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Emergence and Reduction in Science. A Case Study

Alexandru Manafu
The University of Western Ontario

Supervisor
Dr. Robert Batterman
The University of Western Ontario

Graduate Program in Philosophy

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EMERGENCE AND REDUCTION IN SCIENCE.
A CASE STUDY

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by

Alexandru Manafu

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CERTIFICATE OF EXAMINATION

Supervisor	Examiners
Dr. Robert Batterman	Dr. Sandra Mitchell
Supervisory Committee	Dr. Marc-André Lachance
Dr. Gillian Barker	Dr. Gillian Barker
Dr. Christopher Smeenk	Dr. Christopher Smeenk

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Alexandru Manafu

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Abstract

The past decade or so has witnessed an increase in the number of philosophical discussions about emergence and reduction in science. However, many of these discussions (though not all) remain too abstract and theoretical, and are wanting with respect to concrete examples taken from the sciences. This dissertation studies the topics of reduction and emergence in the context of a case study. I focus on the case of chemistry and investigate how emergentism can help us secure the autonomy of this discipline in relation to the underlying microphysics. I develop an account of emergence (called *functional emergence*) that is, I argue, capable of answering the question of why we have chemistry instead of just applied quantum mechanics. I argue that functionally emergent properties in chemistry – properties that are defined by their behaviour, not by some shared microphysical constituent – can help us defend the autonomy of chemistry; they allow for the existence of *sui generis* chemical regularities, which can be used in *sui generis* chemical explanations. Functional emergence generates difficulties for some accounts of inter-theoretic reduction, but unlike other theories of emergence it is compatible with weaker forms of reductionism.

Keywords: emergence, reductionism, ontological autonomy, functional properties, constitutive properties, functional kinds, multiple realization, physics, chemistry, special sciences, micro-reduction, functional reduction, chemical properties, chemical laws, chemical explanations.

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Chapter 1

Introduction

1.1 The question

If all there is consists of the kinds of entities that microphysics talks about, why do we have sciences other than microphysics? This thesis is an attempt to answer a question of this sort. But why should this question even be taken seriously, let alone be considered worthy of investigation? What are the *prima facie* motives for asking it in the first place?

There are two motives for asking this question. First, there is an *ontological* motive, which rests on the asymmetry between the objects that form the subject matter of microphysics and the objects that form the subject matter of the other sciences (the special sciences). The asymmetry is this: if all the objects that form the subject matter of microphysics (elementary particles, fields, etc.) were to vanish, there would be nothing left; the objects that form the subject matter of the special sciences (molecules, organisms, etc.) will also vanish. They will necessarily disappear, for they are composed of the kinds of entities that microphysics talk about. However, if the objects that form the subject matter of the special sciences were to vanish, the objects that form the subject matter of microphysics may persist (e.g., as plasma).

This asymmetry results simply from the direction of the composition relation: the objects that form the subject matter of the special sciences are composed of the objects that form the subject matter of microphysics, but not viceversa. As a result, the latter may exist even in the absence of the former.

In this narrow and precise sense then, the microphysical has ontological primacy. This prompts the following question. If one had a complete science of the microphysical (i.e., a complete inventory of all the microphysical entities and properties, and the laws governing them) couldn't one just deduce the claims made by the special sciences? This is the other motive underlying the question formulated at the beginning, and I will call it the *epistemological* motive.

As it stands, the question formulated above is too general. If the question is to be investigated in detail, it needs further specification. I will specify the question by referring to a couple of specific sciences that are usually perceived as adjacent, such as quantum mechanics and chemistry. Our question then becomes: If the entities forming the subject matter of chemistry consist of the kinds of entities that quantum mechanics talks about, why do we have chemistry instead of just applied quantum mechanics? I will call this *the specific question*, to distinguish it from the more general question from which it arises. This goal of this thesis is to investigate the specific question, and argue for a certain way of answering it.

The prospects of deducing all of the claims made by the special sciences from microphysics appears to threaten the autonomy of the special sciences. For example, if all chemical truths are obtainable from quantum-mechanical truths, then how can the belief in the autonomy of this discipline be maintained? What justifies belief in *chemical* properties, or belief in *chemical* truths? What justifies the belief that there are *chemical* explanations? Are there even such things as *chemical* properties, truths, or explanations as opposed to merely complicated quantum-mechanical properties, truths, or explanations?

Confronted with these sorts of questions, the defender of the autonomy of chemistry may appeal to a variety of possible reasons that would legitimize her position. In the next section I will discuss some of these reasons and briefly evaluate their ability to help us answer the specific question.

1.2 Tentative answers

This section will give a brief presentation and evaluation of the several ways in which an answer to the the specific question could be attempted. It is meant to offer a bird's eye view of the tentative answers and to cursorily expose some of their perceived weaknesses. So why do we have chemistry instead of just applied quantum mechanics?

1.2.1 Historical autonomy

One tentative answer may be this: we have chemistry instead of just applied quantum mechanics for the same reason we had chemistry long before the 20^{th} century when quantum mechanics was discovered. This kind of answer, which points to the fact that historically chemistry has been independent from physics, supports the idea of a historical autonomy of chemistry in relation to physics. This view has been advocated C.D. Broad, among others. Broad remarks that chemistry had become a science "of great extent and certainty" long before we had any mechanistic insight into the internal make-up of the elements. He argues that for a long time, progress in chemistry was possible without using any mechanistic assumptions. He concludes that the possibility of mechanistic explanation is not essential to the progress of chemistry.

> "If then chemistry can be a scientific subject and can make steady progress without using the assumption that a mechanistic explanation of chemical phenomena is possible, it would presumably have made precisely the same progress if in fact no such explanation had been possible." (Broad 1925, p. 74).

While I agree with Broad that progress in chemistry happened long before modern mechanistic explanations of chemical phenomena became available, it is also true that the mechanistic insights that became available in the 20^{th} century have allowed for a great expansion of our chemical knowledge. They allowed us to understand the chemical reactions that we knew about, and to design new reactions. They allowed us to synthesize new molecules, and even new elements, and to design and create new drugs and materials. In other words, chemistry would not have made precisely the same progress if quantum mechanics had not been discovered, although for a long time its own progress was independent from the progress of physics.[1] Therefore, the autonomy of chemistry in relation to physics cannot be based solely on the notion of historical autonomy, which is also only partially defensible.

1.2.2 Methodological autonomy

Another answer to the specific question may be this: we have chemistry instead of just applied quantum mechanics because the methods of chemistry are different from the methods of physics. In general, a chemistry lab looks very different from a physics lab and what goes on in a chemistry lab is different from what goes on in a physics lab. One may respond to this by saying that while physics and chemistry differ with regard to their methodologies in general, the methods of some branches of chemistry are in fact physical in nature. For example, the bond length and angles of molecules are determined using various types of spectroscopy. Spectroscopy is used in physical and analytical chemistry to identify the composition of substances or to assess the concentration of a given chemical species; computational methods that make use of quantum mechanics are used to determine the structure of compounds. Although in general the methods of chemistry and physics are quite different, this does not demonstrate that chemical properties are not physical properties in disguise. That is, *methodological* autonomy – if it obtains – is not tantamount to *ontological* autonomy. I will say more about what ontological autonomy requires in the last section of this introduction, but for now I will just say that chemistry and physics may have different methods of learning about their subject matter even if the subject matter of the former is coextensive with a part of the subject matter of the latter.

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[1] Broad's views will be discussed in more detail in the section on the British emergentist view of chemistry.

1.2.3 Antireductionism

Another tentative answer may be this: we have chemistry instead of just applied quantum mechanics because chemistry does not reduce to quantum mechanics. There are several accounts of reduction, and three of the most important ones will be discussed in detail in chapter 4. For now, I will say that chemistry would reduce to quantum mechanics if one could deduce all chemical truths from the truths of quantum mechanics. But this has not been achieved yet. Many kinds of difficulties stand in the way of such deductions:

i) Chemical terms that don't have a quantum-mechanical reference: chemical bond (Primas 1983), chemical structure (Woolley 1978), orbital (Scerri 1991, Scerri and McIntyre 1997, Post 1974)

ii) Computational difficulties: analytical solutions to the Schrödinger equation can only be obtained for hydrogenic atoms (Scerri 1991; 1994, Scerri and McIntyre 1997)

iii) Appeal to approximations and idealizations: Born-Oppenheimer approximation (Hendry 2006), Hatree-Fock (Scerri 1994; 2004)

iv) Appeal to heuristic ingredients for which we don't really possess a quantum-mechanical justification: Madelung rule (Löwdin 1969, Scerri 2003), Pauli exclusion principle (Hall 1986, Scerri 1995)

The difficulties of reducing chemistry to microphysics mentioned by (ii), (iii) and (iv), are, of course, troublesome for those who deny that chemistry is autonomous from microphysics. But they do not guarantee the ontological autonomy of chemistry from physics, as opposed to only methodological, epistemic or pragmatic autonomy. Rather, they reveal problems with *carrying out* the reduction. Unless we conflate epistemological, methodological or pragmatic matters with ontological matters, these difficulties do not conclusively demonstrate that chemical properties are not in fact merely (complex) physical properties. The fact that we cannot derive all chemical truths from physical truths does not mean that these truths are not so derivable in principle (say, by more powerful beings, or by more clever mathematical techniques). In fact, the success of computer-aided *ab initio* methods in chemistry seems to point to the opposite.

As regards the chemical terms mentioned in (i), issues are more complicated. Such terms pose more than a practical difficulty for reductionism. For if there are chemical truths containing terms that don't have a quantum-mechanical (or microphysical) reference, it is hard to see how these truths could be derived from the truths of microphysics. Faced with this situation, those who would deny the autonomy of chemistry have no other option but to deny that these terms have a reference. In other words, they would be hard pressed to be eliminativists about the chemical terms mentioned in (i). They may argue that terms like "chemical bond", "chemical structure", or "orbital" are useful metaphors which are didactically and pragmatically helpful, but in reality they lack a reference. This could be true for the terms mentioned in (i). For example, the eliminativist could point out that the term "orbital", does not have *per se* a physical interpretation; only the product between the amplitude of a wavefunction with its own complex conjugate corresponds to an observable. Perhaps the eliminativist could find similar arguments for the other terms mentioned in (i). However, this leaves open the possibility of there being specific chemical terms that although lack a unique microphysical reference, do nonetheless refer to observable macro-properties (chemical properties). Chapter 3 will consider this possibility. It will be argued that some chemical terms do not have a (single) microphysical reference, yet they do have a *chemical* reference which is observable at the macro-level.

1.2.4 Internal realism

Another tentative answer may be this: we have chemistry instead of just applied quantum mechanics because chemistry is ontologically autonomous from quantum mechanics; this is because there is a plurality of ontologies, none of which is privileged with respect to the others.

Lombardi and Labarca (2005, 2006) have attempted to ground the ontological autonomy of chemistry in a philosophical position called *internal realism* (Putnam 1981). According to internal realism, the question “What objects does the world consist of?” only makes sense to be asked within a conceptual scheme (or theory). On this view, objects depend on theories in a strong sense, which includes existence. In the view of the two authors mentioned, internal realism leads to ontological pluralism; ontological pluralism, in turn, justifies the ontological autonomy of chemistry. In a schematic form, the argument leading to ontological pluralism is this:

1. An ontology is always relative to a conceptual scheme.

2. There exists a plurality of conceptual schemes that apply simultaneously to the same portion of reality.

3. Therefore, there exists a plurality of ontologies.

This argument aims to endorse the idea that there are as many ontologies as there are theories, all equally legitimate. But if that is the case – Lombardi and Labarca suggest – there is a physical ontology and there is a chemical ontology, and none of these two ontologies is privileged with respect to the other. The ontological autonomy of chemistry would thus be secured.

However, there is an ambiguity with respect to the first premise of the argument schematized above. There are two ways in which premise 1 could be interpreted. On one interpretation, premise 1 says that there is no theory-independent ontology. In other words, there is no privileged (or “God’s eye”) point of view which enables us to see ontology “as it really is”, independently of our conceptual schemes. On a second interpretation, premise 1 says that every conceptual scheme brings in its own ontology; as Lombardi and Labarca put it, “different conceptual schemes *define* different ontologies” (2005, p. 138, my italics).

These two interpretations are not equivalent. It is possible to accept the first interpretation and reject the second. But for the conclusion of the argument to follow, the second interpretation is required. However, one may legitimately doubt that if interpreted according to the second interpretation, premise 1 is true. Contrary to what Lombardi and Labarca believe, it could be argued that not every conceptual scheme defines its own ontology. For example, if two conceptual schemes (theories) are related in a certain way (so that one *reduces* to the other), is it really required to postulate two ontologies, one for each theory? If the properties and laws of a theory can be shown to be reducible to the properties and laws of another theory, why couldn't we dispense with the ontology stipulated by the reduced theory in favor of the ontology stipulated by the reducing theory? Of course, there may be good pragmatic reasons for keeping both theories. If working within the reducing theory alone makes calculations or predictions needlessly complicated, we could, of course, hold on to the reduced theory for its instrumental value. But we need not be committed to its ontology as well. I would like to illustrate this with an example, but I am aware that uncontroversial examples of inter-theoretic reduction might not exist. If one accepts (for the sake of the argument) that Newton's mechanics reduces (in the philosophical sense) to Einstein's, the following example could be given to illustrate my point. Despite being superseded by Einstein's theory, we still use Newton's theory, but we do not continue to believe its ontology (absolute space and time, gravity as a force, etc). Rather, we use Newton's theory for its instrumental value, not as a guide to our ontology. Why couldn't we say the same thing about chemistry? Even if chemistry turns out to be just applied quantum mechanics, we may keep the conceptual scheme of chemistry for its instrumental value alone. In order to conclude that the existence of a plurality of conceptual schemes allows for a plurality of ontologies, one needs to argue that all conceptual schemes are equally legitimate and logically independent from one another. But that, obviously, need not be the case. In particular, if one conceptual scheme can be deduced from another, the claim that the two conceptual schemes bring in two distinct ontologies becomes problematic.

Suppose, however, that the argument schematized above is sound, and Putnam's internal realism does lead to ontological pluralism. If so, the conceptual schemes of physics, respectively chemistry, bring in two ontologies – that of physics and that of chemistry. Lombardi and Labarca's tacit assumption is that ontological pluralism automatically secures the ontological autonomy of chemistry. Notice however, that the fact that physics and chemistry have their own ontologies tells us nothing with respect to how those ontologies are related. It only tells us that the entities, properties and regularities of chemistry exist (and so do those of physics). But this claim is compatible with what some philosophers have called *retentive* reduction (e.g., Churchland 1979). Again, examples from science may be controversial, but here's one. Even if we accept that thermodynamics reduces to statistical mechanics, we may continue to think of temperature and pressure as real. Thus, we may keep the ontology of thermodynamics but deny that this ontology is irreducible to that of statistical mechanics. Here's another example, perhaps less controversial: the fact that a table reduces to a collection of atoms arranged in a certain way does not make it less worthy of existence; it's just that the table has a derived, or secondary existence; reduction need not be *eliminative*.[2]

To conclude, I am not convinced that Putnam's internal realism can, all by itself, secure the ontological autonomy of chemistry. At most, it may be able to secure *an* ontology for chemistry, but an argument is needed for the claim that this ontology is autonomous in relation to that of physics.

1.2.5 Emergentism

Another tentative answer to our question may be this: we have chemistry instead of just applied quantum mechanics because chemistry is ontologically autonomous from quantum mechanics; this is because the entities, properties, and regularities (laws) of chemistry are emergent.

Nowadays many philosophers of science agree that reductionism as a philosophical program has not succeeded. The philosophical accounts of inter-theoretic reduction encountered theoretical and practical difficulties. It has been argued that examples of successful inter-theoretic reductions in science are few and far between. As regards chemistry, many have expressed doubts that a complete reduction of this discipline to physics can be had. On the other hand, nowadays almost everyone is a metaphysical naturalist (at least

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[2] For the distinction between retentive and eliminative reduction see Churchland (1979). For the claim that the reduction of chemistry to atomic physics is an example of a retentive reduction see Ney (2008).

about the domain of chemistry). Chemists and philosophers alike contend that our world does not contain vitalistic chemical essences, spooky chemical souls, or chemical entelechies. They agree that if all the elementary entities that microphysics talks about were to vanish, there would be nothing left. This is sometimes referred to as "the generality of microphysics" – all events are, or are exclusively composed out of parts which are, microphysical events, and so fall under microphysical laws (Pettit 1993, p. 217). I will use the terms "generality of microphysics" and "physicalism" interchangeably: both terms refer to the notion that every thing (or at least every thing in the purview of the natural sciences) ultimately consists of the kinds of entities that physics (or microphysics) talks about and that there are no vital substances, entelechies, etc., occurring at any stage of complexity.

It is hard to miss the apparent tension between the two claims made in the preceding paragraphs. If chemical stuff is composed of nothing else except microphysical stuff, how can one justify the belief that there are even such things as *chemical* properties, truths, or explanations as opposed to merely complex quantum-mechanical properties, truths, or explanations? Given the generality of physics, how can the autonomy of chemistry be preserved in a substantial way, i.e., how can chemistry be considered autonomous in a way which goes beyond historical or methodological autonomy? If physicalism is true, can we even speak of the ontological autonomy of chemistry, as opposed to a merely historical or methodological autonomy?

Some philosophers thought that the said tension is only *prima facie.* According to the emergentists, all objects are composed – at their most fundamental level – of microphysical objects; however, some hold that it would be a mistake to conclude from this that all properties are physical properties; similarly, it would be a mistake to think that if all events are governed by physical laws, then all laws must be physical. Emergentists hold that there are chemical entities, properties, and laws that depend on, but do not reduce to physical entities, properties and laws.[3]

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[3] The term "law" could be used in two ways. It could be used to refer to a regularity in nature. Or it could be used to refer to the linguistic form expressing that regularity (a

"Emergence" is a philosophical term of art, with a lot of appeal to philosophically inclined scientists, including chemists. However, the meaning of this term often remains underarticulated and vague. A prominent contemporary philosopher writes:

> "The term "emergence" seems to have a special appeal for many people; it has an uplifting, expansive ring to it, unlike "reduction" which sounds constrictive and overbearing. We now see the term being freely bandied about, especially by some scientists and science writers, with little visible regard for whether its use is underpinned by a consistent, tolerably unified, and shared meaning" (Kim 2006).

I don't think that the use of the term "emergence" is or should be reserved exclusively to philosophers. Also, I am quite skeptical that a unified meaning can be achieved for this term, even amongst philosophers. But I do think that studying how philosophers have thought about emergence in chemistry can help us answer the specific question. That is, if it can be shown that chemistry somehow emerges out of physics then – given the right account of emergence – one could perhaps give a satisfactory answer to the question of what justifies the autonomy of chemistry in relation to the underlying physics.

As Kim noticed, emergentist positions vary from one author to another and therefore emergentism is hard to pin down. However, there are a number of features that many emergentist positions share. Virtually all emergentist positions hold some form of the view that that the world consists of a hierarchy of levels or ontological *strata* (the physical, the chemical, the biological, the psychological) and each level depends on the previous level but it is irreducible to it. Properties at a certain level interact to produce properties at a higher level (emergents). The relation between the lower level and the higher level is usually thought to be supervenience: higher level properties are said to supervene on the lower level properties.[4] These higher level properties

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sentence). I will use the term in both ways, its meaning being determined by the context.

[4] A set of properties H supervenes on a set of properties L if and only if (i) any two

(emergents) arise from those at the lower level, but they cannot be predicted on the basis thereof. Emergents are often deemed to have novel causal powers, i.e., they have the capability to produce effects in a way that cannot be anticipated. Sometimes emergents are said to be capable of downward causation – the ability to influence the basal conditions from which they arise (the underlying dynamics). Also, sometimes it is held that emergents involve global rather than merely local properties, and thus they arise only when the basal conditions are characterized by a certain amount of complexity. Therefore in relation to the entities from which they arise, emergents are usually characterized as novel, irreducible, unpredictable/unexplainable on the basis of the lower level theory, and on some views, capable of downward causation.

Typically, emergence is correlated with some sort of failure of reduction. Depending on how one construes irreducibility, one ends up with different types of emergence. On the classical account of reduction due to Nagel (1961), one theory is irreducible to another if the laws of the higher level theory cannot be deduced from those of a more fundamental theory by employing bridge laws connecting the two levels. For example, if there are chemical truths that cannot be predicted (deduced) from quantum mechanics together with the requisite bridge laws, one would say that chemistry is irreducible to quantum mechanics. However, the notion of predictability is ambiguous; it may refer to predictability in principle or to predictability in practice. If we hold a strong notion of predictability (i.e., predictability in principle) then we end up with strong emergence: chemistry cannot be reduced to quantum mechanics even in principle. If we hold a weaker notion of predictability (i.e., predictability in practice) then some weaker version of emergence obtains; in this case, we would say that chemistry is weakly emergent – chemistry cannot be in practice reduced to physics.

In chemistry, the following have been considered emergent or irreducible: chemical compounds, molecules, secondary properties of compounds such as

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objects x and y that have the same L properties will necessarily have the same H properties (though not necessarily viceversa), and (ii) any two objects z and w that differ in their H properties will also differ in their L properties (though not necessarily viceversa).

their taste and colour, temperature, phases of matter, phase transitions, the shape of the molecules, atomic structure and properties, periodicity, aromaticity, chemical bond, chemical structure.[5]

1.3 What is needed?

A satisfactory answer to our specific question would have to argue for the existence of *sui generis* chemical properties and laws (regularities), which could be used in *sui generis* chemical explanations. By *sui generis* chemical properties, regularities and explanations I mean properties, regularities and explanations that are not identical to (possibly complicated) quantum-mechanical properties, regularities and explanations. The existence of *sui generis* chemical properties and regularities would make chemistry not only historically and methodologically autonomous from physics, but also ontologically.

The idea of the ontological autonomy of chemistry may seem incompatible with the generality of physics. After all, if all chemical entities are composed of nothing else except microphysical entities, doesn't this mean that the ontology of chemistry reduces to the ontology of physics? However, this argument is construes ontology in a restricted way, as referring exclusively to entities. Ontology is concerned not only with entities, but also with properties and laws (regularities). If one distinguishes between a *property* and its *instances* as one should, the fact that every instance of a chemical property is composed of nothing else except instances of microphysical properties does not mean that all chemical properties are in fact microphysical properties in disguise.[6] Similarly, it would be a mistake to think that if all events are governed by physical laws

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[5] For a list of chemical notions that are not amenable to a rigorous quantum mechanical treatment (and thus to reduction) see van Brakel (2000, p. 132).

[6] The distinction made in metaphysics between properties and property instances is usually illustrated with an example like the following. The color red (redness as such) is a property (property-*type*) whereas the redness of my car is an instance of that property (property-*token*). The color of my car is an instance of color red, but it is not identical with it (redness as such will continue to exist even if the redness of my car disappears). For a more comprehensive account of the distinction between properties and instances, see e.g., Swoyer and Orilia (2011).

then all laws must be physical. Although the entities that chemistry talks about are composed of nothing else except microphysical entities, this leaves open the possibility of *sui generis* chemical properties and laws. But if that is the case, there is a sense in which one can talk of the *ontological* autonomy of chemistry. It must be admitted, however, that this ontological autonomy is not radical: if the entities that microphysics talks about were to vanish, there would be nothing left; consequently, there would be no chemical properties, no laws relating these properties, and no explanations employing those laws. However, the fact that the ontology of chemistry depends on the ontology of microphysics does not make the former a subdomain of the latter.[7]

After a brief overview of the various ways in which an answer to the specific question could be attempted, emergentism seems to offer the most promising answer. If it can be shown that chemical properties and regularities are emerging in some sense out of the underlying microphysics then we have a natural answer to the specific question, and chemistry could be thought of as an ontological *stratum* different from the microphysical one.

The purpose of this thesis is to articulate an emergentist account of chemistry that can justify the idea that there are *sui generis* chemical properties and regularities – in other words, an emergentism that preserves the ontological autonomy of chemistry.

1.4 Overview

Chapter 2 critiques some historical and contemporary accounts of emergence in chemistry. I start out with British emergentism, for which the paradigmatic example of emergence was that of chemical compounds. The first section of chapter 2 discusses the views of J.S. Mill (1806-1873) and C.D. Broad (1887-1971) and it investigates whether their views of chemistry are still viable today. In section 2.2 I present and critically assess the "fusion" account of emergence due to Humphreys (1997b, 1997a, 2008), who views covalent bonding as a "core example of fusion emergence" (2008, p.7). The last section of chapter

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[7] For an argument that physicalism does not entail reductionism see Fodor (1974).

2 discusses briefly other emergentist views in chemistry, such as those due to Hendry (2006) and Luisi (2002), but also other views about emergence in science, such as those due to Bedau (2008), Wimsatt (2000, 2008), Mitchell (2010) and Batterman (2002, 2011).

Chapter 3 develops a theory of emergence that is best equipped to provide a satisfactory answer to the specific question. I call this theory "functional emergence". Functional emergence is a departure from the traditional accounts of emergence in that it is committed to the generality of microphysics and does not recognize the existence of non-physical forces. Nonetheless, I will argue, functional emergence is strong enough to justify the idea that there are *sui generis* chemical properties, laws and explanations. The first two sections of chapter 3 are more theoretical, as they introduce an important distinction, that between constitutive and functional properties. Constitutive properties are higher level properties that are in fact identical with certain lower level properties; functional properties are higher level properties that cannot be identified with particular lower level properties. Sections 3.2 and 3.3 are the most technical parts of this dissertation, but also some of the most important. They argue that a number of properties in chemistry, including acids, bases, metals, oxidants, reductants and piezoelectrics are in fact functionally emergent. These are *sui generis* chemical properties that appear in *sui generis* chemical laws, which can be used to provide *sui generis* chemical explanations. The laws in which these properties appear are "indiscriminate" or "promiscuous" in the sense that they express relations between higher level properties, but do not discriminate between (or are insensitive to) the various ways in which those properties are constituted at the lower level. Such properties and regularities ground the ontological autonomy of chemistry.

Chapter 4 examines what the existence of functionally emergent chemical properties entails with respect to the much discussed reduction of chemistry to physics. It present three prominent accounts of inter-theoretic reduction, namely that of Nagel (1949, 1961), that of Kemeny, Oppenheim and Putnam (1956, 1958), and that of Kim (1999, 2005). It is argued that the existence of terms which refer to functionally emergent properties poses problems for the first two accounts, while the third account does not succeed in establishing the kind of reductionism that would endanger functional emergence and the ontological autonomy of chemistry.

Chapter 5 addresses the objections that can be brought against the thesis of multiple realizability, which is an important tenet of functional emergence. This chapter responds to four criticisms that imperil the multiple realizability thesis itself or its efficacy as an anti-reductionist strategy. I critique the arguments provided by Kim (1992, 2010), Shapiro (2005), (Smart 1963) and others. I also give a unitary voice to a concern that many authors including Millikan (1999), Boyd (1999) and Shapiro (2000) share, and label this "the analyticity objection". With the help of examples of chemical functionally emergent properties such as acidity or piezoelectricity, I argue that some of these criticisms do not pose a threat to functional emergence, while the others do not succeed.

Chapter 6 presents the conclusions. It summarizes the most important results of this thesis and argues why the functionalist view of chemistry counts as an emergentist view. I end with some speculations regarding the disciplinary character of chemistry and the validity of the layered view of the world.

Chapter 2

Accounts of emergence in chemistry

2.1 The British emergentist view of chemistry

In recent years, the work of the British emergentists received an increased amount of attention from authors concerned with emergence and reduction in all disciplines, but especially in the philosophy of mind. While it is true that one of the main motivations for the development of what it has been called "the theory of emergence" was to account for the existence or appearance of secondary qualities such as colours and odours (which seem resistant to a purely mechanistic explanation), for most British emergentists the paradigmatic example of emergence was that of chemical compounds. The purpose of this section is (i) to examine and make explicit the British emergentist view of chemistry as the primary example of emergence, and (ii) to investigate whether this view of chemistry could still be upheld today, after more than eight decades of scientific developments in this field. The section will focus mainly on C.D. Broad (1887-1971), as this author's work is considered representative for the current of thought that came to be know as British emergentism and his discussion of chemistry is more ample than that of any other author in the same current.

2.1.1 Broad's view of chemistry

In chapter II of *The Mind and its Place in Nature (1925),* Broad is concerned with the question of whether the apparently different kinds of material objects and their behaviour are irreducibly different. For example, are living things irreducibly different from non-living things in their behaviour? Of course, as the title of Broad's work reveals, Broad's main concern is the mind and how it can be accommodated within a purely naturalistic framework. However, as Broad himself acknowledges, one is much more likely to elucidate this problem if one considers first similar questions about simpler cases of apparently irreducible behaviour. And one of the simplest cases we find is that of chemical compounds. Chemical behaviour appears markedly different from purely mechanical behaviour; substances which interact chemically behave in a very different way from those which merely hit each other, like billiard balls. What can account for such behaviour? Broad considers two competing theories: the theory of emergence, and the mechanism theory.[1]

The mechanism theory attempts to explain all phenomena (including chemical phenomena) by appeal to a very narrow set of elements. Ideally, such a theory will postulate:

(i) a single fundamental kind of stuff, capable of

(ii) a single fundamental kind of change, governed by

(iii) a single elementary causal law which acts between pairs of particles, which is subject to

(iv) a single principle or law of composition.

If a theory satisfies all these conditions it is called Pure Mechanism. As an example of a theory which is very close to this mechanistic ideal, Broad mentions classical mechanics. Mechanics is very close to having a single fundamental kind of stuff (i.e., mass), capable of a single fundamental kind of change (i.e.,

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[1] Broad also considers a third possibility, the theory of a special component, which he dismisses.

change of positions), governed by a single elementary causal law which acts between pairs of particles (e.g., gravity) and which is subject to a single principle or law of composition (i.e., vector addition). Broad admits that a theory can diverge from this ideal and still be mechanistic. For example, a theory that recognizes mass and charge as fundamental can still be called mechanistic, although will not be "pure".

One characteristic of an ontology obeying the mechanism theory is that the behaviour of the aggregates of particles depends only on the forces acting between pairs of such particles – the law that governs the aggregates is quite independent of the configurations and surroundings in which the constituent particles happen to find themselves. On the mechanist view, the properties of the whole are completely determined by the properties of its parts and their relations. Therefore, the behaviour of the whole could, in principle, be deduced from a sufficient knowledge of of how the parts behave in isolation or in other wholes, plus their relations in the whole they form. Mechanical systems like a set of billiard balls or artificial machines are good examples of wholes to which the mechanistic theory applies. For example, a clock is a system whose behaviour can be deduced from the particular arrangement of its parts (spring, wheels, pendulum, etc.) and from the laws of mechanics which apply to all mechanical systems in general (even to those that are not clock parts).

On the other hand, if a system is emergent, its properties cannot be predicted from a knowledge of the properties of its constituents taken separately or in other wholes, and of their proportions and arrangements in this whole. According to Broad, chemistry "seems to offer the most plausible example of emergent behaviour" (Broad 1925, p.65). If chemical compounds are truly emergent, the only way to learn about their properties is to study samples. It is worth emphasizing that, according to Broad, this limitation does not arise because of the lack of sufficient computational resources or limited knowledge of the initial conditions.

> "If the emergent theory of chemical compounds be true, a mathematical archangel, gifted with the further power of perceiving the microscopic structure of atoms as easily as we can perceive hay-

> stacks, could no more predict the behaviour of silver or of chlorine or the properties of silver chloride without having observed samples of those substances than we can at present." (Broad 1925, p. 71)

In fact, according to Broad, not only that we cannot predict the properties of chemical compounds on the basis of the properties of their constituents, but we cannot even predict that two elements would combine chemically with each other (i.e., chemical affinity).

What stands in the way of such predictions? If one knows the properties of silver and those of chlorine and the laws that govern them, and has perfect knowledge of the microscopic structure of atoms and their relations, then – given the infinite computational abilities of a mathematical archangel – it would seem that one must be able to deduce the properties of silver chloride. If one cannot do this, what stands in the way of such deduction? According to Broad, the answer has to do with the fact that the law connecting the properties of the molecule of silver chloride with those of the atoms of silver and chlorine is "so far as we know, *an unique and ultimate law*" (Broad 1925, p. 65). By this, Broad means that it is not a special case which arises through substituting certain determinate values for variables in a general law which connects the properties of any chemical compound with those of its separate elements and with its structure. Such laws, which connect the properties of entities at adjacent orders (in this case the law connecting the properties of atoms to those of molecules) are called by Broad *trans-ordinal* laws.[2] According to Broad, those trans-ordinal laws which cannot be understood as instances of a more general law are indicative of emergence. For example, in the case of silver chloride, the law connecting the properties of silver and chlorine atoms with the properties of the silver chloride would be a trans-ordinal law of an emergent type, since this law connects entities at two adjacent levels (atomic level, respectively the level of the compound) and cannot be understood as a special case of a more general law – according to Broad, this law is an *ultimate*

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[2] By contrast, an intra-ordinal law would be one which connects the properties of aggregates of the same order.

law.

Broad contrasts this state of affairs with that where a mechanistic explanation is possible. In such cases (e.g., a clock), the behaviour of a whole can be predicted using the general laws of mechanics and vector addition – principles that govern the behaviour of the springs and wheels even before they are assembled together to form the clock. By contrast, in chemistry – according to Broad – the properties of an as yet unexamined compound cannot be predicted from a knowledge of the properties of its elements in isolation or from a knowledge of the properties of their other compounds.

As Broad himself acknowledges, those favoring the mechanism theory will feel that there is something radically unscientific and superstitious about trans-ordinal laws. But Broad attempts to dissolve this feeling. He remarks that chemistry had become a science "of great extent and certainty" long before we had any mechanistic insight into the internal make-up of the elements. He argues that for a long time, progress in chemistry was possible without using any mechanistic assumptions. He concludes that the possibility of mechanistic explanation is not essential to the progress of chemistry.

> "If then chemistry can be a scientific subject and can make steady progress without using the assumption that a mechanistic explanation of chemical phenomena is possible, it would presumably have made precisely the same progress if in fact no such explanation had been possible." (Broad 1925, p. 74).

In addition, Broad does not see anything mysterious or unscientific about the trans-ordinal laws. In his view, a trans-ordinal law is as good a law as any other; once it has been discovered empirically it can be used like any other law in science; we may use it to make predictions, to suggest experiments, or for practical purposes. The only thing that is peculiar about such laws is that they cannot be deduced beforehand from the laws governing entities at a lower level.

Why does Broad think that the law connecting the properties of the molecule of silver chloride with those of the atoms of silver and chlorine is unique and ultimate? In the chapter discussing mechanism and its alternatives, Broad claims that this state of affairs can be ascribed either to (i) the existence of innumerable "latent" properties in each element, each of which is manifested only in certain conditions, or (ii) to the lack of any general principle of composition, such as the parallelogram law in dynamics, by which the behaviour of any chemical compound could be deduced from its structure and from the behaviour of each of its elements in isolation (Broad 1925, p. 66-67).

If the first alternative is correct, then emergence differs from mechanism in that the law that governs the behaviour of a compound is sensitive to the configurations its constituents. On this view, the configuration of the constituents forming a compound play a crucial role in determining the properties of the compound. But is this the distinguishing characteristic of emergence? Mechanism also recognizes the fact that configurations are important. In a system of gravitating particles, the behaviour of the whole will depend in part on the configuration in which the particles happen to find themselves. What then is special about the configurations of the components of an emergent system – in this case, a chemical compound? According to McLaughlin's interpretation of Broad, an emergent whole possesses force-generating properties of a sort not possessed by any of its parts (McLaughlin 2008, p. 41). The forces generated by the configurations of particles (which are distinct from the particle pair forces present in mechanism) are called by McLaughlin *configurational forces*.[3] These are forces which arise in a compound only when the components are arranged in certain select configurations, but not in others. On McLaughlin's interpretation, configurational forces are *fundamental* – they are new forces, forces that are not the resultants of any other forces, such as forces that previously existed in the components.

According to McLaughlin's interpretation of Broad, configurational forces in chemistry are higher-order *chemical* forces characterizing the compounds, irreducible to lower level *physical* forces characterizing the components. Nonethe-

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[3] Although Broad does not use this term, McLaughlin interprets Broad in this way. According to McLaughlin, "it is clear that he [i.e, Broad] maintains that certain structures of chemical compounds can influence motion in fundamental ways" (McLaughlin 2008, p. 47).

less, configurational forces are genuine forces; like all forces, they influence "the go of events"; using a more recent terminology, they are capable of downward causation. In fact, they are the forces responsible for the characteristic behaviour of the chemical compounds, i.e., their ability to bond or react – what Broad calls the "ultimate characteristic" of the chemical order. In McLaughlin's interpretation of Broad, configurational forces are what makes possible the existence of emergent behaviour. On this view, the emergent trans-ordinal laws indicate the existence of chemical configurational forces.[4]

If the second of the two previously mentioned alternatives is correct, then chemistry lacks a general principle of composition similar to vector addition that exists in classical dynamics (mechanism's postulate iv). On this view, one cannot learn about the properties of a compound by substituting certain values of the variables in a general law which connects the properties of that compound with those of its constituents, for there is no such general law. This would explain why the trans-ordinal laws that connect the properties of the atoms with those of compounds are *unique* and *ultimate*. They are *ultimate* because in determining the properties of a chemical compound there is no theoretical shortcut, one must study a sample. However, as Broad himself grants, there is no doubt that the properties of silver chloride are completely determined by the properties of silver and the properties of chlorine, in the sense that whenever we have a whole composed of these two elements in certain proportions and relations we have something with the characteristic properties of silver chloride, and that nothing has these properties except a whole composed in this way (Broad 1925, p. 64). Therefore, one may argue that in producing AgCl, nature does follow some rule of composition. Broad's response would be that this rule of composition is not *general* – according to Broad, by studying the rule nature follows when it produces AgCl one cannot learn anything about the rule nature follows when it produces other compounds. In this sense, the

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[4] There is a complication here. Both atoms and molecules are chemical species. Therefore, chemistry will contain at least two types of trans-ordinal laws. There will be trans-ordinal laws connecting the properties of subatomic particles with those of the atomic elements, and there will be trans-ordinal laws connecting the properties of atomic elements with those of molecules they form.

chemical trans-ordinal laws are *unique*.

2.1.2 Evaluating Broad's account of emergence in chemistry

Is the doctrine of configurational forces on which Broad bases his emergentism compatible with the scientific theories that we currently have? Are there any configurational forces, especially in chemistry?

McLaughlin responds negatively to the second question. According to McLaughlin, the fall of British emergentism was caused by advances in science.

> "[Q]uantum mechanical explanations of chemical bonding in terms of the electro-magnetic force, and the advances this led to in molecular biology and genetics render the doctrines of configurational chemical and vital forces enormously implausible" (McLaughlin 2008, p. 49)

I agree with McLaughlin that quantum-mechanical explanations of chemical bonding in terms of the electromagnetic force render the doctrines of configurational chemical and vital forces implausible. In what follows, I will consider three key statements that Broad makes about chemistry, and then I will examine whether these claims could still be upheld today, after more than eight decades of scientific developments in physical chemistry. The three claims are:

1. It is impossible to predict the properties of a chemical compound on the basis of the properties of the components.
2. Chemical affinity cannot be predicted.
3. In chemistry we lack a general principle of composition, such as the parallelogram law in classical dynamics.

To these three claims, one may add a fourth. According to McLaughlin's interpretation, Broad's emergentism is committed to the existence of chemical configurational forces.

Does chemistry lack a general principle of composition, such as the parallelogram law in classical dynamics, by which the behaviour of any chemical compound could be deduced from its structure and from the behaviour of each of its elements in isolation? Admittedly, if we apply the laws of classical physics to atomic or molecular systems, we get predictions that are incompatible with the observations. This was the situation that the scientific community faced around 1911 when trying to understand the structure of hydrogen – a situation that most certainly Broad knew about. As it happens, if the atom obeys the laws of classical physics, the electron orbiting the nucleus will emit radiation, since it is an accelerating charge. This means that the electron will rapidly loose its kinetic energy and it will spiral down into the nucleus.[5] Therefore, classical physics (in which the forces are subject to vector addition) cannot explain the behaviour of atoms and molecules they form. Since the behaviour of atoms and molecules is part of the subject matter of chemistry, Broad could have been right in thinking that chemistry lacks a general principle of composition similar to the one we have in mechanics.

However, as we now know, it is not true that the entities that form the subject matter of chemistry obey classical mechanics, in which the dynamical law is Newton's second law. But from this does not follow that these entities do not obey a principle of composition similar to the law of parallelogram in dynamics. Chemical compounds are complex quantum-mechanical systems. In the formulation of quantum mechanics developed by Dirac and von Neumann, the possible states of a quantum-mechanical system are represented by vectors in a Hilbert space associated with the system. A vector space is a mathematical structure in which the entities (vectors) are subject to operations such as vector addition and multiplication. The entities that form the subject matter of chemistry, insofar they obey quantum mechanics, are sub-

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[5] If the electron-nucleus distance was originally on the order of an angstrom, it will become zero in $t = 10^{-10}$s.

ject to vector addition. To illustrate vector addition in quantum chemistry, consider an electron of an atomic element. When one calculates the electron's total angular momentum, one treats the electron's orbital angular momentum L and its internal angular momentum S as vectors and adds them using vector addition. Of course, in this context, vectors are subject to quantization. Nonetheless, the entities that form the subject matter of chemistry do obey the sort of compositional principle Broad thought chemistry is missing.

But perhaps this is not what Broad meant when he claimed that in chemistry we lack a general principle of composition. What he had in mind, perhaps, was something along the lines of his predecessor, J.S. Mill. In *A System of Logic,* Mill distinguishes between two modes of causation: a *mechanical mode* and a *chemical mode.* In the mechanical mode of causation, the effect produced by two causes acting together is *the sum* of the effects of each cause acting independently. Mill calls this the principle of Composition of Causes, which in his view, just like in Broad's, is akin to the principle of composition of forces in classical dynamics. On this mode of causation, the effect of the two causes acting in conjunction can be predicted deductively, from the effects of separate causes acting separately. The chemical mode of causation, on the other hand, does not obey the principle of Composition of Causes.

> "The chemical combination of two substances produces, as is well known, a third substance, with properties different from those of either of the two substances separately, or of both of them taken together. Not a trace of the properties of hydrogen or of oxygen is observable in those of their compound, water." (Mill 1882, p. 267)

In Mill's view, chemical compounds have properties that are not "the sum" of the properties of their components taken separately or simply juxtaposed, as in a mixture. Besides the example of water, Mill gives additional examples: the sweet taste of sugar of lead (lead diacetate, $Pb(C_2H_3O_2)_2$) is not the sum of the tastes of its component elements, acetic acid and lead or its oxide; the color of blue vitriol (copper sulfate, $CuSO_4$) is not a mixture of the colors of sulfuric acid (transparent) and copper(II) oxide (black), from which it is produced. Those effects whose properties do not resemble the properties of their causes are called by Mill *heteropathic*; the laws governing the production of these effects are called heteropathic laws. For Mill, the laws of chemistry are heteropathic, since they govern the production of substances whose properties do not resemble those of the reagents.

If this is what Broad had in mind, then he was right: the properties of chemical compounds are not "the sum" of the properties of their components. But why should we expect them to be? A deductive explanation of the properties of chemical compounds in terms of the properties of their atomic constituents could still be possible even if the manifest properties of these compounds are not "the sum" of the manifest properties of their components. For Mill such an explanation was out of sight, but Broad contended that this may be due to a limitation of our present state of knowledge.

Was the impossibility of chemical prediction that Mill and Broad talked about due to a limitation of their present state of knowledge? I join McLaughlin in thinking that the answer is affirmative. Today's theoretical chemists have managed to determine the properties of a number of molecules in an *ab initio* manner, using quantum mechanics to approximate various quantities such as dipole moments, bond energies, bond lengths and angles. Although the *ab initio* methods work only approximately for large molecules, it is nevertheless true that chemical affinity and the properties of molecules can be understood as resulting from molecular structure, which is itself determined by quantum mechanics.

This brings us to Broad's claim that until we try and perform the reaction, we cannot predict that two elements would combine chemically with each other. One of Broad's examples is that of hydrogen and oxygen:

> "Oxygen has certain properties and Hydrogen has certain other properties. They combine to form water, and the proportions in which they do this are fixed. Nothing that we know about Oxygen by itself or in its combinations with anything but Hydrogen would give us the least reason to suppose that it would combine with Hydrogen at all. Nothing that we know about Hydrogen by itself

> or in its combinations with anything but Oxygen would give us the least reason to expect that it would combine with Oxygen at all. And most of the chemical and physical properties of water have no known connexion, either quantitative or qualitative, with those of Oxygen and Hydrogen." (Broad 1925, p. 63)

With the knowledge that physical chemistry has given us about the structure of hydrogen and oxygen, this claim is difficult to maintain. By solving the Schrödinger equation for the hydrogen atom, the electron configuration of hydrogen has been determined as $1s^1$. That is, hydrogen has one electron on its electron shell (the 1s orbital). Through various quantum chemistry methods and the analysis of atomic spectra, the electron configuration of oxygen has been determined as $1s^2 2s^2 2p^4$. Oxygen has been determined to have two electrons on the 2s orbital and four on the 2p orbital; this brings the total number of electrons on the outermost shell to six. It has also been determined that atoms tend to combine in such a way that they each have eight electrons in their last shell (the maximum that quantum mechanics allows). This fact is also known as the *octet rule*. An electron configuration of $\mathrm{n}s^2\mathrm{np}^6$ is very stable energetically (here n represents the principal quantum number which gives us the last shell); this electron configuration characterizes all noble elements with the exception of He, which are known for their very low chemical reactivity. Having six electrons on the last shell, oxygen can have a double covalent bond with one atom of another element that has two electrons on the last shell (e.g., iron(II) oxide, FeO) or a simple covalent bond with two atoms of another element which has one electron on the last shell (e.g., hydrogen oxide, H_2O). Therefore, contrary to what Broad claimed, one must expected that oxygen will bind with hydrogen, forming a relatively stable compound. Similarly, one must expect that Ag will form compounds with Cl, for Ag has one electron on the last shell while chlorine, a halogen, has one missing electron.[6]

What about Broad's claim that the chemical properties of a compound

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[6] Unlike hydrogen oxide, silver chloride is an ionic compound, like most metal-nonmetal compounds. This is explained by the fact that chlorine is has a higher electronegativity than silver.

cannot be determined on the basis of the properties of the components? For the sake of simplicity, let's stick to the examples that Broad himself uses, namely water and silver chloride. One of the chemical properties of water is that it is a good solvent, and neither oxygen nor hydrogen are. This property derives from the polar nature of the water molecule. The H_2O molecule is a v-shaped molecule with oxygen at the vertex and the two hydrogens forming a bond with a 105° angle between them. The relatively high electronegativity of the oxygen pulls the hydrogen electrons away from the hydrogen nuclei, leaving them with a partial positive charge; at the same time, the oxygen becomes more negative. The unequal sharing of electrons and the asymmetric molecular shape result in the H_2O molecule having an electric dipole. The electric dipole is responsible for the effect that water has on ionic compounds such as NaCl. The polarity of the ionic compounds (which due to the nature of the ionic bond) in conjunction with the polarity of water result in an electrostatic attraction between those parts of different compounds that have opposite charges: negatively charged oxygen atoms attract positively charged sodium atoms, while positively charged hydrogens attract negatively charged chlorine – the ionic bond of NaCl is thus broken. To this effect also contribute the short-lived but numerous hydrogen bonds that form between the H_2O molecules. The strong cohesion between water molecules, which is due to these hydrogen bonds, explains why water is a liquid at room temperature, while other substances with similar or even higher molecular weight are gases. Other properties of water are also explained by the underlying quantum mechanics (e.g., water has a high surface tension, 71.97 dyne/cm (at 25°C, 100 kPa), the highest of the non-metallic liquids).

A similar argument can be made for the properties of silver chloride. Broad claims the properties of this substance cannot be predicted in advance; the only way to learn about the properties of silver chloride is by observing a sample. A property for which silver chloride is known is its photo-sensitivity: in the presence of light, the substance darkens. This is why it has been used in photography, where is an important ingredient of the emulsion that is coated on photographic paper. Neither silver nor chlorine has this property. Can this property of silver chloride be deduced from quantum mechanics? If we know the electron structure of silver and that of chlorine and enough quantum mechanics we can in fact deduce this behaviour. Silver chloride is an ionic compound, consisting of silver cations bound to chlorine anions. When light is shone on the sample, the electrons in the chlorine atoms absorb electromagnetic radiation emitted by the light source, becoming excited. If an electron is excited, it leaves the valence band (one of the energy levels allowed by quantum mechanics in which the electron is still bound to its atom and it participates in the lattice bonding of the AgCl crystal structure) and it enters the conduction band (the electron leaves its atom and travels freely through the crystal lattice). The excited electron may give off its energy as heat and relax back to its original state; or it can bind to a silver cation to form an electrically neutral silver atom. If this happens, the ionic compound dissociates into a silver powder (black) and chlorine, and this dissociation is responsible for the darkening of the sample.

But do these quantum-mechanical explanations render Broad's view untenable? Broad's point was that chemical properties cannot be *predicted* on the basis of atomic structure. Most quantum-mechanical explanations of chemical properties are obtained only *a posteriori*. Quantum chemists often know what the target macro-property is, and this makes their job a lot easier. Usually, pure *ab initio* calculations are difficult to carry out due to the complex mathematics and limited computational resources. However, this would not be a problem for a mathematical archangel, who would not be the subject of such limitations.

As mentioned, McLaughlin thinks that the advancements in the understanding of the atomic and molecular structure that took place during the 20^{th} century make Broad's claims regarding emergence in chemistry implausible. However, when it comes to answering if the doctrine of configurational forces on which Broad bases his emergentism is *compatible* with the scientific theories that we currently have McLaughlin claims:

> "So far as I can tell, British emergentism does not rest on any "philosophical mistakes". It is one of my main contentions that

> advances in science, and not philosophical criticism, led to the fall of British Emergentism." (McLaughlin 2008, p. 50)

While McLaughlin is right that advances in science led to the fall of British emergentism, it would be an exaggeration to claim that this doctrine is free of philosophical problems. Insofar as it subscribes to configurational forces, Broad's emergentism supports the idea that there are *sui generis* chemical forces, which are distinct from those within the purely physical domain. Thus, this type of emergentism denies the causal closure of the physical world, for if there are *sui generis* chemical forces able to influence "the go of events", the causal closure of physics (i.e., the idea that every physical effect has a physical cause) is not respected. Chemical configurational forces are both irreducible and efficacious in the physical world; therefore some physical events will have higher level (i.e., *chemical*) causes. Thus, there will be a class of physical events whose causes will not be physical. As a result, physics is not causally closed: there are causal factors which are not described by physics, or for whose description physics defers to another science (in this case, chemistry).

The denial of the causal closure of physics is far from being philosophically innocuous. The reason is that the causal closure of physics came to be viewed as one of the tenets of modern science – a tenet which is grounded in conservation laws. The worry, therefore, is that the denial of the causal closure of physics to which the doctrine of fundamental configurational forces is committed is in fact in tension with modern science.

McLaughlin does not have this worry. He thinks that configurational forces can be easily accommodated in the framework of classical mechanics and even of relativity. He takes the laws of mechanics one by one and argues that all these laws (the law of inertia, Newton's second law, the conservation of momentum) are indifferent to the nature of the force they talk about (whether it is particle-pair force or configurational). He then moves to examining the compatibility of configurational forces with the conservation principles of classical mechanics. He argues that the mass of a system of particles exerting a configurational force could be the sum of the masses of the constituents in the configuration. McLaughlin concludes that there is no conflict between configurational forces and the principle of the conservation of mass.

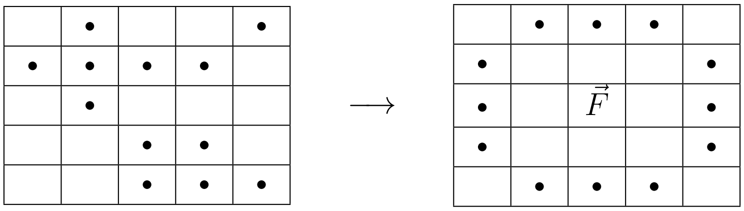
What about the conservation of energy? Is the doctrine of fundamental configurational forces compatible with this principle? If configurational forces exist, they are not idle or epiphenomenal forces – they do mechanical work. But work requires energy. Where does this energy come from? According to McLaughlin, it is possible for it to be the case that particles contain a certain kind of potential energy that can be released only when they figure in appropriate configurations. So for McLaughlin, there need be no conflict between configurational forces and the principle of the conservation of energy. Configurational forces may very well respect the conservation of energy, just like the other forces accepted in physics.

This sort of argument is also presented by Papineau:

> “After all, the conservation of energy in itself does not tell which basic forces operate in the physical universe. Are gravity and impact the only basic forces? What about electromagnetism? Nuclear forces? And so on. Clearly the conservation of energy as such leaves it open exactly which basic forces exist.” (Papineau 2002, p. 249).

McLaughlin and Papineau are right that the conservation of energy is indifferent to the kind of forces it talks about. If configurational forces are just another kind of force among others (gravitational, electromagnetic, etc.), there is no reason to suppose that their mere existence would violate the conservation of energy. However, configurational forces are not like the gravitational or the electromagnetic force – they occur only at certain moments in time. They come into existence as a consequence of particles assuming certain configurations, and they go out of existence when the configurations disappear. So these forces are “special forces” in the sense that they occur only after certain conditions are met, unlike the gravitational or electromagnetic forces, which are not subject to this constraint to the same extent. Nonetheless, configurational forces are supposed to be fundamental, i.e., not derivative or resultant from other kinds of forces.

I worry that the fundamental character of configurational forces cannot be easily reconciled with the principle of the conservation of energy if their "special" nature is to be preserved. I believe the defenders of configurational forces are facing a dilemma: either these forces are not truly fundamental, or their existence violates the conservation of energy. The argument may look as follows. Suppose that we have an energetically isolated system of particles S that assumes the right configuration at time t_c and as a result of this a configurational force F emerges in S at t_c. If the energy characterizing the configurational force can be traced back to some potential energy stored by the particles and released when the right configuration obtains, then the configurational force is not truly fundamental: it is derivative or resultant – it comes from the potential energy of the particles in the configuration. But this goes against the definition of configurational forces, which are supposed to be fundamental.



$$\mathbb{E}S_{t<t_c} < \mathbb{E}S_{t_c}$$

Figure 2.1.1: Configurational forces and the conservation of energy. If the configurational force is fundamental, the energy of system S increases when the configuration obtains.

However, suppose these forces *are* fundamental. Since they are not epiphenomenal, they are able to do work, which requires energy. If this energy is not already in the system as potential energy and released when the configuration obtains (the force is assumed to be *fundamental*!), then the conservation of energy is violated, for the system was assumed to be energetically isolated, yet its total energy increases as a result of its components assuming a certain configuration. Thence the dilemma: either the configurational forces respect the conservation of energy, or they are not truly fundamental.

2.1.3 Conclusion

It has been argued that the advancements in the understanding of the atomic and molecular structure that took place during the 20^{th} century make Broad's claims regarding emergence in chemistry implausible. Broad was aware of this possibility:

> "Now of course it may be true as a matter of fact that the atoms of the various elements are wholes composed of various numbers of similar particles with various arrangements and movements. And it may be true as a matter of fact that the laws of chemical combination, the properties of compounds and so on, are mere consequences of the laws of electro-magnetics and of the particular number, arrangement and movements of the particles which compose each kind of atom" (Broad 1925, p. 73).

Given that Broad was aware of this possibility, one may legitimately ask why he maintained that chemistry is an example of emergence. The reasons are philosophical, but also historical.

Broad developed his theory of emergence primarily to account for the existence or appearance of secondary qualities such as colours and odours, whose integration into a naturalistic framework is not straightforward. But presumably, Broad did not want to see the mind as very different from other natural phenomena. His theory of the mind as an emergent phenomenon would appear more plausible if it could be shown that emergence occurs in "lower" ontological strata, such as the vital or the chemical. If emergent behaviour first occurs at the level of chemical compounds, then it is more plausible and perhaps even expected that emergent behaviour should appear at higher levels as well.

Another reason why Broad thought that chemistry seems to offer the most plausible example of emergence (as he conceived it) is more historical. Broad presented his views about emergence in chemistry as part of the Tarner Lectures in the philosophy of science he delivered at Trinity College, Cambridge in 1923. Two years later, he published *The Mind and its Place in Nature*, a monograph based on these lectures. Although the chemical bond and the properties of compounds were understood in terms of electronic structure since at least the early 1900's by Gilbert N. Lewis and others, this sort of understanding came of age only after 1926, the year when Schrödinger discovered of the equation that governs the dynamics of quantum systems. An abundance of applications to chemistry – many of which consisted in the derivation of chemical facts from the underlying physics – followed immediately thereafter.[7] Couldn't Broad have foreseen such successes? Any attempt to answer this question would be highly speculative, but the fact that Broad published his book one year before Schrödinger discovered the wave equation is most certainly an aspect that played an important role.

The British emergentist view of chemistry can hardly be upheld today. It receives no support from contemporary chemistry, and it seems to be at odds with the conservation of energy. This, however, need not mean that chemistry is not emergent. Emergence is often associated with the occurrence of novel properties, the existence of distinct ontological strata, with irreducibility and disciplinary autonomy. Chemistry may exhibit all these characteristics of emergence even though it does not have the features that Broad associated with emergence (i.e., configurational forces, or the lack of a principle of composition). This leaves open the possibility of coming up with a view of chemistry on which chemical properties and laws are still emergent, however not in the traditional sense. On this view, emergence in chemistry need not necessarily

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[7] In 1927, the philosopher-turned-physicist Fritz London and the physicist Walter Heitler used the new quantum mechanics to formulate the Valence Bond theory, which enabled them to calculate the bonding properties of the hydrogen molecule. In 1929, Sir John Lennard-Jones introduced another method of calculating the molecular structure that used quantum mechanics: the linear combination of atomic orbitals molecular orbital method (LCAO). Lennard-Jones worked on the derivation of the electronic structures of molecules of fluorine and oxygen from first principles, i.e., from quantum mechanics. Other quantum chemistry methods such as the Hartree-Fock or the functional density method have been subsequently developed and used to calculate the structure of molecules. With the advent of modern digital computers, these methods could handle satisfactorily an increasingly large number of electrons and nuclei. In some cases, such as the case of the case of disilyne, Si_2H_2, the computational methods have predicted the correct structure of the molecule before the experiments confirmed it.

be a rival of what Broad called "mechanism"; emergence in chemistry may, for example, be thought of along the lines of *non-reductive physicalism* in the philosophy of mind – that is, as compatible with physicalism but incompatible with reductionism.

2.2 The prospects for fusion emergence in chemistry

In a number of articles, Paul Humphreys (1996, 1997a, 1997b, 2008) has offered an account of emergence which aims to provide the grounds for an ontology of the special sciences. Humphreys' account (called *fusion emergence*) presents a series of challenges to at least three widely accepted assumptions about ontology: (i) that the right way to represent the relation between lower level and higher level properties is supervenience, (ii) that our world's ontology is wholly compositional, and (iii) that the physical domain is causally closed. If sound, Humphrey's account offers an interesting answer to our specific question.

Humphreys has argued not only that fusion emergence can be consistently described (1997b), but also that our own world exhibits cases of this kind of emergence (2008). According to Humphreys, covalent bonding is a "core example of fusion emergence" (2008, p. 7). The purpose of this section is to raise some concerns about Humphreys' account in general and about his core example of fusion emergence in particular. It will be suggested that the extent to which covalent bonding undermines the second assumption mentioned above has been overstated.

2.2.1 Humphreys' fusion emergence

Humphreys' account of emergence was motivated by the desire to avoid the exclusion argument or a generalized version thereof, whose conclusion is that higher level emergent properties are excluded from affecting lower level properties, since all the causal work is done by the latter (see Kim 1992, 1999, 2006). The exclusion argument has unwelcome consequences for the ontology of the special sciences. If one thinks of the special science properties (e.g., chemical or biological) as occupying higher levels than do physical properties, then the exclusion argument entails that no event involving a special science property could ever causally influence a physical event. The idea of special science causation is thus threatened. Also, the exclusion argument challenges the idea that special science properties deserve a place in our ontology: if special science properties are causally idle, what is the point of having them in our ontology? The exclusion argument has unwelcome consequences for physics, too. If one thinks of physics itself as stratified (e.g., with high energy physics, solid state physics and thermodynamics occupying different strata), the exclusion argument entails that only the most basic physical properties can be causally efficacious, and – as a result – all other causal claims within contemporary physics are false.

While the exclusion argument denies that the higher level properties that special sciences are concerned with are capable of downward causation, emergence seems to require it explicitly. It has been argued that the only way to cause an emergent property to be instantiated is by causing its emergence base property to be instantiated (Kim 1992, p. 136). This is known as the downward causation argument, and it shares with the exclusion argument the assumption that the right way to represent the relation between lower level and higher level properties is supervenience.

In his work, Paul Humphreys challenges both the exclusion argument and the downward causation argument by explicitly denying their common assumption, namely that supervenience is the right way to represent the relation between lower level and higher level properties (1997a). He also argues that thinking of higher level emergent properties in terms of supervenience is mistaken. Instead, he links the possibility of emergence with the existence of a *fusion operation* that operates on i-level properties and outputs $i+1$-level properties, which have novel causal powers.[8]

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[8] For the sake of brevity, sometimes I will use “property” instead of “property instance”. It should be noted however that for Humphreys the arguments of the fusion operation are property instances.

The process of fusion is formally represented as follows. Let $\mathrm{P}^i_m(\mathrm{x}^i_r)\mathrm{t}_1$ represent an *i*-level entity, x_r, instantiating an *i*-level property, P_m, at time t_1. $\mathrm{P}^i_n(\mathrm{x}^i_s)\mathrm{t}_1$ will denote another *i*-level entity, x_s, instantiating another *i*-level property, P_n, at time t_1. Humphreys introduces the *fusion operation* symbolized by $[.*.]$, which takes as arguments the two property instances $\mathrm{P}^i_m(\mathrm{x}^i_r)\mathrm{t}_1$ and $\mathrm{P}^i_n(\mathrm{x}^i_s)\mathrm{t}_1$ and fuses them: $[\mathrm{P}^i_m(\mathrm{x}^i_r)\mathrm{t}_1{*}\mathrm{P}^i_n(\mathrm{x}^i_s)\mathrm{t}_1]$. The fusion operation is an *i*-level operation, i.e., an operation of the same level as its arguments. The result of the fusion operation is the fused property $[\mathrm{P}^i_m * \mathrm{P}^i_n][(\mathrm{x}^i_r)+(\mathrm{x}^i_s)](\mathrm{t}_2)$ at the $i+1$-level, which can also be written as $[\mathrm{P}^{i+1}_l][\mathrm{x}^{i+1}_l](\mathrm{t}_2)$. The fused property is a unified whole in the sense that its causal effects cannot be represented in terms of the separate causal effects of the original property instances. Also, within the fused property instance $[\mathrm{P}^i_m(\mathrm{x}^i_r)\mathrm{t}_1{*}\mathrm{P}^i_n(\mathrm{x}^i_s)\mathrm{t}_1]$, the original property instances $\mathrm{P}^i_m(\mathrm{x}^i_r)\mathrm{t}_1$ and $\mathrm{P}^i_n(\mathrm{x}^i_s)\mathrm{t}_1$ no longer exist as separate entities and they do not have all of their *i*-level causal powers available for use at the $i+1$-level (Humphreys 1997b, p. 10).

Humphreys argues that this particularity of fusion emergence is what enables this brand of emergentism to avoid the threats of the exclusion and downward causation arguments. At the time when the fused property instance $[\mathrm{P}^i_m(\mathrm{x}^i_r)\mathrm{t}_1{*}\mathrm{P}^i_n(\mathrm{x}^i_s)\mathrm{t}_1]$ comes into existence, the original property instances $\mathrm{P}^i_m(\mathrm{x}^i_r)\mathrm{t}_1$ and $\mathrm{P}^i_n(\mathrm{x}^i_s)\mathrm{t}_1$ go out of existence. Therefore, it is *a fortiori* the case that they cannot compete as causes with the emergent property instance. On Humphreys account, emergents don't coexist with their bases, and this feature prevents the exclusion argument from getting off the ground.

Humphreys' fusion emergence also deals with the downward causation argument. This argument is also committed to the idea that emergent properties supervene on lower level properties. The argument assumes that the *only* way to bring about an emergent property instance at time t is by bringing about its subvenience base at time t. But if fusion emergents are not synchronous with their bases, this assumption is unwarranted. There is no reason to suppose that an $i+1$-level property instance could not *directly* produce another $i+1$-level property instance e.g., by directly transforming into it or by transforming another, already existing, $i+1$-level property instance – in both cases, other property instances may contribute (1997b, p. 13; 2008, p. 8).

By avoiding the threats to the ontology of the special sciences posed by the exclusion and downward causation arguments, Humphreys' emergentist account attempts to rescue the autonomy of the special sciences and to depict an ontologically antireductionist image of the world in which the subject matters of the various special sciences correspond to irreducible ontological strata.[9] For Humphreys, there is a hierarchy of levels of properties L_0,L_1, ... L_n... of which at least one distinct level is associated with the subject matter of each special science, and L_j cannot be reduced to L_i for any $i < j$ (Humphreys 1997a, p. 5).

2.2.2 Previous criticisms of fusion emergence

Humphreys remarks that philosophers have long thought of the ontology of the special sciences in terms of supervenience. On this view, the higher level properties are "composed of" or "supervenient upon" lower level properties.[10] But Humphreys finds supervenience unsatisfactory. He complains that supervenience does not provide any understanding of ontological relationships holding between levels. If these levels are emergent, they contain emergent properties. According to Humphreys, an important characteristic of emergent properties is that they result from the interaction between their constituents.[11] However, the level of detail that emergent properties demand makes the use of supervenience relations seem simplistic. This is one of the reasons why Humphreys argues that emergence should not be understood in terms of supervenience. Add to this the threats posed by the exclusion and downward causation arguments, and supervenience seems completely inappropriate for providing the grounds for an ontology of the special sciences.

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[9] Humphreys admits however that the boundary between the physical level and other levels is not sharp (Humphreys 1997a, p.S345).

[10] The notion of supervenience that Humphreys uses is Kim's strong supervenience: "A family of properties M strongly supervenes on a family N of properties iff, necessarily, for each x and each property F in M, if F(x) then there is a property G in N such that G(x) and necessarily if any y has G it has F"(Kim 1993, p.65).

[11] Humphreys sees this interaction as nomologically necessary for the existence of emergent properties (1997a, p.S342).

As mentioned in the previous section, on Humphreys' account, emergents are not co-instantiated with their bases. Wong (2006) has called this the *basal loss* feature of fusion emergentism, and he has claimed that it is both problematic and unmotivated (2006, p. 346). According to Wong, the disappearance of the lower level properties of an entity is problematic for two reasons. First, because it threatens the structural properties crucial to the proper functioning of that entity. The basal properties that fuse to become emergents may also constitute nonemergent, structural properties which may be indispensable to the proper functioning of the system. However, if basal properties are destroyed by the fusion process, then so would the structural properties. Second, the disappearance of the lower level properties generates what Wong calls "the correlation problem". It is empirically established that many special science properties have lower level correlates with which they are copresent (e.g., mental properties are synchronously correlated with neurophysiological properties). However, if we are to treat the special science properties as fusion emergents, then we deny the copresence of their lower level correlates, which Wong sees as empirically implausible.

Wong considers the basal loss feature of fusion emergentism as unmotivated for the reason that on Humphreys' account, basal and emergent properties don't have causal profiles that overlap significantly and thus cannot compete as overdeterminers of their effects. According to Wong, emergents supplement the underlying dynamics rather than merely overdetermine physical effects (2006, p. 361).

In his response to Wong's criticisms, Humphreys (2008) argues that most systems possess multiple properties, some of which are essential to carrying out the system's function, whereas others are not. In general, the fusion process will affect only the latter. If a system's state is given by <P,Q,R,...Z> (x), the fusion between P(x) and Q(x), will leave R...Z unchanged and able to sustain the proper functioning of the system. Also, given that most properties are quantitative, part of P and part of Q will fuse, leaving the remainder to maintain the state. Wong's challenge to Humphreys is to show that this is will *always* be the case (Wong 2006, p. 357). However, Wong's demand is unreasonable. If Humphreys can show that at least some of the special science properties are examples of fusion emergence, then this is enough to challenge the three assumptions mentioned at the beginning. But are Humphreys' examples able to do this? Before addressing this question, a couple of quick general points about Humphreys' account of emergence are in order.

2.2.3 The division of labor between properties and the notion of a physical operation

Although Humphreys does not say it, his distinction between properties which are able to undergo fusion and those which are essential in the functioning of the system does in fact rely on two other dichotomies: first, between properties that are able to undergo fusion (PAUF) and properties that are not (PNAUF); and second, between properties which are essential in the functioning of the system (PEFS) and those that are not (PNEFS). Thus, Humphreys' distinction results from crossing two criteria: first, whether the properties are able to undergo fusion; second, whether the properties are essential in the functioning of the system. Humphreys assumes that the application of these two criteria delivers co-extensive subsets of properties, so that the properties which are able to undergo fusion will also be the ones that are not essential in the functioning of the system.

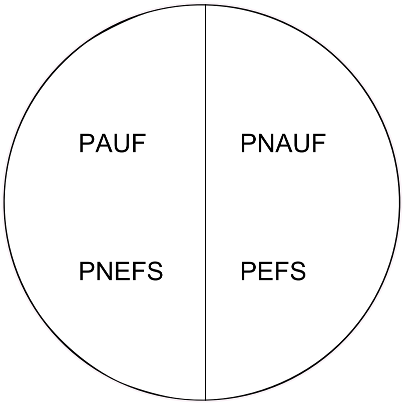

Figure 2.2.1: Two overlapping dichotomies between properties.

The dichotomy between the properties that are able to undergo fusion (PAUF) and those that are not (PNAUF) overlaps with the dichotomy between the properties that are not essential in the functioning of the system (PNEFS) and those that are (PEFS).

Humphreys can, of course, maintain his distinction between properties without threatening the coherency of his account. That is, he can maintain that in any given entity there will be a "division of labor" between properties: some will undergo fusion, while others will preserve the functioning of the system. In this case, the properties to which the emergent character of an entity is due will not also be structural properties with a role in the in the functioning of that entity. Conversely, the structural properties that are crucial to the proper functioning of an entity won't participate in the fusion processes that that entity may undergo. However, these two last claims are far from trivial. Unless we have an independent justification of why the two dichotomies overlap, one may worry that Humphreys' division of labor between properties constitutes an *ad hoc* response to the problem of basal loss.

The other point has to do with the nature of the fusion operation. On Humphreys' account, the fusion operation is not necessarily causal. However, fusion is supposed to operate on real properties in the world, not on their representations. Humphreys claims that the fusion operation is "a real physical operation" as opposed to a merely logical one like conjunction or disjunction (1997b, p. 10).

At this point, one may pause and ask what a *physical* operation is. We know what a *logical* operation like conjunction or disjunction is because there are logical/mathematical theories in which such operations are defined (e.g., sentential logic, predicate logic, Boolean logic, etc.). In the absence of these theories, our understanding of the logical operations will be greatly impoverished. What is the corresponding theory for the fusion operation? Humphreys claims that fusion is a *physical* operation. However, what it means for something to be a physical operation is not entirely clear. For example, in physics textbooks one does not find such an operation being defined. Humphreys may be taken as being uncommitted to the exact nature of the fusion operation pending further empirical work (Wong 2006, p.352). It may turn out that fusion is implemented by single physical process (already discovered or yet to be discovered), or by a host of physical processes. In any case, an understanding of fusion as a physical operation depends on how well one understands its physical implementation. In order to achieve this, one needs to engage with empirical issues. It is to these empirical issues that I will now turn.

2.2.4 Humphreys' examples

Whether the theory of fusion emergence can be coherently formulated is one thing; whether it applies to anything in the world is quite another. The former is a theoretical aspect that can be addressed largely on *a priori* grounds, while the latter is a an empirical issue. To argue that fusion emergence is not a metaphysician's fiction but a real phenomenon, one needs more than appeals to imagined scenarios; one needs concrete examples taken from the sciences. Humphreys presents such examples. According to Humphreys, "the clearest cases of fusion emergence are the entangled states of quantum systems" (2008, p. 4).[12]

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[12] Humphreys' suggestion that the entangled state is an example of fusion emergence has been developed in more detail by Kronz and Tiehen (2002), who also discussed its ramifications and limitations.

According to Humphreys, the existence of such cases of emergence entails that our world's ontology is not wholly compositional. By a compositional ontology Humphreys means an ontology in which "all non-fundamental entities are aggregated or structured collections of other entities that can be generated by the use of explicitly stated rules of combination, where the constituent entities retain their identities within the structure" (2008, p. 2).

Humphreys thinks that the entangled state of a composite quantum system does not conform to the requirements of a compositional ontology because it is non-separable – the state of the system cannot be written as a tensor product of the states of its parts. Although there may be worries that a theory whose physical interpretation is still heavily debated might not be our best guide to ontology, let's grant that the entangled state in quantum mechanics is a *bona fide* example of fusion emergence. The question then becomes whether there are other examples of fusion emergence in our world, preferably in the special sciences.[13] Humphreys' answer is affirmative. The example of fusion emergence that is discussed in most detail by Humphreys is that of the covalent chemical bond. As mentioned, according to Humphreys, covalent bonding is a "core example of fusion emergence" (2008, p. 7).

Why does Humphreys think that the covalent bond exemplifies fusion? Humphreys notes that a covalent bond occurs when a pair of electrons is shared by two atoms; he also notes that the density of the electrons which participate in the covalent bond is distributed over the entire molecule rather than the individual atoms. Humphreys also claims that while some properties remain unchanged after the fusion (e.g., the charge and mass of the nucleons, the total charge of the molecule), others are affected by it; for example, there is a slight lowering of the energy of the combined molecular arrangement compared to the energies of the atoms before fusion. According to Humphreys, this energy that emerges upon fusion is responsible for the characteristic properties of the molecule.

Humphreys contrasts the covalent bond with the ionic bond. He suggests

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[13] The exclusion argument to which fusion emergentism is an objection threatens the special sciences to a greater extent than physics.

that ionic compounds are the result of electrostatic forces between positively and negatively charged ions and can be understood within the framework of a compositional ontology. On the other hand, molecules (resulting from covalent bonding) exemplify fusion and therefore are non-compositional. Humphreys does not elaborate much on why ionic bonding is compositional and covalent bonding isn't. He only claims that there is a contrast between the two types of bonding and that the fact that “the molecule is not simply a spatial arrangement of the two atoms (...) is one of the things that distinguishes fusion from composition” (2008, p. 7).

2.2.5 Questioning the ionic-covalent dichotomy

Insofar as Humphreys takes the two types of bonding as having different ontological requirements (and thus supporting incompatible ontologies), he is committed to a contrast between them that is not simply a matter of degree. However, the sharp contrast between ionic and covalent bonding that Humphreys' example assumes does not receive as much support from physical chemistry as one may think.

Ionic and covalent bonding are viewed as two extreme models of the chemical bond (Atkins and Jones 2002, p. 92). With the exception of the bonds of homonuclear diatomic molecules, all chemical bonds have some ionic character as well. If the electronegativity difference $\Delta\chi$ increases, so does the ionic character of the bond.[14] Generally, if $\Delta\chi > 1.6$, the bond is considered ionic. If $\Delta\chi < 0.5$, the bond is considered covalent non-polar. And if $\Delta\chi$ is between 0.5 and 1.6, the bond is considered covalent polar. However, there is no principled way to choose these values and they may vary slightly from one chemistry textbook to another. There is no sharp distinction between an ionic and a polar covalent bond; rather, the difference between them is a matter of degree. If the difference between the two types of bonding is only gradual,

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[14] On the Pauling scale, the difference in electronegativity between atoms A and B is a dimensionless quantity: $\chi_{\mathrm{A}} - \chi_{\mathrm{B}} = (\mathrm{eV})^{-1/2}\sqrt{E_{\mathrm{d}}(\mathrm{AB}) - [E_{\mathrm{d}}(\mathrm{AA}) + E_{\mathrm{d}}(\mathrm{BB})]/2}$, where $E_{\mathrm{d}}(\mathrm{XY})$ represents the dissociation energy between atoms X and Y in electronvolts. Pauling defined the amount of ionic character of a chemical bond as $1 - e^{-1/4(\chi_{\mathrm{A}} - \chi_{\mathrm{B}})}$ (Pauling 1960, p.98)

then how can they be accommodated within different ontological frameworks? Where should the boundary between compositional and non-compositional be placed?

One may argue that as long as there exist clear cases of covalent and ionic bonding, this should be enough to justify the requirement of different ontological frameworks. However, while pure covalent bonding exists (between the atoms of homonuclear diatomic molecules such as Cl_2, H_2, O_2), pure ionic bonding cannot exist, since it would require that the electronegativity difference $\Delta\chi$ between the atoms be infinite or at least exceedingly large (Carter 1979, p. 124). Therefore, all bonds have some covalent character. Does non-compositionality characterize only those pure cases of covalent bonding, or should all types of bonding be accountable within a single (non-compositional) ontology? If neither, how should the discrete border between two distinct ontological frameworks be superimposed onto the covalent-ionic continuum? These questions are not in themselves sufficient to show that Humphreys' account fails, but they are certainly indicative of a lack of harmony between the sharp character of the boundary between a compositional and a non-compositional ontology and the non-sharp character of the boundary between ionic and covalent bonding.

There is another problem with viewing chemical compounds through the ionic-covalent dichotomy. These two types of chemical bonding are models, i.e., they are idealizations which have their virtues but distort reality in some respect. For example, they represent the pair of electrons participating in a covalent bond as being shared by just one pair of atoms, even when the molecule is polyatomic. Chemical bonds between atoms can be described more accurately using the concept of resonance. Resonance refers to the representation of the electronic structure of a molecular entity in terms of distinct contributing structures (also called resonance structures). Electrons involved in resonance structures are said to be delocalized: for example, in the case of a polyatomic molecule the sharing of an electron pair is distributed over several pairs of atoms and cannot be identified with just one pair of atoms. A resonance hybrid is a blend of the contributing structures.

All compounds, regardless of whether they are considered ionic or covalent, can be viewed as resonance hybrids of purely covalent and purely ionic *resonance structures.* For example, the structure of a homonuclear diatomic molecule, in which two atoms of the same element are covalently bonded to each other, can be described as a resonance hybrid of two ionic structures (Atkins and Jones 2002, p. 93).

$$\mathrm{A{-}A} \longleftrightarrow \mathrm{A}^{\delta-}\mathrm{A}^{\delta+} \longleftrightarrow \mathrm{A}^{\delta+}\mathrm{A}^{\delta-}$$

In the case of homonuclear diatomic molecules, the ionic structures make only a small contribution to the resonance hybrid. Also, the two ionic structures have the same energy and make equal contributions to the hybrid, so the average charge on each atom is zero. In a heteronuclear molecule, the resonance hybrid has unequal contributions from the two ionic structures – the structure with the negative charge on the atom that has a greater electron affinity will make a bigger contribution to the resonance hybrid.

The representation of chemical compounds in terms of resonance structures is more accurate than the ionic-covalent representation but it is strictly speaking incompatible with it. The resonance model challenges the view of chemical compounds as either ionic or covalent because resonance hybrids are a blend of resonance structures rather than the flickering of a compound between different structures, "just as a mule is a blend of a horse and a donkey, not a creature that flickers between the two" (Atkins and Jones 2002, p. 80).

2.2.6 The level-relativeness of fusion

According to Humphreys, the covalent bonding exemplifies a kind of ontological emergence which shows that the ontology of our world is not exclusively compositional. Why does Humphreys think that molecules cannot be understood in the framework of a compositional ontology? Molecules consist of atoms, so at a first glance, the compositionality condition would seem to be satisfied. However, at a closer look, one realizes that molecules are not simply the result of the combination or spatial juxtaposition of atoms. A molecule is the *sharing* of electrons between two or more atoms. Because of this, Humphreys is justified in claiming that the molecule can be described as the *fusion* of two or more atoms, not as a combination or aggregation of atoms.

However, if one thinks of molecules not as collections of atoms but as collections of nuclei and electrons, what looks like fusion between two atoms can be described as composition of nuclei and electrons. I will attempt to show that physical chemistry permits a compositional understanding of atoms and the molecules, in terms of separate but interacting electrons and nuclei. That is, I will attempt to show that atoms and molecules can be generated by the use of explicitly stated rules of combination of separate but interacting electrons and nuclei, which is exactly what fusion emergence denies.

The Aufbau principle consists in a number of explicitly stated rules that allow us to understand the atom (any atom) as a physical system that is build by successively adding electrons around the nucleus.

1. **The principle of the minimum energy.** The electrons occupy atomic orbitals in such a way that the total energy of the atom is a minimum; they fill orbitals starting at the lowest possible energy states before filling higher states.

2. **The Pauli exclusion principle.** Every electron in an atom is described by its own distinct set of four quantum numbers, not shared with any other electron. This entails that a given orbital is to be occupied by no more than two electrons, case in which their spins, denoted by the m_s quantum number, are paired.

3. **The Madelung rule.** Orbitals with a lower $n+l$ value are filled before those with higher $n+l$ values.

4. **Hund's rule of maximum multiplicity**. Electron pairing will not take place in orbitals of the same sub-shell until orbitals are singly filled by electrons with parallel spin.

It should be recognized that the Madelung rule and Hund's rule of maximum multiplicity are not exceptionless. However, they are rules for which the generality of physics entails that there is, nevertheless, a physical reason grounded in physical law (as there is one for the cases when the rules fail), even if discovering this reason is often difficult. What these four rules show is that the atom is a complex physical system in which the nucleus and the electrons are subject to a number of physical constraints and interact with each other according to physical laws. It is these physical laws and constraints that are the more basic rules of composition in the multi-electron atom. The atom appears to be more than just a collection of individual particles because of the complexity of the interactions between these particles.

In contrast with the entangled state, which is non-decomposable into separate states of each of the two electrons and thus cannot be written as a tensor product of the states of the individual electrons, the wavefunction of a multi-electron atom can be thought of as resulting from the separate contributions of each electron wavefunctions, and it can be written as a product of individual atomic orbitals: $\psi(\mathrm{r}_1,\ \mathrm{r}_2, \ldots.\ \mathrm{r}_n) = \phi_1(\ \mathrm{r}_1)\phi_2(\ \mathrm{r}_2)\ldots.\phi_n(\ \mathrm{r}_n)$. This strategy of learning about the wavefunction of a multi-electron atom on the basis of the individual electrons is known as the *orbital approximation* and is a remarkably useful tool in the attempts at solving the Schrödinger equation for atoms that have more than one electron. When applied to multi-electronic atoms, the (atomic) orbital approximation assumes that each electron behaves independently of the others, and thus the electronic Hamiltonian can be separated into as many components as there are electrons: $\hat{H}_e = \hat{H}_1 + \hat{H}_2 + \ldots. + \hat{H}_n$.

The treatment of the multi-electron atom in physical chemistry is, I think, an illustration of compositionality. Admittedly, the orbital approximation is an approximation – the inter-electronic repulsion forces which are due to the Coulomb potential are deliberately ignored, to make the Schrödinger equation more tractable. However, the existence of such forces does not show that the atom cannot be understood compositionally; on the contrary, the inter-electronic repulsion forces are the consequence of the physical laws which are the more basic rules of composition in the multi-electron atom.

Compositionality principles seem to be abundant in the physical chemistry of molecules, too. In contrast to older theories such as the valence shell electron pair repulsion theory (VSEPR), the molecular orbital theory describes the electrons in a molecule as delocalized; they are not confined to pairs of atoms, but are spread over the whole molecule. The central claim of the molecular orbital theory is that molecular orbitals are obtained from *summing up* atomic orbitals. More rigorously, each one-electron molecular orbital ϕ_i is expressed as a linear combination of atomic orbitals (LCAO): $\phi_i = c_{1i}\sigma_1 + c_{2i}\sigma_2 + c_{3i}\sigma_3 + ... + c_{ni}\sigma_n$, where the coefficients represent the weights of the contributions of each atomic orbital to the molecular orbital and are found using the Hartree-Fock method. The wavefunction for the molecule is then written as a product of one-electron wavefunctions. This is the molecular orbital approximation: the wavefunction of a multi-electron molecule is approximated as the product of individual molecular orbitals: $\Psi(\mathrm{r}_1,\ \mathrm{r}_2, ...\ \mathrm{r}_n) = \Phi_1(\ \mathrm{r}_1)\Phi_2(\ \mathrm{r}_2)....\Phi_n(\ \mathrm{r}_n)$. The electron configuration of molecules is obtained from the same set of rules that yielded the electron configuration of multi-electron atoms.

In some sense, Humphreys is justified in thinking of the molecule non-compositionally, for a molecule is not simply the result of the spatial arrangement of atoms. If one descends one ontological level (e.g., from the level of the molecule to the level of atoms), the molecule cannot be described compositionally, in terms of separate but interacting atoms. However, if one descends *two* ontological levels (e.g., from the level of the molecule to the level of nuclei and electrons), the molecule *can* be described in terms of separate but interacting components. What looks like fusion at the *i*-level (molecular level) can be represented as composition at the *i*-2-level (level of electrons and nuclei). For example, in the case of a simple molecule such as the dihydrogen molecule, what looks like fusion between two hydrogen atoms is in fact composition between two nuclei and two electrons.

2.2.7 Entanglement to the rescue?

An argument that challenges this conclusion may in fact be available to the defender of non-compositionality. The argument is based on the remark that the electrons which participate in the covalent bond have opposite spins (are paired), and thus they are entangled (i.e., they form a singlet state, or a state in which their total spin is zero). If the entangled state is a *bona fide* case of fusion and hence it does not conform to the requirements of a compositional ontology, then the molecule must also be an example of fusion. On this view, the fact that the electrons participating in the covalent bond cease to possess separate states is sufficient grounds for concluding that the molecule is a non-separable whole which defies a compositional ontology. The defender of non-compositionality could argue that the covalent bond (and hence the molecule) owes its existence to the entanglement of the electrons constituting the bond. On this view, once two electrons belonging to different atoms have become entangled, a covalent bond occurs between the atoms and a new entity emerges: the molecule.

The problem with the argument above is that it does not give an accurate characterization of the origin and nature of the chemical bond. Chemical bonds are due to the interplay of four sets of forces: the attraction of each electron to the nucleus of its own atom, the attraction of each electron to the nucleus of the other atom, the electron-electron repulsion, and the nucleus-nucleus repulsion. The fact that the electrons participating in a covalent bond are paired is a consequence of their obeying the Pauli exclusion principle. However, the Pauli exclusion principle is not a force, but a constraint that the electrons must satisfy if a covalent bond is to be formed. Consider two hydrogen atoms whose electrons have parallel spins. If the atoms are brought together, the charge density from each electron is accumulated in the antibonding region (i.e., at the extremities of the system), rather than in the bonding region between the nuclei. Therefore, they will not form a dihydrogen molecule. The role of the Pauli exclusion principle is to veto those systems that cannot form a molecule by imposing a constraint on the spin of the electrons participating in the covalent bond. The Pauli exclusion principle tells us that only those hydrogen atoms whose electrons have opposite spins are eligible for forming a bond. The spin entanglement that can be found in a molecule does not play the role of a force holding the molecule together.[15]

In fact, there are molecules in which not all of the electrons are entangled, such as molecules with unpaired electrons or an open shell configuration. Although usually the unpaired electrons are found in the antibonding orbitals and they are expected to lower the bond order and thus decrease the bond energy, there are cases such as the oxygen molecule, O_2, in which the unpaired electrons actually increase the strength of the bond.

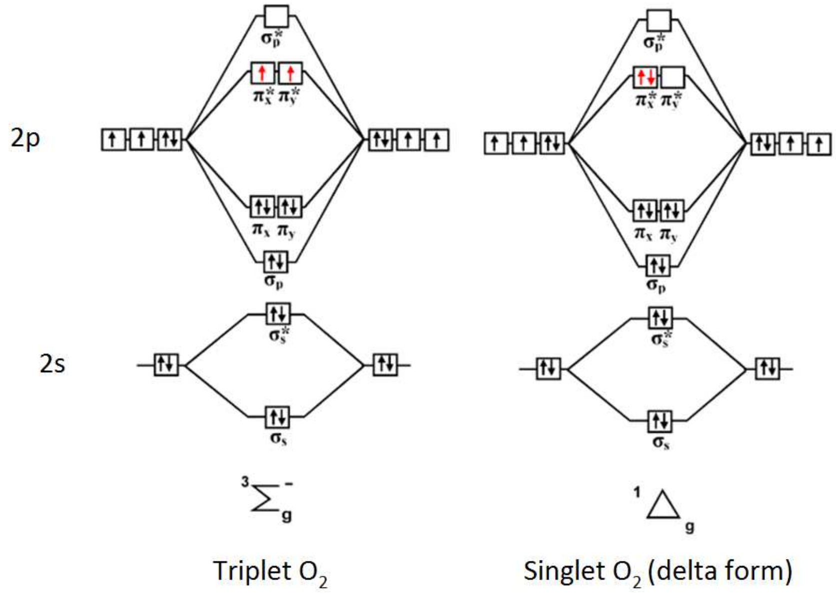

Figure 2.2.2: Triplet oxygen vs. singlet oxygen.

Triplet oxygen is more stable than singlet oxygen, despite the fact that in triplet oxygen there is “less” electron entanglement.

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[15] The so-called “exchange force” or “exchange interaction” which decreases the expectation value of the distance between two electrons (or fermions, more generally) with identical quantum numbers when their wave functions overlap is not a true force and should not be confused with the exchange forces produced by the exchange of force carriers, such as the electromagnetic force produced between two electrons by the exchange of a photon, or the strong force between two quarks produced by the exchange of a gluon.

The ground state of the oxygen molecule is also known as the triplet oxygen because the total spin of the molecule is 1: the electrons occupy two different 2pπ^* molecular orbitals singly and, according to Hund's rule, their spins are parallel (this can also be deduced empirically, from oxygen's paramagnetism). The triplet oxygen is known to be more stable than the singlet oxygen – a diamagnetic form in which the electrons are paired in the same 2pπ^* orbital (Wiberg et al. 2001, p. 476).[16] Another example is that of the molecular hydrogen ion, H_2^+, in which there is no entanglement since there is only one electron. The bond holding together the dihydrogen cation is described as a "one-electron bond", and has a formal bond order of $\frac{1}{2}$ (Pauling and Wilson 1963, p. 362). For this simple system the Schrödinger equation can be solved accurately and the calculations show clearly that the molecular entity possesses a bound state, i.e., it possesses a ground state whose energy is less than that of a hydrogen atom and a free electron. In the case of dilithium, the binding energy is greater for the one-electron Li_2^+ than for the two-electron Li_2, although in the Li_2^+ there is no entanglement involved in bonding, while in the Li_2 there is (James 1935).

These examples show that the connection between the chemical bond and entanglement is not as strong as the argument that is available to Humphreys may assume it to be. They show that i) the chemical bonding of some molecular entities is possible even in the absence of entanglement, as in the case of the one-electron bonds, and ii) the chemical bond of some molecules may actually be stronger if not all electrons are entangled.

2.2.8 Conclusion

Humphreys' fusion emergence is an elegant solution to the exclusion problem, but it is not without its difficulties. There are a couple of general concerns. First, there is the worry that Humphreys' division of labour between properties may be an *ad hoc* response to the problem of basal loss if we don't have independent justification for why the dichotomy between the properties that

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[16] The specific form referenced here is $O_2 a^1 \triangle_g$.

are able to undergo fusion and those that are not should overlap with the dichotomy between the properties that are not essential in the functioning of the system and those that are. Second, the notion of a physical operation plays a crucial role in Humphreys' emergentist account, but it is not clear what this operation means, and how it is implemented at the physical level.

There are also more specific concerns which regard Humphreys' core example of fusion emergence. In developing this example, Humphreys assumes a deep contrast between ionic and covalent bonding that is not warranted by physical chemistry. It is not clear how the the fuzzy boundary between ionic and covalent bonding maps onto the discrete boundary between a compositional and a non-compositional ontology.

Finally, Humphreys' claim that chemistry gives us reasons to reject a compositional ontology is problematic. While it is true that the molecule can be described as the fusion of atoms, if one thinks of the molecule not as a collection of atoms but as a collection of electrons and nuclei, what looks like fusion between two atoms can be described as composition of electrons and nuclei. In fact, chemistry is full of compositional principles: in the molecular orbital theory, each one-electron molecular orbital is expressed as a linear combination of atomic orbitals; the orbital approximation gives us a way of learning about the wavefunction of a multi-electron atom or molecule on the basis of the wavefunctions of the individual electrons; and the Aufbau principle gives us explicit rules of composition for obtaining the electronic structure of atoms and molecules. Given the effectiveness of these rules and principles and the fact that they are compositional *par excellence*, it is premature to conclude that the entities forming the subject matter of chemistry cannot be accommodated within the framework of a compositional ontology.

2.3 Other contemporary accounts

A recent approach to emergence in chemistry is due to Hendry (2006). Hendry's account is based on the classical notion of emergence advocated by Broad. Hendry does not accept McLaughlin's conclusion that there is no scintilla of evidence that there are configurational forces or downward causation in chemistry; he adopts McLaughlin's distinction between resultant and configurational but he formulates it in terms of Hamiltonians, rather than forces. Using the quantum chemistry of the molecule, Hendry aims to show that there is downward causation in chemistry by showing that there are "configurational Hamiltonians" governing the behaviour of molecules.

Hendry asserts that if the behaviour of some systems is governed by configurational (non-resultant) Hamiltonians, then the behaviour of those composite systems is not determined by the more general laws governing their constituents. He argues that to the extent that the behaviour of any subsystem is affected by the supersystems in which it participates, the emergent behaviour of complex systems must be viewed as determining, but not being fully determined by, the behaviour of their constituent parts. This, Hendry contends, is the case in the chemistry of the molecule, where the motions of the atoms are determined by the overall structure of the molecule.

Hendry uses the concrete example of a CO_2 molecule. The motion of the parts of this molecule can be seen as quantum-mechanical harmonic oscillators and rigid rotators. However, this is possible only after we assume a certain structure for the whole molecule. According to Hendry, we use quantum mechanics to explain the motions of parts of the molecule within the context of a given structure for the molecule as a whole (in this case, a linear structure). The problem is that rather than deriving this structure using resultant Hamiltonians, we put it "by hand" – we assume "configurational Hamiltonians". The fact that the motion of the parts of molecule is determined by the overall structure is, according to Hendry, an example of downward causation.

Is the chemical emergence that Hendry's arguments support of a strong kind? If the molecular Hamiltonians are truly configurational and thus fundamental (i.e., not resultant), then the kind of emergence that Hendry's arguments support is strong. If, however, they are resultant, then Hendry's arguments support only weak emergence. The advocate of weak emergence may agree that the molecule as a whole constrains (determines) the motion of its parts. But she may argue that its ability to do so comes from the intrinsic and relational properties of the parts themselves (from the Coulomb attractive and repulsive forces between the parts and various other factors such as gravity, the Pauli principle and relativistic effects). On this view, the use of configurational Hamiltonians is justified for pragmatic reasons (resultant Hamiltonians are just too hard to compute) or epistemic reasons (having to do with their explanatory role), but from an ontological perspective these Hamiltonians are ultimately resultant, albeit often underivable in practice. Nonetheless, Hendry's own view seems to be that the molecular Hamiltonians are not resultant, so in his view the account of emergence that he defends seems to be strong.

Hendry claims that his revision of traditional emergentism is at odds with the causal completeness (or causal closure) of physics – the thesis that "all physical events are determined (or have their chances determined) entirely by prior physical events according to physical laws"(Papineau 1990, p. 67). If chemistry truly denies the causal completeness of physics then it would seem that this constitutes evidence for a strong notion of emergence – presumably, the existence of non-physical but causally efficient properties (such as *sui generis* chemical properties) guarantees that what's true about them cannot be derived from the truths of microphysics. Since the causal closure of physics is grounded in the conservation of energy, it is not entirely clear how a strong version of emergence that denies it may respect this venerable principle of science. Indeed, the argument I brought forward in 2.1.2 against Broad's notion of configurational forces is applicable to Hendry's concept of configurational Hamiltonians as well.

Another emergentist account intended to apply to specifically to chemistry has been offered by Luisi (2002). By the term "emergence" Luisi understands the onset of novel properties that arise when a certain level of structural complexity is formed from components of lower complexity. Luisi emphasizes that molecular sciences, and chemistry in particular, are actually the disciplines in which the notion of emergence has the most obvious applicability. Luisi offers the following examples of emergent properties in chemistry: the aromaticity of a benzene molecule, which is not present in the atoms that form the molecule;

the properties of water and of all other molecules, which are not present in the atomic components; and the oxygen-binding properties of complex chemical structures like hemoglobin or myoglobin which are not present in the single aminoacids.

Luisi considers the following two questions. Can the properties of molecules be explained *a posteriori* from the properties of the components? Can they be foreseen *a priori*? Luisi argues that there are no reasons to think that the liquid properties of water, the aromaticity of benzene, or the folding of myoglobin, cannot be in principle explained or even foreseen on the basis of the properties of the components. Thus, Luisi is entirely committed to token reductionism (explained below). He even goes as far as claiming that the hypothesis that the emergent properties of molecules cannot be explained as a matter of principle on the basis of the components is tantamount to assuming a force of some non-defined nature (Luisi 2002, p. 193). But he points out that in practice, emergent properties are almost impossible to predict. This is especially true for large molecules like myoglobin, in the case of which the 20 different amino acids and a chain length of 153 amino acid residues, gives rise to 20^{153} possible theoretical chains, myoglobin being one of those.

According to Luisi, chemistry offers examples of downward causation, understood as the influence of the relatedness of the parts on the behaviour of the parts themselves. One example that Luisi offers is that of benzene: when a benzene molecule is created, the orbitals of carbon atoms and those of hydrogen are changed; the molecule as a whole affects the properties of its constituents. Of course, it is true that the molecule of benzene could not have emerged if its components did not have the right properties (Luisi does not deny upward causation), but it is also true that once the molecule is formed it constraints the motion of its parts. For Luisi, downward causation is the consequence of upward causation, and once the two exist, they take place simultaneously in a sort of “cyclic” causality. But the kind of downward causation that Luisi endorses differs significantly from the kind of downward causation that the British emergentists talked about; it does not assume any special “configurational” forces at work.

Luisi's account of emergence resembles very much the next account of emergence, due to Mark Bedau (2008), especially when one compares the two authors' views about predictability and downward causation.

A number of contemporary authors have recently proposed concepts of emergence that are applicable to phenomena studied by science in general. Although the examples that these authors refer to come from specific domains (the theory of cellular automata, physics, etc.) these concepts of emergence are applicable to a host of phenomena, including those in the purview of chemistry.

Mark Bedau (2008) thinks that there is not much room for strong emergence in contemporary science, and even if such strongly emergent phenomena existed, they could at best play a primitive role and thus they will be scientifically irrelevant. Bedau defends a version of emergence which he even refers to as "weak emergence". Weak emergence is compatible with the generality of microphysics:

> "Macro entities and their states are wholly constituted by the states and locations of their constituent micro entities, so the causal dynamics involving macro objects is wholly determined by the underlying micro dynamics." (Bedau 2008, p. 161).

But Bedau also recognizes that the global properties of a macro system may influence the behaviour at the micro level. This is a sort of downward causation; however, this kind of downward causation is not the same as the one that is associated with strong emergence. The properties of the macro system (including the causal properties) are a consequence of the properties of the micro systems that compose it, but the derivation is usually hard to obtain. The hallmark of Bedau's weak emergence is that to obtain such a derivation there is no theoretical shortcut: one must resort to simulation. Bedau claims that causal processes in nature are caused by the iteration and aggregation of micro causal interactions. The only way to predict the macro properties of weakly emergent systems is to follow the same steps of iteration and aggregation that nature follows, with the help of powerful computers.

Bedau's examples of weak emergence come primarily from the theory of cellular automata. For example, being a glider gun is a weakly emergent property in the Game of Life – a glider gun is a macro level property, which is realized by a variety of micro level configurations of cells. Thus, Bedau's emergence is compatible with a weak notion of reductionism – *token reductionism*, which claims that all property *instances* are lower level property *instances*; but insofar as it is committed to the idea that the same macro property can be instantiated by a variety of different micro properties (e.g., the glider gun in cellular automata), Bedau's emergence is incompatible with *type reductionism* – the idea that all properties are lower level properties. According to Bedau, explanations that contain emergents (macro explanations) are autonomous in relation to micro explanations – they are overarching explanations that unify an otherwise heterogeneous collection of micro instances.

Concepts of emergence that emphasize context sensitivity, nonlinearity, feedback loops, and the importance of organization between the parts of compositionally complex systems have been presented by William Wimsatt (2000, 2008) and Sandra Mitchell (2010). These accounts of emergence have not been designed to apply to chemistry in particular and they are not at odds with reductionism. This is why those inclined to see reductionism (or at least a strong variant thereof) and emergence as mutually exclusive would not readily embrace these accounts as emergentist. Indeed, what these accounts call "emergence" would in some cases count as "resultance" in the eyes of those who hold more conservative views about what emergence is.[17] However, if one insists on the traditional notion of emergence it may turn out that no phenomena investigated by science meet those strict tenets of emergence, and thus nothing available for scientific study would count as emergent (e.g., see Mitchell 2010). Chemistry is a domain in which a certain type of reductionistic approach has been proven to be tremendously fruitful. But it is also a domain which has been considered as "the embodiment of emergence" (Luisi 2002). Thus, one need not rule out the possibility that the kind of accounts proposed by Mitchell and Wimsatt are applicable to chemistry as well.

Another concept of emergence has been offered by Robert Batterman (2002,

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[17] For a discussion of the distinction between emergence and resultance in the context of British emergentism, see McLaughlin 2008.

2011). Although Batterman's examples of emergence are primarily from physics, his view of emergence could conceivably apply to chemistry as well, and for this reason it is worth mentioning. Batterman distinguishes between two senses of reduction. One may talk of the reduction of one theory to another in the philosopher's sense (e.g., Nagelian reduction, where the laws of a coarse grained theory, are derived from the laws of another theory, which is fine grained); or one may talk of reduction in the physicist's sense (the fine grained theory reduces to the coarse grained theory in the limit of some parameter having a certain value). For example, relativistic mechanics reduces to classical mechanics in the limit in which $\left(\frac{v}{c}\right)^2 \rightarrow 0$. Now, the limiting relations between theories may be *regular* (when the "limiting behaviour" as the parameter tends to a certain value resembles the "behaviour in the limit" where the parameter has that value), or they may be *singular* (when the behaviour in the limit differs markedly from the limiting behaviour). Many pairs of theories are related by singular limiting behaviour: quantum and classical mechanics, the wave and ray optics, statistical mechanics and thermodynamics.

For Batterman, the singular nature of the limiting relations between pairs of theories is indicative of emergence: the behaviour of the system as a certain parameter approaches a certain value is different from the behaviour of the system when that value is reached. When the limiting relations are singular we can expect novel phenomena in the asymptotic regime between the two theories. Often, as in the case of thermodynamics and statistical mechanics, the coarser (higher level) theory can be reduced in the philosopher's sense to the fine grained (lower level) theory only if one makes the assumption that a certain parameter (in this case, the number of particles N) approaches infinity. But real systems are always finite, and a strict derivation obtains only in the thermodynamic limit. As a result, one may speak of the phenomena of thermodynamics as emerging from statistical mechanics. Qualitative changes in the states of matter known as phase transitions (e.g., freezing and boiling water, the transition from the ferromagnetic phase to the paramagnetic phase) are also considered emergent since it proves very difficult (if not impossible) to reduce them to the underlying microphysics if we do not appeal to infinite idealizations.

Batterman's approach pays close attention to mathematical procedures such as renormalization – a mathematical technique for characterizing how the structure of interactions varies with the scale considered. Renormalization reveals how theories at different levels are related, but such relation is not reduction: it turns out that the phenomena studied by the higher level theory are decoupled from those at the lower level.

For Batterman, emergence is also associated with universality or multiple realizability (systems very different at the micro level exhibiting identical macro level behaviour). Multiple realizability shows that lower level explanations cannot adequately account for the convergence of the behaviour of varied systems, and higher level level explanations that ignore the micro-level details are required. In contrast with the classical notions of emergence, Batterman's notion of emergence does not subscribe to the downward causation thesis or to the idea that mereological part/whole relations play a crucial role in emergence.

Chapter 3

Functional emergence

In this chapter I begin to develop a theory of emergence that is, in my view, best equipped to provide a satisfactory answer to the question of what justifies the ontological autonomy of chemistry. For reasons that will become apparent, I will call it "functional emergence". I will begin with a rough and ready characterization of functional emergence and progressively clarify the details of this brand of emergence, including through a number of examples.

The main thesis of functional emergence is the idea that many properties are defined not by a shared microphysical ingredient, but only functionally, by a common behaviour. Take, for example, the property of being an acid (this is one of the examples which will be treated in detail in this chapter). The property of being an acid is defined only functionally, by pointing to a common behaviour of these substances in chemical reactions (the ability to donate a proton) rather than to a shared microphysical ingredient (a H atom, for example).

Functional emergence is committed to the generality of microphysics: e.g, every acidic molecule is a complex microphysical system of interacting electrons, protons and neutrons, all obeying the laws of physics – so unlike more traditional notions of emergence, functional emergence does not recognize the existence of non-physical forces. However, functional emergence agrees that it would be mistake to conclude from this that chemical properties are microphysical properties in disguise.[1] Similarly, functional emergence rejects the idea that if all events are governed by physical laws, then all laws are physical. According to functional emergence, there are genuine chemical properties and laws, which on most accounts of reduction are irreducible to the properties and laws of microphysics (chapter 4 will discuss this in detail). The reason for this is multiple realizability: one and the same chemical property (e.g., acidity) is realized by a variety of microphysical properties (various systems of electrons, protons and neutrons), and thus it cannot be identified with any particular microphysical property. As a result, the laws in which functional chemical properties occur will not be derivable from the laws of microphysics simply because the latter lack the requisite terms. Using the term "emergence" to characterize this kind of functionalism about chemistry is not unjustified: chemical properties are higher level properties, and the general truths about them cannot be derived from the general truths of physics (although this derivation is sometimes available for property *instances*). However, unlike other varieties of emergence, functional emergence does not go as far as to assert the existence of downward causation or deny the causal closure of physics.[2]

The idea that a thing is defined by what it does, and not by what it consists of, was first advocated by Alan Turing, in the foundations of computer science and artificial intelligence (Turing 1950). He thought about it via an analogy with the mathematical concept of a function (Turing 1950, p. 439). Turing's idea was quickly adopted in the philosophy of mind, where it served as a basis for an alternative theory of mind, different from both the identity theory and behaviourism (Putnam 1975b;a, Fodor 1974; 1997). However, functionalism as a theory of the mind has been questioned (starting with Block 1980) and functionalist anti-reductionist strategies in the philosophy of mind encountered a number of complications and obstacles. Among these are the problem of the phenomenal character of experience or *qualia*, the questionable scientific status

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[1] A chemical property is a physical property in disguise if the chemical property is identical with a complex physical property but this identity relation is not obvious.

[2] Downward causation is understood here as the power of a whole to affect its parts that does not originate in the parts themselves.

of folk psychology, and recent empirical findings coming from neuroscience that contradict the multiple realizability thesis in psychology (Bickle 1998, Bechtel and Mundale 1999). The theses of functionalism and multiple realizability have also inspired anti-reductionist arguments in the philosophy of biology (Kitcher 1984; 1999, Kincaid 1990).

This chapter will develop a detailed and rigorous account of functional properties in chemistry – an account that elucidates the nature of functional properties by explicating the contrast between functional and non-functional (constitutive) properties. In this account, the criteria for multiple realizability will be made explicit. The fact that chemical properties can be intersubjectively scrutinized, that they are amenable to measurement, experiment and to a quantitative understanding to a greater extent than those in other special sciences, justifies a more optimistic attitude (see Scerri and McIntyre1997, p. 227; Humphreys 1997b).

Chemistry is the discipline that is in some sense closest to physics, and therefore it is the first domain outside physics itself where we should be able to observe functional properties and irreducibility/emergence, if these truly exist. Despite this, the philosophers interested in the autonomy of chemistry have not given consideration to functionalism and multiple realizability. For example, the volume which was published as a result of the 3rd Erlenmeyer Colloquy for the Philosophy of Chemistry, titled "The Autonomy of Chemistry" (Janich and Psarros 1998) does not even mention functional chemical properties, despite the broad consensus and shared anti-reductionist attitudes among the participants. Other arguments for the autonomy of this discipline (Bunge 1982, van Brakel 2000, Lombardi and Labarca 2005, Scerri and McIntyre 1997) also omit multiple realizability or functionalism. In fact, the idea of multiple realizability that often goes hand in hand with functionalism has been regarded with distrust in the philosophy of chemistry, one major author referring to it as "wishful thinking" (Scerri 2000, p. 406).

These attitudes about functionalism and multiple realizability in chemistry are, in my view, mistaken. In fact – as I will argue – many chemical properties are defined *functionally*, in terms of their efficient roles, and not in terms of their physical constitution. The form of emergence that I defend recruits functionalism's anti-reductionist capacities and is rich enough to justify the ontological autonomy of chemistry.

Unlike psychology, where the multiple realization thesis is a hypothesis (the claim being that properties like pain are multiply realizable), chemistry presents us with properties that are multiply realized.[3] If it can be shown that there are chemical properties that can be defined adequately only functionally, then we have a strong and clear case against property reductionism in chemistry. If there are functional properties in chemistry, they cannot be said to reduce to any constitutive properties, and therefore must be considered as they are, namely *sui generis*, higher-order chemical properties in their own right.

However, a success against reductionism need not mean a success against physicalism. Although chemical functional properties may not be themselves reducible, any *instantiation* of such a property is identical with an *instantiation* of some physical property. This way, physicalism (token physicalism) is preserved, while reductionism (or type physicalism) is resisted.

3.1 Constitutive vs. functional properties

3.1.1 The distinction between constitutive and functional properties

Some properties are defined by "what they are", i.e., by pointing to an intrinsic feature (i.e., a constituent) present in all instances of that property and which explains their distinguishing characteristics. I call these properties and the definitions that such properties receive *constitutive*. A constitutive definition

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[3] In fact, it has been argued that a multiple realizability of psychological states is not well supported by empirical findings. Bickle (1998, ch. 4) emphasizes that most experimental results in contemporary neuroscience indicate continuity of underlying neural mechanisms, both within and across species. Positron emission tomography (PET) and functional magnetic resonance imaging (fMRI) reveal common areas of high metabolic activity during psychological task performance, both across and within individual humans.

is a definition that points to a lower level constituent (a part) that is common to all the entities to which the *definiendum* applies, and explains their behaviour. Showing that a property can be given a constitutive definition is showing that the following steps can be followed.

1) Obtain a description of each type of entity instantiating the property in question in terms of its lower level constituents.

2) Look at the descriptions obtained at step 1 and identify those constituents that a) are common to all entities instantiating the property in question and b) are not shared with any other entities.

3) Find a principled way of explaining how these shared constituents determine the features that characterize the property in question.

4) Only after steps 1-3 are completed can one formulate the constitutive definition and assert the identity of the property in question with the property of being a system possessing the constitutive features found at step 2.

The features that define the property in question mentioned at step 3 are known by consulting the common definition for the property in question. Step 3 is required to ensure that the microphysical features identified at step 2 are not accidental features that just happen to be possessed by all the physical systems in question and only by them. If step 3 is completed then the microphysical features identified at step 2 can be called *microconstitutive*: they are microphysical features that are constitutive of all the systems instantiating the property in question.

To illustrate how a property can be given a constitutive definition, consider the property of being a mammal. The commonly existing definition of a mammal such as the one provided by the Oxford English Dictionary states that a mammal is “a warm-blooded vertebrate animal of a class that is distinguished by the possession of hair or fur, females that secrete milk for the nourishment of the young, and (typically) the birth of live young.” Now let us examine whether one can give a constitutive definition for the property of being a mammal. Being a mammal is a constitutive property if and only if the following steps can be completed.

1) Obtain a description of each type of mammal in terms of its lower level constituents.

Various animals belong to the class of mammals (mammalia). The science of biology can give us a description (an analysis) of each element in this class in terms of its anatomico-physiological features. There is one anatomico-physiological description for dogs, another for humans, another for bats, another for whales.

2) The second step in providing a constitutive definition for the property of being a mammal is to look at the descriptions obtained at step 1 and identify those anatomico-physiological features that a) are shared by all mammals and b) distinguish them from other organisms.

The property that meets both criteria is the property of having mammary glands. Any organism that has mammary glands is a mammal, and any mammal is an organism that has mammary glands.[4]

3) Find a principled way of explaining how having mammary glands determines the features that define or characterize the property of being a mammal.

We need to be sure that the anatomico-physiological features identified at step 2 (mammary glands) are not accidental features that just happen to be possessed by all mammals and only by them. To do this, it is required to show that having mammary glands is related to the features that define or characterize (according to the commonly existing definition) the property of being a mammal. According to the commonly existing definition (be it scientific, from a biology textbook, or lexical, from the dictionary) mammals are distinguished

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[4] Given that in males mammary glands are typically absent, the term “organism” in this sentence should be interpreted as including the male of the pair as well.

from other classes by the fact that the females nourish their young with milk. Milk is a product of the activity of mammary glands. Normally, the mammary glands are fully functional only in females.

4) Only after steps 1-3 are completed can one formulate the constitutive definition and assert that a mammal is an organism that has mammary glands.

Any organism that has mammary glands is a mammal, and any mammal is an organism that has mammary glands. Therefore, the possession of mammary glands is both necessary and sufficient for instantiating the property of being a mammal.[5] Indeed, one can say that the property of being a mammal just is (or reduces to) the property of being an organism that has mammary glands.

One may raise the following question. Commonly existing definitions (be they lexical or scientific) aim to provide the necessary and sufficient conditions for the property defined. But constitutive definitions also claim to isolate the necessary and sufficient conditions. Does this mean that the necessary and sufficient conditions stipulated by the two types of definition are the same? If so, what distinguishes constitutive definitions from commonly existing definitions, be they lexical or scientific?

In response, it should first be recognized that many commonly existing definitions are in fact characterizations or descriptions of the property defined. This is true especially of lexical definitions. In the dictionary definition of mammals mentioned above, some characteristics mentioned in the definition are not necessary. For example not all mammals have their skin covered with hair or fur, monotremes lay eggs, etc. Other characteristics which uniquely

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[5] One may worry that the controversy in the philosophy of biology regarding species as natural kinds prevents us from defining mammals constitutively, as those organisms that have mammary glands. In particular, the worry may be that if biological *species* are defined by a common history (and not by some features present in all members) then the same thing could be said about biological *classes* as well (mammalia included). While there may be ways to defuse this objection (for example, by arguing that the worry does not necessarily extend to biological classes, which are far more general than biological species, being separated from them by three taxonomic ranks), I will instead restrict the scope of my discussion of mammals to currently existing ones. It is then uncontroversially true that, *among currently existing animals,* all mammals and only them have mammary glands.

pick out mammals are not mentioned: two bones in the middle ear called *incus* and *malleus* occur only in mammals. In contrast, constitutive definitions always isolate the necessary and sufficient elements.

Second, even if both the constitutive definitions and the commonly existing ones provide the necessary and sufficient conditions to uniquely pick out the property denoted by the definiendum, it does not follow that the two definitions are identical. This is because they may provide different sets of necessary and sufficient conditions. Take the following two definitions of a square.

> Definition 1: The square is the geometrical figure with four equal sides and a right angle.
>
> Definition 2: The square is the geometrical figure with an area equal to the length of any of its sides multiplied by itself.

Both definitions list properties that are necessary and sufficient to define the square. But these properties mention different things (Definition 1 mentions the right angle, whereas Definition 2 mentions area). However, the two definitions are in a sense equivalent: they pick out the same object, the square. So the definientia of the two definitions are intensionally distinct but extensionally equivalent. The same may happen with constitutive definitions and commonly existing ones.

Third, even if a commonly existing definition provides the necessary and sufficient conditions that uniquely pick out the property denoted by the definiendum, it does not follow that this definition is constitutive: the necessary and sufficient conditions may refer to abstractions or relations, to functions to be fulfilled, or conditions to be met (as in the case of operational definitions), not to microconstitutive features.

Finally, in some cases the commonly existing definition may be in fact constitutive; if this is the case, then we already have a constitutive definition and there is no need to follow the steps above.

Not all properties can be given constitutive definitions. Some properties are defined not by what they are, but by what they do, i.e., they are defined functionally. Functional properties proper are those that can be given only functional definitions. Functional definitions are those definitions that pick out the property denoted by the definiendum via a specification of the efficient role played by that property in the entity instantiating it. The idea is that what makes a functional property the property it is, is the causal role associated with it, and not some constituent shared by all instances of that property. In this respect, functional properties differ fundamentally from constitutive properties, and of course, so do their respective definitions. For every functional property there can be more than one kind of particulars that can carry out the causal role defining that property. Such particulars are the realizers (or implementers, or instantiations) of the considered functional property.

A classic example of a functional property is the property of being a mousetrap. There are many types of mousetraps: springloaded bar mousetraps, "mouth" mousetraps, electric mousetraps, bucket mousetraps, glue mousetraps, etc. There is no microconstitutive property shared by all these devices (so there will be difficulties with step 2). But they are all mousetraps inasmuch as they successfully accomplish the role of trapping mice. The functionalist story has it that anything (any device) that successfully accomplishes this role is a mousetrap – the property of being a mousetrap is said to be multiply realizable.

Functional properties can be seen as second-order constitutive properties, as many philosophers adopting a functionalist view of mental properties prefer to see them. For example, the property of being a mousetrap is a second-order property, namely the property of having some constituent or another that results in mice being trapped. Thus, functional properties are higher-order properties, not reducible to (identifiable with) a particular implementation or realization; the "essence" of being a mousetrap consists in the possession of the ability to realize the relevant causal role, and not in the possession of a constitutive feature shared by all individual realizers.

By contrast, a constitutive property can be reduced to a certain constituent of the things instantiating it, because that constituent is shared by all the instances of the considered property, and possessing that constituent is both necessary and sufficient for instantiating the property in question. Being a mammal reduces to being an organism that has mammary glands, but being a mousetrap does not reduce to being a device that has a spring-loaded bar, for example. To highlight the distinction between properties that are defined by "what they are" and those that are defined by "what they can do", consider this: being a mammal reduces to being an organism that *is* mammary-glanded, whereas being a mousetrap is any device that *can* trap mice.

A couple of things need to be clarified with regard to the type of definition that I propose. First, there is an ambiguity with the word "constitutive". The word may be used to describe the property as such (e.g., as in "Being a mammal is a constitutive property") or the characteristic in virtue of which the property obtains (e.g., as in "Having mammary glands is constitutive of being a mammal").[6] This ambiguity has the potential of obscuring the arguments I will be putting forward and for this reason it must be dealt with. For the sake of clarity, I will continue to refer to the properties that are defined with reference to a common ingredient as *constitutive* properties, but I will use the term *microconstitutive* to refer to those shared features in virtue of which the property obtains. Thus, being a mammal is a *constitutive* property that obtains in virtue of the *microconstitutive* feature of having mammary glands. This choice of terminology is largely conventional as in many cases (including the case of mammals) the shared feature (viz. mammary glands) is not necessarily microphysical.

Second, there is the question of the exact nature of the microconstitutive features that figure in a constitutive definition. What sort of features may be properly considered microconstitutive and what sort of features are excluded? If we pick sufficiently abstract microconstitutive features, couldn't we provide constitutive definitions even for functional properties? In this case, wouldn't the distinction between constitutive and functional collapse? These are all genuine concerns. This is why the features identified at step 2 must meet some

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[6] The distinction between "the property as such" and "the caracteristic in virtue of which the property obtains" matches the distinction between a property and its essential constituents. For example, in the case of mammals, the property of being a mammal is what I call "the property as such", whereas having mammary glands is the characteristic in virtue of which a creature is a mammal.

constraints: they have to be intrinsic and concrete. They cannot be relational or abstract.[7] The constitutive features (or the candidates thereof) must be constituents, i.e., *things* (not relations or abstract features). Discerning when these constraints are met is not easy. However, judging whether a certain feature is an appropriate candidate for being a microconstitutive property can be judged more effectively in the context of concrete situations. The details of the concrete situations that I will be considering will, I hope, make it easier to ascertain whether a certain shared feature is truly microconstitutive.

3.1.2 Functional properties and multiple realization

Equipped with these concepts, we can attempt the following definition of multiple realization. A property T is multiply realized when it has two or more distinct realizations, where distinct realization can be spelled out as follows. Two lower level properties N and M are distinct realizations of a higher level property T if and only if i) the instantiation of either N or M in an individual S is sufficient for the instantiation of T in S (REALIZATION), and ii) there is no microconstitutive property P such that the instantiation of P is sufficient for the instantiation of either N or M (DISTINCTNESS). In other words, a property is multiply realized when it is not constitutive. The existence of a common microconstitutive feature P shared by the lower level realizing properties is determined according to the best mature scientific theories that are applicable to that level.

Since this definition appeals to a scientific theory for ascertaining the distinctness of the realizer properties, a number of examples of multiple realizability that have been traditionally offered could be reevaluated. For example, the claim that psychological properties like pains or beliefs are multiply realized is plausible only to the extent to which there is a mature human and animal neuroscience. The same with the property of being a mouse trap. The prop-

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[7] This must be the case if the property that we are defining is concrete; this requirement does not apply to the case in which the property that we are defining is itself abstract or relational. This proviso is required to allow the possibility of providing constitutive definitions for abstract properties such as mathematical properties.

erty of being a mouse trap has didactical value when it comes to illustrating the thesis of multiple realizability to someone who has never heard of it. But if one adopts the definition of multiple realizability presented above, it could become problematic. Given the definition above, the claim that the property of being a mouse trap is multiply realized receives as much support as the notion that there is a scientific theory that deals with the construction of mice catching devices. While springs and glues may be (and indeed are) of scientific interest (for sciences such as mechanics and chemistry, respectively) one may question that the *devices* that employ them to catch mice hold significant scientific interest. Rigorous talk of multiple realization is best conducted within the framework of an empirical science, and the more established this empirical science is, the more legitimate the talk of multiple realizability becomes.

3.1.3 Constitutive vs. dispositional, constitutive vs. relational

How do functional properties compare with dispositional properties? It may be tempting to think of functional properties as dispositions (in the sense that both are defined by their behaviour). However, this is misleading for the following reason. Many of those who discuss dispositions defend the idea that dispositional properties supervene on intrinsic properties. If one accepts that dispositional properties supervene on intrinsic properties, then this could be incompatible with what I mean by a functional property. Functional properties are multiply realizable, whereas dispositions need not be. For example, the property of being a noble gas is could be considered dispositional (noble gases are disposed to being chemically inert), but it is not functional. Rather, as I will show in the next section, the property of being a noble gas is a constitutive property.

Also, the distinction between constitutive and functional properties does not overlap with the distinction betweeen relational and intrinsic. While some functional properties are relational, not all relational properties are functional. For example, the property of being an object less massive than a given object

X is a relational property, but it need not be functional. It could very well be constitutive: it could turn out that all objects less massive than X are constitutively identical.

3.2 Constitutive properties in chemistry

In chemistry, constitutive properties are those that are given constitutive definitions. Showing that a certain type of chemical property can be given a constitutive definition is showing that the following steps can be followed.

1) Obtain a purely microphysical description of each type of physical system instantiating the chemical property in question.

2) Look at the descriptions obtained at step 1 and identify those microphysical features that a) are common to all physical systems instantiating the chemical property in question and b) are not shared with any other physical systems.

3) Find a principled way of explaining how these shared microphysical features determine the features that define or characterize the chemical property in question.

4) Only after steps 1-3 are completed can one formulate the constitutive definition and assert the identity of the chemical property in question with the property of being a system possessing the microphysical features found at step 2. These features can be now called microconstitutive: they are microphysical features that are constitutive of all the entities to which the definiendum applies.

Step 3 is required to ensure that the microphysical features identified at step 2 are not accidental features that just happen to be possessed by all the physical systems in question and only by them. If step 3 is completed then the microphysical features identified at step 2 can be called *microconstitutive*: they are microphysical features that are constitutive of all the systems instantiating the chemical property in question.

Important chemical properties like being a noble gas, a halogen, an alcohol, an oxide, as well as other chemical properties are defined via constitutive definitions, therefore all such chemical properties can be said to reduce to microphysical properties in this precise sense: they are *identical* with the systems in which a certain microphysical property plays a defining role.

Consider the property of being a noble gas. It can be shown that the property of being a noble gas is nothing more than the possession of a micro-constitutive (quantum-mechanical) property – having a "full" set of electrons on the outer electron shell. Noble gases (helium, neon, argon, krypton, xenon, radon, and the synthesized element ununoctium) are a group of chemical elements that have similar chemical properties: under standard conditions, they are all monoatomic gases with very low chemical reactivity. They occupy group 18 (8A) of the periodic table. In order to show that the chemical property of being a noble gas is identical to a physical property, the steps above can be described more precisely and it can be shown how their completion leads to a constitutive definition for the property of being a noble gas atom.

1) For an isolated atom of each particular noble gas, one needs to obtain a purely microphysical (i.e., quantum-mechanical) description of the nucleus-electrons system representing that atom.

For simple atoms like hydrogen, this quantum-mechanical description can be obtained by solving the Schrödinger equation for the binding energy E and then for the wavefunction ψ. We start out with the (time independent non-relativistic) Schrödinger equation for the hydrogen atom:

$$\hat{H}\psi = E\psi$$

We find that

$$E = -\tfrac{1}{n^2}\tfrac{me}{8\varepsilon_0^2 h^2}$$

where m is the electron mass, e is the electron charge, ε_0 is the permittivity of the vacuum, h is Plank's constant, and n is the first quantum number –

the principal quantum number. By solving Schrödinger's equation for the binding energy we find the value of n. The same procedure can be applied for finding the binding energy for all hydrogenic atoms (e.g., He^+, Li^{++}). The principal quantum number n is the first of the four numbers describing the quantum-mechanical makeup of an atom, and it gives us the binding energy of the electron to the nucleus (it tells us in which "shell" the electron is). An n value of 1 is associated with the ground state of the hydrogen atom. Solving the Schrödinger equation for the wavefunction ψ, we find three more quantum numbers: the angular momentum quantum number, l, that gives us the "shape" of the wavefunction, the magnetic quantum number, m_l, which gives us the energy levels available within a subshell, and the spin quantum number, m_s, which describes the unique quantum state of an electron. Using these four quantum numbers, one can write down the quantum-mechanical description of any nucleus-electrons system – the electronic configuration.

The Schrödinger equation gives us the electronic configuration of all atoms, but as already mentioned, when the number of electrons increases the equations become increasingly difficult to solve exactly and approximate methods are being used. The atoms of noble gases are not simple hydrogenic systems, and except for the simplest noble gas atom, helium, there is no analytical way of solving the Schrödinger equation. Nonetheless, the ground state energy levels of the electrons of the helium atom can be known very accurately using approximate methods like Hartree-Fock and Thomas-Fermi theory (also known as density functional theory). But for our current purposes, how we obtain the quantum-mechanical description of a noble gas atom, is less important. It is perfectly acceptable if the electron configurations are determined experimentally, through the analysis of the atomic spectra. This can be done accurately for the atoms of noble gases, and one way or another we end up with the following quantum-mechanical descriptions:

He	$\mathbf{1}\mathrm{s}^{2}$
Ne	$1\mathrm{s}^{2}\mathbf{2}\mathrm{s}^{2}\mathbf{2}\mathrm{p}^{6}$
Ar	$1\mathrm{s}^{2}2\mathrm{s}^{2}2\mathrm{p}^{6}\mathbf{3}\mathrm{s}^{2}\mathbf{3}\mathrm{p}^{6}$
Kr	$1\mathrm{s}^{2}2\mathrm{s}^{2}2\mathrm{p}^{6}3\mathrm{s}^{2}3\mathrm{p}^{6}\mathbf{4}\mathrm{s}^{2}3\mathrm{d}^{10}\mathbf{4}\mathrm{p}^{6}$
Xe	$1\mathrm{s}^{2}2\mathrm{s}^{2}2\mathrm{p}^{6}3\mathrm{s}^{2}3\mathrm{p}^{6}4\mathrm{s}^{2}3\mathrm{d}^{10}4\mathrm{p}^{6}\mathbf{5}\mathrm{s}^{2}4\mathrm{d}^{10}\mathbf{5}\mathrm{p}^{6}$
Rn	$1\mathrm{s}^{2}2\mathrm{s}^{2}2\mathrm{p}^{6}3\mathrm{s}^{2}3\mathrm{p}^{6}4\mathrm{s}^{2}3\mathrm{d}^{10}4\mathrm{p}^{6}5\mathrm{s}^{2}4\mathrm{d}^{10}5\mathrm{p}^{6}\mathbf{6}\mathrm{s}^{2}4\mathrm{f}^{14}5\mathrm{d}^{10}\mathbf{6}\mathrm{p}^{6}$
Uuo	$1\mathrm{s}^{2}2\mathrm{s}^{2}2\mathrm{p}^{6}3\mathrm{s}^{2}3\mathrm{p}^{6}4\mathrm{s}^{2}3\mathrm{d}^{10}4\mathrm{p}^{6}5\mathrm{s}^{2}4\mathrm{d}^{10}5\mathrm{p}^{6}6\mathrm{s}^{2}4\mathrm{f}^{14}5\mathrm{d}^{10}6\mathrm{p}^{6}5\mathrm{f}^{14}6\mathrm{d}^{10}\mathbf{7}\mathrm{s}^{2}\mathbf{7}\mathrm{p}^{6}$

2) The second step in providing a constitutive definition for the property of being a noble gas is to look at the description obtained at step 1 and identify those quantum-mechanical features that a) are common to all noble gas atoms and b) are not shared with any other atom of a different element.

By examining the electron configurations above and comparing them with those of the other elements in the table, it becomes clear that what fits both conditions is the fact that the atoms of noble gases have their outermost shell (given by the maximum value of the principal quantum number n) filled with electrons (in boldface above).[8] Therefore having a full outer shell is a constituent of all noble gases and only of them.

3) The next step is to find a principled way of explaining how this shared quantum-mechanical feature (having the outermost electron shell filled) determines the features that characterize noble gases (viz., their low reactivity).

As it can be observed from the electronic configurations above, it turns out that the atoms of all noble gases with the exception of He, which has two electrons, have exactly two subshells on the last shell: s and p (second quantum number l is 0, respectively 1). These subshells being both filled, bring up the number of electrons on the last shell to 8, which makes the noble gas atoms conform to the *octet rule*. This rule asserts that atoms tend to be most stable when the

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[8] This is because an s orbital can hold maximum 2 electrons, while a p orbital can hold a maximum of 6 electrons.

outermost electron shells of their constituent atoms contain eight electrons. The octet rule (and the analogous rule for the He atom, the *duet* rule) provide a principled explanation for the very low reactivity of the noble gases: noble gas atoms do not require any more electrons to complete their outer shell.

4) After the steps above have been completed, one can finally assert the identity of the property of being a noble gas atom with the quantum-mechanical property of being an atom with a complete outer shell. One is thus able to formulate the constitutive definition of the noble gas that is found in chemistry textbooks.

One may have a lingering suspicion that the property of having a full outermost electron shell is itself a functional property. This is because the notion of an outermost electron shell sounds functional, due to the adjective "outermost". However, the property of being a full outermost electron shell is in fact a microconstituent of noble gases: a full electron shell is something pretty concrete, that is shared by all noble gases and only by them, that explains their behaviour, and that can be physically removed from the system. Second, even if the property of *being* a full outermost shell were a functional property, it would not follow that the property of *having* a full outermost shell (i.e., the property of being an atom with a full outer shell) is itself a functional property. Consider the property of being a glue, and suppose this property is functional – different glues having different microconstituents (say, made of different chemicals) have the same macro-level property, i.e., they are all sticky. The property of being a glue mouse trap may still be a constitutive property (the shared constituent that plays a crucial role in the functioning of the property being *glue*), despite the fact that this constituent is itself a functional property. The same with mammals: the mammary glands of species X (say, bats) may be truly different in their realization from the mammary glands of species Y (say, whales); thus, being a mammary gland may be a functional property. But this does not entail that the property of being a mammal is itself a functional property: at the anatomical level of analysis, all mammals really do have a constituent in common, namely mammary glands.

At lower levels of analysis, the shared constituent may turn out to depend on heterogeneous mechanisms: the constituents may not consist of the same sub-constituents. But this does not mean that the property originally analyzed is functional. Thinking otherwise may result in a fallacy similar to the fallacy of composition: a forest may be big even if all of its trees are small. I will return to this sort of objection in the first section of chapter 5.

Similar constitutive definitions can be found for the other name-bearing individual groups in the table. Halogens are elements whose atoms have exactly seven electrons on the outermost shell; alkaline earth metals are elements whose atoms have two more electrons on their outermost shell relative to the previous noble gas, etc. The atoms of the elements in these groups show patterns in their electron configuration, and these patterns are responsible for their similar chemical behaviour.

For numerous other chemical properties (especially compounds), providing constitutive definitions is even easier. For such chemicals, one need not look at the quantum-mechanical description of the system, since it is sufficient to examine the molecular structure and identify the individual atoms or functional groups in its constitution. For example, alcohols are those compounds containing the group hydroxyl, OH, which is bound to a saturated carbon atom; sulphones are those compounds containing the functional group sulphonyl, RSO_2R'; carbonates are those compounds containing carbonate ester, ROCOOR', etc.[9] The existence of a functional group in the constitution of the molecule will typically ensure similar chemical properties for all compounds having that group. In general, the same functional group will undergo similar chemical reactions regardless of the molecule to which it belongs.

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[9] The term "functional group" has no semantic connection with "functional property" as described here. In organic chemistry, functional groups are specific groups of atoms within molecules that are responsible for the characteristic chemical reactions of those molecules. In fact, the terminology can be misleading: the presence of a functional group in the constitution of a chemical property instance (a molecule) makes the chemical property in question non-functional in our sense, i.e., it makes it constitutive.

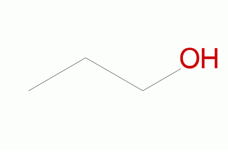
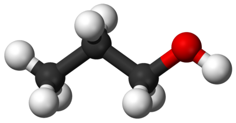
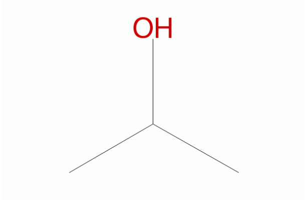
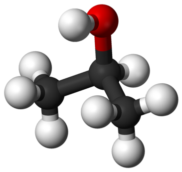
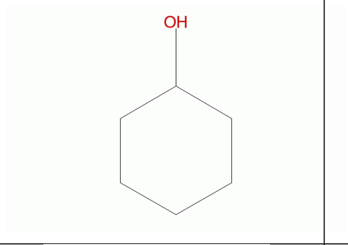
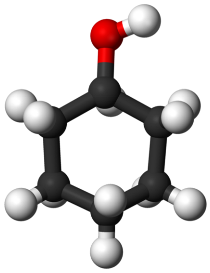
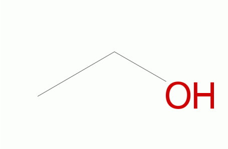
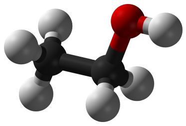
Alcohol	Formula	Structure	Stick-and-ball model
1-Propanol	C_3H_8O		
Isopropyl alcohol	C_3H_8O		
Cyclohexanol	$C_6H_{12}O$		
Ethanol	C_2H_6O		

Table 3.1: Microphysical description of alcohols.

> All alcohols and only alcohols have a hydroxyl group bound to a saturated carbon atom.

3.3 Functional properties in chemistry

3.3.1 Acids and bases

Now consider definitions of chemical properties such as the property of being an acid. According to the Brønsted-Lowry definition, which is the most used, an acid is any compound that can donate a proton to other compound in chemical reactions. Consequently, the Brønsted-Lowry base is defined as a proton receiver.

We first notice that this definition does not resemble a constitutive definition. Unlike noble gases or alcohols, acids and bases are defined not by pointing to a certain microconstitutive feature, but by pointing to what they do in reactions; they are defined by their chemical behaviour relative to the participants in the reaction: acids donate protons, bases accept them. Therefore, the definitions for acids or bases that can be found in chemistry textbooks are functional definitions *par excellence*. But perhaps they need not be; perhaps the property of being an acid (or a base) is defined functionally merely for convenience. Let us see whether acidity and basicity can be given constitutive definitions by following recipe that gave us the constitutive definition for noble gases.

The first step is to obtain a microphysical description of an isolated acidic compound in terms of its constituents, and do so for all acidic compounds. Why does the acid have to be isolated? To be sure that the properties we identify do not depend on the relations of the chemical species in question with whatever is external to it. So the task looks simple: first, make a list of all acids; second, give their microphysical descriptions. In our case, this description may be their structural chemical formula (the Lewis dot-diagram), which gives us the kind, number and charge of the atoms in composition and which also tells us how they are arranged.

Given the requirement that the compound to be described has to be considered in isolation to guarantee that we are investigating constitutive properties, making a list of all acids is not as simple as it sounds. This is because acids are characterized by what they do in chemical reactions, i.e., by their behaviour in relation to the substances to which they react, or in relation to the results of their reaction. For example, Arrhenius acids are defined as those substances which, in aqueous solutions, increase the concentration of hydrogen ions (H^+), bases being those substances that increase the concentration of hydroxide ions (OH^-). Of course, the Arrhenius definition limits acids and bases to substances in aqueous solutions. The Brønsted-Lowry definition does not have this limitation (it includes water-insoluble substances), but ultimately it does not solve our problem. The Brønsted-Lowry acids and bases are defined with reference the products of their reaction: the acid (on the right hand side of the equation) and the corresponding base (on the left side) are referred to as the conjugate acid-base pair. The solvent-system definition of acids does not solve our problem either. According to this definition, an acid is a substance that, when dissolved in an auto-dissociating solvent, increases the concentration of the solvonium cations, and a base is a substance that increases the concentration of the solvate anions. Just like the Brønsted-Lowry definition, this definition extends acid-base reactions to non-aqueous systems, but it does not yield categorical (non-relational) properties: a compound acting as an acid in one solvent may act as a base in another. In fact, the Brønsted-Lowry definition does not yield categorical properties either; amphoteric substances can behave both as an acid and as a base, depending on the substance they react with. The most used example of an amphoteric substance is water, but even substances that are commonly considered strong acids, like sulfuric acid, H_2SO_4, become bases in reaction with super-acids (also known as “magic acids”).

But let’s grant for the sake of the argument that we have a comprehensive and precise list of all acids, and we also possess the microphysical description of each compound on the list. The next step would be to look at these descriptions and identify those intrinsic microphysical features that a) are common to all acids and b) are not shared with any other chemical species. If we take the Brønsted-Lowry definition of acids, the only intrinsic microphysical feature that these compounds have in common is the presence of a hydrogen atom – after all, the ability of donating a hydrogen nucleus presupposes the possession of the nucleus in question. Many 19th century English chemists including Sir Humphry Davy thought this, and for Brønsted-Lowry acids this is correct. But the presence of one (or more) hydrogen atoms in a chemical compound does not guarantee that that compound is a Brønsted-Lowry acid – non-acidic compounds, such as sodium hydride (NaH, a strong base), also have a hydrogen atom. So having a hydrogen atom is a necessary, but not a sufficient condition for being a Brønsted-Lowry acid. Similarly, one may think that Brønsted-Lowry bases have in common the possession of a hydroxyl functional group (OH), consisting of an oxygen and a hydrogen atom connected by a covalent bond. But, while many strong bases have this functional group (e.g., sodium hydroxide, NaOH, potassium hydroxide, KOH, barium hydroxide, $Ba(OH)_2$, other bases don't have it (e.g. weak bases like ammonia, NH_3, methyl-amine, CH_3NH_2, pyridine, C_5H_5N). All that Brønsted-Lowry acids have in common is not a *thing*, but a behaviour:

A1) Acids donate protons in chemical reactions.

A2) Acids in reaction with metals produce a metal salt and hydrogen.

A3) Acids in reaction with metal carbonates produce water, CO_2 and a salt.

A4) Acids in reaction with metal hydroxides and metal oxides produce water and a salt.

This behaviour is shared among all Brønsted-Lowry acids despite the fact that each acid consists of different systems of electrons and nuclei. Similar arguments can be made for substances that qualify as acids according to the other definitions of acidity. Lewis acids, which are defined as any substance that can accept a pair of electrons from another compound which donates it (called a Lewis base), are even more heterogeneous than the Brønsted-Lowry acids. For example, boron trifluoride, BF_3, tin tetrachloride, $SnCl_4$, and even the proton, H^+, are all Lewis acids, although they don't appear to have anything microconstitutive in common. The same thing can be said, *mutatis mutandis*, about bases.

3.3.2 Oxidants and reductants

Another examples of functional properties are the property of being an oxidant and that of being a reductant. Oxidants (also named oxidizing agents, or oxidizers) are substances that accept electrons from another substance in chemical reactions (redox reactions), while reductants (also called reducing agents, or reducers) are substances that donate electrons. The substance that loses electrons (the reductant) is said to be oxidized by the oxidizing agent. The substance that gains electrons (the oxidant) is said to be reduced by the reducing agent. As a result of the oxidation process, the oxidation state of the reducing agent (i.e., the hypothetical charge that an atom would have if all bonds to atoms of different elements were completely ionic) increases, and the oxidation state of the oxidizing agent decreases.

Take, for example, the combustion of hydrogen in oxygen.

$$2\,H_2 + O_2 \longrightarrow 2\,H_2O + \text{Heat}$$

To make the oxidation numbers explicit, the equation is rewritten as

$$2\,H_2^0 + O_2^0 \longrightarrow 2\,H_2^{+1}O^{-2} + \text{Heat}$$

This is a redox reaction. Hydrogen, which on the left side of the equation has the oxidation state of 0 loses electrons to oxygen and acquires the oxidation state of +1.

$$2\,H_2^0 \longrightarrow 2\,H_2^{+1} + 4\,e^-$$

Hydrogen has been oxidized by oxygen, which in this particular reaction acted as an oxidant.

Oxygen, on the other hand, has gained electrons. It moves from the oxidation state of 0 to an oxidation state of -2.

$$O_2^0 + 4\,e^- \longrightarrow 2\,O^{-2}$$

Oxygen has been reduced by hydrogen, which in this particular reaction acted as a reductant.

Originally the term oxidation was used to refer to a reaction in which a chemical substance combined with oxygen; oxidation meant the formation of oxides. However, the term came to refer to a general process that happens when a chemical species combines with a range of substances of which oxygen is one example. It is true that when a chemical species combines with oxygen, it tends to loose electrons to the oxygen. But this process of electron loss may also happen in the absence of oxygen; many different substances have the ability to remove electrons from other chemical species.

For example, in the reaction above the role of oxygen as an oxidizing agent may be played by another substance, e.g., chlorine. It is true that hydrogen burns in oxygen, but it also burns in chlorine:

$$2\,H_2 + Cl_2 \longrightarrow 2\,HCl + \text{Heat}$$

which is also a redox reaction:

$$2\,H_2^0 + Cl_2^0 \longrightarrow 2\,H^{+1}Cl^{-1} + \text{Heat}$$

In this case hydrogen has been oxidized not by oxygen, but by chlorine, which acted as an oxidizing agent. Chlorine has been reduced by hydrogen, which acted as a reducing agent. Therefore the term oxidation no longer means the formation of oxides, but the loss of electrons. Similarly, the term reduction originally meant a reduction in the amount of oxygen in a substance (e.g., the removal of oxygen from cupric oxide when cupric oxide and hydrogen react to form copper and water). The term reduction also came to refer to the general process of gaining electrons in a chemical reaction, whether or not oxygen itself was the substance which gained them. As mentioned, different substances play the role of oxygen in redox reactions, i.e., there are other oxidizing agents besides oxygen:

- Halogens such as F, Cl, I, Br
- Acids such as nitric acid, HNO_3, sulfuric acid, H_2SO_4, peroxymonosulfuric acid, H_2SO_5, peroxydisulfuric acid, $H_2S_2O_8$
- Salts like permanganate, MnO_4
- Oxides like nitrous oxide,N_2O or silver oxide Ag_2O

Despite having heterogeneous microconstitutive features, oxidants behave similarly in chemical reactions:

O1) Oxidants accept electrons from the chemical species to which they react.

O2) Oxidants react with metals, producing oxide(s) and/or salt(s) of the original metal; this process is known as corrosion.

O3) Oxidants degrade the substances that come in contact with (this is especially of concern in biology, since they damage large molecules like DNA and promote ageing).

O4) Oxidants make possible the combustion of chemical substances. They react with hydrogen or hydrocarbons to give off carbon dioxide or water and heat; once a metal is ignited, oxidants promote its combustion, the result being a metal salt.

3.3.3 Piezoeletrics

When subjected to mechanical stress, some materials generate an electric potential on their surface (polarization) or undergo a change in polarization direction. This is called the direct piezoelectric effect. Conversely, if an electric field is applied on their surface, they experience a deformation (strain). This is called the converse piezoelectric effect.[10] One notices right away that piezoelectricity is defined functionally, by pointing to a common behaviour of certain materials when they are subjected to certain conditions: a material is said to be piezoelectric if it “experiences mechanical deformations when placed in an electric field and becomes electrically polarized under mechanical loads” (Yang 2005, p.10).

The piezoelectric effect is defined by the following equations:

$$P = dT \tag{3.3.1}$$

$$S = dE \tag{3.3.2}$$

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[10] Most of the time, the term “piezoelectricity” is used to refer to the direct effect.

The first equation says that that the polarization of a material (P) depends on the stress applied (T) and on some piezoelectric coefficient (d). The second equation says that the strain (S) experienced by the material depends on the piezoelectric coefficient and on the intensity of the electric field applied (E). Polarization is the charge per unit area developed on the surface: $P = Q/A$. Stress is the force per unit area acting within a material: $T = F/A$. Stress can be thought of as the internal resistive response of a material to an externally applied pressure. Strain is the change in shape of an object in response to stress. Strain is defined as the change in length relative to the original length of an object: $S = \triangle L/L$.

It is important to point out that the definition above is phenomenological (it describes the observed relations between magnitudes like the intensity of the electric field, stress, strain and polarization) and it is completely agnostic regarding the mechanism that may be responsible for such relations; in principle, the same relations could be rendered true by different microphysical mechanisms. In this sense then, piezoelectricity can be characterized as a quite general electromechanical phenomenon.

Piezoelectricity is exhibited by a number of materials with diverse physicochemical constitutions, such as natural and synthetic crystals, and materials of biological or synthetic origin. I will investigate how piezoelectricity arises in crystals and in materials of biological origin such as bone and argue that piezoelectricity cannot be reduced to a particular micro-constitutive property shared by all these materials. If this is the case, then piezoelectricity should be regarded as a functional, higher level property of material systems, irreducible to other (lower level) properties.

Discovered by the Curie brothers in 1880, the theory of piezoelectricity underwent a development reverse to that of most fields of physics. While the phenomena in most fields of physics were explained successfully by corpuscular assumptions, piezoelectricity did not reveal any direct relation to microphysical processes (Katzir 2003). In fact, the attempts to explain piezoelectricity in microphysical (molecular) terms were largely unsuccessful because they did not save the phenomena. In 1890 the early molecular model of piezoelectricity was superseded by a phenomenological theory. According to Woldemar Voigt, who developed it, in such a theory "a small number of principles, i.e., rules derived from experience and ascribed hypothetical general validity, support an edifice of mathematical conclusions that yields the laws of the phenomena in the field concerned".[11] Eventually, the microphysical approaches caught up in terms of empirical adequacy with the phenomenological one, and today we have a good understanding of the microphysical processes that give rise to this phenomenon in various materials. However, as I will be showing later on, these microphysical explanations of piezoelectricity differ from material to material.

3.3.3.1 Piezoelectricity in crystals

I will start by examining how the piezoelectric effect arises in quartz. Quartz exhibits significant piezoelectric properties. If a force of 2 kN (500 lbf) is applied to a 1 cm^3 piece of quartz, a voltage of 12500 V will be produced. How can this be explained?

Quartz is a mineral composed of silicon and oxygen and it belongs to the trigonal crystal system, trigonal-trapezohedral class. In a quartz crystal, for every silicon atom, there are two oxygen atoms, so quartz's overall chemical formula is SiO_2. Every oxygen atom is connected to two silicon atoms, and every silicon atom is surrounded by (and connected to) four oxygen atoms. The oxygen atoms form tetrahedra which include a silicon atom at their center. These are the referred to as the SiO_4 tetrahedra. A network of tetrahedra (a motif) forms the crystal unit cell – a unit whose repetitive translation in three dimensions generates the crystal.

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[11] Woldemar Voigt, "Phänomenologische und atomistische Betrachtungsweise," in Katzir (2003, p. 70).

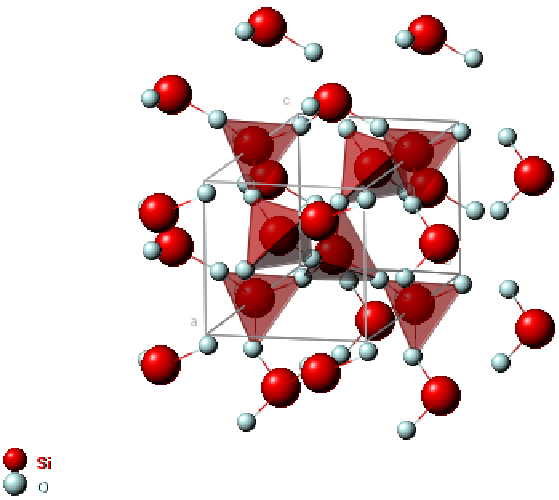

Figure 3.3.1: Quartz unit cell.

Rendered at webmineral.com.

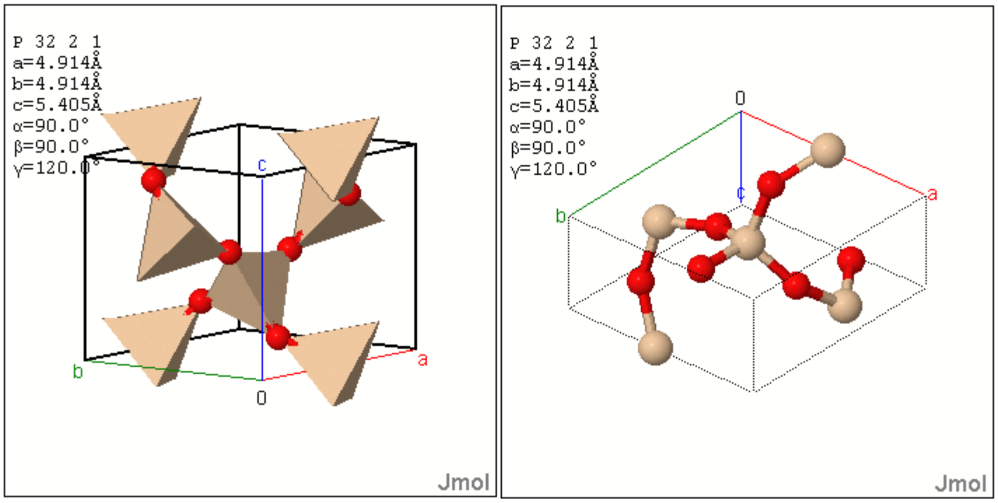

Figure 3.3.2: Different views of a quartz unit cell.

View of a quartz unit cell with emphasis on tetrahedra (left) or with an emphasis on chemical structure (right). Rendered with Jmol.

Unlike other piezoelectric materials (e.g., Rochelle salt), quartz is not ferroelectric, i.e., it does not have a spontaneous electric polarization. Oxygen is more electronegative than silicon but the fact that the oxygen atoms are equally distant from one another and from the central silicon atom does not allow the formation of a net dipole moment in the individual tetrahedra. From an electrical point of view, each SiO_4 group may be seen as a sphere that has a negatively charged shell (due to the four electronegative oxygens) and a positively charged core (the silicon atom that has lost some of its negative charge to the four oxygens and it has become a cation).

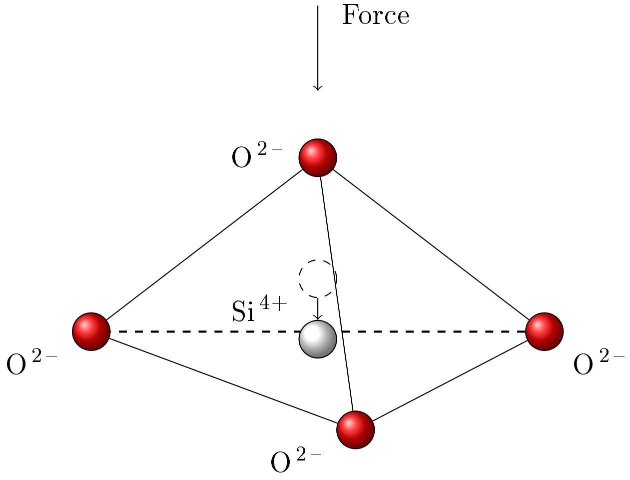

Figure 3.3.3: A deformed SiO_4^{4-} tetrahedron.
The central Si^{4+} ion is moved from the center closer to the base.

If, however, mechanical stress is applied, the tetrahedra become deformed.[12] The central silicon atoms are pushed away from the centre and closer to one of the four sides of the SiO_4 tetrahedron, creating a net dipole moment in each tetrahedron. This takes place in all the tetrahedra of the crystal unit cell. In quartz the dipole moment of one tetrahedron is not cancelled out by the dipoles of the other tetrahedra in the unit cell, and a net induced dipole moment arises in each unit cell. By summing up the dipole moments per unit cell, one may calculate a net polarization for the macroscopic crystal sample.

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[12] At this point the SiO_4 tetrahedra become SiO_4 polyhedra, as the edges become unequal under stress. However, for the sake of clarity and simplicity, I will continue to refer to the deformed SiO_4 tetrahedra as SiO_4 tetrahedra.

In quartz, therefore – as well as in all other piezoelectric crystals – piezoelectricity is realized by a displacement current which arises in the crystal as a consequence of the displacement of atoms (ions) under the application of an external mechanical stress (Tichy et al. 2010, p. 1). Displacement current does not involve a flow of charged particles (a current flow), but the formation of electric dipoles which create an effect similar to the flow of charges.

Another example of piezoelectric crystal is sphalerite (Zn,Fe)S. Sphalerite contains neither silicon nor oxygen. Also, sphalerite differs from quartz in that it crystallizes in the isometric system, hextetrahedral class. Unlike quartz, the unit cell of sphalerite is a cube. Nonetheless, when subjected to mechanical stress, sphalerite exhibits electric polarization.

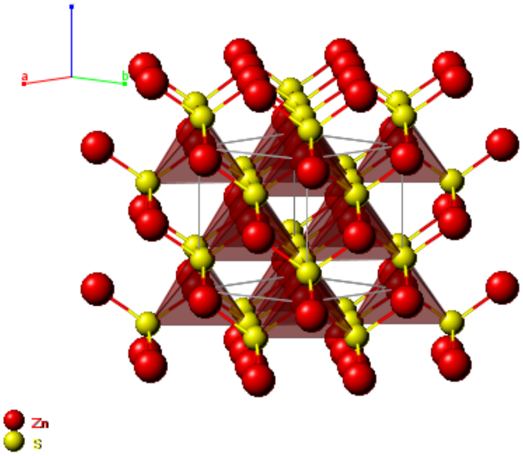

Figure 3.3.4: Sphalerite unit cell.

3D model rendered at webmineral.com.

Yet another example of piezoelectric crystal is hilgardite, $Ca_2B_5O_9Cl(H_2O)$. Hilgardite crystallizes in the triclinic system, pedial class. Unlike quartz or sphalerite its atoms do not form tetrahedra, but more complex polyhedra. Despite all these differences, hilgardite is piezoelectric.

Out of the 32 crystal classes, 20 exhibit piezoelectricity. Now one may ask the following question: why, despite all these differences in structure and constitution, these crystals exhibit similar electrical behaviour (electrical displacement) under stress? It is obvious that the type of the elements in the constitution and structural aspects such as the shape of the crystal unit or the shape of polyhedra that atoms form are not relevant. What is relevant is certain symmetry aspects that obtain in all piezoelectric crystals: they are all noncentrosymmetric. Noncentrosymmetry is the absence of an inversion center in the crystal. More precisely, the condition that for every point (x, y, z) in the in the space group of the crystal there is an indistinguishable point (-x,-y,-z) to which the original point can be mapped, fails to be satisfied. If the crystal is centrosymmetric, the charges developed as a result of strain cancel each other and the result is a zero net dipole moment. So noncentrosymmetry is a *sine qua non* condition for being a piezoelectric crystal.

Then haven't we succeeded in reducing the piezoelectricity of crystals to the property of being noncentrosymmetric? Can't we formulate a constitutive definition of piezoelectricity, at least for crystals? I think that an affirmative answer is problematic. First, although centrosymmetry is a sufficient condition for the absence of piezoelectricity, noncentrosymmetry is not a sufficient condition for piezoelectricity. Crystal class 432 (isometric hexoctahedral) is noncentrosymmetric, but it is not piezoelectric. The reason is that the class still has a sort of symmetry (axial symmetry) that forbids a net polarization: the charges developed along certain axes in the crystal cancel each other. Second, noncentrosymmetry, like symmetry, refers to the relations between the constituents of a crystal, not to the constituents themselves; it is a structural property that occurs at the scale of the crystal unit cell, not at the scale of the atomic microconstituents of the crystal (nodes). For this reason, there are many ways in which a crystal can fail to be centrosymmetric. The structure of quartz is very different from the structure of sphalerite, for example, but both are noncentrosymmetric; both quartz and sphalerite fail to satisfy the condition above, but each does it in its own way. Noncentrosymmetry is not a microconstitutive property; it is a structural/relational property which is multiply realized.

This mechanism that gives rise to polarization in crystals (i.e., electric displacement) is what some authors call "classical" piezoelectricity. The hallmark of classical piezoelectricity is the occurrence of a displacement current as a consequence of applying mechanical stress. The definition of piezoelectricity formulated by authors like Yang certainly covers "classical" piezoelectricity, but need not be restricted to it. Moreover, for our purposes, it is important not to confuse piezoelectricity as a phenomenological occurrence with the mechanisms that give rise to it, displacement current being the most widely known mechanism and the first to be investigated in solids.

3.3.3.2 Streaming current as a source of piezoelectricity

When a solid (e.g., a piece of metal) is placed into a liquid (e.g. an electrolyte), the surface of the solid becomes charged.[13] This charged layer electrostatically attracts oppositely charged ions (counterions) from the liquid, and a second layer forms – the diffuse layer, which is like a cloud of ions and counterions. The concentration of counterions in the diffuse layer decays with distance from the surface: the part of the diffuse layer that is adjacent to the surface charge contains predominantly counterions; as one moves away from the surface charge and towards the bulk of the liquid, regions with mixed charges will be encountered. The two parts of the diffuse layer are separated by the "slip plane" – a plane separating the relatively stationary counterions adjacent to the surface charge from the mixed mobile charges in the rest of the diffuse layer. The potential difference between the bulk of the liquid and that which exists at the hydrodynamic slip plane is termed the zeta potential.

If pressure is applied to the liquid, the motion of the ion-containing liquid along the slip plane produces an electric potential, which is called the streaming potential. Conversely, when an electric potential is applied across a porous material or a capillary tube, the liquid filling that material or tube is set in motion (the process is called electroosmotic flow).

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[13] The mechanism responsible for this is either ion dissociation, complexation or adsorbtion.

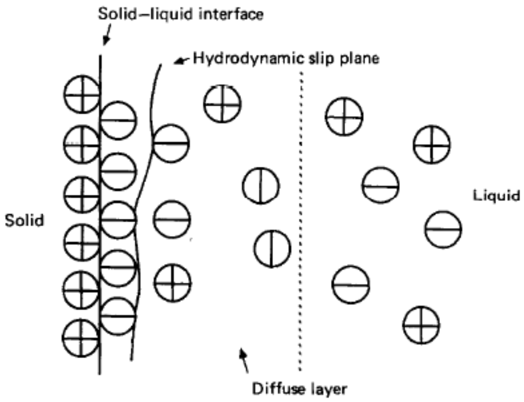

Figure 3.3.5: The electric double layer.

From Hastings and Mahmud (1988).

The potential associated with the the electric double layer has been found responsible for the piezoelectric response of some polymeric materials, gels and liquids (Lewis 1994, Fukada 2000, Lewis et al. 1992). In experiments with liquids like glycol, glycerin, or gels such as agarose (a polysaccharide polymer), both the direct and the converse piezoelectric effect have been detected.

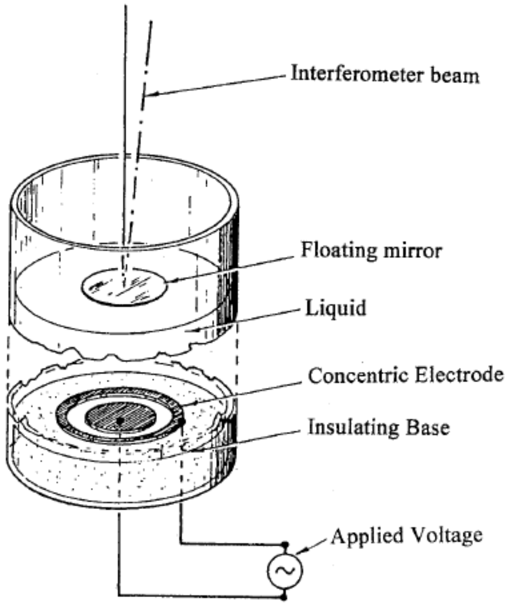

Figure 3.3.6: An experimental setup to show interfacial piezoelectricity due to the streaming current in gel or liquid.

From Lewis et al. (1992), Fukada (2000).

When the liquid or gel is subjected to an applied voltage using circular metal electrodes, the mobile ions in the diffuse layer of the liquid are set in motion along the field lines connecting the inner and outer electrodes.

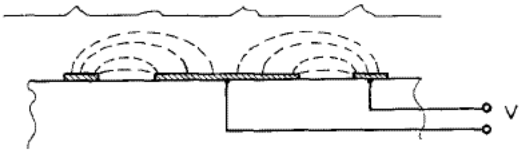

Figure 3.3.7: The electric field pattern between the electrodes generated in the gel or liquid.

From Lewis et al. (1992).

As a result of this motion, a shear wave is generated in the liquid or gel. The mechanical disturbance is propagated throughout the rest of the medium. The displacement of the medium is measured with the use of an interferometer beam and a mirror that floats on the medium's surface. If an alternating voltage from a variable-frequency generator is applied to the electrodes, a cyclic movement of the liquid or gel is registered.

Conversely, mechanical disturbances (vibrations) in the medium result in the occurrence of an electrical potential between the electrodes that can be measured. When vibrations are applied to the gel, the ions in the diffuse layer move relative to the slip plane of the double layer, thereby inducing a current in the electrode circuit. As expected, transverse shear vibrations will be particularly effective in inducing currents. All this shows that the charged double layer can be the source of piezoelectricity (Fukada 2000, p. 1280).

The solid-liquid interface presented above is an integral aspect of the microscopic structure of many natural or artificial composite materials that are classified as solids. Sun et al. (2004) have investigated the piezoelectric properties of hardened cement paste. The mechanism that they found responsible for the piezoelectricity of cement is the streaming current of ions (Ca_2^+, Na^+, K^+, OH^-, SiO_4^{2-}, etc.) present in the water flowing through the capillary pores of the specimens.[14] When compressive stress is applied to the specimen, water is forced through microchannels of the material. The ions in the mobile part of the electrical double layer flow along micropores, which causes the streaming current which results in the polarization of the specimen. Sun et al. concluded that "the mechanism of piezoelectric effect in hardened cement paste is different from that in other piezoelectric materials such as piezoelectric ceramics" (Sun et al. 2004, p. 719).

The examples examined so far show something interesting about the nature of piezoelectricity. They show that one and the same macroscopic phenomenon is carried out by different microscopic mechanisms in different materials. In solid-liquid interfaces and in composite materials in which such interfaces are an integral part, the electric dipole arises as a result of a streaming current of ions. In crystals, on the other hand, the electric dipole arises as a result of a displacement current which is in turn caused by atomic displacement. Unlike

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[14] Water is an integral part of hardened cement. The specimens analyzed by Sun et al. were hardened cement cubes kept in air for a year before testing.

streaming (conduction) currents, displacement currents do not involve the flow of ions. However, the net result of the existence of displacement currents is identical to the effect which arises from the existence of streaming currents: they both generate electric dipoles in the material when it is subjected to mechanical stress. In materials whose microstructure contains solid-liquid interfaces the piezoelectric effect depends crucially on the existence of an electric double layer. However, the electrical double layer does not play a role in the piezoelectric effect in crystals simply because in crystals it does not occur. The piezoelectric mechanism in materials like cement is genuinely different from the piezoelectric mechanism in crystals or ceramics.

3.3.3.3 Piezoelectricity in bone

Bone too exhibits electrical surface polarization if placed under mechanical stress. Bone is a biphasic material whose structural complexity extends down to the molecular level. One phase is organic, consisting of collagen fibrils – long-chain fibrous proteins produced by the bone cells (osteocytes) and deposited in a highly organized pattern that determines the gross structure of each bone. The other phase is inorganic, consisting of hydroxylapatite $Ca_{10}(PO_4)_6(OH)_2$ – a microcrystaline mineral that is deposited naturally on the collagen fibers. The piezoelectric effect in bone cannot be attributed to the hydroxylapatite, which is centrosymmetric (Marino et al. 1971). Instead, the piezoelectricity of bone has been linked to collagen (Fukada and Yasuda 1957).

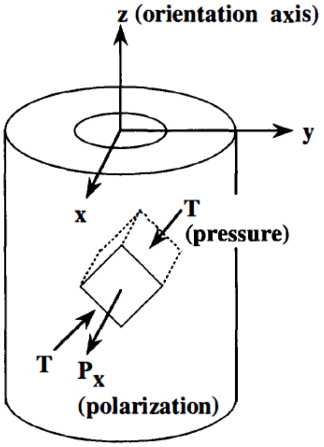

Figure 3.3.8: A cubic sample cut from a long bone.

The pressure, T, in the yz plane produced the polarization along the x-axis . FromFukada (1995).

The collagen molecule is made up of three polypeptide strands (alpha chains), each having the conformation of a left-handed helix. The three helixes form a right-handed triple helix which is held together by hydrogen bonds. These triple helixes make up the collagen molecule. Collagen molecules are arranged in a five-stranded pattern to form a microfibril. An ordered array of these microfibrils makes a collagen fibre. In bone the fibres are mineralised with hydroxylapatite which is cemented to the collagenous surface.

The origin of the piezoelectric effect of collagen is similar to that of other polypeptide molecules. Inside the molecule, the dipoles of the CO and NH groups point roughly in the same direction. If the helix is sheared, the direction of each dipole makes a slight rotation, and the polarization direction changes.This results in electric polarization in the direction perpendicular to the shearing plane (Fukada 1968, p. 229).

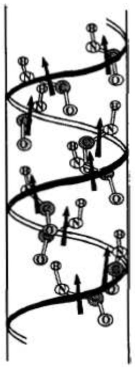

Figure 3.3.9: The alpha-helix of polypeptides.

From Fukada (1995). The piezoelectric effect results from dipole rotations.

The piezoelectric properties of wet bone differ from those of dry bone. In wet (or *in vivo*) bone the presence of water increases the symmetry of the collagen molecules and thus decreases the piezoelectric response of collagen. Nonetheless, the piezoelectric properties of bone collagen persist even in fresh, physiologically wet, bone. This is because the hydroxylapatite crystals prevent access of water to parts of the collagen fibers. Thus the collagen in bone is considered to retain a lower symmetry and to continue to show some piezoelectricity even when the bone is fully hydrated (Anderson and Eriksson 1970). However, the magnitude of the signals observed in bent wet bone have been found to be several orders of magnitude larger than one would expect from the piezoelectric properties of collagen fibers (Johnson et al. 1980). The mechanism responsible for this difference has been found to be streaming potential (Anderson and Eriksson 1970, Gross and Williams 1982, Otter et al. 1985). The occurrence of streaming potentials in bone is made possible by the electrical double layers which occur in the channels and micropores of bone. When pressure is applied, the electrolytic fluid that is naturally present in the bone is forced through the capillaries of the bone, giving rise to a streaming current which leads to the separation of charge. Studies have found that the magnitude of the stress-generated potentials in bone depends on the type of fluid in the capillaries, thereby confirming the presence of streaming potentials

(Pienkowski and Pollack 1983).

If a living bone (e.g., femur) is bent in cantilever mode, the transverse capillaries are inhomogeneously strained. On the convex surface of the bone that results from bending they are subjected to tensile stress, while on the concave surface, they are compressed. As a result, the transversely running channels will increase in diameter (they will open) on the convex side and will decrease in diameter (they will close) on the concave side. This will force the extracellular fluid contained within the capillaries toward the convex surface. Because the extracellular fluid in bone carries a positive charge, the convex surface will become positively charged with respect to the concave surface (Eriksson 1974).

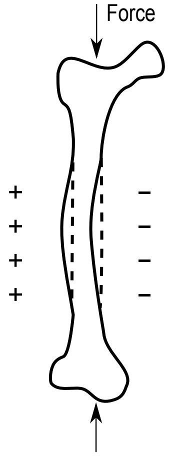

Figure 3.3.10: Bent femur bone.

Bent bone develops positive charges on the convex side and negative charges on the concave side.

Despite the fact that the main mechanism of piezoelectricity in wet bone is very different from that of crystals, the electrical response to mechanical stress is similar from a phenomenological point of view. The similarity becomes striking when one considers that, in addition to the direct effect, wet bone exhibits the converse effect: electric potential applied on surface of fresh femur bone make it deform, just as crystals do (Aschero et al. 1996).

3.3.3.4 A philosophical disagreement among scientists

In a study of viable human cortical bone maintained *in vitro*, Black (1974) referred to the electric potential of mechanically deformed bone not using the term "piezoelectricity" but that of "strain-related potential". In the discussion period following a presentation of this study, Dr. Black was questioned by Dr. Williams about the use of this terminology. I find the discussion illuminating with respect to the concept of piezoelectricity and I reproduce it below (excerpted from Black and Korostoff 1974, p. 199-120).

> DR. W. S. WILLIAMS: You state that the strain, rather than the stress, is correlated with the voltage. Is it really necessary to apply a new term when the mechanism of production, in fact, seems to be piezoelectric?
>
> DR. BLACK: Yes, this is one of my pet peeves. I have spent a few years reading in this field and am now convinced that we have become very sloppy in the jargon. I would suggest that we retain the term piezoelectric for Voight's (sic) original classical definition. That is, if one can find a crystalline repeating phase in which potential is generated as a result of strain due to separation of the apparent charge centers, I'm perfectly happy to call that phase piezoelectric. For other phenomena, my temptation is to invent new words. I believe that confusion has resulted because Dr. Fukada originally described the effect phenomenologically, with the general idea that one applied strain and saw resultant polarization. I don't think he intended to imply a detailed knowledge of the mechanism at that time. In fact, I don't believe that the mechanism he reported for this behaviour in synthetic membranes, for example, was theorized by Voight when he originally wrote his treatise in piezoelectricity. I think we do both the biologists and the physicists disservice by using the word carelessly, so I would much rather use the term "strain-related" in cases where we do not understand exactly what is occurring.

> DR. WILLIAMS: The word, however, derives from pressure, which suggests a wide variety of possible responses. Indeed, Voight's calculations apply strictly to mineral crystals. Conversely, we have heard much evidence that other materials do exhibit this same general effect. Probably, with a very slight modification, this concept could be encompassed within the term piezoelectricity, which specifies and carries more information than strain-related potential. It does suggest a mechanism, namely, the separation of charge in some sense.
>
> DR. B. ROSENBERG: May I suggest that the history of science indicates that difficulties of nomenclature should always be relegated to a committee to resolve rather than be discussed.

Rather than being something like an administrative issue, capable of being resolved by a committee (possibly by mere convention), the "difficulty of nomenclature" would benefit from philosophical attention. In truth, the disagreement between Dr. Black and Dr. Williams is a little deeper than merely terminological – it is conceptual. Dr. Black's reluctance of using the term "piezoelectricity" for the polarization of mechanically deformed bone stems from adopting a constitutive view of piezoelectricity. For Dr. Black, piezoelectricity refers to a mechanism (conduction current resulting from the separation of charge centers), and not to a phenomenological occurrence; for him, piezoelectricity means "classical" piezoelectricity, namely piezoelectricity as it occurs in crystals. For this reason, the polarization produced by any other means would not count as piezoelectric. Dr. Black would rule out that the electromechanical behaviour of polymers (as investigated by Fukada) and that of materials rich in solid-liquid interfaces (such as bone) is in fact piezoelectric, even if the mathematical aspects of this behaviour obeys the same equation that governs the electromechanical behaviour of crystals. Dr. Williams, on the other hand, entertains a functional concept of piezoelectricity. For him, piezoelectricity is primarily a phenomenological occurrence (a phenomenon, a behaviour), not a mechanism; for him, piezoelectricity is defined functionally, as the separation of charge under applied mechanical pressure. Dr. Williams would have no problems classifying the electromechanical behaviour of materials other than crystals as piezoelectric.

Unless we want to conflate a phenomenological occurrence with the mechanism producing it, the point made by Dr. Williams stands. Consider the electromechanical properties of wet bone. They are due to the superposition of two distinct mechanisms: dipole rotation in the collagen molecules and the streaming potential in bone micropores. It is remarkable that despite the different nature of the two mechanisms and the differences in magnitude between them, the phenomenological characteristics of these two mechanisms are essentially identical, making it difficult to discern between them – both mechanisms relate the predicted voltage to the same component of the stress tensor, and both produce currents that are proportional to the strain rate (Gross and Williams 1982, p. 277).

3.3.3.5 "Promiscuous" laws

It has been long known that bone is an adaptable tissue, able to being remodeled by mechanical forces. If loading on a particular bone is increased, in time the bone will adapt as to resist the increased loading. Conversely, if the loading on a particular bone is decreased, the bone becomes weaker.[15] This empirical regularity was first theorized in the 19^{th} century by the German anatomist and surgeon Julius Wolff, and it came to be known as Wolff's law. According to Wolff's law, bone is deposited and reinforced at areas of greatest stress. Wolff's law is an empirically observed regularity which seems intuitive from a clinical point of view. From an engineering point of view, however, it implies that bone has some sort of transduction mechanism that connects the mechanical stress experienced by the bone with the osteogenic activity. Piezoelectricity is a mechanism that is fit for this task. The magnitude of polarization depends on the amount of stress experienced by the bone; in turn, many cellular activities depend by the electrical environment at the

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[15] The increase in bone strength occurs in the racket-holding arm of tennis players and the decrease of bone strength occurs in astronauts who have spend considerable amounts of time in space.

cell's membrane.[16]

Studies have confirmed the formation of new bone close to areas where a steady electrical negative charge is maintained (Rubinacci and Tessari. 1983, Friedenburg et al. 1971). As mentioned, the streaming potential in living bone bent in cantilever mode results in a negative charge on the concave side of the bone and a positive charge on the convex side. A similar polarization of bone may be caused by the mechanical deformation of collagen. Studies have shown that the compressed internal surface of the demineralized bone (collagen) attract calcium ions which leads to subsequent nucleation and crystallization of hydroxylapatite; no bone growth was observed on the tensed, positively charged side of collagen (Noris-Suarez et al. 2007).

The consensus among scientists seems to be that the mechanism of bone growth and remodeling depends on both the electromechanical properties of collagen and the streaming potential of bone (Ahn and Grodzinsky 2009). Thus, bone growth does not discriminate between the negative charges due to the mechanical deformation of the collagen fibers and the ones due to the streaming potential. For this reason, Wolff's law may be characterized as "indiscriminate" or "promiscuous". Promiscuous laws are regularities that correlate two properties, at least one of which is (or is the result of) a heterogeneously realized functional property. Wolff's law correlates bone osteogenic activity with the presence of negative charges induced by mechanical stress, but it is insensitive to how these stress-induced charges are brought about; it links bone growth to electric charges, but it is indifferent to the mechanism that gives rise to the latter (i.e., whether it is dipole rotation or streaming potential).

Promiscuous laws enjoy a degree of independence from the basal conditions that the laws of microphysics typically do not. They are higher level laws which help secure the ontological autonomy of the discipline formulating them. Wolff's law, for example, is a phenomenological regularity that does not rely on a single microscopic regularity – it is not a micro-level law in disguise, but a genuine physiological law.

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[16] Cells have a net surface charge which is due to the protein contents of their membrane.

The equations of piezoelectricity are also promiscuous in the sense explained above. They claim that mechanical stress is correlated with polarization in various materials, but they may be agnostic with respect to the mechanisms that produce polarization in these materials. Voigt's general theory of piezoelectricity, which is the basis of the theory we have today, is a phenomenological approach that was elaborated independently of the molecular approach (Katzir 2003; 2006).

3.3.3.6 Conclusion

Because of the diverse nature of the mechanisms responsible for the piezoelectric behaviour of various materials (e.g., ionic displacement in crystals, dipole rotation in polymers, streaming current in interface materials like cement or bone) it becomes obvious that piezoelectricity is a multiply realized functional property. In other words, being a piezoelectric is defined by the behaviour of the material in certain conditions, not by a microconstitutive feature that is possessed by all piezoelectrics and only by them. For this reason, piezoelectricity is a higher level property which cannot be identified with a particular microphysical property. This lends support to the idea that the field of science that studies piezoelectricity (solid state chemistry, which has a strong overlap with solid state physics) enjoys a degree of ontological autonomy relative to the underlying microphysics. This conclusion is further supported by the existence of "promiscuous" laws – regularities correlating two properties, at least one of which being (or being the result of) a functional property which is multiply realized.

3.3.4 Other functional properties in chemistry

Arguably, the properties discussed so far are not the only chemical properties that are functional. The property of being a metal is also functional. Just like in the case of the noble gas atoms, metal atoms can be given precise quantum-mechanical descriptions. More than 70% of existing chemical elements are metals (91 elements out of 117). Twelve out of eighteen groups in the periodic table are occupied exclusively by metals – alkali elements, alkaline earth elements, lanthanides, actinides, and the transition elements, are all metals. Some elements in group 13 to group 16 are metals too. As one can expect, the quantum-mechanical description for all these atoms will look messy. Physical chemistry has not revealed any microphysical constituent that is shared by all metal atoms and only by them. Despite the fact that their microphysical descriptions are wildly heterogeneous, metals have interesting chemical properties in common: their atoms readily lose electrons to form positive ions; they form metallic bonds with other metal atoms and ionic bonds with nonmetal atoms. Since the property of being a metal is defined with reference to what the entities instantiating the property can do, this property is functional.

3.3.5 Are constitutive definitions impossible?

One may resist the idea that the properties mentioned above (acids, bases, oxidants, reductants, metals, piezoelectrics etc.) are non-constitutive. One argument may be the following. These properties are defined functionally, but merely for convenience. They do have a microconstitutive feature in common, just one that is not of the sort you might have expected. Consider the prototypical case of acids. Admittedly, concrete constituents like a hydrogen nucleus cannot be identified with the common microconstitutive feature of acids. But perhaps more general constituents should be considered. Why not take the physical features shared by different acids that make them suitable for proton donation (such as the proton dissociation energy) as the relevant constituents? Why these physical features can't be microconstitutive, but just more general?

Couldn't we identify acids with those hydrogen-containing molecules whose proton dissociation energy has a certain value (or maybe fits within a value interval)? Couldn't we define acids as those substances that have a labile proton? This seems like a plausible possibility. However, there are a couple of problems with it. First it should be pointed out that even if one could define acids as those H-containing molecules whose proton dissociation energy has a certain value, it is not clear that this definition would be constitutive in the same way as the definitions of mammals, alcohols, or noble gases are. Having a bond dissociation energy of a certain value is not a constituent of acids in the same way as having mammary glands is a constituent of mammals, or having a carbon-bound hydroxyl group is a constituent of alcohols. In all these cases the constituent is a concrete property (an ingredient, a part, something that could be physically removed from the system) whereas having a certain value of the proton dissociation energy is a more abstract physical characteristic – it is not a thing, but a magnitude.

However, there is a much more serious concern about this proposal. Whether a chemical species gives off a proton to another chemical species in a chemical reaction (i.e., whether it behaves as an acid or not) does not depend exclusively on the proton dissociation energy; it depends on the nature of the chemical species to which the acid reacts. In principle, any hydrogen-containing compound could become an acid if the reagent is protophilic enough. Also, the strength of an acid (the extent to which that molecule dissociates) is not dictated by the proton dissociation energy of that species, but by the stability of the reaction products it forms. So the problem is that while the proton dissociation energy for a molecule is a fixed quantity, the strength of the acid consisting of that molecule is not a fixed quantity, but is relative to the chemical species to which that molecule reacts; the strength of the acid is relative to the stability of the reaction products. So the property of being an acid is a relational property. This is often overlooked because of the habit of judging the acidity of a compound by comparison to that of water, or thinking about the behaviour of the compound in an aqueous solution.

$$\mathrm{HA} + \mathrm{H_2O} \longrightarrow \mathrm{A}^- + \mathrm{H_3O}^+$$

$$\mathrm{Acid} + \mathrm{Base} \longrightarrow \mathrm{Conjugate{-}base{-}of{-}acid} + \mathrm{Conjugate{-}acid{-}of{-}base}$$

But consider the case of CH_3COOH. If the solvent is water, CH_3COOH is an acid, although a weak one: its conjugate base, CH_3COO^-, is not a stable compound and it reacts with the conjugate acid, the hydronium ion.

$$\mathrm{CH_3COOH} + \mathrm{H_2O} \rightleftharpoons \mathrm{CH_3COO}^- + \mathrm{H_3O}^+$$

In reaction with metals CH_3COOH is also an acid, the result of the reaction being a salt (acetate) and hydrogen gas (standard acid-metal reaction).

$$2\,CH_3COOH + Mg \longrightarrow (CH_3COO)_2Mg + H_2$$

So we tend to think of CH_3COOH as an acid, and we even call it *acetic acid*, because when we think of it we tend to think of its behaviour in aqueous solutions or relative to metals. However, if the solvent is not water, but H_2SO_4, CH_3COOH is a base.

$$CH_3COOH + H_2SO_4 \rightleftharpoons CH_3COOH_2^+ + HSO_4^-$$

The chemical species that can either donate or receive a proton are called amphiprotic (or amphoteric). Amphoterism challenges the idea that there could be a microconstitutive physical feature shared by all acids and only by them. If the acidic character of a compound varies depending on the reagent (sometimes dramatically, as amphoterism shows) then candidates like the proton dissociation energy (which do not vary depending on the reagent) cannot be the microconstitutive features of acids.

Amphoterism is not a rare phenomenon. Substances commonly considered bases that act as acids (or viceversa) should not be viewed as exceptions, or as odd, isolate cases. Amphiprotic substances include: self-ionizable compounds, such as water or ammonia; substances which have amine and carboxylic acid groups such as amino acids and proteins; the hydroxides of most metals. In fact, most chemical species having a hydrogen atom could become acids given the right reagent. Also, chemicals that are habitually referred to as as acids become bases given the right reagents (stronger acids).

$$HNO_3 + H_2SO_4 \longrightarrow H_2NO_3^+ + HSO_4^-$$

Therefore, instead of mistakenly treating amphoterism as exceptional in order to rescue the idea that acidity is constitutive, it is preferable if we give up on thinking about acidity as an absolute (or categorical) property. It is best to talk about acids in the context of a chemical reaction. Talking about acidity in the absence of the context of a chemical reaction (dissociation reactions included) becomes strictly speaking illegitimate.

Another argument against the idea that the properties mentioned in the previous sections are non-constitutive could be formulated as follows (again, let us consider the case of acids, although exactly the same things can be said about any other functionally-defined chemical property). It is hard to prove that a concrete microphysical property that is present in all acids and only in them which is responsible for the similar behaviour of these substances does not exist. You cannot prove a negative, as they say. Therefore, one cannot conclusively assert that acids are not in fact constitutive.

Of course, it is hard to prove that all these functionally-defined chemical properties are not in fact constitutive. However, there are no compelling reasons to believe that acidity is due to some microphysical property that is present in all acidic molecules and only in them, determines their behaviour, yet so far has not been discovered; or it has been discovered, but it never made it into the definition of acids. On the other hand, there are excellent reasons to believe that there is no such microphysical property. Contemporary chemistry is a mature science. While it is true that some chemical phenomena are not well understood, acidity is not one of them. Contemporary chemistry does have a good understanding of acids and how they work. An acid is a compound in which a hydrogen nucleus dissociates and then combines with a chemical species. This behaviour is explained successfully by an exclusive appeal to general thermodynamic principles having to do with the minimization of energy in the context of the chemical reaction. There are no good reasons to suspect that this behaviour is the result of some microconstitutive physical property which has not yet been discovered.

A related argument that could be made for the idea that acidity is functional is based on naturalism. If one accepts that science is the best way to learn about the material world, then one should also accept that the kinds of things that exist in the material world are best defined by science. As mentioned, the definitions of acids accepted by the scientific comunity are functional *par excellence*. Given that chemistry is a mature science, it is difficult to explain why a constitutive definition for acids has not emerged so far, if such a definition is possible.

These arguments suggest that the definitions of acids (and those of bases, oxides, reductants, etc.) offered by contemporary chemical science should be taken at their face value: these definitions are functional because the properties that they define are themselves functional.

Chapter 4

Functional emergence and reductionisms

What does the existence of functionally emergent chemical properties entail with respect to the much discussed reduction of chemistry to physics? In this chapter I present the most prominent accounts of inter-theoretic reduction and argue that the existence of terms which refer to functionally emergent properties poses problems for two of these accounts, while the third account does not succeed in establishing the kind of reductionism that would endanger functional emergence.

The motives for developing a philosophical account of inter-theoretic reduction have their roots in the ideal of the unity of science held by logical positivism. According to the logical positivists, reduction would foster this ideal by providing a single universal language that would allow the expression of all empirical statements and the formulation of intersubjectively understandable explanations and predictions, and a single method for the investigation of all states of affairs (Carnap 1934). Inter-theoretic reduction was seen as desirable because it could help in the elaboration of a complete picture of reality that is ontologically parcimonious and free of gaps, redundancies or hidden contradictions (Neurath 1983).

4.1 Nagelian reduction

One of the most prominent accounts of inter-theoretic reduction has been formulated by Ernest Nagel (1949, 1961). By the term "reduction", Nagel understands "the explanation of a theory or a set of experimental laws established in one area of inquiry, by a theory usually though not invariably formulated for some other domain" (1961, p. 338). The model of explanation that Nagel assumes in his reductionist account is essentially the deductive-nomological model of explanation. According to this model, an explanation is a deductive inference in which at least one of the premises states a law of nature, while the others state the initial conditions that obtain in the given situation. Nagel shares with the logical positivists the view that reduction is a means of achieving the ideal of the unity of science – "a comprehensive theory which will integrate all domains of natural science in terms of a common set of principles" (1961, p. 336).

Nagel distinguishes between two kinds of reduction. If all terms in the vocabulary of the theory to be reduced are also present in the vocabulary of the reducing theory, and these terms have similar meanings in both theories, the reduction is *homogeneous*. If the theory to be reduced includes terms that do not occur in the vocabulary of the reducing theory, the reduction is *heterogeneous*. It is a logical fact that in order to derive a conclusion from a set of premises, the conclusion must not include terms that are not mentioned in the premises. Therefore, heterogeneous reductions are more challenging than homogeneous reductions since between the reduced theory and the reducing one there is a terminological gap that must be bridged before reduction can happen. Nagel is well aware of this fact. He writes:

> "If the laws of the secondary science contain terms that do not occur in the theoretical assumptions of the primary discipline ..., the logical derivation of the former from the latter is prima facie impossible" (Nagel 1961, p. 352).[1]

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[1] By "secondary science" Nagel means the reduced science or theory, while by "primary science" Nagel means the reducing science or theory.

For the reduction to be even possible, the vocabularies of the reduced theory must be appropriately connected with the vocabulary of the reducing theory. Nagel sees this requirement as a formal condition that is necessary for reduction. He calls it the connectability condition.

- *Connectability*: "Assumptions of some kind must be introduced which postulate suitable relations between whatever is signified by 'A' [term of the reduced theory that does not occur in the reducing theory] and traits represented by theoretical terms already present in the primary science" (1961, p. 353-354).

This necessary condition is supplemented by another, which Nagel calls the derivability condition:

- *Derivability*: "With the help of these additional assumption, all the laws of the secondary science, including those containing the term 'A', must be logically derivable from the theoretical premises and their associated coordinating definitions in the primary discipline"

How does Nagel's account apply to the reduction of chemistry to physics? If T_2 is a theory of chemistry and T_1 is a theory of physics, then on Nagel's schema T_2 reduces to T_1 if and only if the following conditions are met:

1. For every theoretical term C that is present in T_2 but not in T_1, there is a theoretical term P in T_1 such that for all entities x, x is C if (and possibly only if) x is P.

2. All the laws of T_2 must be derivable from T_1 together with the bridge laws.

The first condition states the requirement of connectability via what's been called "bridge laws" connecting the vocabulary of chemistry with that of physics. I will leave aside problems with the second condition above (they have been discussed by Luisi 2002 for example). Instead, I will focus on the first condition.

Given that the vocabulary of chemistry contains terms that are not present in the vocabulary of physics (e.g., terms like "acid", "base", "reductant", "oxidant", etc.), it appears that the reduction of chemistry to physics would be of the heterogeneous kind. Therefore, bridge laws must be found for these terms. Consider, for example, the following chemical law, which contains terms that are not present in the vocabulary of physics:

A) Acids in reaction with metals produce a metal salt and hydrogen gas.[2]

This chemical law is instantiated, for example, when H_2SO_4 reacts with metals, or when HCl reacts with metals. These two cases are particular instantiations of the chemical law A, but they must not be confused with the law A itself, which is more general. The possibility of deriving chemical law A from the laws of physics depends on the existence of a bridge law connecting the term "acid" with a term present in the vocabulary of physics. But in order to derive the chemical law A (not just one of its instantiations), the bridge law must be stronger than a one-way conditional. If the bridge law expresses a one way conditional, such as "For all x, if x is H_2SO_4 then x is an acid", one could derive at most a particular case of law A: "Some acids in reaction with metals produce a metal salt and hydrogen gas".[3] But the sentence expressing chemical law A is a universal statement – it talks about all acids. And universal statements cannot be derived (i.e., logically deduced) from particular statements. Therefore, in order to derive the universal statement expressing chemical law A, the bridge law must be stronger than a one-way conditional; it must be a biconditional.[4]

The reductionist could reply by saying that a universal statement could be derived from a set of particular statements if that set is exhaustive. That is, one could derive the claim "Acids in reaction with metals produce a metal salt

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[2] The conception of acids and bases assumed is that of the Brønsted-Lowry theory.

[3] In the hypothetical bridge law mentioned here a H_2SO_4 molecule is construed as a physical system which consists of electrons and nuclei.

[4] Some authors like Richardson (1979) have argued that the suitable relations demanded by Nagel's connectability condition need not be biconditional (p. 548). For a response, see Marras (2005, p. 356).

and hydrogen gas" from of an exhaustive conjunction of particular statements, such as "H_2SO_4 in reaction with metals produce a metal salt and hydrogen gas" and "HCl in reaction with metals produce a metal salt and hydrogen gas" and "H_3PO_4 in reaction with metals produce a metal salt and hydrogen gas", and so on until the the class of physical systems composed of electrons and nuclei that constitute the extension of the term "acid" is exhausted. Of course, in order for the derivation to be possible, one must also add the premise that the extension of the chemical term "acid" is exhausted by H_2SO_4 , HCl, H_3PO_4, and so on. This premise would amount to the following tentative bridge law: "For all x, x is an acid if and only if x is H_2SO_4 or HCl or H_3PO_4 or ...".

There are a few problems with this strategy. One problem is that the members of the biconditional above denote properties that differ in some significant way, and this difference may be important enough as to preclude relating the properties via a biconditional. Being an acid is a relational property: a system of electrons and nuclei behaves as an acid or as a base (i.e., donates protons or accept them) depending on the nature of the other participants in the reaction.[5] On the other hand, being a molecule of H_2SO_4 or HCl or H_3PO_4 or ..., is not a relational property. Rather, if this disjunctive property is a property at all, it is an intrinsic property – something is on the list (or not) regardless of that thing's relationships with other things. If one sees a problem with equating an intrinsic property with a relational property one should also see a problem with the tentative bridge law above. The reductionist may attempt to circumvent this problem by ammending the tentative bridge law as follows: "For all x, there is an y, such that x is an acid in reaction to y if and only if x is H_2SO_4 or HCl or H_3PO_4 or ...". However, chemistry is in the business of synthesizing new substances, and the list of physical systems composed of electrons and nuclei to which the term "acid" applies may never be completed. As a result, the bridge law may never be completed and the gap between the chemical and the physical vocabulary may never be closed.

But perhaps a better strategy is available. Can't our Nagelian bridge law be something like "For all x, x is an acid if and only if x is a proton donor"?

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[5] Section 3.3.5 offered a detailed discussion of amphoterism.

According to the Brønsted-Lowry definition, acids are those substances that donate protons in chemical reactions. Therefore, this candidate bridge law expresses a true statement. But is this statement fit for functioning as a bridge law in the Nagelian reduction of chemical law A? Is the term "proton donor" truly a term of physics? It should be noted that term "proton donor" is not a theoretical term that habitually occurs in the vocabulary of physics (unlike the term "mean molecular energy" in the case of the prototypical reduction of temperature offered by Nagel). The problem is not with the term "proton", which is – of course – part of the standard vocabulary of physics, but with the term "donor". The term "proton donor" is a functional term, i.e., it describes acids by pointing to their causal role in chemical reactions. Like other functional terms, this term denotes a higher level property, capable of being carried out (or realized) by a variety of lower level physical systems – in our case systems of electrons and nuclei such as H_2SO_4, HCl or H_3PO_4. Each of these lower level physical systems of electrons and nuclei belongs to a certain set of entities that are grouped together according to a natural/objective criterion (relevant physical similarities) rather than an artificial/subjective one. In other words, each of these systems instantiates what philosophers have called a "natural kind" (more precisely, a *physical* natural kind, or physical kind for short).[6] For example, all H_2SO_4 molecules belong to the same physical kind, which is distinct from the physical kind to which H_3PO_4 molecules belong. However, the set of molecules that can donate protons does not form a *physical* kind – the members of this set are just too dissimilar from the point

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[6] The philosophical literature on natural kinds is vast and many authors have expressed skepticism towards the idea that the kinds talked about in science are natural kinds in the philosophers' sense. The topic of natural kinds remains full of controversies also because there are competing philosophical accounts of what the term "natural kind" should mean. In my discussion of natural kinds I assume a metaphysically modest notion of natural kinds. By the term "natural kind" I mean the kinds that the sciences talk about, whatever those might be. For my purposes, "natural kind" need not mean more than just "scientific kind". The two terms are obviously not coextensive: the term "20^{th} century Canadian immigrants" expresses a natural kind on my view (a sociological kind), but it certainly does not express a natural kind in the traditional philosophical sense. In fact, in the rest of this section I will phrase my arguments in terms of "physical kinds" or "chemical kinds", as opposed to the more controversial "natural kinds".

of view of their physical characterization. So the problem with our tentative bridge law appears to be the following. Either "proton donor" is a term of physics, or it is not. If it is not truly a term of physics, our tentative bridge law is not really connecting the vocabulary of physics with that of chemistry, so it is not truly a *bridge* law. On the other hand, if "proton donor" is a term of physics, its extension is too disunified and context dependent (see section 3.3.5) to form a physical kind. But bridge laws are supposed to be *laws*, and laws are supposed to connect kinds to kinds (see, e.g., Fodor 1974). Thus, if "proton donor" does not refer to a physical kind, then the tentative bridge law above is not *a law.*[7] Therefore, our tentative bridge law is either not a *bridge* between the two vocabularies, or it is not a *law.* Either way, there is a problem for the Nagelian reduction of chemistry to physics.

One may object to the argument above by questioning the idea that the connectivity condition must be substantiated by bridge *laws* chemical physical kinds to physical kinds. Why can't we have bridge *principles* instead, which do not necessarily connect kinds to kinds? (Kim 1992, p. 10).[8] However, this strategy prompts the following questions: what would be the nature of these bridge principles, and why should they be allowed among the premises of the derivation? The motivation for bridge laws connecting (through identification) natural kinds to natural kinds seems pretty obvious – reductions must reduce, i.e., they must ensure ontological parsimony. In order to achieve this, the connectivity condition must require identities.[9] But in this context, identities are identities of *kinds.* If acids are a chemical kind and Nagelian reduction

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[7] This is also a problem for the tentative bridge law that was considered previously.

[8] Kim finds the following answer plausible: "if M is identified with non-kind Q (or M is reduced via a biconditional bridge principle "M↔Q", where Q is a non-kind), M could no longer figure in special science laws; e.g., the law, "M→R", would in effect reduce to "Q→R", and therefore loses its status as a law on account of containing Q, a non-kind" (Kim 1992, p. 10).

[9] Mere correlations won't do, as Sklar (1967, p. 119) has argued. Sklar offered the example of the Wiedemann-Franz law, which expresses a correlation between the thermal conductive properties of a material and its electrical conductivity properties. Despite this, no one has ever maintained that this law establish the reduction of the theory of heat conduction to the theory of the conduction of electricity. The reason is that the Wiedemann-Franz law expresses a correlation between two properties, not an identity. Thus, the Wiedemann-Franz law is not truly a bridge law in the sense that Nagelian reduction demands.

obtains, there must be a physical kind to which the property of being an acid could be identified. Bridge laws express such identities, and thus they are, in principle, able to bridge the gap between the two domains. It is not clear on what basis could bridge principles accomplish this task.

The idea that the laws of nature state relations between natural kinds gives rise to another concern. A reduction of chemistry to physics would amount to the derivation of chemical laws from physical *laws.* If the physical entities that form the extension of the chemical term "acid" do not form a physical natural kind, the concern is that there would be no physical laws from which the chemical law A could be derived. This idea can be illustrated with an example. Consider again chemical law A.

A) $\text{Acid} + \text{Metal} \longrightarrow \text{Metal}{-}\text{Salt} + H_2\uparrow$

The number of reactions rendering A true is vast. Consider the following two examples.

A1) $H_2SO_4 + Fe \longrightarrow FeSO_4 + H_2\uparrow$

A2) $2\,HCl + Zn \longrightarrow ZnCl_2 + H_2\uparrow$

As one can see, every property mentioned in statement A with the exception of hydrogen can be realized by various nuclei-electrons physical systems (representing a particular acid, metal, and metal salt, respectively). Of course, any particular chemical reaction (like A1, A2) is nothing but a physical process involving nuclei and electrons, as well as some other physical parameters (temperature, pressure, etc.). Quantum physics could offer an explanation in terms of atomic and molecular wavefunctions for each of the reactions exemplifying our chemical statement. Thus, each of the particular reactions exemplifying A can be regarded as a physical truth having nomic character – A1 and A2 are only two examples. Now we can paraphrase Fodor (1974, p. 405) and say that while it is a law that sulfuric acid in reaction with iron produces iron sulfate and hydrogen, and it is a law that hydrogen chloride in reaction with zinc produces zinc dichloride and hydrogen, it is not a *law* that *either* sulfuric acid *or* hydrogen chloride in reaction with *either* iron *or* zinc produces *either* iron sulfate *or* zinc dichloride and hydrogen. In other words, heterogeneous kinds (or disjunctive properties) are unfit for laws. Nonetheless, the more general claim, asserting that acids in reactions with metals produce a metal salt and hydrogen *is* a law. Statements like A constitute *knowledge*. This knowledge is not physical knowledge; it is *sui generis* chemical knowledge, which is as such unavailable to the physicist, whose vocabulary does not include terms like "acid".

Similar difficulties in finding bridge laws occur for other specific chemical terms, such as base, metal, reductant, oxidant. Take the chemical term "metal", for example. "Metal" is a specific chemical term, which is defined with reference to the periodic table of elements, a chemical theoretical device *par excellence* (metals are those elements that occupy a certain part of the periodic table). What would a bridge law for this term look like? The possibility of coming up with a bridge law for the term "metal" depends on the possibility of finding a microphysical constitutive definition for the property of being a metal. But, as argued in section 3.3.4, the property of being a metal is functional. Physical chemistry has not revealed any particular microphysical constituent that is shared by all atoms of metallic elements and only by them. Nonetheless, metallic elements have interesting chemical properties in common: metal atoms readily lose electrons to form positive ions; they form metallic bonds with other metal atoms and ionic bonds with nonmetal atoms. In the case of metals it is hard to see how even a tentative bridge law would look like.

What does the existence of chemical terms for which bridge laws are not available entail with respect to the notion that chemistry is Nagel-reducible to physics? If bridge laws are not available for functional terms this means that for the laws in which these terms occur the connectability condition is not met; consequently, the derivability condition is not met. As a result, the laws in which these terms occur are not reducible to the laws of physics, although they depend on them; they must be considered *sui generis* chemical laws (see Table 4.1).

There is an objection to the antireductionist stance above that I would like to consider. The objection is this: one may accept that properties like being an acid, a metal, a piezoelectric, etc. can't be given constitutive definitions and still reject that the truths in which these properties figure cannot be construed as truths of microphysics.

So far, my argument against Nagelian reduction has been that statements like those expressed by law A can't be reduced to some unique microphysical process because the properties mentioned by them cannot be given constitutive definitions. But perhaps the strategy of finding bridge laws connecting chemical terms with physical terms is not the best move that the reductionist can make if he wants to reduce law A. Perhaps the reductionist would be more successful if he attempted to reduce law A *in toto*, as a whole, without the mediation of bridge laws connecting the chemical terms occuring in this law with their physical referents. Indeed, why can't the reductionist say that even if the chemical properties appearing in law A cannot be identified with physical properties, chemical law A does nevertheless refer to a certain physical process, A*. So even if the chemical properties appearing in A are not physical properties in disguise, perhaps chemical law A is in fact a physical law in disguise (i.e, A*).

What might A* be? A* might be something like "the giving up of protons by certain physical systems in the presence of certain other physical systems". But how do we specify "certain physical systems" and "certain other physical systems" without using the terms "acid" and "metal"? As argued in 3.3.1, and 3.3.4, the terms "acid" and "metal" do not have unique physical references. If we can't specify "certain physical systems" as to refer exclusively to acids and "certain other physical systems" as to pick out metals, then A* is not the equivalent *of A*.

One may object by saying that construing A* as "the giving up of protons by certain physical systems in the presence of certain other physical systems" does not abandon thinking about A* as we thought about A, i.e., as a process involving different *properties*. Rather, to find A* we need to construe it as a single, unitary process, and give up the idea that it is about the interaction of properties. On this view, what needs to be done is to find a physical replacement for A *as a whole.* Thus, on this view, we need to switch to the *chemical reaction* as basic (rather than chemical *properties*) and try to find the physical process A* that chemical law A expresses. This version of reductionism departs from Nagel's in that the bridge laws are assumed to connect whole statements and not terms (alternatively, one could think of this version of reductionism as connecting types of chemical reactions with types of physical processes).

Suppose we regard chemical law A as basic. If so, what physical process A* could we identify it with? The following answer is appealing: "the giving up of protons". Now we can construe chemical law A (acids in reaction with metals produce metal salts and hydrogen) as the physical process A* – the giving up of protons. But there is a problem with this strategy. If we construe chemical law A as "the giving up of protons" simpliciter, we lose the distinction between the various types of chemical reactions in which acids participate. For example, acid-metal reactions are different from acid-base reactions – the first produce hydrogen gas, the second water. However, they both involve the giving up of protons; from a microphysical stance, they are both instances of A*. Therefore, thinking of A* as the giving up of protons does not allow us to differentiate between the various types of chemical reactions.

What if we ammend A* by further specifying it? What if we construe A* as "the giving up of protons *that form hydrogen gas*"? But this answer won't work either: this answer does not allow us to differentiate acid-metal reactions from dissociation reactions such as the following:

$$\mathrm{CH_4} \longrightarrow \mathrm{C} + \mathrm{H_2}\uparrow$$

Both acid-metal reactions and dissociation reactions like the one above involve "the giving up of protons that form hydrogen gas". To be able to distinguish acid-metal reactions from dissociation reactions like the one above, one has to abandon the microphysical stance and revert to the chemical vocabulary of acids and metals. To paraphrase Dennett, we need to adopt a "chemical stance" (as opposed to a microphysical one) and see the "real patterns" of chemical behaviour.[10]

To conclude, switching to the chemical reaction as basic does not appear to be an effective strategy to establish the reduction of chemistry to microphysics along Nagelian lines, i.e., using some sort of bridges between the two domains.

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[10] The phrase “chemical stance” is a paraphrase of Dennett’s “intentional stance” (see Dennett 1987) while the phrase “real patterns” is the title of one of his papers (Dennett 2008).

Acids	A) Acids in reaction with metals to produce a metal salt and hydrogen gas. B) Acids in reaction with metal carbonates to produce water, CO_2 and a salt. C) Acids in reaction with metal hydroxides and metal oxides to produce water and a salt.
Bases	B1) Bases accept hydrogen ions from the chemical species to which they react. B2) Bases donate electron pairs in chemical reactions. (This is the Lewis definition of bases.) B3) Bases react with triglycerides to produce soaps (reaction known as saponification). B4) Bases react with acids to produce salts and water. B5) Bases can act as insoluble heterogeneous catalysts for chemical reactions.
Oxidants	O1) Oxidants accept electrons from the chemical species to which they react. O2) Oxidants react with metals, producing oxide(s) and/or salt(s) of the original metal; this process is known as corrosion. O3) Oxidants degrade the substances that come in contact with (this is especially of concern in biology, since they damage large molecules like DNA and promote ageing). O4) Oxidants make possible the combustion of chemical substances. They react with hydrogen or hydrocarbons to give off carbon dioxide or water and heat; once a metal is ignited, oxidants promote its combustion, the result being a metal salt.
Reductants	R1) Reductants react with metal oxides to produce metals. R2) Reductants make possible the combustion of chemical substances. R3) Reactions involving reductants are typically reversible under appropriate circumstances.
Metals	M1) Metals in reaction with acids produce a metal salt and hydrogen gas. (A) M2) Metals in reaction with oxidants produce oxide(s) and/or salt(s) of the original metal. M3) Metal atoms readily lose electrons to form positive ions. M4) Metal atoms form metallic bonds with other metal atoms and ionic bonds with nonmetal atoms.

Table 4.1: List of *sui generis* chemical laws.

4.2 Micro-reduction

Another account of reduction has been offered by Kemeny and Oppenheim in their 1956 paper “On Reduction” and by Putnam and Oppenheim in their 1958 article titled “The Unity of Science as Working Hypothesis”. The approach to reduction advocated by Kemeny, Oppenheim and Putnam (henceforth KOP) is in some respects a reaction to another model of reduction, advocated by Nagel (1949, 1961). KOP’s account is not as widely known as Nagel’s, and it has not been discussed to the same extent. Nonetheless, KOP’s account has its virtues and its authors argue that it is superior to that of Nagel.

In their treatment of inter-theoretic reduction KOP distinguish between what they call *internal reduction* (when the vocabulary of the base theory, T1, is a subset of the vocabulary of the target theory, T2) and *branch reduction* (when the two theories, T1 and T2, belong to two distinct branches of science, B1 and B2) (Kemeny and Oppenheim 1956, p. 9). Branch reduction is also called *micro-reduction* (Putnam and Oppenheim 1958, p. 6).

How does KOP’s model apply specifically to the reduction of chemistry to physics? Since chemistry and physics are two branches of science, the issue becomes whether chemistry micro-reduces to physics. According to KOP, this happens if the following conditions are met:

1. The objects in the universe of discourse of chemistry are wholes which possess a decomposition into proper parts all of which belong to the universe of discourse of physics.

2. Given a physical theory T_1, a chemical theory T_2, and some observational data O:

   (a) The vocabulary of the chemical theory T_2 contains terms that are not in the vocabulary of the physical theory T_1.

   (b) Any part of O explainable by means of T_2 is explainable by T_1.

   (c) T_1 is at least as well systematized as T_2.

One of KOP's motivations for reduction is the elimination of unnecessary theoretical terms, or ontological parsimony.

> "Nevertheless, since theoretical terms are in a sense a luxury, we want to know if we can get along without some of them. It is, then, of considerable interest to know that a set of theoretical terms is superfluous since we can replace the theories using these by others in which they do not occur, without sacrificing the degree of systematization achieved by science to this day". (Kemeny and Oppenheim 1956, p. 12)

Two characteristics of KOP's model distinguish it profoundly from Nagel's model. The first is the absence of bridge laws and the relativization of inter-theoretic reductions to observational data. The second is the requirement that the base theory is at least as well systematized as the target theory.[11]

Let us now consider the first difference between the two models in the context of the reduction of chemistry to physics. In Nagel's model, the reduction of chemistry to physics is accomplished when the laws of chemistry are derived from the laws of physics. This derivation cannot obtain unless the theoretical terms that occur in the vocabulary of chemistry are translated via bridge laws into terms present in the vocabulary of physics. Bridge laws, if they can be found, guarantee a direct connection between chemistry and physics. But KOP would deny that a direct connection between chemistry and physics is necessary for reduction. They argue that the connection between two theories may be effected indirectly, via their respective connections with the observational data. For KOP, theories are practical theoretical devices for explaining and predicting observations. They claim that any theory

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[11] The post-positivist philosophy of science has raised serious doubts with respect to the dichotomy between theoretic and observational terms. However, it is worth considering the issue whether the spirit of the KOP's model really requires maintaining this discredited distinction. It has been claimed that, likely, a version of the view could be refined that replaced the notion of explaining observations with an appeal to explaining phenomena more generally (Ney 2008). In my discussion of KOP's model I will continue to employ their terminology. The goal is to see whether KOP's model is viable independently of what views on the theoretic-observational dichotomy one may hold.

can be replaced, for the purposes of explanation and prediction, by the set of all observational statements that follow from it. KOP emphasize that a theory cannot add anything to the set of observational data that follows from it. A theory is nothing over and above a set of observations, and for this reason the two are cognitively equivalent. Admittedly, the set of observations to which a theory is equivalent is infinite. But it is recursively enumerable. A theory organizes these observational facts into a practically manageable form; a theory is just a simple, economical and systematic proxy for a set of observations. For KOP, a theory has the same explanatory ability as the long (or infinite) list of statements, but it is much more simple and therefore preferable to such a list.

The need for introducing theoretical terms is justified only insofar as it makes the body of observations more manageable for the purposes of explanation and prediction. KOP emphasize that anything that can be said about actual observations can be said without theoretical terms, but their introduction allows a much more systematized treatment of our total knowledge.

Since chemistry and physics are theories in KOP's sense, each is equivalent with a set of observations. As a result, chemistry is replaceable by physics insofar as the set of observations to which it is equivalent is explainable by means of physics alone. The connection between chemistry and physics can be effected indirectly, without translating chemical terms into physical terms via bridge laws.

> "If one theory is to follow from another, it must be translatable into the vocabulary of the latter. But it is entirely possible that a theory should be able to explain all facts that another can, without there being any method of translation. Of course, each set of theoretical terms must be connected to observational terms, and hence to each other, but this connection is normally much weaker than a full translation." (Kemeny and Oppenheim 1956, p. 16).

KOP argue that the requirement of direct connections between theories has the unavoidable consequence of producing a very narrow definition of reduction.

This is what they find unsatisfactory about Nagel's definition of reduction. Nagel's definition of reduction, KOP suggest, is too narrow in that excludes most actual cases of reduction, including the reduction of chemistry to physics (quantum mechanics, to be precise). KOP claim that "while some attempts have been made to show that something like biconditional translation does exist, this certainly is not the case if quantum mechanics is taken as the reducing science" (Kemeny and Oppenheim 1956, p. 16).[12] KOP do not exclude the possibility that some reductions may be accomplished by means of a translation of theories via bridge laws, *à la* Nagel. But they claim that Nagelian reductions cover what is an extremely special case of reduction. Therefore, in KOP's view, their model is more comprehensive than Nagel's as it applies even to cases in which bridge laws cannot be found, such as the case of the reduction of chemistry to physics.

Before examining some aspects of the reduction of chemistry to physics according to KOP's model, it is worth noting that KOP's model of reduction is deeply eliminativist. If the reduction of chemistry to physics is successful, chemistry is replaced by physics, allowing us to effect an economy in the theoretical vocabulary of science. Kemeny and Oppenheim would relate the reduction of chemistry to physics to the possibility of forming a theory in physics which can take the place of the totality of chemical theories.[13] They would argue that such a theory would have to explain all phenomena explainable by means of chemical theories, without introducing undue complexity into the theoretical structure of science. Kemeny and Oppenheim would claim that if this is achieved, then all the theoretical terms of chemistry could be eliminated from the vocabulary of science. Given this extreme eliminativism, it appears that the hope for the ontological autonomy of the chemistry in relation to physics vanishes.

Let us now turn to the issue of how the existence of specific chemical terms

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[12] According to KOP, another case of actual reduction in which there is nothing that even remotely resembles the translation by means of biconditionals is the reduction of Newtonian mechanics to relativity theory.

[13] The case that Kemeny and Oppenheim consider explicitly is the reduction of biology to physics, but their remarks equally apply to the reduction of chemistry.

impacts KOP's theory of reduction. If chemistry employs terms that do not occur in the vocabulary of physics, could it micro-reduce to physics in the sense KOP argued?

Let us grant that the first condition of KOP's definition of micro-reduction is met. That is, let us grant that the concrete objects in the universe of discourse of chemistry (atoms, ions, molecules) are wholly composed of objects that belong to the universe of discourse of physics (protons, neutrons and electrons). The issue now becomes whether the second condition of KOP's definition obtains. If one grants the that the first condition is met, the issue of whether chemistry micro-reduces to physics boils down to conditions (b) and (c):

(b) Any observation that is explainable by a theory of chemistry is explainable by a theory of physics.

(c) That theory of physics is at least as well systematized as the theory of chemistry.

Neither of these claims is uncontroversial. The belief that for any observation that is explainable by chemistry there is a correct quantum-mechanical explanation is often an act of faith, given that such explanations are usually difficult to obtain in practice. The defenders of reductionism would argue that in this case, faith is grounded in reason: the fruitfulness of the quantum-mechanical approach in chemistry is undeniable, and if empirical success is the mark of truth, then any particular chemical truth is in fact a complicated quantum-mechanical truth – in some cases perhaps too complicated to be ever known. I do not wish to enter the debate about the truth of condition (b) here. Instead, I will focus on condition (c), namely the requirement that the theory of physics that explains an observation should be at least as well systematized as the chemical theory that explains the same observation.

Kemeny and Oppenheim conceive of the systematic character of a theory as a combination of that theory's simplicity and its explanatory power. The systematic character of a theory may be unchanged or it may even increase if any loss in simplicity is compensated for by a sufficient gain in its explanatory and predictive strength. Putnam and Oppenheim require that the “ratio” of simplicity to explanatory power should be at least as great in the case of the reducing theory as in the case of the reduced theory (Putnam and Oppenheim 1958, p. 5).

Kemeny and Oppenheim do not say much about what motivates subcondition (c). But they say that replacement of one theory by another should not be regarded as progress unless the new theory compares favorably with the old one in systematicity. Presumably, the requirement of systematicity originates in the need for ontological parsimony.

Kemeny and Oppenheim admit that the concept of simplicity is in need of a precise definition. They claim that simplicity is a purely syntactic concept applicable to theories as a whole, and they want to distinguish it from certain nonsyntactic concepts. In a footnote, Kemeny and Oppenheim write:

> “In some cases there will be complete agreement among scientists as to which of two theories is simpler; for example, if one can be stated in a single line, while the other – using the same vocabulary – requires several pages to state, then there would be little room for argument” (Kemeny and Oppenheim 1956, p. 18).

I agree that in the case of internal reductions, where the two theories share the same vocabulary, judging which theory is simpler can be a purely syntactical matter. The issue, however, is to determine which of two theories is simpler in the case of micro-reductions, i.e., when the two theories do not share the same vocabulary. In such cases, it is at least conceivable that there could be disagreement about which theory is simpler. And if there could be disagreement about which theory is simpler, there could also be disagreement about which theory is more systematized. Given that the presumed reduction of chemistry to physics is a case of micro-reduction, let us ask the following question: could it be that the chemical theory which explains a certain observational data is in fact more systematized than the physical theory which explains the same data?

As far as I was able to determine, the only philosopher of science who approached this question was Klee (1997). He argued for an affirmative answer:

> "Consider the reduction of chemical theory to quantum physical theory. This is surely a reduction going in the correct direction; yet, it is just as surely a reduction of a fairly well systematized body of theory to one that is notoriously, if not infamously, conceptually problematic and simply not as well systematized." (Klee 1997, p. 88)

Although I agree with Klee that the answer to our question should be in the affirmative, I find Klee's argument not entirely convincing. Quantum mechanics may be fraught with interpretational problems, but it is not at all clear that these problems make the theory unsystematized in the sense of KOP. In particular, it is hard to see how the lack of a widely accepted interpretation of the quantum-mechanical formalism affects its ratio of simplicity to explanatory power. I think that an affirmative answer to our question could be supported by a more elaborate argument, one that does not hinge upon controversies in the foundations of quantum mechanics. I will now attempt to present such an argument.

The argument starts with the following scenario. Suppose that a chemist working in a chemistry laboratory needs some hydrogen gas for a combustion reaction. The power is off and he cannot use the electrolysis device to produce hydrogen by splitting up water; he has to find another solution. Luckily he has some sulfuric acid and iron filings lying around and he decides to generate hydrogen gas by performing the following reaction:

A1) $\mathrm{H_2SO_4} + \mathrm{Fe} \longrightarrow \mathrm{FeSO_4} + \mathrm{H_2}\uparrow$

At the point when the chemist confirms the presence of hydrogen gas in the flask, a physicist steps in the lab and asks him why did hydrogen gas appear in the flask. The chemist gives him a chemical explanation:

P1) Acids in reaction with metals produce hydrogen gas.[14]

P2) In this flask, an acid reacted with a metal.

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[14] The conception of acids and bases assumed here is that of the Brønsted-Lowry theory.

C) This is why hydrogen gas appeared in the flask.

This is a simple but perfectly valid explanation for why hydrogen gas appeared in the flask. The explanation above is a standard deductive-nomological explanation, and as far as deductive-nomological explanations go, it is perfectly acceptable. However, it relies on concepts that are not in the vocabulary of the physicist. Both "acid" and "metal" are concepts whose meaning is made precise in the context of chemistry. Acids are defined in the context of chemical reactions as proton donors, while metals are elements that readily lose electrons and can be identified by looking at the periodic table, which is a chemical theoretical device *par excellence*.

But if condition (b) is true, the physicist could offer a different explanation, one that is deeper in that it involves quantum mechanics and references to atomic and molecular wavefunctions. If the physicist has enough knowledge of the initial state of the system and sufficient mathematical skill and computing power, he could give an alternative explanation as to why hydrogen gas appeared in the flask; or so reductionists would argue.

Now suppose the chemist needs more hydrogen gas, but he has used up his supply of sulfuric acid and iron filings. He looks into his chemical cabinet and he finds some hydrochloric acid and zinc pellets, some acetic acid and calcium and some phosphoric acid and magnesium. He decides to generate more hydrogen gas by performing the following reactions:[15]

A2) $2\,\mathrm{HCl} + \mathrm{Zn} \longrightarrow \mathrm{ZnCl_2} + \mathrm{H_2}\uparrow$

A3) $2\,\mathrm{CH_3COOH} + \mathrm{Ca} \longrightarrow \mathrm{Ca(OOCCH_3)_2} + \mathrm{H_2}\uparrow$

A4) $2\,\mathrm{H_3PO_4} + \mathrm{Mg} \longrightarrow \mathrm{Mg(H_2PO_4)_2} + \mathrm{H_2}\uparrow$

Now the physicist asks a different type of why-question: "Why did hydrogen gas appear in all four reactions? Why, despite of the diversity of the reactants, all these reactions lead to the formation of hydrogen gas?"[16] The chemist's

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[15] All reactions below take place in aqueous solutions.

[16] This distinction between two types of why-questions is very similar to the one made by Batterman (2002, p. 23).

answer is straightforward: “Because all these reactions are in fact acid-metal reactions and it is a chemical law that acid-metal reactions generate hydrogen gas.”

The chemist’s explanation of why hydrogen gas appeared in all four reactions is *unified*: despite the fact that the reactants in each reaction are different, the chemist’s explanation recognizes these reactions as instances of *a single type of reaction* (i.e., acid-metal reactions).

The physicist’s explanation, however, is not unified. Since the physicist does not have the concept of an acid, he will also lack the concept of acid-metal reactions. Therefore, he will not realize that the four different reactions are in fact instances of the same type of chemical reaction, one which produces hydrogen gas. To answer the question of why hydrogen gas appeared in all four reactions, the physicist must apply the principles of the physical theory to each chemical reaction; he will have to consider each pair of reactants individually and calculate what the reaction products will be. Grant that after a complicated and resource-demanding process, the physicist will eventually arrive at an explanation of why hydrogen gas appears in reaction A1, for instance. But he will not be able to use that explanation to account for the occurrence of hydrogen in the other three cases, for the initial conditions in are different in each case. To explain the occurrence of hydrogen gas when phosphoric acid reacts with magnesium (reaction A4), the physicist will have to start “from scratch” so to speak, and go through another resource-demanding process.

The chemist, on the other hand, is not confined to the vocabulary of the physicist. By classifying entities not according to their physical characteristics (e.g., charge, mass, spin, etc.) as the physicist does, but according to their behaviour in reactions, the chemist is able to talk about acids, metals, and acid-metal reactions.

Many terms in the chemist’s vocabulary, including “acid”, “base”, “oxidant”, “reductant”, refer to substances that are defined by their behaviour in chemical reactions, not by some shared physical constituent possessed by them and only by them. For example, according to the Brønsted-Lowry theory, the term “acid” denotes those compounds that donate protons in chemical reactions. In the same theory, the term “base” refers to proton acceptors. Reductants are defined as those substances that donate electrons to another chemical species, while oxidants are those that receive them. All of these types of substances are defined functionally, by reference to their role in chemical reactions. In order to be able to recognize the existence of properties like acidity, one needs to take a step back and notice similarity in behaviour among systems whose physical descriptions are very different.

The existence of specific chemical terms allows for the possibility of unified, overarching chemical explanations, like the one offered by our chemist. In our lab scenario, the unified character of the chemist’s explanation is made possible by the existence of chemical terms like “acid” and "metal". If the unified chemical explanation was possible, it was because the chemist recognized H_2SO_4, HCl, CH_3COOH and H_3PO_4, on the one hand, and Fe, Zn, Ca, Mg, on the other, as entities belonging to certain classes of substances that have certain functional descriptions (acids, respectively metals). This is *chemical* knowledge, which is as such unavailable to the physicist, whose vocabulary does not include terms like “acid”.

One may object. Couldn’t the physicist give an equally unified explanation that doesn’t use specific chemical terms? Couldn’t he give an explanation identical to the one given by the chemist, but in which the terms “acid” and “metal” are replaced with expressions containing purely physical terms?

There are several problems with this suggestion. First, it is hard to see how a strategy that relies on translating specific chemical terms into purely physical terms can be accommodated within KOP’s model of reduction given this model’s explicit disavowal of bridge laws. If the micro-reductionist insists that the physicist could give an equally unified explanation if he is allowed to translate the specific chemical terms into expressions that do figure in the physicist’s vocabulary, then it looks like KOP’s micro-reduction is after all not that different from Nagelian reduction. Both models of reduction would embrace the use of bridge laws, although they would disagree about which stage in the reduction process the bridge laws would come in – the advocate of Nagelian reduction appeals to bridge laws in the early stages of reduction process, before the crucial explanatory step takes place, whereas the advocate of micro-reduction would appeal to bridge laws in the final stage, after this step would have occurred.

Another problem is that of actually finding translations of the specific chemical terms into purely physical terms. As mentioned, metals are defined with reference to the position they occupy in the periodic table of elements, a chemical theoretical device par excellence. However, leading philosophers of chemistry have argued that the periodic table continues to resist physical axiomatization (Scerri 1997). Finally, even if the physicist could find such translations, it could be argued that by using them he would be expanding the conceptual inventory of physics. In other words, he would not be doing just physics anymore. Moreover, if the physicist decided to use these translations in his explanation, it could be argued that he would be doing this in an *ad hoc* manner, prompted by the challenge ahead of him, and not by independent reasons having to do with furthering the goals of his discipline.

I take it that the unity of the explanations given by a theory is an important aspect of the systematicity of that theory. It is hard to consider a theory systematized if some of the explanations that it offers are disunified. But does the disunified character of the physicist's answer to the second why-question pose a problem for the idea that chemistry is micro-reducible to physics as KOP hoped? Micro-reduction demands that any observational data that is explainable by chemistry is also explainable by physics. Notice however that by "observational data" one can mean two things: an observable *instance* of a phenomenon (e.g., the occurrence of hydrogen gas in any of the reactions above), or an observable *pattern* (e.g., the occurrence of hydrogen gas in all of the reactions above). If the explanandum is an observable instance, then one could perhaps argue that the physical explanation is at least as systematized as the chemical explanation; one could say that although it may be more complicated than the chemical explanation, the physical explanation is deeper and more powerful, so any loss in simplicity is compensated by a gain in explanatory power. However, if what needs to be explained is the occurrence of an observable pattern (in our case the occurrence of hydrogen gas in all four reactions), then there are reasons to question the idea that a similarly systematized physical explanation is possible. This is because there are reasons to think that the physical explanation is less unified than the chemical explanation, as the lab scenario shows.

As mentioned, the model of reduction that KOP propose is deeply eliminativist. If the reduction of chemistry to physics is achieved, then all the theoretical terms of chemistry are superfluous and should be eliminated from the vocabulary of science. Terms like “acid”, “base”, “oxidant”, “reductant”, etc. will become otiose, since whatever can be done with these terms (e.g., explaining) could be done just as well if not better with a more fine-grained theory in which these terms do not figure.

I argued that some things that are in need of explanation (i.e., patterns of chemical behaviour) cannot be explained in a unified manner by physics, but they can be so explained by chemistry. What seems to be required for a unified explanation of patterns of chemical behaviour is not knowledge of the micro-details that the fine-grained physical theory provides, but quite the opposite: abstraction from those details, which enables one to see similarities between systems that are regarded as different by the fine-grained theory. If for some explananda the chemical explanantia are more unified than the corresponding physical explanantia, the idea that physics and chemistry are equally well systematized becomes problematic. But if this is the case, there are grounds to question that subcondition (c) of KOP’s account of reduction is met. This result, in turn, raises doubts that KOP’s account of reduction can be effectively applied to chemistry.

4.3 Functional reduction

The next model of reduction that I will be examining is the one elaborated by Kim (1999, 2005). Kim suggests that his model is distinct from Nagel’s and superior to it insofar as it does not require bridge laws to connect the vocabularies of the two theories. Although Kim’s model is aimed at the reduction of the mental properties to the neurophysiological ones, it is intended to apply more generally to the reduction of the special sciences to physics. Here's a general formulation of Kim's functional model of reduction: if E is a higher level property that is a candidate for reduction and B is the domain of properties serving as a reduction base, the functional reduction of E to B involves three steps (Kim 1999, p. 10-11).

> **Step 1**: E must be functionalized – that is, E must be construed, or reconstrued, as a property defined by its causal/nomic relations to other properties, specifically properties in the reduction base B.
>
> **Step 2**: Find realizers of E in B. If the reduction, or reductive explanation, of a particular instance of E in a given system is wanted, find the particular realizing property P in virtue of which E is instantiated on this occasion in this system; similarly, for classes of systems belonging to the same species or structure types.
>
> **Step 3**: Find a theory (at the level of B) that explains how realizers of E perform the causal task that is constitutive of E (i.e., the causal role specified in Step 1). Such a theory may also explain other significant causal/nomic relations in which E plays a role.

Let's see how this model of reduction is supposed to apply to chemistry. Consider the property of being an acid. The first step consists in construing acidity as a property defined by its causal/nomic relations to physical properties in the reduction base.

> **Step 1***: Acidity = the ability of some substances to donate protons in chemical reactions.

The second step would be to find those physical properties that realize the causal role that defines acidity; that is, find those systems of electrons and nuclei that donate protons in chemical reactions. Step 2 above explicitly considers the reduction of a particular instance of E to a particular realizing property P. Applied to our case, step 2 tells us that in order to to reduce a particular instance of acidity (i.e., a particular acid) we need to find a particular physical system of electrons and nuclei. So applied to our case, step 2 will be

> **Step 2***: Acid A is realized by system of electrons and nuclei P.

Step 3 tells us that we need to find a physical theory that explains how these physical systems of electrons and nuclei donate protons to other systems of electrons and nuclei. So applied to our case, step 3 will be

> **Step 3***: How system of electrons and nuclei P donates protons is explained by quantum mechanics.

As a result of applying these steps, acid A is said to be reduced to its realizer P. But it is worth emphasizing: the functional model of reduction allows us to reduce an *instance* of a higher level property to an *instance* of a lower level property. It does not does not allow us to reduce a higher level property simpliciter to a lower level property. For example, if the property candidate for reduction is pain, the functional model of reduction would – at best – allow the identification of pain as instantiated in some type of organism (or species) with some neurophysiological property that is characteristic of that organisms or species. Therefore, functional reduction delivers at most "local" or "species-specific" reductions: e.g., it allows us to reduce human pain to one neurophysiological property N_h, reptilian pain to another neurophysiological property N_r, etc. It does not allow us to reduce the general property of being in pain to a certain lower level property common to all beings that can experience pain.

If the functional model of reduction is applied to chemical properties like acidity, it allows us to reduce an *instance* of a higher level property (acid A) to an *instance* of a lower level property (physical system P). According to this model of reduction, the general property of being an acid (i.e., acidity simpliciter) would be fragmented into multiple species of acidity, each of which could be reduced to a certain physical property. For example, Kim's model implies that there must be a hydrochloric-acid type of acidity, a sulfuric-acid type of acidity, etc., and each of these types would be reducible to a certain physical property (e.g., being an HCl molecule, or being an H_2SO_4 molecule, etc.). This model would imply that beyond these species-specific notions of acidity, there is no notion of acidity as such.[17]

In order to evaluate the consequences of Kim's model of reduction for functional emergence, it is worth pointing out to the distinction between physicalism and reductionism. Fodor (1974) argued that physicalism (the idea that all that the sciences talk about are physical events, even if they are not using the physical vocabulary) is a thesis weaker than what he called reductivism (what I called reductionism), reductivism being the conjunction of physicalism with the assumption that there are natural kind predicates in an ideally completed physics which correspond to each natural kind predicate in any ideally completed special science. The distinction was also recognized by Hellman and Thompson (1975):

> "Traditionally, physicalism has taken the form of reductionism – roughly, that all scientific terms can be given explicit definitions in physical terms. Of late there has been growing awareness, however, that reductionism is an unreasonably strong demand." (1975, p. 551).

It seems pretty clear now that if functional reduction can be obtained, it proves something that is closer to physicalism (or token reductionism), rather than full fledged reductionism. Kim's model of reduction may be successful in providing local or species-specific reductions, but it does not deliver the reduction of properties simpliciter. It may be able to reduce human pain, reptilian pain, etc., to corresponding neurophysiological properties, but it is incapable of reducing pain as such. Similarly, it may be able to reduce the acidity of the various chemical species into as many physical properties, but it is incapable of reducing acidity itself. Therefore, this model of reduction leaves open the possibility of there being *sui generis* chemical properties (or *sui generis* special science properties, more generally).

Functional emergence embraces physicalism while at the same time maintaining that chemical properties are irreducible to physical properties because

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[17] In the next chapter I will argue that this claim is not warranted by the theory and practice of the science of chemistry.

the former are multiply realizable across various types of physical systems. Kim's functional reduction does not establish reductionism about the special science properties unless it is complemented by an argument to the effect that the properties that are the objects of study for the special sciences are not multiply realizable. Indeed, Kim offers an argument to the effect that multiply realizable properties cannot be legitimate objects of a unified scientific inquiry (Kim 1992). In Kim's view, there can be no science of pain. If Kim's reasoning is followed consistently, it leads us to the perplexing conclusion that there can be no science of acidity. I will discuss Kim's arguments in the next chapter, which will be dedicated to the evaluation of the various philosophical arguments against the thesis of multiple realization.

Chapter 5

A defense of functional emergence

Since multiple realizability is an important ingredient in functional emergence, challenges to the multiple realizability argument against reductionism are also challenges to functional emergence. This chapter responds to the various criticisms that have been brought to multiple realizability as an anti-reductionist strategy or to the multiple realizability thesis itself. With the help of examples of chemical functionally emergent properties such as acidity or piezoelectricity, I argue that some of these criticisms do not pose a threat to functional emergence, while the others do not succeed.

5.1 Shapiro's challenge

Shapiro (2000) claims that the thesis that a given kind is multiply realizable has been accepted too uncritically by philosophers. He complains that despite its wide acceptance, the thesis of multiply realizability is not precise. This, in Shapiro's view, is because it is not clear what the satisfaction conditions for the multiple realizability thesis are. Shapiro notices that the philosophical discussion of the multiple realizability thesis is dominated by examples that appeal to the intuitive force of the thesis, such as mousetraps, carburetors and minds. However, he points out that a rigorous formulation of the multiple realizability thesis is lacking. He complains that so far, no philosopher has ever tried to complete the sentence, “N and M are distinct realizations of T when and only when ...” (Shapiro 2000, p. 636).

Shapiro’s concern is twofold. He demands an answer to the question of how different two realizations have to be before we call them *distinct* realizations of a certain kind. But he also asks the question of how much similarity must realizers bear to each other to justify the claim that they are realizations of the *same* kind. Shapiro argues that once various conceptual issues are clarified, the task of demonstrating multiple realizability leaves this thesis far more difficult to establish than philosophers have thought.

My goal in this section is to propose a way of completing the sentence that Shapiro talks about and put it to the test. I will use the notion of a microconstitutive property developed in chapter 3 to provide the precise definition of multiple realizability that Shapiro requires and I will investigate whether this definition delivers the same (correct, I agree) conclusions about the different cases that Shapiro considers. In addition, I will show how the various chemical functional properties examined meet the criteria of multiple realizability that I put forward and why they should be considered genuine cases of multiple realizability.

Let’s consider the first of Shapiro’s concerns: how different two realizations have to be before we call them *distinct* realizations of a certain kind? Shapiro asks:

> “Are corkscrews that differ in composition only – one is made of steel and the other of aluminum – different realizations of the same kind? Are corkscrews which are identical in composition but which differ only in color – one is painted yellow and the other red – different realizations of a corkscrew? Are corkscrews that differ in mechanism as well as in composition – a waiter’s corkscrew relies on a simple lever whereas a "winged" corkscrew utilizes a rack and pinion – different realizations of the same kind?”(Shapiro 2000, p. 636).

Shapiro’s conclusion is that showing that a kind is multiply realizable, or that two realizations of a kind are in fact distinct, requires some work. In particular, one must show that the realizations in question differ in causally relevant ways. For example, he denies that two corkscrews that differ only in color are different realizations of a corkscrew because color is not a property that contributes to their capacity to remove corks. On the other hand, a waiter's corkscrew and a winged corkscrew do count as distinct realizations of a corkscrew because they accomplish their function in non-identical ways. The moral, according to Shapiro, is that multiple realizations count truly as multiple realizations when they differ in causally relevant properties – in properties that make a difference to how they contribute to the capacity under investigation.

How about two corkscrews that differ in composition only? Does a corkscrew made of aluminum and one made of steel count as a different realizations of the kind corkscrew? Shapiro's answer is negative. He writes:

> "Steel and aluminum are *not* different realizations of a waiter's corkscrew because, relative to the properties that make them suitable for removing corks, they are identical. The fact that one corkscrew is steel and the other aluminum is no more a reason to characterize them as different realizations than the fact that one might be yellow and the other red." (Shapiro 2000, p. 644).

I think that Shapiro's claim that a difference in composition is no more reason to characterize two corkscrews as different than a difference in color needs to be qualified. Although I agree with Shapiro that differences in composition and differences in color are not sufficient to establish differences in realization, such differences are not on a par. The reason is that color does not play any role in how well a corkscrew accomplishes its function, whereas the material a corkscrew is made of does. Corkscrews of any color do an equally good job at removing corks (provided that color is the only difference between them), whereas corkscrews made of different materials (steel and aluminum, for example) may differ in their performance (e.g., if a corkscrew is made of a type of a steel that has an extremely high strength due to an extremely high carbon concentration, the corkscrew may break more easily than an identical one made of aluminum). So while Shapiro is right to claim that the material composition does not make a difference in the *function* of a corkscrew (function depends primarily on design/form, not on composition), it could make a difference in the *how well* that function is carried out.

That being said, I think that Shapiro's argument is correct: unless two realizations of a kind carry out their functional role in distinct ways there is no reason to consider them different realizations of that kind. Corkscrews that differ only in the material they are made of or in color should not be considered different realizations of a corkscrew because material composition and color do not make a real difference in the way the corkscrew accomplishes its functional role. On the other hand, a waiter's corkscrew and a winged corkscrew are considered by Shapiro as truly distinct realizations of a corkscrew:

> "The waiter's corkscrew relies on a lever to pry the cork out of the bottle whereas the winged corkscrew uses a rack and two pinions to do the same job. Levers and rack and pinions are different mechanisms that require different manipulations, they are described by different laws, and so on. The causally relevant properties of these two devices differ; a fortiori they qualify as different realizations of a corkscrew." (Shapiro 2000, p. 644).

Now let's see if the the notion of a microconstitutive property developed in chapter 3 can be used to provide a precise definition of multiple realizability that would deliver the same (correct) verdict about the cases discussed by Shapiro. I suggest the following definition of multiple realization. Two lower level properties N and M are distinct realizations of a higher level property T when and only when

1) The instantiation of either N or M in an individual S is sufficient for the instantiation of T in S. (REALIZATION)

2) There is no microconstitutive property P such that the instantiation of P in an individual S is sufficient for the instantiation of either N or M in S. In other words, N and M have no microcon-

> stitutive feature in common (simply put, T is not a constitutive property). (DISTINCTNESS)

As discussed in chapter 3, a microconstitutive feature of a property is a feature that is possessed by all the instantiations of that property and only by them, and which determines the characteristics that define the property in question (e.g., the microconstitutive feature of the property of being a mammal is the possession of mammary glands, the microconstitutive feature of the property of being an alcohol is the possession of a hydroxyl group bound to a saturated carbon).

The first condition (REALIZATION) is broadly compatible with both accounts of realization currently on the market (the standard account and the subset account). According to the standard account, a property realizes another just in case it fills the causal role that defines the realized property. If the instantiation of a property in an individual is sufficient for the instantiation of another property in the same individual, then it is also the case that the causal profile of the latter obtains in virtue of the instantiation of the former. On the subset account, a property realizes another if and only if its causal powers include the causal powers of the realized property as a subset (Shoemaker 2007). If the instantiation of either N or M in an individual S is sufficient for the instantiation of T in S, and N and M are distinct, then the set of causal powers of T cannot be coextensive with the set of causal powers of either N or M – it must be a subset of the causal powers of either of them.

Does this definition of multiple realization deliver the correct conclusions about the different cases considered by Shapiro? Let's see. Consider the case of two corkscrews that differ only in material composition. Say, we have two waiter's corkscrews similar in all respects with the exception of the material they are made of: one is made of steel, the other is made of aluminum. Are they distinct realizations of a waiter's corkscrew according to the definition of multiple realization just proposed?

According to the definition of multiple realization above, a waiter's corkscrew made of aluminum and one made of steel are distinct realizations of a waiter's corkscrew when and only when:

1) The instantiation of either of them is sufficient for the instantiation of the kind waiter's corkscrew.

2) There is no microconstitutive property P such that the instantiation of P in an individual S is sufficient for the instantiation of either the property of being an aluminum or a steel waiter's corkscrew in S. In other words, there is no microconstitutive feature common to both an aluminum waiter's corkscrew and a steel one.

In this case, 1 is satisfied: if you have either an aluminum waiter's corkscrew or a steel one then you have a waiter's corkscrew. But condition 2 is not met: both the aluminum and the steel corkscrew are systems consisting of a helix (worm) and a class 2 lever.[1] Thus, the property of being a worm + class 2 lever system is a microconstitutive property of the waiter's corkscrew: the presence of a worm + class 2 lever system explains the ability of the waiter's corkscrew to remove corks. In explaining the ability of the waiter's corkscrew to remove corks, the explanation stops at the description of the worm + class 2 lever system and need not mention what the worm or the lever are made of. As Shapiro would put it, the shared microconstitutive feature of being a worm + class 2 lever *screens off* the differences between steel and aluminum relative to their function in a waiter's corkscrew. Therefore, a waiter's corkscrew made of aluminum and one made of steel are not distinct realizations of the kind waiter's corkscrew.

A similar argument can be made for the idea that two corkscrews that differ only in color are not distinct realizations of the kind they realize. Two corkscrews that differ only in color share the same microconstitutive feature – a feature that explains the ability of the type of corkscrew in question to remove corks. The explanation of how the corkscrew achieves its function stops at this shared microconstitutive feature, and need not go further and mention the color; nor should it, because the color is not part of the shared

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[1] In the case of class 2 levers, the load is situated between the fulcrum and the applied force. In class 1 levers the fulcrum is situated between the applied force and the load.

microconstitutive feature.

How about a waiter's corkscrew and a winged corkscrew? Are they distinct realizations of the kind corkscrew? According to the definition of multiple realization above, a waiter's corkscrew and a winged corkscrew are distinct realization of a corkscrew when and only when:

1) The instantiation of either of them is sufficient for the instantiation of the kind corkscrew.

2) There is no microconstitutive property P such that the instantiation of P in an individual S is sufficient for the instantiation in S of either the property of being a waiter's corkscrew or that of being a winged corkscrew. In other words, there is no microconstitutive feature common to both a waiter's corkscrew and a winged one – the property of being a corkscrew is not constitutive.

In this case, both 1 and 2 are satisfied. A waiter's corkscrew is realized by a system consisting of a worm and a class 2 lever, whereas a winged corkscrew is realized by a system that ultimately consists in a worm and two class 1 levers. In the case of the lever of the waiter's corkscrew, the load is situated between the fulcrum and the force (class 2 lever), whereas in the case of the levers of the winged corkscrew the fulcrum is located between the applied force and the load (class 1 lever). This results in a different operation of the two corkscrews: the waiter's corkscrew needs a pulling motion to remove the cork, whereas the winged corkscrew needs a pushing motion. What about the worm? The worm is present in both the winged corkscrew and in waiter's corkscrew. Isn't the worm a microconstitutive feature of both corkscrews? It is not. Despite being a constituent of both types of corkscrew the worm alone does not amount to a microconstitutive property of corkscrews: the presence of the worm alone cannot explain how each of the two types of corkscrew can remove corks; it explains how the cork is gripped, but it does not explain how the cork is extracted (the lever or the rack and pinions do). So the presence of the worm is not sufficient to explain the function of either corkscrew. Therefore the worm is not (by itself) a microconstitutive feature shared by the two corkscrews.

Thus, a waiter's corkscrew and a winged corkscrew have no microconstitutive feature in common (and thus being a corkscrew is not a constitutive property). As a result, a winged corkscrew and a waiter's corkscrew are truly distinct realizations of the kind corkscrew.

Do the functional properties considered in chapter 3 meet the criteria of multiple realizability that I put forward? Are acids, bases, reductants, oxidants, piezoelectrics genuinely multiply realized? The answer is affirmative because in all these cases both conditions are met. First consider acids and bases. As argued in chapter 3, there is no microconstitutive feature that is shared by all acids and only by them. Acids are not defined as those substances that contain a H atom. Bases are not defined as those substances that have a hydroxyl group. Thus, the second condition is met.[2]

The same with the property of being an oxidant: both oxygen and fluorine are good oxidants. But does this ability derive from a common microconstitutive property? This can be investigated by looking at their microphysical descriptions. Oxygen has 8 protons in its nucleus and 6 electrons on the last shell, whereas fluorine has 9 protons in its nucleus and 7 electrons on the last shell. Admittedly, both oxygen and fluorine have the first shell full (2 electrons on the 1s orbital), but so does any other element in the periodic table with the exception of hydrogen. Thus, having a first shell full is not a microconstitutive property. Also, having the first shell full does not explain the oxidizing properties of oxygen and chlorine. What does explain these properties is their ability to accept electrons, which is related to a magnitude called the redox potential. In aqueous solutions, the redox potential is a measure of the tendency of the solution to either gain or lose electrons when it is subject to change by introduction of a new species. A solution with a higher (more positive) reduction potential than the new species will have a tendency to gain electrons from the new species (i.e. to be reduced by oxidizing the new species) and a solution with a lower (more negative) reduction potential will have a tendency to lose electrons to the new species (i.e. to be oxidized by reducing the new

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[2] In all cases considered, the first condition is met in an uninteresting way. The contentious condition that is related to Shapiro's criticisms is condition 2.

species). Thus, there is an important relational aspect to this ability, which further prevents the possibility of attributing it to a microconstitutive property. Therefore, the ability to gain electrons is not the result of a microphysical ingredient common to both oxygen and fluorine, but that of an interplay of various forces such as the electrostatic attraction of the nucleus and the electron shielding. For this reason, the property of being an oxidant and that of being a reductant should be regarded as genuinely multiply realized.

The same holds for piezoelectrics. Because of the diverse nature of the mechanisms responsible for the piezoelectric behaviour of various materials it becomes obvious that piezoelectricity is a multiply realized property – the mechanism of piezoelectricity of crystals (ionic displacement) is distinct from that of polymers (dipole rotation), which is distinct from that of interface materials like cement and bone (streaming current).

Two questions remain, however. The first is this: admittedly, piezoelectricity is realized by three categories of phenomena, but couldn't we reduce the piezoelectricity of crystals to ion displacement, that of polymers to dipole rotation, and that of interface materials to streaming currents? Take the case of crystals: couldn't we define the piezoelectricity of crystals microconstitutively, with reference to the creation of a dipole moment which is caused by ion displacement in noncentrosymmetric crystals? As argued in chapter 3 (subsubsection 3.3.3.1), noncentrosymmetry is not a microconstitutive property because there are various nonequivalent ways in which a crystal can fail to be centrosymmetric (noncentrosymmetry is itself functional). However, what about those piezoelectric crystals that are structurally identical? Why claim that two crystals that have the same structure are different realizations of the property of being a piezoelectric crystal? Take, for example quartz (SiO_4 tetrahedra) and gallium orthophosphate, which is structurally identical but the silicon atoms are alternately substituted with gallium and phosphorus ($GaPO_4$ tetrahedra). Why claim that quartz and gallium orthophosphate are distinct realizations of the property of being a piezoelectric crystal? Since the piezoelectricity of crystals is mainly the result of their structural properties, Shapiro would probably argue that two piezoelectric crystals that are structurally identical should not count as different realizations of the property of being a piezoelectric crystal. I suspect that in Shapiro's view, the differences between a quartz and a gallium orthophosphate crystal would be as relevant as the differences between a steel corkscrew and one made of aluminum; in both cases, Shapiro would argue, the properties that make them suitable for accomplishing their role (producing piezoelectricity, respectively removing corks) are identical. So Shapiro may agree that piezoelectricity can be multiply realized, but he would probably deny that the piezoelectricity of structurally identical crystals is multiply realized.

The stance that Shapiro would take is tempting. Agreeing with it would not be a major concession: even if structurally identical crystals are not different realizations of crystal piezoelectricity, piezoelectricity as a general property is still multiply realized (i.e., Shapiro would most certainly grant that the mechanism of piezoelectricity in cement or wet bone is not similar with the one in crystals, and even that the piezoelectricity of crystals with dissimilar structures is multiply realized). However, it is worth investigating whether the case of structurally identical crystals parallels the case of corkscrews identical in all respects but composition. So are quartz and gallium orthophosphate different realizations of crystal piezoelectricity any more than a waiter's corkscrew made of aluminum and one made of steel are different realizations of the kind waiter's corkscrew?

To answer this question, we need to see whether the way in which these objects (i.e., aluminum vs. steel corkscrew, respectively quartz vs. gallium orthophosphate) accomplish their respective functions is genuinely different. Take the case of corkscrews first. Do we have a satisfactory explanation of the way in which a waiter's corkscrew made of aluminum accomplishes its function of removing corks? It turns out that we do. A waiter's corkscrew made of aluminum is able to remove the cork from a bottle by a two-step process: 1) *the grip*, which happens when the worm penetrates the cork; 2) *the pull*, which happens when the class 2 lever is deployed on the lip of the bottle and the waiter pulls the handle of the corkscrew, thereby removing the cork. This is a perfectly satisfactory description of the way in which a waiter's corkscrew made of aluminum works. But how does a waiter's corkscrew made of steel work? It turns out that the process is identical. The two explanations are identical, and neither of them makes reference to the material from which the corkscrew is made. The words "aluminum" or "steel" do not occur in the description of the ways in which these corkscrews accomplish their function. In explaining the ability of the waiter's corkscrew to remove corks, the explanation does not mention what the worm or the lever are made of; it only mentions how the grip and the pull are realized (the grip is realized by the worm penetrating the cork, and the pull is realized by the class 2 lever system). For this reason, any corkscrew (regardless of the kind of material it is made of) that removes corks precisely in the way described above would not count as a different realization of a waiter's corkscrew.

To what extent does this analysis carry over to the case of a piezoelectric made of quartz and one made of gallium orthophosphate? What is the way in which a quartz crystal converts mechanical stress into surface charge, and does it differ from the way in which gallium orthophosphate accomplishes the same thing? The mechanism of quartz piezoelectricity has been described in detail in chapter 3. For our purpose here it is important to recall that an explanation of quartz's piezoelectric properties makes a reference to silicon and oxygen atoms, as well as to the geometrical structure whose nodes these atoms occupy (tetrahedra). Similarly, an explanation of the way in which a gallium orthophosphate converts mechanical stress into surface charge will make a reference to the same type of geometric structure (tetrahedra), but it will also mention the atoms that occupy the center and the tips of the tetrahedra (alternating gallium and phosphorus in the centers, and and oxygen at the tips). Therefore, despite being very similar, the two explanations are not quite identical: the explanation of quartz's piezoelectricity mentions silicon and oxygen, while that of gallium orthophosphate mentions gallium and phosphorus as well as oxygen. This is where the case of quartz and gallium orthophosphate differs from the case of aluminum and steel corkscrews. This difference shows that the case of crystals is not as simple as the case of corkscrews, and it lends some support to the idea that quartz and gallium orthophosphate are distinct realizations of the property of being a piezoelectric crystal.

To conclude, Shapiro's remarks do indeed discipline the talk of multiple realizability that philosophers have been engaged in. In truth, the thesis of multiple realizability had been accepted too uncritically by philosophers. But in this section I have attempted to show that the talk of multiple realization can be made rigorous. Using the notion of a microconstitutive property developed in chapter 3, I suggested a criterion for multiple realization and I showed that the chemical properties considered in chapter 3 meet it.

5.2 Kim's argument from two metaphysical principles

As stated in the previous chapter, Kim's functional reduction does not establish reductionism about the special science properties unless it is complemented by an argument to the effect that the properties that are the objects of study for the special sciences are not multiply realizable. Indeed, Kim offers arguments to the effect that multiply realizable properties cannot be legitimate objects of a unified scientific inquiry (Kim 1992). In this section I will present Kim's arguments and evaluate them.

Kim takes issue with a claim shared by functionalists about special science properties. The claim is that disjunctions of heterogeneous kinds (or disjunctive properties) are unfit for laws (Kim 1992, p. 10). In section 3.1 I illustrated this claim with the following example: while it is a law that sulfuric acid in reaction with iron produces iron sulfate, and it is a law that hydrochloric acid in reaction with zinc produces zinc dichloride, it is not a *law* that *either* sulfuric acid *or* hydrochloric acid in reaction with *either* iron *or* zinc produces *either* iron sulfate *or* zinc dichloride. I claimed that nonetheless, the more general claim, asserting that acids in reactions with metals produce a metal salt *is* a law. The general idea here is that the kinds that the special sciences talk about are natural kinds which figure in true universal generalizations but they are realized by a variety of lower level kinds which cannot replace them in those generalizations. Being an acid is a genuine property which can figure in true chemical generalizations, but being a molecule of H_2SO_4__or__HCl is a disjunctive property which cannot. Kim's problem with this claim is this: if the kinds that the special sciences talk about are realized by wildly disjunctive and obviously nonnomic lower level kinds, why aren't themselves equally heterogeneous and nonnomic?

Kim thinks that this question is prompted by examining the case of jade. It turns out that being jade is a disjunctive property: all samples of jade are either samples of jadeite or nephrite. Kim argues that since jade is disjunctive, it cannot be a mineral kind – jade does not pass the projectibility test. If we discovered (suppose) that all the millions of observed samples of green jade turn out to have been samples of jadeite, and none of nephrite, we clearly would not, and should not – Kim argues – continue to think of the universal generalization "Jade is green" as well confirmed (Kim 1992, p. 12). Therefore there can be no laws about jade; the universal generalization "Jade is green" lacks nomic character, since it is just the conjunction between two other claims, which admittedly do have nomic character: "Jadeite is green" and "Nephrite is green". As a result, there can be no science of jade (or at least no unified science of jade).

Kim thinks that there is a strong and instructive analogy between jade and multiply realized special science properties (Kim's favourite example is pain). Kim argues that just like jade and because of the same reason, the multiply realized properties cannot be the object of a unified science. Kim further supports this conclusion by invoking two principles.

- **The Principle of Causal Individuation of Kinds:** Kinds in science are individuated on the basis of causal powers; that is, objects and events fall under a kind, or share in a property, insofar as they have similar causal powers (Kim 1992, p. 17).

- **The Causal Inheritance Principle:** If a higher-order property M is realized in a system at t in virtue of physical realization base P, the causal powers of this instance of M are identical with the causal powers

> of P (Kim 1992, p. 18).

Applied to the case of jade, these two principles lead to the conclusion that samples of jade that consist of nephrite must be grouped under one kind and those that consist of jadeite must be grouped under another (By the Causal Inheritance Principle, samples of jade that consist of jadeite have the causal powers of jadeite and those that consist of nephrite have the causal powers of nephrite; and by the Principle of Causal Individuation of Kinds, $\text{jade}_{jadeite}$ and $\text{jade}_{nephrite}$ have different causal powers and thus fall under distinct kinds.) The upshot is that the disjunctive nature of jade prevents the possibility of there being laws about it – as a result, there can be no science of jade.

According to Kim, the same fate befalls all special science kinds that are multiply realized (including mental kinds M).

> "The reasoning is simple: instances of M that are realized by the same physical base must be grouped under one kind, since ex hypothesi the physical base is a causal kind; and instances of M with different realization bases must be grouped under distinct kinds, since, again ex hypothesi, these realization bases are distinct as causal kinds. Given that mental kinds are realized by diverse physical causal kinds, therefore, it follows that mental kinds are not causal kinds, and hence are disqualified as proper scientific kinds. Each mental kind is sundered into as many kinds as there are physical realization bases for it, and psychology as a science with disciplinary unity turns out to be an impossible project." (Kim 1992, p. 18).

If correct, Kim's arguments show that the multiply realized properties cannot as such be legitimate objects of scientific inquiry. If Kim is right, there cannot be a unified science of jade or a unified science of pain, or a science of any multiply realized property, in point of fact.

> "There are no scientific theories of jade, and we don't need any; if you insist on having one, you can help yourself with the conjunction of the theory of jadeite and the theory of nephrite. In the same

> way, there will be theories about human pains (instances of N_h), reptilian pains (instances of N_r), and so on; but there will be no unified, integrated theory encompassing all pains in all pain-capable organisms, only a conjunction of pain theories for appropriately individuated biological species and physical structure-types. Scientific psychology, like the theory of jade, gives way to a conjunction of structure-specific theories." (Kim 1992, p. 17).

Consequently, the autonomy of the special sciences is threatened:

> "If this is right, the correct conclusion to be drawn from the MR-inspired antireductionist argument is not the claim that psychology is an irreducible and autonomous science, but something that contradicts it, namely that it cannot be a science with a unified subject matter." (Kim 1992, p. 17).

According to Kim, the thesis of multiple realizability seriously compromises the disciplinary unity and autonomy of the special sciences. If Kim's reasoning is followed consistently, it leads us to the perplexing conclusion that there can be no science of acidity (or at least not a unified one). So if we follow Kim's reasoning, either there is no science of chemistry or chemistry is fragmented into as many chemistries as kinds of acids there are. This conclusion is indeed puzzling. Before we turn to evaluate this possibility, let us first ask the following questions. Could the case of psychology that Kim discusses be relevantly different from that of other special sciences such as chemistry? Or perhaps the kind that Kim relies on in his analogy (jade) is fundamentally different from the kinds of both psychology and chemistry?

I think that the analogy between special science properties (pain, acidity) and jade is not justified, let alone strong and instructive as Kim believes. The reason is simple: jade is not a functional kind, despite the fact that it is multiply (or rather, doubly) instantiated. Although jade artifacts have a role (i.e., an ornamental role), the property of being jade is not itself defined by a functional role. Jade is not defined by the way it reflects light, for example. If you cook up something that reflects light like jade, and is in its macroscopic appearance indiscernible from jade, you have not made jade (unless you have made either jadeite or nephrite). If you try to sell it as jade, you risk getting arrested.[3] However, if you invent something that traps mice, you have made a mousetrap. Selling the mice-catching device that you invented as a mouse trap will make you a legit enterpriser, while selling something that has the macroscopic appearance of jade as jade will make you a counterfeiter.

Now, the functional properties of chemistry are more like mousetraps than like jade. If you cook up a substance that plays the causal role of acids (donates protons in chemical reactions), you have made an acid. This is what people working in synthetic chemistry do, and they get paid for it. Kim's mistake is that he conflates disjunctive properties like jade with functional properties, like acidity: the latter are disjunctively-based, but not disjunctive. This is why I think it is improper to say that jade is multiply realized; saying this implies that jade is a functional property when it is not. Unlike the property of being an acid, being jade is not defined by a certain causal role (say, the ability to reflect light in a certain manner). Being jade is simply a disjunctive property (being either jadeite or nephrite), not a multiply realized one. For this reason, there is no wonder that there are no laws about jade, and thus there is no wonder that there is no science of jade. However, there are laws about acids and there is a unified science of acidity, or at least it appears that way.

Shapiro (2005) has argued that even if one accepts The Principle of Causal Individuation of Kinds and The Causal Inheritance Principle the conclusion that the special sciences which talk about multiply realized kinds are disunified still does not follow. This, in Shapiro's view, is because The Principle of Causal Individuation of Kinds does not entail that kinds with distinct causal powers cannot realize the same higher level kind (Shapiro 2005, p. 957). Interestingly, Shapiro invokes the case of acids: "Sulfuric acid and deoxyribonucleic acid differ in their causal powers. One has the causal powers of a gene and the other does not. However, it does not follow from this difference that they do not share a scientific property – they are both acids after all" (Shapiro 2005, p.

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[3] This argument is due to Fodor (1997).

957). According to Shapiro, if Kim maintains that every difference in a kind's substrate implies a difference in kind, this leads to an absurd consequence: that *acid* is not a kind. Shapiro writes:

> "Because acids can be multiply realized, the reasoning of the Master Argument [Kim's argument] leads to the rejection of chemistry as a unified science. There must, it turns out, be at best local chemistries: a chemistry in which sulfuric acid is an acid; a chemistry in which hydrochloric acid is an acid; a chemistry in which DNA is an acid. There will be as many chemistries as there are, not just actual acids, but nomologically possible acids. I was pretty good at chemistry in high school, but of course those were the days when there was only one chemistry." (Shapiro 2005, p. 957).

Shapiro finds it absurd that chemistry is a disunified science and thus he constructs a *reductio* against Kim's argument. But is the idea that chemistry is a disunified science absurd? Not if acidity is a fragmented property, as Kim's principles would seem to entail. Let us now examine the possibility that for various reasons (social, institutional, etc.) people mistakenly believed that chemistry is a unified science. Let us not dismiss out of hand what Kim suggests, namely that the sciences that talk about multiply realized kinds are in fact fragmented or disunified, and hence unprojectible. If we stick to the case of chemistry, Kim's reasoning leads us to the conclusion that chemistry is a disunified science because it talks about properties like acidity, which are realized by a variety of nuclei-electrons systems. But is this conclusion right?

The claim that the property of being an acid, for example, can be fragmented into a HCl acidity, a H_2SO_4 acidity, a HNO_3 acidity and so on depending on its physical realization base is without theoretical support. Chemists would balk at this idea, as Shapiro in fact does. They would be entitled to do so because such subdivisions lack any theoretical grounding and they are unwarranted by scientific practice. According to Brønsted-Lowry theory of acids and bases, substances like HCl, H_2SO_4, HNO_3 are all acids because they donate protons in chemical reactions. The substances we call acids are composed of different elements, and they have different chemical structures, but they are unified by a certain behaviour which can be objectively determined. Even if acids were to be subdivided along some criteria, the subdivisions would not be made using constitutive criteria, but functional ones. For example, depending on what is the functional property considered as defining acidity we have Lewis acids (electron-pair acceptors), Brønsted-Lowry acids (proton donors), Arrhenius acids (increase the concentration of the hydronium ion when dissolved in water). In the case of the Brønsted-Lowry acids, depending on how much they dissociate and whether they stay like that, we have weak acids and strong acids. Depending on the number of protons donated by each acidic compound, we have monoprotic acids or polyprotic acids.[4]

The fragmentation of acidity that Kim's argument commends would not be motivated by scientific considerations, but by a commitment to *a priori* metaphysical principles. As discussed above, Shapiro claims that Kim's two principles do not jointly entail that kinds that are multiply realized must be disunified. The Causal Inheritance Principle is relatively unproblematic, so the point of contention is The Principle of Causal Individuation of Kinds. Shapiro is of the view that this principle does not entail that every difference in a kind's physical substrates implies a difference in kind. I agree with Shapiro, but I am not sure Kim would. As stated by Kim, The Principle of Causal Individuation of Kinds is compatible with two readings, depending on how "similar causal powers" is understood. One possible reading is this:

- **The (Strong) Principle of Causal Individuation of Kinds:** Kinds in science are individuated on the basis of causal powers; that is, objects and events fall under a kind, or share in a property, insofar as they have the same (i.e., *identical*) causal powers.

On this interpretation, if two objects fall under a kind they have all of their causal powers in common. Conversely, if two objects share some of their causal powers but not others, the two objects will fall under two different kinds. Another possible reading is this:

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[4] A similar point was made in the philosophy of biology by Kincaid (1990).

- **The (Weak) Principle of Causal Individuation of Kinds:** Kinds in science are individuated on the basis of causal powers; that is, objects and events fall under a kind, or share in a property, insofar as they have most (or their most relevant) causal powers in common.

On this interpretation, if two objects have most (or their most relevant) causal powers in common then the two objects may be legitimately grouped under the same kind. Likewise, if two objects belong to the same kind, the they share most of their causal powers (or at least a sufficient number of their most relevant causal powers).

The second (weak) interpretation is more charitable than the first. Two objects that are classified as belonging to distinct kinds according to the strong formulation of the Causal Individuation of Kinds Principle could very well be classified as belonging to the same kind according to the weak version. Since Shapiro is of the view that The Principle of Causal Individuation of Kinds does not entail that every difference in a kind's physical substrates implies a difference in kind, it is pretty obvious that he endorses the weak reading of this principle (differences in a kind's physical substrate determine some differences in causal powers).

But the weak version defines sameness of kind in terms of the causal powers that are deemed relevant. And when talking about causal powers, relevancy may differ in accordance to our interests. Consider Shapiro's example: if you are a biologist, DNA and sulfuric acid belong to different kinds (one has a role in biological heredity, the other doesn't). But if you're a chemist, DNA and sulfuric acid belong to the same kind (both donate protons). The strong version of the principle does not allow this sort of relativization.[5] At the same time, the strong version of the principle has some undesirable consequences. It entails that any difference, no matter how small or irrelevant, suffices to establish a difference in kind. For example, two individuals of the same biological species would fall under different kinds if one is heavier, or more aggressive, or has a darker coat than the other. Samples of two different substances be-

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[5] This sort of relativization is neither dangerous nor should it be avoided; in fact, it is productive for the sciences.

longing to a certain group of the periodic table (group 11) would fail to be classified as belonging to the same kind (metal) if they consist of atoms having different atomic numbers (e.g., silver has atomic number 47 and gold has atomic number 79).

Another reason why the weak version of the principle is to be preferred is its compatibility with the idea that kinds could be individuated on the basis of the causal role they perform, and this sort of individuation is to be preferred in many contexts (including in science). Imagine a hardware store organized according to Kim's principles. Such a store would go out of business pretty quickly, for mousetrap buyers will have hard times finding an electric mousetrap in the electric-circuitry based devices section of the store, on the same aisle where photo cameras and telephone sets would be located. If the buyer is cautious and they want to shop-around and compare the different types of mousetraps available in the store, they will give up pretty quickly, for spending a full day criss-crossing a hardware store from the electric-circuitry-based devices aisle to spring-based devices aisle to glue-based-devices aisle is not fun. Of course, mousetraps are not scientific kinds, and hardware stores are not research institutions. But this does not affect the point I am making, namely that kinds in general may be individuated not on the basis of their constitution, but on the basis of their causal roles, i.e., functionally. This allows individuating kinds on the basis of a relevant subset of the causal powers of the entities instantiating that kind. Thus, two objects belonging to different physical kinds may be legitimately grouped under the same chemical kind if they share a relevant subset of their causal powers, namely those causal powers that are deemed as defining the chemical kind in question. Fodor was entitled to ask: "Why... should not the natural kind predicates of the special sciences cross-classify the physical natural kinds?" (1974, p. 408). There is no reason why, and in my view chemical kinds like *acid* are the living proof of this.

In my view, these are pretty compelling reasons to reject the strong version of the principle in favor of the weak version. But if the weak version is preferred, Kim's argument does not succeed and his conclusion that there cannot be a science whose kinds are multiply realized does not follow.

5.3 The argument from the general failure of special-science causal closure and the argument from the idiosyncratic nature of special science properties

More recently, while maintaining his old argument that multiply realizable properties/kinds cannot figure in laws, Kim (2010) argued that there can be no strict laws in the special sciences. Presumably, this weaker claim is intended to support Kim's views about the impossibility of a science whose kinds are multiply realized.[6] In this section I will present Kim's arguments and argue that they do not support this conclusion.

One of the arguments that Kim presents is inspired by Davidson's view on mental anomalism. Davidson was of the view that the mental was anomalous, i.e., there can be no laws connecting mental phenomena with other mental phenomena. This is because every instance of mental to mental causation is vulnerable to disruption by the occurrence of a nonmental (physical) event. Kim calls this the "massive failure of causal closure for the mental":

> "Let M and M* be mental event kinds and consider a putative causal relation from an M-event to an M*-event. Then there always is a physical event kind P such that if a P-event were to occur along with the M-event, that would prevent the M*-event from occurring. That is, every mental-to-mental causal relation is liable to disruption by the occurrence of a physical event." (Kim 2010, p. 292)

Kim believes that this sort of argument generalizes to the special sciences:

- **General failure of special-science causal closure**: For any putative causal relation from an S_1-event to an S_2-event, involving special-science kinds S_1 and S_2, there always is a lower level condition C such that if

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[6] It should be noted however that Kim does not make this argument explicitly.

> C were to occur along with the S_1-event, that would disrupt the causal process and prevent the S_2-event from occurring. (Kim 2010, p. 292)

According to Kim, the general failure of special-science causal closure entails the nonexistence of strict special-science laws: for any special science kinds S_1 and S_2, there is no strict law of the form kinds $S_1 \rightarrow S_2$. Because the causal/nomological relations at higher levels studied by the special sciences are always susceptible to disruption from below (i.e., to interference from events occurring at a lower level) it follows that strict laws can be found only in fundamental physics, where the danger of disruption from below does not exist because at the most fundamental physical level there is no "below". Kim claims that the physical level being the bottom level, physical causal relations at the fundamental level suffer no similar vulnerability, and this allows for the possibility of strict physical laws.

The other argument presented by Kim is based on an argument made by J.J.C. Smart (1963). In his book *Philosophy and Scientific Realism*, Smart argues for the same conclusion as Kim, namely that there are no strict laws in the special sciences. Like Kim, Smart thinks that physics is the only science in the business of discovering and formulating laws. He writes:

> "Not only do I deny the existence of emergent laws and properties, but I even deny that in biology and psychology there are laws in the strict sense at all. There are, of course, empirical generalizations. There are not any biological laws for the very same reason that there are not any laws of engineering. Writers who have tried to axiomatise biological and psychological theories seem to me to be barking up the same gum tree as would a man who tried to produce the first, second, and third laws of electronics, or of bridge building. We are not puzzled that there are no laws of electronics or of bridge building, though we recognize that the electronic engineer or bridge designer must use laws, namely laws of physics...I shall try to show that the important analogy is not between biology and the physical sciences but between biology and the technologies, such as electronics." (Smart 1963, p. 52)

By “laws in the strict sense” Smart means laws that are universal in the sense that they apply everywhere in space and time.[7] Therefore, strict laws are exceptionless. According to Smart, examples of strict laws are the laws of motion in classical mechanics, the laws of electrodynamics, and the equations of quantum mechanics. Interestingly, Smart does not think of chemistry as different from physics with respect to the kind of laws that it affords (1963, p. 53). The two sciences are viewed as being on the same side of the fence, so to speak, in contradistinction to sciences like biology or psychology, which cannot afford strict laws. So in Smart’s book, chemistry is not quite a special science. On the other hand, biology and psychology are. Their relation with the former emulates the relation between physics and engineering. For Smart, biology is related to physics and chemistry the way radio-engineering is related to the theory of electromagnetism. He claims that just as the radio-engineer uses physics to explain why a circuit with a certain wiring diagram behaves as it does, so the biologist uses physics and chemistry to explain why organisms or parts of organisms with a certain natural-history description behave as they do (Smart 1963, p. 57). For Smart, therefore, biology is “applied” chemistry and physics in the same way in which engineering is “applied” physics: the laws of chemistry and physics explain the behaviour of biological entities in the same way the laws of physics explain the workings of a radio receiver.

Even if one grants that the special sciences are like engineering, why should one accept that they cannot have strict laws, like physics? Smart’s answer is this. Both engineering and biology involve complex systems and entities – much more complex than those of the basic science, physics (or physico-chemistry). For this reason, the entities of the special sciences are highly idiosyncratic. For example, no two cells are exactly alike, even those accomplishing the same function in the same organism. From this it follows that no two cells behave exactly the same way. As a result – according to Smart – we cannot expect to find strict laws about them. So according to Smart, the

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[7] Smarts adds here the condition that proper laws should be able to be expressed in perfectly general terms without making use of proper names or tacit reference to proper names.

individual variability among the kinds of any given special science preclude the possibility of strict laws in that science.

Unsurprisingly, Kim supports Smart's argument. Kim thinks that the similarity in the behaviour of some entities (that the nomological character of the claims about those entities requires) is determined by the similarity in the microphysical constitution of those entities, and conversely, the greater the dissimilarity in microphysical constitution, the greater the behavioural dissimilarity. Kim's argument is basically a version of the one presented in the previous section, where I also pointed out what's wrong with it. But it is worth noting a difference between Kim and Smart. While Smart argues that there are no strict laws in the special sciences, Kim wants to go further. He argues not only that there are no strict laws in the special sciences (2010), but also that the so-called special sciences are not in fact sciences (1992). Kim insists that this does not have to be taken as a negative message. Special sciences can still flourish if they turn to providing explanations of the phenomena they study at a more basic level. In Kim's view, a special science like psychology remains *scientific*, though perhaps not *a science* (Kim 1992, p. 26). It is not a science because the kinds that it talks about are too dissimilar from the point of view of their realizations to be legitimate objects of scientific inquiry. It remains scientific insofar as it dedicates its research programs to elucidating the more basic mechanisms that make the species-specific kinds possible.

Before evaluating the arguments inspired by Davidson and Smart we should look at two claims that Kim isn't very careful to distinguish – indeed, one may argue that Kim is in fact interested to blur the distinction between them and to take both of them as supporting his view of the special sciences: it is one thing to claim that the special sciences cannot afford strict laws and quite another to claim that the kinds that the special sciences talk about cannot be legitimate objects of scientific inquiry because they are too disunified to be laws about them. The former claim states something about the nature of the special-science laws, while the latter calls into question the very possibility of there being special-science laws. The former claim is about the nature of the special sciences *qua* sciences, while the latter doubts that the special sciences can be that – namely sciences.

In the light of the clarification above, one may see that Kim's general failure of special-science causal closure supports at most the idea that the laws formulated by the special sciences are not exceptionless. The same with Smart's argument based on the idiosyncratic and complex nature of the special science kinds. Neither argument purports or is able to show that there can be no science whose kinds are multiply realized. At best, they show that the character of a science whose kinds are multiply realized is somewhat different from the character of a science whose kinds are not. But neither argument intends or has the force to show that the only science which deserves to be called like that is physics.

Now let's turn to Kim's arguments inspired by Davidson and Smart. Does the general failure of special-science causal closure affect the scientific status of the special sciences? I don't see why this should be the case. I don't see why the possibility of disruption from below endangers the nomological status of the relations between higher level properties. Consider this example. Admittedly, an acid and a metal won't react to produce hydrogen if the temperature is near 0 K. This is a standard example of what Kim means by physical conditions disrupting chemical behaviour "from below". Does it follow from here that "acids in reaction with metals produce hydrogen" is not "a real" law, or that it is just a rule of thumb devoid of nomological content? It doesn't. What follows is that the statement in question is susceptible to being interfered with by some factors (which in this case are known, but could be unknown as well) such that if those factors obtain, the antecedent does not give rise to the consequent (acids and metals may come in contact, but hydrogen will not be produced). But this possibility arises with respect to the laws of physics as well. For example, if you wait long enough, heat may "flow" from a cooler body to a hotter one, thereby violating the second law of thermodynamics.[8]

Of course, one may object by saying that thermodynamics is not a fundamental theory in the sense in which Kim or Smart use the word. But are

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[8] I am considering here the Clausius formulation: "No process is possible whose sole result is the transfer of heat from a body of lower temperature to a body of higher temperature".

there any more reasons to consider the laws of fundamental physics as strict? Even if we grant that the danger of disruption from below does not arise in relation to the causal/nomological relations between entities populating the most fundamental physical level, these relations may still be sensitive to other factors. For example, the notion that the laws of basic physics are changing with time is currently being taken seriously by particle physicists, astronomers and cosmologists. There is evidence that the coupling constant characterizing the strength of the electromagnetic interaction (the so-called fine structure constant) may not actually be a constant. If this is the case, *pace* Smart, the laws of the electrodynamics are not strict – they did not apply in the present form to the early universe, and they may cease to hold in the future. Does the fact that the laws of basic physics evolve with time threaten the scientific character of fundamental physics? It does not. Fundamental physics remains a science even if there are no strict laws in the sense of Kim or Smart; physicists can still formulate explanations and predictions using these laws, even if they do not hold universally in time. Similarly, researchers in any of the special sciences can still formulate explanations and predictions with the laws available in their own domains, even if these laws are not exceptionless – that is, they can still do *science*. The exceptional "disruptions from below" that Kim talks about are just that – exceptions. They do not threaten the scientific character of chemistry any more than the evolving nature of physical laws threatens the scientific character of physics. The low frequency of these disruptions in the laws of a given domain allows for reliable explanations and predictions using those laws; and this is what is required from a science. If one demands that the laws of a domain be exceptionless in order for them to be considered "real laws" (and in order for that domain to be considered "scientific") then not only is one setting the bar of what it means to be scientific unreasonably high so that no actual science can reach it, but one is also misrepresenting the nature of science.

What about Smart's claim that the special sciences resemble more technologies or engineering than they resemble physics? This claim, as well as the claim that the laws of the special sciences are not strict, are intended to depict a certain image of the special sciences as significantly different from physics (or from fundamental physics). According to this image, physics affords strict laws, the special sciences do not. Physics alone is science, biology and other special sciences are just engineering; the special sciences involve applications of the laws of physics but they do not have laws of their own. Smart says that "there are no real laws of biology for the very same reason that there are no special laws of engineering". He suggests that trying to find laws in the special sciences is as futile as trying to find laws in electronics. However, as a matter of fact, *there are* laws in electronics:

- **Ohm's law**: in a circuit, the amount of current flowing between two points is directly proportional to the potential difference across the two points, and inversely proportional to the resistance between them.
- **Kirchhoff's current law**: in a circuit, the sum of the currents flowing to a point is equal to the sum of the currents flowing away from that point.

These laws are *not* laws of physics.[9] These laws are neither laws of classical mechanics, nor of electromagnetism or quantum mechanics, or of any other branch of physics, although they, like any other regularity, are the result of the existence of such laws.[10] These laws are grounded in Maxwell's equations, but they are not themselves the laws of electromagnetism. The laws mentioned above are not as much about the physical behaviour of the elementary particles known as electrons as they are about the properties of circuits (they are also called "circuit laws"). Indeed, these laws apply *mutatis mutandis* to hydraulics as well; thus, they are about electrons as much as hydraulics is about water (hydraulics is not about water, it is about the properties of *fluid flow*).

What if one insists that my notion of "physics" is too narrow and that the laws of electronics mentioned above should in fact be also considered laws of physics? If that is the case, then Smart's distinction about science and

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[9] The term "electrical circuit" which is referenced in these laws belongs to engineering, not to physics as such.

[10] E.g., they depend on the conservation of electric charge, a conservation law.

engineering cannot be maintained and his claim that special sciences like biology are more like engineering than like physics loses its support. But even if the laws of electronics are considered to be laws of physics, they are certainly not the exceptionless laws of *fundamental* physics that Smart and Kim talk about; they admit of exceptions just like the laws of the special sciences do. For example, Ohm's law fails to obtain if there are temperature or conductivity fluctuations across the circuit, Kirchhoff's law fails if the charge density fluctuates at the point to which it is applied, etc. The fact that Kirchhoff's laws fail in certain circumstances while Maxwell's laws of electromagnetism continue to hold in those circumstances further supports the previous argument that the laws mentioned above are not the laws of electromagnetism under a different guise.

The arguments above aimed to show that even if the special sciences are like engineering (in the sense of their domain being populated by complex entities whose parts obey more fundamental physical laws), this does not necessarily preclude the possibility of laws existing in their restricted domains (special science laws). On this view, there could be laws in biology or in any other special science just as there are laws in some branches of engineering such as electronics. There is no reason to believe that the special sciences cannot be nomic or that they cannot use laws formulated in their own restricted domains to propose explanations and make predictions, or to formulate and test hypotheses. In short, there is no reason to think that at least some of these engineering analogues cannot be *sciences*.[11]

I do not claim that all engineering is like electronics. Most certainly, there are branches of engineering in which rigorous mathematical laws are replaced by rough and ready empirical generalizations or even heuristic rules (just think of social engineering).[12] There could be branches of engineering with few rigorous laws or no rigorous laws at all, and branches in which even the much

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[11] If Smart's reasoning is followed consistently, it leads to the paradoxical conclusion that legitimate branches of physics such as thermodynamics are in fact engineering.

[12] In my opinion, the difference between the former and the latter is not sharp. Indeed, why can't nomicity come in degrees? Laws express interdictions, thereby placing constraints on the logical space of events. Why can't some of these constraints be stronger than others?

less rigorous heuristic rules are scarce. But as long as some branches of engineering afford some sort of nomicity, the argument put forward by Smart and endorsed by Kim does not work as intended.

5.4 The analyticity objection

A number of authors including Millikan (1999), Boyd (1999), Shapiro (2000) have expressed similar concerns about the possibility of a science whose kinds are functional. Like Kim (1992), they doubt that functional kinds that are multiply realizable will figure in any interesting generalizations. However, there is a point that these authors are explicitly making that Kim doesn't – namely, that the laws (or universal generalizations if you prefer) in which functional kinds or properties figure would be analytic and thus uninformative.[13] As a result, any science talking about functional kinds would be *a priori*. If one holds the requirement that natural sciences are by their very nature empirical investigations of the world, the same concern voiced by Kim emerges: there can't be a science of multiply realized kinds. In this section I will try to formulate the concerns that these authors have univocally, as similar instances of what I will call the "analiticity objection". In formulating the analyticity objection I may ignore the possible differences between these authors. My goal is to give a clear and unambiguous formulation of a problem that arises with respect to functional kinds, and then see how one can respond to it.

The analyticity objection can be seen as related to the objections put forward by Kim and presented in section 2 of this chapter. Perhaps it could even be seen as a special case of Kim's argument. In any case, the analyticity objection shares with Kim's argument two crucial premises. Each starts from the observation that functional kinds are heterogeneous in their realizations. And each agrees that as a result of this heterogeneity, the instantiations of these kinds will differ in their causal properties. From these premises Kim concluded that functional kinds are too disunified to be of scientific interest:

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[13] Some of these authors are more clear than others. It is not clear whether Millikan is making the same point as Shapiro and Boyd.

they are fragmented, they are unprojectible, so they can't figure in laws. The analyticity objection contends that even if there are laws in which functional kinds figure, these laws will be analytic.

The reasoning behind the analyticity objection is as follows. Functional kinds are heterogeneous in their realizations. As a result, they differ in their causal properties. But if they are so different in their causal properties, there is not much that can be said about them *as a kind*. Take mouse traps as an example. There are spring-loaded bar mouse traps, electric mouse traps, glue mouse traps, etc. All these devices are truly different in their causal properties (i.e., spring-loaded bar mouse traps store mechanical energy and kill the mouse by releasing it suddenly, electric mouse traps use electrical energy and kill the mouse by electrocuting it, while glue mouse traps use natural or synthetic adhesive to immobilize the mouse). Now the following question may be asked, and it has been: "Given that different realizations of mousetraps have different causally relevant properties, what more can be said about mousetraps other than that they are all used to catch mice?" (Shapiro 2000, p. 649). By contrast, consider the macro-level laws about scientifically legitimate kinds, such as water. The macro-level law that water freezes at 0 degrees Celsius derives from empirical investigation, but it can conceivably be challenged and found to be false. The fact that water freezes around 0 degrees Celsius in normal conditions cannot be found by simply reflecting upon the concept of water; on the other hand, the fact that mouse traps kill or trap mice can be found by simply reflecting on the concept of a mouse trap. The worry is that while laws about kinds that are not multiply realizable such as water are genuinely empirical, laws about kinds that are functional are not.

The laws about water obtain in virtue of the uniformity of the microphysical description of all samples of water. Any instance of water has *a lot* in common at the level of its microphysical constitution with any other instance of water. Thus, it is to be expected that macrolevel regularities will obtain in virtue of the microlevel commonalities. As Shapiro puts it, "macrolevel laws about water are true because certain microlevel laws about water are true. But, more significantly, macrolevel laws about all samples of water are possible because the same microlevel laws are true of all samples of water" (Shapiro 2000, p. 649). From this, the following worry emerges: if the microlevel uniformities across instances of a kind are few or absent, then the macrolevel laws about that kind will be few or absent:

> "There exist laws about the viscosity, specific gravity, freezing point, and so on of all samples of water, because all samples of water are composed of H_2O and are thereby determined, according to the microlevel laws that describe the behaviour of H_2O, to exhibit similarities in their viscosity, and so on. Contrast this now with so-called functional kinds like eyes. We can say nothing more about what camera eyes and compound eyes have in common other than that they have the function to see; this is because they differ in their causally relevant properties. Because, that is, microlevel laws about camera eyes and compound eyes are very different, there is no reason to expect that there will be any interesting macrolevel generalizations common to both." (Shapiro 2000, p. 650)

This worry has also been recognized by Boyd:

> "The various different realizations of such kinds are too diverse for there to be any *a posteriori* laws about them. They are not projectible, so any "laws" applying to all instantiations of such functional kinds would not be *a posteriori* – they would follow just from the analytic functional definitions of the kinds in question." (Boyd 1999, p. 68)

For many philosophers (including Shapiro), the laws about functional kinds must do more than simply state the capacity in virtue of which a functional kind is the kind that it is (Shapiro 2000, p. 649). To be considered legitimate scientific kinds, functional kinds should support more than a single generalization – namely, what can be said about them should not be limited to the description of their functional role. But if there isn't anything to say about functional multiply realizable kinds other than they all carry out the functional role that defines them, why think of them as legitimate scientific kinds?

If there aren't any *a posteriori* laws about them, what justifies the belief that there can be sciences about them? As Millikan puts it,

> "No science consists of a single generalization, nor of a heap of generalizations about different kinds of things. A science begins only when, at minimum, a number of generalizations can be made over instances of a single kind." (Millikan 1999, p. 48)

So if there aren't enough interesting (i.e., empirical) generalizations about functional multiply realizable kinds, they are not legitimate objects of scientific inquiry – they are not really *scientific* kinds, just as mouse traps are not scientific kinds. They may still hold some interest for science, but only insofar as scientists are interested in elucidating the various microphysical constituents that make the functional kind possible.

In order to examine how the analyticity objection could be responded to let's first see how this objection applies to the kinds/properties that I discussed in detail in chapter 3. If we consider acids as an example, the analyticity objection could be formulated as follows: acids do not form a genuine chemical kind because there isn't anything to be said about them besides that they all have the property that defines them (that they all donate protons in chemical reactions). The same for piezoelectrics: if piezoelectrics are to be accepted as a genuine scientific kind, there should be more to be said about them other than they all generate electricity when subjected to mechanical stress. If functional kinds like acids, oxidants, piezoelectrics are like mouse traps in that all that can be said about them is that they all have the property that defines them, then the laws in which these kinds would figure will be all analytical (they will be nothing more than statements expressing the definitions of these terms). But if that's the case, then there is no real science of these kinds, nor could there be one. For example, if all that can be said about piezoelectrics is that they generate electricity when subjected to mechanical stress, then they do not hold any more interest for science than mouse traps do. Thus, the analyticity objection brings forth the same old worry about the possibility of there being a science whose kinds are multiply realized: given that there is no science of mouse traps, why should there be a science of piezoelectricity?

Before seeing how this question could be answered, I want to pause for some reflection. Insofar as the analyticity objection places a restriction on the kinds or properties that can be of interest for science, it is an instance of philosophy being prescriptive towards science – it tells science which kinds or properties are legitimate objects of scientific inquiry and which are not. But can philosophy be prescriptive towards science in this way? Isn't philosophy overstepping its boundaries when it tells science what is scientifically interesting and what is not? In the case of acids, oxidants, piezoelectrics, the fact of the matter is that they – unlike mouse traps – are regarded as scientifically interesting by chemists, regardless what philosophers may think is or should be the case. So perhaps it would be a good idea if our philosophical reflections started with this brute fact, rather than deny it based on philosophical argument.

Now back to responding the objection. One possible strategy to deal with the analyticity objection is pointed out by Funkhouser (2007):

> "Jaegwon Kim (1993), Ruth Millikan (1999), and Richard Boyd (1999) have even argued that there cannot be a science of multiply realized (functional) kinds. They claim that we should not expect any generalizations/explanations to hold for such kinds, except for those captured by their functional specification. For such generalizations are blocked by the very diversity of lower level realizations. Their claim certainly runs counter to standard methodological assumptions of functionalists and cognitive scientists. The best way to refute their position, and certainly the most straightforward, is simply to discover such interesting generalizations." (Funkhouser 2007, p. 308)

I agree with Funkhouser that in order to address the analyticity objection it is a good idea to take a look at the actual science – in our case chemistry. In the case of acids, what more can be said about them except that they donate protons in chemical reactions? In the case of piezoelectrics, what more can be said about them that they generate electricity when subjected to mechanical stress? As it turns out, there are laws about piezoelectrics and acids that are genuinely empirical. Most of the laws enumerated in Table 1 (chapter 3) are in fact empirical. Consider the laws about acids:

A) Acids in reaction with metals produce a metal salt and hydrogen gas.

B) Acids in reaction with metal carbonates produce water, CO_2 and a salt.

C) Acids in reaction with metal hydroxides and metal oxides produce water and a salt.

None of these laws is true in virtue of the meaning of term "acid". Consider law A. Nowhere in the concept of a proton donor (acid) can be found that it produces a metal salt and hydrogen gas when it reacts with metals. The same with laws B and C. Unlike "Acids donate protons in chemical reactions" which is in fact the definition of acids and thus analytical, all three laws above are genuinely empirical.

Now consider the laws about bases.

B1) Bases accept hydrogen ions from the chemical species to which they react. (Brønsted-Lowry definition)

B2) Bases donate electron pairs in chemical reactions. (Lewis definition)

B3) Bases react with triglycerides to produce soaps (reaction known as saponification).

B4) Bases react with acids to produce salts and water.

B5) Bases can act as insoluble heterogeneous catalysts for chemical reactions.

If we assume the Brønsted-Lowry definition of bases, then B1 is analytical, but B2 isn't. Nowhere in the concept of proton acceptor can be found the concept of electron-pair donor. Conversely, if we assume the Lewis definition

B2 will be analytical but B1 won't be. Regardless of the adopted definition, the laws B3, B4, B5 are all empirical. Nowhere in the concept of a base can be found the ability to react with triglycerides to produce soaps. Nowhere in the concept of a proton acceptor can be found the ability to react with proton donors to produce salts and water. And nowhere in the concept of a base can be found that it may catalyze chemical reactions. The same with the laws about oxidants, reductants, and metals – most of them are empirical.

What about piezoelectrics? What more can be said about piezoelectric materials except that they all have piezoelectric properties, which is not at all informative? It turns out that there are interesting universal generalizations which are not accidental about piezoelectrics:

P1) All piezoelectrics are dielectric, but not all dielectrics are piezoelectric. (Tilley 2004, p. 344)

P2) All piezoelectrics are temperature-dependent. (Broch 1980, p. 108)

P3) All piezoelectrics are anisotropic. (Park and Lakes 2007, p. 85)

To the truths above one may add the following:

P4) Not all piezoelectric materials are pyroelectric, but all pyroelectric materials are piezoelectric.

P5) Not all piezoelectrics are ferroelectric, but all ferroelectrics are piezoelectric.

All these truths are genuinely empirical. If a material produces electricity when subjected to mechanical stress it is still an empirical question whether that material is an insulator that can be polarized by an applied electric field. Nowhere in the concept of a piezoelectric can be found that its piezoelectric properties vary with temperature. And one cannot infer that piezoelectric materials are anisotropic by simply reflecting on the fact that they produce electricity when subjected to mechanical stress; in other words, whether the structure of piezoelectric materials is direction independent or not remains an empirical question. Thus, the fact of the matter is that there are plenty of empirical laws in which functional kinds figure. This shows that the analyticity objection is *de facto* untenable. It also indicates that something must be wrong among the premises of the analyticity objection. But what?

The supporters of the analyticity objection appeal in their argument to the principle that the macrolevel regularities obtain in virtue of the uniformity existing at the microlevel (I will call this the Macro-Micro Principle). Shapiro is one of the proponents of the analyticity objection who are endorsing the Macro-Micro Principle (without naming it so). As already mentioned, Shapiro thinks that macrolevel laws about the instances of a kind are uniformly true because certain microlevel laws about those instances are uniformly true. He gives the example of the laws about water (the laws regarding viscosity, specific gravity, freezing point, etc.) and he argues that they are true because all samples of water are composed of H_2O molecules, which obey the same set of microlevel laws.

As in the case of the Principle of Causal Individuation of Kinds to which it resembles, the Macro-Micro principle is compatible with two readings. On one reading, the principle is saying that if microlevel uniformity is present, macrolevel regularities obtain. On another reading, the principle is saying that macrolevel regularities *require* microlevel uniformity. What the supporters of the analyticity objection need for their argument is not the idea that microlevel uniformity makes possible macrolevel regularities, but the idea that in the absence of microlevel uniformity, macrolevel regularities cannot occur. The supporters of functional kinds may well agree that the more uniformity there is at the microlevel, the more macrolevel regularities there will be. What they would deny, however, is that microlevel uniformity is *the only* source of macrolevel regularities. But this is exactly what the proponents of the analyticity objection need to argue if they want to show that the absence of microlevel uniformity prevents the formulation of interesting macrolevel laws.

The analyticity objection claims that in the absence of commonalities in the microphysical constitution of the instances of a functional kind, there won't be any empirical truths to be said about that kind at the macrolevel. But this ignores the fact that most of the laws in which functional kinds figure obtain not in virtue of the microlevel commonalities among the instances of those kinds, but in virtue of how those instances are *relating* to other instances; it ignores the fact that one and the same kind of behaviour can be exhibited by entities that are diverse from the point of view of their microphysical description. The laws about acids, for example, are true not because all acids are similar at the microphysical level (they aren't!) but because they all behave similarly towards other chemical species – they all donate protons in chemical reactions. For example, the macrolevel law that acids in reaction with metals produce hydrogen is true not because acids are uniform with respect to their microphysical constitution, but because they are uniform with respect to their behaviour despite being non-uniform in constitution. The proponents of the analyticity objection cannot see why there should be any similarities in behaviour unless there is similarity in constitution. But as the examples considered in chapter 3 show, the fact of the matter is that there are such similarities.

Now, the fact that such similarities obtain despite the lack of uniformity at the microconstitutive level has been considered by some "a metaphysical mystery" (Fodor 1997). Batterman (2000) has showed that this need not be a mystery at all: there are principled (mathematical) reasons why there are macrolevel similarities despite microlevel heterogeneity – why, for example, fluids behave similarly despite having different molecular constitutions.

I agree that in many cases the explanation for the similarity in behaviour despite dissimilarity in constitution (what I will call *behavioural convergence*) can be be given a principled explanation that is elegant (e.g., Batterman appeals to the mathematical tool of renormalization). Wherever such principled explanations are available, they should be sought. But are such explanations always available? Consider the cases studied in chapter 3. Why do molecules as varied as H_2SO_4, HBF_4 and HCl donate protons in chemical reactions (while molecules like HNa don't)? Why do materials as varied as cement, collagen and quartz exhibit a surface charge when placed under mechanical stress? In such cases there does not seem to be a unique explanation for the sameness of behaviour. There doesn't seem to be a single argument explaining the behaviour of all acids or all piezoelectrics. In the case of acid molecules, they all donate protons in chemical reactions because of thermodynamic reasons having to do with the minimization of energy in the context of the chemical reactions. In every non-reversible chemical reaction the products of the reaction form molecular structures that are more stable than the reagents. Some of the molecules entering the reaction will achieve reaction equilibrium by donating protons to the other species; it is these molecules that we call acids. Asking why acids donate protons in chemical reactions is not the same as asking why various liquids have the same critical exponent – the ability to donate protons is part of the definition of acids, whereas having a certain critical exponent is not part of the definition of liquids. Asking why acids donate protons is more like asking why liquids take the shape of their container – substances that do not take the shape of their container are not called liquids. In the case of materials under mechanical stress, some of them will develop a surface charge, others won't. The first belong to the class of piezoelectrics, the latter do not. Cement, collagen and quartz belong to this class. There isn't a unique reason why these materials develop a surface charge under mechanical stress. But why should there be one? It would be an even greater metaphysical mystery if behavioural convergence would never just happen.[14]

So far I have argued that the functional properties examined in chapter 3 are *de facto* objects of scientific inquiry. If these properties are truly functional, as I have argued, then the issue of whether there could be a science about them is not a matter of philosophical argument – it is a matter of fact. I supported this by showing that there are laws about functional properties studied by chemistry that are genuinely empirical, and I presented a few examples of such laws.

But what if there are properties which do not figure in a great number of laws? If we found a functional property/kind about which not much could be said except what defines it, would we be forced to conclude that there cannot be a science about that kind/property? Even if we accept the analyticity

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[14] A similar point is made by Shapiro (2005).

objection, are we forced to accept its alleged consequence, that there can be no science of functional kinds?

I will try to answer the questions above by considering the example of functional property which I deem the most vulnerable to the analyticity objection – piezoelectricity. Suppose nothing could be said about piezoelectrics aside from the fact that they all generate a surface charge when compressed. Would there still be a science of piezoelectricity? I think the answer is affirmative. The reason is that unlike mouse traps, piezoelectrics are interesting for science – the fact that a certain material develops a surface charge when compressed is a remarkable phenomenon. However, those who argue that there cannot be a science of multiply realized kinds may very well agree with this claim. Kim, for example, would have no problem accepting that the study of piezoelectricity remains scientific; he would claim that piezoelectricity is of interest to science insofar as it is worthwhile elucidating the more basic mechanisms that make this phenomenon possible in various materials. But he would deny that beyond the reductionistic inquiry into the lower level mechanisms that give rise to it, piezoelectricity holds any interest for science in and of itself. To paraphrase Kim, the study of piezoelectricity may remain scientific, but there could be no science of piezoelectricity (Kim 1992, p. 26). The reason behind this conclusion is the heterogeneous nature of piezoelectric materials. Kim's would think that piezoelectricity is just as disunified as its realizers, and hence there isn't much to say about piezoelectrics except that they all have the property in virtue of which they are called so. In an argument of this sort, one makes implicit use of the idea espoused by Millikan (1999, p. 48) that "a science begins only when, at minimum, a number of generalizations can be made over instances of a single kind". I will call this *Millikan's dictum*.

Two points can be made in response to Millikan's dictum, but both stem from the realization that it assumes a certain view about the nature of science (a view which has become entrenched). First, it could be argued that science begins not only after one has gathered a hefty number of generalizations over the instances of a single kind, but when one can make successful predictions and explanations about a certain property using even a single such generalization. Consider mass in Newtonian mechanics. What more can can be said about mass in Newtonian mechanics other than it is the property of a body in virtue of which that body accelerates when a force is applied to it? The fact that there aren't a great number of different generalizations that can be made about mass in Newtonian mechanics does not rule out – as Millikan's dictum would – the possibility of a science about mass (viz., mechanics).

There is a second problem with Millikan's dictum: it stems from a certain view about the nature of science according to which the goal of science is to describe reality by inventorying a great number of laws. This view about the nature of science is the consequence of a philosophy of science that takes physics as its central reference point. But this philosophical view of the goals and methods of science is not as readily applicable to chemistry. Unlike physics, which aims primarily at describing the world by inventorying its laws, chemistry focuses on changing the world by producing new substances. It is not a great exaggeration to say that the rule of the game in physics is the discovery of new laws, whereas the rule of the game in chemistry is the synthesis of new compounds (just compare the kind of research that has been awarded the Nobel prize in chemistry with the kind of research that has been awarded the Nobel prize in physics, especially in more recent decades). The following quote from Schummer (2006) makes this point convincingly:

> "While philosophers of science have been telling us that scientists aim at a true theoretical description of the natural world, the great majority of chemists (which also means the great majority of scientists) have actually been engaged in synthesizing new substances, i.e., changing the natural world. Chemical synthesis is, to be sure, the most obvious peculiarity of chemistry, albeit the most neglected one because it is foreign to any received idea of philosophy of science." (Schummer 2006, p. 32-33)

If we turn to the example of piezoelectricity, the following point can be made. Even if nothing could be said about piezoelectrics aside from the fact that they all generate a surface charge when compressed, there would still be a science of piezoelectricity: predictions and explanations could still be made about piezoelectrics (e.g., the prediction that piezoelectric properties would be found in amorphous and polycrystalline materials (Shubnikov), the explanation of the transition from the piezoelectric paraelectric phase to a ferroelastic phase (Swada and Nakamura), and the explanation of relaxation in piezoelectric materials (Arit)).[15] But, perhaps more importantly, there is a science of piezoelectricity because because there are a lot of scientists that spend their time in the lab investigating and producing new piezoelectric materials (e.g., materials with remarkable piezoelectric properties like lead zirconate titanate (PZT), a man-made ceramic, or polyvinylidene fluoride (PVDF), a synthetic polymer whose piezoelectric properties exceed several times those of quartz).

In conclusion, even if nothing could be said about a kind except that it has the property that defines it, this does not by itself undermine the possibility of a science of that kind. A systematic investigation of the kind in question that involves successful explanations and predictions could still be possible even with a modest number of “laws”. More importantly, if one uses the methods of science not merely to describe the natural world but also to change it by producing new entities (as chemistry does), then the label “science” should equally apply to this sort of creative activity. Millikan’s dictum does not take into account the disciplinary specificity of sciences like chemistry, and for this reason it does not express a condition of scientificity *tout court*. Contrary to what Millikan thinks, we have a science of chemistry not just because we have laws about acids, bases, oxidants, reductants and piezoelectrics, but also because (or, I should say *mainly* because) scientists spend their time discovering new acids, bases, oxidants, reductants and piezoelectrics, often by synthesis. Thus, even if the analyticity objection is true (which in the case of chemical functional properties isn’t, as I have argued) the conclusion that there cannot be a science of multiply realized kinds does not follow.

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[15] For a more comprehensive description of the science of piezoelectricity see Taylor (1985).

Chapter 6

Conclusions

This thesis was motivated by the following question: “If all there is consists of the kind of entities that microphysics talks about, why do we have sciences other than microphysics?” I have considered a specific version of this question, namely why do we have chemistry instead of just applied quantum mechanics, and I have argued for a certain way of answering it.

I approached the specific question through a case study. I looked at the case of chemistry and investigated whether there are even such things as *chemical* properties, truths, and explanations as opposed to merely complex quantum-mechanical properties, truths, and explanations. I have argued for an affirmative answer. With the help of a distinction introduced in chapter 3 (that between constitutive and functional properties), I argued for the existence of *sui generis* chemical properties, laws and explanations. By *sui generis* chemical properties, laws, and explanations I meant properties, laws and explanations that cannot be construed as (possibly complex) quantum-mechanical properties, laws, or explanations. The reason for this was the existence of properties which are defined by their functional role, and not by a shared microphysical constituent. I have argued that properties like acidity, being an oxidant, a metal or a piezoelectric, are properties defined by a common behaviour, which is carried out by a variety of quantum-mechanical systems of electrons and nuclei. Thus, properties like acidity are higher level properties, which cannot be reductively identified with a unique lower level (microphysical) property.

I called such properties *functionally emergent* and I claimed that they can ground the ontological autonomy of chemistry in relation to the underlying microphysics.

Why is the term "emergence" suitable to characterize the functional properties that chemistry talks about? What makes the functionalist view of chemistry that I defended in this thesis an "emergentist" view? As mentioned in chapter 1, the term "emergence" does not have a unified meaning amongst philosophers. However, there are several features that the emergentist accounts typically share. The first is a layered view of the world. As mentioned in 1.2.5, virtually all emergentist positions hold some form of the view that the world consists of a hierarchy of levels or ontological *strata* (the physical, the chemical, the biological, the psychological, and so on). The second feature of emergentism is that each ontological stratum depends on the previous one. Thus, the chemical level depends on the physical level, the biological depends on the chemical, and so on, such that if a certain level were to disappear, all the subsequent levels will vanish as well – biology would not be possible without chemistry, chemistry would not be possible without microphysics. The third feature that many emergentist accounts share is a conflict with certain notions of reductionism – the higher levels are viewed as dependent on, but not wholly reducible to the lower levels.

The functionalist view of chemistry that I advocate has all three features discussed above. As argued in chapter 4, functional chemical properties pose problems for the reduction of chemistry to physics on some accounts of intertheoretic reduction, such as that of Nagel and that of Kemeny, Putnam and Oppenheim. For Nagel's account the problems arise with regard the connectability condition. Terms like "acid" or "metal" are terms that do not occur in the vocabulary of physics; therefore "bridge laws" are needed to connect the vocabulary of chemistry with that of physics. But, as argued in 4.1, the heterogeneous nature of the physical descriptions of acids does not allow one-to-one connections between the terms present in the vocabulary of chemistry and terms or expressions referring to physical kinds; moreover, the relational nature of many chemical kinds further prevents construing them as physical kinds. As a result, the connectability condition is not met; consequently, the derivability condition cannot be met. This shows that the laws in which functional chemical terms occur are not Nagel-reducible to the laws of physics, although they are made possible by them.

For the account of reduction advocated by Kemeny, Putnam and Oppenheim the problems arise with the condition asking that the theory of physics be at least as well systematized as the theory of chemistry that we want to reduce. But the unity of the explanations given by a theory is an important aspect of the systematicity of that theory. In 4.2. I argued that the existence of specific chemical terms allows for the possibility of chemical explanations that are more unified than the rival physical explanations with the same explanandum. I argued that some things that are in need of explanation (i.e., patterns of chemical behaviour) cannot be explained in a unified manner by physics, but they can be so explained by chemistry. I claimed that what is required for a unified explanation of patterns of chemical behaviour is not knowledge of the micro-details that the fine-grained physical theory provides, but quite the opposite: abstraction from those details, which enables one to see similarities between systems that are regarded as different by the fine-grained theory. Therefore, if for some explananda the chemical explanantia are more unified than the corresponding physical explanantia, the idea that physics and chemistry are equally well systematized becomes problematic. But if this is the case, the account of reduction advocated by Kemeny, Putnam and Oppenheim cannot be effectively applied to chemistry.

The second feature of emergence mentioned above is also possessed by the functionalist account I advocate. Chemistry is made possible by the underlying physics, such that if the underlying physics were to disappear, chemistry and everything that depends on it would disappear as well. This is indeed a kind of reductionism. But it is a different kind of reductionism than the one defended by Nagel or Kemeny, Putnam and Oppenheim. Those two accounts aimed for ontological parsimony; their goal was to effect an economy in the ontology of science. But the kind of reductionism that characterizes emergence does not have such goals or consequences. The kind of reductionism that most emergentist accounts embrace and even require is what philosophers have called *token* reductionism (or physicalism) – the notion that every thing or process consists ultimately of the kinds of things or processes that microphysics talks about and that there are no non-physical property instances, vitalistic substances, entelechies, etc., occurring at any stage of complexity. However, physicalism is a relatively modest thesis. Given the naturalist worldview that became established with the advent of modern science, the thesis of physicalism as it applies to chemistry appears quite indisputable; today, everyone accepts that there are no chemical souls or vitalistic chemical essences and that all chemical substances and processes consist exclusively of microphysical substances or processes. From the perspective of scientific naturalism, the thesis of token reductionism appears quite uninteresting. Of course, there remains the problem whether given a certain instance of a chemical property (say, a molecule) one could predict all its intrinsic properties (e.g., bond energies, dipole moments, etc.) on the basis of *ab initio* quantum-mechanical calculations (i.e., calculations from first principles). For most systems such a task requires not only computing power but also mathematical flair and creativity. Of course, there are practical and theoretical obstacles to full fledged *ab initio* derivations. But the success physical chemistry has had so far (see the case of disilyne mentioned in 2.1.3) reveals the unquestionable truth of physicalism. The difficulties that the *ab initio* derivations encounter do not tell against the modest form of reductionism that some philosophers have called *token* reductionism (or physicalism).

But the truth of this modest form of reductionism does not entail that chemistry is just applied quantum mechanics. If various systems of electrons and nuclei display the same behavioural pattern in spite of having disparate microphysical constitutions, the pattern is real and should be treated as such. In chemistry, patterns of chemical behaviour such as those exhibited by acids, bases, oxidants, reductants, metals, piezoelectrics are just as real as those exhibited by noble gases and alcohols. But, as I argued in chapter 3, there is an important difference between the former and the latter. The latter are just microphysical properties in disguise, whereas the former are chemical properties in their own right, which cannot be reductively identified with physical properties. Chemistry is not just applied quantum mechanics also because it has its own laws, which are not reducible to the laws of physics (what I called *sui generis* chemical laws). Of course, given the truth of physicalism, these laws are made possible by the laws of physics, which govern all events (including chemical events). However, it would be a mistake to think that if all events are governed by physical laws, then all laws must be physical. The law that acids in reaction with metals produce hydrogen gas is made possible by the laws of quantum mechanics (the electrons and nuclei from which acids and metals consist of obey the Schrödinger equation), but, as argued in 4.1, this law has no quantum-mechanical derivation. As argued in 4.2., the *sui generis* laws of chemistry can be used in chemical explanations which are more unified and overarching than the rival physical explanations.

As argued in chapter 3, the *sui generis* chemical laws are "indiscriminate" or "promiscuous", i.e., they are indifferent to the various ways in which the properties they relate are constituted at the lower level of description. For example, the first equation of piezoelectricity relates mechanical stress to electric polarization in various materials, but is insensitive to how the latter is constituted at the microphysical level (ion displacement in crystals like quartz, dipole rotations in polymers like collagen, streaming potential in interface materials like bone or cement). The law does not "care" how polarization is brought about in various materials, it only "cares" about its relation to stress. In the same way, the *sui generis* laws of chemistry mentioned in Table 4.1 are also promiscuous. For example, the chemical law stating that acids in reaction with metals produce a metal salt and hydrogen gas is promiscuous because it could be rendered true by a great variety of physical systems composed of electrons and nuclei. Similarly, the chemical law that oxidants corrode metals is promiscuous because the physical systems of electrons and nuclei that serve as an oxidizing agent, respectively a metal are wildly heterogeneous from the point of view of their microphysical makeup. As mentioned in 3.3.3.5, promiscuous laws enjoy a degree of independence from the basal conditions that the laws of microphysics typically do not. For this reason, they should be regarded as higher level laws which are not just complex physical laws in disguise; such laws should be regarded as chemical laws in their own right.

The *sui generis* nature of the functional properties, laws and explanations justifies the idea that chemistry investigates its own stratum of reality or domain, distinct from the domain of microphysics. Thus, the first feature of emergence mentioned earlier is also possessed by the functionalist view of chemistry I advocate. Therefore, the functionalist view of chemistry qualifies as an emergentist view because it is committed to the idea that chemistry has its own ontology, which depends on, but is irreducible to the ontology of physics. However, the functional emergentist view of chemistry differs markedly from the more orthodox accounts of emergence in chemistry. For example, unlike Broad's account based on non-physical configurational forces (1925), or the recent account based on configurational Hamiltonians (Hendry 2006), functional emergence is not at odds with the conservation of energy. Also, unlike the emergentist account based on fusion defended by Humphreys (1997b, 1997a, 2008), functional emergence does not threaten the idea of a compositional ontology. But despite being less ambitious than other emergentist accounts, functional emergence can still justify the ontological autonomy of chemistry in relation to the underlying microphysics insofar as it acknowledges the existence of *sui generis* chemical properties and regularities. The existence of *sui generis* chemical properties and regularities makes chemistry autonomous from microphysics not merely in an epistemic or pragmatic sense, but also in an ontological one. I admitted, however, that the ontological autonomy of chemistry from microphysics is not radical: if the entities that microphysics talks about were to vanish, there would be no chemical properties, no laws relating these properties, and no explanations employing those laws.

Is the kind of emergence defended in this thesis weak or strong? In the introduction, where I made the distinction between strong and weak emergence, I suggested that if the kind of reductionism with which a given account of emergence is deemed to be incompatible is reductionism *in practice,* then that account of emergence would be considered weak. If, however, that account of emergence presupposed irreducibility *in principle*, the account would be considered strong. However, the answer to the question is complicated by the existence of another distinction, that between properties and property instances (section 1.3). So the question of whether functional emergence counts as weak or strong depends on whether we talk about *type* or *token* reductionism (see 2.3). Functional emergence qualifies as strong if we talk about the reduction of properties as such (type reductionism), but it qualifies as weak if we talk about the reduction of property instances, with which it is compatible (token reductionism).

As I noted in chapter 3, not all chemical properties are functionally emergent. What does this situation tell us with respect to the nature of chemistry as a science? In my view, this situation reflects the status of chemistry as "the first" of the special sciences. Chemical substances are made of microphysical systems that consist of electrons and nuclei; hence, many of their chemical properties are the reflection of commonalities in their physical makeup, as illustrated in the case of alcohols or noble gases. As a result, some chemical properties will receive constitutive definitions and thus they will be reductively identified with physical properties. Others, however, are able to receive only functional definitions, and they will not be identifiable with particular physical properties. This depicts an image of chemistry as a "mixed" science – a science that is close enough to physics so that some of the properties it talks about are physical properties, but also a science that begins to emancipate itself from the base, and deals with genuinely new properties. The "mixed" character of chemistry further qualifies how the notion that chemistry is ontologically autonomous from physics should be interpreted. Nonetheless, the ontological autonomy of chemistry persists because the *sui generis* properties and regularities that chemistry talks about are sufficiently numerous and pervasive. It would be wrong to conclude that the mixed character of chemistry makes the ontology of this discipline as a whole a sub-domain of the ontology of physics.

This image of chemistry as a "mixed science" offers only a partial support to the classical *layer-cake* model of science that has been assumed by many reductionists, anti-reductionists and emergentists alike. In the light of section

5.3, where I discussed the argument from the general failure of special-science causal closure and the argument from the idiosyncratic nature of special science properties, it becomes apparent that chemical properties and regularities are always susceptible of disruptions “from below”. In other words, chemical properties and regularities can always be affected by physical or microphysical factors. The most simple and clear example is the influence of temperature on chemical reactions, but numerous other examples could be found. Physical factors such as electromagnetic fields, pressure, even gravity may affect chemical properties and regularities, no matter how *sui generis* these are. Thus, chemistry, although ontologically autonomous from physics, is not “insulated” from physics. To express this in the terms of the layer-cake metaphor, chemistry is not a perfectly distinct layer that lays flat on top of the physical layer. Instead of the layer-cake model, perhaps a better model could be suggested, one which captures more accurately the relationships between the various sciences. For the lack of a better metaphor, this could be called the “Easter-bread” model. In the Easter-bread model, the sciences are not arranged neatly in distinct layers, with physics at the base and then followed by chemistry, biology, psychology, etc.; rather, they interweave and penetrate each other globally, although locally they typically retain their distinctness.

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Alexandru Manafu

Education

Ph.D. in Philosophy, The University of Western Ontario, 2011

> Dissertation: *Emergence and Reduction in Science. A Case Study.* Advisor: Robert Batterman. Committee: Christopher Smeenk, Gillian Barker. Internal: Marc-André Lachance (Biology). External: Sandra Mitchell (HPS Pittsburgh).

M.A. in History and Philosophy of Science, University of Calgary, 2006

> Thesis: *Non-locality and Non-separability in Quantum Mechanics.* Advisors: Elaine Landry, Dean Rickles. Internal: Jack MacIntosh. External: David Hobill (Physics)

In-depth Studies in Theoretical Philosophy, University of Bucharest, 2003

> Thesis: *Realism, Non-locality and the Interpretation of Quantum Mechanics.* Advisor: Ilie Pârvu

B.A. in Philosophy, A.I. Cuza University, 2001

> Thesis: *Realism and Anti-realism in Quantum Theory.* Advisor: Theodor Dima

Awards and Distinctions

Ontario Graduate Scholarship (OGS), 2010. Value: $15,000 CAD

Social Sciences and Humanities Research Council of Canada (SSHRC) Fellowship, 2009. Value: $20,000 CAD

Distinction, History of Philosophy Comprehensive Examination, UWO, 2007

Harry and Laura Jacques Scholarship, Open Scholarship Competition, University of Calgary, 2004. Value: $3,500 CAD

Dean's Award, UAIC, GPA-based, 2001

Merit Bursary - 7/8 semesters of my undergraduate studies, GPA-based, 1997-2001

Publications

Concepts of Emergence in Chemistry. In Llored, J.P., editor, *Philosophy of Chemistry: Practices, Methodologies and Concepts*. Cambridge Scholars Publishing, forthcoming.

Presentations

"Multiple Realization: Some Lessons from Solid-State Theory"

> Canadian Society for the History and Philosophy of Science, May 2011, University of New Brunswick and St. Thomas University, Fredericton

"The Prospects for Fusion Emergence"

> International Society for the Philosophy of Chemistry, August 2010, University College, Oxford
>
> Canadian Philosophical Association, June 2011, University of New Brunswick and St. Thomas University, Fredericton

"The British Emergentist View of Chemistry"

> International Society for the History of Philosophy of Science, June 2010, Central European University, Budapest
>
> Canadian Society for the History and Philosophy of Science, May 2010, Concordia University, Montreal

"Two Notions of Emergence"

> European Philosophy of Science Association, October 2009, Free University, Amsterdam
>
> International Society for Philosophy of Chemistry, August 2009, Philadelphia

"Configurational Forces and the Emergence of the Chemical"

Canadian Society for the History and Philosophy of Science, May 2009, Carleton University, Ottawa

"How Not to Think About Emergence"

Philosophy Graduate Student Association Colloquium Series, February 2009, UWO

"The Role of Light in Special Relativity"

Philosophy of Physics Graduate Conference, November 2008, State University of New York at Buffalo

"Enantiomorphy, Symmetry and the Reality of Space"

Canadian Society for the History and Philosophy of Science, June 2008, University of British Columbia, Vancouver

"What's Wrong with the Zombie Argument"

Canadian Philosophical Association, June 2008, University of British Columbia, Vancouver

"Strawberries, Stoplights and Reflectance Physicalism"

Philosophy Graduate Student Association Colloquium Series, 2008, The University of Western Ontario

"More Difficulties for the Indispensability Argument"

Yale & UConn Philosophy Graduate Conference, October 2006, Yale University

Graduate Students' Colloquium Series, 2005, University of Calgary

Public Lecture: "Could Science Prove the Existence of God? (Or, Must Science Be Naturalistic?)", Polaris 25, July 2011, Toronto

Teaching

In 2009 I completed the Advanced Teaching Program, offered by UWO's Teaching Support Centre.

I am expecting to complete the Western Certificate in University Teaching and Learning in January 2012.

Lecturer:

- Biomedical Ethics (PHIL 2071), The University of Western Ontario, Fall-Winter 2011-12
- Epistemology (PHIL 2500), The University of Western Ontario, Winter 2011
- Philosophy of Science (PHIL 2030), The University of Western Ontario, Fall 2009
- Introductory Logic (200-level), Ovidius University, Fall 2003 – Winter 2004
- Introduction to Philosophy (100-level), Ovidius University, Fall 2003 – Winter 2004

Tutorial leader:

- Big Ideas (PHIL 1130), The University of Western Ontario, Winter 2008
- Basic Logic (PHIL 2020), The University of Western Ontario, Fall 2008
- Critical Thinking (PHIL 1200), The University of Western Ontario, Fall 2006–Winter 2007
- Ethics (PHIL 249), University of Calgary, Winter 2005
- Ethics (PHIL 249), University of Calgary, Fall 2005
- Introductory Logic (PHIL 275), University of Calgary, Winter 2004
- Problems of Philosophy (PHIL 201), University of Calgary, Fall 2004

Professional Activities

Committee work: editorial committee for the Rotman Institute of Philosophy blog

Referee for the Logic, Mathematics and Physics philosophy graduate conference at UWO in 2008, 2009, 2010, 2011

Referee for the graduate conference in the Philosophy of Mind, Language, and Cognitive Science at UWO in 2008, 2011

Workshop on “Emergence and Reduction in the Sciences”, Center for Philosophy of Science, University of Pittsburgh, December 2009 (invited)

Research Assistant for Dr. Robert Batterman. Project: “Idealizations, Singularities, and the Applicability of Mathematics”. Funded by the Social Sciences and Humanities Research Council of Canada, 2008-2009, Value: $84,984 CAD

Summer school on “Reduction and Emergence” with Nobel laureate physicist Robert B. Laughlin, Tübingen, Germany, May 2008

Resident member of the Rotman Institute of Philosophy 2009-2011