

Chapter 6

The Inadequacy of Husserlian Formal Mereology for the Regional Ontology of Chemical Wholes

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1. Introduction

In his book, *History as a Science and the System of the Sciences*, Thomas Seebohm articulates the view that history can serve to mediate between the sciences of explanation and the sciences of interpretation, that is, between the natural sciences and the human sciences. Among other things, Seebohm analyzes history from a phenomenological perspective to reveal the material foundations of the historical human sciences in the lifeworld.¹ As a preliminary to his analyses, Seebohm examines the formal and material presuppositions of phenomenological epistemology, as well as the emergence of the human sciences and the traditional distinctions and divisions that are made between the natural and the human sciences.

In his examination of the formal methodological presuppositions of phenomenological epistemology, Seebohm begins by outlining the history of the development of the human sciences and by considering the dominance of psychologism in the late nineteenth and early twentieth centuries. One of the paradoxes of psychologism is that the epistemology of the formal sciences, that is, of the sciences concerned with ideal objects, would have to become a branch of empirical science. As Seebohm points out, naturalistic psychologism chooses to live with this paradox. Edmund Husserl, on the other hand, rejects this psychologistic approach, since it would entail that mathematics should become a branch of empirical psychology. Instead, Husserl chooses to apply phenomenological descriptions immediately to epistemology. In fact, the second volume of the *Logical Investigations* directly concerns the application of phenomenological descriptions to epistemology. As Seebohm notes, Husserl seeks to demonstrate that “the assumption that phenomenology can be applied in epistemological investigation about the formal sciences and, in general, to ideal objects implies that phenomenology cannot be understood as descriptive psychology” (2015, 14). The relevance of Husserl’s task for Seebohm’s thesis is that Husserl shows that “phenomenology is in this phase of its development the method not only of epistemology, but also of all other disciplines of philosophy” (14). Thus, just as Husserl’s phenomenological epistemology reveals the foundations of the formal sciences within eidetic structures, Seebohm seeks to show that a reflective phenomenological attitude with respect to the historical sciences will reveal their material foundations in the lifeworld.

In his discussion of Husserl’s application of phenomenology to the epistemology of the formal sciences, Seebohm devotes a section of his book to Husserl’s theory of parts and wholes, that is, to mereology, as it is developed in the second volume of the *Logical Investigations* and later in *Experience and Judgment*.

¹ This paper is dedicated to the memory of Professor Lester Embree, who was my respected colleague of many years and whose advice and support were always generous and invaluable to the progress of my work.

Understood as a general theory of parts and wholes, mereology has a long history that can be traced back to the early days of philosophy. As a formal theory of the part-whole relation—or rather, as a theory of the relations of part to whole and of part to part within a whole—it is relative recent and came to us mainly through the writings of Edmund Husserl and Stanisław Leśniewski. [Husserl’s work was] part of a larger project aimed at the development of a general framework for formal ontology . . . [and it] finds its fullest formulation in the [second volume] of his *Logical Investigations*. (Gruszczyński and Varzi 2015, 409–410)

For Husserl, ontology is to be understood in the old sense of a theory of being and “its task is to lay bare the formal structure of what there is *no matter what it is* . . . For instance, it would pertain to the task of formal ontology to assert that every entity, no matter what it is, is governed by certain laws concerning identity, such as reflexivity, symmetry, or transitivity” (410). Identity, reflexivity, and transitivity are formal relations since they may be said to apply to anything that might exist, and Husserl believed that the part-whole relation is also formal in this sense. “Parthood seems to apply to entities as different as material bodies (the handle is part of the mug), events (the first act is part of the play), geometrical entities (the point is part of the line), etc. Even abstract entities such as sets, appear to be amenable to mereological treatment” (411). Thus, Husserl believed that “a purely formal theory of wholes and parts was possible” (Simons 1982, 114) and would serve as the foundation of the mereology of regional ontologies.

In fact, Seeböhm devotes a section to discussing Husserl’s formal mereology precisely because he understands that a reflective analysis of the foundations of the historical sciences requires a reflective analysis of the objects of the historical sciences, that is, of concrete organic wholes (i.e., social groups) and of their parts. Thus, Seeböhm is first concerned with discussing Husserl’s mereological ontology of the formal sciences and then with examining whether this extensional mereology suffices to properly describe the relations between the organic wholes and their parts that form the objects of the historical sciences. Seeböhm concludes that Husserl’s mereological ontology needs to be altered with regard to the historical sciences because the relations between organic wholes and their parts are not the kinds of summative relations that exist between, for example, mugs and their parts or sets and their parts. Seeböhm’s conclusion is relevant for the issue of the reducibility of organic wholes such as social groups to their parts and for the issue of the reducibility of the historical sciences to the lower-order sciences, that is, to the sciences concerned with lower-order ontologies.

In this paper, I propose to extend Seeböhm’s conclusion to the ontology of chemical wholes as objects of quantum chemistry and to argue that Husserl’s formal mereology is descriptively inadequate for this regional ontology as well. This may seem surprising at first, since the objects studied by quantum chemists are not organic wholes. However, my discussion of atoms and molecules as they are understood in quantum chemistry will show that Husserl’s classical summative and extensional mereology does not accurately capture the relations between chemical wholes and their parts.

I will begin by examining the principles of Husserlian mereology for formal ontology, then focus on Seeböhm’s critique of the applicability of Husserlian mereology to the higher-order regional ontologies of social groups, and I will conclude by arguing that this same critique can be extended to the lower-order regional ontology of chemical wholes and parts. To support my arguments, I will discuss concrete examples from the field of quantum chemistry, albeit in a non-technical manner, to show that the summative extensional mereology developed in the *Logical*

Investigation and Experience and Judgment cannot successfully capture the distinctive relations that exist between molecules and their atomic parts. Again, this conclusion is relevant for the question of the reducibility of chemical wholes to their parts and of the reduction of chemistry to physics, issues that have been of central importance within the philosophy of chemistry for the past several decades.

2. The Principles of Husserlian Mereology for Formal Ontology

Husserl devotes a generous part of the second volume of the *Logical Investigations* and, later, of *Experience and Judgment* to the theory of wholes and parts because he considers mereology as fundamental to the phenomenology of the formal sciences. This is because he understands pure logical grammar as “the theory of apophantic forms of complex independent unified wholes of meaning, *Bedeutungskomplexionen*” (Seebohm 2015, 16). Seebohm points out that, certainly, the formal ontological theory of wholes and parts that is developed in the *Logical Investigations* suffices for the analysis of apophantic forms and of “the hyletic correlates of passive synthesis in primordial sensual experience,” (19) what he refers to as first-order wholes. In the *Logical Investigations*, Husserl concludes that the formal ontology of parts and wholes is analogous to that of units and manifolds so that, just as manifolds are additive collections of units, wholes are analyzed as additive collections of parts (see Simons 1982).

For our discussion, it is important to note that one significant aspect of the Husserlian theory of parts and wholes is his extensive discussion of the notions of dependent parts (moments) and independent parts (pieces).

Each part that is independent relatively to a whole W we call a Piece (Portion), each part that is non-independent relatively to W we call a Moment (an abstract part) of this same whole W . It makes no difference here whether the whole itself, considered absolutely, or in relation to a higher whole, is independent or not. Abstract parts can in their turn have pieces, and pieces in their turn abstract parts. (Husserl 1970, §17, 29)

This aspect of Husserl’s theory is crucial for our discussion because, to answer the question of the reduction of a higher-order ontology to a lower-order ontology, one must examine whether the parts of the wholes that constitute the objects at the higher level are pieces of the whole (in which case reduction is materially possible) or moments of the whole (in which case reduction is not materially possible). This is the case because, although pieces of wholes can exist independently of the whole of which they are independent parts, moments of wholes cannot exist independently of the whole of which they are dependent parts. One possible example of this distinction is given by Peter Simons: “The board which makes up the top of the table is a piece of the table [while] the surface of the table, or its particular individual color-aspect, are moments of it” (1982, 115). Husserl believes that this distinction can be extended from the psychological sphere to objects in general, which is why it becomes a general component of his formal ontology. Husserl also specifies that he is using the term “part” in a wide sense that includes not only detachable pieces of wholes but also “anything that is a constituent of it, apart from relational characteristics [including] so-called accidents and also boundaries” (120).

Husserl distinguishes three different sorts of wholes and this distinction is also important in our consideration of reductionism. The first sort is a whole considered in the narrow sense or

what Barry Smith calls a “narrow” whole (Smith and Mulligan 1982, 121). This is one in which entities have come together by virtue of the kinds of entities that they are, without anything else joining them together apart from a “unifying moment,” which is itself not another entity.² Are the entities that come together to form “narrow” wholes to be considered pieces or moments of the whole? From a formal perspective, the existence of such entities is independent of the whole because their existence as the kinds of entities they are is not dependent upon their existence within the whole. Instead, it is their intrinsic nature as certain sorts of individuals that necessarily binds them together to form the whole, which is extrinsically unified. So, the answer to the question above would have to be that the parts of “narrow” wholes are to be considered as pieces of the whole, rather than as moments (Husserl 1970, §22–24, 37–40).

The second sort is a whole considered in the “wide” sense or what Smith calls a “wide” whole, which can be regarded as a single thing, regardless of how scattered its parts are or how tightly or loosely connected they are. This allows the inclusion both of unities and pluralities, since “any plurality may be taken together as something unitary, thereby founding a new higher unity, whose unity is, however, extrinsic to it, in the collective act” (Simons 1982, 122). In this case, it is obvious that the parts of a wider whole are pieces, that is, independent parts of the unity or plurality of which they are parts. In fact, what is regarded as a “wide” whole seems to be a factor of some decision to trace the boundaries of the whole at one place rather than another, whether the decision is arbitrarily made or not. As Simons points out, one can “allow as individuals anything which can possess a (singular) proper name. This will include arbitrary *collectiva*. This liberality is reflected in extensional mereologies by allowing that arbitrary sums of individuals are themselves individuals. The reason for this is . . . that it is not clear in advance where to draw the line between things which are wholes in this widest and weakest sense, and those which have some more intrinsic unity”(122).

The third and more interesting sort of whole is a “pregnant” whole, which Husserl defines as “a range of contents which are all covered by a *single foundation* without the help of further contents. The contents of such a range we call its parts. Talk of the *singleness of the foundation implies that every content is foundationally connected whether directly or indirectly, with every content . . . without external assistance*” (Husserl 1970, §21, 34). Unlike mere sums or aggregates (“narrow” and “wide” wholes) whose unity is extrinsic, the unity of pregnant wholes is intrinsic but the parts of such wholes are still to be considered as pieces. It is the relations between those parts that are, for Husserl, to be considered as moments. Such relations can be either ideal or real relations. Ideal relations are such that they do not alter their terms in any way nor do they bring their terms into any real connection to each other. For example, if A is the same height as B, both A and B remain unaffected by their being in this relation to each other. Ideal relations are often equivalence relations and are, thus, reflexive, which is why ideal relations cannot “engender genuine foundation relations” (Simons 1982, 154).³ Real relations, on the other hand, are such that they alter or affect their terms in some way. For example, if magnet A attracts metal B, both A and B are affected by this magnetic attraction. Thus, the most obvious example of a real relation is one

² Husserl is here trying to avoid the regress, discussed by F. H. Bradley in *Appearance and Reality*, that is generated when one requires a third entity to join the first two so that: “if A and B are bound together by U, then A and U must be bound together by U¹, and so on *ad infinitum*” (Simons 1982, 121).

³ Simons regards the whole notion of a relation that holds between a thing and itself as suspect, especially in cases such as identity which can only hold between a thing and itself. Thus, Simons considers reflexive relative terms to be “ontologically sterile” since “nothing intrinsically relational is represented” by such terms.

that involves a causal link (154). Real relations are clearly not reflexive and can serve to engender genuine foundation relations. When they do so, such relations can be described as moments of the whole that unite the parts (154). Some foundation relations are symmetric (*two-sided* or *mutual* foundations), such as the foundation relation between color and extension which are mutually founding. Other foundation relations are asymmetric (*one-sided*), such as the foundation relation between a lake and the dry land upon which the lake is one-sidedly founded.⁴

These are the three types of wholes discussed by Husserl within the context of formal ontology. However, if ontology is to be understood in the old sense of a theory of being whose “task is to lay bare the formal structure of what there is *no matter what it is*” (Gruszczyński and Varzi 2015, 410) and if mereology reveals the fundamental principles of such formal structure, the question is what constitutes natural wholes and whether the mereology of the *Logical Investigations* and *Experience and Judgment* suffices to adequately describe the whole-parts relations of the categorial objects within the regional ontological spheres of the material world. When we are considering natural wholes or systems, it is the causal integrity of such systems that binds them together (Simons 1982, 150), and we may ask whether the parts of such wholes are to be considered as independent parts (pieces) or as dependent parts (moments). Husserl regards objects in the world as being naturally organized in many different ways, so that the distinction between lower-order and higher-order objects is not absolute. From one point of view, an object may be “a natural unit, from another it may coincide with an aggregate of differently organized units, or again be a moment of a greater whole” (150). However, the relativity described here “is not the mere imposition of a conceptual scheme on an otherwise unstructured world, but cuts along natural seams in reality.” It would follow from this that, at least for Husserl, the parts of even higher-order wholes are to be considered pieces rather than moments. Yet, both Seeböhm’s discussion of organic wholes and my discussion of chemical wholes will call this into question, since Seeböhm challenges the idea that the parts of organic wholes are independent parts, while I will challenge the idea that the parts of chemical wholes are independent parts.

As Rafał Gruszczyński and Achille Varzi have recently pointed out, “the general applicability of the part-whole relation is controversial . . . [David] Lewis himself famously argued that entities such as universals *cannot* be structured mereologically, short of unintelligibility” (2015, 409–10). To illustrate this point Lewis, interestingly, uses an example taken from chemistry: “Each methane molecule has not one hydrogen atom but four. So, if the structural universal methane is to be an isomorph of the molecules that are its instances, it must have the universal hydrogen as a part not just once, but four times over. . . . But what can it mean for something to have a part four times over?” (Lewis 1986, 34). This difficulty concerns the bounds of mereology as formal ontology, but there are also other difficulties that concern its content. “Consider, for instance, the question of whether there are mereological *atoms* (i.e., entities with no proper parts), or of whether everything is ultimately *composed* of atoms. Clearly any answer to such questions would amount to a substantive metaphysical thesis that goes beyond a ‘pure theory of objects as such.’” (Gruszczyński and Varzi 2015, 412). In the words of Gruszczyński and Varzi, “taken together, then, these two sorts of difficulty represent a serious challenge to the idea that mereology can form a genuine piece of formal ontology” (413).

This paper will not be concerned with this second difficulty but will focus only on the first, that is, does Husserl’s conception of the parts-whole relation as formal ontology extend to all regional ontologies as he believed? The paper will argue that the answer to this question is negative

⁴ The terms “narrow” whole and “wide” whole are coined by Barry Smith, while “pregnant” whole is Husserl’s own term.

to the extent that the formal principles of Husserlian mereology do not, in fact, extend either to the higher-order ontologies of organic wholes discussed by Seebohm or to the lower-order regional ontology of chemical wholes as these are conceived in quantum chemistry. I will first examine Seebohm's arguments regarding organic wholes, then I will examine chemical wholes as they are conceptualized but also manipulated and transformed by chemists. Here, I will show that, for the purposes of quantum chemical calculations, chemists must conceptualize subatomic "entities" in ways that violate the principles of standard mereology such as transitivity, unrestricted composition, and uniqueness of composition. For example, Kit Fine discusses a fundamental principle of standard mereology, with which Husserl would agree, according to which "the same parts cannot, through different methods of composition, yield different wholes" (1994, 138). That is, according to this principle, the same composition of parts structured differently will yield the same whole, with the same properties. As well, Lewis explains another fundamental principle, that is, although any two or more individuals constitute a mereological sum or fusion, inclusion in such a sum or fusion does not alter the individuals that are included (1986, 25–26). The mereological sum or fusion has no causal effectiveness as such or as separate from the causal effectiveness of its parts.

As we shall see in this essay, however, it is precisely these aspects of classical extensional mereology that render it inadequate for describing the whole-parts relations both of organic wholes but also of chemical structures as understood in quantum chemistry. I now turn to Seebohm's discussion of the whole-parts relations for the higher-order ontologies of organic wholes as it appears in his book *History as a Science and the System of the Sciences*.

3. The Application of Husserlian Mereology to the Higher-Order Regional Ontologies of Organic Wholes

As Seebohm points out, the mereological theory of the *Logical Investigations* and *Experience and Judgment* is a "general ontological theory of wholes and their parts" (2015, 20) that presupposes an abstractive reduction that focuses on first-order wholes with parts that are "held together by unifying foundations" (20), in other words, pregnant wholes. However, there are more complex types of wholes and parts that are referred to in natural language, what Seebohm calls "wholes of a higher order" (19). Among higher-order wholes are included the solar system, organisms of varying degrees of complexity, and social groups and communities. Such wholes are of a higher order precisely because their constituent parts are themselves wholes rather than simple parts. However, Husserl does not offer a formal account of such structures, precisely because he is only concerned with developing a mereology for the formal ontology of pure logical grammar, not with the mereologies of categorial objects of a higher order. Seebohm raises the question of "whether some types of such categorial objects of a higher order can have formal ontological structures that count as the formal structures of the wholes of a higher order" (20). Certainly, as Seebohm points out, Husserl's discussion in the *Logical Investigations* begins in the psychological sphere but is intended to be valid and applicable to all objects, psychological or not, because it appeals only to properly generalizable features.

For Seebohm, then, the question is really "whether such a theory can admit additional categorial structures for wholes with parts [that are not parts of a unifying system of *foundations* but] that are already themselves wholes connected by unifying systems of relations" (20). As he emphasizes, "going beyond *Experience and Judgment* it can be said that the differences between

collections as categorial forms of a higher order are determined by structured systems of relations” (20). In a series of specific comments on this point, Seebohm proposes that the criterion for demarcating “between the unifying systems of parts in wholes of the first order and wholes of higher order is the difference between foundations and relations. Foundations share some of the formal properties of relations, but foundations are ‘relation’ between dependent moments that cannot be given only in the context with other moments and between pieces as relative independent parts of wholes” (21). To clarify this passage, foundations concern parts that can be given independently of the context with other moments. On the other hand, relations as they pertain to the formal ontological theory of categorial structures of higher-order wholes are “relations between independent wholes” (22). In other words, we are not talking here about relations between n -adic predicates that refer to individual objects but about relations between parts that are themselves independent wholes.

There is another distinction that needs to be made, however, when one considers the mereology of higher-order wholes. This is the distinction between inorganic and organic wholes of a higher order, and it is a distinction that is extremely relevant when one reflects upon those wholes that are the objects of the life sciences and of the human and social sciences. Seebohm clarifies that phenomenological epistemology is not concerned with answering the empirical question of whether and of how organic wholes can emerge from inorganic matter. Rather, phenomenological epistemology

is restricted to the analysis of the cognitive attitude of the life sciences and their intentional correlate, the ontological region of organic entities. It includes in addition the analysis of the relations between the categories of the ontological region of organic life and the categories of the ontological region of inorganic matter. Such analyses are, however, able to decide the question of whether the reduction of the life sciences to the hard sciences is an ideal formal ontological possibility and then a material ontological possibility. This will be the case if it can be shown that the ontological region of inorganic matter is the static and genetic foundation of the ontological region of organisms. (242)

Regarding the phenomenological epistemology of the life sciences, Seebohm establishes that it is not enough to simply analyze the formal categorial structures of the formal ontology of the wholes and parts. One must also analyze the formal ontological theory of unit and manifold and establish what the relation is between the theory of wholes and parts and the theory of units and manifold (242–243). “*Either* they are two independent formal ontological theories on the same level of universality *or* one of them belongs to a higher logical level of universality . . . It is obvious that the reduction of organic life to inorganic matter is a priori a formal ontological impossibility if the answer is ‘yes’ to the first horn of the dilemma and ‘no’ to the second. The reduction is, however, an ideal possibility if the answer is ‘no’ to the first and ‘yes’ to the second horn of the dilemma” (243). The question, therefore, really turns on whether organic wholes can be treated like collections and, therefore, analyzed as manifolds, which are additive collections of units. If so, then one can answer yes to the first horn of the dilemma and no to the second.

According to Seebohm, the latter is in fact the case so that reduction is an ideal possibility. He states that

Measuring as counting of units and numbers as units in measuring can be applied to all dependent parts that belong to the genus extension. But this means that all entities under

the formal ontological categories of the whole and the parts can be considered as units and collections of units if the formal ontological differences pertaining to the categories of the theory of the whole and parts are excluded with the aid of a generalizing abstraction determining a realm in which all of them, including the wholes themselves, are mathematical units in collection that can be themselves considered as units, etc. . . . The formal ontological theory of unit and manifolds is, hence, one-sidedly founding for the formal ontological category of the whole and the parts. Manifolds of concrete wholes as well as independent parts can be counted. A reduction of the material ontological structures of organic entities is, hence, an ideal possibility. (243–244)

Lest the reductionist declare victory at this point, Seebohm stresses that a reduction of the material ontological structures of organic entities is “only an *ideal* possibility [and not a material one] because a genetic foundation of B in A requires, beyond A, the additional structures of properties C for B” (244). The additional structures of properties C for B are discovered by carrying out an analysis of the structures of the material regional ontology to which B belongs. Thus, in the case of organic wholes, “the second dimension of the description of phenomena that are necessary for the explication of the material categories of organic life and organisms has to determine the material characteristics of the parts of organic wholes. The independent parts of organic wholes cannot be simultaneously parts of other organic wholes, and they cannot exist independently outside the system of their functions in the organic whole. They will decay if they are separated from the wholes without providing an artificial environment that can substitute for the whole or stop the process of decay” (245).

Seebohm also says something very important about the role that an analysis of environment must play in the phenomenological epistemological analysis of organic wholes.⁵ He states that “the description of the environment of a species and the ecological relation of the species to the environment is not of immediate significance for the simple recognition of the species of an individual organic being or for the development of taxonomies of organic species. It is, however, of significance for experimental research and for the discovery of causal relations between organisms as concrete whole (or their parts) and certain properties or aspects of their environments” (245). Thus, although a description of the environment is not part of the first dimension of the description of organic wholes, it is crucial for the second dimension of the phenomenological description since it pertains to the structures of properties C for B that are discovered through an analysis of the material regional ontology of B. Ultimately, however, the material ontological categories of organic wholes are . . . in the last instance one-sidedly founded in the categorical system of the ontological region of the hard sciences” (248), that is, physics and chemistry. But, this “does not mean that organic life can be *reduced* to the system of the categories of the hard sciences. What is again in question is the factor C that must be added to the founding material ontological region A for the emergence of entities belonging to the material ontological region B” (249).

Accepting Seebohm’s argument that the regional ontologies of organic wholes cannot be materially reduced to the ontologies of inorganic wholes, I wish to address another question in the

⁵ This attention to the relation between organism and environment was emphasized in the late nineteenth century by Louis-Adolphe Bertillon, who coined the term mesology to refer to what he called “*la science des milieux*,” a concept that he later expanded to the field of sociology. The focus on mesology has recently been resurrected by Augustin Berque to, once again, call attention to the importance of milieu in the study of organisms and as part of a proposal for overcoming modernist reductionism. See Berque 2010.

rest of this paper, the question of whether Husserlian mereology can properly describe the whole-parts relations in the system of categories of the hard science of chemistry. The answer to this question is pertinent to the question of whether or not the reduction of chemistry to physics is possible. If it is not possible to reduce chemistry to physics, then this would establish that each regional ontology requires formal ontological theories on the same level of universality.

4. The Application of Summative Extensional Mereology to the Lower-Order Regional Ontology of Chemical Wholes

One of the fundamental questions in contemporary philosophy of chemistry is that of the autonomy of chemistry as a science, an issue that is directly related to the reduction of chemistry to physics. In fact, the issue of the reduction of chemistry to physics has been called “one of the main areas in which philosophical interest in chemistry should be directed” (Scerri and McIntyre 1997, 214). Since the ontological dependency of chemical properties on fundamental physical states is not at issue, the sort of reduction meant here is epistemic, rather than ontological, and the question is “whether our current description of chemistry can be reduced to our most fundamental current description of physics, namely quantum mechanics—and with its explanatory consequences” (215). To put this differently, the issue here is not whether the reduction is an ideal possibility since, as Seeböhm states, “all entities under the formal ontological categories of the whole and the parts can be considered as units and collections of units” (2015, 243). Thus, a reduction of the material ontological structures of chemical entities is an ideal possibility. However, as with organic entities, the issue is whether such a reduction is a material possibility and this question is what the rest of this essay will address, focusing on the mereology of whole-parts relations for chemical structures.

Despite the received view among many philosophers of science (see, e.g., Hilary Putnam and Paul Oppenheim 1958), quantum chemists and philosophers of chemistry have serious doubts about whether the ontological dependency of chemical states upon physical states undermines the epistemological and explanatory autonomy of chemistry as a science. The hope for such reduction

seems to have been abandoned and . . . all that remains is the possibility for approximate reduction. However, criteria for approximate reduction have not been put forward and the notion remains vague . . . the calculation of the ground state energies of atoms has been achieved to a remarkable degree of accuracy and similarly calculations on small or even medium-sized molecules have given encouraging results. However, whether one can draw the conclusion that chemistry has been reduced rather depends on one’s criteria of reduction. If we are to define approximate reduction as has been suggested . . . then it must be concluded that *chemistry is not even approximately reduced to quantum mechanics*. (Scerri 1994, 168)

As far back as 1939, Linus Pauling claimed that “[a] small part of the body of contributions of quantum mechanics to chemistry has been purely quantum mechanical in character: only in a few cases, for example, have results of direct chemical interest been obtained by the accurate solution of the Schrödinger wave equation . . . The principal contribution of quantum mechanics to chemistry has been the suggestion of new ideas, such as the resonance of molecules among several electronic structures with an accompanying increase in stability” (1960, vii). However, regarding

the chemical concepts of valence and bonding, there is a great deal of doubt about the possibility of reduction.

As well, the conceptual reduction of notions such as composition and molecular structure is also in serious doubt, in part because these concepts do not represent ontological features of the world. When it comes to such concepts, reduction is just not possible even in principle (i.e., it is not even an ideal possibility) “due to the very nature of the concepts themselves. That is, the concepts of composition, bonding, and molecular structure cannot be expressed except at the chemical level . . . we can calculate certain molecular properties, but we cannot point to something in the mathematical expressions which can be identified with bonding. The concept of chemical bonding seems to be lost in the process of reduction.” (Scerri and McIntyre 1997, 218–219). There is also doubt regarding the amount of insight that quantum theory can provide for understanding such chemical concepts. “Many calculations have been extremely sophisticated, designed by some of the foremost researchers in this field to extract a maximum of insight from quantum theory. For simple molecules, outstanding agreement between calculated and measured data has been obtained. Yet, the concept of a chemical bond could not be found anywhere in these calculations. We calculate bonding energies without even knowing what a bond is” (Primas 2013, 5).

Robert Mulliken, who was actively involved in the development of quantum chemistry, claims that “attempts to regard a molecule as consisting of specific atomic or ionic units held together by discrete numbers of bonding electrons or electron-pairs are considered as more or less meaningless, except as approximations in special cases, or as methods of calculation” (1932, 55). For Mulliken, the atom does not exist in a molecule because each orbit is delocalized over all the nuclei and can contribute a stabilizing or destabilizing energy contribution to the total energy of the molecule (see Banchetti-Robino and Llored 2016). “A molecule is here regarded as a set of nuclei, around each of which is grouped an electron configuration closely similar to that of a free atom in an external field, except that the outer parts of the electron configurations surrounding each nucleus usually belong, in part, jointly to two or more *nuclei*” (Mulliken 1932, 55). Thus, there is a key semantic shift here from the concept of molecular *orbit* to that of molecular *orbital*, which takes its meaning from Max Born’s probabilistic interpretation according to which the square of a molecular orbital corresponds to the probability density of finding a particular electron within the molecular space. Molecular orbitals have a wave function that contains one electron and that can be delocalized either over all the nuclei or simply over a set of particular nuclei. Thus, the complete electronic wave function is restricted to one of several types that depend upon the symmetry of the nuclear skeleton.

Besides the concepts of molecule and chemical bond, at least two other chemical concepts resist reduction. The first of these is the concept of molecular shape, which cannot be reduced in principle because it is a “mere” concept, albeit one with strong heuristic power. Molecular “shape is metaphorical in virtue of being only chemical . . . Molecules can lack an orientation in three-dimensional space, and a particular shape is dependent on the way that the molecule is picked out in measurement. . . . Whether we need to employ the fixed nucleus picture, separate nuclear and electronic ‘clouds’, or interacting clouds depends on the particular molecule chosen for study, the experimental technique we employ and the questions we ask. As it turns out, there are many different representations of the same property.” (Ramsey 1994, 234–248). The second concept that resists reduction is that of chemical composition, a concept related to that of bonding and molecular structure. Chemical composition cannot be reduced because “what is physical about a chemical system are its components rather than the system itself [*qua* chemical system] which possesses emergent (though explainable) properties in addition to physical properties” (Bunge 1982, 210).

As Jeffry Ramsey states, “the fundamental idea that molecules are constructed additively of atoms, which retain their essential identity within the molecule, is brought into question” (1994, 233). This irreducibility of chemical systems to their physical components is best understood by examining the mereology of systems such as molecules, for example. As Rom Harré and Jean-Pierre Llored explain, “constituent atoms of molecules are not parts of those molecules when we look at the total entity in the light of molecular orbitals. Unlike chair parts which preserve their material properties whether in the chair or on the bench” (2011, 73). It is also questionable whether molecules have definitive physical component parts in such a way that the concept of molecule could be reduced to the concept of physical components without remainder. According to chemist and philosopher of chemistry Joseph Earley, for example, “Na and Cl ions are not parts of salt lattices after that salt has been dissolved. Being in the solution determines that the solution will afford salt as a mass substance on the carrying out of certain operations on sea water, and not something else. Thus, they are at best potential material parts of salt” (2008b, 71).

Harré introduces the concept of “affordance” to capture this idea so that, although there is not salt as such in the sea, the sea “affords” salt under certain conditions and via certain procedures that are carried out on sea water. Philosophers of chemistry argue that, in the same way, there are no atoms in molecules, although “molecules afford atoms in the context of certain manipulations as studies of molecular reactivity have shown us. The material content of a molecule can only by a fusion of atomic potentials, not of atoms [and] affordances are not simple conditional properties . . . they incorporate the procedure or method used to display their empirical manifestations . . . the parts of chemical wholes like molecules and atoms are affordances, not themselves concrete entities” (Harré and Llored 2011, 69). This implies that the concept of molecules cannot, therefore, be reduced to the concept of constituent atoms, because these parts of the whole are not concrete entities as such and, in some cases, may be “ephemeral” individuals. For example, “the swiftly composing and decomposing hydrogen-oxygen structures of which real water is really composed are ephemeral individuals. Water is made up of these beings. As such they are [ontological] constituents of a certain whole” (73). But water, as a chemical composition, cannot simply be reduced to these ephemeral parts or occurrences.

As Early states, “most philosophers have yet to recognize that, when components enter into chemical combination, those components do not, in general, maintain the same identity that they would have absent that combination” (2003, 89). Simple examples that illustrate this point are H₂O and silver chloride. While the property of being H₂O or of being silver chloride “supervenes on the features of the constituent atoms, the features of the atoms on which it supervenes includes features that the atoms have only by virtue of being parts of that compound. The atomic interrelations that give rise to the compound would not obtain if the atoms were parts of a different molecular type” (Francescotti 2007, 58). Molecules themselves are defined in accordance with chemical reaction networks and not vice versa.⁶ Since the emergent properties of the whole affect the properties of the constituent parts so that these parts are different than they would otherwise be, the emergent property not only displays novel causal powers, but it very specifically displays downward causal influence. In fact, the causal influence between parts and whole in chemical systems is not asymmetrical. That is, it is neither wholly upwardly directed nor wholly downwardly directed but is, instead, symmetrical in that there is both upward and downward causal influence. As Harré and Llored suggest, this symmetrical causal influence between chemical whole and parts is best accounted for through the notion of relationality, because the relations of the parts to one another, as well as the relations of their properties to one another, and the relation of the

⁶ I am grateful to Jean-Pierre Llored for suggesting this useful example.

whole system to its environment are what account for the emergent properties of the whole and its parts. An analysis of relationality in this context, however, requires the development of an adequate mereology that accounts for the fact that, once individuals have entered combinations of interesting sorts, they are no longer the same individuals that existed prior to the combinations.

The classical extensional and summative mereology advocated by Husserl for formal ontology is not adequate for this sort of account, because, in its theory of wholes and parts, classical mereology does not consider the relationality of the parts nor does it consider the environment in which parts and wholes exist as something to be factored into the analysis of parts and wholes. In fact, “the standard mereology for chemical compounds involves the presupposition that just as molecules are ultimate constituents or parts of material things, so atom-cores are parts or constituents of molecules” (Harré and Llored 2013, 133). According to Harré and Llored, the conceptualization of electrons as entity-like beings involves two mereological fallacies. The first of these is the fallacy of applying to a part a predicate designed to ascribe an attribute to the whole. “A holistic predicate is not necessarily a part predicate, the notion of use is crucial because . . . predications are context-sensitive” (133). The second mereological fallacy involved in this sort of predication is that of “inferring that substantive products of an analytical procedure are parts of the substance on which the procedure was performed” (134).

Given the discussion above, we note that chemical wholes violate the classical principle discussed by Lewis, which requires that a mereological sum or fusion has no causal effectiveness apart from the causal effectiveness of the parts. As well, quantum chemists consider the classical mereological principle of uniqueness of composition to be “unintuitive and inadequate to those rules for chemical parts-whole reasoning that are required to accommodate the role of chemical entities in structures, such as atoms in ‘polyatomic’ ions. [Quantum chemists] are likely to question the relevance of transitive mereology whenever the whole molecule and the parts are co-dependent and relative to a specific environment or action” (Llored 2014, 159). Regarding the classical principle of standard mereology discussed by Fine, that different methods of composition do not yield different wholes, we must point out that Fine himself admits that mereology must recognize relationships, as well as other sorts of parts, in a way that does not conflate relations between parts with properties of parts. This is important, for example, in order to accommodate the mereology of structured wholes, such as chemical molecules, since these “generally have causal efficacy in virtue of their ‘connectivity’—in addition to the causal powers of their constituent atoms, levorotatory amino acids are nutritious [but] the corresponding dextrorotatory amino acids are poisonous—although both sorts of molecules have exactly the same component parts” (Earley 2008a, 9). However, in addition to optical activity and chirality, we find that the structural arrangement of the parts of chemical wholes also contributes to the properties of the whole. Thus, different structural arrangements of the same parts will yield different chemical wholes. This characteristic of molecules, which is known as structural isomerism, was first discovered in 1827 by Friedrich Woehler, when he prepared cyanic acid and noted that although its elemental composition was identical to fulminic acid, its properties were quite different. This find challenged the prevailing chemical understanding of the time, which embraced the classical mereological principle that chemical compounds could be different only when they had different elemental compositions.

It is, therefore, clear that the properties of chemical wholes are not merely a function of the properties of their parts. As well, once we examine closely the way quantum chemists conceive of molecules, atoms, and subatomic “parts,” we notice that they think of these in terms of chemical relations and *relata* at different levels of organization that co-define each other. What is needed

then is a non-standard mereology that captures this co-defining and co-constituting feature of chemical whole-parts relations. To the extent that parts and whole co-constitute each other and to the extent that parts and whole are co-dependent, the parts must be considered as moments of the whole rather than as pieces.

But there is more. Chemical mereology must also capture the way the environment (or milieu) of the chemical experiment contributes to constituting chemical whole-parts relations. Such a mereology challenges the assumptions of classical summative mereology since, in quantum chemistry, it is clear that the parts do not define the whole but, rather, the parts and the whole co-define each other in the context of chemical activity within a given environmental context. Yet, for such a mereology to succeed, our understanding of chemical parts and wholes as independent concepts must itself be altered and, to do this, we turn to the way in which quantum chemists involve different levels of organization in their daily experimental practice, in their syntheses and analyses of chemical structures, and in their calculations.

Developments in quantum chemistry have shown that the constituents of atoms and molecules should not be described as entity-like or as having clear boundaries in the way in which atoms or molecules were traditionally conceived as bounded and entity-like (e.g., ball and stick models). In fact, as Harré and Llored emphasize, “it is a mistake to treat electrons as constituents of anything” (2013, 159). Thus, the classical summative mereology advocated by Husserl in the context of formal ontology is not only inadequate for describing whole-parts relations for organic wholes as Seebohm argues, it is also inadequate for describing whole-parts relations for the regional ontology of quantum chemistry, which deals with “such structured entities as molecules, where the whole is not merely the sum of its parts” (Sukumar 2013, 303).

At best, then, “the part-whole relation . . . may behave according to such principles as [discussed by Husserl]. But there is a growing consensus that this is the best one can say, and that mereology is best understood as a theory—or a plurality of theories—whose fundamental truths do not reflect the properties of the part-whole relation itself but the nature of the entities to which it applies” (Seebohm 2015, 16). If this is the case then, the analysis of the part-whole relation with regard to both the higher-order ontologies of organic wholes and the lower-order ontology of chemical wholes serves to illustrate the inapplicability of formal mereology to all regional ontologies, thus calling into question Husserl’s belief that mereology is an element of formal ontology. As well, these discussions draw attention to the need for developing non-summative and non-extensional mereologies that are tailored to describe whole-parts relations in the various regional ontologies studied by the natural, human, and social sciences.

Reference List

- Aimable, A., R. Brayner, J. P. Llored, S. Sarrade, and M. Rozé. 2013. Chemistry and interfaces. In *Philosophy of Chemistry: Practices, Methodologies and Concepts*, ed. J. P. Llored, 172–201. Newcastle Upon Tyne: Cambridge Scholars Publishing.
- Bader, R. F. W., and C. F. Matta. 2013. Atoms in molecules as non-overlapping, bounded, space-filling, open quantum systems. *Foundations of Chemistry* 15(3): 253–276.
- Banchetti-Robino, M. P., and J. P. Llored. 2016. Reality without reification: Philosophy of chemistry’s contribution to philosophy of mind. In *Essays in the philosophy of chemistry*, ed. Eric Scerri and Grant Fisher, 83–110. Oxford: Oxford University Press.

- Berque, A. 2010. *Milieu et identité humaine. Notes pour le dépassement de la modernité*. Paris: Donner lieu.
- Bunge, M. 1982. Is chemistry a branch of physics? *Journal for General Philosophy of Science* 13: 209–223.
- Earley, J. E. 2008a. How philosophy of mind needs philosophy of chemistry. *HYLE - International Journal for the Philosophy of Chemistry* 14: 1–26.
- Earley, J. E. 2008b. How chemistry shifts horizons: Element, substance and the essential. *Foundations of Chemistry* 11: 65–77.
- Earley, J. E. 2005. Why there is no salt in the sea. *Foundations of Chemistry* 7: 85–102.
- Earley, J. E. 2003. Varieties of properties: An alternative distinction among qualities. *Annals of the New York Academy of Science* 988: 80–89.
- Fine, K. 1994. Compounds and aggregates. *Noûs* 28: 137–158.
- Francescotti, R. M. 2007. Emergence. *Erkenntnis* 67: 47–63.
- Gruszczyński, R. and A. Varzi. 2015. Mereology then and now. *Logic and Logical Philosophy* 24: 409–427.
- Harré, R. and J. -P. Llored. 2013. Molecules and mereology. *Foundations of Chemistry* 15: 127–144.
- Harré, R., and J. -P. Llored. 2011. Mereologies as the grammars of chemical discourses. *Foundations of Chemistry* 13: 63–76.
- Hettema, H. 2013. Austere quantum mechanics as a reductive basis for chemistry. *Foundations of Chemistry* 15: 311–326.
- Husserl, Edmund. 1970. *Logical investigations*, 2 vols. Trans. J. N. Findlay. New York: Routledge & Kegan Paul.
- Lewis, D. 1986. Against structural universals. *Australasian Journal of Philosophy* 64: 25–46.
- Llored, J. -P. 2014. Whole-parts strategies in quantum chemistry: Some philosophical and mereological lessons. *HYLE - International Journal for the Philosophy of Chemistry* 20: 141–163.
- Mulliken, R. S. 1932. Electronic structures of polyatomic molecules and valence I. *Physical Review* 40: 55–62.
- Pauling, L. 1960. *The nature of the chemical bond and the structure of molecules and crystals*, 3rd edition. Ithaca, NY: Cornell University Press.
- Popelier, Paul. 2000. *Atoms in molecules*. London: Prentice Hall.
- Primas, H. 2013. *Chemistry, quantum mechanics and reductionism: Perspectives in theoretical chemistry*. Berlin: Springer-Verlag.
- Putnam, H., and P. Oppenheim. 1958. Unity of science as a working hypothesis. In *Minnesota Studies in the Philosophy of Science*, Volume II, ed. H. Feigl, M. Scriven, and G. Maxwell. Minneapolis: University of Minnesota Press.
- Ramsey, J. 1997. Molecular shape, reduction, explanation and approximate concept. *Synthese* 111: 233–251.
- Scerri, E. R. 1994. Has chemistry been at least approximately reduced to quantum mechanics? *PSA: Proceedings of the Biennial Meeting of the Philosophy of Science Association* 1994: 160–170.
- Scerri, E. R., and L. McIntyre. 1997. The case for the philosophy of chemistry. *Synthese* 111: 213–232.
- Schummer, J. 1998. The chemical of chemistry I: A conceptual approach. *Hyle* 4: 129–162.

- Seebohm, T. M. 2015. *History as a science and the system of the sciences: Phenomenological investigations*. New York: Springer.
- Simons, P. M. 1982. Three essays in formal ontology. In *Parts and moments: Studies in logic and formal ontology*, ed. Barry Smith, Analytica Series, 111–260. Munich: Philosophia Verlag.
- Smith, B., and K. Mulligan. 1982. Pieces of a theory. In *Parts and moments: Studies in logic and formal ontology*, ed. Barry Smith, Analytica Series, 15–110. Munich: Philosophia Verlag.
- Sukumar, N. 2013. The atom in a molecule as a mereological construct in chemistry. *Foundations of Chemistry* 15: 303–309.