

Prospects for Strong Emergence in Chemistry

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ABSTRACT – Chemistry and physics are so closely intertwined that for many philosophers it hardly seems possible that chemistry should be autonomous in any ontologically serious way. Firstly, chemistry itself individuates substances by their microstructural properties. Secondly, during the twentieth century chemistry and physics worked closely together to provide physical explanations of the structure, bonding and behaviour of molecules. I argue that each of these facts is fully consistent with the existence of strongly emergent chemical properties, understood as involving downward causation. The prospects for strong emergence in chemistry are at least as good as those of reduction.

1. Introduction.

How is it possible that there could be downward causation in chemistry? Since the chemical revolution chemists have pursued a research programme which has successively identified the elemental constitution of compound substances, and explained their behaviour in terms of that constitution. In the nineteenth century they began to think of elemental composition in terms of atomic constitution, and devised *structures* at the atomic scale, diversity among which accounted for the existence of distinct substances (isomers) that have the same elemental composition. In the twentieth century the relationship was deepened further by discovering the structure of atoms themselves, and how *their* parts (electrons and nuclei), and the interactions between *them*, underpin the structures that individuate substances and explain their behaviour. At the same time the structures themselves were fleshed out using the joint resources of theory and experiment. Thus classical mechanics, the structural theories of the nineteenth century, the ‘old’ quantum theory, quantum mechanics, X-ray crystallography, spectroscopy, and dear old chemical inference all pulled together to provide, by the early twenty-first century, detailed theories of how nuclei and electrons are arranged within substances, how they move and interact, and how these structures and processes give rise to the phenomena that chemists and physicists study.

Does this undoubted intellectual achievement not amount to a reduction? It does not, I argue. Chemistry supplied the atoms, and initially the physicists took some persuading of their existence: the physicists came late to *chemical* atomism.¹ Furthermore, *chemistry’s* distinct perspective on structure at the molecular scale was an indispensable part of the development of structural explanation in both physics and chemistry. The whole enterprise was a collaboration, and it is perhaps surprising that it is not seen that way more widely in philosophy and physics, and indeed chemistry itself. We should regard the process as a synthesis of chemistry and physics, not a reduction of one to the other. But the reductionist will say, quite correctly, that these are merely historical points. We have a theory of everything (non-relativistic quantum mechanics), at least for chemistry, that can, in principle, explain everything about molecules. My question is: let’s examine the assumption that such a theory exists, and examine what the theories that we *know* to exist can, and cannot, do for us.

2. Setting Up the Question.

Many philosophers and scientists are convinced that there can be no strong emergence in chemistry, and that this view is supported by evidence from physics and chemistry. In this paper

¹ It is important to distinguish between the atoms of Boyle and of Dalton. For Boyle, atoms may play this or that explanatory role, but there is no assumed connection between the number and diversity of atoms and the identity of chemical substances known in the laboratory. For Dalton, there is one distinct kind of atom for each chemical element, and so a clear relevance to chemical explanation.

I will argue that they are mistaken in believing the second part of that sentence to be true. I am not going to argue against reductionism: my aim is the weaker epistemic one of convincing the reader that the scientific evidence for the existence of strong emergence in chemistry is at least as good as the evidence for reductionist positions that rule it out. I want the reductionists to stop thinking not only that their position is forced on us by the evidence, but also that it is in any way more plausible or better supported by the evidence than the strong emergentist's. To do that I have to explain what I mean by strong emergence, and also set some terms for the debate: what should and should not count as an appropriate source of evidence.

It is common to make a distinction between weak and strong emergence. For a property to be weakly emergent from physics requires that physics provides insufficient resources to make a practical basis for predicting or explaining a system's possession of that property, and the causal powers it confers. Strong emergence requires that the failure to predict and explain is there in principle. In metaphysics and the philosophy of mind, it has been common recently to use causal efficacy as a mark of reality, following either Plato's Eleatic stranger (Colyvan (2001: Chapter 3)) or Samuel Alexander (Kim (1998: 119), (2005: 159)), according to preference. To exist requires the possession of causal powers. Applied to the case of reduction and emergence, one might use the conferment of additional causal powers as a mark of the *distinct* reality that is characteristic of something that is strongly emergent. Now the possession of novel causal powers does *not* require the violation of more fundamental laws. Strong emergence requires not that these laws be broken, but only that they fail to determine what happens. This will be the case where, for instance, fundamental laws fail to favour one of a number of different possibilities, with the missing determination provided by the strongly emergent property.

In other papers (Hendry (2006a), (2010a), (2010b)) I have attributed to Broad (1925) the view that strong emergence involves downwards causation: that the subsystems of an emergent supersystem sometimes do something different to what they would do if the causal structure of the world were as imagined by the reductionist. In short, the strong emergentist makes a counternomic claim. Filling out this bare sketch of the emergentist position then requires one to identify just how, in particular scientific cases, the reductionist imagines the causal structure of the world to be.

Evidence: I will assume in what follows that philosophical intuition is an unreliable guide to composition and reduction. Reasons to regard X as reducible to Y should come from science, not from *a priori* argument.

3. Chemical Substances.

One reason why many philosophers reject the idea that there can be any strong emergence in chemistry is that they think that the reducibility of chemical entities and properties to physical entities and properties, or their identity with physical entities and properties, has been established through such theoretical identities as "water is H₂O". The argument is supposed to be that "water is H₂O" should be read as "water = H₂O". In short, to be H₂O *just is* to be composed of H₂O molecules. This settles the reduction issue as we have framed it for the purposes of this paper, because if the contents of a particular jug have any causal powers in virtue of being water (e.g. the power to quench thirst, or to dissolve salt), then those contents have those powers in virtue of their being composed of H₂O molecules. I will not challenge the claim that "water is H₂O", so long as that claim is properly construed.² I have argued elsewhere that chemical substances are

² For a range of different reasons, the identity is challenged by Barbara Malt (1994), Paul Needham (2000), (2002), (2011), Jaap van Brakel (2000) and Michael Weisberg (2006).

individuated by their microstructural properties and relations (see Hendry (2006b), (2008)), and have more recently come to the view that a substance's structure at the molecular scale *is what makes it the substance that it is*, from a chemical point of view (Hendry (2016)). However, I will argue that the widespread idea that the identity "water is H₂O" establishes reducibility, or some chemical analogue of the mind-brain identity theory, is the product of a straightforward misreading.

What is the scientific basis of a theoretical identity such as "water is H₂O"? Historically, it was established via a number of distinct steps, the first being the compositional claim that water is a compound of hydrogen and oxygen. The eighteenth-century chemists did not content themselves with giving a hypothetical explanation of water's behaviour in terms of its elemental composition. Rather, they took known weights of water, decomposed them into hydrogen and oxygen, weighed the separate elements to establish that their combined weights were (roughly) the same as those of the decomposed water, then recombined them, recovering close to the original weights of water. Later, in the nineteenth century, they introduced quantitative compositional formulae, which represented the proportions between the constituent elements: H₂O in the case of water.³ Finally, the compositional formulae came to be interpreted as embodying molecular facts (in some cases): for water, that its characteristic molecule contains two atoms of hydrogen and one of oxygen (however, such atomist interpretations were controversial for much of the nineteenth century). All this should be salutary for materialist philosophers of mind who would wish to use parallels between "water is H₂O" and "pain is c-fibres firing" as a guide in developing a materialist theory of the mind. Establishing that water is H₂O was a detailed process, whose first step involved the analysis of water into its proposed constituents, and then a re-synthesis from them. It does not seem unreasonable to withhold one's assent to "pain is c-fibres firing" until something analogous has been achieved.

That point made, how should "water is H₂O" be construed? To survey the alternatives we need to identify the relata (water and H₂O) and the relation itself.⁴ First consider the relata: following Paul Needham, we can treat "water" and "H₂O" as predicates, or more likely a range of predicates. We can discuss whether these predicates correspond to properties later. What does it mean to say that something is water? First note that some substance names—"ice" or "diamond" for instance—refer only to specific states of aggregation: the name determines whether the relevant stuff is solid, liquid or gas. Other substance names are used independently of state of aggregation, which must be added explicitly if it is to be specified, as in "liquid nitrogen" or "solid carbon dioxide". "Water" has a phase-neutral use, in which we may ask (for instance) how much of it there is in the solar system.⁵ A comprehensive answer will include the solid water in the polar icecaps of various planets,⁶ liquid water in their seas (perhaps only in the case of the Earth), water vapour in their atmospheres and also isolated water molecules strung out in interplanetary space. In the case of hydrogen one would have to include the large quantities present as plasma in the interior of the sun. Clearly, nothing of interest depends on whether one

³ Note that the proportions were not between the weights of the elements, but between equivalents, thus "water is H₂O" represents the fact that it contains twice as many equivalents of hydrogen as of oxygen, although the oxygen-hydrogen weight ratio in water is more like 8:1.

⁴ In the following discussion I am indebted in many ways to Paul Needham ((2000), and many conversations), although we are in clear disagreement on some of the issues.

⁵ Note that various chemical processes produce and consume water. Hence the total amount of water in the solar system will vary, so the question must be asked with reference to some period of time.

⁶ In fact John Finney (2004) identifies sixteen distinct structures for ice, which form under different thermodynamic conditions.

allows the phase-neutral scientific usage, or insists on the supposed “ordinary language” usage (I use scare quotes because I am highly sceptical that there *is* an ordinary language usage that is consistent enough to be said to have an extension). From the chemists' point of view, since there is something important that all water's different states of aggregation share, it makes sense to have one name for all these forms.

Now consider “being H₂O”. People who know little of chemistry may take this simply to be a molecular condition (something like “being composed of H₂O molecules”), but in general a chemical formula need not convey much information at the molecular level: it may, for instance, specify just the elemental composition of a substance, which may be shared by more than one substance. The formula “C₂H₆O”, for instance, applies both to ethanol (often written CH₃CH₂OH) and dimethyl ether (sometimes written CH₃OCH₃), which are distinct compounds with very different physical and chemical properties. So we must ask, is “H₂O” intended to specify the molecular make-up of water, or merely its elemental composition?

Finally we come to the relation itself. It is well known that “A is B” bears interpretation in terms of either identity or predication. In the present case two such interpretations suggest themselves: clearly “water” and “H₂O” are not the same predicate, though they may correspond to the same property. A weaker interpretation involves a relation of coextension or containment between the two predicates or properties: all A is B. If a necessity operator is envisaged (and on my view, one is required), then the source of the necessity is important. On the strongest microstructural essentialist view, which I would endorse, the relationship could be put in one of two ways: (identity) to be water is to be composed of H₂O molecules; (coextension) necessarily, all samples of water are samples of stuff composed of H₂O molecules, with the necessity in question being full metaphysical necessity. Putting this all together, “water is H₂O” could mean either (i) “to be water is to be made up of two parts of hydrogen to one part (by equivalents) of oxygen”; (ii) “to be water is to be composed of H₂O molecules”; (iii) “every sample of water is made up of two parts of hydrogen to one part (by equivalents) of oxygen”; and (iv) “every sample of water is composed of H₂O molecules”. Different versions of (iii) and (iv) also result if modal operators are appended, and also if one attends to the source of such modality (see van Brakel (2000)).

Even if one takes the *strongest* essentialist reading, according which to be water *is to be* H₂O, then on the only scientifically plausible reading of what it is to be H₂O, reductionism does not follow. Why? Hilary Putnam once said that the extension of “water” is “the set of all wholes consisting of H₂O molecules” (Putnam (1975: 224)). If a “whole” is taken to be a mereological sum, or any other composition operation in which the components are assumed to survive, this is straightforwardly false according to chemistry. Being a whole that consists of H₂O molecules may well be sufficient to be a quantity of water, but it is not necessary. Pure liquid water contains other things apart from H₂O molecules: a small but significant proportion of H₂O molecules (at room temperature, about 1 in 10⁷) dissociate (or self-ionise) forming H₃O⁺ and OH⁻ ions:



Furthermore, H₂O molecules are polar and form hydrogen-bonded chains which are similar in structure to ice. One might regard the ionic dissociation products and chains as impurities, but the presence of these charged species is central to understanding water's electrical conductivity. Since chemists regard the electrical conductivity they measure as a property *of pure water*, it seems gratuitous for we philosophers to interpret it instead as a property of an aqueous solution of water's ionic dissociation products. Looked at this way, liquid water can at best be considered to be composed of some diverse and constantly changing population of species at the molecular

scale, including H_2O molecules, H_3O^+ and OH^- ions, and various oligomolecular species. Can we defend the claim that water is H_2O ? Yes, by considering water in all its forms to be the substance brought into being by interactions among H_2O molecules (see Hendry (2006b)).⁷

One way to summarise all this is to regard being water as a distinct property that both molecular species and macroscopic bodies of stuff can have. H_2O molecules have it merely in virtue of being H_2O molecules. Larger bodies of stuff get it by being composed of (possibly diverse) populations of molecular species of kinds which are produced when H_2O molecules interact. Given the assumption that every part of water is water, this means that molecular species (such as H_3O^+ and OH^- ions) can be water in virtue of being part of a diverse population of molecular species which is produced when H_2O molecules interact. Hence they acquire the property of being water by association. There is nothing strange in this. If we consider the protons in water to be part of the water, they acquire their wateriness by association too.

In a less exciting sense, wateriness is therefore an emergent property because nothing below a particular size (that of an H_2O molecule) can be water on its own account, and some smaller fragments acquire the property by association. But that doesn't tell us whether being water is a *strongly* emergent property, i.e., whether or not being water confers additional causal powers. This is where the standard argument I mentioned earlier comes in, except we can now see that it runs into difficulty. Consider all the different kinds of thing that, we have agreed, count as quantities of water, from mereological sums of water molecules, through steam, liquid water and (the various forms of) ice. Trivially, a mereological sum of water molecules is no more than the sum of its parts. Any powers it has are acquired from its constituent H_2O molecules. But it has no bulk properties, so there is no distinction to be made between its molecular and its bulk properties. Steam, liquid water and (the various forms of) ice do have bulk properties, each bearing distinct sets of properties produced by the distinct kinds of interactions between their parts. Wherever there is significant interaction between the H_2O molecules, there is scope for that interaction to bring new powers into being. This is particularly obvious if that interaction includes self-ionisation and the formation of oligomers: the excess charge of solvated protons can be transported across a body of liquid water without the transport of any matter to carry it, via what is called the Grotthuss mechanism. This, in fact is why water conducts electricity so well, unlike other, similar hydrides. The power to conduct electricity is not possessed by any sum of (neutral) H_2O molecules. The mechanism by which that power is exercised requires some part of the molecular population to be charged. It therefore depends on a feature of a diverse *population* of molecular species.

The reductionist will say at this point that the water can only acquire its causal powers from its parts, and interactions between them. So no novel causal powers have been introduced. The strong emergentist will ask why, when it is being decided whether they are novel, the powers acquired only when the molecules interact are already accounted for by the powers of H_2O molecules. If the rule is that any power possessed by any molecular population produced by any interaction between H_2O molecules is included, and we know this rule to apply independently of any empirical information we might ever acquire about what water can do and how it does it, then it seems that we know *a priori* that there will be no novel causal powers, which violates the rules of our discussion. This does not of course mean that the strong emergentist wins the argument by default: only that in the absence of a specific scientific argument, the reductionist

⁷ Note that I have ignored the token identity question, which I take to be an irrelevance from the point of view of science.

and the strong emergentist conclude this discussion honours even. Anti-reductionists need not fear theoretical identities, and should even learn to love them.

4. Molecular Structure and Quantum Mechanics.

Our other possible locus for emergence in chemistry is molecular structure. Are molecules anything more than systems of charged particles, interacting according to the laws of quantum mechanics? I seem to be in a minority of one in giving that question an affirmative answer, and certainly so when I defend the idea that molecular structure is strongly emergent. Yet I think the unanimity on the other side is baseless, as I have argued elsewhere (see Hendry (2006a), (2010a), (2010b)). Because this is familiar territory, I will give these issues a fairly brisk treatment here.

Textbooks of physical chemistry often present the application of quantum mechanics to chemistry as a process that begins with the writing down of a Schrödinger equation for an isolated molecule, purely in terms of the electrons and nuclei present. The aim is to solve the equation and thereby explain the characteristic structures of molecules, which chemists have used to explain the chemical behaviour of substances since the 1860s. When it appeared on the scene in the mid-1920s, quantum mechanics was widely expected to provide a complete account of chemistry. Just a few years later, Paul Dirac famously wrote:

“The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble. It therefore becomes desirable that approximate methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation”. (Dirac (1929: 714))

Here, non-relativistic quantum mechanics is assumed to be a sort of “theory of everything” for the motions of electrons and nuclei, and therefore for any molecule. Physicists and philosophers who use that phrase usually mean a theory that could—in principle—explain everything that happens in a system to which it is applied, to the extent that it can be explained. Think of Newton’s laws applied to the planetary motions: natural philosophers since Newton’s time have imagined a God’s-eye-view application of his laws which could be used to predict all future planetary positions, if only we had accurate enough access to their current positions and momenta, plus large enough computers to cope with very detailed and accurate mathematical models of the solar system. A more formal way to put this is to say that in a multi-dimensional configuration space representing the dynamical state of the solar system, the laws governing planetary motions uniquely specify its future evolution, given only its current state. The question of whether molecular structure is strongly emergent is, I think, best understood as the question of whether we have good reasons to think that, from a God’s-eye-view, non-relativistic quantum mechanics is a “theory of everything” in this sense, or whether some looser relationship between the dynamics and the evolution of the system is better supported.

The problem raised by Dirac is that for any chemical system bigger than a hydrogen atom, the Schrödinger equation, the central equation of this theory of everything, is insoluble analytically. This means that approximations must be introduced: known falsehoods that will affect the calculations in well-understood ways. For molecules, this means the Born-Oppenheimer or ‘small oscillation’ approximation. It is worthwhile separating this into two separate moves. First, nuclear and electronic motions are considered as separate (even though electrons and nuclei are known to interact), yielding an overall wavefunction that is a product of nuclear and electronic wavefunctions. In the second step the nuclei are then assumed to be at rest, on account of their

much higher masses, and therefore slower motion. The problem of calculating the wavefunction for the electrons can now be addressed on its own, and the molecule's energy calculated from that. In the last twenty years or so this problem has increasingly been addressed through density functional theory (DFT), in which the aim is to calculate the electron density, rather than the molecular orbitals of yore. The electronic energy can be calculated for a few nuclear configurations near the (empirically given) equilibrium configuration, and the fact that it is the equilibrium configuration is thus explained, after a fashion: it is the local minimum in a particular region of the potential-energy surface. The problem is that it is explained in a way that seems to undermine the status of non-relativistic quantum mechanics as a theory of everything for molecules, and therefore for chemistry.

Brian Sutcliffe and Guy Woolley (2012) argue that the Born-Oppenheimer approximation should not be called an approximation, because it fundamentally alters important mathematical properties of the equations and their solutions. Sutcliffe and Woolley raise two difficulties, concerning isomers and symmetry properties. Turning to isomers first, the Schrödinger equation for a molecule is fully determined once the nuclei and electrons present are enumerated. This means that isomers, such as ethanol ($\text{CH}_3\text{CH}_2\text{OH}$) and dimethyl ether (CH_3OCH_3), mentioned earlier, will share the same Schrödinger equation. But the Born-Oppenheimer equations for ethanol and dimethyl ether are quite different. In applying the Born-Oppenheimer approximation we have moved straight from an equation that applies to both of these molecules to a *different* equation that applies to just one of them and not the other. How, from a mathematical point of view, did we do that? By putting in *by hand* the parameters that specify an important difference between the two cases: the nuclear positions. We have explained the geometrical configuration of an ethanol molecule as a local minimum on a particular potential-energy surface. We have explained the geometrical configuration of a dimethyl ether molecule as a local minimum on *its* particular potential-energy surface. But can we say we have a “theory of everything” that encompasses all of this? We have an equation that, in a sense, *allows* both possibilities. But that is a very weak way of being a theory of everything. We cannot say that it determines the different possibilities to arise when they do arise. Do we have good reasons to say that quantum mechanics is any more than this, unless supplemented with structural insights from chemistry?

The second problem concerns symmetry. For good physical reasons, the only force appearing in molecular Schrödinger equations is the electrostatic or Coulomb force: other forces are negligible at the relevant scales. But the Coulomb force has spherical symmetry. How, from this slim basis, do we get the great variety of different symmetry properties (chiral (asymmetrical), cylindrical, hexagonal and many more) exhibited by real molecules? In practice the lower symmetries are introduced as part of the Born-Oppenheimer approximation. Surely ‘approximation’ is a misnomer for a procedure that changes the symmetry properties of the problem, introducing the specific symmetry properties we need to understand the behaviour of each kind of molecule on a case-by-case basis.

I now turn to the strong emergentist interpretation of this situation, which I offer not because I am committed to it, but to establish the plausibility of an alternative to ontological reductionism, and its strong interpretation of what it is to be a “theory of everything.” The strong emergentist sees the role of quantum mechanics as much closer to that of thermodynamics: its universal laws deepen our understanding of the behaviour of the systems to which we apply it, but it cannot explain everything. Thermodynamics must always be applied in tandem with other information about the system. Likewise, the Schrödinger equation provides an important framework for studying molecules, because it encompasses all the possibilities, but for that very reason it is

implausible to see it as fully specifying the dynamical behaviour of every kind of molecule, given only the charges and masses of the constituent particles. It is too abstract on its own, and far removed from the particular structures we study in chemistry. It allows too many other, un-chemical possibilities, and we have no general account of the different classes of solutions it does allow, or of the relationships between them. So instead we simply assume that the known structures exist, and explore the energetic landscape around them to provide an understanding of their dynamical behaviour.

5. Objections and Replies.

In this section I respond to some common objections to the idea that chemical substances and molecular structure could be strongly emergent.

Objection 1: The chemical bond is “just a model”

One response to the foregoing arguments, available to the philosopher or scientist who is temperamentally disposed to physicalism, is to deny the reality of anything which is irreducible to physics, arguing that anything which cannot be reduced to the physical is of dubious physicalistic respectability. To the emergentist this is a cheap move, since it begs the question by declaring unreal anything that doesn't fit within the physicalist's philosophy. And a cheap move it is, unless it is backed up with independent grounds for denying the reality of the items in question. In the case of abstract objects such as numbers, independent grounds for questioning them might be that they are not located in time and space, raising the question of how we can know anything of them. A more detailed and interesting version of this kind of response would draw upon independent *scientific* considerations in the case against the dubious items. Alexander Rosenberg (1994) has argued that biology studies properties and processes which have been honed by natural selection. They are highly complex and multiply realised, so it is beyond human cognition to grasp the underlying (chemical and physical) reasons why these processes work in just the ways they do. Instead, biology must fashion *functional* explanations which Rosenberg proposes to interpret instrumentally, since they do not latch on to the fundamental (physical) forces that drive things. Even in this case the independent grounds for doubting the reality of functionally-characterised properties and processes are only semi-scientific. There have long been worries within biology that function has a whiff of teleology, but Rosenberg's argument also depends on the presumption that the underlying reasons why biological processes work the way they do can only be found in the chemical and physical realisers.⁸ That is a different objection (see below, Objection 3).

In the case of chemistry, the scientific pedigree of instrumentalism about structure is quite as long as that of structural explanation itself. Around the mid-nineteenth century, chemists were divided on whether or not chemical formulae should be used; they were divided on whether or not chemical formulae should be given an atomistic interpretation, and what this involved; and they were divided on whether, under an atomistic interpretation, chemical formulae should be interpreted literally (see Rocke (1984)). This can be read partly as reasonable caution. Structural explanation was purely hypothetical in the 1860s and 1870s. Chemists constructed a range of possible structures which both respected the elemental composition of the substance, and were “legal” by valence rules,⁹ to borrow a phrase from Alan Rocke (2010: 132). They then selected from among these possibilities on the basis of chemical evidence. It was only in the twentieth

⁸ For this reason John Dupré (1995: 283) identifies Rosenberg as a ‘frustrated reductionist’.

⁹ The ‘valence rules’ determined, for each type of atom, how many other atoms it could be linked to by bonds.

century that X-ray crystallography and various kinds of spectroscopy allowed structural theory and experiment to become more closely integrated, with the measurement of (for instance) bond lengths and (vibrational) force constants. A second problem was that molecular structures consisted of atoms connected by bonds, but the bond was no more than an explanatory role in a theory. There was no account of what bonds were, or how they attached one atom to another. G. N. Lewis identified paired electrons as the realisers of this role, but given that Lewis' atom was static while physics seemed to demand constant motion, it was far from clear how the physicists' and the chemists' models could both be true (see Arabatzis (2006: chapter 7)), with Lewis even querying whether chemistry would require a revision of Coulomb's law at short distances (Lewis (1917)). By the mid-1920s quantum mechanics had come into being, a theory which seemed to pose severe difficulties for Lewis' conception of structure, because electrons ought to be delocalised: smeared out across the whole molecule, rather than held static between two atoms.

As we have already seen, the advent of quantum mechanics in the 1920s brought in its train fundamental equations describing molecules which could not be solved exactly. The chemists and physicists who faced this situation in the early days of quantum mechanics developed semi-empirical models. They interpreted the situation in quite different ways (see Hendry (2003)). Linus Pauling saw quantum chemistry as a synthesis of quantum mechanics and autonomous structural insights provided by chemistry. John Clarke Slater, who was, with Pauling, one of the founders of the valence-bond method for constructing semi-empirical models of bonding, saw that method instead as something that stood proxy for the exact equations which Dirac had recognised to be "much too complicated to be soluble". On this view, quantum chemistry should be much less autonomous, with every explanatory step justified as one that could also be made in the exact theory. The problem is that these strictures have only rarely ever been met. The explanatory and predictive successes of quantum mechanics in chemistry, including the novel predictions provided by the Woodward-Hoffmann rules (see Brush (1999)) were achieved through simplified models which neglected the quantum-mechanical character of parts of the molecules whose behaviour they predicted, assuming them instead to be classical. Quantum chemistry seems more like Pauling's synthesis than Slater's reduction.

All this motivates the following argument, which I have heard in different forms from chemists, physicists and philosophers. The chemical bond is a theoretical figment. It was useful in the 1860s, and remains useful now, for predictive and heuristic purposes. But bonds are not real. Quantum mechanics, which provides the best description of the world at the atomic level, has shown the structural theories of the 1860s to be at best naive portrayals of molecular reality.

I do not find this argument convincing, and more generally I am at a loss to understand why philosophers and scientists alike are so ready to approach the results of the special sciences in a spirit of ontological non-seriousness, yet the craziest ideas from physics are taken much more seriously.¹⁰ The argument for instrumentalism about molecular structure can be resisted in a number of different ways. Firstly, structural theory has been around for a very long time—some sixty years longer than non-relativistic quantum mechanics—and its development has been cumulative: the theory itself, and the structures assigned to substances within it, have been retained or extended, our understanding of them deepened by the interaction with physics. I cite two scientific authorities in support of this claim. In a systematic presentation of his views on structure and bonding, Lewis said that

¹⁰ Consider the existence of multiverses and realist interpretations of N-particle wavefunctions propagating in 3N-dimensional space.

“No generalization of science, even if we include those capable of exact mathematical statement, has ever achieved a greater success in assembling in simple form a multitude of heterogeneous observations than this group of ideas which we call structural theory.” (Lewis (1923: 20-21))

In his presidential address to the Annual General Meeting of the Chemical Society (later to become the Royal Society of Chemistry) in April 1936, Nevil Sidgwick rejected the idea that new scientific theories must always overthrow the conceptions of their predecessors (Sidgwick (1936)). A detailed examination of the development of chemistry, he argued, revealed that although “the progress of knowledge does indeed correct certain details in our ideas”, the structural theory of Kekulé, laid down in the 1860s, had “undergone no serious modifications” (Sidgwick (1936: 533)). As we have seen, the chemists of the 1860s had assigned molecular structures to substances so as to account for isomerism, and Sidgwick confidently asserted that “[a]mong the hundreds of thousands of known substances, there are never more isomeric forms than the theory permits” (Sidgwick (1936: 533)). Subsequent developments had clearly enriched the theory, in two ways. On the one hand, Kekulé’s theory “assumes that the molecule is held together by links between one atom and the next,” but in that theory “[n]o assumption whatsoever is made as to the mechanism of the linkage” (Sidgwick (1936: 533)). A proposal as to *how* molecular structure is realised came only later, in Lewis’ theory of the electron-pair bond. On the other hand, later developments enriched structures with detail:

“To Kekulé the links had no properties beyond that of linking; but we now know their lengths, their heats of formation, their resistance to deformation, and the electrostatic disturbance which they involve.” (Sidgwick (1936: 533-534))

He concluded:

“I hope I have said enough to show that the modern development of the structural theory, far from destroying the older doctrine, has given it a longer and a fuller life.” (Sidgwick (1936: 538))

A second argument against an instrumentalist interpretation of structural theory is that its development has been extremely fruitful from an empirical point of view: structural theory has underwritten the design and synthesis of many thousands of new substances; the theories of reaction mechanisms developed from the 1920s onwards depended on Lewis’ insight that the chemical bond is realised by pairs of electrons. If longevity, theoretical continuity and fruitfulness are hallmarks of the real, then structure has a claim on our commitment, and perhaps a stronger one than quantum mechanics, on the basis of which it is called into question. Thirdly, the conflicts with quantum mechanics are often overstated. To be sure, Lewis’s static electron pairs seem naive, but within theoretical chemistry the attempt to recover different aspects of ‘classical’ structure and Lewis’ account of bonding remain important (see for instance Bader (1990)), for the explanatory successes of these theories must be accommodated somehow within the theory which replaces them. I think these considerations should give us pause before we sweep away these intellectual achievements of chemistry with the wave of an instrumentalist hand.

Objection 2: Chemistry doesn’t study properties

Famously, Fodor presented multiple realisation as a sign of the autonomy of the special sciences (Fodor (1974)). Special sciences find “higher-level” (in this case, functional) properties, such as being in pain, indispensable in predicting and explaining how things go, yet such properties

cannot be identical with any group of physical properties if they are realised by different groups in different organisms. It is now quite common to respond to this argument by arguing that the autonomy of the special sciences may only be in the eye of the (scientific) beholder, masking a deeper ontological unity in the world. Perhaps the special sciences do not study properties at all, but instead functionally-defined *predicates*, and the relationships between them. Here is one argument to that effect, adapted from John Heil (2003), (2012): to call something a ‘property’ is to treat it with full ontological seriousness. But it cannot be assumed that special-science predicates should be approached in this way merely because they are useful, or even indispensable in predicting and explaining how things go. Such an abundant view of properties could be assumed if they were just the intensions of the worldly shadows of meaningful predicates, but there are many reasons to set the bar higher than that. Heil (2012) proposes a less serious stance toward special-science categories, allowing that statements involving special-science predicates have truthmakers among the real. In this way the physicalist can get vanishingly close to taking the special sciences (ontologically) seriously without actually doing so, even endorsing semantic realism.

The emergentist can reply as follows. One can think that special sciences study properties without committing the fallacy of adopting the abundant theory of properties (if fallacy it is). As we have seen, causal efficacy is often identified as a mark of reality. Being water confers on a body of matter the power to quench thirst or dissolve salt. A water molecule’s structure confers on it powers to interact in distinct ways with other species at the molecular scale. As we have seen, there is an argument about whether these powers are really inherited from physical properties, but when the Eleatic principle or Alexander’s dictum is applied, this is an argument about whether or not water is a distinct reality over and above its physical basis, or merely a dependent reality. In either case it is a part of reality.

Consider optical activity: in the early nineteenth century, chemists and physicists noticed that some crystals possess the power to rotate plane-polarised light by a characteristic angle. Strikingly, these optically active crystals came in two forms, one which rotates light in one direction, the other rotating it in the opposite direction, by the same angle. The dissymmetrical behaviour was presumed to arise from some internal dissymmetry, but in the particles themselves, or in the way they combine to make up the crystal? In 1849, Louis Pasteur separated, by hand, crystals of the L- and D- forms of the salt of an optically-active acid, sodium ammonium tartrate, which he had obtained from a racemic solution (an equal mixture of the two). Pasteur then dissolved the L- and D- crystals, and showed that they retained the rotatory power in solution, a power which must therefore reside in the individual particles of the tartrate. In the 1870s, Jacobus van 't Hoff and Joseph Achille Le Bel independently proposed that the optical activity arises when four different functional groups are attached to a single (chiral) carbon atom, giving rise to two possible structures which are non-superimposable mirror images of each other: incongruent counterparts, like right and left hands. A full physical explanation of *how* the structural asymmetry gives rise to the power had to wait until the 1930s (for details see Needham (2004)). I have told this scientific story as if complex objects—chiral molecules, or molecular populations—can (irreducibly) possess powers, such as to rotate plane-polarised light or conduct electricity. Our other candidate locus of emergence in chemistry—the emergence of a macroscopic body of stuff from its molecular constituents—we illustrated with water, and its power to conduct electricity.

Heil points out that the classes of things that fall under some special-science predicates do not exactly resemble each other. Thus, for instance

“biologists ‘abstract away’ from physical differences that would be blindingly salient from the point of view of physics, or chemistry, or, for that matter, molecular biology.” (Heil (2012: 195))

Yet it is not clear that *all* special-science predicates can be dismissed in this way. ‘L-tartaric acid’ is not a functional category, and the fact that it can be individuated by the structure of its molecules does not establish its reducibility, as we saw in the case of water. Nor is it clear why *only* special-science predicates can be dismissed in this way. The point about abstraction seems unfair on the special sciences because *all* sciences, including fundamental physics, engage in abstraction, that is, partial consideration of the similarities among a class of objects, and ignoring the differences. Now it might be said that fundamental physics abstracts away only from *relational* differences in the complex causal situations in which its objects participate. Perhaps so, but the emergentist will ask again why such relational differences cannot be irreducibly causally relevant.

For Heil, causal efficacy is not sufficient for being a property: properties can only be instantiated by substances, and substances must be simple. He does not rule out strong emergence, but properties require substances to instantiate them. In short, strongly emergent properties require emergent substances.¹¹ This is not the place for a detailed examination of Heil’s interesting and heterodox ontological views, but I do find the idea that complex entities should be excluded *a priori* from ontological seriousness merely in virtue of their complexity a deeply unscientific one. The ways that complex chemical objects and situations are, in virtue of which they have causal powers, are as good a candidate as anything in science for being properties. Scientific metaphysics, it seems to me, has no business denying this. Metaphysics should not stray too far from science in what it will countenance, in the direction either of permissiveness or restriction.¹²

Objection 3: The causal closure of physics

A third and final objection I will consider is that chemical substances or structures cannot be strongly emergent because their being so would entail the possibility of downward causation. But downward causation is not possible, because the physical is causally closed. One must admit that the existence of strong emergence in chemistry is incompatible with the causal closure of the physical. Closure is widely assumed by philosophers, and is an essential part of the problem of causal exclusion (a philosophical pseudoproblem if ever there was one). Closure is hardly ever argued for however, honourable exceptions being the arguments offered by Brian McLaughlin (1992) and David Papineau (2002: 232-256), which I have responded to elsewhere (Hendry (2006a), (2010a), (2010b)). This is not the place for a general review of evidence for closure, but I will conclude with the following argument.

Closure is a thesis that concerns the relationship of physics to everything else, so to find evidence for it we must look beyond the internal structure of physical theories, and see how they are applied to the special sciences. Of all the special sciences, chemistry has the closest relationship to physics, which as we have seen is embodied in two great scientific achievements. Firstly there is the twentieth-century discovery that chemical substances can be individuated, and their behaviour understood, in terms of their structures at the atomic scale. Secondly there is the

¹¹ If this sounds like a contradiction, because a strongly emergent substance would need to be both dependent and independent, Heil can point to a distinction between (causal) maintenance and ontological dependence.

¹² Peter van Inwagen (2014: 1-14) has recently described the ‘ontology room’, where existence can be discussed. My hope is that the ontology room can overlap with the science room, where actual existence is discussed, not merely what is possible or necessary.

fact that non-relativistic quantum mechanics provides a “theory of everything” for molecules, an all-encompassing framework within which to understand their dynamical behaviour. Yet neither of these facts entails closure. In short, chemistry is where one might expect to find the imperial ambitions of physics fully played out, if they are played out anywhere. It is where we might expect to see some evidence for closure. Yet as I have argued above, strong emergence is a plausible interpretation of the evidence offered by the explanatory relationships between physics and chemistry, which must surely weaken the case for closure.

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