

The philosophy of chemistry

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Although chemistry is by far the largest scientific discipline according to any quantitative measure, it had, until recently, been virtually ignored by professional philosophers of science. They left both a vacuum and a one-sided picture of science tailored to physics. Since the early 1990s, the situation has changed drastically, such that philosophy of chemistry is now one of the most flourishing fields in the philosophy of science, like the philosophy of biology that emerged in the 1970s. This article narrates the development and provides a survey of the main topics and trends.

Until recently, philosophers stubbornly neglected chemistry as if it were virtually non-existent. There have been many attempts to explain this strange fact. Is it the lack of 'big questions' in chemistry, its close relationship to technology or the historically rooted pragmatism of chemists and their lack of interest in metaphysical issues? A widely held view sees the alleged reduction of chemistry to physics (quantum mechanics) as the main obstacle. If chemistry were only an applied branch of physics, there would be no genuine philosophical issue of chemistry. Indeed, some prominent theoretical physicists as well as some followers of logical positivism fostered that view by making bold reductionist claims since the early 1930s.

The philosophy of chemistry before 1990

The philosophical neglect of chemistry

Historical reasons for the neglect of chemistry by philosophers are both deeper and more trivial. First, the rise of early-modern epistemology, both of the rationalist and the empiricist branch (with the exception of Francis Bacon), was closely connected to the rise of mechanical philosophy, which strongly opposed various kinds of chemical philosophy. Second, because modern physics has its theoretical roots in analytical mechanics, which still in 1800 did not belong to the physical sciences but to applied mathematics, 19th-century philosophical debates over scientific method were essentially about establishing mechanics as a physical science. Kant's former dictum that only mechanics is a science proper because it has an *a priori* foundation in mathematics was an early and influential view in these debates. That made it easy for Kantians to focus on mechanics and ignore the rest of the sciences. Third, most of the members of the Vienna and Berlin Circles (e.g. Moritz Schlick, Rudolf Carnap, Hans Reichenbach and Carl Gustav Hempel), who would become extremely influential in creating a discipline of philosophy of science, were philosophically minded physicists who shaped the

field by reflections on relativity theory and the notion of probability in statistical mechanics. Following the example set by their 'founding fathers', the next generation of philosophers of science, particularly in the USA and in Germany, made a name for themselves with their numerous dissertations on relativity theory and quantum mechanics. Philosophers of theoretical physics soon occupied virtually all of the newly established chairs in philosophy of science – a situation that has not much changed since.

The obsession of philosophers of science with theoretical physics led them to neglect not only chemistry but also every other branch of the sciences, including experimental physics. Relicts of the older meaning of 'physics', as the generic term for the natural sciences still in the 19th century, and the ambiguity of the English term 'physical' contributed to the confusion of philosophy of physics with general philosophy of science. It was not until the early 1970s that biologists first reacted to the narrow focus and established their own groups together with biologically minded philosophers. It took another two decades for a similar movement to emerge in chemistry. In some sense, philosophy of science now repeats the 19th-century process of the ramification and professionalization of the natural sciences.

The exception: philosophy of chemistry in dialectical materialism

There is only one remarkable exception to the rule of philosophical neglect. In Engel's dialectical materialism, chemistry featured prominently as a case against what he called vulgar or French materialism. Not only did Engels, like Comte, claim that 'chemical forms of movement' were distinct from mechanical, biological and social forms, but chemical phenomena also served to illustrate universal laws of his doctrine. For instance, acid–base-reactions could be used to exemplify his 'law of contradictions' and, when performed by titration with some colourful indicators, they wondrously visualized his 'law of change from the quantitative to the qualitative'. With their established role in tertiary science education and their official task to interpret particular scientific facts, problems and developments within the general framework of dialectical and historical materialism, philosophers of science in Marxist countries produced a wealth of studies on modern chemical phenomena, laws, theories and sub-discipline formation. It is impossible to review the material here, as there are studies on virtually every philosophical issue [1]. At least it might be said that Engels' 19th-century framework was liberal enough to elaborate on such sophisticated topics as the relationship between quantum chemistry and quantum mechanics, but epistemologically too naive to deal

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with quantum chemical concepts such as Pauling's resonance structures.

The vacuum filled from various sides

As long as professional philosophers did not care about chemistry in western countries, scholars from various disciplines approached the field from different angles, each from their own perspective and with specific questions. In particular, scholars of chemistry education have always recognized the need to reflect on methods and to work on the clarification of concepts, such that most of their journals are still a rich source for philosophers. Working chemists usually stumbled on philosophical issues when their own research challenged them to reflect on received notions or methodological ideas (Fig. 1). Prominent examples included Benjamin Brodie, Frantisek Wald, Wilhelm Ostwald and Pierre Duhem, but the series of philosophizing chemists did not stop in the early 20th century. For instance, Friedrich Paneth's work on isotopy made him think about the concept of chemical elements [2]; and Alwin Mittasch's reflection on the notion of causation in chemistry arose from his studies on chemical catalysis [3]. Faced with the reluctance by established scientists to accept his own theories and based on his detailed experience in laboratory practice, Michael Polanyi challenged received rationalist methodologies of science by calling for social factors and the role of tacit knowledge [4]. Edward T. Caldin, who as any other chemist primarily worked in the laboratory, argued that the then prevailing Popperian methodology simply failed to grasp the role of experiments in the experimental sciences and the way scientists deal with theories [5].

Since the late 1970s theoretical chemists, who worked hard on the development of quantum chemical models for chemical purposes, also began to question the naive reductionist, albeit common, view among western philosophers of science, according to which chemical concepts and laws could simply be derived from quantum mechanical principles. Guy Woolley, in a seminal paper [6], argued that the concept of chemical structure cannot be deduced

from quantum mechanics. Hans Primas [7] devoted a whole book to the issue of reductionism, arguing that quantum mechanical holism does not allow the derivation of statements about chemical objects without further assumptions. Giuseppe Del Re and Christoph Liegener considered chemical phenomena to lie on a higher level of complexity that emerges from but does not reduce to the quantum mechanical level [8].

Because the border between philosophy and history of science has never been sharply drawn, not surprisingly many historians of chemistry approached the field by dealing with philosophical issues of the past, of which two for some time ranked so high among historical topics of chemistry that it is impossible to review the literature here. These are the metaphysical issue of atomism and the methodological issue of conceptual change and theoretical progress exemplified by Thomas Kuhn's treatment of the 'chemical revolution'. Of course both topics also attracted many philosophers, especially the second topic, which initiated collaboration and competition, and a flood of case studies. Challenged by the historiographic rigor of their colleagues, the philosophers' case studies frequently did not differ much from historical work, except by their greater ambition to make them a case for or against a general methodological position, such as pro or con Popper, Kuhn, Lakatos and so on. Yet, picking up chemical stories as evidence for one or the other general methodology in science is hardly a conclusive argument, nor can it count as philosophy of chemistry proper. This has never been better criticized than by chemist-philosopher Elisabeth Ströker in one of the most detailed historical accounts of the 'chemical revolution' [9].

More than in other historical branches, historians of chemistry approached philosophical issues with a wealth of fine studies on the history of ideas, theories, and methods and the mutual impact between chemistry, on the one hand, and its neighbouring disciplines, philosophy, humanities, religion and the general society, on the other [10]. Insofar as their goal was a better understanding of our present intellectual culture and the role of chemistry therein, they did a job that professional philosophers refused to do.

Interestingly, the few western philosophers who dealt at book-length with chemistry (e.g. Gaston Bachelard, François Dagonet and Elisabeth Ströker [11]) were strongly historically minded. I will come back to this point which is by no means pure chance.

The emergence of the philosophy of chemistry since 1990 *Establishing socially*

The most obvious distinction between the previous period and the emergence of the philosophy of chemistry in the 1990s was its social establishment. Whereas former scholars worked in relative isolation, the new generation sought contact with each other and the exchange of ideas. Since the late 1980s, chemists, philosophers and historians of chemistry began to gather in more or less formal working groups with regular meetings in many countries. In addition, there was a call from the chemical industries to build bridges between chemistry and the humanities at a time when the public image of chemistry was at its worst [12]. In 1994, national meetings grew to a series of international

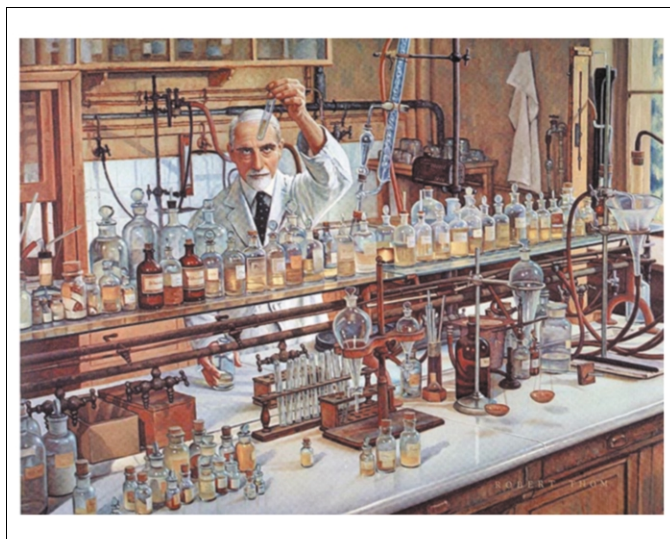


Fig. 1. The French chemist Ernest Fourneau (1872–1949) in his laboratory. Reproduced, with permission, from the Edgar Fahs Smith Collection at the University of Pennsylvania Library.

conferences in London (March), Karlsruhe (April), Marburg (November) and Rome (December). By 1997, international ties enabled the formal establishment of an International Society for the Philosophy of Chemistry with annual summer symposia (Bradford, UK, 1997; Cambridge, UK, 1998; Columbia, SC, USA, 1999; Poznań, Poland, 2000; Loughborough, UK, 2001; Washington, DC, USA, 2002). Two journals were launched, *Hyle: International Journal for Philosophy of Chemistry* (since 1995, edited by the author) and *Foundations of Chemistry* (since 1999, edited by Eric Scerri). The parallel rise of internet technologies, which were soon employed for many purposes (e-journal, e-mail discussion forum, regularly updated bibliography, information boards for conferences, syllabi and so on) has essentially helped establish a community and attract a wider audience.

Rediscovering the philosophical classics

The historical neglect of chemistry is, in part, also an artefact of historians of philosophy who simply ignored what philosophical classics had to say about chemistry. This has been brought to light in a growing number of recent studies. A prominent example is Kant's *opus postumum*, which was not published before the early 20th century (with an English translation as late as 1993), although it contained a complete revision of his former theoretical philosophy against the background of the new Lavoisian chemistry [13]. Also Hegel's extensive writing on chemistry, albeit placed in his most famous books, became subject to scholarly investigations only recently [14]. And whilst Duhem's *La Théorie Physique. Son Objet – sa Structure* (1905–1906) has long been a classic in the philosophy of science and translated into many languages, his *Le Mixte et la Combinaison Chimique* (1902) was translated into English only in 2002 [15]. Even Rousseau had written a book on chemistry [16]. It is up to historians of philosophy to explore further writings on chemistry in philosophical classics such as Leibniz, Schelling, Schopenhauer, Herschel, Comte, Peirce, Broad, Alexander, Mill, Cassirer and Bachelard.

Struggling with reductionism

Still an important topic in today's philosophy of chemistry is reduction (Box 1) – not of biology to chemistry but of chemistry to physics. Criticism of reductionism plays different roles.

First, it provides a more precise and technical understanding of the limits of quantum-mechanical approaches to chemistry, and thereby defines independent areas for the philosophy of chemistry. For instance, in a series of papers, Eric Scerri [17] has convincingly argued that quantum-mechanical approaches are not able to calculate the exact electronic configuration of atoms. Since Bohr's early atomic theory, it has been taken for granted that the electronic configuration of atoms determines the chemical properties and thus the place of each element in the periodic table. The reduction of the periodic system to quantum mechanics was claimed on the basis that the exact electronic configuration could be calculated for each atom, such that the complete chemical order of the periodic system could be derived from first principles. Since that

Box 1. Versions of reductionism

Metaphysical or ontological reductionism claims that the supposed objects of chemistry are actually nothing else than the objects of quantum mechanics and their relations governed by quantum-mechanical laws. In its strong, *eliminative* version, ontological reductionism states that there are no chemical objects proper. *Microstructural essentialism* à la Hilary Putnam and Saul Kripke reformulates metaphysical reductionism in semantic terms. It employs a certain meaning theory, which is tailored to the needs of metaphysical reductionism, to claim that the proper meaning of chemical substance terms, such as 'water', is nothing other than the (quantum-mechanical) microstructure of the substance. *Epistemological or theory reductionism* claims that all theories, laws and basic concepts of chemistry can be derived from first principle quantum mechanics (or quantum electrodynamics) as the more basic and more comprehensive theory. *Methodological reductionism*, whilst acknowledging the present failure of epistemological reductionist claims, recommends applying quantum-mechanical methods to all chemical problems, because that would be the most successful approach in the long run (*approximate reductionism*).

In addition, the popular notion that 'the whole is nothing but the sum of its parts' has frequently been related to reductionism, but it remains obscure what 'the sum of parts' means. In more articulated forms, the relationship between the properties of the parts and the properties of the whole are discussed. *Emergentism* claims that new properties of wholes (say, of water) emerge when the parts (say, oxygen and hydrogen) are combined. Although emergentism frequently comes with an antireductionist attitude, it can be a firm part of ontological and epistemological reductionism if the properties of the whole are explained or derived from the relationships between the parts. In recent times, many weaker versions of reductionism have been formulated under the label of *supervenience*. In a simple version, supervenience means that, although epistemological reductionism might be wrong, the properties of a whole asymmetrically depend on the properties of the parts, in such a way that every change of the properties of the whole is based on changes of the properties of or the relationships between the parts, but not the other way round.

has now turned out to be too hasty a claim, the periodic system is open to new philosophical analysis. Similar arguments can be found with regard to the concept of molecular structure, for which correspondingly reductionist claims were made before.

Second, the criticism of reductionism at the 'lowest' level of chemistry to quantum mechanics challenges microreductionism as a general metaphysical, epistemological or methodological position and thus contributes to general philosophy. In the most detailed philosophical study on various forms of reductionism (including supervenience and microstructural essentialism à la Putnam and Kripke), Jaap van Brakel [18] has made chemistry a case to argue for a kind of pragmatism in which the 'manifest image' of common sense and empirical sciences has primacy over the 'scientific image' of microphysics. For Nikos Psarros [19], rejection of reductionism is even a necessary presupposition of his extensive work on the culturalist foundation of chemical concepts, laws and theories that he seeks in pre-scientific cultural practices, norms and values. For many others, including myself, it supports a pragmatist and pluralist position about methods that distinguish clearly between fields of research where quantum-mechanical approaches are poor or even useless compared to other approaches, and those where they are strong and even indispensable.

Third, once reductionism had lost its credibility to secure the unity of the sciences, new relationships between the autonomous sciences, such as structural similarities and interdisciplinarity, became subject to both philosophical and historical investigations [20].

Adapting philosophical concepts

Because of their narrow focus on theoretical physics, concepts of mainstream philosophy of science frequently require considerable revision before they can shed light on chemistry. It is the gap between what Thomas Kuhn has called the 'mathematical' and the 'Baconian sciences' that philosophers of chemistry must bridge. Because chemistry is by far the largest scientific discipline, with enormous impact on every other experimental science, philosophers of chemistry also make valuable contributions to our philosophical understanding of the sciences when they adapt classical concepts for an understanding of chemistry. Examples, which are scattered around in the two journals (*Hyle* and *Foundations of Chemistry*) and in numerous general anthologies [21], include: the concepts of experiment, law, model, prediction, explanation, natural kinds, substance and process; the scientific approaches to concept building, model building and classification; the treatment of competing theories; methods of research in the sense of exploring the new; the role of instruments in research; and the distinction and relationship between science and technology. Also, the topic of scientific realism, sometimes misused to distinguish theoretical physics from the rest of the sciences that are thereby discredited as 'immature sciences', appears in new light if applied to chemistry, and even becomes a research methodological concept if applied to synthetic chemistry [22]. Whilst philosophers of mathematical physics have confined methodology to the 'context of justification', if not to proof theory, philosophers of experimental sciences like chemistry put emphasis on the 'context of discovery' (i.e. on scientific research methodology).

Analysing the structure of chemistry

Since each scientific discipline has its own fundamental concepts, methods and theories, philosophy of chemistry reaches a state of maturity, so to speak, when it focuses on peculiarities of chemistry. This not only requires a double competence in chemistry and philosophy but also a deep understanding of the history of chemistry because our present scientific disciplines, with all their peculiarities, are historical entities, snapshots in a process of development. Thus, unlike general philosophers of science, with their eternal, albeit personal, ideas of 'general science', philosophers of chemistry do merge with historians of chemistry to analyse fundamental concepts, methods and theories in modern chemistry. It is in these areas where much work has been done in the past decade, such that I can give only a brief list of the most important topics.

Philosophical and historical analyses have covered several fundamental concepts including chemical element, pure substance, chemical species, compound, affinity, chemical reaction, atom, molecular structure and aromaticity [18,19,22–24]. Recent interest in chemical methods has focused both on practical methods, such as

experimentation and instrumentation [25] and chemical synthesis [22,26], and on cognitive methods, such as the pictorial language of chemistry [27] and the various forms of model building and representation [28]. Still neglected are methods of classification – probably a legacy of the traditional focus on the 'classification-free' physics before the rise of the particle era – although recent studies on the periodic system combine classificatory and theoretical aspects [29]. With respect to chemical theories, the axiomatic mathematical structures of physics with their apparently universal validity made philosophers reluctant to accept what chemists, virtually without any difference in meaning, call theories, models or laws. Thus, save the aforementioned studies on models in chemistry, most of the present work on chemical theories is strongly historically orientated or about quantum chemistry and physical chemistry [30].

Transcending boundaries

Ironically, philosophy of chemistry emerged at a time when scientific activities increasingly transcended disciplinary boundaries towards problem-orientated research. Chemistry is heavily involved in these activities, from environmental science to nanotechnology, such that philosophers of chemistry have been challenged to take them seriously. Three recent books, each of which combine their own philosophical and historical analyses of transdisciplinary research, have taken up this challenge. Hans-Jörg Rheinberger [31] analyses the experimental settings, epistemological conditions and the transdisciplinary culture in which cancer research moved in the 1950s towards protein synthesis as the chemical background of molecular biology. Applying ideas from ancient philosophy of nature and technology, Bernadette Bensaude-Vincent [32] investigates modern materials science which has shifted from pure materials to composites that are individually designed for various technological purposes. With a critical view on classical approaches in the philosophy of science, Maureen Christie [33] examines the methodological basis on which theories of ozone depletion have actually been accepted in the atmospheric sciences since the 1970s.

Besides disciplinary boundaries of the sciences, there are also disciplinary boundaries within philosophy that philosophers of chemistry are about to transcend. If 'philosophy of science' means philosophical reflection on science, there is no need to restrict that to epistemological, methodological and metaphysical reasoning, as philosophers of physics have done. Philosophy is a much richer field, and sciences like chemistry have many more interesting, sometimes even more pressing, aspects that philosophers can deal with. For instance, although moral issues concerning chemistry have been vividly debated in public, from chemical weapons to environmental issues, the first collection of essays on ethics of chemistry was not published until 2001 [34]. And although it is well-known that chemists make heavy use of all kinds of means of visualization, from simple drawings to virtual reality, systematic investigations of the role aesthetics play in chemical research will appear only in 2003 [35]. Once the full scope of philosophy is acknowledged, topics in the philosophy of chemistry spring up abundantly [36]. This

might be at the expense of simple paradigms of the field, but the intellectual profit will be incomparably richer.

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