Reframing the Reduction-Emergence Debate around Chemistry¹

Abstract

The study of molecular structure has played a central role in the debate around chemistry's reduction to quantum physics. So far, this case has been invoked to support the non-reducibility of chemistry. However, recent papers claim that there might not be any structure to be assigned to isolated molecules, thus prompting a deeper investigation of the nature of molecular structure. To this end, this paper explores two alternative accounts of structure: the relational and dispositional accounts. Each metaphysical account has interesting implications for the reduction debate and opens news ways of arguing for (but also against) the reducibility of chemistry. The aim is to show that the debate around chemistry's reduction needs to be radically reframed so as to include a rigorous metaphysical analysis of the nature of molecular structure.

1. Introduction

Molecules are central to chemistry. Yet when it comes to describing them quantum mechanically, there is no specific structure assigned to them from first principles. Various interpretations have been offered, including that this is evidence of strong emergence, ontological pluralism or at least the non-reducibility of chemistry to quantum physics (Chang 2015; González et al. 2019; Hendry 2010a; 2010b; Hendry and Needham 2007; Lombardi and Labarca 2005; Scerri 1991; 1994). A more recent reply by Franklin and Seifert (2024) focuses on the role of the measurement problem. They argue that a specific structure cannot be identified by quantum mechanics (from first principles) because in isolated contexts a molecule's stable state (sometimes) corresponds to a superposition of structures, rendering this situation an instance of the measurement problem.

This paper explores the potential implications of Franklin and Seifert's response to our metaphysical understanding of molecules and in particular of molecular structure. According to Franklin and Seifert, under at least certain interpretations of quantum mechanics, it would be mistaken to assume that isolated molecules exhibit the structure assigned to them by chemistry. Put differently, isolated molecules should perhaps be construed as quantum objects which- as such- cannot be expected to instantiate this classical property.

If they are correct, then what sort of property is molecular structure? That is, how should we metaphysically understand the property of structure if - under isolation- this property is not instantiated by molecules? To answer this, I present and critically analyse two alternatives; the relational and dispositional view. On the relational view, structure is understood as a property that comes about *only* in relation to some environment or interaction. So, strictly speaking, there is no structure in isolation. Given that in chemistry structure determines the identity of molecules, this

¹ Preprint of book chapter to be published In: Bryant, A. and Yates, D., (eds.) *Rethinking Emergence*. Oxford University Press (In Press)

implies that in isolation there are no molecules the way chemistry conceptualises them. On the dispositional view, isolated molecules maintain their structure but *only* as dispositions. In this context, one can understand a superposition of molecular structures as identifying all the possible structures the system is disposed to exhibit *after* collapse of its wavefunction. More importantly, molecules are objects which maintain - in a thinner sense- the classical properties that, according to chemistry, are essential to their identity.

Regardless of which view one adopts, this analysis shows that the discussion around chemistry's relation to quantum physics needs to be radically reframed. How one understands the nature of molecular structure (as a relational, dispositional or other sort of property) affects the stance one holds about structure's reducibility. For example, under the relational view, the chemical description of molecules becomes irrelevant to isolated systems, thus undermining the empirical basis of existing antireductionist and emergentist accounts. Nevertheless, one could propose alternative forms of emergence that are based on a broader examination of the classical-quantum divide. On the other hand, under the dispositional view one can maintain a sense of reducibility that does not require (as previously thought) the instantiation of structure in isolated systems. This is because, even though quantum physics does not identify the specific observable structure of a system, it does map the range of possible structures an isolated molecule can instantiate after collapse of its wavefunction.

Note that apart from an informed understanding of the metaphysical nature of structure, the reframing of the reduction-emergence debate requires an additional amendment. As Franklin and Seifert show, the issue cannot be discussed independently of the different interpretations of quantum physics. How exactly that is, I leave it for another occasion.

Section 2 presents how considerations around molecular structure have so far guided philosophical discussion around chemistry's reduction. Section 3 presents how to understand the nature of molecular structure, if we accept that there is no structure in isolation. Specifically, it spells out two alternative views: the relational and dispositional accounts of structure. Section 4 sketches how each of the two accounts may change our views on chemistry's reduction. This analysis shows that any account of chemistry's relation to quantum physics which is based on the examination of molecular structure, needs to include a rigorous analysis of the nature of structure.

2. The situation so far

Until late in the 20th century, it was more or less accepted in general philosophy of science that chemistry is one of the least problematic examples of successful reduction to physics (Hendry 2012: 369). This was in large part due to the empirical success of quantum physics which led scientists such as Paul Dirac, to famously exclaim that "(t)he underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known" (1929: 714). This was reinforced by the subsequent formation of quantum chemistry; a field that has developed various quantum models with growing precision so as to describe the chemical behaviour of different types of molecules (including organic molecules and metallic

compounds). In addition, models of reduction which to this day are deemed standard or classic reductionist theses in the literature took chemistry to represent an uncontroversial example of reduction, thus contributing to this overarching impression that chemistry is successfully reduced to physics (e.g. Nagel 1979; Oppenheim and Putnam 1958).

However, when philosophy of chemistry was organised as a separate field of study, several of its representatives took it to be of perennial importance to resist this reductionist stance towards chemistry (Chang 2015; Lombardi and Labarca 2005; Scerri and Fisher 2015; Schummer 2014; van Brakel 1999). It was believed that resisting the reducibility of chemistry to quantum physics is central in order to safeguard the autonomy of chemistry but also that of the philosophy of chemistry. It is no surprise that in the relevant literature, chemistry's reduction to quantum physics was presented as the defining issue of philosophy of chemistry. As Chang states:

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. (2015: 193)

In this context, one of the most compelling cases that have been invoked to reject chemistry's reduction, is that of molecular structure. In particular, the apparent inability of quantum physics to identify a molecule's structure from first principles, is taken as evidence of some form of irreducibility (of the epistemic and/or metaphysical form).

Interestingly, the empirical evidence that is most standardly invoked in this discussion is drawn from the work of quantum chemists R. Guy Woolley and Brian Sutcliffe who in the 1970s pointed out that:

(..) if one starts from a description of a molecule as an isolated, dynamical system consisting of the number of electrons and nuclei implied by the stoichiometric formula that interact via electromagnetic forces, one cannot even calculate the most important parameters in chemistry, namely, those that describe the molecular structure. (Woolley 1978: 1074)

The next subsection spells out the alleged problem with quantum physics' description of molecular structure, and presents some of the most representative antireductionist views that have been prompted by this putative problem.

2.1 The anti-reductionist camp

In order to appreciate how molecular structure is invoked in the debate about chemistry's reduction, it is helpful to offer first some scientific and terminological background. A molecule is

"(a)n electrically neutral entity consisting of more than one atom" (IUPAC 2014: 958).² It is stable (under particular thermodynamic conditions) when it is found in its "state of lowest Gibbs energy" (IUPAC 2014: 646).

A molecule's structure refers to the spatial arrangement of the atoms that constitute it. While it prima facie seems like a very intuitive and easy to grasp property (often referred to as the 'shape' or 'geometry' of a molecule), structure is a tricky concept. This is for two main reasons. First, it is a collective term: there is no single empirically measurable (chemical or physical) property which corresponds to a molecule's structure (Seifert 2020a: 23). Instead, there are a number of empirically measurable chemical and physical properties that collectively specify a molecule's structure.³ These include the properties that are assigned to the intramolecular interactions of atoms (such as bond types, bond lengths, angles, dipole moments, and so on); the properties that are based on the quantum mechanical description of molecules (including the electronic configuration of the relevant atoms); and, the properties which specify structural differences between distinct kinds of molecules (such as isomerism- more on this later).

Secondly, in chemistry structure is represented statically, as if a molecule and its constituting atoms are not continuously moving and rotating in space. However, this is an idealisation as structure is a dynamic property (Seifert 2020a: 25; see also Hendry 2021). There is no such thing as a static and unchanging structure to a molecule. The particles that comprise a molecule interact with each other and move in space. Intramolecular interactions persist even when the total energy of the system is constant, since the angular momentum of its comprising entities is non-zero. That is, the structure of a molecule is dynamic: a molecule possesses different conformations in time as a result of the continuous interactions of the electrons and nuclei that comprise the system (e.g. Longuet-Higgins 1963: 446).

Moving on to quantum physics, any collection of particles can be studied either in isolation or with respect to how it interacts with its environment, and it can be in a number of different possible dynamical states (Bransden and Joachain 1989: 189). In order to find the wavefunctions that represent all the states of a system, one solves the Schrödinger equation for that system. The Schrödinger equation is the "equation of motion for the wave function" which describes "the state of a quantum-mechanical system, and (more generally) for the corresponding state-vector ψ " (Palgrave Macmillan Ltd 2004: 2029). The time-dependent Schrödinger equation is a linear partial second-order differential equation with respect to position and a partial first-order differential equation, it is possible to formulate the time-independent Schrödinger equation, which is an

² To avoid potential disagreements on terminology, I employ (to the extent possible) the definitions and terminology offered by the International Union in Pure and Applied Chemistry (IUPAC 2014).

³ Hendry (2016) is particularly helpful in understanding the concept of structure.

⁴ I only focus on the non-relativistic Schrödinger equation of a quantum system since this is the one that is standardly employed for the description of a molecule.

equation independent of time and whose solutions are a system's time-independent wavefunctions, $\psi(x)$. These wavefunctions correspond to the stationary states of the system under examination.

The time-independent Schrödinger equation does not yield one unique solution; i.e. one wavefunction. It yields an infinite number of solutions ($\psi(x1)$, $\psi(x2)$, ...), each of which corresponds to a different state of the system under examination. Note that, in accordance with the superposition principle, any linear combination of the solutions of the time-independent Schrödinger equation is also regarded as a wavefunction that represents a possible state of the system (Griffiths 2005: 27). The wavefunction that is associated with the minimum total energy corresponds to the ground state of the system, whereas the wavefunctions whose total energies are larger correspond to the excited states of the system. The ground state of a molecule is taken to correspond to its stable state (where stability is understood in a manner consonant with chemistry's understanding- see above).

The quantum mechanical description that philosophers focus on in the debate about reduction, is that which is developed for a single *isolated* molecule. Standardly, a molecule is considered to be in isolation if it does not interact with other entities (such as electrons, ions, atoms or molecules) and if its total energy is conserved (i.e. there are no energetic exchanges with its environment that lead to a change in its total energy) (Seifert 2020a: 21). In this context, the time-independent Schrödinger equation for an isolated molecule provides an infinite number of solutions (i.e. wavefunctions) each of which corresponds to different stationary states of the molecule. The state with the minimum total energy is the ground state of the isolated molecule; i.e. the state in which it is stable (under specific conditions).

The Hamiltonian operator plays a central role in the solution of the time-independent Schrödinger equation for isolated molecules (and quantum systems more generally). The Hamiltonian operator is the sum of two operators; the kinetic energy operator and the potential energy operator. With respect to a molecule, the Hamiltonian operator corresponds to its total energy (i.e. its eigenvalue is the total energy of each state of the molecule); hence it is called the molecular Hamiltonian. In principle, the molecular Hamiltonian operator should include all the factors that determine the kinetic and dynamic energy of the molecule. That is, it should take into account the kinetic energy of each nucleus and electron in the system; the repulsion between each pair of electrons and between each pair of nuclei; and the attraction between each pair of electron and nucleus.

Because of the mathematical complexity involved in the formulation of the Hamiltonian operator, molecules are examined in the framework of the Born-Oppenheimer (BO) approximation.⁵ The BO approximation is a "(r)epresentation of the complete wavefunction as a product of an electronic and a nuclear part" (IUPAC 2014: 179). The validity of the BO approximation is "founded on the

⁵ This section does not consider cases where the approximation is not justified (e.g. IUPAC 2014: 179).

fact that the ratio of electronic to nuclear mass (..) is sufficiently small and the nuclei, as compared to the rapidly moving electrons, appear to be fixed" (IUPAC 2014: 179).

Within the BO approximation, one can in principle formulate the Hamiltonian operator by positioning the nuclei at all the different possible fixed positions. Each set of nucleonic positions corresponds to different quantum states of the system (hence to different wavefunctions) and to different values of the total energy, E, of the molecule. However, in practice this process is not followed. By having prior knowledge of the quantum system that is under examination (in this case, by knowing the chemical and structural properties of a molecule) only particular nucleonic conformations are considered when constructing the Hamiltonian operator.

Note that even when the nucleonic conformation is fixed (in the manner represented by the BO approximation), calculating the solution of the Schrödinger equation remains a complicated task. First, each nucleonic conformation is compatible with different quantum states of the system (and thus different wavefunctions). This is to be expected as chemistry tells us that even if the nuclei in a molecule are fixed at particular positions, the electrons may behave in more than one way within that molecule. Secondly, solving the Schrödinger equation and finding the wavefunction that corresponds to the ground state of the system (i.e. the state of the stable isolated molecule) is not straightforward for one additional reason. There are two unknowns in the equation; namely the total energy of the system, E, and the wavefunction of the corresponding quantum state of the system. That means that one must solve one equation with two unknown variables. In light of the above, the Schrödinger equation is not solved analytically for almost any molecule. As Hendry states:

There is an exact analytical solution to the non-relativistic Schrödinger equation for the hydrogen atom and other one-electron systems, but these are special cases on account of their simplicity and symmetry properties. (2010a: 212)

Instead, various approximate methods have been developed to solve it, most of which employ the BO approximation. In general, the development of computation has led to the proliferation of complex computational methods that solve the equation by following different mathematical strategies and by making different sorts of assumptions.

In the above situation, the alleged problem for Woolley and Sutcliffe (and later on for antireductionists) is that quantum physics cannot identify a molecule's structure from first principles, i.e. without making any ad hoc assumptions about that structure. The assumptions that they focus on are those implemented via the BO approximation, as they take that by assuming that nuclei hold fixed positions, one imposes the structure that quantum mechanics is supposed to derive for the system it describes. In addition, they claim that the implementation of the BO approximation is not just an epistemic necessity; i.e. something that quantum chemists do in order to surpass the mathematical complexity involved in solving the equation. Rather, there is a more substantial reason why the BO is used. Namely, if scientists did not apply this approximation and

instead solved the equation from first principles, they wouldn't derive any structure for the system in question.⁶

Hendry explains this problem in terms of the distinction between the resultant and configurational Hamiltonian (Hendry 2010a: 208–213). A resultant Hamiltonian is defined as the complete description of all the interactions that occur in a molecule, and it is constructed using as input the fundamental physical interactions and the value of the physical properties of the quantum entities comprising a molecule. However, the Coulombic Schrödinger equation, which is defined in terms of a resultant Hamiltonian, is almost never used. Instead, what is standardly used in order to construct the Schrödinger equation and to describe a system, is the configurational Hamiltonian. The configurational Hamiltonian is constructed on the basis of ad hoc assumptions about the nuclear geometry of the examined molecule (via the BO approximation). Based on this distinction, Hendry claims that, regardless of the mathematical complexity involved in solving the Coulombic Schrödinger equation, the resultant Hamiltonian is *in principle* unable to provide information regarding a molecule's structure.

This is taken to be empirically supported by two examples from chemistry. The first concerns the quantum mechanical description of isomers (Hendry 2010a: 213; Hendry 2010b: 186; Woolley 1998: 11). Isomers are sets of molecules which are all constituted by the same number and kinds of atoms, but that differ in the way that these atoms are connected to each other. Distinguishing between isomers is particularly important in chemistry as substances comprised of different isomers can exhibit quite different physical and chemical properties. According to Hendry, Woolley and Sutcliffe, distinct isomers are described by one identical resultant Hamiltonian and therefore an identical Coulombic Schrödinger equation. Therefore, it is not possible to use the resultant Hamiltonian to differentiate molecules that differ in terms of their isomerism. Instead, it is the configurational Hamiltonian that can differentiate systems which differ only in terms of their structure.

The second example concerns the quantum mechanical description of any non-symmetric isolated molecule (Hendry 2010b: 186; Woolley and Sutcliffe 2012: 409). The quantum mechanical description (in terms of the resultant Hamiltonian) does not describe the asymmetries in the structure of a particular molecule (as specified, for example, by the dipole moment). This is because "arbitrary solutions to the Coulombic Schrödinger equations should be spherically symmetrical" (Hendry 2010a: 213). However, "polyatomic molecules cannot be spherically symmetrical, for their lower symmetries are important in explaining their behaviour" (Hendry 2010a: 213). Therefore, one inserts information regarding such asymmetries into the configurational Hamiltonian (via the BO approximation) in order to construct an accurate description of a molecule's structure.⁷

⁶ How Woolley and Sutcliffe themselves interpret this situation is discussed in the next section.

⁷ A quantum mechanical description is understood here as being accurate if it agrees with how the structure of a molecule is experimentally identified.

In the philosophy of chemistry, the above situation is taken to suggest that chemistry is somehow irreducible to physics, if not also autonomous in some substantial way.⁸ Initially, it was argued that this situation shows that chemistry cannot be epistemologically reduced to quantum mechanics, in the Nagelian sense of epistemological reduction. Scerri (1991; 1994) who was the main advocate of this view, thought that a Nagelian form of reduction required the deduction or derivability of higher level properties from the lower level theory without the use of ad hoc assumptions. He claimed that a successful reduction of chemistry can be supported only if quantum physics can (at least in principle) describe the chemical properties of a system "entirely from first principles, without recourse to any experimental input whatsoever" (Scerri 1994: 162). Regardless of whether this is an accurate or even sensible rendering of Nagel's account of reduction, he concluded that the way in which quantum physics describes molecules and their chemical properties is evidence of chemistry not being reduced to quantum physics.9 Note that a similar point against physicalism is presently formulated by Robin Hendry and Thomas Rossetter against physicalism in chapter [..]. They take the inability of quantum physics to derive chemical facts from first principles as evidence for the failure of the causal closure of the physical, which is a key principle not just of Nagelian reduction but of physicalism too (as advocated for example by Papineau 2002).

Moving on, another response that has been offered in light of this situation is that this is an instance of strong emergence (Hendry 2010a; 2010b; 2017). Strong emergence consists of three main claims, which can be spelled out as follows (see Seifert 2020b: 44-45). First, there is a hierarchy of levels in which things in the world are found. 'Levels' are understood here as referring to partially distinct scales of energy, length, and/or time. On this view, there is the physical scale in which quantum entities and their properties are found; chemical entities that are found at the chemical level; and so on. Secondly, the chemical properties of a molecule (including its structure) supervene on its physical constituents (Hendry 2010b: 185). That is, whenever there is some change in the chemical properties of a molecule, there is always some change in the way its physical constituents interact. Thirdly, molecular structure is causally autonomous from the molecule's physical entities and interactions. Its causal autonomy is spelled out in terms of 'downward causation' (Hendry 2010b: 185). That is, structure is causally autonomous in the sense that it exerts downward causal powers to the physical entities that make up the molecule. What this means in more crude terms is that the structure of a molecule partially determines how (a stable) molecule's physical entities interact with each other.

Another interesting antireductionist response that has been offered (though it will not be further discussed here) is ontological pluralism (Lombardi and Labarca 2005; Fortin, Labarca and Lombardi 2020). This account is perhaps the strongest metaphysical account advocated on the basis of analysing molecular structure. On the one hand, Scerri's account of antireductionism is primarily epistemological in that it concerns how chemical and quantum descriptions relate to

⁸ Autonomy can be spelled out in various ways. The two forms of autonomy I have in mind are those spelled out in terms of strong emergence and ontological pluralism (see below).

⁹ Hettema (2017) for example argues that Scerri is too strict in his interpretation of Nagelian reduction.

each other. Hendry's account of strong emergence- though metaphysical- retains some form of dependence relation between the chemical properties of a molecule and its physical constituents (namely, in terms of supervenience). On the other hand, under ontological pluralism, no dependence relation is maintained. As Fortin, Labarca and Lombardi state:

the admission of a multiplicity of ontologies, not necessarily linked by hierarchical connections, cancels the need of finding a relation of dependence between the molecular level and the quantum level. (2022: 1)

These are the most representative antireductionist accounts that have been offered in the literature and which have been supported or at least prompted by considerations around the quantum physical description of molecular structure. Of course, this is not a complete overview of the relevant literature, and some reductionists have attempted to resist these views (Lombardi et al. 2022 for a detailed overview; see also Hettema 2017; Needham 2006). I do not delve into these responses here. Instead I focus on one assumption that is common to all the aforementioned antireductionist accounts and which has been largely overlooked by both sides of the debate. This is the assumption that there is structure in isolation.

All antireductionist theses which invoke the apparent inability of quantum physics to identify a molecule's structure make one crucial (though implicit) assumption: that there is such structure to be found in isolation.¹⁰ If they did not make this assumption, then the question of recovering structure through the quantum physical description of molecules would not arise in the first place. Put differently, the aforementioned antireductionist claims all hinge on the assumption that there is such a property to be found somewhere. If molecules did not exhibit such a property in isolation, then the question of its reducibility would be moot.

However, recent analyses by Seifert (2020a; 2022) and Franklin and Seifert (2024) offer arguments against the tenability of this assumption. That is, perhaps molecules in isolation do not exhibit any structure. If this is indeed the case, then- as is shown in the next two sections- this completely reframes the debate around chemistry's reduction. Before explicating this, the next subsection briefly presents the arguments supporting that there is no structure in isolation.

2.2 Could there be no structure in isolation?

There are convincing epistemological and theoretical reasons to believe that there is no structure when a molecule is in isolation. The epistemological grounds are based on how we observe structure. As Seifert (2022) notes, the conditions under which we empirically identify a molecule's structure are always conditions under which the molecule is not isolated. It is only recently that chemists have started to develop experimental techniques that try to empirically observe single

¹⁰ Recall, quantum physics describes a molecule which is in isolation: that is, it assumes that there are no other entities in the close vicinity that interact with the system in question, and the total energy of the system is conserved (Seifert 2020a: 21).

molecules (this emerging field is called 'single molecule chemistry'). In general however, it is standard to infer the properties of a single molecule by examining it as part of a chemical species; namely as part of an ensemble of entities (usually of the same type). More importantly, the chemical investigation of molecules has shown that their structure is not only determined by the interactions of its constituents, but also by the interactions of the system with its environment. Therefore, whatever structure chemists observe and subsequently assign to a single molecule, it is always one which it instantiated when examined as part of an ensemble.

Moreover, note that the mere act of experimentally interacting with a system automatically renders the system in non-isolation. Even if we could single out a molecule, any observation requires that some form of interaction takes place between the system and a device. So strictly speaking, whenever scientists assign any property to isolated molecules, it is not the case that they have observed isolated molecules having this property.

However, the most compelling reason to believe that there is no structure in isolation is offered by a close examination of quantum physics. Franklin and Seifert (2024) offer theoretical grounds to the claim that there is no structure to isolated molecules by looking at their predicted ground state. They note that in isolation, the ground state of many molecules (in particular those that exhibit different isomeric structures) corresponds to a superposition of structures. They claim that this explains why - without applying the BO approximation- one cannot derive molecular structure. More importantly, they take this to suggest that the alleged problem of identifying molecular structure though quantum physics is just an instance of the measurement problem.

In this context, any suggested solution to the measurement problem also offers an explanation of why quantum physics does not assign a specific structure to a molecule from first principles (i.e. without applying the BO approximation). More importantly, they claim that under certain interpretations of quantum mechanics, the superposition of structures indicates that isolated molecules may not have structure in the way chemistry purports (Franklin and Seifert 2024: 47). For example, according to the Everrett interpretation of quantum physics, superpositions of distinct atomic configurations are interpreted physically, suggesting that there may not be any structure to isolated molecules prior to interaction with an environment (or measurement device) (Franklin and Seifert 2024: 49).

Of course, their claim is contingent on a specific interpretation or theory of quantum physics, and there are certain theories (such as the de Broglie-Bohm theory) that do not seem to imply that there is no structure in isolation (Franklin and Seifert 2024: 52). Nevertheless, they do offer evidence that at least in the context of some of the most prominent realist interpretations of quantum physics, structure may not be a property that we can meaningfully assign to isolated molecules.

The above arguments provide sufficient grounds to seriously discuss the idea that isolated molecules do not have structure, and explore its potential implications for the reduction debate around chemistry. The next section explores how the idea of molecules without structure affects our metaphysical understanding of this chemical property. In particular, I present two alternative

views: the relational and dispositional view of structure. As will be shown in section 4, each metaphysical account has interesting implications for the reduction-emergence debate, thus showing the need to reframe this debate so as to include a detailed analysis of the metaphysics of molecular structure.

3. Making sense of structure in a metaphysically informed way

There are different accounts of properties available in metaphysics and different proposed distinctions between kinds of properties, including between simple and complex properties, natural and non-natural, intrinsic and relational (or extrinsic) properties, but also dispositional properties, sortal properties, potencies and so on (see Orilia and Paolini Paoletti 2022). There are also different ways to understand the metaphysical nature of molecular structure, and different metaphysical accounts to chose from. Moreover, structure in general (construed more commonly as shape or geometry) has been examined in philosophy extensively, and considered in the context of different metaphysical frameworks.¹¹ For example, Locke (1847) argued that shape is one of five primary qualities of material objects (see also Orilia and Paolini Paoletti 2022). Another example is Lewis who took 'shape properties'- such as 'being a triangle'- to be intrinsic (though this was later contested; e.g. Skow 2007). In fact, it is interesting to note that in metaphysics, shape is considered as one of the most paradigmatic examples of intrinsic properties. As Ott recently stated, "shape is an intrinsic property if anything is" (2022: 89).

So there are various ways to metaphysically construe the nature of molecular structure and different accounts that one could apply to the case in question. By no means do I offer such a complete account here. In fact, I do not defend a particular metaphysical account of the nature of molecular structure; the choice of the examined accounts should be viewed as merely instructive. This is because the aim here is to show that the reduction- emergence debate around chemistry should consider the metaphysical nature of molecular structure. Which specific metaphysical account is most tenable, is an issue that requires separate investigation elsewhere.

This section examines the nature of molecular structure within the framework of the intrinsic/ relational distinction of properties. The reason for this choice is the following. When Woolley and Sutcliffe argued that quantum physics does not identify structure for isolated molecules (from first principles), they claimed that this is evidence of structure not being an intrinsic property.¹² They stated:

¹¹ Of course this is a brief overview of a vast literature in philosophy that discusses and examines shape in the context of the metaphysics of properties. By this sketch I merely wish to point out some metaphysical ideas that are associated with structure.

¹² Primas (2013) also denies that structure is an intrinsic property. His claim is based on his more general view that molecules are hierarchical systems which, as such, have properties that arise "from a particular way we interact with the system" (i.e. the molecule) (2013: 321).

The central dogma of molecular science is the proposition that all experiments involving molecules can be understood in terms of molecular structure; the *shape* of a molecule is universally held to be an *intrinsic property* which can be characterised by definite numerical quantities such as the "equilibrium" bond lengths and angles. We have argued in this letter and in previous publications (..) that this view is not consistent with the requirements of the quantum theory (Woolley and Sutcliffe 1977: 397)¹³

Elsewhere, Woolley is even more explicit about structure not being an intrinsic property:

The idea of molecular structure is discussed from the point of view of the quantum theory: we show that the modern picture of a molecule as a bound collection of electrons and nuclei is not invariably equivalent to the classical molecular model of atoms joined by bonds, and hence molecular structure is not an intrinsic property. (1978: 1073)

Jeffry Ramsey caught on Woolley and Sutcliffe's ideas on the non-intrinsic nature of structure and was- perhaps one of the first- who offered a philosophically informed analysis of structure vis-a-vis its non-intrinsic nature. In particular, he agreed with them on the idea that structure is not intrinsic and further claimed that structure is a 'response property' which depends "on the way the molecule is picked out in measurement" (1997b: 247).¹⁴

While Woolley and Sutcliffe do not offer a precise or philosophically informed definition of intrinsic properties, I take that their understanding of 'intrinsic properties' is consonant with the general philosophical understanding of 'intrinsic', namely as "properties objects have just in virtue of how they are in themselves, not how they are in relation to other things" (Ney 2014: 285; also Lewis 1983: 197). Consequently, relational (also called extrinsic) properties are understood here as properties objects have "in relation to other things" (Ney 2014: 285; also Lewis 1983: 197).¹⁵

Subsection 3.1 follows the spirit of Woolley, Sutcliffe, and Ramsey's views and outlines how structure can be construed as a relational property. Subsection 3.2 examines how one can retain some sense of intrinsicality with respect to molecular structure, by conceiving it as a dispositional property.

3.1 The Relational view of molecular structure

¹³ Italics in original text.

¹⁴ I briefly return to Ramsey's views in subsection 3.1.

¹⁵ This basic distinction between intrinsic and relational properties has been further elaborated on and critically examined in the literature (e.g. Marshall and Weatherson 2018 for an overview). I do not consider these issues here; I merely employ this distinction to showcase two basic ways in which structure can be construed.

First, consider molecular structure as a relational property of molecules. We could argue that structure is a relational property of molecules in the sense that it comes about only when there is an energetic exchange of the system with its environment, or when the molecule interacts with some other entity. This implies that, unless such interactions occur that by definition render a molecule in non-isolation, a molecule does not have any structure.

What does it mean that an isolated molecule does not have structure, if the latter is viewed from such a relational perspective? Consider as an analogy Alan's politeness. How polite Alan is, is empirically identified when one examines Alan with respect to the presence of people P in an environment C. In this context, the fact that Alan is polite/rude is determined with respect to whom Alan interacts within a particular environment. Now consider Alan in isolation. One could argue that it doesn't make sense to talk about Alan's politeness independently of other people and of the context in which he is considered.¹⁶ This is not merely because one cannot empirically verify whether Alan is polite in such a context, but because being rude or polite is partially determined by the environment and the people with which Alan interacts. Similarly, just like Alan is neither polite nor rude when he sits in a room by himself, so a molecule is neither structured nor unstructured when in isolation.

This is indeed a strange way to conceive of isolated molecules, or any material object for that matter. Nevertheless, there is empirical evidence that molecules exhibit such a 'strange' nonclassical behaviour when in isolation. Under conditions which resemble the conditions of isolation, molecules have been empirically observed to exhibit non-classical behaviour in the sense of exhibiting interference effects, non locality, and entanglement (Chatzidimitriou-Dreismann and Arndt 2004: 144). Moreover, as Franklin and Seifert point out, such behaviour is theoretically predicted by certain interpretations of quantum physics. All in all, understanding structure as a relational property is in line with viewing it as a classical property that strictly speaking does not apply with reference to quantum objects (in this case isolated molecules). This implies that we cannot meaningfully assign structure to a molecule in isolation.

Interestingly, one need not commit to a particular interpretation of quantum physics in order to think that structure is a relational property. Instead, one can adopt an empiricist attitude towards structure and take as decisive the lack of empirical evidence that supports the existence of structure with reference to an isolated molecule. Recall, there is no empirical evidence of a single isolated molecule with structure (Seifert 2020a: 22-25). Science has only experimentally identified these properties in a non-isolated and time-dependent manner. More than that, the experimental identification of these properties suggests that the environment and conditions in which a molecule is examined partially determines its structure. This challenges the assumption that

¹⁶ Obviously this analogy can be debated. Nevertheless, this doesn't undermine the possibility of understanding molecular structure in this manner.

structure can be instantiated by an isolated molecule. Put differently, it challenges the assumption that structure is an intrinsic property.¹⁷

Of course, the tenability of this view depends on what one precisely means by 'existence', 'property' and 'relational'. Ney's definition of relational properties is a rather general statement and other definitions- such as Lewis' paradigmatic formulation- have been extensively scrutinised (e.g. Marshall 2016). Among other things, we need to specify what renders a molecule in relation to something else. For example, 'Elliot is in love with Helen' posits the existence of a relational property (i.e. being in love with) between two objects (i.e. Elliot and Helen). Can we construe in a similar manner a molecule's relation with its environment? This is a particularly pressing question that may even pose a challenge to the view that structure is a relational property. This is because a system's wavefunction may not collapse only when it interacts with an environment or measurement device. Wallace (2018) points out that decoherence can also happen to an isolated molecule without interaction with an environment (see also Franklin and Seifert 2024: 50). If this is the case for certain isolated molecules then it is not clear how we can coherently spell out the relevant relata that figure in the posited relation.

3.2 The Dispositional view of molecular structure

An alternative way to construe the nature of molecular structure is by claiming that structure is a dispositional property of molecules.¹⁸ Dispositional properties are kinds of properties that a system possesses even when it is under conditions where it does not actualise them. A classic example of dispositional property is that of fragility. A glass is said to possess the property of fragility: if it were to fall down with sufficient force, it would break. However, this is a possibility; it is permissible that we never observe the glass breaking.¹⁹ As Mumford (1998) puts it:

¹⁷ As mentioned above, a similar claim is made by Ramsey (1997a; 1997b) who takes that structure depends on measurement. He believes structure- or rather, shape- to be a non-intrinsic approximate concept that "refers to a causal property, rigidity, which most molecules display under most experimental conditions" (1997a: 320). For Ramsey the role of measurement is crucial: whether or not a molecule has shape depends in part by the measuring apparatus. However, note that he understands shape slightly differently as only referring to the separability of nuclear and electronic motions, rejecting the idea of shape as a classical concept (1997a: 320).

¹⁸ Whether or not dispositional properties are intrinsic is an open question. On the one hand, Lewis maintained that "if two things (actual or merely possible) are exact intrinsic duplicates (and if they are subject to the same laws of nature) then they are disposed alike" (1997: 147). Many philosophers seem to agree that dispositions are intrinsic properties. On the other hand, Contessa claims that there are intrinsic and extrinsic dispositions, where extrinsic are those which do not supervene only on an object's intrinsic properties (2015: 163). While I present this account in order to offer an alternative view of structure that may maintain some idea of intrinsicality to structure, I leave open whether this is in fact tenable.

¹⁹ I do not delve into issues of modality here.

The general criterion for something to be a disposition is that the appropriate kind of behaviour, the so-called manifestation, need not be actual. Hence, something can be disposed to break though it is not broken now. The disposition is thought to be a persisting state or condition that makes possible the manifestation.

As shown by Mumford's quote, it is common to distinguish between dispositions and their manifestations. That is, it is assumed that a disposition manifests itself under specific stimulus conditions, and observed via its manifestation.²⁰ As McKitrick puts it "a manifestation is *an effect* of a disposition being activated" (2010: 81).²¹

From this perspective, one could claim that being-structured is a disposition that molecules have even when they do not instantiate that property (i.e. including when found in isolation). Put crudely, being-structured is a disposition that may not be actualised when the system is in isolation but is nevertheless in some sense still there via the expression of the superposition of all possible structures. Of course, the sense in which 'structure is still there' depends on how we understand superpositions and on whether we interpret superpositions in some metaphysical way, but this needs separate investigation elsewhere.

In any case, when the ground state of an isolated molecule corresponds to a superposition of structures, this could be understood as providing all the possible structures the system is *disposed* to exhibit after collapse of its wavefunction. The theory of decoherence can be viewed as explaining how we arrive at the 'characteristic manifestation' of structure under specific stimulus conditions, which is consonant with what is sometimes expected of dispositional properties (contrary to categorical ones; see Choi and Fara 2021). Then the structure of a molecule is a disposition that is manifested via the observation of its characteristic responses to, say, x-ray or nuclear magnetic resonance techniques which in turn act as the stimulus conditions that trigger, in accordance to quantum physics, the collapse of the molecule's wavefunction.²²

²⁰ There is no consensus on this. For example, Engelhard (2021) contests that we should distinguish between dispositions and their manifestations as they are partially identical.

²¹ Italics in original text. In metaphysics, there is no consensus as to whether a disposition is activated by a single manifestation or whether dispositions can be multi-track (e.g. Vetter 2013). Prima facie, being-structured is a multi-track disposition to the extent that there are different ways (by means of different measurements, observations, etc.) by which a molecule's wavefunction reduces to a single eigenstate.

²² I take 'stimulus conditions' to refer to whatever mechanisms are taken to lead to the collapse of the wavefunction, whether these have to do with measurement devices, the effects of the environment or the size of the system itself (e.g. Wallace 2018). Of course, this needs more unpacking as the specification of such mechanisms is to some extent contingent on a specific interpretation of quantum mechanisms.

To appreciate how structure is construed in dispositional terms, let us recast the analogy of Alan's politeness. Contrary to the relational view, one could argue that Alan has a disposition to be polite (or rude) regardless of whether he ever gets the opportunity to interact with other people. This allows us to maintain the idea that Alan is disposed to behave in a certain way- or a range of ways-regardless of whether he ever does so. Similarly with structure. Whether or not a molecule manifests a specific structure, a molecule is disposed to instantiate some structure under appropriate conditions. What these structures are (for a stable molecule) is identified via the predicted superposition of structures of its ground state.

The main advantage of the dispositional view of structure is that it retains structure as essential to a molecule's identity; i.e. as something a molecule maintains even when it does not instantiate it. This is consonant with the importance that chemists assign to molecular structure. In chemistry, structure is not just another property of molecules; it forms part of the identity of molecules, explaining to a large extent their chemical and physical properties. In fact, as the case of isomers illustrates, one cannot even distinguish between distinct kinds of molecules without specifying their structure. Put differently, structure in chemistry is a defining characteristic of molecules, without which chemists cannot identify and distinguish between different kinds of molecules.

However, one should also be careful before definitively endorsing this view as it is crucial to examine whether it is coherent with the different available interpretations of quantum physics and with how they construe superpositions. Moreover, the problems and questions that are raised with respect to dispositional properties in general, carry over and need to be addressed relative to the special case of molecular structure. For example, are dispositions reduced away or grounded by-say- tropes or universals? If they are, does this imply that we should reject the existence of structure as a genuine property of molecules (e.g. Tugby 2016: 75-98)?

Admittedly, this is a brief analysis of how to construe the nature of molecular structure from each of the two metaphysical perspectives. One needs to spell out in detail what each account involves and how the nature of structure is precisely specified under each framework. In addition, one could formulate an account which combines the basic ideas of both views; one need not adhere strictly to one or the other. This also needs further inquiry. Moreover, one needs to pursue an interdisciplinary analysis by considering foundational issues in quantum physics. Whatever the results of such analyses, the next section shows that such a project is important to the debate about chemistry's reduction-emergence, as each metaphysical account affects differently how we understand chemistry's relation to quantum physics.

4. Implications for the reduction-emergence debate around chemistry

This section presents how the existing antireductionist ideas about chemistry which have been prompted by an analysis of molecular structure, are affected if structure is considered under the

relational and dispositional framework respectively.²³ Moreover, it briefly sketches how alternative accounts of emergence and reduction that have not been previously considered in this debate, can be supported by these new metaphysical frameworks.

First, recall that under the relational view of structure, in isolation there are no molecules as construed and described in chemistry. That is, molecules with structure do not exist in isolation; something else exists in their place. If this is correct, then chemistry and quantum physics each describe distinct target systems. Chemistry describes structured entities that exhibit classical behaviour; whereas quantum physics describes (at least prior to collapse) non-classical objects. Put differently, the things which in non-isolation are described as chemistry's molecules do not belong within the purview of chemistry when considered in isolation. Therefore, looking for an epistemological or metaphysical connection between the two descriptions is misguided from the perspective of the reductionist debate as each description concerns a distinct target system.

From this it follows that any antireductionist view which invokes the apparent inability of quantum physics to identify an isolated system's structure is undermined. For example, if structure is a relational property which- as such- cannot be instantiated by an isolated molecule, then this undermines the claim that structure is a strongly emergent property. If there is no structure to be assigned to isolated molecule, then strictly speaking, the system described by quantum physics (i.e. the isolated molecule) is a different system from that which is described by chemistry (i.e. the non-isolated structured molecule). Looking for structure to emerge is simply misplaced in the isolated case; this is not a property held by an isolated molecule, regardless of the scale at which the molecule is found. The same response can be given against epistemological anti-reductive arguments (namely Scerri's argument against Nagelian reduction). Given that quantum physics aims at describing a distinct system from that which is described by chemistry, there is no reason why the inability of the former description to identify the system described by the latter is evidence of the failure of epistemic reduction.

Of course, this does not imply that advocating for some (other) form of emergence is no longer an option. While existing antireductionist and emergentist accounts are undermined, one could still argue that a different form of emergence is well-supported within the relational perspective of structure. One such example is contextual emergence as advocated by Barbara Drossel (ref) and by Michael Silberstein (ref). Silberstein's account of contextual emergence is consistent with the relational view of structure because it is incompatible with the existence of intrinsic or essential properties. It also brings forward the importance of scale and rejects the standard view of a strict and static hierarchy of levels. For Silberstein, contexts are multiscale and are characterised by stability conditions set at different scales. The relation between larger and smaller things is not asymmetric or bottom-up; things interact with each other in different multiscale contexts. While

²³ Note that a similar analysis is pursued by Franklin and Seifert (2024: section 4). Their analysis and revision of anti-reductive views is spelled out and supported within the framework of three standard realist interpretations of quantum physics. Here, the analysis is based on the investigation of two standard interpretations of the metaphysics of properties.

there is a lot to unpack here in order to decide whether this version of emergence fits the particular case study, it is worth noting that a similar view about the important of scale-relativity (though not in defence of contextual emergence) is made by Robin Hendry (2021) for the case of molecular structure.

More relevant to the present case is Drossel's account which is based on four case studies; namely, quantum measurement processes, quasiparticles (as studied in condensed matter physics), thermodynamic systems and cosmological phenomena. The first example is particularly relevant to the case of molecular structure because, as Drossel rightly points out, it is a special case of how we construe the quantum-classical divide and deal with the measurement problem. I agree with Drossel that the context in which a system is considered plays a major part in understanding its behaviour and, to that extent, I believe the relational view of molecular structure illuminates this, even if by spelling it out in different terms. However, I am not convinced that this implies the causal closure of the physical, as Drossel (but also Hendry and Rossetter (ref)) advocates. Drossel believes that multiple realisability together with the explanatory value of higher level facts undermines the causal closure of the physical, thus challenging physicalism. Indeed, the explanatory value of higher level facts seems ineliminable in areas such as cosmology and thermodynamics, but I am not sure the same applies to how quantum chemistry studies and explains molecules. Given how important quantum physics is in the explanation of molecules and their properties, this argument is harder to maintain for the case at hand.

Overall, I suspect that whatever the precise form of a candidate emergentist view is, it is an account which will be based on a close examination of the classical-quantum divide. This is because the relational view of structure illustrates that the debate regarding chemistry's reduction or emergence should be recast as a special case of how the classical reduces to or emerges from the quantum (see Bokulich 2010). Interestingly, such accounts of emergence have already been proposed in the literature. For example, in the context of the Everettian interpretation of quantum physics, Wallace (2012) argues for "the existence of an emergent branching structure in physical reality" where classical objects are construed in terms of Dennett's real patterns (2012: 46-63; see also Dennett 1991; Wallace 2003). If we were to accept this interpretation of quantum physics, we could subsequently argue that-just like tigers- molecular structure is an emergent real pattern.

Moving to the dispositional view, existing antireductionist accounts are similarly undermined as it seems that one can again resolve the putative problem that was initially directed towards reductionism (though in a different manner). Recall that according to antireductionists, quantum physics could not assign a specific structure to isolated molecules from first principles. However, if we construe structure as a dispositional property then the reductionist could maintain that there is a sense in which the structure identified by chemistry is identified by quantum physics as well. This is because quantum physics identifies all possible structures a system is disposed to instantiate after the collapse of its wavefunction, including that which is finally observed by chemists.

This line of thought undermines the antireductionist argument, however it does not tell us what form of reduction is achievable within this framework. My suspicion is that it would require formulating a thinner sense of reduction; one which does not (among other things) require a oneto-one relation between the quantum and chemical description (but rather a one-to-many). I do not pursue this investigation further, and leave open how such an account of reduction could be spelled out.

On the other hand, there are also alternative emergentist accounts which hinge on a dispositional view of properties and are thus worth considering in the present context. For example, in chapter [..] Paul Humphreys discusses synchronic and diachronic emergence.²⁴ I have argued elsewhere against the coherence of synchronic emergence, so I only focus on diachronic emergence (also called 'transformational emergence' by Humphreys) (Seifert 2020b). Transformational emergence is understood in terms of changes to some essential property of a system, leading the former to its transformation. As Humphreys states, "(a) change from an entity O to an entity O' is a transformation just in case at least one essential property differs between O and O''' (page?). In this context, we could view the manifestation of a specific structure after the collapse of a molecule's wavefunction, as a change in its essential property ('having structure') and thus as an instance of diachronic emergence. The molecule (as construed and described in chemistry) diachronically emerges in the sense that it transforms from a system O with no structure to a system O' with structure.

More precisely, under the influence of an environment or interaction, the system which is in the ground state corresponding to a superposition of structures transforms into a system with definite structure. This counts as a change in the essential properties of the system because a molecule (as construed in chemistry) is by definition an entity with structure. Following Humphreys, we could count this as a case of genuine transformation and of emergence of a novel entity, namely the structured molecule. The structured molecule emerges from its previous quantum state because it possesses four features: it is 'developed' from its predecessor; it 'depends' on it; it is autonomous from it; and, it possesses novel properties (namely 'being structured'). In this context, 'being structured' is a dispositional property possessed by the (classical) non-isolated molecule O'. This is a novel property with respect to the properties possessed by the isolated molecule prior to collapse (system O) because 'being structured' has at least one type of manifestation in some context that cannot be the manifestation of any property of the system O prior to collapse (under any contexts). Once again there is a lot to unpack here but this seems like an interesting way to spell out the emergence of molecular structure without recourse to downward causation. More importantly, it is an account of emergence that hinges on viewing structure as an essential, dispositional property which- as explained above- has specific advantages.

All in all, a lot more should be said about how to defend the reduction or emergence of chemistry through the consideration of the nature of molecular structure. The above analysis is far from a

²⁴ The purpose of Humphrey's analysis in this chapter is to see how these two versions of emergence can overcome the so-called collapse problem, I do not consider this here.

complete defence of such an account. This is to be expected as it would be mistaken to assume that a specific metaphysics of molecular structure could fully determine whether and in what way chemistry relates to quantum physics. Nevertheless, I take the intended purpose to be fulfilled. Namely, I showed that pursuing a metaphysics of molecular structure can lead to substantial revisions in our existing views and inform in novel ways our understanding of the relation of chemistry and quantum physics.

5. Conclusion

Recent arguments have suggested that there is no structure to molecules when the latter are found in isolation. If this is indeed the case, then this leads to substantial changes in our views about chemistry's reduction, but also in the manner in which we defend these views. To illustrate this claim, I present two alternative accounts of the nature of molecular structure; namely the dispositional and relational accounts of structure. Each account interprets differently how we should understand the claim that there is no structure in isolation. I show that both accounts undermine existing antireductionist arguments that have been prompted by considerations of molecular structure. Moreover, I briefly present how these metaphysical frameworks can prompt novel views about chemistry's reduction or emergence. Whichever position one maintains about chemistry's relation to quantum physics, a radical reframing of this discussion has to take place; one which involves a much more informed and thorough analysis of the metaphysics of molecular structure.

Acknowledgements

This work is supported by the European Research Council project CReaCaL: Chemical Reactions as Causes and Laws (project number 101064082).

References

Bird, A. (2009). "Structural properties revisited". In *Dispositions and causes* (pp. 215-241). Oxford University Press.

Bokulich, A. (2008). *Reexamining the Quantum-Classical Relation: Beyond Reductionism and Pluralism*. Cambridge: Cambridge University Press. doi:10.1017/CBO978051175181

Bransden, B.H., and C.J. Joachain. 1989. *Introduction to quantum mechanics* (Essex: Longman Scientific & Technical)

Chang, H. (2015). Reductionism and the relation between chemistry and physics. *Relocating the history of science: Essays in honor of Kostas Gavroglu,* 193-209.

Chatzidimitriou-Dreismann, A., and M. Arndt. 2004. 'Quantum Mechanics and Chemistry: The Relevance of Nonlocality and Entanglement for Molecules', *Angewandte Chemie International Edition*, **43**: 144-145

Choi, Sungho and Michael Fara, "Dispositions", The Stanford Encyclopedia of Philosophy (Spring 2021 Edition), Edward N. Zalta (ed.), URL = https://plato.stanford.edu/archives/spr2021/ entries/dispositions/>.

Contessa, G. (2015). Only powers can confer dispositions. *The Philosophical Quarterly*, 65(259), 160-176.

Dennett, D. C. (1991). Real patterns. The journal of Philosophy, 88(1), 27-51.

Engelhard, K. (2021). Dispositions manifest themselves: an identity theory of properties. *Synthese*, *199*(5), 13497-13522.

Fortin, S., Labarca, M., & Lombardi, O. (2022). On the ontological status of molecular structure: is it possible to reconcile molecular chemistry with quantum mechanics?. *Foundations of Science*, 1-17.

Franklin, A., & Seifert, V. A. (2024). The problem of molecular structure just is the measurement problem. *The British Journal for the Philosophy of Science*, *75*(1), 31-59.

González, J. C. M., Fortin, S., & Lombardi, O. (2019). Why molecular structure cannot be strictly reduced to quantum mechanics. *Foundations of Chemistry*, 21, 31-45.

Griffiths, David J.. 2005. Introduction to Quantum Mechanics, 2nd edn (USA: Pearson Education International)

Hendry, R. F. (2010a). Emergence vs. reduction in chemistry. *Emergence in mind*, 205-221.

Hendry, R. F. (2010b). 'Ontological reduction and molecular structure', *Studies in History and Philosophy of Modern Physics*, **41**: 183–91

Hendry, R. F. (2012). Reduction, emergence and physicalism. In *Philosophy of chemistry* (pp. 367-386). North-Holland.

Hendry, R. F. (2016). Structure as abstraction. *Philosophy of Science*, 83(5), 1070-1081.

Hendry, R. F. (2017). Prospects for strong emergence in chemistry. In *Philosophical and scientific perspectives on downward causation* (pp. 146-163). Routledge.

Hendry, R. F. (2021). Structure, scale and emergence. *Studies in History and Philosophy of Science Part A*, *85*, 44-53.

Hendry, R. F., and P. Needham (2007), "Le Poidevin on the Reduction of Chemistry", *The British Journal for the Philosophy of Science*, 58(2): 339–53

Hettema, H. (2017). The union of chemistry and physics. *Cham: Springer International*.

IUPAC. 2014. *Compendium of Chemical Terminology: Gold Book*, Version 2.3.3, Available at: http://goldbook.iupac.org/pdf/goldbook.pdf [accessed 3/05/2018]

Lewis, D. (1983). Extrinsic properties. *Philosophical Studies: An International Journal for Philosophy in the Analytic Tradition*, 44(2), 197-200

Lewis, D. (1997). Finkish dispositions. *The Philosophical Quarterly*, 47(187), 143-158.

Locke, J. (1847). An essay concerning human understanding. Kay & Troutman.

Lombardi, O. and M. Labarca. (2005). The Ontological Autonomy of the Chemical World. *Foundations of Chemistry* 7: 125–148.

Longuet-Higgins, H. C. (1963). The symmetry groups of non-rigid molecules. *Molecular Physics*, *6*(5), 445-460.

Marshall, D. (2016). The varieties of intrinsicality. *Philosophy and Phenomenological Research*, 92(2), 237-263.

Marshall, Dan and Brian Weatherson, "Intrinsic vs. Extrinsic Properties", The Stanford Encyclopedia of Philosophy (Spring 2018 Edition), Edward N. Zalta (ed.), URL = https://plato.stanford.edu/archives/spr2018/entries/intrinsic-extrinsic/.

McKitrick, J. (2010). Manifestations as effects. In *The metaphysics of powers* (pp. 81-91). Routledge.

Mumford, Stephen. Dispositions, 1998, doi:10.4324/9780415249126-N116-1. Routledge Encyclopedia of Philosophy, Taylor and Francis, https://www.rep.routledge.com/articles/thematic/dispositions/v-1.

Nagel, Ernest. 1979. The Structure of Science: Problems in the Logic of Scientific Explanation, 3rd edn (Hackett Publishing)

Needham, Paul. 2006. 'Ontological Reduction: a comment on Lombardi and Labarca', Foundations of Chemistry, 8(1): 73-80

Ney, Alyssa. 2014. Metaphysics: an introduction (Oxon: Routledge)

Oppenheim, P., and H. Putnam. 1958. 'The unity of science as a working hypothesis', in Minnesota Studies in the Philosophy of Science vol. 2, ed. by H. Feigl et al. (Minneapolis: Minnesota University Press) pp.3-36

Orilia, Francesco and Michele Paolini Paoletti, "Properties", The Stanford Encyclopedia of Philosophy (Spring 2022 Edition), Edward N. Zalta (ed.), URL = https://plato.stanford.edu/archives/spr2022/entries/>.

Ott, Walter. (2022). *The Metaphysics of Laws of Nature: The Rules of the Game* (Oxford: Oxford University Press)

Palgrave Macmillan Ltd. (2004) *Dictionary of Physics* (UK: Palgrave Macmillan)

Papineau, David. (2002) Thinking about Consciousness. Oxford University Press. https://doi.org/ 10.1093/0199243824.001.0001

Primas, H. (2013). *Chemistry, quantum mechanics and reductionism: Perspectives in theoretical chemistry* (Vol. 24). Springer Science & Business Media.

Ramsey, J.L. (1997a). A Philosopher's Perspective on the "Problem" of Molecular Shape. In: Calais, JL., Kryachko, E. (eds) Conceptual Perspectives in Quantum Chemistry. Springer, Dordrecht. https://doi.org/10.1007/978-94-011-5572-4_9

Ramsey, J. L. (1997b). Molecular shape, reduction, explanation and approximate concepts. *Synthese*, 233-251.

Scerri, E. R. (1991). The electronic configuration model, quantum mechanics and reduction. *The British Journal for the Philosophy of Science*, *42*(3), 309-325.

Scerri, E. R. (1994). Has chemistry been at least approximately reduced to quantum mechanics?. In *PSA: Proceedings of the biennial meeting of the philosophy of science association* (Vol. 1994, No. 1, pp. 160-170). Philosophy of Science Association.

Scerri, E., and G. Fisher (ed.). (2015). *Essays in the Philosophy of Chemistry*. Oxford: Oxford University Press

Schummer, J. (2014). Special Issue on 'General Lessons from Philosophy of Chemistry'on the Occasion of the 20th Anniversary of HYLE. *HYLE–International Journal for Philosophy of Chemistry*, 20, 1-10.

Seifert, V. A. (2020a). The role of idealisations in describing an isolated molecule. *Foundations of Chemistry*, 22, 15-29.

Seifert, V. A. (2020b). The strong emergence of molecular structure. *European Journal for Philosophy of Science*, *10*(3), 45.

Skow, B. (2007). Are shapes intrinsic?. *Philosophical Studies*, 133, 111-130.

Tugby, Matthew, 'What are Dispositional Properties?', in Mark Jago (ed.), *Reality Making*, Mind Association Occasional Series (Oxford, 2016; online edn, Oxford Academic, 24 Mar. 2016)

Van Brakel, J. (1999). On the neglect of the philosophy of chemistry. *Foundations of Chemistry*, 1(2), 111-174.

Vetter, B. (2013). Multi-track dispositions. The Philosophical Quarterly, 63(251), 330-352.

Wallace, D. (2003). Everett and structure. Studies in History and Philosophy of science Part B: Studies in History and philosophy of modern Physics, 34(1), 87-105.

Wallace, David. (2012). *The Emergent Multiverse: Quantum Theory according to the Everett Interpretation* (Oxford: Oxford University Press)

Wallace, D. (2018). Spontaneous symmetry breaking in finite quantum systems: a decoherenthistories approach. *arXiv preprint arXiv:1808.09547*.

Woolley, R. G. (1976). Quantum theory and molecular structure. *Advances in Physics*, 25(1), 27-52.

Woolley, R. G. (1978). Must a molecule have a shape?. *Journal of the American Chemical Society*, 100(4), 1073-1078

Woolley, R. G. (1998). 'Is there a quantum definition of a molecule?', *Journal of Mathematical Chemistry*, **23**: 3–12

Woolley, R. G., & Sutcliffe, B. T. (1977). Molecular structure and the born—Oppenheimer approximation. *Chemical Physics Letters*, 45(2), 393-398.

Woolley, R. G., & Sutcliffe, B. T. (2012). 'Atoms and Molecules in Classical Chemistry and Quantum Mechanics', in *Handbook of the Philosophy of Science. Volume 6: Philosophy of Chemistry*, ed. by Robin F. Hendry, Paul Needham and Andrea I. Woody (Amsterdam: Elsevier BV) pp. 387-426