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The Chemical Bond is a Real Pattern

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Abstract

There is a persisting debate about what chemical bonds are and whether they exist. I argue that chemical bonds are real patterns of interactions between subatomic particles. This proposal resolves the problems raised in the context of existing understandings of the chemical bond and provides a novel way to defend the reality of chemical bonds.

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Ostensibly, it (Dennett's "Real Patterns") is prompted by questions about the reality of intentional states. (…) But these are pretexts: the issue is not intentionality at all, but rather being (…) Intentional states are just a special case, and there can be other special cases as well. (Haugeland 1993, 53)

We might say that the description of a bond is essentially the description of the pattern of the charge-cloud. (Coulson 1955, 2070)

1. Introduction

In both science and philosophy, understanding chemical bonds is a persisting problem (see for example Esser 2019; Hendry 2008, 2010b; Needham 2013, 2014; Sutcliffe 1996; Weisberg 2008). Even though quantum physics has enhanced our understanding of them, there is still disagreement about what chemical bonds are and whether they exist. I resolve this by showing that chemical bonds are real patterns of interactions between subatomic particles. Specifically, I present Dennett's account of real patterns and show that it fits the case of chemical bonds. In addition, I consider a standard objection to Dennett's account; namely that this account implies instrumentalism or pluralism about patterns. I show that by incorporating ideas about patterns from structural realism, we can circumvent instrumentalism and pluralism and maintain the reality of bonds as patterns.

Section 2 presents the different definitions, classifications and methods of describing the chemical bond. This shows the ambiguity that exists around the chemical bond. Section 3 presents Dennett's account of real patterns and shows that it successfully applies to chemical bonds. Section 4 presents a central challenge raised against the realist feature of Dennett's account and considers how it can be formulated for the case of chemical bonds. Section 5 argues that adopting a structural realist understanding of real patterns circumvents this challenge, but also correctly identifies important features of the chemical bond.

2. The Ambiguity around Chemical Bonds

The chemical bond is a central concept whose explanatory and descriptive value in science cannot be easily overstated. However, despite its wide use, it is unclear what exactly the chemical bond is. As Weisberg states:

> Once one moves beyond introductory textbooks to advanced treatments, one finds many theoretical approaches to bonding, but few if any definitions or direct characterizations of the bond itself. While some might attribute this lack of definitional clarity to common background knowledge shared among all chemists, I

> believe this reflects uncertainty or maybe even ambivalence about the status of the chemical bond itself. (2008, 932-933)

This is not just a philosophical worry. Chemists and quantum chemists also admit that there is an ambiguity around chemical bonds:

> Later studies showed that the nature of the chemical bond is far more complicated than initially thought and that the connection between the Lewis model and the physical nature of chemical bonding is quite intricate. (Zhao et al. 2019, 8782)

One way to illustrate this ambiguity is by looking at how the chemical bond is defined and classified in science.[1] For example, the International Union for Pure and Applied Chemistry (IUPAC), which is the leading authority on chemical nomenclature and terminology, defines the chemical bond as follows:

> When forces acting between two atoms or groups of atoms lead to the formation of a stable independent molecular entity, a chemical bond is considered to exist between these atoms or groups. (IUPAC 2014, 257)

[1] One could also consider different scientific representations of the chemical bond.

This definition does not state what chemical bonds are; rather it states the conditions that hold when a chemical bond is considered to exist. This unclarity about the exact nature of bonds is not resolved by the definitions of the types of bonds posited in chemistry. Even though most definitions identify a specific referent for chemical bonds, the referent is each time something else, further confusing what chemical bonds are.[2] For example, the covalent bond is defined as a "*region of relatively high electron density* between nuclei" (IUPAC 2014, 344); the ionic bond "refers to the *electrostatic attraction* experienced between the electric charges of a cation and an anion" (2014, 767); the hydrogen bond refers to a "*form of association"* (2014, 697); whereas multi-center bonds refer to "electron pairs" that "occupy orbitals encompassing three or more atomic centres" (2014, 968).[3]

One would expect that quantum chemistry resolves this ambiguity by revealing what underwrites all types of bonds. However, this is not the case because "the need for approximate (quantum) methods greatly complicates the explanatory relationship" (Hendry 2010b, 124).

Specifically, the complication stems from the fact that there is no unique way of solving the molecular Schrödinger equation. The Schrödinger equation provides a quantum mechanical description of atoms and molecules in terms of the interactions between their

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[2] For example, dative bonds don't identify a referent for bonds (IUPAC 2014, 374).

[3] Italics added.

composing parts. However, the equation cannot be solved analytically for almost any molecule. So, different computational methods are developed that solve the equation by following different mathematical strategies and making different assumptions.

Two are the main methods of solving the Schrödinger equation: the Valence Bond (VB) and the Molecular Orbital (MO) approach. Each approach encompasses more than one methods of solving the Schrödinger equation.[4] More relevantly, each implies a different understanding of what chemical bonds are. Under the VB approach, chemical bonds are taken to refer to the "change in electron distribution and the resulting energetic stabilization from this change" (Weisberg 2008, 935). The methods that fall under the VB approach understand chemical bonds as directional, identify them with subatomic regions of high electron density, and take the electrons that participate in a bond to exhibit increased delocalisation (Weisberg 2008, 939). On the other hand, the MO approach takes chemical bonds to refer to phenomena which, due to delocalisation effects, are neither directional nor subatomic (Weisberg 2008, 941-43).

In addition to solving the Schrödinger equation via these approaches, quantum chemists have developed methods that connect the numerical results of quantum calculations to

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[4] Most notable is the Density Functional Theory (DFT) which is a "parametrised variant" of the MO approach (Zhao et al. 2019, 8788). Currently, the DFT is the most used method in quantum chemistry.

chemistry's tools of describing bonds (Zhao et al. 2019, 8790). Each of these methods is used in conjunction with the most appropriate method of solving the Schrödinger equation. In this way, quantum chemists acquire additional information about the chemical bonds posited in a system. Specifically, there are three main methods used for such purposes: the Natural Bond Orbital Method (NBO), the Quantum Theory of Atoms in Molecules (QTAIM), and the Energy Decomposition Analysis and Natural Orbitals for Chemical Valence (EDA- NOCV).[5]

The NBO and the QTAIM are charge-partitioning methods (Zhao et al. 2019, 8790-92). The NBO divides the molecular wavefunction into atomic regions in a way that corresponds to chemistry's understanding in terms of localised bonds and lone pairs of electrons (IUPAC 2014, 980; Zhao et al. 2019, 8791). The QTAIM offers a topological analysis of electron density and identifies chemical bonds in terms of "well-defined atomic regions and interatomic bond paths" (Zhao et al 2019, 8791). Both methods illuminate the role of subatomic charge in the description of chemical bonds. In contrast to the NBO and the QTAIM, the EDA-NOCV analysis is an energy-partitioning method that focuses on the interaction energy of a bond and on the bond dissociation energy (Zhao et al 2019, 8792). As such, this analysis illuminates the role of energy in the formation and stability of chemical bonds.

[5] Note that there are different variants to these methods (Zhao et al. 2019).

It is also worth looking at the history of quantum chemistry, in particular with respect to how the chemical bond has been understood throughout the field's development. Scientists, historians, and philosophers have pointed out that the way in which the MO and VB methods were developed has affected not only how the chemical bond is understood, but also explains the persistent ambiguity around its nature (Gavroglu and Simões 2011; Needham 2014).

Very briefly, the VB and MO methods were initially developed in competition and scientists participating in their development took their preferred quantum method to infer a substantially different understanding of the chemical bond. The VB approach got a head's start through Heitler and London's work who were the first to solve Schrödinger's equation for specific chemical systems (1927). They developed a mathematical method of solving the Schrödinger equation for the hydrogen ion and hydrogen molecule and showed that in the hydrogen molecule there is a covalent bond which is manifested by the sharing of two electrons between the two hydrogen atoms.

Pauling took up the work of Heitler and London and set to show how, through the VB approach, quantum mechanics can become relevant to chemists (Pauling 1960).[6] In particular, Pauling's goal was to show that the VB approach retains chemistry's image of

[6] This was motivated by chemists' less than enthusiastic reaction towards the purported role of quantum mechanics in chemistry (see Gavroglu and Simões 2011).

chemical bonds as real parts of molecules that partially determine their structural and chemical properties (Needham 2014, 2). This project was strongly motivated by the work of Lewis whose discovery and explanation of covalent bonds (in terms of an electron pair connecting two atoms) was (and still is) considered as one of the most important achievements in chemistry.[7] Lewis's view on the nature of chemical bonds illuminates the spirit underlying the development of the VB approach:

> (…) in the mind of the organic chemist the chemical bond is no mere abstraction; it is a definite physical reality, a something that binds atom to atom. (Lewis [1923] 1966, 67)

On the other hand, the MO approach was taken to support a completely different understanding of chemical bonds. Some of its central proponents, Coulson and Mulliken, took the development of the MO approach to challenge not only the Lewisian understanding of chemical bonds but also its reality (Weisberg 2008, 933). As Coulson stated:

> a chemical bond is not a real thing: it does not exist: no-one has ever seen it, no-one ever can. It is a figment of our own imagination. (1955, 2084)

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[7] In fact, Pauling spelled out the connection between Heitler and London's results and the Lewis's electron-pair bonding model (Needham 2014, 2).

This was not without empirical warrant as the development of MO methods lead to higher predictive accuracy and revealed previously unknown factors that explained chemical behaviour. For example, modern versions of the MO approach showed that the repulsion of electrons, the ionic character of chemical bonds, and the mixing of higher energy states play an important role in correctly describing the structure of specific types of molecules (Weisberg 2008, 939-943; Needham 2013, 54).

To recapitulate, different ideas about the chemical bond have resulted from the use of different quantum chemical methods and chemical classifications. That different methods and types of bonds have been developed is in turn explained by the fact that each accommodates the description of specific molecules and serves specific aims (such as predictive success, agreement with chemistry's conceptual understanding of bonds, etc.).

Of course these features of scientific practice are absolutely reasonable, and it is not my intention to contest such practice. Nevertheless, when it comes to understanding chemical bonds this situation is not particularly helpful. First, if we take ontologically literally what existing understandings of bonds state, then we arrive at the impossible result that the chemical bond is at the same time a *region* of high electron density (as per the covalent bond's definition), an *electrostatic attraction* (as per the ionic bond), *a form of association* between atoms (as per hydrogen bonds), and *the overlapping atomic wavefunction* (as per

the VB approach). Secondly, none of the existing definitions are general enough to capture all cases of bonding. For example, some definitions require for there to be two electrons for a bond to exist between two atomic centres, even though there are cases of bonding between two atomic centres with just one electron (de Sousa and Nascimento 2019). Additionally, certain types of bonds (such as covalent bonds) imply that the bond is a localisable thing materialised in a particular region, even though there are molecules that exhibit resonance structures due to electron delocalisation.[8] So despite the many ideas on the chemical bond, it is an open question how to spell out its nature in a way that accommodates all existing accounts of it.

Before concluding this section, it is worth considering how the philosophy of chemistry has dealt with this ambivalence around the chemical bond. I focus here on one of the most clear expressions of this ambivalence, given by Hendry's two conceptions of the chemical bond. Hendry distinguishes between what he calls the structural and the energetic conception of the chemical bond (2008). These two conceptions highlight the main features of the chemical bond (as outlined above), and group them in terms of two candidate understandings of the chemical bond.

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[8] Resonance structure refers to the interchangeable structures of certain molecules due to their electrons moving around (IUPAC 2014, 388).

The structural conception takes chemical bonds to be "material parts of the molecule that are responsible for spatially localized submolecular relationships between individual atomic centers" (Hendry 2008, 917). It encompasses the postulations of chemical theory about there being a bond between two atoms that share electrons, without however always necessitating such a pairwise relation. It encompasses all chemical classifications, including the different types of chemical bonds mentioned above. More importantly, this conception implies that chemical bonds are "a *submolecular* phenomenon, confined to regions between the atom"; "(t)his eliminates the possibility that bonds are a molecule-wide phenomenon" (Weisberg 2008, 935).[9]

The energetic conception takes chemical bonding to signify "facts about energy changes between molecular or supermolecular states" (Hendry 2008, 919). It explains why a bond is formed in terms of the energetic stabilisation of the molecule, rather than defines what the chemical bond is. It doesn't require that there are bonds in a molecule but rather remains agnostic with respect to their existence. The molecule is regarded as a set of nuclei and electrons that all together interact and form a stable entity. The structural features of the chemical bond are no longer required. Instead, what is necessary is a loose notion of bonding that is described in terms of the energetic stabilisation of the whole system.

[9] Italics in original.

Hendry's two conceptions don't provide a way out of the ambiguity around chemical bonds. Instead, they summarise and highlight the main points of disagreement around the chemical bond. The structural conception is consonant with chemistry's standard way of defining, classifying and representing the chemical bond. As such, it is in line with the VB approach and how it recovers the chemical bond (namely as a localised material thing between atoms). The energetic conception is in line with modern approaches in quantum chemistry (namely the MO approach and its variants) and is consistent with views that reject the existence of chemical bonds (at least) as material parts of molecules (see Coulson 1955).[10]

Another reason why the two conceptions aren't suitable candidates to account for chemical bonds is because neither does justice to the results of both chemistry and quantum chemistry. On the one hand, the structural conception implies that bonding is always confined in a sub-molecular region despite evidence from quantum chemistry that this is not always the case.[11] On the other hand, the energetic conception dismisses some of chemistry's most accepted insights and says nothing of the nature of chemical bonds: as Hendry states, it is more of "a theory of chemical bonding than a theory of bonds" (2008, 919).

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[10] This doesn't necessitate antirealism. The energetic conception is also consistent with understanding chemical bonds as properties.

[11] See Weisberg 2008 for a critique of the structural conception.

So it is an open question what chemical bonds are and even though one could explore this question by arguing in favour of the structural or energetic conception, I follow a different strategy. The next section draws inspiration from Dennett's paper *Real Patterns* and argues that chemical bonds are patterns of subatomic interactions.[12] This proposal offers a novel solution to the ambivalence around chemical bonds.

3. Chemical Bonds are Real Patterns

In his paper *Real Patterns*, Dennett presents six frames each made of black and white dots (figure 1).[13] According to Dennett, one way to describe each frame (say frame A in Fig.1) is to state its bit map: that is, specify the position of each and every black and white dot

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[12] In the philosophy of chemistry, patterns have been examined before but neither in connection to Dennett's work nor to chemical bonds. For example, Primas claims that molecular structure is an "asymptotic pattern" that is derived by quantum mechanics via the Born-Oppenheimer approximation (2013, 335). He argues that structure emerges as a pattern after the molecule's interaction with the environment (see also Hendry 1998). Primas's claim is motivated by foundational issues in quantum mechanics and specifically the quantum-classical divide (1975, 140).

[13] Dennett has presented this idea in earlier works (for example 1981) but I focus on the 1991 paper as this is considered his most representative formulation (Ross 2000, 149).

that makes up the frame. The bit map is the least efficient description of the frame because it specifies all the properties of all the dots that make up that frame (it identifies "each dot seriatim" (Dennett 1991, 32)). There are however alternative ways of describing the frame that don't require identifying the position of each and every dot. For example, one can describe the frame by specifying the number, size, and position of five black boxes. Given that such a description can be offered then, according to Dennett, this means that there is a pattern in how the black and white dots are positioned in the frame. Put differently, since frame A can be described in a manner that is more efficient than the bit map, this suffices to argue that a real pattern exists.

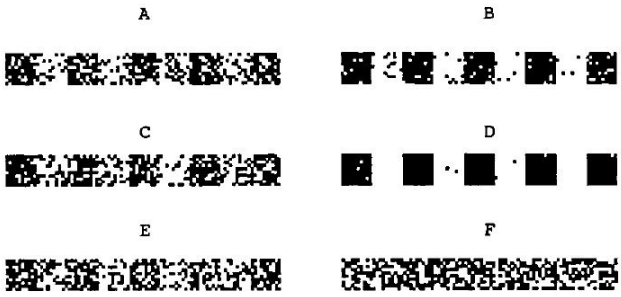

Figure 1. Dennett's Six Frames (1991, 31)

As Dennett has famously stated:

> a pattern exists in some data- is real- if there is a description of the data that is more efficient than the bit map, whether or not anyone can concoct it. (1991, 34)[14]

[14] I don't consider whether Dennett's account should be construed as one about patterns in the data (for example Suñé and Martínez 2019) or about patterns in the world. I follow McAllister who interprets Dennett's account as one about patterns in the world (2010, 804).

A similar claim can be made about chemical bonds. Specifically, I argue that Dennett's method of identifying real patterns applies to how subatomic interactions are described in terms of chemical bonds, thus showing that chemical bonds are real patterns of subatomic interactions.[15]

I provide support to this claim by examining how a common molecule- methane (CH_4)- is described in chemistry and quantum chemistry. Methane consists of one carbon atom and four hydrogen atoms (i.e. 10 electrons and 5 nuclei). In principle, methane can be described by solving the Schrödinger equation from first principles. Solving the Schrödinger equation from first principles amounts to identifying *the interactions of each and every electron and nucleus* that comprises the molecule; this implies that none of the entities or interactions that are postulated at the quantum scale are disregarded. As such, solving the Schrödinger equation from first principles amounts to providing the bit map

[15] I assume Dennett's account is a valid way of identifying patterns so I don't offer any support. Whether these patterns should be deemed real is discussed in later sections.

description because this description identifies “each dot seriatim” (Dennett 1991, 32).[16] Specifically, the bit map is the description of the quantum state which is produced by solving the Schrödinger equation from first principles.[17]

However, there are more efficient ways of describing methane. For example, it can be described via the QTAIM which calculates the electric field at carbon nuclei, the electron density, and the energy density of the carbon and hydrogen bonds (Macedo and Haiduke

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[16] Dennett’s definition of the bit map implies that it is a complete description in the following sense: there is no entity, property, etc. at the relevant energy, length and time scale which is not taken into account. This shouldn’t be conflated with reductive or physicalist notions of completeness, such as the causal closure of the physical which claims that “physical effects are brought about solely by physical causes via physical laws” (Hendry 2010a, 185).

[17] Solving the Schrödinger equation from first principles leads for some molecules to a set of possible quantum states as the most energetically stable. What this means metaphysically and which state obtains, has to do both with the environmental conditions the system is placed in as well as with foundational problems in quantum mechanics (see Franklin and Seifert 2020). However, this isn’t a problem for satisfying Dennett’s account. Given that the bit map corresponds to the description of the quantum state we are interested in, it does not matter that it has resulted from or is part of a description that describes other quantum systems (i.e. produces other bit maps) too.

2020). Others, like Mendoza et al. 2013, calculate methane's electron charge distributions by applying the kinetic theory to the DFT method (figure 2).

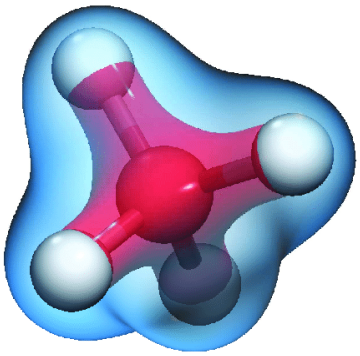

Figure 2. A pictorial representation of methane where the blue and red surfaces denote the low and high electron charge distributions that are calculated by applying a version of the DFT (Mendoza et al. 2013, 1). The red surfaces correspond to chemical bonds.

In general, there are different quantum methods that describe subatomic interactions and identify chemical bonds in terms of electron clouds, bond paths and electron charge distributions. These represent a set of descriptions that, in the spirit of Dennett's account, are more efficient than the bit map: they are more efficient ways of describing subatomic interactions than by solving the Schrödinger equation from first principles.

Similarly, chemistry has its own method of identifying subatomic interactions which is more efficient than using the bit map.[18] This method involves positing specific numbers and types of bonds and stating their properties (such as bond angles, bond length, etc). For

[18] Whether chemistry provides a more efficient description compared to the models of quantum chemistry is irrelevant to Dennett's account (1991, 33).

example, methane's subatomic interactions are described by positing four covalent bonds between the carbon atom and each hydrogen atom (figure 3).

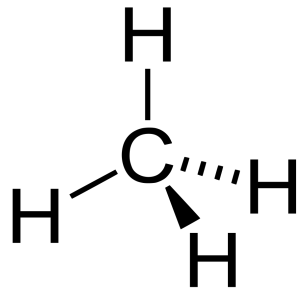

Figure 3. A three-dimensional representation of methane which shows the number, type and orientation of four covalent bonds.[19]

So there are chemical and quantum chemical descriptions that are more efficient ways of describing subatomic interactions than by solving the Schrödinger equation from first principles (i.e. solving the bit map). Therefore Dennett's account is satisfied and there are real patterns of subatomic interactions which are identified as chemical bonds.[20]

For this claim to be convincing, one needs to specify efficiency. Dennett employs 'compressibility' as a means to specify efficiency, by explaining how compression algorithms are efficient ways of describing a system (1991, 34). For example, frame D (in Fig. 1) "can be described as "ten rows of ninety: ten black followed by ten white, etc., with

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[19] Image from Wikipedia: https://en.wikipedia.org/wiki/Methane

[20] Chemical and quantum chemical methods are often used in tandem to describe a molecule. This doesn't undermine Dennett's account as the latter only focuses on how descriptions compare with the bit map.

the following exceptions: dots 57, 88, ….”” (1991, 32-33). This is a more efficient description than specifying the position of every black and white dot because it is much shorter than its bit map in the sense that it requires less storage space in a computer (i.e. number of bits) (1991, 33).

In the case of chemical bonds, calculating the number of bits of chemical and quantum chemical descriptions doesn't seem like a sensible way to understand (let alone measure) their efficiency.[21] So I present two alternative (and compatible to each other) understandings that capture Dennett's general idea about efficiency and can be easily grasped for the case of chemical bonds.

First, efficiency can be understood in a naive heuristic way. One could argue that chemical and quantum chemical methods are more efficient methods than the bit map if they are regarded as such by the scientific community. Indeed chemical and quantum chemical descriptions are used almost exclusively compared to solving the Schrödinger equation

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[21] Ross 2000 and Ladyman et al. 2007 precisify Dennett's notion of compressibility by employing notions from computer science and information theory. However, Millhouse argues against information-theoretic understandings of compressibility because "high-level models cannot be interpreted as compressing information about the fine-grained behaviour of their target system" (2021, 24). I circumvent such objections by proposing an understanding of efficiency that is not information-theoretic.

from first principles. This is because chemical and quantum chemical descriptions are computationally less complex and more tractable. On this view, one needs not to specify efficiency more precisely. The exact way in which scientists regard these methods as being more efficient is not important. As long as scientists regard them as such, this suffices to accept them as more efficient descriptions and thus as descriptions that identify real patterns.

However, one may find such an understanding of efficiency anthropocentric, contingent on science's changing computational abilities or just ambiguous (see for example discussion in Ross 2000, 160). After all, scientists may in the future develop their computational means to such an extent that they solve the Schrödinger equation from first principles just as easily as they do through approximations.

To avoid such objections, I propose further specifying efficiency in terms of the degrees of freedom of the relevant descriptions. I base this idea on Wilson's account of degrees of freedom, though there are other accounts one could alternatively employ.[22] A degree of freedom is "an independent parameter needed to characterise an entity as being in a state

[22] For example, Ladyman and Ross accept understandings of efficiency expressed in dynamical or statistical terms (Ladyman and Ross 2013; Ladyman 2017, 153). Interestingly, Ladyman accepts Wilson's account as a tenable way of spelling out efficiency (2017, 157).

functionally relevant to its law-governed properties and behaviour" (Wilson 2010, 281). Wilson claims that there are three ways that the degrees of freedom required to describe special sciences entities relate to the degrees of freedom for physical ones: she calls these relations "restriction", "reduction", and "elimination" (2010, 281).[23] Based on this, I take a description to be more efficient than the bit map if it "restricts, eliminates or reduces" the number of variables required in order to sufficiently describe a system. That is, if a description can be formulated by specifying less variables than those required by the bit map, then the former is more efficient than the latter.

There are two advantages to understanding efficiency this way. First, this is not an anthropocentric understanding. The number of variables required to formulate a description is constrained by the system under investigation (namely, by the properties and the number of entities that comprise it). While scientists chose the entities and/or properties that will be disregarded, such a choice is always justified on empirical grounds and is constrained by

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[23] She argues that elimination is the best way to understand how special science entities are "both physically acceptable and irreducible to physical entities" and proposes a novel account of non-reductive physicalism (NRP) for the special sciences (Wilson 2010, 281). I don't examine whether NRP applies to chemical bonds. I only employ Wilson's idea to the extent that it specifies how chemical and quantum chemical methods are more efficient than the bit map, leaving open the possibility that there may not be elimination but rather restriction or reduction in degrees of freedom.

what is physically possible. For example, almost all quantum chemical methods make the Born-Oppenheimer approximation. This approximation assumes that nuclei hold fixed positions relevant to the electrons, and thus disregards certain of the interactions that the bit map description would specify. Scientists justify this approximation "on the fact that the ratio of electronic to nuclear mass ($m/M \cong 5 \times 10^{-4}$) is sufficiently small and the nuclei, as compared to the rapidly moving electrons, appear to be determinate" (IUPAC 2014, 179).

The second advantage of this understanding of efficiency is that it is not connected to a subjective notion of simplicity. Simplicity is often conflated with efficiency and this is the source of many apparent ambiguities around Dennett's account (see Beni 2017; Willard 2014). Very crudely, what is simple in one context may be complicated in another or regarded as such by someone else. So if we understand efficiency in such terms then it becomes just as amenable to subjective interpretations. However, in the context of degrees of freedom, there is no room for this. It is a matter of fact that the number of variables required by one description is smaller or larger than the number of variables required by another. Thus understood, efficiency is not vulnerable to problems raised against simplicity.

In the context of my proposed understanding of efficiency, it is evident why chemical and quantum chemical descriptions are more efficient than the bit map. Solving the Schrödinger equation from first principles requires specifying the interactions of each and

every subatomic particle that makes up a molecule. However, quantum chemical descriptions solve the equation by disregarding some of the interactions between certain pairs of subatomic particles, thus reducing the number of variables requiring specification. The most widely used assumption in these descriptions is the BO approximation. It leads to the reduction of the degrees of freedom because it disregards the interactions between the nuclei that comprise the examined molecule.

Of course applying the BO approximation doesn't suffice to specify quantum chemically a molecule's bonds. This approximation is just one of the multiple steps taken so as to arrive at a description which- among other things- identifies chemical bonds. The previous section explains how different quantum chemical methods identify bonds by calculating the bond dissociation energy, bond paths, etc. Given that the BO approximation is applied in all these models, and that the BO leads to a reduction in degrees of freedom, this suffices to argue that these models are more efficient descriptions of molecules and bonds.

Similarly chemistry doesn't specify the interactions of each and every subatomic particle but instead employs a smaller number of variables to formulate its description. Specifically, chemistry focuses on the electrons that occupy the outer shell orbital of each composing atom. The rest of the electrons that make up each atom are disregarded because it is the outer shell electrons that determine how the specific atom tends to bond. For example, carbon has 4 electrons in its outer-shell. Given that hydrogen has just one,

chemists infer that in methane carbon shares one of its outer shell electrons with the electron of each hydrogen atom, thus forming four covalent bonds. So, chemistry describes methane more efficiently than the bit map because it disregards the electrons that occupy the inner orbitals of methane's constituting atoms.

In sum, neither chemical nor quantum chemical methods require specifying the interactions between all subatomic particles. In contrast, the bit map requires specifying the interactions between all subatomic particles. This suffices to show that the former descriptions are more efficient than the bit map.

4. The Challenge from Pluralism and Instrumentalism

As with any account in philosophy, objections have been raised against Dennett's real patterns. A central objection is that it is not a genuinely realist thesis (most notably raised by Fodor 1985). Dennett's account seems to allow all efficient descriptions to identify real patterns and critics interpret this to imply either instrumentalism or pluralism about patterns.[24] This section formulates this objection with respect to chemical bonds.

[24] This objection is primarily raised with respect to intentional states though more general formulations are also offered (see Dahlbom 1995; McAllister 2010; Viger 2000).

For a clear formulation of this objection, it is instructive to return to the example of methane. Chemists describe subatomic interactions by identifying four covalent bonds between carbon and each hydrogen atom. This means that chemists only identify as bonds some of the interactions within the molecule; the interactions between hydrogen atoms aren't identified as bonds, despite the fact that chemists acknowledge that such interactions take place (see Bader 2009).

Given this, it is sensible to expect that there is a principled difference between those interactions that are referred to as bonds and those that aren't. One might even expect that Dennett's account provides a criterion that discerns between the two. However, this is not the case. Dennett's account is consistent with there being more than one ways to describe a frame efficiently and admits that there are different patterns within a single frame (1991, 33).[25]

This feature of Dennett's account becomes apparent via the notion of noise. Noise refers to the information about a frame which is disregarded or eliminated by an efficient description (Dennett 1991, 32-35). According to Dennett, noise is to be expected as not all information about a frame can be compressed by an efficient description, and there will inevitably be some information that is left out. Moreover, each description describes the

[25] A frame corresponds to the specific molecule one aims to describe.

same frame by compressing the information differently. So what is regarded as noise under one description, may be part of a pattern by another.[26]

A similar case can be made about methane. For example, the DFT method describes surfaces of electron charge distributions not only between carbon and hydrogen atoms, but also between the hydrogen atoms (recall the blue surfaces in Fig.2). This implies that unlike the chemical description, the DFT describes methane (i.e the frame) by identifying a pattern not only between carbon and hydrogen, but also between the hydrogen atoms. It is only after calculating the intensity of electron charge distributions that one posits a bond just in the regions with high electron charge (namely between carbon and hydrogen). However, in Dennett's account, this is irrelevant: there is also a pattern between the hydrogen atoms because there is a method which describes more efficiently than the bit map the interactions between them.

Critics to Dennett interpret this situation in two alternative ways (for example McAllister 2010, 810-812; Brading 2010). On the one hand, if something is part of a pattern under one description and noise under another, then the patterns aren't real. In the context of chemical bonds this could be stated as follows: there is no principled reason why specific subatomic interactions qualify as patterns, therefore there are no real patterns and thus no chemical

[26] Different patterns in a system can also be identified because the system is described at different scales (Dennett 1991, 44; Ladyman et al. 2007, 203).

bonds. Alternatively, one could interpret this situation from a pluralist perspective. Specifically, *all* subatomic interactions which are efficiently described are patterns irrespective of whether chemical and quantum chemical descriptions identify them as bonds. While pluralism maintains that chemical bonds are real patterns, it undermines their special status relevant to subatomic interactions which aren't regarded as bonds.

Neither the instrumentalist nor the pluralist interpretation is appealing for a scientific realist. This is because both interpretations dismiss (in different ways) the special status that chemical bonds hold in scientific practice. Bonds are essential in the explanation of chemical, biological and physical phenomena. Disregarding their success in science is not in line with the commitment to take seriously the success of scientific concepts when evaluating the existence of relevant entities.

So even though I don't offer evidence against instrumentalist and pluralist interpretations, there is an incentive to clarify Dennett'a account in a way that does justice to the scientific success of bonds. To do so, I incorporate ideas about real patterns that have been presented in structural realist positions.

5. Structural Realism to the Rescue

Among realist accounts in the literature, structural realism is the only position that explicitly draws inspiration from Dennett's account of real patterns.[27] So it is natural to examine it in order to overcome an objection that undermines the reality of bonds as patterns. This section shows how incorporating ideas from structural realism circumvents instrumentalism and pluralism about chemical bonds.[28]

The most detailed contribution to clarifying the realist feature of Dennett's account is by Ross who on his own and jointly with Ladyman, has argued for an amendment to Dennett's account in order to overcome instrumentalist objections and advocate a universal thesis about the reality of special science entities (Ladyman et al. 2007; Ross 1995, 2000). Ladyman and Ross, based (in part) on their analysis of Dennett's account, defend a form of non-reductive unity which doesn't eliminate special science entities from our ontology

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[27] There are forms of structural realism which imply eliminativism about special science ontology (see French 2014). Given that I propose a realist understanding of chemical bonds, these are disregarded.

[28] My discussion of structural realism only focuses on how specific ideas can accommodate our understanding of chemical bonds as patterns. A lot more can be said about metaphysical and epistemic versions of structural realism, and about how such accounts inform our understanding of chemistry's relation to quantum physics.

(called ontic structural realism (OSR)).[29] OSR circumvents pluralist and instrumentalist interpretations of real patterns, by understanding them as follows:

> real patterns are those that indispensably figure in projectable generalisations that allow us to predict and explain the behaviour of the world. (Ladyman 2017, 157)

On this view, special science descriptions identify real patterns not only because they are more efficient than the bit map but because they make counterfactual and nomological generalisations that are highly successful in explaining and predicting phenomena

[29] Ladyman and Ross's account has prompted debates, including about the role of science in metaphysics, the existence of a fundamental level, and the information-theoretic approach on projectibility (for example Hettema 2017, 256-258; Frigg and Votsis 2011; Psillos 2001). I focus only on those parts of their account that are related to defending the reality of chemical bonds as patterns; the aforementioned issues are disregarded. Moreover, as with Wilson's account, the present *partial* use of Ladyman and Ross's account doesn't imply the full acceptance of their views.

(Ladyman 2017, 154; Ladyman 2011, 100).[30] This is what qualifies only some efficient descriptions as correctly identifying real patterns and stands as the criterion to discern those patterns.

That this is the appropriate way to pick out real patterns becomes also apparent by Wallace's similar understanding of them:

> Dennett's criterion: A macro-object is a pattern, and the existence of a pattern as a real thing depends on the usefulness — in particular, the explanatory power and predictive reliability — of theories which admit that pattern in their ontology. (2010, 6)

So Ladyman, Ross, and Wallace take the explanatory, predictive and heuristic success of the special sciences to be the appropriate means to discern descriptions which identify real patterns. And indeed, applied to chemical bonds, this criterion explains why only some patterns of subatomic interactions are identified as chemical bonds in science.

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[30] Ross requires counterfactual generalisations to be true in physically possible worlds, in particular those worlds that are physically similar to ours (Ross 2000, 161-63). French investigates dispositionalist, Humean, and potentiality understandings of modality (2020, 13-17). I leave this issue open and only require that counterfactual generalisations are true in the actual world.

Consider for example covalent bonds. By positing such bonds, chemistry describes a large class of molecules and makes counterfactual and nomological generalisations about how these molecules react and why they are stable. For example, carbon atoms are taken to be bonded to each other via covalent bonds. This explains the stability of the resulting molecules and the formation of large macromolecules. Moreover, that large amounts of energy are produced when hydrocarbon molecules react with oxygen is also explained by the covalent bonds that make up these molecules.

So only some sets of subatomic interactions are referred to as chemical bonds because only these figure in empirically successful counterfactual and nomological generalisations. That aromatic compounds are unusually stable is explained by the covalent bonds formed between the carbon atoms; that water boils at a high temperature is explained by the hydrogen bonds that are formed between H_2O molecules; and, that metals conduct electricity is explained by their ionic bonds.

Only specific interactions figure in counterfactual and nomological generalisations because it is those that play the largest role in a molecule's behaviour. For example, the subatomic interactions between carbon and hydrogen determine to the largest extent how methane is structured and reacts. This doesn't mean that other subatomic interactions don't occur within methane, nor that these don't have some effect on its behaviour. However, such

interactions are negligible and therefore rightly don't figure in counterfactual and explanatory generalisations.

This also becomes apparent if we consider why similar subatomic interactions are identified in certain cases as patterns and in others as noise. For example, chemical bonds usually refer to subatomic interactions among entities that form part of the *same* molecule. However, there are specific atoms which are posited to form a bond (called hydrogen bond) even if they are parts of neighbouring molecules. So while chemistry doesn't standardly identify subatomic interactions among neighbouring molecules as bonds (because they play no substantial role in explaining and predicting molecules's behaviour), the case of hydrogen bonds illustrates that such interactions aren't always negligible. Hydrogen bonds determine how some molecules behave and this is why they are included in explanations and predictions, and are identified as bonds.

One could accept the above as an accurate rendering of how science posits bonds, yet maintain that this illustrates that bonds are just useful tools for describing specific phenomena. For example, Beni argues against Ladyman and Ross's understanding of real patterns because the usefulness of a specific method is not an "objective notion, and the decision about usefulness or uselessness of patterns may well depend on the cognitive and practical interests of the investigator" (2017, 298).

In the case of bonds, the previous examples show that the usefulness of positing chemical bonds and the choice of which subatomic interactions are identified as such are based on the explanatory and predictive success that is produced by their use. Their explanatory and predictive success is in turn evaluated in terms of well-confirmed empirical evidence drawn from the experimental manipulation and measurement of molecules. So, even when there is subjectivity about which method is employed and what assumptions are made, the usefulness of positing chemical bonds is evaluated by looking at how their use fares with empirical evidence.[31]

6. Advantages

Requiring efficient descriptions to be part of successful counterfactual and nomological generalisations is a sufficient amendment to Dennett's account so as to circumvent instrumentalism and pluralism about chemical bonds as patterns. However, there are additional advantages to accepting such an understanding of patterns, which this section briefly presents.

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[31] If one assumes that the results of empirical observation and experimental manipulation are open to subjective interpretation then no amount of well-confirmed empirical evidence would suffice to convince them otherwise.

First, the proposed account implies an understanding of composition which is in line with the physical underpinning of chemical bonds. Ladyman states that in the context of real patterns, composition:

> is a real feature of the world and is in general *diachronic, dynamical,* and domain specific, since it depends on the relevant kinds of interaction among parts. (2017, 152)[32]

This "diachronic and dynamical" feature of real patterns is particularly appealing because it is consonant with the scientific understanding of chemical bonds. Electrons and nuclei that form a bond are dynamic: subatomic particles move around the molecule and occupy different positions and orbitals at different times.[33] By advocating a non-static understanding of the composing entities of a pattern, we illuminate an important (yet neglected) feature of chemical bonding; namely that it is a diachronic and dynamic process during which subatomic particles interact via (mostly) Coulomb forces.

Secondly, this proposal resolves the ambiguity around chemical bonds without undermining or dismissing any scientific classification or method of describing them. Under the framework of real patterns, all scientifically-admissible methods and

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[32] Italics added.

[33] Hendry similarly points out the dynamic character of bonded structure (2016, 1072).

classifications of bonds identify real patterns. The proliferation of methods is partially due to the specific aims that are in play, but also due to the characteristics of the molecule that is under examination. Given that each molecule differs in the number and mass of subatomic particles that constitute it, it is only natural that the resulting patterns of interactions exhibit different characteristics, even though all interactions are the result of Coulomb forces among negatively and positively charged entities (as well as of their relativistic effects). For example, some patterns of interactions involve transferring an electron to one nucleus (as per the ionic bond), while others involve sharing two (or more) electrons between two nuclei (as per the covalent bond or multicenter bonds). Each type identifies the unique way a chemical bond is instantiated in a molecule, without this undermining that all types correspond to patterns of interactions among subatomic particles.

Regarding the structural and energetic conceptions, when it comes to specifying the metaphysical nature of bonds both conceptions become obsolete within the proposed account. Chemical bonds are real patterns of subatomic interactions; they are neither material things (as per the structural conception) nor energetic facts (as per the energetic conception). However, there is still value in talking of bonds in terms of the two conceptions. Each conception illuminates features of chemical bonds that are relevant to the description and explanation of some set of molecules. For example, the structural conception is helpful in understanding the role of bonds in chemical reactions: given that

reactions are standardly explained in terms of the formation and breaking of bonds, the structural conception helps understand the result of a chemical reaction but also the mechanism by which it is realised. Nevertheless, this doesn't mean that the structural conception captures what chemical bonds are. As stated in section 2, both conceptions are incomplete descriptions that identify some (though not all) features of chemical bonds.

Moreover, the proposed account explains the use of approximations and idealisations in chemical and quantum chemical descriptions, without undermining the reality of bonds. Recall that when a description is more efficient than the bit map, it inevitably disregards some of the entities and/or properties that are part of the system. The entities, properties and interactions which are disregarded via idealisations and approximations correspond to what Dennett calls noise. In the case of chemical bonds, some descriptions involve idealisations or approximations that don't affect the accuracy with which they describe bonds (i.e. the pattern).[34] This is because they disregard factors that are negligible with respect to how the molecule is bonded (for example this is the case with the BO approximation). Other descriptions make idealisations that include information a more efficient description would regard as part of a pattern. This explains why the MO approach is preferred over the VB (at least for a class of molecules), as the former doesn't disregard interactions which play a determinant role on how some molecules are bonded (such as the

[34] Weisberg discusses the role of idealisations in the quantum chemical descriptions of chemical bonds (2007).

delocalisation of electrons). However, it is not the case that a description accompanied by any amount of noise, is qualified as identifying real patterns. Science decides on empirical and theoretical grounds whether a specific idealisation is acceptable and whether the relevant description adequately agrees with empirical evidence.

All this shows that the proposed account is constrained, compatible, and informed by scientific practice. That chemical bonds are real patterns is justified by the relevant chemical and quantum chemical methods and classifications, and by how chemical bonds are understood in science. In addition, this proposal is a novel contribution to the question of the reality of chemical entities. This becomes apparent if one takes into account that the reality of chemical entities is standardly defended within anti-reductionist, pluralist and emergentist contexts (for example Hendry 2006).

Lastly, this proposal opens new avenues for understanding how chemical bonds are related to their lower-level constituents.[35] While Dennett does not provide a complete account of inter-theory relations, subsequent talk of real patterns (such as within OSR or Wilson's NRP) explores how patterns are related to their constituents. While some initial conclusions are drawn by my present analysis, a lot more has to be said about how

[35] Primas examines the relation of chemical entities with their quantum mechanical constituents in terms of a non-Denettian understanding of patterns (1975; 2013).

chemical bonds (as patterns) relate to subatomic interactions. Nevertheless, understanding bonds as real patterns encourages studying this issue in more detail.

7. Conclusion

I argue that chemical bonds are real patterns of subatomic interactions. Arguing for the reality of chemical bonds as patterns may not convince instrumentalists or pluralists about patterns. To overcome such worries, I propose an understanding of real patterns which includes ideas about patterns from structural realism. For the specific case of chemical bonds, this proposal (i) is well-supported by scientific evidence; (ii) does not undermine the special status of chemical bonds in science; and (iii) captures important features of bonds, including the fact that they are dynamic and diachronic.

More importantly, it is a metaphysical account that resolves existing ambiguities around the nature of chemical bonds, without- as was previously done- undermining or dismissing any of the existing methods of describing and classifying chemical bonds. Put differently, this proposal hits two birds with one stone: it correctly identifies the physical nature of chemical bonds, while proposing an understanding of chemical and quantum chemical methods that is in line with how science is actually done.

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