

Structure, essence and existence in chemistry

Robin Findlay Hendry 

Department of Philosophy, Durham University, Durham, UK

Correspondence

Robin Findlay Hendry, Department of Philosophy, Durham University, 50 Old Elvet, Durham DH1 3HN, UK.
Email: r.f.hendry@durham.ac.uk

Abstract

Philosophers have often debated the truth of microstructural essentialism about chemical substances: whether or not the structure of a chemical substance at the molecular scale is what makes it the substance it is. Oddly they have tended to pursue this debate without identifying what a structure is, and with some confusion and about what a chemical substance is. In this paper I draw on chemistry to rectify those omissions, providing a pluralist account of structure, clarifying what (according to chemistry) a chemical substance is and defending microstructural essentialism, as I understand that position. I then give an account of the existence of composite substances and objects in chemistry, an issue that goes back to Aristotle.

KEYWORDS

chemical substances, composition, essentialism, existence, natural kinds, structure

1 | INTRODUCTION

In this paper I explore the central role of structure in the metaphysics of chemistry. By 'the metaphysics of chemistry,' I mean the account that chemistry gives us of the particular aspects of the world that it studies. It is the *metaphysics* of chemistry because it focuses on how things would be if chemistry's account of those aspects of the world that it studies is broadly correct. I begin by developing a broadly pluralist, yet still realist, account of what structure is. It is pluralist in two ways: there is more than one kind of structure, and the structure of a substance can, in important respects, be dependent on scale (of length, time and energy). I then argue that the centrality of structure to chemical classification, nomenclature and explanation underwrites a good argument for microstructural essentialism in chemistry, the thesis that the structure of a chemical substance at the

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molecular scale is what makes it the substance that it is, rather than any other. I conclude the paper with an account of existence in chemistry, giving an analysis of when, according to chemistry, two objects can be said to come together to form something new. This account is scale-relative too, a feature that enables us to answer a foundational puzzle concerning the existence of chemical elements, and the atomic nuclei that ground their existence.

2 | WHAT IS A STRUCTURE?

I will begin by identifying what, for the purposes of chemistry, a structure is. This is a deceptively simple question: although easily asked, the nature of reality at the molecular scale means that there are complications in giving it a scientifically literate answer. A natural way to approach structure *in chemistry* is via composition: a structure is how some parts fit together to form a complex whole.¹ Now chemistry deals with composition at three levels: how sub-molecular parts (electrons and nuclei) compose molecules (for instance, how two protons, an oxygen nucleus and 10 electrons compose an H₂O molecule); how molecules and ions compose substances (for instance, how H₂O molecules compose water); and how substances compose other substances (for instance, how hydrogen and oxygen compose water). For most of this paper I focus on the first topic, only turning to the others when necessary.

How electrons and nuclei compose molecules is a matter of the relationships between them, but these are not static geometrical relationships. Geometrical relationships at the molecular scale are typically dynamic, changing over time. Philosophers who think about structure and the metaphysics of composition sometimes use the word 'arrangement' to describe the kind of geometrical relationship among parts that is involved in composition (see for instance Sider, 2013; van Inwagen, 1990). It is important to avoid that word, however, because 'arrangement' suggests a static configuration, something that could not be robust with respect to motion among the parts, which would take the parts into a different arrangement. However, one thing we know is that at the molecular scale everything is always in motion. Thermal energy has the atoms within molecules bobbing around, the bonds between them vibrating and whole molecules rotating.² Quantum mechanics takes this Heraclitean picture to be a matter of physical necessity: even at absolute zero there is a minimal random zero-point motion associated with the lowest possible energy state of a quantum-mechanical system. Whatever we say about structure must be consistent with this constant motion. My response to these issues will be to appeal to abstraction. To think about structure through change, we must attend to what is preserved across those changes, to what is shared across difference.

One can discern two distinct kinds of structure that chemists apply to substances: geometrical structure and bond structure (Hendry, 2016). *Geometrical structure* is simply the disposal of atoms or ions in space, or the attribution of geometrical relationships between them. It is attributed (for instance) in descriptions of the structures of crystals, such as common salt (sodium chloride), which crystallographers describe as being formed from sodium (Na⁺) and chloride (Cl⁻) ions close-packed so as to minimise the energy of the whole crystal (see Greenwood, 1968, chapter 1). Since the ions are in motion, they must be assigned *loci* rather than positions: small regions of space explored by their random motions. The size of these regions depends on temperature, and if the crystal is warmed up sufficiently the ions will acquire enough energy to overcome the forces holding them in the structure, which at that point will break down and be replaced by a liquid consisting mostly of dissociated ions. The liquid has geometrical

¹Note that this allows us to think of structure in two ways: inclusively, so as to include the parts, or more abstractly excluding them. Thus 'the structure of methane' might mean a carbon atom connected to each of four hydrogen atoms in a tetrahedral geometry or, abstracting away from the parts, it might mean just the connectivity plus the tetrahedral geometry, which methane shares with (for instance) silicon tetrachloride.

²The compositional relationship between substances and their parts at the molecular scale raises a separate problem: not only do relations among the parts undergo change; some of the parts themselves disappear and are replaced by others. As we shall see, this is a particular issue for liquid water.

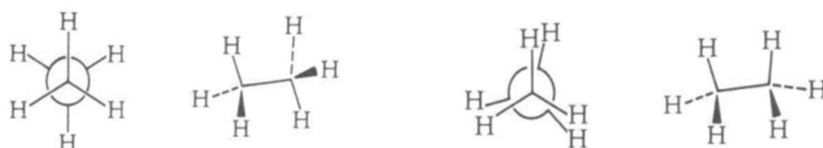


FIGURE 1 Newman and sawhorse projections of staggered and eclipsed ethane (from Bassindale, 1984, p. 50).

structure too, of a looser sort, which can be described statistically in terms of correlations between the positions of atoms or ions.

The second kind of structure that chemists attribute to molecules is *bond structure*. Historically, the need for a theory of bond structure arose in response to the phenomenon of isomerism, in which two or more distinct substances are formed from the same elements in the same proportions: were it not for isomerism, the elemental composition of a substance would be sufficient to identify it. For instance, ethanol ($\text{CH}_3\text{CH}_2\text{OH}$) and methoxy-methane (dimethyl ether, CH_3OCH_3) are both formed from carbon, hydrogen and oxygen in the ratios 2:6:1. Ethanol boils at 78.4°C , is widely used as a solvent and is an important component of certain drinks. Dimethyl ether boils at -24.9°C , and is sometimes used as an aerosol propellant. Because they are different substances, isomers must differ in the ways in which those elements are combined. Thus bond structure originally emerged as the hypothetical core of a detailed account of the different ways in which elements can be combined into compounds, building on the chemical atomism that had been proposed by John Dalton at the beginning of the nineteenth century (see Brock, 1992, chapter 4).³ The first theories of bond structure in chemistry, developed in the 1860s, were combinatorial: supposing that hydrogen can link to one other atom, oxygen two and carbon four and so on, how many different ways can a given set of atoms be connected together?⁴ These different ways would correspond to the possible isomers. At this earliest stage the atoms were not thought of as being arranged in space: that came later when, in the 1870s, structural theory was extended to account for optical isomerism (see Ramberg, 2003).

A bond structure is formed from pairwise relationships between atoms (bonds). The bond structure of an ethane molecule is simply two linked methyl groups, each consisting of a carbon atom linked to three hydrogen atoms ($\text{CH}_3\text{-CH}_3$). Now ethane molecules have a geometry too: the bonds around a carbon atom are roughly tetrahedral, with an angle between bonds of about 109° . If we imagine looking down the end of such a molecule along the axis of the carbon-carbon bond (this is called a Newman projection - see Figure 1), the two methyl groups might either be arranged such that the hydrogen atoms are staggered (offset) or eclipsed (aligned).

How does such a bonded structure move? According to Bassindale (1984, p. 25), ethane 'can be thought of in terms of two linked CH_3 propellers, with each CH_3 rotating rapidly'. The two methyl groups rotate around the bond between them, but the staggered configuration is of lower energy than the eclipsed one so the rotation is bumpy. The molecule explores the different geometrical configurations available to it (called conformations), rotating many millions of times a second. The different conformations are characterised by different geometrical relationships between the parts of the molecules, but the bond structure is a constant throughout, and prior, since it constrains which geometrical configurations are available. Interestingly, the bonded structure was first supported by complicated inferences based on the chemical behaviour of organic molecules (see above). The conformations

³Chemical atomism is the claim that the chemical elements are individuated by distinct species of atom. It should not be confused with earlier atomist theories, which made no direct connections between the identity of substances and species of atoms (see Hendry, 2020b; Klein, 1994; Roche, 1984).

⁴Mathematically minded readers will realise that such structures can be described in terms of undirected graphs. In fact, the early history of bond structure and graph theory were closely intertwined (see Biggs et al., 1976).

were added only later, when chemists began to think about how such bonded structures could be embedded in space (Ramberg, 2003). In the twentieth century, chemistry's close interaction with physics produced direct methods for accessing the structure of substances, including X-ray crystallography, and infrared, ultraviolet, mass, and nuclear magnetic resonance spectrometry. However, abstraction takes us from the multiplicity of conformations back to the simple bonded structure as 'the' structure of ethane, because this is what survives throughout the constant transitions between different conformations.

Before we move on to the next section, it is worthwhile taking stock and drawing a few consequences. I started with the idea of building something complex up from its parts. A structure is just the way this is done. We noted that chemists appeal to two different kinds of structure: geometrical structure and bond structure, involving different families of relations among chemical parts. Neither of these families of relations is plausibly regarded as being prior to the other (Hendry, 2016). Some substances, including such ionic crystals as solid sodium chloride, can be described without appeal to bonds between the constituent ions, which suggests that geometrical structure cannot be dependent on bond structure. But where a substance has both (e.g. ethane), bond structure can survive change in geometrical configuration, and even acts as a constraint on which geometrical configurations are possible. This suggests that in such cases the bond structure cannot be dependent on geometrical structure.

A principled way to deal with the incessant diversity and change is again via abstraction: to get a structure that persists over a longer timescale we attend to what they have in common. This is how we go from ethane's conformations to its bond structure. It is also how we can accommodate the fact that ethane (for instance) can exist in different states of aggregation (i.e. as a solid, a liquid and a gas). These are just different ways that ethane molecules come together under different conditions. What these states of aggregation share is being formed from ethane molecules. Allotropy, the phenomenon in which the same chemical element (e.g. carbon) can exist in different chemical forms (e.g. graphite and diamond), is dealt with in exactly the same way: they are the same element combined with itself in different ways.

The relativity of structure to scale, whether of length, time or energy, is another pluralistic feature of this dynamic picture. Consider ice, the H_2O molecules in which undergo vibrational, rotational and translational motions, the molecules vibrating much faster than they rotate or move through the lattice. At very short timescales (shorter than the period of vibration), the structure of ice is a snapshot in which the molecules are caught in mid-vibration. It will be disordered because different molecules will be caught at slightly different stages of the vibration. As the timescales get longer, the structure averages over the vibrational motions, and then (at yet longer scales) the rotational and translational motions. This yields successively more regular but diffuse structures (see Eisenberg & Kauzmann, 1969, pp. 150–152). Cyclobutadiene presents a more exotic example: the molecule is unstable except at very low temperatures, and the reasons why it presents different structures at different scales are quantum mechanical. Cyclobutadiene is a planar hydrocarbon with alternating single and double bonds. It tunnels between two distinct structures. Sampled at a lower (infrared) frequency, the molecule presents a square shape, which one might regard as an average over, or smoothing between, two distinct rectangular structures which can be sampled at higher (ultraviolet) frequencies. What is interesting is that, in order to describe this molecule, we need to appeal to more than one bonded structure (see Schoonmaker et al., 2018).

Another example of scale relativity concerns the sameness and difference of structures. Biphenyls are molecules consisting of two benzene rings attached by a single bond, about which the two rings rotate (see Figure 2).

If some of the hydrogens on each ring are replaced by other atoms or groups of atoms (shown as X and Y) then, if X and Y are bulky enough, they interfere with each other, restricting rotation around the single bond. This can give rise to a form of isomerism (atropisomerism) that only appears below a certain temperature, when the molecules no longer have enough energy to overcome the barrier to rotation around the single bond. At this point each molecule becomes trapped, in either configuration (a) or configuration (b). What was a single substance has now

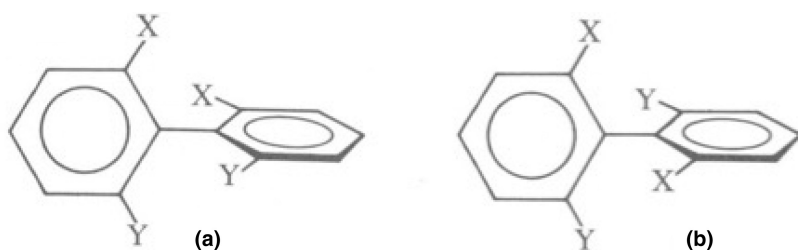


FIGURE 2 Biphenyl atropisomers, from Bassindale (1984, p. 58). Hydrogen atoms are omitted for clarity.

become two distinct and separable substances, distinguishable by their physical properties.⁵ The work of Louis Pasteur involves a similar case, but at the level where molecules compose substances. Pasteur showed that optical activity is a molecular phenomenon by manually separating crystals of the L- and D-forms of sodium ammonium tartrate, obtained from a racemic solution (an equal mixture of the two). Among chemists this is a famous example of structural explanation and its experimental demonstration, for the L- and D-forms are enantiomers. A very interesting fact is that, if Pasteur had attempted to separate the crystals at a higher temperature than he did, he would likely have failed: above 26°C the L- and the D-salts form a *single* racemate crystal (see Kauffman & Myers, 1975). Like in the case of the atropisomers, as temperature (or energy) increases, two distinct possibilities become one.

In summary, structures are abstractions from molecular species instantiating structural properties and relations over particular time, energy or length scales. 'Abstraction' suggests a mental operation: does this undermine realism about structure? Not if abstraction is a form of partial consideration, or selective attention (see Heil, 2003, p. 172), for we are selectively attending to genuine physical properties and relations such as charge, mass, and spatial proximity. Even if we are selecting, we are selecting only from among what is robustly real and physical. One final observation is that in the foregoing account there seems no reason to think of chemical structures as substantial forms, as in Aristotelianhylomorphism. In processes of structural change, structures themselves can be ephemeral. There is no need to see them as continuants, uniting the stages of a process into a whole. Structures *in chemistry* seem more like complex modes: ways for the parts of a whole collectively to be.

3 | DEFENDING MICROSTRUCTURAL ESSENTIALISM

Microstructural essentialism about chemical substances is the thesis that the structure of a chemical substance at the molecular scale is what makes it the substance that it is, and not another one. I will begin with some clarificatory remarks about this thesis.

Natural kinds are classes of thing or stuff about which it is possible to make reliable inductive inferences. Philosophical theories of natural kinds offer explanations of that possibility. Essentialism is a particular metaphysical explanation of that type, to the effect that there is a property shared by members of the kind the having of which is essential, in the sense that it is (at least part of) what makes them members of that kind and not another. A property being essential entails that (and therefore explains *why*), members of the kind necessarily have the property. Essentialism explains the possibility of reliable inductive inferences because

⁵The two distinct structures are enantiomers: mirror images that cannot be superimposed on each other. If molecule (a) rotates plane polarised light on one direction, molecule (b) rotates it in the opposite direction but to the same degree (*ceteris paribus*), which is why they are sometimes called 'optical isomers'.

possession of the essential property explains why members of the kind have many other properties associated with the kind.⁶

Microstructural essentialism is the claim that *microstructural* properties, i.e. features of the structure at the molecular scale, make a substance the substance it is. Microstructural essentialism may not apply to other natural kinds: it seems quite likely to me, for instance, that microstructural essentialism may provide the correct account of our ability to make inductive inferences about chemical substances, but not for biological species. For that reason I also defend metaclassificatory pluralism, the thesis that different philosophical accounts of natural kinds apply to different natural kinds. Philosophers sometimes declare themselves to be for or against essentialism about natural kinds *simpliciter*. To me this seems an odd thing to do: we should judge each case on the particular scientific facts relevant to it.

Some essentialists deny that there is any such *thing* as an essence. For instance, Lowe (2018) attributes to Locke the mistaken view that a hidden structure is a *thing* which could itself be a real essence. I take it that the danger of this kind of confusion is particularly severe in chemical examples. Consider the view that containing ethanol is (part of) what makes something whisky. Then consider the view that the ethanol in whisky is an active ingredient that enables that mixed substance to do what it does, and which could in principle be extracted. Dictionary definitions of 'essence' bear reading in terms of both the former (i.e. drawing on technical uses of 'essence' developed by metaphysicians) and also the latter (more like a quintessence). Neither, I take it, implies the other. Relatedly, Oderberg (2011) argues that it is a confusion to see essences as properties. Now there is, I will argue, a (complex structural) property the having of which is essential to water,⁷ but that claim need not entail that that complex structural property is 'the essence' of water in any other sense. I assume that the essentialism I sketch here, and which I take to be a fairly standard one, need not be viewed as committing either of the errors identified by Lowe and Oderberg.

A last clarification point concerns chemical substances. Chemical substances are natural kinds of stuff, but not every natural kind of stuff is a chemical substance: some stuffs are mixtures of different chemical substances, and their chemical composition—that is, the chemical substances they contain—may vary. Thus, for instance, milk and wool are stuffs that are produced by particular biological species, and may have particular functions. Their chemical composition varies, depending on the genetic background and environment of the particular organisms producing them. Microstructural essentialism about chemical substances does not imply microstructural essentialism about these other kinds of stuff. In fact, given their compositional variability, microstructural essentialism about milk and wool seems highly implausible. Chemists may well investigate the chemical composition of particular samples of milk or wool, but chemistry is not the discipline that decides what counts as milk or wool.

Putting these points together, it is clear that some criticisms of microstructural essentialism in chemistry fail to hit the mark, because they base criticisms of essentialism on non-substances. Thus for instance LaPorte (2004, chapter 4) has criticised microstructural essentialism on the basis that jade has no single microstructure. However, the term 'jade' is not used by chemists; jade is not a chemical substance but a gemstone; and jade's chemical constitution is variable. Hence it belongs with milk and wool, outside the scope of microstructural essentialism about chemical substances. Havstad (2018, section 6) uses concrete and other mixtures as part of a criticism of the version of microstructuralism I developed to cover the case of water (see below), but her argument makes the assumption that mixtures are a kind of chemical substance. In fact mixtures having a variable composition disbars them from being substances: they are less confusingly thought of as being composed of multiple chemical substances. Acidity is a different kind of case, for 'acid' is surely a chemical category. Stanford and Kitcher (2000) argue that there is no microstructural essence for acidity, but think mistakenly that this is relevant to a broader critique of essentialism in chemistry. I would summarise the case of acidity as follows: from the late eighteenth century until the early twentieth century, chemists considered and

⁶Other accounts of natural kinds provide quite different explanations of this possibility. Applied to biological species, for instance, homeostatic property cluster (HPC) accounts explain similarities between members of a species via homeostatic mechanisms including environmental selection and breeding between members of the species.

⁷Some metaphysicians also worry about whether complex structural 'properties' can be genuine properties (see for instance Heil, 2003), but that is a different worry.

abandoned various hypotheses that could have supported essentialist claims about acidity. Given that series of failed hypotheses, one might view acidity instead as a syndrome: a kind of chemical *behaviour* rather than a kind of chemical *substance* (see Finston & Rychman, 1982, chapter 1). Even if microstructural essentialism fails for acidity, that failure has no tendency to undermine essentialism about (for instance) the chemical elements.

I find strong support for the microstructural part of microstructural essentialism in three immanent arguments drawing on the practice of chemistry, concerning (i) the centrality of structure at the molecular scale to chemical classification and nomenclature, and the complete absence of any *non*-microstructural criteria; (ii) the role of microstructure in explaining and predicting the chemical and physical behaviour of substances, and (iii) the fact that no other systematic basis for individuating substances is consistent with chemical practice, and the epistemic interests that underlie it. I will develop those three immanent arguments in turn.

The case for microstructuralism is particularly strong in the case of the chemical elements. Since 1923, the International Union of Pure and Applied Chemistry (IUPAC) has quite explicitly identified nuclear charge as what characterises each chemical element (see Kragh, 2000; van der Vet, 1979). I have argued that the historical record supports realism about the elements as natural kinds, because the IUPAC change reflected a discovery (Hendry, 2006, 2010a). I correspondingly disagree with LaPorte (2004, chapter 4), who has argued that, prior to the twentieth century, it was indeterminate whether the names of the chemical elements referred to classes of atoms which are alike in respect of their nuclear charge, or to classes of atoms alike in respect of their atomic weight, or to classes of atoms alike in both respects. For LaPorte, IUPAC's 1923 decision had the character of a stipulation. I think it is quite natural to see the extensions of the names of the elements as being determinate before 1923, and IUPAC's identification as simply the recognition of determinate membership (see Hendry, 2006, 2010a). Silver, which has been known since ancient times, always consisted of roughly equal mixtures of two isotopes of silver (^{107}Ag and ^{109}Ag), differing in respect of their atomic weight. (That is, unless some miracle occurred changing the isotopic composition of silver.) What makes those diverse atoms count as silver is what they share, namely their nuclear charge (47), a property that explains why these diverse atoms behave in chemically very similar ways. The twentieth-century identification of nuclear charge as what individuates the elements was a discovery of this fact, rather than a stipulation or a convention.

There are good grounds for extending microstructuralism to *compound* substances, because the rules for chemical nomenclature that IUPAC has developed over the years are based entirely on microstructural properties and relations. Consider for instance 2, 4, 6,-trinitrotoluene, better known as trinitrotoluene, or TNT (see Figure 3).

For the purposes of nomenclature this compound, which was first synthesised in the nineteenth century, is regarded as a derivative of methylbenzene (toluene): counting clockwise from the methyl ($-\text{CH}_3$) group at position 1, there are three nitro-groups ($-\text{NO}_2$) at positions 2, 4 and 6, replacing three hydrogen atoms (conventionally the remaining hydrogen atoms at positions 3 and 5 are left out for clarity). Evidently, TNT is named purely on the basis of its bond structure. Now it is true that there are alternative ways of generating names for compounds (see Leigh

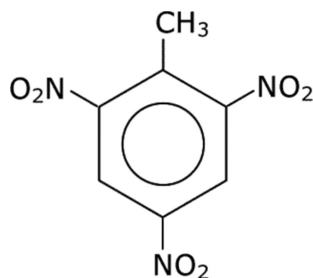


FIGURE 3 2, 4, 6,-trinitrotoluene, or TNT.

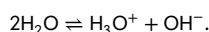
et al., 1998), but IUPAC's various systems of nomenclature are all based on microstructure. This important fact has escaped the attention of the critics of microstructural essentialism in chemistry.

A second immanent argument for microstructuralism concerns explanation. Understanding the chemical behaviour of a compound substance—its chemical reactivity—is a matter of understanding how its structure transforms into the structure of other substances under various conditions. This involves the study of chemical reaction mechanisms, which break such transformations into series of steps, starting from the reagent structures and ending with the product structures (see Goodwin, 2012; Hendry, 2017b). Similarly, understanding the physical behaviour of a substance, including its melting and boiling points and its spectroscopic behaviour, is a matter of understanding how, given their structure, its constituent molecules interact with each other and with radiation respectively.

A third argument for microstructuralism concerns the fact that no other group of properties provides a systematic framework for naming and classifying substances, or understanding their behaviour, that is consistent with chemical practice. What are the alternatives? Needham (2011) has argued that classical thermodynamics provides macroscopic relations of sameness and difference between substances, acknowledging that his macroscopic perspective is revisionary of current chemical practice, in that it divides substances more finely than chemists do. On Needham's view, different isotopes of the same element are distinct substances even though chemists lump them together when thinking about the elements. Moreover he describes IUPAC's identification of nuclear charge as what characterises the elements as a 'convention' (Needham, 2008, p. 66). I think that is too thin a description, and historically misleading. The adoption of nuclear charge was a considered choice, reflecting the *discovery* that the elements occur in nature as mixtures of different isotopes. The names of the elements *as they were currently being used* had been *discovered* to refer to populations of atoms which are alike in respect of their nuclear charge, while diverse in respect of their weight. The identification of nuclear charge as what characterises the elements was therefore simply a recognition of the real basis of the periodic table (see Hendry, 2006, 2010a). Further objections to Needham's thermodynamic criteria are provided by other examples. Orthohydrogen and parahydrogen are spin isomers of the hydrogen molecule that readily interconvert on thermal interaction: in orthohydrogen the spins are aligned, while in parahydrogen they are opposed. Orthohydrogen and parahydrogen count as different substances on the thermodynamic criteria. The same holds for populations of atoms in mutually orthogonal quantum states, such as the two streams of silver atoms emerging from a Stern-Gerlach apparatus. A natural conclusion is that Needham's proposed thermodynamic criteria for sameness and difference of substance track differences of physical state, without regard for whether those differences correspond to distinctions of chemical substance (for detailed discussion see Hendry, 2010b).

I believe that these three immanent arguments together constitute a strong positive case in favour of taking microstructuralism to be the prevailing classificatory ideology of the discipline of chemistry, and also that chemistry's adoption of it is well motivated as a natural 'carving' of chemical reality. Before I move on to arguing for the more robustly metaphysical claim of microstructural *essentialism*, it's worth responding to a common objection to microstructuralism: that the molecular heterogeneity of water undermines microstructuralism because it resists microstructural analysis.⁸

Like many other substances water is heterogeneous at the molecular scale, which is ironic, given that the slogan 'water is H₂O' has been so central to discussions of the microstructural essentialism associated with Saul Kripke and Hilary Putnam. In liquid water H₂O molecules self-ionise, forming hydronium (H₃O⁺) and hydroxyl (OH⁻) ions:



The proportion of water molecules that do this is small but significant, and they also form themselves into oligomolecular chains that explain water's physical properties. Water is a good electrical conductor, for instance, because excess electrical charge at one end of such an oligomolecular chain can be transferred to the other end in a concerted mechanism, without any material particles having to make that journey. Moreover the equilibrium between

⁸See Needham (2000, 2002), Havstad (2018), Häggqvist and Wikforss (2018). Lively debate on the example of water continues: see Hofer and Martí (2019) and Raatikainen (2021) on the essentialist side; Häggqvist (2022) against.

H₂O molecules, hydronium and hydroxyl ions and oligomolecular chains is dynamic: all these items are constantly disappearing and being replaced by new ones. This means that the molecular-scale parts of water are constantly changing.

I would resist the rather sweeping responses that some philosophers make in response to this example. One misguided response is to reject the identity of water and H₂O as scientifically illiterate and outdated: according to the critics, twentieth-century physical chemistry has shown that things at the molecular scale are more complicated than can be captured by the simple formula 'water is H₂O'! But this heterogeneity is not sufficient reason to reject microstructural essentialism. What, exactly, is the form of argument? Water is complex at the molecular scale *therefore* it is not H₂O? What, exactly, is water supposed to be instead? Chemists know just what liquid water is made of at the molecular scale: dynamic congeries of H₂O molecules interacting together, a process which involves some of them going out of existence. Rather than a sweeping rejection of the identity, I suggest that we think carefully how to construe the identity so that it is consistent with the science. This is a project on which I have been engaged for some time (see Hendry, 2006, 2017a).

Paul Needham and Jaap van Brakel have argued that water the macroscopic substance is distinct from its constituents at the molecular scale (see Needham, 2000, 2002; van Brakel, 2000, chapter 3). I have a lot of sympathy with this claim, but it is consistent with microstructural essentialism. We can still identify (for instance) liquid water as the macroscopic substance to which H₂O molecules give rise. Elsewhere (2006) I have developed a *productive* view of the relationship between a molecular species and the substance of which it is characteristic, one that is consistent with both the molecular heterogeneity of water and the unique place that the H₂O molecule has in chemists' conceptions of what makes something water. The first step is to correct the hidden assumption that identifying water as H₂O involves the claim that water is simply a collection of H₂O molecules. This claim has been made by both critics and friends of 'microessentialism'. Duhem (2002, p. 86) and Timmermans (1941, chapter 8) criticised the closely related thesis of chemical atomism on the grounds that it must characterise pure chemical substances as collections of qualitatively identical atoms or molecules. Hilary Putnam identified the extension of 'water' as 'the set of all wholes consisting of H₂O molecules' (Putnam, 1975, p. 224). Now unlike Needham and van Brakel, I would admit mereological sums of H₂O molecules as quantities of water. Mereological composition is, after all, composition. But physical chemistry tells us that not every quantity of water is a mereological sum of water molecules, because some of them are diverse molecular populations. So let us dispense with the molecular homogeneity requirement. Chemical substances can sometimes be regarded as collections of molecules with the same structure (the different [solid, liquid and gas] states of ethane for instance) but water, we must admit, is more complex. When its characteristic molecules come together and interact, some of them are used up in the process. Water must therefore be what you get when H₂O molecules are brought together and interact. Note that if we allow transworld variation in the processes through which these molecules interact, we can recover the intuition, associated with Kripke and Putnam, that neither the appearance nor the behaviour of a substance are metaphysically necessary: in nomologically different worlds H₂O molecules might interact quite differently, yielding water with quite different appearance and behaviour.

This last point allows microstructural essentialism to issue its own challenge to Needham's macroscopic view of water. If Needham is correct, and chemical substances are characterised by their thermodynamic similarities and differences from other chemical substances, it is difficult to see how the identity of a chemical substance can be pulled apart (even in thought) from its thermodynamic behaviour. But this is just what chemists seem to allow. For example, chemistry textbooks describe the boiling points of ammonia, water and hydrogen fluoride (NH₃, H₂O and HF, respectively) as 'abnormally high' (Cotton & Wilkinson, 1988, p. 91), 'unexpectedly high' (Gray, 1994, p. 205) and 'anomalously high' (Greenwood & Earnshaw, 1997, p. 53) in comparison to those of the hydrides of the other elements in relevant groups of the periodic table. The explanation for the departure from the expected behaviour involves hydrogen bonding, which is a stronger kind of interaction than the weaker van der Waal's interactions that occur between (for instance) hydrogen sulphide

molecules (see Hendry & Rowbottom, 2009 for the example).⁹ An obvious way to construe comments such as these is that, were it not for the hydrogen bonding, ammonia, water and hydrogen fluoride would melt and boil at much lower temperatures than they actually do. But this kind of counternomic claim would be nonsense if the actual thermodynamic behaviour were metaphysically necessary. Microstructuralism is compatible with water's thermodynamic behaviour being metaphysically contingent. In contrast, Needham's proposal for a macroscopic view of chemical substances, in which thermodynamic behaviour is part of what makes a substance the substance that it is, has a harder task in this respect. The macroscopic view would surely take the actual thermodynamic behaviour as necessary, holding it fixed in counterfactual contexts (or more importantly counternomic contexts, as above). What else is to be kept fixed in a counternomic context, to anchor thinking about what *water* would do, if facts (or laws) were slightly different? For this reason I do not think that Needham's proposal is consistent with the way that chemists think about the identity of substances: chemists hold structure fixed and allow thermodynamic behaviour to vary.

How do we go from microstructuralism about chemical substances to microstructural essentialism about chemical substances? This is a pertinent question because some philosophers of science are wary of essentialism about classification even if they admit the centrality of microstructure (see for instance Bursten, 2014). I think we can get to microstructuralism, but that we should avoid the linguistic route widely associated with Putnam (1975). The idea of the linguistic route is as follows: the names of chemical substances such as 'gold' and 'water' are used in ordinary language, and have extensions. Chemists have examined what falls within these extensions, finding gold to be the element with atomic number 79, and water to be H_2O . I am sceptical about this route to microstructural essentialism for two kinds of reason. One problem is that chemists did not simply investigate the extensions of ordinary-language substance names. The route to those chemical discoveries was more complicated, involving conceptual clarification along the way. This makes it harder to say that the chemists are investigating the same things as non-scientific folk talk about. Moreover it seems implausible that the names of many substances, as used in ordinary language, have extensions at all, because they are used in too many mutually incompatible ways (for both points see Hendry, 2012). A second problem concerns the claim that water's microstructure is what makes it the substance it is. The linguistic route is unsatisfying in this respect: we say, in effect, that scientists have checked the extension of 'water' and found H_2O there. That is true enough, but chemists have identified many other properties that water has. Why aren't these equally good candidates for being essential? In this vein, Needham might ask why it is not the thermodynamic behaviour of water rather than its microstructure that makes it what it is. Similarly, van Brakel (2000, p. 109) challenges the microstructural essentialist to say why it is the atomic number of krypton (36) that makes it the element that it is, rather than (say) its ground-state electronic structure or its spectroscopic behaviour.

These are good questions, but I think the microstructural essentialist has good answers to them. Drawing on my earlier answer to Needham, the thermodynamic behaviour of water is not necessary to it, because chemists consider the behaviour of water in counternomic contexts in which it behaves differently. The same applies to van Brakel's candidates. A deeper answer is that the microstructure is causally upstream from these other properties. Water's molecular structure is part of the reason why it has the thermodynamic behaviour it has, but the converse is not true. Similarly, gold's atomic number being 79 is part of the reason why its ground-state electronic structure and spectroscopic behaviour are what they are, and the converse is not true. The microstructure is what grounds the behaviour, but not vice versa. A separate argument draws on chemistry's interest in synthesis. When chemists make some gold they bring into being something with the atomic number 79, and when they make water they bring into being a population of interacting H_2O molecules. Note that in defending essentialism this way I am basing it not on language, but rather on causal priority and production (which is, after all, what synthesis is).

⁹The two kinds of bonding are closely related. Hydrogen bonding arises between molecules with permanent dipoles (asymmetrical charge distributions), whereas van der Waal's forces arise when random fluctuations in an atom's or molecule's charge distribution give rise to dipoles in its neighbours, and resultant attractive forces between them.

4 | EXISTENCE AND COMPOSITION IN CHEMISTRY

The most enduring philosophical question about chemical combination is the Aristotelian problem of mixture (see Wood & Weisberg, 2004). Aristotle rejected the atomist account of chemical combination, because in his view it could not distinguish between a true chemical combination of elements from a mere mixture of them. Atoms would retain their existence and identity across chemical change, so processes of combination could not amount to anything more than a reshuffling of atoms. How could this result in anything more than a very intimate mixture of the elements? Aristotle concluded that elements cannot survive true chemical combination, during which they must disappear and be present in the product only *in potentia*, in the sense that there are processes of separation that will regenerate them (see Needham, 2006, 2009). The problem of mixture raises two distinct, but complementary ontological questions: one concerns whether, and under what conditions, something can enter into a more complex whole while itself persisting, rather than being 'used up' in the process; a second question concerns whether, and under what conditions, a collection of objects *whose persistence is assumed* can form a new complex whole.

Modern chemistry gives qualified support to atomism on the first question. Elements are regarded as surviving in their compounds, an assumption that has underwritten a research programme into the composition of substances since before Lavoisier (see Hendry, 2021b). Yet chemical combination between elements is more than a mere juxtaposition of their atoms. Atoms are known to be complex, consisting of electrons and nuclei, and quantum mechanics regards electrons as being either transferred or shared as part of the process of combination. The survival of the nuclei underwrites the survival of elements across chemical change, but the pooling of electrons means that, if we follow a body of matter through the process of combination followed by separation, we can recover the 'same' elements only to a limited extent (the limitation is not merely an epistemic one). Some sodium and some chlorine combine to form salt, and the same weights of the two elements can be recovered, but the quantities of elemental matter before and after will not be the same: we recover the same nuclei, not the accompanying electrons (for detailed discussion of these points see Needham & Hendry, 2018).

The second ontological question raised by the problem of mixture is what van Inwagen (1990) has called the 'special composition question' (hereafter SCQ). Following van Inwagen, many discussions of the SCQ apply a rather abstract classification of possible answers. The SCQ asks when (i.e. under what conditions) a group of things forms another thing. We might answer 'always,' 'sometimes' or 'never': these answers correspond respectively to universalism, moderation and nihilism about composition. Chemistry seems to care about the SCQ: undergraduate courses and textbooks on theoretical chemistry show how quantum mechanics provides a simple contrastive explanation for why the hydrogen molecule (H_2) exists, while the helium molecule (He_2) does not (see for instance Atkins, 1986, pp. 379–380). The H_2 molecule exists because it is of lower energy than two separate hydrogen atoms, and so is stable with respect to separation. This is not true of He_2 , which is unstable with respect to separation. Note that neither universalism nor nihilism are promising as models for composition in chemistry because they are not set up to provide contrastive explanations of existence, for they take exactly the same stance towards every composite object. For that reason I set those two kinds of position aside and turn to moderate answers to the SCQ (for more extended discussions of the SCQ in chemistry, and the different kinds of answer, see Hendry, 2020a, 2021a).

McKenzie and Muller (2017) respond to the SCQ as follows: '[Physical] objects form a composite object iff these physical objects interact and are in a common bound state, where 'common bound state' means that the composing objects are in the potential well that results of their mutual physical interaction (McKenzie & Muller, 2017, p. 234). This is a moderate answer, as befits one that draws on an empirical science such as physics, and moreover it fits the contrastive explanation of the existence of H_2 versus the non-existence of He_2 . The answer is not yet complete however: the parts of a (putative) composite object being in a potential well is insufficient to entail that it really hangs together robustly. We can see the problem if we return to the example of He_2 . The above discussion is incomplete, for it leaves out the much weaker van der Waals' forces,

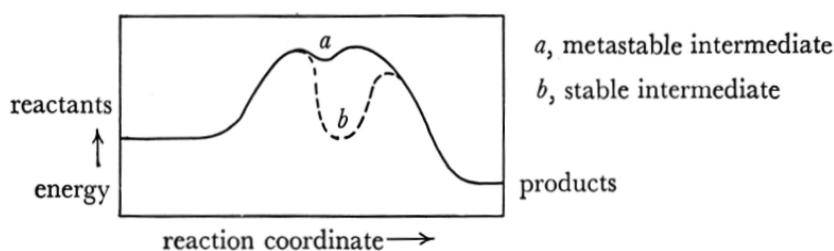


FIGURE 4 Energy profiles for reactions proceeding through intermediates, from Gould (1959, p. 130).

which arise between the randomly fluctuating electronic charge clouds of atoms and molecules. Imagine two helium atoms approaching each other: as they do so, their charge clouds will mutually adjust, giving rise to spontaneous attractions between them. As the two atoms get really close, the overall interaction between them will come to be dominated by repulsion between their nuclei, and the atoms will rebound. The van der Waals' forces are present, and give rise to a potential well, but one which at room temperature is too shallow to constrain the relative motions of the two helium atoms. Close to absolute zero, however, the two atoms are unlikely to have enough thermal energy to escape this shallow well: they are trapped. I would say that the helium dimer exists when the two cold atoms meet (this is confirmable by the singular physical behaviour of helium at very low temperatures). In the warmer case, the potential well is a shallow dip in an energy landscape traversed quickly, like a rut in the road. The two warmer atoms briefly being in the potential well that results of their mutual physical interaction is therefore insufficient for them to compose a dimer. McKenzie and Muller do not address this issue in their discussion, partly because they speak of a composite object's parts being 'trapped' in a potential well, which they refer to as a 'bound state.' But saying that the system is 'bound' or 'trapped' is simply helping ourselves to the modal language that needs to be explained. What does it take to be trapped in a potential well? How long does the complex entity need to reside in it? The answer to that question requires that we address the dynamics of existence. I believe chemistry has the resources to do this.

Chemical reactions involve one or more structures (the reactants) transforming into one or more different structures (the products; for discussion see Hendry, 2017b). Intermediate structures are often formed during chemical reactions, which are typically less stable and more shortlived species than the reactants and products. They are often too unstable to be isolated. However, even if that is true, distinctions can be made among them (see Figure 4). A *metastable* intermediate (*a*) is more of a dip in the path from reactants to products than a distinct existence, like the room-temperature helium dimer. A *stable* intermediate (*b*), in contrast, may be detected spectroscopically: the energy dip corresponding to its stability is deep enough for the species to go through a few cycles of its typical vibrations, because at the furthest point of each vibration there is a strong enough restoring force pulling the parts back into their equilibrium position. In Aristotelian terms one might say that the existence of (*b*) is robust enough for it to display one of its characteristic powers (absorbing and emitting radiation at characteristic frequencies), which is how it can be detected. The restoring force is what explains both the stability of the species and its ability to vibrate. The explanation is scale-relative, because it depends on the size of the energy dip, and it is kind-relative because the powers (to vibrate and therefore to absorb or emit radiation) are typical of the species.

These insights furnish us with a response to a conceptual conundrum in chemistry. As atomic nuclei get heavier, they tend to become less stable, and their lifetimes correspondingly shorter.¹⁰ This trend comes to a head with the superheavy elements (SHEs), including oganesson (Og, with atomic number 118) the most recently discovered of them. The nuclei of SHEs are so unstable that they pose some interesting questions. In a recent book,

¹⁰In fact there is a peak of stability around the middle of the periodic table: an isotope of iron (⁵⁶Fe, or iron-56), is the most stable nuclear species, as measured by the binding energy per nucleon (nucleons being the constituents of nuclei, i.e. protons and neutrons).

Helge Kragh (2018) explores some of the historical issues around credit for the discovery of SHEs: what experimental proof is required? In an accompanying paper (Kragh, 2017), he argues that SHEs put pressure on the very concept of a chemical element: as we have seen, IUPAC individuates elements in terms of nuclear charge, but some chemists worry that the existence of a nucleus with a particular charge is not necessarily sufficient for the existence of the corresponding element. An element must have a chemistry (that is, a set of typical reactions and compounds), but SHEs are too short-lived for that.

Now a term like 'superheavy element' seems somewhat vague, but as Kragh points out (Kragh, 2017, p. 9), in practice it refers to elements whose atomic number is above 103. What is so special about this class of elements? They are very heavy compared to other nuclear species; they do not occur naturally; they tend to be very unstable, and have correspondingly short lifetimes; for any given space in the periodic table, such elements might be merely possible existences, rather than actual existents. I think that Kragh raises an interesting philosophical question: how is it possible that a sample of a nuclear species has been brought into existence, yet this does not entail that there exists a chemical element corresponding to this species?

Here is what I take to be a plausible answer to that question (for further detail see Hendry, 2020a): a nucleus can be said to exist when its lifetime is long enough for it to be detected in a high-energy experiment in which nuclei of some kind are bombarded with particles of some other kind (typically other nuclear species). The energy scales at which these interactions occur (gigaelectron volts, or GeV) are very high compared to those at which the interactions governing chemical reactions typically occur (involving electrons and nuclei). This entails that the nuclear reactions occur much more quickly than the chemical reactions. Hence a nuclear species may come into existence and quickly decay into a different species before it could possibly have had time to acquire a stable electronic structure. If the lifetime of a nuclear species is in the femtosecond range (i.e. 10^{-15} s), while the time it would take for electrons to relax into a stable electronic structure corresponding to a neutral atom might be of the order of picoseconds or nanoseconds (10^{-12} s or 10^{-9} s), then the existence of the nucleus may be thousands or millions of times too brief to allow the formation of a neutral atom with a determinate chemistry. Thus there can be nuclear species that live long enough to be detected but which *cannot*—owing to their own instability—live long enough to have a stable and determinate electronic structure. So in some important sense they cannot have a chemistry. If they cannot have a chemistry, then they cannot be chemical elements. The point is not merely that these nuclei lack electrons. The same is true of α -particles, which are ${}^4\text{He}$ (helium-4) nuclei without any electrons. Despite lacking electrons, α -particles clearly have a chemistry. It is that of helium, associated with the stable electronic structure they *would* have if they were supplied with electrons.

Overall, I would argue that the above discussion of existence and composition in chemistry supports a broadly Aristotelian view of composition: bringing some things together results in the formation of a new complex whole when that process brings with it distinct additional powers and susceptibilities. The difference between the hydrogen and helium dimers, and the stable and metastable intermediaries, was not only that the stable complexes were tightly enough bound, but also that the binding *ipso facto* brought with it characteristic powers (of the complex species to vibrate at typical frequencies and absorb or emit light of particular frequencies). Moreover the stability and the exertion of typical powers have the same explanation. Turning now to the foundational question about the existence of superheavy elements, the kind-relativity of existence was expressed most interestingly in the contrast between oganesson the nuclear species and oganesson the element. Oganesson the nuclear species lives long enough to display some of its typical powers: to interact with radiation in characteristic ways, and thereby be detected. According to microstructural essentialism, oganesson the element can exist only if its characteristic nuclear species do, but their existence is not sufficient: they would have to exist long enough to allow it to display *its* characteristic powers. These include chemical powers requiring its characteristic atoms to have stable electronic structures. This requirement they cannot meet because, as a matter of physical necessity, their nuclei transform into other nuclear species too quickly. Hence oganesson the element does not exist even though its characteristic nuclei do exist, because they live too briefly for it to display the powers typical of being an element, that is, having a particular chemistry. This echoes the distinction drawn by van Brakel and Needham

between a substance and its constituent species at the molecular scale, and shows that even a microstructural essentialist can accommodate that distinction.

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ORCID

Robin Findlay Hendry  <https://orcid.org/0000-0002-1043-5177>

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