

Linking chemistry with physics: arguments and counterarguments

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Abstract The many-faced relationship between chemistry and physics is one of the most discussed topics in the philosophy of chemistry. In his recent book *Reducing Chemistry to Physics. Limits, Models, Consequences*, Hinne Hettema (Reducing chemistry to physics. Limits, models, consequences, Rijksuniversiteit Groningen, Groningen, 2012) conceives this relationship as a reduction link, and devotes his work to defend this position on the basis of a “naturalized” concept of reduction. In the present paper I critically review three kinds of issues stemming from Hettema’s argumentation: philosophical, scientific and methodological.

Keywords Ontological reduction · Quantum mechanics · Quantum chemistry · Molecular shape · Unity of science

Introduction

In his recent book *Reducing Chemistry to Physics. Limits, Models, Consequences*, Hettema (2012) addresses the issue of the many-faced relationship between chemistry and physics from a reductive viewpoint. He devotes his work to defend this position on the basis of a “naturalized” Nagelian concept of reduction, which admits a number of modifications that significantly weaken the original schema.

The book is a very fruitful contribution for those interested in understanding the subtleties and complexities underlying the loose and indirect links that interconnect chemistry, quantum chemistry and quantum mechanics. However, there are some considerations that deserve to be made for a balanced assessment of the work. I will critically review three kinds of issues stemming from Hettema’s argumentation: philosophical, scientific and

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methodological. The aim that underlies the present work is to contribute to the general discussion about the relationships between chemistry and physics, by stressing the many difficulties that must be faced to insist on the reduction of chemistry to physics.

Philosophy: ontological reduction and grounding

In the second chapter of the third part of his book (Chapter 10), Hettema focuses on ontological matters from the traditional viewpoint of the so-called “received view” in the philosophy of science. In particular, he addresses the problem of scientific realism in the light of the question about the reference and the eliminability of the theoretical terms of science¹ as introduced by Hempel’s “*theoretician’s dilemma*”: under the assumption that the only purpose of theoretical terms is to establish predictive and explanatory connections among observables, then if they serve their purpose, they are unnecessary, and if they don’t serve their purpose, they are surely unnecessary; but theoretical terms either serve their purpose or they don’t; hence, they are unnecessary (Hempel 1958, pp. 49–50).

The simple realist answer to the dilemma consists in contesting the premise of the argument: to establish predictive and explanatory connections among observables is not the only purpose of theoretical terms, since they have ontological import, that is, they refer to existing items. As a consequence, according to the realist, theoretical terms cannot be removed from the discourse of science. Although this answer seems plausible, Hettema correctly identifies the trouble with it when applied to the case of the theories of chemistry and physics: “*Chemical theories often refer to entities, such as atoms, chemical elements, electrons and orbitals that have some counterpart of the same name in theories of physics. [...] Yet it is also the case that the uses of such terms in the theories of chemistry are in many cases inconsistent with how these same terms are conceived in physics. Even worse, it is not clear at the outset that the manner in which these terms are used in both the theories of chemistry and physics are even compatible. Hence for the theoretical terms in use in chemistry, it is not that easy to show that they actually do more than connect observations to each other.*” (pp. 365–366). The ontological consequence of this fact is what the author calls “*ontological discontinuity*” between the terms of chemistry and those of physics: certain terms used both in chemistry and in physics seem to refer to different items in the two disciplines. Moreover, such a discontinuity is considered as “*one of the central problems in the philosophy of chemistry, around which many other problems, such as that of reduction, revolve.*” (p. 368) and, as a consequence, has to be resolved prior of those other problems.

Hettema considers three possible ways out of ontological discontinuity: ontological reduction, internal realism and his own position based on the notion of grounding. Ontological reduction would solve the challenge by showing that discontinuity is only apparent because theoretical terms refer to the same item both in chemistry and in physics. In spite of the defense of reductionism that underlies the rest of his book, Hettema rejects this solution, and claims that “*philosophers of chemistry better rid themselves of the concept of ‘ontological reduction’.*” (p. 409). Nevertheless, the reason for adopting this stance is not completely clear. He considers ontological reduction in the light of a quantification reading of the reduction postulates in Nagelian heterogeneous reduction

¹ Here I will not discuss the traditional distinction between theoretical terms and observational terms, a distinction that was challenged not only by the so-called “new philosophy of science” (at present not new anymore), but also by the structuralist view of scientific theories that he himself seems to advocate.

(Nagel 1961): if those postulates are of a form ‘ $\forall x, y : Px \rightarrow Py$ ’, then they are ontologically committed with the existence of the items denoted by x and by y , corresponding to both poles of the reductive relation (pp. 381–382). However, it is not clear why Nagelian-type reduction cannot be read from a different perspective: if considered as logical identities that assimilate the referents of the related terms, reduction postulates would endow ontological reduction with a precise formulation.

With respect to this issue, Hettema seems to agree with Needham (2006, 2010) in judging that the notion of ontological reduction is not sufficiently clear and that the burden of proof shifts to the ontological reductionist, who must first clarify the notion. In fact, he claims that “[t]he notion of ‘ontological reduction’ standing on its own is nonsensical” (p. 382). However, this position ignores the venerable history that the idea of ontological reduction has in the development of philosophy, a history that begins with the Presocratic philosophers and the reduction of all things to a single substance (water, air, apeiron), the reduction of sensible properties to the movement of atoms in vacuum in the atomist philosophy, and arrives to the Modern Age with corpuscularism and with the relationship between primary qualities, endowed with ontological priority, and secondary qualities, conceived as merely subjective and depending on the primary ones.² Perhaps the disregard of the history of philosophy is what leads Hettema to assert that “[o]ntological reduction is a concept that is somewhat peculiar to the philosophy of chemistry. It was for example introduced by LePoidevin (2005)” (p. 381), and that it was even invented by philosophy of chemistry: “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.” (p. 2). My above comments do not amount to a defense of ontological reductionism; by contrast, I advocate an anti-reductionist ontological pluralism. However, the rejection of ontological reduction does not require the rejection of the concept itself; on the contrary, who wants to argue against the ontological reductive link between two domains needs to use the concept in a meaningful way to support his argumentation.

The second possible way out of ontological discontinuity, internal realism, is not seriously considered by Hettema. This is rather curious since a Kantian-rooted ontological pluralism, inspired by Putnam’s internal realism (Putnam 1981), has been discussed in detail in the recent literature on the philosophy of chemistry. In particular, that position has been wielded against reductionism to support the ontological autonomy of the chemical world (Lombardi and Labarca 2005, 2006). It is true that Hettema devoted the previous chapter (Chapter 9) to criticize the arguments presented by Labarca and Lombardi (2010), based on their ontological pluralism, regarding the existence of orbitals.³ However, the assumption that the case of orbitals is not a good argument for ontological pluralism does not yet invalidate ontological pluralism as a whole: since the concept of orbital is very peculiar, it could be considered as a candidate not good enough to serve as a paradigm for the relation between chemistry and physics. In short, Hettema acknowledges that internal realism is a possible way out of ontological discontinuity, but it is not easy to find the explanation of why he decides to discard it.

In spite of his decision of dismissing internal realism, Hettema takes into account some Kantian elements to build his notion of chemical object. Of course, there is a wide spectrum of interpretations of Kant’s philosophy, from the most idealist interpretations to

² This answer to Needham’s (2006) non-sense objection was already given in Lombardi and Labarca (2006).

³ These criticisms will not be considered here but will be discussed in a future work.

the readings coming from the analytic thought. However, the reading proposed by the author sounds rather strange. Following Langton (1998), he endows the noumenal realm with causal power, in clear opposition to Kant's view of causality as one of the categories of human understanding. By considering the Kantian influence on Paneth's conception of a chemical element (Ruthenberg 2009, 2010), he identifies noumenal and unobservable, forgetting that, whereas we have direct knowledge of observable items and indirect knowledge of unobservable items, Kant's noumenon is not an object of knowledge at all. As a consequence, Hettema's reading of Kant's theses deprives them from their philosophical specificity.

Since Hettema believes that it is necessary to set aside the concept of ontological reduction, he proposes a different concept, the relation of "*grounding*", to understand the links between chemical objects and physical objects. Grounding is initially defined as "*a metaphysical relationship expressing how things are in virtue of something else that grounds them*" (p. 380). Following Schaffer (2008), '*x grounds y*' means that *x* is ontologically prior to *y*, or that *y* depends on, or derives from, *x*: *y* exists and has its nature in virtue of, on the basis of, or because of, *x*. In other words, *x* is the fundamental, basic, independent and primary item, as opposed to the derivative, dependent and secondary character of *y*. From this characterization, it is clear that grounding is a relationship between ontological items (objects, properties, facts, etc.) and, precisely for this reason, "*introduces an ordering on what there is in the world, in Schaffer's words, a great tree of being*" (p. 380). In the picture of reality resulting from grounding, the ontology of chemistry is preserved—unlike in the ontological reductionist picture—, but it is derived, dependent and secondary with respect to the fundamental ontology of physics—unlike in the ontological pluralist picture. This is an interesting view that has strong points of contact with emergentism, a position that finds its roots in the so-called "British emergentism" (Alexander 1920; Lloyd Morgan 1923; Broad 1925), and "reemerges" in the seventies as a consequence of the collapse of the received view (Kim 1999; Cunningham 2001; Philström 2002; El-Hani 2002) and the development of interdisciplinary fields of study related with the phenomenon of complexity (Emmeche 1997). Hettema's argumentation in favor of grounding and a hierarchical view of reality would greatly benefit from connecting and comparing the proposed stance with the already traditional discussions about emergence.

The relation of grounding, as initially introduced, is a relationship between ontological items that leads to a hierarchical picture of reality. However, the nature or the relation suffers a gradual transmutation through the pages. For instance, before its explicit characterization, grounding is preannounced as a relation between a theory and certain entities: "*theories are ontologically committed to their theoretical entities and have a grounding relation to other entities*" (p. 350). But, after its characterization, grounding turns out to be a relation between theoretical terms and intertheoretic links: "*The notion of grounding seems to be capable of at least providing us with a number of hints as to what theoretical terms actually do in our theories: theoretical terms, on this view, may be said to provide grounds to a critical sort of linkage between the apparatus of one theory to that of another*" (p. 382). Later, grounding operates as a relation between concepts: "*the concept of a chemical element as a 'simple substance' is grounded in a concept of a chemical element as a 'basic substance'.*" (p. 393); "*A 'grounded' concept, in this sense, is one that satisfies the criterion that it is capable of being 'imported' from a neighboring science*" (p. 395). Even later, grounding seems to be a relation between certain entities and the facts that lead us to believe in their existence: "*Chemical elements, conceived as 'simple' substances are grounded in how they appear to our senses, even though this grounding is somewhat trivial. 'Basic' substances were initially grounded in the observation that*

certain types of ‘stuff’ cannot be decomposed by chemical means.” (p. 394). The fact that the notion of grounding does not find a univocal characterization in Hettema’s argumentation hinders the understanding of the links that the author tries to establish between his proposal and the recent work of other authors in the philosophy of science, as Ladyman et al. (2007), Wimsatt (2007) and Strevens (2008) (pp. 396–400).

Hettema says that the ontological relation of grounding “*is not capable of further analysis*”, but in the context of the discussion about ontological reduction, it “*is analysable roughly in terms of scientific explanation and theory formation*” (p. 382). It is true that, although there are no definitive criteria to decide the applicability of ontological relations, what happens in the epistemic domain can nevertheless help us to find good arguments to support conclusions in the ontological domain.⁴ However, this argumentative strategy should not lead us to conflate an ontological relation with an epistemic relation. In summary, the loose use of a concept as grounding, which intends to play a central role in Hettema’s argumentation, threatens the whole ontological proposal: many different conclusions can be drawn from the different faces that the notion shows throughout the text.

Science: what quantum mechanics we are talking about?

Hettema devotes a large part of his book to develop two formal reconstructions. Firstly, he reconstructs quantum chemistry as a Lakatosian program (Lakatos 1970) that can consistently integrate ab initio calculations and semi-empirical methods. Then, on the basis of the canonical work of Balzer et al. (1987), he supplies a structuralist reconstruction of two versions of quantum mechanics, a “simple” quantum mechanics and a “complex” quantum mechanics, and then proceeds to reconstruct quantum chemistry. The main contribution of these reconstructions is that they accurately bring to light the assumptions needed to link chemistry, quantum chemistry and quantum mechanics. However, at the same time, when carefully analyzed these reconstructions operate as a counterargument to Hettema’s own reductionist stance about the relationship between chemistry and physics. In the following subsections I will consider two points that threaten the supposed reduction.

A one-observable quantum mechanics

The second part of the book is devoted to the problem of the relations between chemistry and physics with the tools supplied by structuralism. In the first chapter of this part (Chapter 6), Hettema begins by supplying an overview of the structuralist reduction concepts, and then emends the original structuralist proposal by conceiving intertheoretic links as key elements in the reduction relation. On the basis of this initial task, in the following chapter (Chapter 7) Hettema undertakes the reconstruction of quantum mechanics and quantum chemistry, in order to clarify the relationships between these two disciplines. The final aim is to consider *how* quantum chemistry can be classified as quantum mechanics and *whether* quantum chemistry can also be classified as chemistry (p. 256). Here I will only focus on the first issue, which clearly manifests the author’s presupposition that quantum chemistry “*is a member of quantum mechanical theories*” (p. 256).

In order to analyze, from a structuralist viewpoint, how quantum chemistry can be considered quantum mechanics, the first step is to supply a structuralist reconstruction of

⁴ Lombardi and Labarca (2006) also appeal to epistemic facts to find good arguments for supporting ontological claims, but in those epistemic facts they find support for ontological pluralism.

quantum mechanics. Hettema distinguishes between a “simple” form and a “complex” form of quantum mechanics (p. 255). The simple form differs from the complex form in the fact that the first one does not include the concepts of quantum state and of probability. According to the author, a large part of quantum chemistry can be characterized in terms of the simple form of quantum mechanics. In turn, the interpretive problems that are usually conceived as obstacles to reduction emerge only in the complex form: “*the concerns expressed especially by Primas (1981) about the reducibility of chemistry instead relate to a ‘complex’ form of quantum mechanics, in which the matters of a state function and acceptable probability distribution play a major role.*” (p. 255). Therefore, Hettema begins by the reconstruction of the simple form, and then adds the “*components that ‘complete’ the simple quantum mechanics into a ‘full’ version of quantum mechanics*” (p. 264). On this basis, the aim of the referred chapter is to show that quantum chemistry can be reconstructed in terms of the simple version of quantum mechanics and, therefore, it can be viewed as an “application” or “modification” of the reducing theory (p. 258).

One might call into question a view that conceives a theoretical structure as the simple version, lacking the concepts of state and probability, as quantum mechanics. This viewpoint would be a difficulty for Hettema’s proposal, based on reducing quantum chemistry to that simple version. However, the problem is logically previous, since it affects likewise both the simple and the complex versions: it is related not with the quantum state or the probabilities, but with the selection of the observables of the quantum system.

The question about whether all operators on the Hilbert space represent physical observables or not is an unsolved interpretive problem. Nevertheless, no matter how much one is willing to restrict the space of observables, such a space must preserve a minimal structure that includes, at least, certain basic physical observables as energy, position, momentum, angular momentum, etc. Moreover, as Ballentine (1998) points out, the relevant observables of the system, endowed with a clear physical meaning, are closely related to space–time transformations, and can be defined in terms of the Galilean group, that is, the symmetry group of the theory. On the contrary, in Hettema’s reconstruction, the structures that characterize quantum mechanics (p. 264 the simple form, pp. 264–265 the complex form) incorporate a *single operator* \hat{A} , instead of the whole set of operators on the Hilbert space representing the observables of the system. This strategy deprives quantum mechanics of meaningful physical content, since many relevant magnitudes cannot be even expressed in the proposed reconstruction.⁵

Of course, the result of this move is that, not only in the simple form, but also in the complex form of the theory, the interpretive problems derived from the incompatibility between non-commuting observables suddenly disappear. But, at the same time, this kind of reconstruction also cancels one of the foundational features of quantum mechanics. It is quite clear that the Uncertainty Principle, which prevents two commuting observables from having definite values simultaneously, cannot even be formulated in a one-observable theory. And not only the Uncertainty Principle is affected. As Hughes (1989, pp. 109–110) emphasizes, in the absence of non-commuting observables there may be no way to distinguish a superposition of two pure states from a mixture of them; therefore, it is precisely the existence of non-commuting observables what gives empirical content to the Superposition Principle. Furthermore, the contextuality of the theory, as resulting from the

⁵ It is interesting to point out that there is a structuralist reconstruction of quantum mechanics without this limitation in the works of Lastiri (2011, 2012).

Kochen-Specker theorem (Kochen and Specker 1967), also vanishes in a one-observable theory.

Hettema adds that, in the cases in which the simple form of quantum mechanics is sufficient for reducing quantum chemistry, in practice “*the operator \hat{A} will be the Hamiltonian operator \hat{H}* ” (p. 264). It is true that in quantum chemistry the Hamiltonian plays a central role, since the main task is to solve the time-independent Schrödinger equation. But, in the framework of quantum mechanics, such an equation is better viewed as the eigenstate-eigenvalue equation for the Hamiltonian, and the Hamiltonian is one of the many physically meaningful observables of a quantum system: the analog eigenstate-eigenvalue equation can be formulated for any observable, since all the observables of the system are on a par. This means that the privilege of the Hamiltonian, as presupposed by quantum chemistry, does not derive from the formalism of quantum mechanics, but has to be added to the quantum context as an interpretive postulate and has to be argued for in terms of its fruitfulness for solving the traditional conceptual problems of the theory. This is precisely the perspective adopted by one of the members of the modal family of interpretations of quantum mechanics (see survey in Lombardi and Dieks 2012): the modal-Hamiltonian interpretation endows the Hamiltonian with a leading role both in the definition of quantum systems and subsystems and in the selection of the definite-valued observables (Lombardi and Castagnino 2008; Lombardi et al. 2010).

These considerations lead us to ask whether what is reconstructed as quantum mechanics, even in its complex version, is quantum mechanics in a strict sense. The restriction to a single privileged observable seems to point to a negative answer: in Hettema’s reconstruction, quantum chemistry is linked to a theoretical structure that lacks the essential features of quantum mechanics, precisely those features that give rise to the conceptual obstacles to the desired reduction.

The problem of molecular shape

In the last chapter of the first part of the book (Chapter 5), Hettema undertakes the reconstruction of quantum chemistry as a Lakatosian program. This task is guided by two purposes. The first one is to determine whether quantum chemistry can be seen as a research program, and whether the research program is progressive or degenerative. The second one is to analyze the kind of explanations offered by quantum chemistry.

In this chapter the author addresses the relation between quantum chemistry and classical chemistry. The final conclusion is that the two disciplines can be viewed as independently progressive research programs (p. 201). This reconstruction work is highly valuable, since it explores in detail the many different approximations, methods and auxiliary assumptions that constitute the Lakatosian protective belt (see Subsections 5.4.3 and 5.4.4, pp. 192–200). Moreover, the analysis brings to light the subtle relations between quantum chemistry and classical chemistry, which do not admit a simple reductive reading. Nevertheless, I will not focus on the interesting issue of the relation between quantum chemistry and classical chemistry, but on the reconstruction of quantum chemistry itself, in order to assess the author’s claims about the reduction of quantum chemistry to quantum mechanics.

In the Lakatosian reconstruction of quantum chemistry proposed by Hettema, the assumption of a nuclear framework with its geometrical structure belongs to the hard core: “*The (isolated) molecule can be characterised as having a ‘frame’ in the first instance, by assuming that the position of the nuclei is fixed while that of the electrons is not.*” (p. 189). This is one of the idealizations “*inherent in the specification of the hard core, which limits*

the hard core to non-relativistic space-fixed electronic structure theory" (p. 191). It is clear that, if the concept of molecular structure belongs to the hard core of the program, the reducibility of quantum chemistry to quantum mechanics will strongly depend on the possibility of defining that concept exclusively in quantum mechanical terms.

Wolley (1976, 1978, 1998) is one of the first authors who address the problem of linking molecular structure with quantum mechanical concepts. From a reductionist viewpoint, he claims that molecular structure is not an intrinsic property of molecules because it is not definable in quantum mechanical terms. More recently, Hendry (2004, 2008, 2010) also focuses on the issue of molecular structure in the context of the problem of reduction. According to the author, reduction must be discussed in the ontological domain, since the epistemological irreducibility of chemistry to physics is indisputable: even the reductionist knows that the exact equations are insoluble, "*the semi-empirical models are approximations to rigorous treatments, standing in for them in explanations of special-science phenomena.*" (p. 184). On this basis, the relation between chemical theories and quantum mechanics, embodied in the way in which molecular structure is explained, must be conceived in terms of emergence and not of reduction: molecular structure is a property that emerges from the underlying quantum mechanical realm.

Although very representative, Woolley and Hendry are only two of the many voices that raise worries about the possibility of explaining molecular structure in the quantum mechanical domain. Hettema admits that "*it is sometimes argued that fixing the nuclear framework in space imposes a specific shape on the molecule from the outset*", but justifies this move by saying that "*practising quantum chemists have to start with some notion of molecular shape, though the starting shape of a calculation does not have to correspond to the chemical equilibrium state of the molecule*" (p. 178). However, from the viewpoint of quantum mechanics the problem here is not the arbitrary selection of a particular framework to begin the computation, but the concept of nuclear framework itself, which seems to be at odds with Heisenberg's Uncertainty Principle.

The assumption of a nuclear framework of fixed nuclei depends on the application of the Born–Oppenheimer approximation, which is consistently also placed in the hard core of the research program (pp. 188–191). According to Hettema, this hard core should be viewed primarily in terms of a model of the molecule, which "*allows us to temporarily bracket some of the principled worries that emerge from the application of quantum theory to chemistry*" (p. 190). In fact, the model brackets the fact that the Born–Oppenheimer involves a step that is not supported by quantum mechanics: the assumption of the definite value of the energy of the molecular system. Such an assumption is what allows us to accept that, in the limit of infinite nuclear mass, the nuclei have a definite value of position. However, the definite value of the total energy in a stationary state does not derive from the formalism of quantum mechanics, but is a consequence of a particular interpretive assumption, the eigenstate-eigenvalue link, which leads to difficulties when applied to some well-known situations (see Lombardi and Castagnino 2010). Therefore, the Born–Oppenheimer approximation is not at all an innocuous postulation when the question of reduction is considered.

It is true that the aim of the Lakatosian reconstruction undertaken in this chapter is to study the links between quantum chemistry and classical chemistry. Nevertheless, the position of the concept of molecular structure and the Born–Oppenheimer approximation in the hard core of the quantum chemistry research program is relevant to the discussion about the links between quantum chemistry and quantum mechanics. In fact, in Chapter 3 Hettema offers an incisive analysis of the concept of molecular structure and a detailed presentation of the history and the meaning of the Born–Oppenheimer interpretation, with

the purpose of defending the reductionist view. He claims that the worries about the non-reducibility of molecular structure in the philosophy of chemistry are generally misplaced, because they wrongly take the description of a molecule with a certain shape as the theory to be reduced, and a form of principled quantum mechanics as the reducing theory. According to the author, on the one hand, molecules are not committed to have a particular shape to possess a chemical structure and, on the other hand, it is not necessary to take “principled quantum mechanics” as the reducing theory. This claim might be accepted even by the non-reductionist, since it highlights the highly indirect links that connect quantum chemistry with structural chemistry and with quantum mechanics. But it is this same claim what calls into question Hettema’s own reductionist conclusion: the problem of reducing chemistry to physics is “*whether chemical structures can be reduced to a set of properties derived from a pragmatic Born–Oppenheimer dependent, not so principled quantum calculation. The latter is all that may be required to make Dirac’s optimistic quote true and reduction a reality*” (p. 126).

Summing up, the Lakatosian reconstruction of quantum chemistry of Chapter 5, combined with the very detailed study presented in Chapter 3, far from supporting a reductive view, seem to point to the opposite direction. The question is, then, why, after so valuable and deep analysis, Hettema insists in defending a reductionist stance regarding the relationship between chemistry and physics. This question leads us to the reflections contained in the next section.

Method: the cart and the horse

It is quite clear that the general aim that underlies Hettema’s work is to argue for a reductive relationship between physics and chemistry. The global conclusion can be expressed by the last sentence of the book: “*The reduction of chemistry to physics is in this sense indeed a paradigm case for the notion of reduction*” (p. 410). However, in reaching this conclusion, the author has driven us a long way fraught with the intricacies of the supposed reduction.

In fact, the intertheoretic links do not supply a global reduction of chemistry to physics, but only local and partial reductions of particular theories or even of specific concepts: “*reduction becomes a local, rather than global affair. While the necessary links do exist between the various levels of theory, they exist between versions of theory and observation that have a somewhat limited local range of application*” (p. 330). Those links require the introduction of relevant idealizations and approximations that establish loose and non-continuous connections between theories. Moreover, the “unprincipled” models required for reduction “*make a number of assumptions that are inadmissible from a principled point of view*” (p. 341). The general strategy needs to weaken the Nagelian model of reduction sufficiently to still consider the connections so established as reductive. These links supply a notion of reduction so liberal that it could even be made compatible with non-reductionist positions: “*there is scope for the view that the reductive view as advocated by Nagel is capable of accommodating some of the non-reductive views*” (p. 47).

Hettema introduces the notion of composite theory as a theory capable to act as an agent of reduction. A composite theory usually “*draws concepts and observations from a larger body of other theories and fields in a usually pragmatic fashion*” (p. 337). In this way, some of the original theoretical complexity is hidden from sight in the composite theory, which in many cases ignores not only the details, but also the principles of the original composing theories. Therefore, composite theories, in their reductive function, “*may draw*

concepts out of context, and re-use the concept in a manner not admissible to the theory in which the concept was first introduced." (p. 337). But once the concept of reduction has been relaxed in such a way, we are entitled to ask why the relationship is still called 'reduction' instead of 'inter-theory link', and how to justify Hettema's insistence on conceptualizing this kind of loose links as reductive in the Nagelian sense.

Perhaps the answer to these questions can be found in the "naturalistic" or "pragmatic" stance adopted by the author, according to which "[t]he reduction between chemistry and physics should be the hallmark of what we would expect a successful reduction to accomplish" (p. 8), and "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" (p. 4). However, some might consider that this move puts the cart before the horse: the reduction of chemistry to physics is postulated from the very beginning, and on this basis the notion of reduction is adapted and made "flexible" as much as needed to agree with the original postulation. This strategy leaves no room for conceiving different kinds of inter-theory relations; furthermore, it might be argued that it renders the very concept of reduction vacuous.

What is the reason that leads Hettema to take this strategy? Many passages of the book point toward a strong link between reduction and unity of science: "*the (programmatic) notion of 'unity of science' is intimately connected with the notion of reduction*" (p. 2). And although the author acknowledges the existence of non-reductionist approaches to the unity of science, as that of Darden and Maull (1977) (see Section 1.4), he directs his efforts to argue for the compatibility between those non-reductionist views and Nagelian reduction. This seems to suggest that reduction is considered indispensable to the unity of science: "*reduction originated as a primary glue in the unity of science. Hence reduction has a strongly programmatic aspect, which has consequences not only for the individual status of theories, but also for how theories hang together*" (p. 42). However, the unity of science may still be considered a desirable goal from a non-reductionist perspective. In fact, different theories may be interconnected through symmetric links, which do not lead to a hierarchy or a "tree", but to a net where each theory is connected in different ways with many others. This picture, which leads to a non-reductive unity of science, is completely alien to a perspective that makes reduction the primary intertheoretic glue.

Conclusions

What is reduction? According to Hettema, "[r]eduction is a particular formal rendering, or paraphrase, of what happens when we claim that one theory explains another." (p. 2). However, throughout the pages of the book, this initial asymmetric characterization suffers a progressive transmutation, which turns the concept of reduction into a notion so liberal that it is difficult to see the difference between the meanings of the terms 'reduction' and 'intertheoretic link'. The arrival point of this journey will please the defenders of the various pluralist views that populate the present-day philosophy of science (for just some of the many examples, see Cartwright 1999; Torretti 2000; Hacking 2002; Lombardi and Labarca 2005, 2006; Chang 2012) but, at the same time, will disappoint the reductionists, who expect to find in the book arguments in favor of their own position.

Leaving aside some philosophical disagreements, this is the only essential shortcoming that I find in Hettema's book. Furthermore, this is an issue that could be easily removed from the argumentation by giving up the idea of reduction and its supposedly fundamental role in the unity of science. Once this aspect of the author's position is removed, we are left

with a highly valuable work, written by somebody who has a thorough knowledge of the subject matter. It is precisely his deep scientific training, in particular in quantum chemistry, what allows Hetteema to face the details of the different methods used in the practice of chemistry, and to analyze some recent developments in the area from a technical viewpoint. For this reason, Hetteema's book cannot be overlooked: it deserves to be carefully read, since it contains many fruitful insights about the relationships between chemistry and physics. As a consequence, the work will take a central place in the debates of the philosophy of chemistry over the next years.

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References

- Alexander, S.: *Space, Time and Deity*. Macmillan, London (1920)
- Ballentine, L.: *Quantum Mechanics: A Modern Development*. World Scientific, Singapore (1998)
- Balzer, W., Moulines, C.U., Sneed, J.D.: *An Architectonic for Science*. The Structuralist Program. Reidel, Dordrecht (1987)
- Broad, C.D.: *The Mind and its Place in Nature*. Kegan Paul, New York (1925)
- Cartwright, N.: *The Dappled World: A Study of the Boundaries of Science*. Cambridge University Press, Cambridge (1999)
- Chang, H.: *Is Water H₂O? Evidence, Pluralism and Realism*, Boston Studies in the Philosophy of Science. Springer, Dordrecht (2012)
- Cunningham, B.: The reemergence of 'emergence'. *Philos. Sci.* **68**, S62–S75 (2001)
- Darden, L., Maull, N.: Interfield theories. *Philos. Sci.* **44**, 43–64 (1977)
- El-Hani, C.N.: On the reality of emergents. *Principia* **6**, 51–87 (2002)
- Emmeche, C.: Autopoietic systems, replicators, and the search for a meaningful biologic definition of life. *Ult. Real. Mean.* **20**, 244–264 (1997)
- Hacking, I.: *Historical Ontology*. Harvard University Press, Cambridge, MA (2002)
- Hempel, C.: The theoretician's dilemma. In: Feigl, H., Scriven, M., Maxwell, G. (eds.) *Concepts, Theories, and the Mind-Body Problem*, Volume 2 of Minnesota Studies in the Philosophy of Science. University of Minnesota Press, Minneapolis (1958)
- Hendry, R.F.: The physicists, the chemists, and the pragmatics of explanation. *Philos. Sci.* **71**, 1048–1059 (2004)
- Hendry, R.F.: Two conceptions of the chemical bond. *Philos. Sci.* **75**, 909–920 (2008)
- Hendry, R.F.: Ontological reduction and molecular structure. *Stud. Hist. Philos. Mod. Phys.* **41**, 183–191 (2010)
- Hetteema, H.: *Reducing Chemistry to Physics. Limits, Models, Consequences*. Rijksuniversiteit Groningen, Groningen (2012)
- Hughes, R.I.G.: *The Structure and Interpretation of Quantum Mechanics*. Harvard University Press, Cambridge, MA (1989)
- Kim, J.: Making sense of emergence. *Philos. Stud.* **95**, 3–36 (1999)
- Kochen, S., Specker, E.: The problem of hidden variables in quantum mechanics. *J. Math. Mech.* **17**, 59–87 (1967)
- Labarca, M., Lombardi, O.: Why orbitals do not exist? *Found. Chem.* **12**, 147–157 (2010)
- Ladyman, J., Ross, D., Spurrett, D., Collier, J.: *Every Thing Must Go: Metaphysics Naturalized*. Oxford University Press, Oxford (2007)
- Lakatos, I.: The methodology of scientific research programmes. In: Lakatos, I., Musgrave, A. (eds.) *Criticism and the Growth of Knowledge*. Cambridge University Press, Cambridge (1970)
- Langton, R.: *Kantian Humility: Our Ignorance of Things in Themselves*. Clarendon Press, Oxford (1998)
- Lastiri, M.: *Una Reconstrucción Estructuralista de la Mecánica Cuántica*. Doctoral Dissertation. Universidad Nacional de Tres de Febrero, Buenos Aires (2011)

- Lastiri, M.: Aplicaciones intencionales de la mecánica cuántica. *Agora. Papeles de Filosofía* **31**, 271–285 (2012)
- LePoidevin, R.: Missing elements and missing premises: a combinatorial argument for the reduction of chemistry. *British J. Philos. Sci.* **56**, 117–134 (2005)
- Lloyd Morgan, C.: *Emergent Evolution*. Williams and Norgate, London (1923)
- Lombardi, O., Castagnino, M.: A modal-Hamiltonian interpretation of quantum mechanics. *Stud. Hist. Philos. Mod. Phys.* **39**, 380–443 (2008)
- Lombardi, O., Castagnino, M.: Matters are not so clear on the physical side. *Found. Chem.* **12**, 159–166 (2010)
- Lombardi, O., Castagnino, M., Ardenghi, J.S.: The modal-Hamiltonian interpretation and the Galilean covariance of quantum mechanics. *Stud. Hist. Philos. Mod. Phys.* **41**, 93–103 (2010)
- Lombardi, O., Dieks, D.: Modal interpretations of quantum mechanics. In: Zalta, E.N. (ed.) *Stanford Encyclopedia of Philosophy* (Winter 2012 Edition). <http://plato.stanford.edu/archives/win2012/entries/qm-modal/> (2012)
- Lombardi, O., Labarca, M.: The ontological autonomy of the chemical world. *Found. Chem.* **7**, 125–148 (2005)
- Lombardi, O., Labarca, M.: The ontological autonomy of the chemical world: a response to Needham. *Found. Chem.* **8**, 81–92 (2006)
- Nagel, E.: *The Structure of Science: Problems in the Logic of Scientific Explanation*. Routledge and Kegan Paul, London (1961)
- Needham, P.: Ontological reduction: a comment on Lombardi and Labarca. *Found. Chem.* **8**, 73–80 (2006)
- Needham, P.: Nagel's analysis of reduction: comments in defense as well as critique. *Stud. Hist. Philos. Mod. Phys.* **41**, 163–170 (2010)
- Philström, S.: The re-emergence of the emergence debate. *Principia* **6**, 133–181 (2002)
- Primas, H.: *Chemistry, Quantum Mechanics and Reductionism*. Springer, Berlin (1981)
- Putnam, H.: *Reason, Truth and History*. Cambridge University Press, Cambridge (1981)
- Ruthenberg, K.: Paneth, Kant, and the philosophy of chemistry. *Found. Chem.* **11**, 79–91 (2009)
- Ruthenberg, K.: Das Kant'sche Echo in Paneths Philosophie der Chemie. *Kant-Studien* **101**, 465–479 (2010)
- Schaffer, J.: Truth and fundamentality: on Merricks's truth and ontology. *Philos. Books* **49**, 302–316 (2008)
- Strevens, M.: *Depth: An Account of Scientific Explanation*. Harvard University Press, Cambridge, MA (2008)
- Torretti, R.: Scientific realism and scientific practice. In: Agazzi, E., Pauri, M. (eds.) *The Reality of the Unobservable: Observability, Unobservability and their Impact on the Issue of Scientific Realism*. Kluwer, Dordrecht (2000)
- Wimsatt, W.C.: *Re-engineering Philosophy for Limited Beings: Piecewise Approximations To Reality*. Harvard University Press, Cambridge, MA (2007)
- Wolley, R.G.: Quantum theory and molecular structure. *Adv. Phys.* **25**, 27–52 (1976)
- Wolley, R.G.: Must a molecule have a shape? *J. Am. Chem. Soc.* **100**, 1073–1078 (1978)
- Wolley, R.G.: Is there a quantum definition of a molecule? *J. Math. Chem.* **23**, 3–12 (1998)