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Reducing Chemistry to Physics

Limits, Models, Consequences

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Durch den ganzen logischen Apparat hindurch sprechen die physikalische Gesetze doch von den Gegenständen der Welt.

Ludwig Wittgenstein, 'Tractatus Logico Philosophicus' 6.3431.

... all quantum-mechanical set-structures float in a sea of stories ...

Fred Muller (2003), 'Refutability revamped: how Quantum Mechanics saves the phenomena', p. 198.

It is a familiar fact that theories in the sciences (especially though not exclusively in mathematical physics) are generally formulated with painstaking care and that the relations of theoretical notions to each other (whether the notions are primitives in the system or are defined in terms of the primitives) are stated with great precision. Such care and precision are essential if the deductive consequences of theoretical assumptions are to be rigorously explored.

Ernest Nagel (1961), 'The Structure of Science', p. 99.

What is important to the modern temperament is that scientific speculations be taken straight as conjectures, not mixed and served in metaphysical cocktails of suspect ingredients. So one of the puritanical themes of this book is that scientific reduction is hard work.

Patrick Suppes (2002), 'Representation and Invariance of Scientific Structures', p. 467.

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Preface

The topic of the following pages is the interrelationship between theories of chemistry and theories of physics and the role played by quantum chemistry as a theory ‘in between’. Traditionally, this relationship was thought to be one of reduction. More recently, the nature of this putative reduction relation has become a contested topic in the philosophy of chemistry. At the moment the emerging consensus suggests that the application of reductionist principles in chemistry is problematic at best and impossible at worst. My aim in what follows is to critically re-evaluate that position.

The reduction of chemistry to physics was once thought to be a simple textbook case of how these things ought to be done. Philosophers have generally accepted the reduction of chemistry to physics as a fact requiring little further comment, or requiring far less comment than the problems surrounding the potential reduction of biology or the potential reduction of mental events to physical events. Outside the somewhat narrow confines of philosophy of chemistry, the reduction of chemistry to physics is still usually seen as a paradigmatic, but also ultimately uninteresting example of scientific reduction.

One of the early achievements of philosophy of chemistry was its contention that this reduction relationship was not so simple after all. Early philosophers of chemistry argued that the casebook on the reduction of chemistry to physics should be reopened, and re-examined as a philosophical ‘cold case’ that is not only interesting in its own right, but also (still) potentially paradigmatic for the reduction of other sciences. Significant problems exist around a number of issues such as the notion of molecular structure, and the exact role played by quantum chemistry in the reduction of chemistry to physics. The early philosophers of chemistry pointed out that these issues could not just be overlooked when claiming a reduction, and moreover, that the obvious *success* of quantum theories in the explanation of chemical phenomena could not be taken as outright support for a reductive relationship. A somewhat unfortunate corollary of the early discussions in the philosophy of chemistry was however that the notion of reduction itself was seen as hopelessly flawed, a corollary with which I largely disagree.

The claim of reduction now stands with many questions attached. Yet the reduction of chemistry to physics is still paradigmatic for, or at least fundamental to, the notion of reduction *per se*: as reduction relations go, the domains of chemistry and physics are close and significantly overlapping, there is a lot of theoretical and ontological ‘borrowing’ and a significant amount of continuity between the two sciences. If a claim of reduction cannot stand here, there is little or no hope ‘higher up’ for similar claims between biology and chemistry, or mental and physical events. Hence, the notion of reduction finds itself in an unenviable spot here: it is problematic on the one hand, and paradigmatic on the other.

The approach I take in addressing these issues tries to navigate between a normative and a naturalistic strategy.

In the normative strategy one investigates what sort of minimal logical connections are required to uphold a particular conception of the ‘unity of science’ project, and then proceeds to investigate whether these conditions obtain in actual practice. The two main problems with this strategy are that (i) there is no clear-cut and universal conception of the ‘unity of science’, and (ii) this approach attempts to ‘read in’ some set of necessary preconditions for a particular conception of the unity of science in actual scientific practice. Also, the normative strategy is in significant danger of being married off quickly to the (much stronger) claim of metaphysical reductionism.

In opposition, the naturalistic strategy is to investigate the sort of relationships that obtain in the actual practice of science, and then proceed to conclusions about the sort of ‘unity of science’ that these relationships will support. Despite looking more charitable to the scientific endeavour, the main danger of this approach is that the actual practice of science needs to be understood in significant detail for the conclusions to be robust. Underestimate the amount of scientific work involved, make a mountain out of a few philosophical molehills, and the disunity of science appears as more or less the default solution.

At the moment, the tendency in the philosophy of chemistry is to be dismissive of the normative approach, and to use the naturalistic approach to argue for some sort of autonomy of chemistry from physics.

The main reason for the dismissal of a reduction relation between chemistry and physics, as I see it, is that the normative approach is frequently confused with a metaphysical reductionist approach on the one hand and a ‘tutelage’ interpretation of its consequences on the other. Hence the contrast between the (primarily metaphysical and normative) thesis of *reductionism* on the one hand and a more moderate (naturalistic) notion of *reduction* on the other forms one of the key elements of my analysis. The conditions that were originally specified by Nagel (1961) are akin to naturalistic conditions for reduction, though they are often read as enablers for a much stronger metaphysical *reductionism*. As has been argued by Causey (1977), the unity

of science conceived along reductionist lines requires stronger conditions. Specifically, reductionism requires that the reduction postulates be identities.

But the unity of science does not depend on reductionism. The claim that reduction can exist without reductionism has recently been made by Klein (2009), Dizadji-Bahmani, Frigg, and Hartmann (2010) and van Riel (2011), who argue for what might be called a ‘naturalised’ interpretation of the Nagelian conditions.

By confusing the notions of reductionism and reduction, many philosophers of chemistry have jumped to the conclusion that a moderate view of reduction between chemistry and physics was impossible. Additionally, some philosophers of chemistry have tended to render the naturalistic approach nonviable by a lack of the sort of sensitivity that is required to understand both the theories involved as well as the motivations and inclinations of actual scientists. In brief, another one of my gripes with the current tendency to dismiss reduction in the philosophy of chemistry is that autonomy is claimed too quickly and too easily, on the basis of insufficient evidence. Moreover, the reductionist’s main contender programme, disciplinary autonomy, is not usually well developed and clearly stated.

As a complicating factor, the sort of unity of science that might be supported by a moderate view of reduction is largely open. In this area, the philosophy of chemistry occupies a rather unique position. In some sense, theories of chemistry are also theories of physics, since modern chemistry has ‘borrowed’ concepts from the theories of physics rather freely. Moreover, the sort of competition that might result from an overly eliminative view of reduction is largely absent between chemistry and physics. Hence my contention that the sort of interrelationships that we might find between the theories of chemistry and the theories of physics will tell us much about the ‘unity of science’ and about the potential for fruitful cooperation between the sciences.

In developing my argument, I employ a somewhat heavier technical and mathematical apparatus than is common in most philosophical studies of quantum chemistry, even though for most quantum chemists the material does not extend beyond what may be found in most textbooks. This situation has arisen partly because of my expertise and inclination, but also because I believe that the mathematical apparatus serves a function. Quantum chemistry is a field that relies on significant quantities of the stuff, and in my opinion the current philosophical literature has overlooked too many mathematical realities that are part and parcel of scientific practice in quantum chemistry. Even the relatively simple textbook equations that are given can clarify philosophical issues which otherwise would have remained obscure. I have therefore used mathematics freely, but restricted its application to make philosophical points.

I have also, as much as possible, resisted the urge to recast the historical

mathematical notations in modern language, or to (re)present old arguments in the language of second quantisation (which I believe to be more efficient for many purposes in quantum chemistry), mostly because the existing notations proved to be sufficient for my purpose, which is specifying the operation of quantum chemistry. Especially in cases where the historical notation is sufficient to bring out the structure of the philosophical argument (and this proved to be the case in a surprising number of cases), I have resisted the urge to do the same thing 'better' as much as possible. Readers who are interested in a modern representation of the various approaches in the framework of second quantisation (which is a useful exercise if one wants to bring out the specific interrelationships between them) are encouraged to consult the book by Helgaker, Jørgensen, and Olsen (2000) which contains more about these issues than I could convey in the context of a philosophical specification of quantum chemistry. However, the recently popular Density Functional Theory is not treated in this resource, and for the discussions on this theory the reader should consult Engel and Dreizler (2011).

Acknowledgements

Though writing is a lonely task, it does not happen in a vacuum. This acknowledgements section is an effort to acknowledge the web of dependencies that has built up around the project, a task which is impossible but can only be tried as best one can.

My working relationship with Theo Kuipers now stretches back into the last century, and dates from shortly before the paper we wrote together on the Periodic Table in 1988. It has survived numerous missed deadlines (on my part) and a physical distance which spanned half the globe. It has now finally seen the completion of a thesis that was planned, at least in my mind, more than twenty years ago. Theo's kind patience is mainly responsible for the fact that it all worked out in the end.

Ria Broer was always willing to give guidance on matters of organisation and quantum mechanical detail as well as provide encouragement along the way. She has provided a firm hand in quantum chemical matters, particularly in drawing my attention to density functional theory, and correcting a large amount of obscurity in my writing. At various points her criticism drew me back from 'philosophy' to science, which was not only beneficial to the end result, but also provided a pleasant re-confrontation with my past.

Paul Wormer has, now and in the past, been very instrumental to my development as a quantum chemist. Throughout, the work has benefited in various places from his historical knowledge and continuing interest in matters historical.

I would also like to thank the members of the manuscript committee, who did an impressive job assessing a long and complex manuscript in a brief span of time.

Quantum chemistry is not an easy subject, and commenting on someone else's mistakes is not an easy task. Of course I am solely responsible for those that remain, despite the best efforts of the three people mentioned above.

Some of the ideas developed in this work have benefited significantly from brief email conversations with Fred Muller, Paul van der Vet, Eric Scerri, Josef Paldus, Bogumil Jeziorski, Brian Sutcliffe, Guy Woolley and Adrian Currie. Each of them has kindly let me pick their brains for little

nuggets of information on little known theorems and other obscure points of the history of quantum chemistry, aspects of reduction, unity of science, and formal approaches to quantum mechanics. They have also, in more or less severe degrees, put up with my lengthy ramblings and various half-baked ideas. These sort of little gems make the life of the philosopher of science a lot more attractive and matter enormously to the final product. I would in particular like to thank Brian Sutcliffe and Guy Woolley for reading and commenting on an early draft of Chapter 3.

Many of the ideas presented in this thesis developed more fully during an afternoon spent with Richard Bader in the lobby of a hotel in Auckland. This discussion, though it may not have appeared so at the time, significantly sharpened my sensitivity to some of the issues discussed, as well as to the depth of feeling about reductionism that is felt by some members of the quantum chemistry and chemistry community. It does maybe not always appear so, but chemists *do* care.

I would also like to thank the members of the Department of Philosophy at The University of Auckland for providing me with support in the form of a continuing honorary fellowship. Most of the work reported in this thesis utilised the excellent library resources at The University of Auckland. Various heads of department have been very helpful in setting me up with the little and sometimes not so little things I have needed at times. I especially thank John Bishop for taking me on, on that fateful day somewhere in April 1997, when I finally made the intellectual transition from chemistry into philosophy (and a work transition from academia into the ‘real world’ and so became an ‘indie’ scholar).

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This book was written and typeset in Eclipse / TeXLipse on Ubuntu Linux using JabRef and Zotero as reference managers. The amount of technical effort and expertise that has gone into the creation of such a massive platform often goes overlooked. To the many unnamed developers of this platform: thanks! You’ve made my life so much better.

Some of the material was published previously as early drafts. Parts of Chapter 5 have been published previously in Hettema (2008b). Most of Chapter 4 was published as Hettema (2009), though modifications have been made to make the paper better fit as a chapter in the current project. The formalisation of the periodic table was published previously as Hettema and Kuipers (1988), and slightly revised in Hettema and Kuipers (2000). Chapters 9 and 10 are expanded versions of Hettema (2012).

Roadmap for busy readers

While of course everyone is invited to read this thesis cover to cover, there are many people with little time. The following two sections contain a roadmap for busy chemists and a different one for busy philosophers which should assist in grasping the main arguments quicker.

Philosophy of chemistry is a small field and the number of people equally proficient in philosophy and chemistry is limited. Reading this work requires quite a bit of schooling in both fields. Chemists tend to be pragmatic people who generally do not have a solid grasp of some of the intricate details of philosophy. Some of these details matter in the argument. Similarly, philosophers have tended to have a much looser grasp of chemical theories than of either physical or biological theories, having decided for some unknown reason that the latter two fields are ‘more interesting’ than chemistry. Some philosophers will be taxed by the mathematics involved. It is thus possible to provide a roadmap, but there are not too many shortcuts.

Roadmap for busy chemists

In setting out a roadmap for busy chemists, I assume that ‘chemists’ know their chemistry and are conversant to a significant degree with the basic tenets of quantum chemistry. The roadmap for busy chemists is therefore dependent, in significant measure, upon whether the chemist is a theoretical chemist or not. For many theoretical chemists, the material presented here is pretty commonplace, for many non-theoretical chemists, it is outlandish and comes across just as arcane as the philosophy itself. There is no remedy for this. I am also going to assume that chemists are less familiar with philosophy, and may not even be interested in all of the finer philosophical details of some of these issues, which they may perceive as useless hair-splitting.

Chemists that have no philosophical interests are advised not to read this work at all, but spend their time more productively. There is not much new chemistry here, and there certainly is no new chemical work that has any relevance to what happens on the ‘bench’. This work is primarily in the philos-

ophy of chemistry, focusing on the (philosophical) foundations of chemical theories and its target is a characterisation of theories of chemistry in terms of theories of philosophy of science.

Busy chemists that have a moderate level of philosophical interest are advised to read those parts of Chapter 1 that interest them and most of Part I, before moving on to the Summary. Some of the materials in Part I, especially Chapters 2, 3, and 5 can be used to develop a sense of how some of the theories of chemistry ‘fit’ with non-formal, but reasonably precise, philosophical notions of explanation, research programmes and reduction. It is possible to be a philosopher of science and not do any formal work, and this part gives an example of what may be achieved in the philosophy of chemistry without getting overly formal. This material will also assist in getting an appreciation of current topics in the philosophy of chemistry, especially on previous work in the philosophy of explanation in chemistry.

The formal part of the book, Part II, may be confusing for chemists if they are not introduced into formal aspects of philosophy of science (as most chemists are not). At this stage in the book, the busy chemist will have to make some decision on precisely how deep their interest in philosophy goes. If not very deep, busy chemists may read the introductions and conclusions to these chapters, and sample the rest. The part is reasonably self-contained in that all the notions are explicitly introduced and explained, but the chemist may want a somewhat gentler introduction to the details of the structuralist theory. The main reference on this theory, the book by Balzer, Moulines, and Sneed (1987), should be of assistance, but may also prove frightening. It will help at this point to realise that most members of the general public are somewhat intimidated by chemical notations. Chemists know that these things can be mastered over time, and the structuralist framework for scientific theories falls in the same category of things that can be mastered with some time and patience.

The upshot of this part is that the reduction relations that exist between chemistry and physics make specific ‘linking’ commitments that tie chemical and physical concepts together. The ‘linking’ commitments are sufficient to defend the notion of *explanation* of chemistry by physics, but it is argued that the explanations are by no means straightforward and ‘one to one’. While this may not come as a surprise to many chemists, it is nevertheless an interesting philosophical conclusion.

Busy chemists are again advised to sample some pieces of Part III to get a handle on a philosophical topic most nebulous: ontology. Ontology makes for good party small-talk if there are no philosophers around, but the busy chemist is well advised make certain of this fact before engaging in it. Finally, the busy chemist is advised to read the Postscript to get a sense of the philosophical progress made, and my personal interpretation of what I believe the future issues in the philosophy of chemistry will be.

Finally, the discussion given here may convince some chemists to dabble or engage in serious work in philosophy of chemistry themselves. Such activities are highly encouraged, but in that case it will be wise to read the relevant references as well.

Roadmap for busy philosophers

Busy philosophers can skim most of Chapter 1 to get a sense of the particular take on reductionist concepts on which the further argument in this book is based, but need not read this chapter in detail.

Philosophers are again advised to read most of Part I. Part I of this work revises a number of the scientific and philosophical arguments on which dearly held convictions in the philosophy of chemistry are based – hence it is important for philosophers to get a sense of the science involved in these debates and see how this influences the philosophical thinking on these matters. Especially around the topic of molecular structure, the science is currently unsettled and completely satisfactory explanations do not exist. However, that does not necessarily mean that issues affecting the foundation of quantum theory intrude deeply in its capability for explanation. From this perspective, philosophers are highly encouraged to try and follow at least the basic line of argument in the ‘science’ sections of Part I.

Not all philosophers of science are familiar with the structuralist framework on theories on which Part II is largely based. Despite the technical complications, the structuralist framework is sometimes described as putting angle brackets around one’s philosophical intuitions, a description which at times is disturbingly apt. However, the structuralist framework lets us re-engage with the Nagelian concept of reduction in ways which are not only refreshing, but also required if we are to make meaningful progress in the philosophy of chemistry. My contention is that the structuralist framework is capable of providing formal foundations to a ‘naturalised’ Nagelian model of reduction. Moreover, while philosophers of science may not be universally familiar with the structuralist approach, they should be sufficiently familiar with the *semantic* approach to see what is going on in broad outline. The first and last sections, as well as the introduction and summary to this part, should convey a sense of the issues and the proposed solutions which avoids reliance on technical notation.

Philosophers are also advised to read Part III and the Postscript to place the results discussed in this work in wider context. Not much of a shortcut, I’m afraid, but hopefully an enjoyable journey.

Introduction

My aim is to explore the reduction of chemistry to physics from the viewpoint of quantum chemistry, using a suitably liberal form of reduction, and to discuss the consequences of this reduction for the philosophy of science.

The debate around reduction in the special sciences is generally framed around three separate notions of ‘reduction’ which are not usually distinguished: the notion of scientific explanation, some logical notion of reduction (which in turn has an epistemic and ontological component), and a sociological component. These positions track more or less closely the role of reduction in the original unity of science project, where the ‘unity of science’ was conceived as containing an explanatory, ontological and sociological component. As Reisch (2005) outlines in his study of the demise of the Received View, the concept of unity of science changed considerably over time, from Neurath’s programme, in which the unity of science was conceived mainly as a coordination among the sciences in order to achieve a social goal, to, towards the end, a philosophical position that was largely decoupled from active collaboration with scientists themselves. The latter approach runs the risk of degenerating into a simplistic, overly metaphysical, ‘nothing but’ sort of reductionism that, in my opinion, has made philosophers of chemistry overly wary of the concept of reduction.

I argue that the best thinking on how to relate chemistry to physics may be found in a creative re-confrontation with Nagel’s theory of reduction of the sciences. To sum up my position at the outset: I believe that chemistry can be *explained* by physics, that its *reduction* is more problematic but not impossible (assuming a moderately relaxed notion of reduction), that chemistry however has a separate *ontology*, and, finally, that any sort of sociological ‘takeover’ is simply out of the question.

One of the leading themes of this book is that the failure to distinguish properly between explanation, Nagelian or other forms of reduction, ontological reduction and finally sociological reduction has led to significant confusion in the debate on reduction in the philosophy of chemistry. Chapter 1 will contain more details on the various philosophical positions regarding the unity of science and reductionism, but it is useful to set out the general

framework of the discussion before embarking on the details, and especially to make clear the distinction between explanation and reduction.

Explanation applies in cases where one scientific theory explains another theory or empirical law. Thus explanation is a matter of scientific fact. The notion of explanation is an epistemological one, but does not commit one at the outset to a deductive nomological scheme. There are other explanatory schemes that do not involve derivation in a strict sense. In fact, as will be discussed in much more detail in Part I, the explanation of chemistry by physical theory has many complications, and the physical foundations of chemistry are found in a multitude of physical theories, patched together with assumptions, approximations and special applications.

Reduction is a particular formal rendering, or paraphrase, of what happens when we claim that one theory explains another. As will be discussed in more detail in Chapter 1, the (programmatic) notion of ‘unity of science’ is intimately connected with the notion of reduction, and one’s conception of the unity of science has a significant bearing on one’s notion of reduction. The philosophy of chemistry has employed a number of notions of reduction, and is perhaps notable for its invention and significant subsequent use of ‘ontological reduction’ as a separate form of reduction, which can be decoupled from theory reduction. The idea is that ‘ontological reduction’ is what remains of the putative reduction relationship once ‘epistemological reduction’ has proved impossible. It will be my aim in this book to clarify the issues around ontological reduction in more detail.

This book has three parts. The first part, called ‘Limits’ is a non-formal discussion and introduction of the issues as well as an outline of possible solutions. In this part I discuss two specific cases of explanation and theory formation in quantum chemistry: the formation of the chemical bond and molecular structure in Chapters 2 and 3. I also discuss how quantum chemistry might be reconstructed as a Lakatosian research programme in Chapter 5. Part I also contains a chapter, Chapter 4, which focuses on its specific explanatory structure.

The main aim of this part is to argue that the accounts of reductionism that are at present fairly current in the philosophy of chemistry, and which focus on the lack of ‘derivability’ of chemical concepts from the notions of quantum theory, short-change the philosophical analysis of the issues. In particular, the subject matter of explanation and reduction has a greater variety than is contained in mere concepts of identity and deduction. In turn, quantum chemistry is significantly more diverse in its outlook and approach than its current implementation in terms of easily used ‘black box’ computer programs might suggest.

Specifically, the characterisation of quantum chemistry as a research programme in Chapter 5 is attractive in this context, because quantum chemistry contains a number of distinct methods, which (from the viewpoint of a re-

search programme) can be characterised as a succession of theories. Moreover, quantum chemistry makes a number of programmatic claims, such as its applicability to chemistry, which can be fruitfully evaluated with a suitably enriched concept of research programmes such as those of Kuipers (2007) or Zandvoort (1986).

The material in Chapter 5 will also form a core part of the foundations for Part II. This part, called ‘Models’ is a more formal overview and evaluation of quantum chemical theories in a structuralist (or set-theoretic) approach in the philosophy of science. In this part, I employ the structuralist conception of theories to gain an understanding of how quantum theory and chemistry might be related. The structuralist approach to theories is arguably one of the most fruitful approaches in the philosophy of science in the sense that this approach does not suffer from some of the main drawbacks of the linguistic approach that characterised the ‘Received View’. The main advantage of the structuralist approach, the fact that it allows for a relatively clear statement of notions that are close to the hearts and minds of philosophers of science, such as scientific paradigms, scientific change, and theoretical terms, is the main motivating factor for putting up with what in the eyes of some is tiresome hairsplitting.

Its main weakness in the present context, though here turned to strength, is that notions of inter-theory reduction are thoroughly problematic in this framework. In the original formulation of Suppes (1957), the reduction relation is one of structural isomorphism. This form of reduction is too weak to support the Nagelian conditions of connectibility and especially derivability, and also suffers from a significant underspecification of the issues. I will argue for a significantly more liberal reading of the work of Nagel, supported by a detailed return to Nagel’s original text, and a subsequent recasting of the Nagelian conditions in terms of the structuralist framework. Since in the case of quantum chemistry the strict Nagelian conditions are problematic, this weakness of the structuralist framework turns out to be advantageous: while various authors have proposed additional conditions on the isomorphisms to furnish a fully fledged reduction relation, the case of quantum chemistry that we discuss is one of the first examples that allows us to evaluate how these additional conditions track under actual conditions of scientific explanations, conditions that we might want to argue should be properly called reductions. The remainder of this part deals with specific formal reconstructions of the theories of quantum chemistry and especially their interrelationships.

The third part, called ‘Consequences’ consists of two chapters, Chapter 9 and Chapter 10, that focus on chemical ontology and the somewhat hairy topic of ontological reduction. In the philosophy of chemistry, ontological reduction seems to originate in the notion that, at the end of the day, chemistry and physics deal with the ‘same’ matter, and hence must therefore be ontologically compatible. From this perspective, ‘ontological reduction’ is

what remains of reduction after the hope of achieving theory reduction has been given up: it tries to save the intuition by writing, so to say, a blank cheque to metaphysics. The contention I will develop in this part is that this approach misunderstands ontology. I argue from the viewpoint that ontology is the end result of the ontological commitment of our theories, and is hence dependent on epistemology to some degree. Specifically, from the viewpoint of ontological commitment, commitment to a single or at least compatible ontology in chemistry and physics is commitment to a concept of the unity of science. On this basis, I develop a specific ‘chemical ontology’ in this part which is compatible with the view on reduction offered in Part II. Part III furthermore underpins this specific view on ontology by situating it in the historical context of a Kantian theory of objects, and proposes a number of twenty-first century emendations to this theory.

The Postscript aims to situate philosophy of chemistry in the broader context of philosophy of science and philosophy proper by locating the topic of reduction within the wider context of the unity of science. By doing so, it also locates the extent to which chemistry can be classified as an autonomous science. It argues that while chemistry is somewhat special as a science, it is not so special that it needs to be insulated from wider philosophical concerns. There is a fruitful approach in which the peculiarities of chemistry can be addressed from a wider philosophical scope. The viewpoints that are useful here are methodological pragmatism, scientific autonomy and inter-theory reduction. These three viewpoints form a field in which chemistry as a science can be usefully triangulated.

While the book contains a complex argument, the conclusion of it all is that chemistry is actually not that special. Chemistry is a science and as such, amenable to the theories and frameworks developed by philosophers of science, or at least, it *should be*. Philosophers of science have not always been sensitive to the theories of chemistry. They have overlooked many of the small and not so small peculiarities which make chemical theories special.

Hence there is something interesting to learn for philosophers as well. The fact that a reduction relation with the theories of physics should exist provides the philosopher with a useful, but generally overlooked, opportunity to investigate reduction relations where they are still *simple*: as daunting as the problems with this reduction are, they are in all probability still less daunting than the reductions of other sciences.

The attitude I will take with respect to reduction relations is pragmatic: reduction conditions are what has to be *proven* in actual cases of reduction (such as the one from chemistry to physics), rather than imposed from the outset. This study thus takes an *experimental* approach to the topic of reduction: using the formalism of structural links between theories, it investigates which reduction conditions actually apply in practice, and then evaluates the prospects for the project of unity of science on that basis.

Broadly speaking, the present book may be read as a defence of reduction in the sciences, even while it focuses specifically on the relationship between physics and chemistry. It will be obvious at this point (even if only judging from its size) that this defence is a bit more involved than we were inclined to believe initially. Early literature on the topic (specifically from the late 1950s and early 1960s, for instance Nagel (1961) or Kemeny and Oppenheim (1956)) concluded that the reduction of chemistry to physics was more or less achieved successfully and therefore lacking of the sort of problems that should interest philosophers of science.

Part of what I aim to achieve is to prove this wrong: if one is sufficiently sensitive to some of the problems posed by the respective sciences, the reduction relation becomes very interesting indeed.

Before concluding this introduction it is necessary to deal with one possible objection. The objection is quite simply this: if *this* is what it takes to discuss the reduction relationship between simple sciences ('this' being the considerable complexities in the pages that follow), why bother?

This objection can be answered in several ways. The first one is a simple platitude: it takes what it takes. While intuitive appeal, simplicity and directness is a laudable feature of concepts, it is not a required feature. If the reduction relation between chemistry and physics proves to be in some ways indirect and more roundabout than initially expected, this is not in itself a reason to give up on the concept altogether.

A second answer is a bit more substantial. The reduction between chemistry and physics is intuitively one of the more credible cases of reduction between two disciplines: both sciences deal with matter, both sciences express their views on that matter in more or less compatible theories, and there are few who doubt that physical theories such as quantum mechanics or statistical mechanics yield plausible *explanations* that can be patched into chemical theories at the appropriate places. Hence one would expect this situation to give rise to a paradigmatic sort of reduction. Giving up hope for reduction entirely at this stage therefore amounts to giving up hope altogether. If this is the required outcome, let the argument for it at least be robust.

A third answer is a consequence of the second. It consists merely in the claim that the resolution of the problems associated with reduction between chemistry and physics should be instructive for the concept of reduction itself.