(22)*. This news rapidly pervaded the scientific community *(23)*; for instance, some authors stated that such an experimental work had to be considered as the first step toward the understanding of high-temperature superconductivity *(24)*. Some months later, another research team claimed to have obtained an image of molecular orbitals *(25)*. However, some authors immediately opened the debate by claiming that the interpretation of those experimental results was conceptually mistaken *(26–27)*: since quantum mechanics only includes the concept of wave function, the concept of orbital is deprived of reference in the real world; therefore, it is not possible to obtain an image of an nonexistent entity.

Although this debate may seem rather technical and specialized, it is a manifestation of a problem that has deep consequences for chemistry education. In fact, the concept of orbital is a key concept in teaching: it is used to explain bonding, chemical structure, and reactivity. Therefore, chemistry educators cannot do without such a concept in their teaching. For this reason, educators naturally accept orbitals as real entities existing in the world. But this position clashes with

the assumption according to which we have to follow what quantum mechanics has to say about the subject: only the concept of wave function is legitimate; the term "orbital" has no reference in the real world. In particular, the realistic viewpoint about orbitals adopted by chemistry teachers turns out to be incompatible with their own position when introducing quantum mechanics as the underlying explanatory theory of chemical phenomena. This problem is explicitly pointed out by Scerri *(4)* in an article published in this *Journal,* when he raises the question: "Can orbitals be real in chemistry but not in physics?". It seems quite clear that this paradoxical situation has negative consequences for a deep understanding of the discipline: students are faced with the alternative of living in a sort of conceptual schizophrenia or accepting that chemistry describes mere apparent or "metaphorical" phenomena.

This serious pedagogical problem can be avoided by adopting a well-founded philosophical position. Once we have recognized that each accepted theory constitutes its corresponding ontology through its own conceptual scheme, all so constituted ontologies have the same metaphysical status and are equally objective. In other words, since there is not a single "true" ontology, the chemical world is as real as the physical world. As a consequence, the chemical concept of orbital does not need to be referred to quantum mechanics to acquire legitimacy: orbitals are real entities belonging to the chemical ontology. Therefore, it is possible to speak about orbitals in the ontological level of chemistry and about wave functions in the ontological level of physics with no contradiction and without being forced to confine orbitals to the realm of illusion. Summing up, we believe that this philosophically founded ontological pluralism can overcome many conceptual difficulties that chemistry teachers have to face in the classroom, because ontological pluralism provides philosophical support for the realistic position, usually adopted in a naive or pre-reflexive way.

Conclusions

Research in chemistry education in recent years has made important advances by introducing the use of technology in the classroom and of models of information processing, by proposing changes in chemistry content, by improving laboratory activities, and so forth. However, little attention has been paid to the question of the nature of chemistry as a scientific discipline and, in particular, to the relationships between chemistry and physics. In this context, it is necessary to emphasize that philosophical issues of epistemology and ontology are essential for an in-depth understanding of the discipline.

For these reasons, we do believe that the philosophy of chemistry should become a new pedagogical tool that can guide educators in deciding how to balance descriptive and theoretical chemistry and what approaches to use in teaching chemical concepts. Since history and philosophy of science are implicit in chemistry itself *(28),* teachers should be capable of facing philosophical issues at their classes. As it has been empirically shown, not only in chemistry *(13, 29–31)*, but also in other scientific disciplines *(32–33)*, philosophical thinking contributes to the students' comprehension of science. In Scerri's words *(30):*

> It is not enough to train chemistry teachers about just the contents of chemistry courses and perhaps a little educational psychology. Chemical educators need to be introduced to the study of the nature of chemistry.

In summary, gaining insight on topics of the philosophy of chemistry has positive effects on the way that chemistry is taught and learned, and also leads educators to reach a better understanding of their own scientific discipline.

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