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Philosophy of Chemistry

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The emergence of the field and key issues

The philosophy of chemistry began to develop in earnest in the mid 1990s following the efforts of a number of individuals who were initially working and publishing independently, before joining together to form the *International Society for the Philosophy of Chemistry* (ISPC). Of course, some isolated authors had already stressed the philosophical aspects of chemistry and the need for such a sub-discipline (van Brakel and Vermeeren 1981). However, the International Encyclopedia of Unified Science of logical empiricism had a volume of many disciplines but nothing on chemistry since it was considered to be reduced field.

This chapter will not be concerned with what may be termed the pre-paradigmatic phase which has been reviewed by van Brakel (van Brakel, 2012). Returning to the field's more recent emergence, one should mention the efforts of Michael Akeroyd, who organized the first two meetings of the burgeoning society, the second of which witnessed its formalization in 1997 (Ruthenberg 1997). Moreover, two international journals were soon established. The first one in print was the *Foundations of Chemistry* published by Kluwer and now Springer, which appeared in 1999. The other journal, *Hyle*, was privately published by Joachim Schummer beginning in 1997, initially in an on-line format but later also in print. Unfortunately, this second journal has now ceased to exist.

A major issue from the inception of the field has been the question of whether chemistry reduces to physics and more specifically to quantum mechanics. This issue strikes at the raison d'être of the field since it had hitherto been generally thought that chemistry does indeed reduce fully and that there were subsequently no foundational issues in chemistry to be dealt with.

As is well known, post-positivist philosophy of science resulted in a questioning of reductionism in all areas of science, partly in opposition to the unity of science movement that the positivists had promoted. Authors in current philosophy of chemistry generally dispute the notion that chemistry does indeed reduce to quantum mechanics and claim that there are genuinely fundamental ideas in chemistry that deserve philosophical scrutiny. These scholars have also made a distinction between epistemological or theoretical reduction on one hand, and ontological reduction on the other. The first category, which is more clearly specified, involves the question of whether current theories in chemistry have been reduced to current quantum mechanical theories.

An alternative but related approach among philosophers of chemistry is based on the view that there are some genuinely foundational ideas, such as the existence of the periodic system and the phenomenon of chemical bonding, which deserve philosophical scrutiny regardless of the question of reduction (Scerri 2019; Weisberg 2008).

The reduction of chemistry to quantum mechanics

There are many ways that the question of reduction has been explored. First of all, Nagel's criteria for reduction (Nagel, 1961) have been applied, namely attempts to axiomatize the theory to be reduced as well as the more fundamental theory, followed by the attempt to establish bridge principles (Hettema and Kuipers 1988). These attempts are generally considered to fail in the case of chemical theories because it is not clear what an axiomatization of chemical theories might consist of.

More naturalistic approaches which move beyond the formal Nagelian approach have examined the calculations that are used in quantum chemistry in an attempt to establish whether there is a seamless connection with fundamental quantum mechanics. For example, quantum chemistry and indeed general chemistry traditionally uses the concept of atomic orbitals in order to explain many chemical phenomena. Here the issue centers on whether atomic orbitals genuinely reduce to quantum mechanics (Scerri 1991). Such discussions were greatly enlivened starting in 1999 when it was reported that atomic orbitals had been experimentally observed for the first time (Scerri 2001; Mulder 2010).

Other contributions to the question of reduction have centered around the Born-Oppenheimer approximation which is generally applied in calculations involving molecules. The simplest of all molecules, or strictly speaking the simplest ion, consists of the H_2^+ system, will be used to explore some of the details of how the Born-Oppenheimer is used in quantum mechanical calculations.

The central equation in quantum mechanics, the time independent Schrödinger equation, is shown below as equation (1).

$$H\Psi = E\Psi \qquad (1)$$

It consists of a Hamiltonian operator, H, which acts on the wavefunction for the system Ψ and thereby yields a set of possible discrete energy values denoted by E. The Hamiltonian itself contains operators specifying the kinetic and potential energies of every single particle in the system. In the case of the H_2^+ system there are two protons and just one electron. Consequently, there exists two kinetic energy terms, one for each of the protons in addition to a potential energy term due to their mutual repulsion. In the case of the electron there is a kinetic energy term and two potential energy terms, one for each attraction between the electron and each of the protons. The mathematical expression for the Schrödinger equation in which the Hamiltonian is shown explicitly is,

$$\left[-\tfrac{1}{2} M \nabla_A^2 - \tfrac{1}{2} M \nabla_B^2 + \frac{e.e}{R_{AB}} - \tfrac{1}{2} m \nabla^2 - \frac{e.e}{r_A} - \frac{e.e}{r_B} \right] \Psi = E\Psi \qquad (2)$$

where ∇ is the Laplacian differential operator, M and m are the masses of the proton and the electron respectively, R_{AB} the distance between the protons, r_A and r_B the distance of the electron from each of the nuclei A and B and e is the charge on the electron. Expressed otherwise, each of the operators in (1) corresponds to the following kinetic energy (KE) and potential energy terms (PE),

$$KE_{\text{proton A}} + KE_{\text{protonB}} + PE_{AB} + KE_{\text{electron}} + PE_{Ae} + PE_{Be}$$

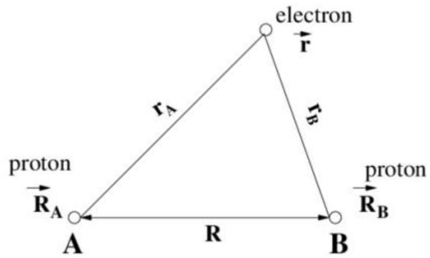

Figure 1. The H_2^+ system consisting of two protons and one electron.

The application of the Born-Oppenheimer approximation (BOA) consists in recognizing the fact that electrons are so much lighter than protons, or more specifically, 9.1093819 x 10^{-31} kg as compared with 1.6726216 x 10^{-27} kg, or a ratio of 1 to 1836. If one assumes that an equal momentum is given to a proton and an electron, it follows that the relative speeds of the particles is 1 to 1836 in favor of the electron from the following simple argument. If M and m are the masses of the proton and the electron respectively,

$$\begin{aligned} \text{Momentum} &= M\,v_{\text{proton}} = m\,v_{\text{electron}} \\ &= 1836 \times v_{\text{proton}} = 1 \times v_{\text{electron}} \\ v_{\text{electron}} / v_{\text{proton}} &= 1836 / 1 \end{aligned}$$

According to the BOA this discrepancy in velocities is taken to the limit, in that protons are assumed to have a velocity of zero as compared to that of electrons. It follows that their kinetic energies (1/2 mv^2) will also be zero. Consequently, all kinetic energy terms for protons can be neglected under the BOA scheme and quation (2) therefore reduces to equation (3).

$$\left[+ \frac{e.e}{R_{AB}} - \tfrac{1}{2} m \nabla^2 - \frac{e.e}{r_A} - \frac{e.e}{r_B} \right] \Psi = E\,\Psi \qquad (3)$$

Furthermore, the first term in (3) takes on a constant value for any particular fixed inter-proton distance. What remains is therefore three operators, all referring to the electron which operate on the wavefunction to determine the allowed eigenvalues for the system. Such an equation does not involve any electron-electron repulsion terms, since there is only one electron present, and can be solved analytically, meaning exactly.

The result computed in this way for the ground state energy of the H_2^+ system is –0.602342 Hartrees, as compared with the experimentally obtained value of –0.596689 Hartrees, or a difference of approximately 1%. Clearly the BOA is justifiable for this system, at least in numerical terms. Moreover, the error decreases when one considers molecules with heavier nuclei. For example, in the case of the C_2 molecule, the nuclei concerned are tweleve times as heavy as the proton which means that the error will be reduced to at least 1/12th of the value for the H_2^+ system.

So much for the technical aspects of the BOA. Let us now turn to what some philosophers of science, and of chemistry in particular, have made of this situation. In what is perhaps a more extreme position, some authors have claimed that the use of the BOA results in a treatment of particles in a fundamentally non-quantum manner, because fixed positions are assigned to the nuclei and that this step represents a violation of the Heisenberg Principle. These same authors frequently go on to claim that without such classical "scene setting" the quantum calculations are quite impossible.

However, the notion that denying any motion to nuclei in a molecule represents a violation of the Heisenberg Principle ignores the fact that scientific theories frequently contain internal inconsistencies. Stated otherwise, scientific progress is not restricted by matters of principle. Numerous instances from the history of science show that progress is achieved by violating what may hitherto have seemed to be inviolable restrictions. For example, the Bohr model contains several apparent inconsistencies and yet it represented a major step forward and the beginnings of the quantum theory of atoms which culminated in the discovery of quantum mechanics (Vickers 2007). What matters most in scientific practice is obtaining a result. If an approximation provides a calculation that falls short of the experimental value by 1%, or less for heavier systems, it is considered perfectly reasonable, even if it may appear to violate a central principle of the theory that is being utilized.

Furthermore, the apparent violation of principles is a frequent occurrence in the practice of science. For example, the use of electronic configurations of atoms, that are ubiquitous in chemistry and physics, and which specify which electrons are in which particular orbitals, represents a violation of the Pauli Principle, which asserts that electrons are completely indistinguishable. And yet electronic configurations are routinely and successfully used in chemical reasoning as well as calculations.

More importantly perhaps, there is a significant sense in which the use of the BOA does *not* in fact represent a violation of the Heisenberg Principle. Solving equation (3) above involves obtaining many solutions for the total electronic energy, one for each particular chosen internuclear distance. It is only by doing so that a graph of the potential energy of the nuclei can be plotted against distance (Figure 2), in order to obtain the minimum in the plot and thereby the ground state energy and bond length of the system in question. In other words, even though each particular solution involves keeping the nuclei stationary, the fact that one is considering many different inter-nuclear distances serves to restore the motion of nuclei. The Heisenberg Principle could only be said to be violated if one were to focus on just a single data point on the energy graph shown below.

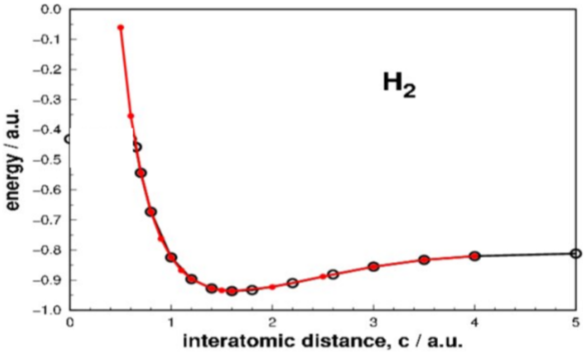

Figure 2. Potential energy of nuclei against inter-nuclear distance.

A third point to emerge from these more extravagant views is the notion that quantum chemists are somehow obliged to use the BOA. In fact, there has long existed a thriving branch of quantum chemistry which specializes in non-Born-Oppenheimer calculations (Agostini and Curchod 2022). Such calculations have a wide variety of applications in chemistry such as the interaction between light and matter and ensuing ultrafast, out-of-equilibrium nuclear dynamics. This work includes the photochemistry of isolated and solvated molecules and excited-state dynamics with long timescales.

Other philosophers of chemistry do not draw such categorical conclusions from the use of the BOA in quantum chemistry. For example, Lombardi and her co-authors appear to accept the usefulness of the BOA in the name of pragmatic realism (Lombardi 2023).

Another frequently made, and perhaps a more valid, claim among the philosophy of chemistry community is that quantum mechanical calculations using the Born-Oppenheimer approximation do not allow one to distinguish between isomers, such as CH_3CH_2OH and CH_3OCH_3, which share the same molecular formula of C_2H_6O. This state of affairs occurs because the Hamiltonian, as discussed above, is concerned only with the number of protons and electrons in a molecule, as well as the interactions between them. Without specifying the positions of the nuclei or without distinguishing between the two above isomers, solving the Schrödinger equation results in precisely the same energy for both molecules.

The claim that quantum mechanics does not distinguish between isomers is countered by other authors who point to the well-known measurement problem in quantum mechanics. The wavefunction for any particular system consists of a superposition of various states until an observation is made, which results in the collapse of the wavefunction and the actualization of one particular state, rather than a superposition of several of them. Just as the mechanism of quantum decoherence has been invoked in attempts to solve the measurement problem in the foundations of quantum mechanics, some philosophers of chemistry have claimed that it can be brought to bear on this question of isomers. The claim is that a molecule with the molecular formula of C_2H_6O is in a superposition of its various isomers and only actualizes to form one particular isomer following quantum decoherence. However, the details of this proposal remain controversial and have not yet been fully elaborated (Franklin and Seifert, 2020).

Other areas of interest to philosophers of chemistry

Elements

The nature of elements, which are of course central to the discipline of chemistry has been another main theme which many philosophers of chemistry have considered. In several languages, including English, the term “element” has two distinct senses which are not always differentiated by chemists at large or by chemical educators. One may speak of elements in the sense of simple substances that can be isolated and that have specific properties such as the yellow element sulfur or the green gas chlorine. In addition, the same term element is used in a more abstract sense to denote substances that persists in chemical reactions. For example, when sodium reacts with chlorine to yield sodium chloride, each of these two elements cease to exist as simple substances but persist as what is sometimes termed elements as basic substances (Scerri and Ghibaudi 2020). Somewhat paradoxically, Mendeleev, the leading discoverer of chemical periodicity, claimed that his periodic table was primarily a classification of the elements in the latter more abstract sense, which are characterized by their atomic weights rather than by their properties as simple substances.

The theme of elements is also at the center of many studies on natural kinds. Indeed, it would appear that elements have become increasingly important examples of natural kinds given that biological species are no longer considered to be so among philosophers of biology, as well as in philosophy of science in general. Needless to say, there is no widespread consensus as to whether elements are indeed natural kinds, although it is a question which philosophers of chemistry may be in a better position to answer than philosophers at large (van Brakel 2000).

The Periodic Table

A central idea in chemistry, as mentioned earlier, consists of the periodic table of the elements which has received considerable philosophical attention in the community. Such studies have included attempts to categorize the periodic table as a classification, a model, a theory or a scientific domain (Shapere 1984). Meanwhile others have drawn on historical and philosophical aspects of the periodic system in attempting to answer questions which appear to be intractable within mainstream chemistry. These include the possible existence of an optimal periodic table, attempts to understand the basis for the Madelung or n + l rule for electronic configurations, the membership of group 3 of the periodic table etc. (Scerri 2019).

Emergence

The question of emergence looms large in the philosophy of chemistry. It seems to be broadly accepted that many aspects of chemistry are emergent in the sense that they cannot be explained from the constituent components of the substances concerned. An obvious example would be the fact that the properties of compounds appear to be greater than the sum of the properties of the elements from which they are comprised. This notion has also been taken up by researchers in the field of chemical education who advocate a systems approach to chemistry (Tumai 2016).

Some writers in the philosophy of chemistry have attempted to identify the occurrence of emergence in more specific ways, including an analysis of the Hamiltonian operator in quantum mechanical calculations (Hendry 2010). Not surprisingly, this question has led to a considerable amount of debate (Scerri 2023).

Supervenience

The appeal to emergence is one aspect of the alleged failure of the reduction of chemistry to physics and more specifically to quantum mechanics. Another response and indeed an alternative to reduction, which was very prevalent for a while in mainstream philosophy of science, has been the notion of supervenience which has received attention from philosophers of chemistry. Although there is notoriously no unanimous agreement on what the supervenience relationship is, the most popular view is that supervenience is a relationship of asymmetric dependence. Two macroscopic systems which have been constructed from identical microscopic components are assumed to show identical macroscopic properties, whereas the observation of identical macroscopic properties in any two systems need not necessarily imply identity at the microscopic level. In simpler terms, the phenomena we study in some secondary sciences? are thought to be ontologically dependent upon relationships at the primary level. This argument has been widely used throughout the philosophy of science (and the philosophy of mind) as a rescuing maneuver from the impasse produced by the failure to establish the epistemological reducibility of any of the special sciences. This is because supervenience is taken to make no guarantee about the epistemological or explanatory consequences which would necessarily follow from even a strong ontological dependence between two different descriptive levels. Thus, the claim has been that supervenience allows us the virtue of ontological dependence, without the vice of explanatory reduction (Scerri and McIntyre 1997)

Causation

Turning to another important theme in mainstream philosophy of science, namely causation, surprisingly little attention seems to have come from philosophers of chemistry. One important exception has been the view that the electronic configurations of atoms play a causal role in chemistry and more specifically in explaining the behavior of elements in the context of the periodic table (Ross 2021). Whereas it is generally claimed that the periodic table does not figure in causal explanation because it does not reveal causal structure, Ross takes seriously the commonplace view that the periodic table explains the properties of the elements through their electronic configurations and draws on the interventionist account of causation to make such arguments.

Meanwhile another author takes the view that chemical behavior is governed as much by the nuclear charge of an atom as it is by its electronic structure and that an adequate analysis requires attention to the dynamical interactions between nuclear charges and those of electrons, as typically carried out through the application of the Schrödinger equation. This author concludes that electronic configurations can only be said be causal in a weak sense that is somewhat analogous to the causal arguments that are invoked in folk physics (Scerri 2021).

Revolutions in chemistry

Meanwhile it has been gratifying to see that general philosophers of science appear to be taking a greater interest in the fertile ground that the field of chemistry offers to them. For example, the Kuhn expert Wray has proposed that the change that occurred when elements became ordered according to their atomic numbers, rather than their atomic weights, might be said to represent a scientific revolution (Wray 2017). The issue concerns the fact that the elements in the periodic table were originally ordered according to their increasing atomic weights. This practice resulted in some anomalies, including the reversal of tellurium and iodine, which were originally carried out because they were demanded by the chemical properties of these elements. The discovery of atomic number provided an independent and more fundamental justification for making such reversals. It also meant that the identification of elements changed from the use of atomic weight to atomic number and helped to incorporate another discovery, that of isotopy, that occurs in the majority of the chemical elements.

As in the cases of most examples cited here there is some debate over these questions, which may be indicative of the fact that the philosophy of chemistry has yet to reach any substantial degree of maturity, while at the same time serving to invite contributions from philosophers in search of new pastures.

Predictivism

A long-standing debate in general philosophy of science concerns the relative virtue of predictions and accommodations (retrodictions) in the acceptance of scientific theories or concepts. Chemistry in the form of the periodic table has provided one of the main examples that have been discussed by proponents of both positions. For example, Stephen Brush has argued that the periodic table was accepted primarily because of its ability to explain facts about numerous elements that were already known, rather than because of Mendeleev's well-known and dramatic successful prediction of a few elements (Brush 2007; Scerri, Worrall, 2001)

Laws

The nature of laws of science has generated a large literature in the philosophy of science but surprisingly little attention from philosophers of chemistry with a few exceptions (Christie and Christie 2000). Indeed, there appears to be something of a gulf between the manner in which laws are regarded by philosophers, who have focused on the need to distinguish genuine laws from accidental generalizations, either through Humean or no-Humean approaches, and chemists who do not consider this to be an urgent issue. Indeed, many chemists appear to deny any role whatsoever for laws in agreement with philosophers such as Giere and van Fraassen.

Alternatives approaches to reduction

The attention to micro-structure and quantum mechanics, which some philosophers of chemistry regard as excessive, receives an interesting counterbalance from authors including Needham (2013) who favor a more macroscopic approach provided by the field of thermodynamics. Under the same umbrella, which eschews the discussion of chemistry through the lens of quantum mechanics, several authors have written about the role of 'stuff' in chemistry (Schummer 1998; Ruthenberg and van Brakel 2008).

In addition, several authors have focused on some specifically chemical themes which are neither concerned with reduction or with concepts that are typically discussed by general philosophers of science. For example, William Goodwin (2012) has published a number of interesting articles which examine the role of mechanism in organic chemistry.

An area that is rather unique to chemistry and that has not been discussed by philosophers at large in the question of chemical synthesis, which is addressed in some stimulating papers in the philosophy of chemistry literature (Bhushan and Rosenfeld 2000).

Similarly, nanochemistry, which has been examined by Bursten (2018), offers new vistas to general philosophers of science. As this author explains, classification in nanoscience differs from classification in chemistry because the latter relies heavily on compositional identity, whereas the former must consider additional properties, namely, size, shape, and surface chemistry.

Some scholars in the philosophy of chemistry have begun to develop sub-field such as the philosophy of biochemistry while invoking a process ontology (Stein 2006). The general idea they have proposed is to think of macromolecules as relational and processual entities, such as in the case of ligand receptors and receptor-mediated biosignaling (Alassia 2022).

Historical aspects

Needless to say, the philosophy of chemistry draws heavily on the history of the field and vice versa. One may cite such scholars as Rocke, Kim and Banchetti who frequently cross between historical and philosophical aspects of chemistry while spanning different time periods. For example, Rocke has written widely on atomic theory and has recently published a thoroughgoing rehabilitation of the 19th-century chemist Lothar Meyer (Boek, Rocke, 2022). Even more broadly, the past 50 years or so wave witnessed a reappraisal of the value of alchemy which had previously been deemed to be of little scientific value (Principe 1998; Newman 2006).

Ethical aspects

Perhaps the most unfortunate aspect of chemistry is that it has been partly responsible for a variety of environmental problems including climate change. It therefore behoves chemists to address its ethical dimension with some urgency. Such a mission has been undertaken within the mainstream chemical community under the banner of Green Chemistry which seeks to design chemical products and processes that reduce or eliminate the use or generation of hazardous substances. Several philosophical commentaries and analyses on these initiatives have been provided by some philosophers of chemistry (Linthorst 2010; Llored and Sarrade 2016).

A somewhat different though related approach, known as sustainable chemistry, seeks to transcend the narrow focus on chemical synthesis, while embracing a more holistic view of chemical activities, including social responsibility and sustainable business models. This sub-discipline too has received attention within the philosophy of chemistry (Krasnodębski, 2023)

Chemical Education

One of the fields that can most obviously benefit from a deeper conceptual analysis of all aspects of chemistry is chemical education research. The majority of research in this field consists in devising new forms of computer visualization or new methods of assessing students' abilities rather than focusing on the subject matter of chemistry itself. It has been gratifying to see a number of chemical educators who have embraced some of the work in philosophy of chemistry in order to redress this imbalance with the aim of improving the teaching of chemistry (Erduran and Mugaloglu 2014; Taber 2003).

Closing remarks

This entry intends to end on a cautionary note. Given the recent arrival of the philosophy of chemistry onto the philosophical scene, it is especially important that the field remain cognizant of technical issues in mainstream chemistry (Ruedenberg 1962). Only by doing so can the field hope to compare with the philosophy of physics which is nowadays taken seriously by physicists working on more foundational issues. For example, one of the most active debates among theoretical chemists consists in trying to establish the relative importance of potential and kinetic energy of electrons and their role in the formation of chemical bonds. This issue and several others have been almost completely neglected by philosophers of chemistry while they retreat into discussions as to whether chemical bonds are 'real'.

Nevertheless, one may also report that a certain rapprochement does seem to be occurring between the analysis of issues in the philosophy of chemistry and the philosophy of physics in some recent work (Miller, 2023, Sebens, 2021). Finally, just as one can do philosophy of physics without a deep knowledge of physics, there continues to be much interesting work that is being carried out in the metaphysics of chemistry, which may also offer new insights to the field of metaphycis in general (Siebert, 2023).

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