PHILOSOPHY OF CHEMISTRY

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Contents

Summary

This chapter presents an overview of some of the most developed topics in contemporary philosophy of chemistry according to current literature. After a brief introduction to the field (Section 1), the obstacles that have prevented the development of the discipline are reviewed as well as its vigorous present (Section 2). Section 3 concerns with the old and complex problem of the relation between chemistry and physics. Two examples that involve these two disciplines −the ontological status of atomic orbitals and the problem of molecular structure− are analyzed in detail in Section 4 and Section 5, respectively. The nature of chemical bond is addressed in Section 6. One of the main categories of the chemical world is the concept of 'element', a notion that shows serious difficulties when has to be defined; this is reviewed in Section 7. Several problems concerning the foundations of the periodic table −the icon of chemistry and, probably, of whole modern science− are developed in Section 8. Section 9 deals with models and explanations. The renewed interest in the study of natural kinds in the world of chemistry is developed in Section 10. Lastly, some other topics under philosophical reflection as well as trends in the field are outlined.

1. Introduction

Chemistry has a venerable history as scientific discipline and is nowadays one of the most important natural sciences together with physics and biology. But what is chemistry about? Even though it seems to be a question, in principle, easy to answer, by exploring the different interpretations it is possible to see that the responses differ: while some authors say that chemistry is the science of substances and their transformations into other substances, it is also claimed that chemistry is the science that studies matter and all its changes, and has also been pointed out that chemistry concerns with the study of molecules. This problem, which concerns to the foundations of the discipline, is a scientific-philosophical problem. Likewise, a new question arises: what is a substance, a molecule, and what is the relation between them?

Philosophy of chemistry is the branch of philosophy of science whose aim is mainly a critical reflection on the chemical world from the viewpoint of the different chapters of philosophy, e.g. metaphysics, epistemology, and ethics. In particular, it involves the study of the concepts, theories, and methods of chemistry, the relationships with and also the differences from the concepts, theories, and methods of other special sciences. The traditional topics in philosophy of science (realism, reduction, modeling, explanation) are analyzed within the realm of chemistry. This chapter offers a survey of the main topics selected from the current literature on the subject matter. The goal then will be present the discussions in each of them.

2. A Brief History of the Philosophy of Chemistry

The history of the philosophy of science of the 20th century, especially the Anglo-Saxon tradition, shows that the philosophical problems of chemistry were virtually ignored or neglected. The obsession of philosophers of science with theoretical physics led them to pay little attention not only to philosophical reflection on chemistry, but also to every other branches of science. In the case of chemistry, this situation is particularly surprising given its rich history as a scientific discipline, and its position in the current context of the natural scmulapalliiences.

Although chemistry has a wide popularity since the mid-nineteenth century, there were only a few isolated publications in the field of the philosophy of chemistry in the first five decades of the twentieth century. In the period from 1949 to 1986, a number of Eastern European magazines published philosophical works on various subjects of the chemical world.

The causes that have hindered the development of philosophy of chemistry are varied. Among them, quantum mechanics has played a decisive role in the relationship between chemistry and physics: the stunning success of the theory led physicists and philosophers of science to accept that chemistry can be completely reduced to physics. This view is best expressed in the famous *dictum* by Paul Dirac in 1929, according to which the whole of chemistry could be deduced from quantum mechanics.

Of course, this traditional assumption not only deprives the philosophy of chemistry of legitimacy as a field of philosophical inquiry, but also counts against the autonomy of chemistry as a scientific discipline: whereas physics turns out to be a "fundamental" science that describes reality in its deepest aspects, chemistry is conceived as a mere "phenomenological" science, that only describes phenomena as they appear to us. This supposed difference between both disciplines agrees with the traditional hierarchy of the natural sciences, rooted in the positivistic thought of the end of 19th century. Due to its fundamental character, physics is at the top of the hierarchy, whereas chemistry is relegated to an inferior position, to the extent that it can be derived from fundamental physical laws.

Closely related to that assumption, it is possible to add a naive externalist realism adopted, in general, by physicists and chemists: the object of our knowledge is a single ontology. That is, on the basis of a reductionist approach to the relation between the chemical world and the physical world on the one hand, and a metaphysical realism, on the other hand, chemistry is considered only a chapter of physics and chemists are perceived as scientists doing 'applied physics'. But, as Nikos Psarros stresses, this leads to the conclusion that chemistry is not susceptible to philosophical analysis, and this is itself a philosophical statement (see Psarros 1998).

In addition, other factors have contributed to the delay of the subdiscipline. The perception that chemistry is closely linked to technology (manufacture of medicines, industrial products, etc.) plus certain anti-scientific, and especially anti-chemical campaigns in the media, along with the current environmental problems, do not favor the image of chemistry in society. Another argument against the existence of an interdisciplinary research field between physics and chemistry is concerned with the absence of a 'crisis' in the chemical sciences to mark the course of its evolution. This crisis is very significant in the development of physics in the late nineteenth and early twentieth century with the advent of quantum mechanics and relativity theory. Similarly, Neo-Darwinian' theories greatly modified the further development of biology, whose space of philosophical thinking began in the 1970s.

The neglect of the philosophy of chemistry as a legitimate field of philosophical inquiry suffered a backlash in the mid-1990s, particularly in Great Britain, United States, and Germany along with some isolated groups in The Netherlands, Belgium, and Italy start to arise from late 1980. Since then, chemists, philosophers, and historians of chemistry began to work in relatively formal ways, holding regular meetings in various countries. In addition, the building of bridges between chemistry and humanities was powered by the chemical industry when the public image of chemistry was at its worst level. In 1994 a series of international conferences were held in London, Karlsruhe, Marburg, and Rome. Since 1997 the International Society for the Philosophy of Chemistry carries out annually symposia. In the last years, the symposia were held in Bogotá (2011) and Montevideo (2013), expanding thus the subdiscipline to South America.

Two journals emerged in this context: *Hyle – International Journal for Philosophy of Chemistry* (since 1995) and *Foundations of Chemistry* (since 1999). Some excellent monographs and anthologies have been published to date by prestigious publishers (Oxford University Press, Boston Studies in the Philosophy of Science, Elsevier). Similarly, an online discussion forum (*Philchem*) is leading the attempt to add a great number of chemists and philosophers to this new subdiscipline.

3. The Problem of the Relationship between Chemistry and Physics

Historians of science know very well that chemistry and physics are inheritors of very different traditions. Modern physics is the result of an unexpected but fruitful combination of the mechanicism propounded by Descartes with the corpuscularism formulated by Robert Boyle and other British thinkers. On the contrary, chemistry can be considered as a derivation of medieval alchemy, from which chemistry inherited a major interest in practical applications. While physics aimed at describing and explaining reality "in itself", the main goals of chemistry always involved the manipulation and transformation of substances. As a consequence, until the second half of the 19th century, chemistry and physics were two independent disciplines, each one with its own purposes and methodologies.

The situation begun to change with the advent of quantum mechanics, whose impressive success supported the idea that chemistry is a branch of physics: chemistry supposedly deals with complex systems and particular processes which, nevertheless, could in principle be described and explained by quantum theory alone. As early as 1929, Paul Dirac expressed the conviction that, since the underlying laws governing the behavior of the atom's components became known, to do chemistry meant to deal with the equations supplied by physics: "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 the exact applications of these laws lead to equations which are too complicated to be soluble" (Dirac 1929, p. 714).

Dirac's words have often been considered the clearest pronouncement about the derivability of chemistry from physics. However, an earlier claim made by the physicist Paul Langmuir in 1921 is scarcely known, although it expresses an even stronger position: "I think that within a few years we will be able to deduce 90 percent of everything that is in every textbook on chemistry, deduce it as you need it, from simple ordinary principles, knowing definite facts in regard to the structure of the atoms" (Scerri 1994, p. 162). This view rapidly acquired the status of a dogma, and was adopted by many authors active in the fields of chemistry, physics, and philosophy.

The problem of the relationship between chemistry and physics, usually known as 'the problem of reduction of chemistry to physics', is probably the most mature topic of the field. This problem can be stated as follows: What is the relationship between the chemical world and the physical world? Is chemistry an autonomous scientific discipline or, by the contrary, is a mere branch of physics? Is there an interdependent relationship between chemistry and physics? To address these questions, philosophers of chemistry take into account the scientific, philosophical, and historical approaches of the problem.

When the problem at issue is reduction, the first step is to distinguish between ontological reduction and epistemological reduction. In its traditional version, 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 some authors have 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. 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 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 (see Vemulapalli and Byerly 1999).

Van Brakel addresses the traditionally alleged reduction of thermodynamics to statistical mechanics from a similar perspective. 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 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 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, the epistemological reduction of chemistry to physics should be avoided (see Scerri and McIntyre 1997).

Summing up, the traditional assumption that chemistry is just a branch of physics has begun to be challenged by noting that chemical concepts and laws can hardly be deduced from physical theories. In particular, crucial chemical notions such as chemical bond, chirality, molecular shape or orbital among others, are not amenable to rigorous quantum-mechanical treatment. Of course, such a failure guarantees the methodological autonomy of chemistry as a scientific discipline: to the extent that there are specifically chemical concepts, chemists can continue with their work with no worry, since physicists will not replace them in the laboratories.

As we have seen, the discussions about the alleged reduction of chemistry to physics follow the traditional philosophy of science of 20th century in focusing on epistemological issues: the conclusion is that not all the chemical concepts and laws can be deduced from the concepts and laws of physics. However, ontological questions usually did not go further than unquestioningly accepting ontological reduction.

By contrast, Lombardi and Labarca claim that when ontological issues are ignored, 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, the notion of molecular shape turns out to be, in the Wooley's words, only a "powerful and illuminating metaphor".

Some philosophers of chemistry have directed their attention to ontological questions related to the referring character of chemical descriptions. One of them is van Brakel who asserts that it is necessary to abandon the paradigm of the mirror of nature, according to which 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 this author, this paradigm should be abandoned by denying the asymmetric relationship between chemistry and physics, and by claiming that no privileged description exists. Furthermore, van Brakel stresses the fact that the failure of epistemological reduction implies nothing about the interpretation of chemical concepts and their relation to what is "real". If there is no privileged description, chemical and quantum-mechanical concepts may be both 'powerful and illuminating metaphors'. On this basis, van Brakel concludes that we should 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.

Lombardi and Labarca have stressed that the failure of epistemological reduction is not strong enough to remove the idea of a hierarchical dependence of chemistry with respect to physics. The rejection of the secondary position of chemistry and the defense of the legitimacy of the philosophy of chemistry require a radically different philosophical perspective, which denies not only epistemological reduction but also ontological reduction. In this sense, they propose a philosophically grounded ontological pluralism to support the ontological autonomy of the chemical world and, with this, to reverse the traditional idea of the “superiority” of physics in the context of natural sciences. This framework allows the coexistence of different but equally objective theory-dependent ontologies interconnected by nomological, non-reductive relationships (see Lombardi and Labarca 2005).

It has also been pointed out that the reduction of chemistry is more ambiguous and multi-faceted than generally supposed. The success or the failure of reduction depends on what one requires from quantum chemistry. Scerri advocates for a dialogue among philosophers of chemistry, and for the engagement in dialogue with theoretical chemists, just as philosophers of physics have maintained a dialogue with contemporary physicists (see Scerri 2007a).

At the same time, notions such as ‘emergence’ and ‘supervenience’ have also been proposed to understand the relationship between the chemical and the physical world. In this complex scenario, it has been argued that given the enormous variety of possible intertheoretical relations, the proliferation of definitions of reduction, supervenience, emergence, unification, and so on, a possible way to follow is give perspicuous renderings of the practice of chemistry, that is, to analyze case studies and further discussions about them, instead of bickering whether chemistry can be reduced to physics, supervenes on it, can be unified with it, and similar “metaphysical” concerns (see van Brakel 2003). According to van Brakel, the question ‘can chemistry be reduced to physics?’ is meaningless because the terms ‘chemistry’ and ‘physics’ are far too vague. Thus, we need more concrete questions such as ‘Can one give a statistical mechanical or quantum mechanical description of the three-phase line between a solid, a liquid, and a vapor phase?’ or ‘Can we understand the notion of ‘chemical substance’ in a quantum mechanical discourse?’ (see van Brakel 2010).

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Biographical Sketch

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