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Philosophy of Chemistry

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Introduction

Chemical ideas about the diversity of matter in terms of elements and compound substances and their transformations have been pivotal to any scientific or pre-scientific approach ever since. From ancient natural philosophy and alchemy to modern 19th-century chemistry, these ideas were made both the basis of philosophical systems and the target of critical reflection. After temporary interruption, when modern philosophy of science materialized as a discourse on mathematical physics, philosophy of chemistry emerged anew in the 1980s and is now a flourishing field in which philosophers, chemists, and historians of chemistry are engaged.

While many of the old philosophical issues have been rediscovered and discussed, new issues have appeared due to shifts of general philosophical foci, alliances with historians and sociologists of science, and the changes of chemistry and its role in society.

Ontological issues

Beyond simple definition issues, the objects of chemistry are subject to many ontological debates, which also impacts epistemological and methodological issues.

Following the example of microphysics, many philosophers and chemists take atoms and molecules as the basic objects of chemistry. Yet, despite numerous techniques to visualize them, molecule is a theoretical concept with many model assumptions that do not apply to non-molecular substances, like water, metals, salts, and so on. It is not so much the lack of optional microstructural descriptions for these substances, but the variety of models, which are continuously refined and adapted to certain contexts and problems, that make such models a weak basis for defining the basic objects of chemistry. The other option is to take material substances, either elementary or compound, as the basic objects. Yet, far from being phenomenologically given entities, pure substances are the final results of infinite purification operation, ideal laboratory artifacts, which in turn has inspired operational definitions. Whether one takes microstructures or pure substances is not an arbitrary decision, but has direct impact on the chemical classification and all derived concepts, because there is no simple one-to-one relationship between both kinds of entities. There are microstructures without corresponding pure substance and there are substances with many different microstructures corresponding.

A second but related ontological issue is about natural kinds in chemistry. Microstructuralist, following Hilary Putnam, claimed that water is a natural kind because it would be determined by a microstructural essence. While this claim is faced with the problems mentioned above, the substance-based approach to natural kinds is confronted not only with a potentially infinite number of possibly essential properties (see below) but also with the artificiality of pure substances. Even if pure substances were stable kinds independent of our conceptualization, they are not independent of laboratory purification. On the other hand, the experimental reproducibility of sufficiently pure substances provides, within limits, a successful operation to ensure relatively stable kinds.

A third ontological issue is about whether substances (or microstructures) or transformations are the basic objects of chemistry, which refers to the general debate between substance and process philosophy. If not closed in bottles, substances continuously undergo chemical reactions, are only intermediate states in an ongoing process; and quantum chemistry describes even these states as processes. Furthermore, classical chemical characterization of substances goes by chemical properties, i.e. by all the dispositions to transform into other substances under certain conditions, including certain other substances as reactants. Substance philosophers define a chemical reaction by the change of certain substances, whereas process philosophers define a substance by its characteristic chemical reactions. A third option, proposed by the author, combines substances and processes in a network of dynamic relations, as the proper object of chemical research, such that substances and reactivities mutually define each other. Answering the ontological question has direct consequences on how chemists best organize their knowledge in the form of either substance, reaction, or combined substance-reaction databases.

Although all substances and transformations are usually considered objects of chemistry, the metaphysical distinction between natural and synthetic pervades both common sense and chemical reasoning. The notion of natural substances, as being isolable from natural resources by purification, is questionable, however. Not only is purification a technical operation, also most elements would have to count as synthetic as long as natural resources are lacking. On the other hand, all substances that are isolable from natural resources can also be synthesized today, which undermines the distinction. Furthermore, we have little evidence to claim that a synthetic substance will never be isolable from natural resources in the entire universe.

Epistemological and methodological issues

A central epistemological issue is whether chemical knowledge can be complete or not. Microstructural essentialists claim that a perfect microstructural description of any substance yields complete chemical knowledge. However, chemical properties are not manifest properties but dispositional relations (e.g., A has under certain conditions the disposition to react with B to form C and D), such that the structure of experimental chemical knowledge is relational, dispositional, and open-ended. Since new contextual conditions and new potential reactants, which are currently produced at 15.5 million per year, define new properties, experimental chemical knowledge can increase infinitely without reaching completeness. It is an open question to what extent theoretical approaches can compensate for the incompleteness on the experimental level.

Chemistry differs from other sciences in that its theoretical concepts need to serve different methodological goals. Besides the classical goals of truthful description, explanation, and prediction of phenomena, theoretical concepts in chemistry also fulfill classificatory and synthetic purposes. By 2003 the chemical classification system has been able to distinguish between 60.5 million different substances and to order them by classes and sub-classes. And beyond mere prediction of phenomena, theoretical concepts provide experimental guidelines for producing millions of new substances and reactions per year. For all three methodological goals, the main theoretical approach has been chemical structure theory that emerged in mid-19th century and which has been influenced and diversified by many different developments since, including quantum chemistry and spectroscopic instrumentation. Apart from that, a multitude of other theoretical concepts and models have been developed for particular substance classes and phenomena and for various purposes.

The main methodological issue in current philosophy of chemistry is to bring order to that complex picture without imposing methodologies tailored to other disciplines upon chemistry. Several case studies have shown that received approaches, like for instance Poppers falsificationism, are rather useless in chemistry. There is some agreement that chemists favor methodological pluralism and pragmatism of models, rather than methodological universalism and the ideal of a single axiomatic theory. A study on scientific realism has suggested that, unlike theory realism, entity realism is a more appropriate methodological ideal in chemistry. The received methodological focus on methods of justification has been widened to include methods for research, i.e. for developing new knowledge. Many detailed studies on the different kinds and uses of models in chemistry, from theoretical chemistry to chemical engineering, have been undertaken. Besides the impact of quantum mechanics (see the Section on Reducibility), the impact of spectroscopic instrumentation on theoretical concepts since the mid-20th century has received considerable attention, such that interest in the "instrumental revolution" has replaced the older focus on the 18th-century "chemical revolution" by Lavoisier and others. The methodological integration of both chemical analysis and synthesis, which is the major experimental activity of chemists, has overcome received distinctions between science and technology. Studies on the formal sign language system of chemistry, consisting of structural formulas and reaction mechanisms, have illuminated its multi-purposed theoretical capacity; but further studies are required to understand its change due to impacts from various theoretical and experimental developments.

Reducibility to physics

Whether chemistry is reducible to physics is a question that could come up only in the mid-19th century when modern physics emerged as an own discipline, because the former meaning of physics, as natural science or natural philosophy, included chemistry as a branch. Before that, mechanical approaches were among several competing approaches within theoretical chemistry, though not very successful. The question became meaningful only with the development of quantum mechanics and its application to chemistry since the late 1920s. Following a speech by Paul Dirac in 1929, many quantum physicists and philosophers of physics have taken for granted that the whole of chemistry would be reducible to quantum mechanics, would be part of physics.

Unlike such bold claims, philosophers have carefully distinguished between different meanings of "reduction". Ontological reductionism claims that the supposed objects of chemistry are actually nothing else than the objects of quantum mechanics and that quantum-mechanical laws govern their relations. In its strong, eliminative, version, ontological reductionism states that there are no chemical objects proper. Anti-reductionists argue that theoretical entities are determined by their corresponding theory, such that theoretical entities of different theories cannot be identified. For instance, from the different meanings of the term "electron" in quantum electrodynamics and in chemical reaction mechanisms they conclude that the term "electron" has different references, which rules out ontological reductionism. Epistemological or theory reductionism claims that all theories, laws, and fundamental concepts of chemistry can be derived from first principle quantum mechanics as the more basic and more comprehensive theory. That claim has prompted many detailed studies (see below). Methodological reductionism, while acknowledging the current failure of epistemological reductionism, recommends applying quantum mechanical methods to all chemical problems, because that would be the most successful approach in the long run (approximate reductionism). However, the mere promise of future success is not convincing unless a comparative assessment of different methods is provided. By modifying the popular notion that "the whole is nothing but the sum of its parts" two further versions of reductionism have been developed. Emergentism acknowledges that new properties of wholes (say, of water) emerge when the parts (say, oxygen and hydrogen) are combined, but does not deny that the properties of the whole can be explained or derived from the relations between the parts (epistemological reductionism). Supervenience, in a simple version, means that, although epistemological reductionism might be wrong, the properties of a whole asymmetrically depend on the properties of the parts, such that every change of the properties of the whole is based on changes of the properties of or the relations between the parts, but not the other way round. If applied to the reduction of chemistry to quantum mechanics, i.e. to chemical entities as wholes and quantum mechanical entities as parts, emergentism and supervenience presuppose elements of epistemological or ontological reductionism, such that criticism of these positions applies accordingly. For instance, denying that chemical electrons are the same as quantum electrodynamical electrons or, more generally, that quantum mechanical entities are proper parts of chemical wholes, rejects supervenience altogether.

Recent criticism has focused on epistemological reductionism by pointing out the technical limits of quantum mechanics with regard to particular chemical concepts, laws, and problems. Two quantum chemists, Guy Woolley and Hans Primas, have shown that the concept of molecular structure, which is central to most chemical theories, cannot be derived from first principle quantum mechanics because molecular structures cannot be represented by quantum mechanical observables. Eric Scerri has argued that current quantum mechanical approaches cannot calculate the exact electronic configuration of atoms, which was considered a successful reduction of the chemical law that underlies the periodic system of elements. Jaap van Brakel has pointed out that the successful applications of quantum mechanics to chemical problems frequently include model assumptions and concepts taken from chemistry. Joachim Schummer has argued that quantum mechanical approaches are almost absent and useless in areas that chemists are mainly concerned with, i.e. chemical reactions, synthesis, and classification.

The criticism of reductionism of chemistry to quantum mechanics, as the “lowest” level in a standard hierarchy of reductions, also challenges microreductionism as a general position and thus contributes to general philosophy. In the most detailed philosophical study on various forms of reductionism, Jaap van Brakel 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, rejection of reductionism is even a necessary presupposition of his extensive work on the culturalist foundation of chemical concepts, laws, and theories, which he seeks in pre-scientific cultural practices, norms, and values. For many others, including the author, it supports a pragmatist and pluralist position about methods that distinguish clearly between fields of research where quantum-mechanical approaches are strong and even indispensable and those where they are poor or even useless compared to other approaches. Once reductionism has lost its function to secure the unity of the sciences, new relationships between chemistry and other disciplines could become subject to philosophical and historical investigations, including studies on multi-disciplinary fields such as atmospheric science, biomedical science, materials science, and nanotechnology.

Further Topics

Current philosophy of chemistry reaches far beyond ontological, epistemological, and methodological issues. On the one hand, there are a strong historical research trends. Pertinent works on chemistry by philosophical classics, such as Aristoteles, Immanuel Kant, Georg Wilhelm Friedrich Hegel, Pierre Duhem, Ernst Cassirer, and Gaston Bachelard, have been rediscovered, allowing reinterpretations of the history of philosophy of science. Philosophical works by historical chemists, such as Benjamin C. Brodie, Wilhelm Ostwald, Frantisek Wald, Edward F. Caldin, Fritz Paneth, and Michael Polanyi, have been rediscovered. Historians and philosophers of chemistry have explored the development of many fundamental concepts in chemistry, such as chemical substance, element, atom, the periodic system of elements, molecular structure, chemical bond, chemical reaction, affinity, and aromaticity. In addition, important historical developments of chemistry have been philosophically scrutinized, such as the transitions from alchemy to modern chemistry, from phlogistic to anti-phlogistic chemistry, the emergence of physical, quantum, and biochemistry, and the development of molecular model building and instrumentalization.

On the other hand, philosophers of chemistry have also applied theoretical insights to practical problems, discovered a wider spectrum of philosophical perspectives on chemistry, and engaged in contemporary issues. Epistemological and ontological studies found most useful applications in chemistry education and information management. Beyond the classical scope of philosophy of science, perspectives on chemistry from philosophy of technology, language, culture, and literature, and from metaphysics, aesthetics, ethics, sociology, and public understanding of science have been exploited. For instance, studies on the role of visualization and aesthetics in chemical research have been undertaken to understand the heuristics and research dynamics beyond epistemic and technological goals within a broader cultural context. Philosophers and historians have investigated the historical roots and the cultural value conflicts underlying the widespread chemophobic attitude of society and the peculiar opposition of natural versus chemical. Apart from general professional ethics, philosophers have questioned the legitimacy of chemical weapon research, the alleged moral neutrality of synthesizing new substances for scientific purposes, discussed the scope of moral responsibility of chemists for their synthetic products, and developed moral frameworks for assessing chemical research practice. Finally, with the rise of nanotechnology, in which chemistry is particularly involved, philosophers of chemistry have taken a leading role in discussing societal and ethical implications of nanotechnology.

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