Philosophy of Chemistry

Concepts, ideas and open questions

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1. Introduction: The field that is called *Philosophy of Chemistry*

Whether one realises it or not, chemistry is everywhere. What we eat; the drugs that cure our diseases; the detergents that we use to clean our clothes and houses, to climate change; the discovery of life in distant planets; understanding brain activity; and, photosynthesis- for everything, the study of chemistry is not just relevant but vital.

So, it should not come as a surprise that phenomena that standardly belong to the subject matter of chemistry have been discussed in philosophy since ancient times. Chemistry is concerned with how matter is composed, its properties, but also more importantly, with how matter transforms from one substance to another. Aristotle did a systematic analysis of phenomena and concepts that nowadays are regarded within the purview of chemistry.[2] The alchemists, at least from the time of ancient Egypt up until Renaissance Europe, built entire metaphysical worldviews based on the study of chemical phenomena.[3]

However, the philosophy of chemistry as an organised research study is relatively new as it flourished the past 30 years. A key event that signified the formation of this field was the foundation of the International Society for the Philosophy of Chemistry (ISPC) which organises annual conferences since 1997 and publishes the journal *Foundations of Chemistry* since 1999. Books and collections of papers are published by publishing houses such as Oxford Universe Press, Springer and Cambridge University Press, and articles are regularly published in general philosophy of science journals such as *Philosophy of Science* (PSA) and the *British Journal for the Philosophy of Science* (BJPS). The presence of the philosophy of chemistry has also expanded online. *Hyle,* which is published in printed and online form since 1997, was the first international journal

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[1] Preprint of chapter to be published in Turkish in the book titled ***Bilimlerin Felsefesi,*** ed. by M. Efe Ateş and Dinçer Çevik.

[2] See in particular the following works of Aristotle: *On Generation and Corruption*, *Meteorology*, *Physics*, and *On the Heavens* (Barnes 1984). See also (Hendry et al. 2011: Section 1.1) and (Needham 2006).

[3] See for example Principe 2012. More on alchemy in section 5.

on philosophy of chemistry (Schummer 2014a). A more recent online contribution is *Jargonium* and there are also entries on philosophy of chemistry in the *Stanford Encyclopedia of Philosophy* and in the *Internet Encyclopaedia of Philosophy*.[4]

In the Stanford Encyclopaedia entry on the philosophy of chemistry, Hendry, Needham and Weisberg state that the field examines two sorts of issues:

> In the first, conceptual issues arising within chemistry are carefully articulated and analyzed. Such questions which are internal to chemistry include the nature of substance, atomism, the chemical bond, and synthesis. In the second, traditional topics in philosophy of science such as realism, reduction, explanation, confirmation, and modeling are taken up within the context of chemistry. (Hendry et al. 2011)

So, there are two complementary ways to understand the subject matter of the philosophy of chemistry. First, it is a subdiscipline subsumed in the more general field of philosophy of science. In this context, any topic within the purview of philosophy of science that is examined from the perspective of chemistry, is essentially part of doing philosophy of chemistry. Secondly, there are matters unique to chemistry and its history which illustrate that chemistry prompts philosophical questions that are autonomous from how we philosophise about the natural sciences in general. This is important to note because chemistry should not be viewed only as a repository of case studies for philosophers.

This article presents some of the main concepts, ideas and open questions that fall within the purview of philosophy of chemistry. It presents the most central debates that have occupied philosophers for the past 30 years and discusses the new avenues of research that are recently being developed. I should note from the offset that this presentation is partial and by no means complete. I present issues that I take to have been mostly discussed in the recent literature (since the formation of the field) and I also focus on matters that I believe can attract new interest into the field (see especially section 6).[5]

2. The place of chemistry among the sciences

[4] Hendry Robin F., Needham Paul, Weisberg Michael, *Philosophy of Chemistry*, (2011), <https://plato.stanford.edu/entries/chemistry/>, 3/11/2017. Seifert, V., *Reduction and Emergence in Chemistry*, (2019) <https://iep.utm.edu/reduction-and-emergence-in-chemistry/>

[5] I also recommend reading the Stanford Encyclopaedia entry on philosophy of chemistry (see footnote 3).

When one talks of chemistry's place among the natural sciences, the first thing that comes to mind is how chemistry relates to physics, and more precisely, to quantum mechanics. There are two ways to pose this question. One can focus on the epistemic aspect and investigate how the descriptions formulated within the two sciences relate to each other. For example, how does the Schrödinger equation describe the properties of molecules, and does this description differ from those offered in chemistry? Secondly, one can pose the metaphysical question of how the entities postulated by the two sciences relate to each other. This concerns the relations we putatively discover in the world through the sciences. For example, how do molecules and chemical bonds relate to the subatomic particles that make them up?

The question of chemistry's relation to quantum mechanics has been viewed as the defining issue for philosophy of chemistry. As Hasok Chang puts it:

> the relationship between physics and chemistry is one of the perennial foundational issues in the philosophy of chemistry. It concerns the very existence and identity of chemistry as an independent scientific discipline. Chemistry is also the most immediate territory that physics must conquer if its "imperialistic" claim to be the foundation for all sciences is to have any promise. (Chang 2015: 193)

In a similar spirit, Eric Scerri and Grant Fisher point out that the defence of the autonomy of chemistry is essential to validate its philosophical analysis:

> the philosophy of chemistry had been mostly ignored as a field, in contrast to that of physics and, later, biology. This seems to have been due to a rather conservative, and at times implicitly reductionist, philosophy of physics whose voice seemed to speak for the general Philosophy of Science. It has taken an enormous effort by dedicated scholars around the globe to get beyond the idea that chemistry merely provides case studies for established metaphysical and epistemological doctrines in the philosophy of physics. These efforts have resulted in both definitive declarations of the philosophy of chemistry to be an autonomous field of inquiry and a number of edited volumes and monographs. (Scerri and Fisher 2015: 3)

Chang's, Scerri's and Fisher's attitude towards chemistry and its relation to physics is a reaction to an assumption that was established at the beginning of the 20th century, namely that quantum physics in principle accounts for all natural phenomena. This was most clearly expressed by mathematician and physicist Paul Dirac in this now infamous quote:

> The underlying physical 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 application of these laws leads to equations much too complicated to be soluble.[6] (Dirac 1929: 714)

In response to this attitude, during the first two decades of the philosophy of chemistry, there was a proliferation of accounts focused on defending what I call disunity theses.[7] Disunity theses include any account which focuses on those aspects of chemistry's relation to quantum mechanics which purportedly illustrate the separateness or autonomy of chemistry. Specifically, disunity has been supported by making at least one of the following claims:

- Explicitly denying the existence of a particular epistemic relation between the two sciences. For example, this includes the claim that chemistry fails to epistemically reduce to quantum mechanics in the way that (most characteristically) philosopher of science Ernest Nagel had envisioned about the special sciences (e..g. Scerri 1994; van Brakel 2000).[8]
- Pointing out the difference in the methodologies, tools or concepts that are employed by chemistry and quantum mechanics, as well as the explanatory and predictive success of chemistry (over quantum mechanics) with respect to a particular set of phenomena (e.g. Schummer 2014b; Llored 2012).
- Denying the existence of a particular metaphysical relation between the two sciences. This includes, for example, the rejection of ontological reduction (e.g. Labarca and Lombardi 2005: 140).

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[6] Whether this should be understood as supporting 'the firm expectation that a "full reduction" of chemistry can one day be achieved' is not examined here (Hettema 2017: 3). For example, Hettema argues that Dirac was not so 'confident' about the epistemic reduction of chemistry to quantum mechanics (Hettema 2017: 3).

[7] Of course, it cannot be argued that any particular disunity thesis has been formulated with such an explicit intention. Nevertheless, the aforementioned quotes illustrate that some of the main representatives of the field have connected the indispensability of the philosophy of chemistry with the success to argue for a disunity thesis. Put differently, there is a general attitude, not necessarily advocated by all representatives of the field, that if the relation between chemistry and quantum mechanics is undermined, then this assures not only the autonomy of chemistry (from quantum mechanics), but also the importance of philosophising about it.

[8] I briefly present Nagel's account below.

- Making a metaphysical claim about chemical entities, properties, etc. For example, Robin Hendry (2006b) claims that the structure of a molecule is distinct from its physical constituents in the sense that it possesses distinct causal powers (This view is called strong emergence; I return to it below).[9] Alternatively, Martín Labarca and Olimpia Lombardi defend chemistry's autonomy in terms of ontological pluralism which "permits the coexistence of different but equally objective theory-dependent ontologies interconnected by nomological, non-reductive relationships" (2005: 146).

Disunity theses do not necessarily reject that chemistry is somehow related to quantum mechanics. Some acknowledge that the two sciences employ concepts in an identical manner, that quantum mechanics has contributed to the better understanding of chemical phenomena, or even that chemical and physical entities are somehow metaphysically related.[10] Nevertheless, all disunity theses primarily focus on presenting the differences or incompatibilities between chemistry and quantum mechanics.

Moving on to unity theses, these include any account that focuses on those aspects of chemistry's relation to quantum mechanics which illustrate the unity or dependence of chemistry to quantum mechanics. In this context, at least one of the following claims are made:

- There exists a substantial epistemic relation between the two sciences. For example, Hinne Hettema spells out this relation in terms of the 'union' of chemistry and quantum mechanics, and proposes an amended understanding of Nagel's reductionism (Hettema 2017). Other accounts point out the methodological, explanatory, heuristic or confirmatory dependence of chemistry to quantum mechanics (e.g. Needham 2010; Seifert 2017).
- There exists an ontological relation between physical and chemical entities, properties, etc. For example, Le Poidevin (2005) claims that chemical entities ontologically reduce to quantum physical ones.

As with disunity theses, 'unity' groups together accounts that differ in various respects. They often propose different understandings of the relation between chemistry and quantum mechanics

[9] For a different account regarding the ontological autonomy of chemistry see Labarca and Lombardi 2005.

[10] For example, Hendry- who defends the strong emergence of chemistry and thus formulates a disunity thesis- accepts that supervenience holds between the chemical and quantum mechanical properties of a molecule (Hendry 2006b: 173-176). Supervenience brings out the idea that whenever there is a change in the higher level (say, chemical) entities or properties in a system, this is always accompanied by some change in its lower level (i.e. physical) entities.

which may not be compatible with each other. Moreover, they do not necessarily reject that chemistry is somehow autonomous or separate from quantum mechanics. For example, there are unity theses which acknowledge that chemistry is autonomous from quantum mechanics in the sense that the former employs distinct methodologies and has independent research goals (e.g. Seifert 2017: 221). Moreover, there are those which accept that chemistry is epistemically distinct from quantum mechanics (in the sense of being non-reducible in a Nagelian manner), but argue that there is a particular metaphysical relation between chemical and physical entities (Le Poidevin 2005). Nevertheless, all unity theses focus on presenting the connections or dependencies between chemistry and quantum mechanics, rather than their incompatibilities or disconnections.

There are two interesting features to unity theses. First, most accept that a Nagelian kind of reduction fails with respect to the examined pair of sciences.[11] Nagel (1961) formulated an account of reductionism that to this day is considered paradigmatic (though for some outdated) of how the special sciences relate to physics. He claimed that a theory reduces to another when the latter is able (at least in principle) to derive the laws of the former. When the descriptive terms of the reduced theory are not contained in the reducing theory, then Nagel further requires the existence of bridge laws which connect these terms and thus allow the derivability of one theory's laws from the other. When bridge laws are required then the purported form of reduction is called heterogeneous.

In the case in question, the candidate reduction of chemistry to quantum mechanics would fall under the case of heterogeneous reductions. This is because "some typically chemical terms cannot be found in the quantum mechanical language", thus requiring the existence of bridge laws (Scerri 1994: 160). For Eric Scerri, a successful reduction would sufficiently be supported if the properties

[11] For example, Hettema states that 'the idea that chemistry stands in a reductive relationship to physics still is a somewhat unfashionable doctrine in the philosophy of chemistry' (Hettema 2017: 1). A possible exception is the position, advocated primarily by Bader, that 'the Quantum Theory of Atoms in Molecules forms a proper, (reductionist) basis for chemistry' (Hettema 2013: 311) (see also (Bader and Matta 2013) and (Shahbazian 2013)). Whether Bader's position should be considered as one that supports strict Nagelian reduction in the sense specified here, is not examined further.

of atoms and molecules can (at least in principle) be calculated "entirely from first principles, without recourse to any experimental input whatsoever" (1994: 162).[12]

However, a Nagelian reduction along these lines has been rejected for a variety of reasons. It is argued that if Nagelian reduction forbids the use of approximations, then it fails for the examined pair because such approximations are prevalent in the quantum mechanical description of chemical phenomena (Needham 2010).[13] Another apparent problem is that "chemistry is a field, whereas reduction tends to be a relation between individual theories, or between laws and theories" (Hettema 2017: 1).

Contrary to the existing disunity theses, unity theses do not take the failure of Nagelian reduction to support the idea that the two science are disunified. Instead they take that there are alternative ways to support unity. For instance, Hettema proposes "a suitable paraphrase of the Nagelian reduction programme" which is "reinforced by a modern notion of both connectibility and derivability" (Hettema 2017: 24). Needham also proposes a more liberal understanding of Nagelian reduction that permits the use of approximations in science (Needham 2010: 168-169). Secondly, there are theses which defend the unity of chemistry with quantum mechanics by defending the existence of an ontological relation that does not require a Nagelian reduction between the respective sciences (Le Poidevin 2005).

Beyond existing unity theses about chemistry there are available non-reductive positions in the philosophy of science literature that, to this day, have not been examined for the case in question. This includes positions such as non-reductive physicalism, ontic structural realism and weak

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[12] The use of the term 'Nagelian' with reference to such an understanding of reduction is to an extent misleading because, as Hettema argues, Nagel was not so strict in his account of reduction: "Reduction is too often conceived of as a straightforward derivation or deduction of the laws and concepts of the theory to be reduced to a reducing theory, notwithstanding Nagel's insistence that heterogeneous reduction simply does not work that way" (Hettema 2017: 1-2). Nevertheless, since this term is often employed with reference to this understanding of (strict) reduction, this section retains it in order to differentiate it from amended understandings of reduction as these are formulated in the philosophy of chemistry literature.

[13] Scerri has argued that even if reduction is understood as allowing the use of approximations, it still fails for the examined pair of theories (1994: 168).

emergence.[14] This is not unexpected given the established attitude in the community to focus on defending (or at least investigating) the autonomy of chemistry from physics. Nevertheless, it also points at how much more can be said about the relation of the two sciences.

Moving on, the most discussed- and for some, most illuminating- case study for understanding chemistry's relation to quantum physics, is molecular structure. The spatial arrangement of the atoms that constitute a molecule is one of the most important properties in chemistry which is invoked to explain physical, chemical and biological properties of matter such as the structure of DNA, the toxicity of drugs and the reactivity of explosives. In the philosophy of chemistry, it has been invoked to show that chemistry is disunified from quantum mechanics.

One important account that examines molecular structure is Robin Hendry's strong emergence. He takes that the inability of quantum mechanics to identify the structure of a molecule through the Schrödinger equation without the use of any assumptions about that structure, is illustrative of its emergence. This is a metaphysical account because it purports a relation in the world; namely between molecular structure and the physical constituents of molecules. It is part of a more general idea in philosophy called emergence, which takes that "the emergent behaviour of complex systems must be viewed as determining, but not being fully determined by, the behaviour of their constituent parts" (Hendry 2006b: 180).[15] In the case of Hendry's account, strong emergence is spelled out in terms of downwards causation. As he puts it:

> a system exhibits downward causation if its behavior would be different were it determined by the more basic laws governing the stuff of which it is made. (Hendry 2010b: 189)

Hendry offers empirical support to the strong emergence of molecular structure by invoking- among other things- the example of isomers. Isomers are sets of molecules that consist of the same number and type of atoms but whose atoms are rearranged differently. There are different types of isomers postulated in chemistry and Hendry focuses on optical isomers, namely those isomers that

[14] For example, this includes 'supervenience-based formulations of physicalism' as per (Wilson 2005), accounts of non-reductive physicalism (Wilson 2010), and 'realization physicalism' as per (Melnyk 2003). It is not argued here that any of these accounts successfully apply to the case in question. These accounts are only mentioned to point out that there is a rich bibliography in the philosophy of science (and other fields of philosophy, such as the philosophy of biology) that could contribute to the examination of unity theses in the philosophy of chemistry.

[15] There are different versions of emergence that one can find in philosophy, see for an overview (Wilson 2021).

have the same kinds of chemical bonds and only differ in terms of the spatial arrangement of their atoms. According to Hendry, if one is to describe in quantum mechanics an optical isomer by taking into account all the interactions that occur in the molecule and by using as input only fundamental physical interactions and the value of the physical properties of the entities, then it would not be possible to distinguish between distinct optical isomers. To do so one has to incorporate ad hoc assumptions about the examined molecule into the Schrödinger equation. According to Hendry, this illustrates that the molecule's behaviour, as this is described "by the more basic laws governing the stuff of which it is made", is different from its behaviour as this is described by assuming its structure (Hendry 2017: 153).

Several responses have been offered against this account (Scerri 2012a; 2023; Seifert 2020b). Most recently, Franklin and Seifert (2024) have pointed out the role of the measurement problem and how this (at least in part) accounts for the inability of quantum mechanics to distinguish between isomers. The measurement problem arises because quantum physics predicts certain systems to be in superposition states relative to a measurement basis, despite the fact that the measurement of those states produces determinate outcomes. If we assume that the Schrödinger equation offers a complete description of a quantum state, this reveals an apparent inconsistency which is referred to as the measurement problem (Maudlin 1995). In the case of optical isomers, quantum mechanics predicts that the ground state corresponds to a superposition of their structures.[16] Franklin and Seifert argue that given we only observe a determinate structure and that the quantum physical description of isomers is assumed to be complete, it follows that this is an instance of the measurement problem. That is, the apparent inability of quantum physics to identify molecular structure from first principles, is just a special case of the measurement problem.[17]

Beyond the case of molecular structure, chemistry's relation to physics has been investigated in the context of macroscopic substances (van Brakel 2014: 34), the periodic table (Scerri 2012b: 75-76), orbitals (Villani et al. 2018), chemical reaction rates (Hettema 2017: 69-86) and the chemical bond (Hendry 2008; Weisberg 2008). Chemistry's place among the other sciences, most notably with respect to biology, has also been investigated but not in the context of the reductionist question. Instead, the relation of chemistry to biology has been addressed in the context of a different issue, namely that of natural kinds. The next section presents the main views around natural kinds in chemistry as well as on the reality of chemistry.

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[16] The ground state corresponds to the stable observable state of a system.

[17] Hendry (2022) has subsequently responded to the criticism. See also Fortin and Lombardi (2021).

3. Taking chemistry to its word

Apart from asking how chemical entities and their properties relate to their physical constituents, there are other questions regarding chemical ontology that have also been raised. These include questions about the reality of chemical stuff: are atoms, molecules, orbitals or chemical bonds real? Relatedly, do chemical classifications correspond to natural kinds? Moreover, are there laws in chemistry and, if so, do they track causal relations? I briefly sketch some of the views that have been proposed around these questions.

The realist question about chemistry, namely of whether and which chemical entities are real, has been posed both in the context of chemistry's relation to physics as well as independently. In the context of chemistry's relation to physics, the defence of a disunity thesis (as outlined above) is usually taken to imply that chemical ontology is distinct for the physical one. That is, chemical stuff are distinct from the physical things of which they are made and by consequence, exists. On the other hand, the defence of a unity thesis (including a reductionist one) does not necessarily imply that chemical stuff does not exist. It has been falsely assumed that the defence of chemistry's reduction implies the elimination of chemical ontology. That is, if atoms, molecules, bonds, etc. are just a collection of physical entities and their interactions, then there is no need to believe they exist (e.g. Labarca and Lombardi 2005: 134). On the contrary, even a strong reductionist position about chemistry that is formulated -say- by positing an identity relation between chemical and physical stuff does not imply an antirealist view about chemistry.

Independently of the question of reductionism, the realist question about chemical stuff has been examined with respect to atoms, molecules, orbitals, chemical bonds and even phlogiston. With respect to atoms and molecules, while John Dalton in the 18th century posited atoms as the constituents of chemical elements, it was Jean Perrin that is said to have established that they exist. This is because he calculated Avogadro's constant by using thirteen different methods and examining a wide range of diverse phenomena (Perrin 1916: 206-207).[18] The agreement between his calculations were taken to empirically establish the reality of these entities and has been invoked in philosophy in support of scientific realism (Achinstein 2001; Chalmers 2011; Hudson 2020; Psillos 2011; Salmon 1985; see van Fraassen 2009 for a criticism of this view).

[18] The Avogadro constant ($6.022\ 140\ 76 \times 10^{23}$ mol^{-1}) is a "(f)undamental physical constant representing the molar number of entities" (IUPAC 2014: 133).

With respect to the chemical bond, there are two conceptions that have been proposed by Robin Hendry (2008) and which purportedly specify its nature and reality. These are the structural and energetic conception. According to the structural conception, the bond is a material entity that connects atoms in a molecule. According to the energetic conception, the bond is best understood in terms of energetic facts around bonding. Each conception implies different metaphysical views around bonds' nature and existence (Seifert 2022b). For example, the structural conception is compatible with a realist view of chemical bonds, whereas the energetic is compatible either with an anti-realist view of bonds or a view of bonds as a property of molecules. More recently, it has been argued that bonds are best understood as real patterns in the spirit advocated by Daniel Dennett in his 1991 seminal paper (Seifert 2022b).

In addition, there are alternative realist views that defend the reality of chemical entities in a way that diverges from the spirit of standard scientific realism.[19] In chemistry, such a view is developed with respect to phlogiston, namely the substance that was posited in the 17th century and whose term was coined by Georg Stahl at the beginning of the 18th century. According to the phlogiston theory, phlogiston is a principle that all substances contain in some degree and which accounts for the phenomena of oxidation (what we call in common parlance, burning). At the end of the 18th century, Antoine Lavoisier successfully denied the existence of phlogiston and explained oxidation in terms of his theory of oxygen.

Nowadays philosopher and historian of chemistry Hasok Chang argues that phlogiston is "as real as tables-and-chairs and cats-and-dogs are in our daily lives" (2016: 118). This claim is part of his more general view called pragmatic realism. On this view, truth is granted not to a set of propositions, but to a scientific practice which succeeds in meeting its aims. In this context, to the extent that the postulation of phlogiston proved successful with respect to the function it served in the phlogiston theory, it should be deemed real.[20]

Apart from scientific realism, chemical entities have been invoked in discussions concerning natural kinds. Very briefly, the topic of natural kinds concerns whether classifications posited in science reflect (part of) the structure of the world. Chemistry is rich in classifications, offering

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[19] Standardly, a realist view takes that an entity to exist independently of how humans conceive it (that is, mind-independently). Chang's pragmatic realism (presented below in the main text) denies mind-independence.

[20] For a criticism of this view see e.g. Blumenthal and Ladyman 2017; 2018.

many examples of candidate natural kinds (i.e. chemical kinds). Elements represent a paradigmatic case for this topic (Bird 2018; Kripke 1972), but other candidates also are compounds, mixtures, chemical bonds, acids and macromolecules, including proteins (Bartol 2016; Bellazzi 2022; Chang 2012a; Havstad 2018; Hendry 2006a; Needham 2011; Tahko 2020; Weisberg 2006).

A standard view about elements as natural kinds is microstructural essentialism.[21] This view consists of two claims: (a) the property which identifies a kind-element is microstructural (in this case, its atomic number), and (b) this property is essential to its kindhood (Hendry 2005: 33). The latter means that all and only members of a kind-element posses the same atomic number. For example, all instances of gold are members of the kind-gold because they all possess the same microstructural property (namely, they have atomic number 79) and this property is essential to them. This view extends to chemical compounds as well, namely entities that are understood as collections of identical molecular entities. In this case, microstructural essentialism takes a chunk of matter to be an instance of a compound-kind (such as, say, water) because it has a particular microstructure that is unique to members of that kind (namely consisting of H_2O molecules).

Several criticisms have been formulated against this view, including that the microstructural properties invoked to pick out members of element-kinds and compound-kinds do not take into account isotopes. Isotopes are sets of entities which have the same atomic number but differ in the number of neutrons in their nuclei. In the context of microstructural essentialism, it follows that different isotopes correspond to the same kind. For example, matter consisting of deuterium oxide D_2O (i.e. heavy water) is a member of the kind-water as is matter consisting of H_2O. This is so despite the fact that macroscopically they exhibit different properties, including that D_2O is highly toxic and undrinkable. According to some philosophers this is a problem because macroscopic differences (including differences in size) should somehow be taken into account when distinguishing between chemical kinds (e.g. Bursten 2016; Needham 2011; Häggqvist 2022: 32).

As mentioned in the previous section, it is in the context of natural kinds that chemistry's relation to biology has been primarily examined. In particular, the question that has been raised is whether there are biochemical kinds, namely classifications that purportedly describe, predict and explain biological behaviour. Candidate biochemical kinds are proteins, genes and vitamins. In this context, philosophers have argued out that chemical entities (such as macromolecules) are

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[21] Chemical elements are entities that contain identical atoms. Atoms are distinguished in terms of the number of protons they contain in their nucleus (i.e. their atomic number).

identified as members of functional kinds because the property which unifies them into a particular class is a biological function that they serve (e.g. Bellazzi 2022; Tahko 2020; Tobin 2010).

One last metaphysical issue around chemistry that is worth mentioning because it is recently gaining growing attention, is that of causation. Rom Harré (2016) was perhaps the first to bring forward the idea that chemical transformations can be thought of as causal relations; namely as relations between causes and effects where the reactants combine together to bring about new products. He considered different accounts of causation for chemical transformations, including the regularity view, the power-based view and the mechanistic view. More recently, the question of whether chemical reactions can be understood as relations between causes and effects has been taken up by some philosophers who argue for example, for the propensity or dispositional view (Suárez and Sánchez Gómez 2023; Zambon 2022). The topic is I'm afraid too complicated to be sufficiently presented here in brief terms, so I direct the reader to Harré 2016, Seifert 2023, Suárez and Sánchez Gómez 2023, and Zambon 2022.[22]

But the investigation of chemistry is not restricted to metaphysical discussions, far from it. There are also epistemological questions with respect to chemistry which receive attention. The next section briefly presents some of them.

4. What and how do we know from chemistry?

Epistemic questions around chemistry have to do with chemical knowledge: how is it produced, what are its limits, and what is its nature. With regard to the nature of chemical knowledge, one question concerns the role of mathematics. In physics, the role of mathematics is taken to be central as it is often taken to account for its immense credibility. However, in chemistry, mathematics' role is not as ubiquitous (at least to the extent it is in physics). While there are areas in which mathematics play a central role (such as in quantum chemistry and thermodynamics), there is also a large part of chemical practice that is much more qualitative or based on the pictorial analysis of chemical phenomena (such as via physical models of atoms and molecules and the pictorial representation of chemical reactions and reaction mechanisms).

[22] Another metaphysical issue which related to the question of causation in chemistry and is now starting to gain attention is that of chemical laws. Specifically, are there laws in chemistry and what is their nature? For an introduction to this topic, see Seifert 2023.

Another important epistemic issue concerns the role of models and idealisations in chemistry. In philosophy of science, the role and function of models has been extensively examined and while a similar level of investigation has not been pursued in the philosophy of chemistry, there is a rich repository of chemical models that can inform such discussions (e.g. Weisberg 2007). There are different kinds of models one can identify in chemistry including physical models of atoms and molecules but also mathematical models of chemical systems that are used in quantum chemistry (such as valence bond, molecular orbital, and semi-empirical models). One question around models is how closely they approach the true nature of the systems they examine, but also the reliability of metaphysical claims that are made based on the study of such models (e.g. Seifert 2020a; 2022a). Philosophers have also questioned the reasons for the development of models in chemistry. Among those is the complexity of the mathematical descriptions developed in quantum physics, the value of simple explanations in the teaching of chemical phenomena, and the models' predictive success and numerical accuracy. Depending on the models' purported function, some philosophers regard the approximations and idealisations made in a particular model to be something that is supposed to be removed eventually (these type of idealisations are called Galilean; McMullin 1985). Others take the role of idealisations to play an ineliminable role in chemical theory and understanding (Hoffman 1998).

Relatedly, a major issue in the epistemology of chemistry concerns scientific explanations. For example, Hoffman (1997) claims that there are two modes of explanations found in chemistry: the vertical and horizontal mode. The vertical mode is based on the idea that explanations are derived by quantum mechanical calculations of chemical phenomena (this is closely related to the Deductive-Nomological explanation developed in general philosophy of science; e.g. Hempel and Oppenheim 1948). The horizontal mode is based on the idea that chemistry employs chemical concepts with which it explains phenomena.

On a different front, the nature of chemical explanations is also investigated with respect to reaction mechanisms. A reaction mechanism is a "detailed description of the process leading from the reactants to the products of a reaction, including a characterization as complete as possible of the composition, structure, energy and other properties of reaction intermediates, products and transition states" (IUPAC 2014: 902). Given their function and nature, they have been examined as paradigmatic examples of mechanistic explanations. For example, Goodwin (2012) argues that there are two notions of mechanisms employed in chemistry. First, the thin notion of reaction mechanisms which consists in specifying the discrete steps through which a reaction occurs. The second is the thick notion which consist in a sort of 'motion picture' of a chemical reaction (Weisberg, Needham and Hendry 2019).

Having briefly presented some of the epistemological issues raised around chemistry, the next section brings forward the idea of how philosophy of chemistry is informed by another discipline, namely the history of chemistry.

5. Thinking philosophically of the history of chemistry

Historical considerations are essential to the philosophical analysis of any natural or social science.[23] With respect to chemistry, this becomes apparent by two characteristics of chemistry. First, chemistry is a special science that is very much driven by the economic and social benefits that can be gained through the discovery of new elements and processes, as well as through the production of novel chemical substances.[24] For example, the need for the production of new materials and drugs determines in a great extent the sort of chemical research that is done at a particular time. Secondly, chemistry is an experimental science in the sense that experimentation is involved not only in the confirmation of a chemical hypothesis, but also in the development of the theories, models and concepts involved. For example, the development of the periodic table and the consequent classification of the elements was very much determined by the particular experimental means that were available at the time, and by the particular classificatory goals of the scientists involved.[25] All in all, history illuminates:

i. the influence of the economic and social context in which chemistry is being practiced at particular times, and;
ii. the role particular chemists have played in the development of chemical theories.

In this context, history plays an important role in the analysis of philosophical issues such as theory change, mereology, conceptual analysis, and the relation of chemistry with other sciences.

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23 Perhaps the most notable example of how central a role history plays in philosophy, is Kuhn's (2012) book on scientific revolutions which has until today a large impact on how one understands theory-change, realism and other philosophical issues.

24 For a very brief overview of how efficient chemistry has been in the production of novel chemical substances, see Madrigal Alexis, *HUMANS HAVE MADE, FOUND OR USED OVER 50 MILLION UNIQUE CHEMICALS*, (2009), <https://www.wired.com/2009/09/humans-have-made-found-or-used-over-50-million-unique-chemicals/>, 2/11/2017. Also, the Chemical Abstracts Service (CAS), a division of the American Chemical Society, has formed the CAS registry which enumerates all the known chemical substances (more than 133 million chemical substances thus far).

25 For a detailed analysis see Scerri 2007.

The understanding of the main chemical concepts has been articulated within historical accounts about the main players involved in the development of those concepts, such as the atom and Perrin's contribution in establishing its existence (see section 3).[26] Also, the understanding of the relation between chemistry and other sciences (i.e. quantum mechanics, thermodynamics, biology, etc.) is accommodated by mapping the historical affiliations between chemistry and those sciences.[27]

The corpus around the history of chemistry is extensive; in fact, the field is much older than that of the philosophy of chemistry. There are societies dedicated to the history of chemistry that have existed for approximately 80 years. For example, the Society for the History of Alchemy and Chemistry (SHAC) was founded in 1935 and publishes the journal *Ambix*. The European Association for Chemical and Molecular Sciences (EuCheMS) founded the Working Party (WP) on History of Chemistry in 1977. The Working Party has organised the International Conference on the History of Chemistry since 1991. The Royal Society of Chemistry has founded the Historical Group which holds annual meetings and publishes newsletters. The History of Chemistry Division of the American Chemical Society first published the Bulletin for the History of Chemistry in 1988. Articles on the history of chemistry are also published in history of science journals, such as the *British Journal for the History of Science* and *Centaurus*.

Several historical episodes in chemistry have influenced philosophers in how they think of not just chemistry but of the sciences in general too. These include the Chemical Revolution, the development of the periodic table of elements, alchemy, and the development of quantum chemistry. I very briefly sketch some of the questions of philosophical significance that have been informed by the historical analysis of chemistry.

First, the Chemical Revolution. By this term we refer to that period in the 18th century when Lavoisier's theory of oxygen was accepted and replaced the up-until-then prevalent phlogiston theory. Phlogiston theory was based on the postulation of an element called phlogiston (from the greek word for flame) and had been developed to explain phenomena such as combustion and the transformation of metals into oxides. Some of the main proponents and developers of the

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[26] For a historical account of the image of the atom see e.g. Pullman 1998. For a historical account concerning the discovery of particular chemical elements, see e.g. Scerri 2013.

[27] For the case of the relation between chemistry and quantum mechanics, see e.g. Gavroglu and Simões 2012.

phlogiston theory were Johann Joachim Becher, Georg Ernst Stahl, and Joseph Priestley.[28] This theory was eventually abandoned in favour of the oxygen theory that was proposed by Antoine Lavoisier and which was based on the postulation of oxygen for the explanation of- among other things- how things burn.

One of the questions philosophers ask about the Chemical Revolution is whether the Kuhnian understanding of theory change and scientific progress in terms of paradigm shifts applies in this instance. For example, was the Chemical Revolution an example of a scientific revolution as Kuhn had proposed? Were the two theories- namely the phlogiston theory and the oxygen theory- incommensurable, and if so, in what ways? How was communication and exchange of ideas achieved (if indeed it was) between defenders of the two camps? Subsequently, some philosophers have defended the successful application of the Kuhnian account to the Chemical Revolution (e.g. Chang 2009; 2012b; Hoyningen-Huene 2008). For example, Hasok Chang defends the methodological incommensurability between the two theories and argues that the chemists of that time did not have good reasons to abandon phlogiston over the oxygen theory. Others, such as Geoffrey Blumenthal (2013) and James Ladyman (Blumenthal and Ladyman 2018), have resisted Kahn's framework by offering historical evidence that phlogistians managed to perfectly communicate and critically analyse their work with chemists who adopted the oxygen theory (thus undermining Kuhn's idea of incommensurability).

Another episode from the history of chemistry which has received attention from philosophy- though admittedly not as much as the Chemical Revolution- is alchemy. Alchemy is the field which preceded the rise of modern chemistry. Its development spans over many centuries and regions. Evidence of alchemical practice is found in ancient Egypt, reach the Arab period in the Middle East and Africa, and goes all the way to Medieval Europe. Alchemy is standardly associated with the idea of the transmutation of metals into gold and the search for the elixir of life (also called Philosopher's Stone). It was believed that there is a way to transform all metals (and possibly any material) into gold through this so-called elixir. The elixir would also be able to cure all diseases, if not grant immortality to its users.

Alchemists were in the business of discovering the elixir and in the process of doing so developed a number of chemical apparatuses and techniques and discovered plenty of chemical elements.

[28] Interestingly, Priestley is credited with being the first who isolated (and thus) discovered oxygen (which he called dephlogisticated air) despite the fact that he never accepted Lavoisier's theory of oxygen and was an ardent proponent of the phlogiston theory.

Due to the mystical nature of their studies (they often used cryptic language to present their recipes and made obscure metaphysical claims), alchemy has been regarded a pseudo-science. This view was in fact promoted by key figures in the history of chemistry- most notably by Robert Boyle during the 16^{th} century- who wanted to separate their study of chemical phenomena from alchemy so as to gain credibility. This inevitably lead to modern discussions about whether indeed alchemy was pseudoscientific, with some historians of chemistry recently arguing that it was not (at least not to the extent that has been standardly believed) (e.g. Newman 2011; Principe 2011).

Another major historical event in chemistry was the development and subsequent acceptance of Mendeleev's periodic table of elements. While the modern table is based on Mendeleev's initial classification, Mendeleev was not the only one to develop a classification of elements. Lavoisier had proposed his own classification and during the time that Mendeleev was developing his table, other classifications were proposed as well. In fact, historical evidence shows that early classifications of chemical elements (as proposed by Meyers, Newlands and Mendeleev) were competing each other. It has been recently pointed out that the way these classifications were developed and defended was based on a set of values that those actors had aimed at meeting. For example, Mendeleev's table aimed at completeness: he wanted his proposed classification to include as many of the known elements as possible (Pulkkinen 2019; 2020). Meyers sought 'carefulness'; that is, he "was the most explicit about the quality of the data that gave rise to his systematisations" (Pulkkinen 2020: 182). Newlands on the other hand, sought out simplicity with his proposed 'Law of Octaves' (Pulkkinen 2020: 176). Discussion of the role values in the formulation of early classifications of chemical elements is closely related to a more general topic in philosophy of science: namely to that of the role of values in science and in theory choice.

In fact, the latter question- namely how scientists choose between competing theories or (in this case) classificatory schemes- is one which has prompted extensive debate. In the case of the periodic table, it is argued that the eventual choice of Mendeleev's periodic table was based on its unique ability to not just include all the known chemical elements of his time but also to predict elements which had not been discovered yet. Lipton has put this quite famously like this:

> When Mendeleev produced a theory of the periodic table that accounted for all sixty [really sixty-two] known elements, the scientific community was only mildly impressed. When he went on to use his theory to predict the existence of two unknown elements that were then independently detected, the Royal Society awarded him its Davy Medal . . . Sixty accommodations paled next to two predictions. (Lipton 1991: 134)

In this context, the choice of Mendeleev's table is invoked as evidence for the view called 'predictivism' according to which, the assessment of scientific theories should be based on their ability to make novel predictions and not on the basis of accommodating already known empirical facts (e.g. Popper 1963).

These are some of the episodes in chemistry's long history which have drawn the attention of philosophers and have informed their analysis. The investigation of chemistry's history for philosophical purposes is part of a wider effort to enrich our understanding of how chemistry has been practiced throughout the centuries.

6. New frontiers in chemistry

While I have covered a broad range of the topics that belong in the purview of the philosophy of chemistry, admittedly there is a lot more that can be said about each of them. In fact, the debate still continues about whether chemistry is reduced to physics, if there are chemical kinds, whether chemical bonds are real, and if the Chemical Revolution was indeed so revolutionary! Beyond these issues, there are also others which I did not mention but that also belong to the subject matter of this field. I am confident that the reader has now sufficient information to discover these topics.

As a form of conclusion to this article, I wish to briefly present three issues that are rarely discussed by the community but which I believe will start to gain considerable attention, and become extremely valuable to our understanding of chemistry and of its role in modern societal problems.

The first issue concerns the role of Artificial Intelligence (AI) in chemistry. Machine learning is a field that is now starting to be applied to chemistry (as well as of course other sciences). The main purposes for which it is used are the discovery of new compounds and substances, the prediction of their properties, as well as the identification of reaction mechanisms by which they can be produced. The predictive ability of Machine Learning has already shown to be of immense power, with unexpected new substances being discovered for uses that sometimes even scientists themselves did not expect (or even want).[29] Given the capabilities of AI and its role in chemistry,

[29] Note that the synthesis of novel chemical substances is closely connected to their aspired use in drugs but also weapons. e.g. https://www.scientificamerican.com/article/ai-drug-discovery-systems-might-be-repurposed-to-make-chemical-weapons-researchers-warn/

one issue that will eventually warrant the insight of philosophers has to do with the nature of chemical knowledge. Will chemical knowledge change in its nature? What will the role of chemical theory be in the discovery of substances via AI? Will the notions of prediction, explanation and discovery in chemistry change in light of the role of AI? It goes without saying that ethical issues also come to the fore and will become more and more pressing. How should scientists handle the vast amount of data produced by AI, and how should that data be disseminated given its potentially sensitive use? Moreover, who should receive credit for the discovery of a substance that was predicted using a tool that in turn employs a vast amount of prior scientific knowledge?

The second issue has to do with the inclusion of women in chemical historiography and practice. The feminist philosophy of science has developed an extensive critique towards the sciences, pointing out the ways in which women scientists have been excluded. First, it is now an established fact that the history of science has not accurately acknowledged the role women in the production of scientific knowledge. In this context, it is an ongoing project to identify the unknown women who have practiced chemistry since the ancient times. For example, it was only recently pointed out that the first known chemist was a woman: around 1230 BCE Tappūtī-bēlat-ekalle was head perfurmer in ancient Assyria (Wills et al. 2023). Secondly, feminist critiques of science have identified the specific ways by which women scientists have been undermined, overlooked, or hampered in their work (e.g. Schiebinger 1991). While Marie Curie may be one of the most celebrated chemists and scientists of all time, unfortunately she is an exception. There are many other women chemists that have remained hidden behind male figures throughout chemistry's history (the story of Marie Lavoisier is one such example).

The third issue has to do with the role of philosophy in chemical education. Sibel Erduran (2001; 2013; 2020) has extensively worked in bringing forward the value of philosophising about chemistry to chemical education. However, a much more systematic and collective effort needs to be made to bring together philosophers and educators of chemistry, and spell out the exact ways by which philosophy can ameliorate the teaching of chemistry at all levels of education.

These are in a nutshell some of the issues I believe will (or at least should) emerge in the philosophy of chemistry in the next few years, and which can further enhance its value both to science and society. The philosophy of chemistry- just like chemistry itself- is a rich and exciting field of study that raises diverse questions about the nature of science, but also - more importantly- about the world and our place in it.

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