



NATIONAL AUTONOMOUS UNIVERSITY OF MEXICO
FACULTY OF CHEMISTRY

“A PRAGMATIST APPROACH TO NEW DYNAMIC ONTOLOGIES IN CHEMISTRY”

THESIS

SUBMITTED IN PARTIAL FULFILLMENT
OF THE REQUIREMENTS FOR THE DEGREE OF
CHEMIST

BY
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MEXICO CITY

2021



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«Except for the point, the still point,

There would be no dance

And there's only dance»

T. S. Eliot



1. Introduction



In contemporary chemistry—and in science more broadly—a reductionist view predominates, largely as a consequence of the success of quantum mechanics during the twentieth century. In the philosophy of science, a realist approach also prevails, assuming that science grants us access to a single, unified reality. This means that reality is conceived as one; that physics describes reality in a more fundamental way than other sciences; and that, therefore, the other sciences are subordinate to physics in the sense that whatever happens is “simply physics,” while the theories and concepts produced in other sciences are considered merely useful theoretical tools to deal with the technological impossibility of treating everything strictly as physical systems. But is this true? How could it be conceived otherwise?

At the beginning of this century, a movement emerged within the philosophy of chemistry that has been grounding chemistry in a pragmatist framework—one that allows alternative conceptions of reality through ontological pluralism. It is argued that reality as it is *in itself* is inaccessible, and that we only perceive what is perceptible to us—redundant though that may sound. This is far from trivial, and the aim of this paper is to begin exploring the implications of adopting such perspectives in chemistry.

Long before the twentieth century, chemistry developed theories to describe chemical phenomena. The observations on which these theories are based typically arise from phenomena unique to chemistry, such as synthesis or chemical reactions in general. And although quantum mechanics has represented an advance in a certain sense, chemical theories—where concepts such as “orbital” emerge—remain valid and widely used in practice, even though under a reductionist lens they may be considered nonexistent.

In this century, moreover, the philosopher of chemistry Rom Harré has pointed out the opportunities offered by three new tools within the field: mereological fallacies, hinge propositions, and Gibsonian properties. These three concepts will be defined later, but for now it is important to emphasize that they make sense in the context of relations or interactions among substances. Chemical identity, in fact, is also a concept that is preceded by interactions—in other words, a substance *is* what it is *because of how it behaves*. This too is nontrivial and constitutes one of the main foundations of this work, as it allows us to begin exploring ontologies in which relations define the object, in contrast with corpuscular ontologies in which the relations objects enter into are predetermined by their intrinsic structure. The latter constitutes the current scientific paradigm—one that is now being questioned even within physics itself.

One concept borrowed from physics and adopted in chemical practice is that of *time*. The predominant framework has been Newtonian: time and space as invisible backgrounds in which objects exist and phenomena occur. This conflicts with chemical identity (and reactivity), which is



preceded by interactions and depends on them in order to emerge. Chemical identity depends—fully or in part—on emergent properties, which are properties exhibited by a whole but not by any of its parts in isolation, and which depend on the interactions among those parts. If interactions occur over time, then a minimal amount of time is required for substances to emerge as such. This means that the static concept of matter (“matter is what it is at every moment in time”) can be questioned and redefined toward a more dynamic concept, where chemical identity as an emergent property is a function of time. One consequence of this reflection is that chemistry may adopt dynamic ontologies, in the sense that they can vary as a function of time—allowing us to conceptualize a chemistry more prepared to accommodate novel or unexpected phenomena, especially in experimental setups involving extremely short or long time intervals.

As chemists, we need a philosophy of chemistry. New technological tools allow us to achieve more, but questioning and grounding chemical practice through our own philosophical framework allows the use of these technologies to make sense in a world dominated by a reductionist conception of reality. I have included the word “toward” in the title to signal that my work—like that of other philosophers of chemistry—aims to support future research that will begin to explore the implications of adopting dynamic, time-dependent ontological frameworks.

2. Theoretical Framework



2.1 The Philosophy of Chemistry

"She's a rum 'un is Natur' (...) Natur' is more easier conceived than described"

- Charles Dickens

This research project falls within the philosophy of chemistry, which for some authors is a field whose purpose is to clarify and analyze the foundations on which chemistry relies in order to construct, validate, and give coherence to the concepts and practices through which knowledge is produced (Harré, 2014, p. 77).

The philosophy of chemistry is a relatively recent undertaking (Scerri, 2015, p. 1), and it is interesting to note that philosophers of chemistry form the smallest group among philosophers of science, while chemists form the largest group among scientists (Schummer, 1998, p. 129).

The assumption that chemistry is reducible to physics and, consequently, that the philosophy of physics is sufficient to ground chemical practice, has resulted in the underdevelopment of the philosophy of chemistry. These assumptions spread after the success of quantum mechanics in the twentieth century. The physicist Paul Dirac (Dirac, 1929, p. 714) stated the following:

"The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble."

From a pragmatist perspective, I will begin this thesis by rejecting this supposed reduction, whose main weakness is that it requires conceiving reality as a single thing and assumes that science grants us access to it, forming a Single and True Theory with which all phenomena that make up reality—including chemical phenomena—could someday be explained. Given the belief that quantum mechanics represents an approximation to this Single and True Theory, and that chemical phenomena can be entirely described in terms of quantum mechanics, it is interesting to note that chemical practice continues to rely on concepts such as orbital, chemical bond, chirality, to name a few—concepts that cannot yet be derived or treated with the rigor of quantum mechanics and that came into use successfully long before its development. A. Manafu (Manafu, 2015, pp. 46–47) poses the following question: *"If the entities spoken of in chemistry are composed of nothing more than the entities spoken of in quantum mechanics, why do we have chemistry and not simply applied quantum mechanics?"*

The prevailing paradigm assumes that there truly is an ontological reduction of chemistry to physics, and that these kinds of concepts, which originate independently of the reducing theory (in this case, quantum mechanics), could be deduced from it if we had epistemological tools with greater



reach—such as better mathematical and computational tools for performing calculations that would confirm the Single and True Theory. In other words, the particular concepts of chemistry, as well as the theories in which they emerge, are considered useful tools that artificially compensate for the fact that we are epistemologically limited, mainly by computational capacity. As a result, what is particular to chemistry is seen as a kind of theoretical “sleight of hand”—useful, but without true existence in the one single reality.

This has already been noted by Labarca and Lombardi (2010), who reflected on the existence of the orbital and observed that reductionism is so widespread that a great number of scientists not only reject the ontological autonomy of chemistry by considering orbitals to be epistemically inaccessible, but even go so far as to claim that they simply do not exist, despite the usefulness of the concept in chemistry (Labarca, 2010, pp. 149–157).

2.1.2 Science

Before delving further into this analysis, it is necessary to recall the criteria by which an activity is classified as science. Below I present the definition of science chosen by Goldstein in *How We Know*, an introductory essay on epistemology in the sciences.

“We have chosen to define science very broadly—as an activity characterized by three features:

It is a search for understanding, in the sense of finding satisfactory explanations of some aspect of reality.

Understanding is achieved through statements of principles or general laws—laws applicable to the widest possible variety of phenomena.

The laws or principles can be tested experimentally.”

(Goldstein, 1978, p. 12)

There are certain subtleties in two of the concepts involved in these criteria: the concepts of *facts* and *reality*, which will be explored below. The third aspect of the definition of science presented here allows us to assert that scientific knowledge is built through experiments, where we make observations and then obtain facts with which we test hypotheses. Quoting Goldstein:

“We are surrounded by facts—the things we can see, feel, hear, and smell.”

(Goldstein, 1978, p. 12)



We only have certainty about our sensations (with which we construct facts), and what we call *reality* is the way we interpret and structure those sensations. On facts, Goldstein reflects:

“We believe in their reality, and at times we even come to suppose that nothing else is real. But the common view of them as inevitable and basic data of existence ignores the strong component of experience and conditioning in even the simplest perceptions.”
(Goldstein, 1978, p. 12)

There are philosophers who argue that human knowledge is connected to effective action. This includes science, which “(...) does not begin with facts; it begins with the perception of a problem and the belief in the possibility of an answer.”
(Goldstein, 1978, p. 19)

Hypotheses, then, are beliefs in the possibility of an answer, given that “(...) a hypothesis is understood as the perception of some pattern in the phenomena, the establishment of some expectation about what will happen next.”
(Goldstein, 1978, p. 24)

Scientific knowledge must be epistemologically accessible to the scientist, and the facts we work with are distinguished or perceived selectively.

Goldstein (*How We Know*, p. 18) argues that conceiving facts in science as “fixed and unchangeable” has led to misinterpretations of their use; for example, that “theories must agree with all the facts and, if they do not, they are wrong.” Such assertions, according to Goldstein, ignore “that the reality of the world is composed of an absolutely enormous number of facts: each grain of sand on a beach is different from another; no two have exactly the same weight or shape. Yet the weight and shape of each are separate facts. No theory can be expected to explain such a multitude of things; we must be content with far less.”
(Goldstein, 1978, p. 18)

To conceive of a single reality in its entirety from a limited set of data—the data we know—is a line of reasoning already criticized by philosophers such as Lee Smolin (Smolin, 2013, p. 13). In this work we will reject this reductionist stance and defend the ontological independence of the concepts upon which chemical practice is based. To this end, we will adopt a pragmatist position, which recognizes the impossibility of accessing reality as it truly is (what Kant calls *noumena*), and we will explore the opportunity represented by pluralist perspectives to conceive, describe, and observe reality—perspectives in which knowledge is acquired by participating in reality and in which the



assumption is discarded that it is possible to acquire knowledge as spectators who do not affect the reality they observe.

Pragmatism

Charles S. Peirce (1839–1914) is considered the founder of philosophical pragmatism, which becomes a fundamental element in resolving current problems in the philosophy of chemistry. In fact, Peirce graduated in chemistry and identified as a chemist throughout his career. (Earley, 2015, p. 73)

Pragmatists point out that we learn about our world, as well as about our own capacities and limitations, by interacting with and exploiting our surroundings, which include members of our own species. (Earley, 2015, p. 75)

Reality, from this perspective, is constructed from the most elementary basis: human sensory experiences.

According to Peirce, pragmatists deny that any conceivable description of the world could be sufficiently complete and accurate to suit all purposes. We cannot access reality as it truly is, which would require what some philosophers call the “God’s-eye view,” referring to a superhuman capacity to conceive reality; such a conception of reality is impossible to experience or corroborate for human beings, who are forced to conceive a more limited reality based on what is indeed accessible to us through our senses. “Peirce argued that we acquire knowledge as participants, not as spectators.” (Earley, 2015, p. 3)

Following this pragmatist approach, we therefore admit that science is an activity inseparable from our human condition, given that any knowledge generated within it involves a chain of interactions that ends in the human sensory experience, even when mediated through sophisticated measuring devices (for example, when viewing a numerical value displayed by a digital instrument). Beyond the question of whether human beings can be separated from this knowledge, I wish to highlight the necessity of their interaction with it in every measurement process.

This has an important implication:

“Since the privileged point of view of the God’s Eye does not exist, there is no ‘true’ ontology: all ontologies have the same metaphysical status because all of them are constituted by equally objective descriptions.”
(Lombardi, 2005, p. 14)

Although at first it may seem unusual to do science while conceiving of non-noumenal realities, or realities other than “reality as it is,” a bit of reflection leads us to notice that this is what has always



been done, but under the assumption that access to the noumenal reality is possible. The discomfort toward the idea of doing science while giving up the description of reality “as it is” originates, according to Putnam, from reasoning through a false dichotomy that divides reality into objective and subjective. Putnam frees us from this false dichotomy through internal realism, a philosophical stance that does not aim to access the One True Theory, but proposes instead that what we might think of as “objective” reality actually emerges when we define objects within a conceptual framework limited by our epistemological capacities. In other words, one can abandon the task of describing reality as it truly is and at the same time be objective with respect to what is epistemologically accessible within certain conceptual frameworks. Although it is acknowledged that this would be an objectivity for the subject who defines the ontological framework, it is the only objectivity to which that subject can aspire in their human condition with epistemological limitations, and it is the maximum possible objectivity once the idea of a “God’s-eye point of view” is rejected. (Putnam, 1981, p. 49 as cited in Lombardi, 2005, p. 14)

Human beings begin with sensory experiences that we organize in order to construct ontological frameworks in which the objects and concepts with which we build and describe reality emerge. In a certain sense, to assume that chemistry reduces to physics is to assume that the ontological schemes used in physics include and surpass the ontological schemes that may be used in chemistry. This stance is rejected in favor of ontological pluralism, “a central feature of Putnam’s internalism.” (Lombardi, 2005, p. 13)

The portions of reality studied by physics and chemistry, although not necessarily required to be mutually exclusive, *can* become so (for example, precipitation reactions cannot be explained by physics), and they can give rise to ontological frameworks that *are* mutually exclusive. This allows us to recognize that the ontological frameworks used to describe physics may turn out to be limited in the practice of chemistry, where new concepts emerge to describe chemical phenomena that cannot be derived from the concepts used to describe the reality addressed by physics. With this in mind, the need to develop a philosophy of chemistry becomes evident, particularly as we explore alternative approaches to those that take for granted chemistry’s subordination to the philosophy of physics.

2.2 Physics and chemistry as sciences that can be approached through essentially different ontological frameworks

A fundamental difference between physics and chemistry concerns reactivity and the way in which the identity and properties of objects are conceived. In chemistry we have the periodic table, as well as other categories used to classify matter, which depend on the kinds of changes in which matter participates. Some authors even prefer to define chemistry as the science that studies change rather



than matter itself (Stein, 2004, p. 5). Since the time of alchemy, the capacity of acids to produce changes in other substances—what we now call *reactivity*—sparked the curiosity of alchemists and made acids some of the first substances to be studied for their potential to bring about transformations in others. Joachim Schummer reflects:

“Is chemistry primarily about things or about processes, about chemical substances or chemical reactions? Is a chemical reaction defined by the change of certain substances, or are substances defined by their characteristic chemical reactions?” (Schummer, 2004, p. 3)

To begin answering these questions, we can recall that the criterion for the existence of chemical species, according to the literature, is that they interact with a measurement system. In fact, the models through which matter is conceived are useful because of their predictive power regarding the reactivity of substances: if we want to know what something is made of, it is because that knowledge will allow us to anticipate what will happen to it and what it will cause in other things, objects, or substances. That is, within an ontological framework concerned with describing reality “as it is,” one can conceive of a static or inherent structure for chemical substances—but such a structure only becomes meaningful at the moment the patterns of behavior of those substances are recognized.

2.2.1 The dynamism of chemical identity

To identify a sample, for example, it is necessary to perform analyses or tests such that the substance is perturbed and reacts in a distinctive way. This activity depends on assuming that every chemical substance has at least one property that makes it unique (Enke 2001, as cited in Ngai, 2016, p. 137). If there is a substance whose behavior has not been previously observed—one for which no record of its existence exists—we could say that a new substance has been discovered, and we would expect subsequent experiments to observe and document its reactivity. “In fact, any chemical substance eventually becomes an encyclopedia of knowledge about itself.” (Laszlo, 2014, p. 99)

Joseph E. Earley provides an example of the criterion of existence used to establish the existence of an unstable van der Waals complex; it was determined that such a species existed because it produced effects that could not be attributed to the chemical species from which it was composed:

“My suggestion would be that anything which possesses any sort of power to affect anything else, or to be affected by anything else, even for a moment, no matter how trivial the cause or how subtle the effect, has real existence; and I maintain that the definition of being is simply power.” (Hamilton & Cairns, 1961, pp. 246–247, as cited in Earley, 1998, p. 107).



This notion forms the basis of the criterion used by chemists to determine the existence of substances and to characterize them, where their reactions correspond to the characteristic reactions of an already identified substance. A pattern is recognized—a kind of puzzle piece within a network that also unfolds over time.

2.2.2 Ontological differences between physics and chemistry: ontologies of internal and external relations

From the behavior of substances, theories have been developed in which such behavior is interpreted as a consequence of the intrinsic or inherent structure of the entities that make up the substance. These entities are atoms and molecules.

Tontini states that the fundamental purpose of chemistry is to understand how the structure of molecules determines the properties of substances (Tontini, 2004, p. 25). This reflects the popularity of a mechanistic view in which the phenomena in which a substance participates depend on intrinsic factors such as structure. More recently, it has been argued that knowledge of molecular structure as a static and real property of objects may not be epistemologically accessible (Ochiai, 2017, p. 202).

Bernal establishes a distinction between chemical atoms and physical atoms: chemical atoms differ from physical ones in being defined as fundamental units of chemical combination. “Their atomic character relates not to their status as indivisible particles but to their appearance as ‘minimal factors’ emerging from the law of proportions.” (Bernal, 2010, p. 88) The properties of chemical atoms “are not specified prior to making them part of a physical theory, but are discerned as the result of chemical investigation” (Chalmers, 2008, p. 162).

2.2.3 Corpuscularism as an example of an ontology of external relations

Andrés Bernal and Edgar E. Daza are two authors who have examined the epistemological and ontological status of chemical relations, including an analysis of corpuscularism:

“Corpuscularism belongs to a class of ontologies that conceives the relations of objects as external to their identity, which means that things have a reality independent of their relations—one that precedes them. Under this view, relations do not fundamentally affect the identity of the things that are related, or that will come to be related. This allows the qualities of things—for example, size and shape—to determine their relations.” (Bernal, 2010, p. 84)



Emphasis is placed on the fact that these approaches become problematic in situations where there is high selectivity, as is the case in chemical reactions, because the complex variety of behaviors becomes impossible to describe simply in terms of the properties of the species. Corpuscularism, and ontologies of external relations more generally, require assigning more and more attributes to species in order to make sense of the observed high selectivity—an approach that violates the principle of Occam’s razor (Bernal, 2010, p. 85).

2.2.4 Ontologies of Internal Relations

In addition to analyzing corpuscularism as an example of an ontology of external relations, Daza and Bernal also examine ontologies of internal relations:

“When relations are conceived as internal, it is assumed that the things that are related are not independent of their relations. Thus, relations do not depend on something ‘internal’ to the things themselves (ibid). In an ontology of internal relations there is no object that precedes its relations, since it is the relations that constitute the object. The qualities of the object cannot have any role in determining its relations, because the latter precede the former. Instead, the relations of the object serve to construct its qualities. A theory of internal relations exploits complex patterns of relations to construct varied characterizations of entities. Therefore, the consequences regarding the effect of selectivity are inverted with respect to the case of external relations: when relations are non-selective, such a theory would tell us nothing except that all objects are similar; but when there is high selectivity, internal relations become a powerful source of knowledge about the entities.” (Bernal, 2010, p. 86)

2.2.5 The Precipitation of Chemical Species: A Case Study

During the seventeenth century, natural philosophers sought to “tame” the field of chemistry and elevate it to a level of legitimacy comparable to Boyle’s corpuscularism. (Bernal, 2010, p. 83) During that century in France, distillation—previously the primary tool for analytical chemistry—was replaced by solution chemistry, which dealt mostly with metallic ions. In keeping with the intellectual framework of the time, an attempt was made to explain the selectivity of reactions in solution on the basis of corpuscularism. This resulted in a complex theory that attributed more and more qualities to matter in order to account for the high selectivity observed. Besides being overly complex, the theory was not very successful in practice.



The essentially different studies of the French chemist Etienne-François Geoffroy were more successful due to his focus on the selectivity of reactions rather than on the composition of matter itself. Through this approach he constructed a table of affinities between different substances, which proved to have great predictive power. Bernal argues that the rejection of corpuscularism and the focus on the “preferences” of substances were fundamental to Geoffroy’s success. (Bernal, 2010, p. 84)

2.2.6 Conclusion: Toward Relational Ontologies

“As both a science and a practical art, chemistry is characteristically concerned with relations—indeed, the focus on relations is arguably a defining feature of chemistry.”
(Earley, 2015, p. 77)

The idea that chemistry is essentially about the transformation of substances and that events are the basic elements of chemical ontology is certainly not new (Van Brakel, 2014, p. 11), yet its implications remain underexplored. Chemistry can begin to be examined without the burden imposed by the conception of reality as something reducible to physics, allowing it to be conceived instead from an ontology of internal relations in which the identity of substances is preceded by their particular relations.

The most useful classifications of chemical substances focus on their functions; concepts such as acids, bases, and even groups or families in the periodic table only make sense when common patterns of behavior are abstracted from the entities that compose these groups. In ontologies of internal relations, there is no object that precedes its relations, since it is these relations that constitute the properties or qualities that give the object its identity. Such ontologies become a powerful source of knowledge about substances, particularly in situations where high selectivity is observed, as in chemistry. Today, there are philosophers directing efforts toward the development of ontological frameworks that focus on relations as the distinctive feature of chemistry. (Earley, 2015, p. 85) One example of such frameworks will be discussed in the following chapter.

2.3 Relational Structure of Chemistry: Schummer’s Network

Having presented in the previous chapter two distinct ontologies through which chemistry and physics can be approached, as well as their fundamental differences, we can now recognize that an important task in contemporary philosophy of chemistry is the structuring of the fundamental and distinctive aspects of chemistry—those that set it apart from other sciences and whose relevance is



justified through ontological pluralism. Joachim Schummer (1998, p. 158) argues that the philosophical study of these distinctive issues would allow us to:

- Better define the scope of chemistry in interdisciplinary applications
- Avoid falling into blind reductionism and overgeneralizations, particularly in relation to physics and biology
- Bring to light those particular problems in the philosophy of chemistry that cannot be addressed from physicalist standpoints

La contribución de Schummer ante esta labor consiste en comenzar a estructurar los conceptos clasificatorios en la química en forma de red, esbozando lo que él llama “el núcleo químico de la Química”, refiriéndose a aquellas partes de la química que pueden ser “claramente distinguibles conceptualmente en la química interdisciplinaria y aplicada, así como en las ramas especializadas, que además resisten la reducción fisicalista”. Esta abstracción se explicará a más detalle a lo largo de este capítulo.

2.3.1 Properties and Chemical Identity

Historically, the exact sciences have adopted a mechanistic stance in their mission to search for the “essence” of matter—something invariant or that remains after material changes. (Schummer, 1998, p. 132) While a physicalist position assumes that the identity and behavior of objects are a function of their internal structure, in chemistry *properties precede identity* and are exhibited *contextually*:

“The concept of ‘chemical identity’ encapsulates the most basic notion of chemistry: *what is this?* The identification of substances has been central to chemistry throughout the entire history of the discipline. Analyzing a sample with the intention of identifying it is, fundamentally, a problem of classification or differentiation. Such activity depends on the assumption that each chemical substance has at least one differentiable property that makes it unique.” (Ngai, 2016, p. 137)

Whereas primary properties (shape, size, composition, etc.) are considered inherent to objects on their own, Schummer defines *material properties* as reproducible behavior under certain reproducible contextual conditions, and emphasizes the importance of recognizing that material properties are attributed not to isolated objects, but to both the objects *and* the contexts in which they occur. These two types of properties—primary and material—are considered orthogonal. (Schummer, 1998, p. 132)



Schummer concludes that *chemical identity* is a concept that makes sense only through interactions. As an example, he notes that toxicity is not a property of a substance by itself, but is exhibited in a context—typically the body of a biological organism. Recognizing that there are several types of important properties in substances (physical, chemical, electromagnetic), Schummer argues that the most essential interactions in chemistry are those through which substances undergo a transmutation or change in chemical identity—that is, chemical reactions. (Schummer, 1998, p. 134) Schummer points out that chemical reactions “connect” certain chemical substances with others, and these connections place them within the chemical network.

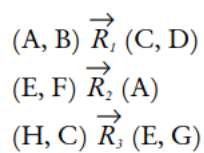


Figure 1 – Substances and Chemical Relations as a Function of Contextual Factors

A, B, ..., H: chemical substances. R_1 , R_2 , R_3 : chemical relations, which are functions of certain contextual conditions.

Schummer's Network

“Chemistry is, at its core, a science about peculiar relationships. Instead of studying isolated objects, measuring them, comparing them, and placing them within a classificatory scheme, the dynamic relationships between objects form the basic body of chemical knowledge and, at the same time, provide the basis for the classification of the objects themselves.” (Schummer, 1998, p. 135)

Reactivity, or the set of chemical properties of a substance, is exhibited in relation to other substances, and through it the substance's identity and its place in the network are defined. Schummer undertakes the task of structuring chemical knowledge in a way that accounts for this peculiarity, arriving at a network-like structure that connects, directly or indirectly, all chemical substances. In this network, the nodes are chemical substances, while the connections represent chemical reactions.

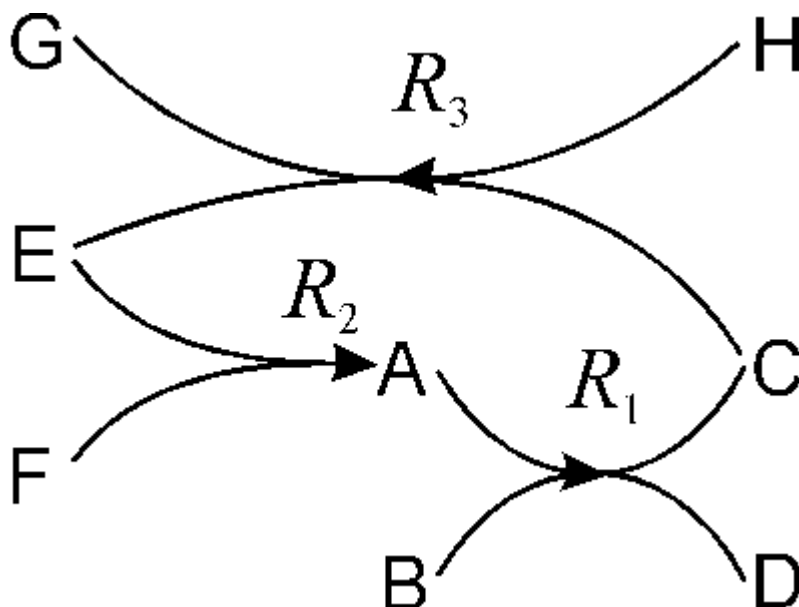


Figure 2 - Scheme of the Chemical Network

In the same way that chemical reactions allow us to assign identity to chemical substances, it is also possible to classify substances into higher-level groups (esters, alcohols, carboxylic acids, etc.) according to their reactivity. The result is another network, whose connections would also be chemical reactions, although more general, and whose nodes would be the functional groups. For example, H could represent the large variety of compounds classified as carboxylic acids, while C could represent, for instance, a metal hydrogen carbonate that, when reacting with a carboxylic acid, would produce a salt represented by G, carbon dioxide represented by E, and water represented by W:

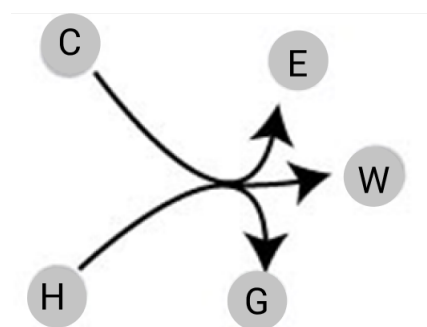


Figure 3 - Example of a Chemical Reaction in Schummer's Network

A concrete example of such a reaction is the reaction between sodium bicarbonate and acetic acid, shown below:

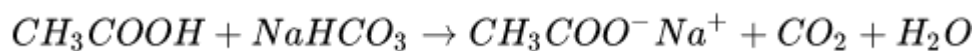


Figure 4 - Reaction of Sodium Bicarbonate with Acetic Acid



It becomes evident that the chemical network is useful for assigning identity to substances, but it also makes it possible to categorize substances at higher levels, which turns the network into a tool with great predictive power in chemical practice.

2.3.2 The Need for Pure Substances

So far, we have mentioned that the nodes of this network are pure substances, not individual atoms or molecules, *and there is a fundamental reason for constructing the network in this way*. Schummer avoids building his network starting from such concepts due to doubts about their validity as representations of reality, although he acknowledges the predictive power of such constructions within certain theories and models.

While the requirement that the nodes be pure substances may seem arbitrary, it is in fact epistemologically necessary. A strong argument in favor of this restriction is that molecular structure makes sense only within contexts or environments; quasi-molecular species are often interpreted as entities that have intrinsic or environment-independent properties (solvents, etc.), which undermines the distinction between pure substances and mixtures. Although it is true that substances are rarely found in a pure state in nature and that purification is an “artificial” intervention on matter, this procedure is not only useful but also *necessary in the sense that it allows us to have controlled and repeatable starting points for structuring a chemical knowledge network*.

Perhaps one day it may be possible to structure a similar network with individual chemical species, but this remains epistemologically inaccessible. Moreover, it is likely that its applicability or predictive power with respect to our reality would be irrelevant or even unobservable, making it difficult to justify such an undertaking with the rigor of the scientific method.



2.4 New Tools for the Philosophy of Chemistry

A man takes the tram after buying the newspaper and tucks it under his arm. Half an hour later, he gets off with the same newspaper still under the same arm.

But it is no longer the same newspaper; it is now a pile of printed sheets that the man leaves on a park bench.

As soon as it is left alone on the bench, the pile of printed sheets becomes a newspaper again, until a boy sees it, reads it, and leaves it as a pile of printed sheets.

As soon as it is left alone on the bench, the pile of printed sheets becomes a newspaper again, until an elderly woman finds it, reads it, and leaves it as a pile of printed sheets. She then takes it home and, on the way, uses it to wrap half a kilo of chard, which is what newspapers are for after these exciting metamorphoses.

“El diario a diario,” Julio Cortázar

As I hope this epigraph has suggested, this chapter will introduce some key concepts for contemporary philosophy of chemistry that relate to dispositional properties of objects. We can begin by reflecting that what happens with chemical entities, like with the newspaper, also depends on factors external to them (and on time). These are three concepts that have recently been included in the philosophy of chemistry and that offer scholars an opportunity to explore and restructure chemical knowledge (Harré, 2014, p. 77). These three concepts are:

- Affordances
- Hinge propositions
- Mereological fallacies

As Harré argues, these concepts are tools to broaden and structure knowledge of chemistry and are fully compatible with the ontology of internal relations. Each of these concepts will be contextualized below, as well as located within Schummer’s network.

2.4.1 Affordances



The concept of Gibsonian affordances was introduced by Gibson and later developed in his studies on perception (Gibson, 1967) (Harré, 2014, p. 78). This concept arose from studying visual perception and noticing that seeing something is not merely a physical phenomenon; it involves a type of perception in which attention is focused according to the purpose the actor has or the ways in which objects can be used. For example, a frozen lake has the Gibsonian affordance of being walkable for a wolf, but not for a moose, whereas a knife has the affordance of cutting in a context where there is bread.

“Gibson rejected the idea that these properties were merely phenomenal qualities without classificatory significance outside subjective experience. On the contrary, he assumed that they were real properties of the environment relative to an animal (or person, or measuring device, etc.)” (Turvey, 1965, p. 175, as cited in Harré, 2014, p. 78).

In the context of the philosophy of science, it can be said that nature and experiments must, at some point, involve measurements that in practice are also Gibsonian affordances that transform into data: taking a position compatible with Gibson’s, we recall that physical measurements necessarily involve a perceptible change for the observer, either directly through the senses or indirectly through some measuring device. The affordances that define objects within a conceptual framework are also, and have always been, interactions that provide the observer with classificatory data; they are responses to measurements interpreted through the observer’s conceptual framework. There is, therefore, a fundamental relationship between sensitivity and the conceptual construction of reality for the human as an observer.

Regarding the usefulness of these concepts in the philosophy of chemistry, we argue that they support the foundation of its practices through the construction of conceptual tools, such as Schummer’s network presented earlier. This network, for example, structures hinge propositions as “C has the affordance to become E thanks to H, which in turn became G when reacting with C.” One could also say something like “C + H as a conglomerate has the affordance to produce G + E.” In this structuring of chemistry, it makes sense to assume that chemical properties do not have to be attributed to a substance in isolation, but rather are derived within a context: the set of objects from which the properties emerge, a set that also includes the observer, not only the actors (chemical substances), at the moment of observation.

The identity of chemical species takes place within a network, since chemical species are distinguished and identified by their affordances, or in other words, by the way they react with the rest of the species.

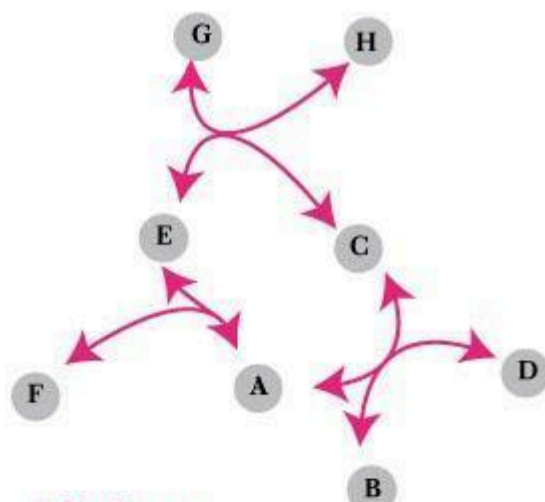


Figure 5 - Schummer's network (relations represented as Gibsonian affordances)

In this network, affordances are shown as red arrows in both directions, although this does not mean that the reactions are always reversible or equally so. In fact, we consider affordances to be temporally unidirectional, as illustrated in Figure 6.

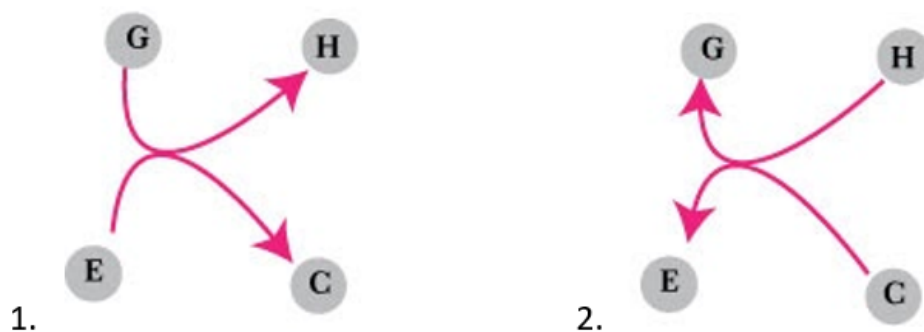


Figura 6

For example, a combustion reaction can be modeled using this graphical representation of affordances. Here, G and E could be the fuel and oxygen, while H and C could be the products of combustion, assuming CO_2 and water. In this case, the affordance would be valid in this direction: fuel and oxygen generate H and C, whereas the affordance in the opposite direction is not valid: “ CO_2 and water generate fuel and oxygen” is a false statement. On the other hand, there are also reversible reactions that would involve affordances occurring in both directions, but this does not mean that the magnitude of one direction is comparable or indistinguishable from its inverse. It should be noted that affordances make sense in a temporal dimension from the perspective of a scientist.

While in physics the equations used to describe systems are often temporally symmetric, meaning that the future and the past are equivalent (indistinguishable), chemistry is strongly linked to the



temporal evolution of its phenomena. This begins to reveal that there is an evolutionary aspect in Schummer's network, in the sense of evolving over time. This topic will be addressed further later.

Finally, it is necessary to clarify that chemical substances can have distinctive affordances that do not involve chemical reactions and, consequently, no changes in chemical identity. A substance, for example, can be characterized or assigned a certain identity based on its interactions with light in a spectrophotometer, without any change in identity being involved.

2.4.2 Hinge propositions

Hinge propositions are statements that arise from the scientist's interpretation of the Gibsonian affordances obtained through experimentation. These affordances, depending on how they are interpreted, become valid assertions for describing, for example, the fact or phenomenon of combustion (such as "oxygen plus fuel produces water, carbon dioxide, and related products").

Harré introduces Wittgenstein's concept of hinge properties (hinges) by inviting us to recognize that even the simplest pictures of knowledge include conceptual relations presented as *a priori* truths, such as "causes precede their effects" or "an acid reacts with a base to produce a salt and water." Hinge propositions are simple certainties that function like axioms when structuring scientific knowledge. A Wittgensteinian hinge proposition is not an object of knowledge; rather, it expresses that about which we can be certain (Harré, 2014, p. 81).

The philosophical stance we adopt in this work, pragmatist in nature, accepts without difficulty that knowledge may be limited to that about which we can have certainty. Within a pluralist perspective, hinge properties are those that—without needing to be true from the standpoint of the "God's-Eye View"—provide us with a kind of objectivity accessible to humans, and which is also compatible with the scientific method.

Recognizing that knowledge requires a human participant, we can also situate the concept of hinge properties in relation to Schummer's network within the lived reality of the scientist.

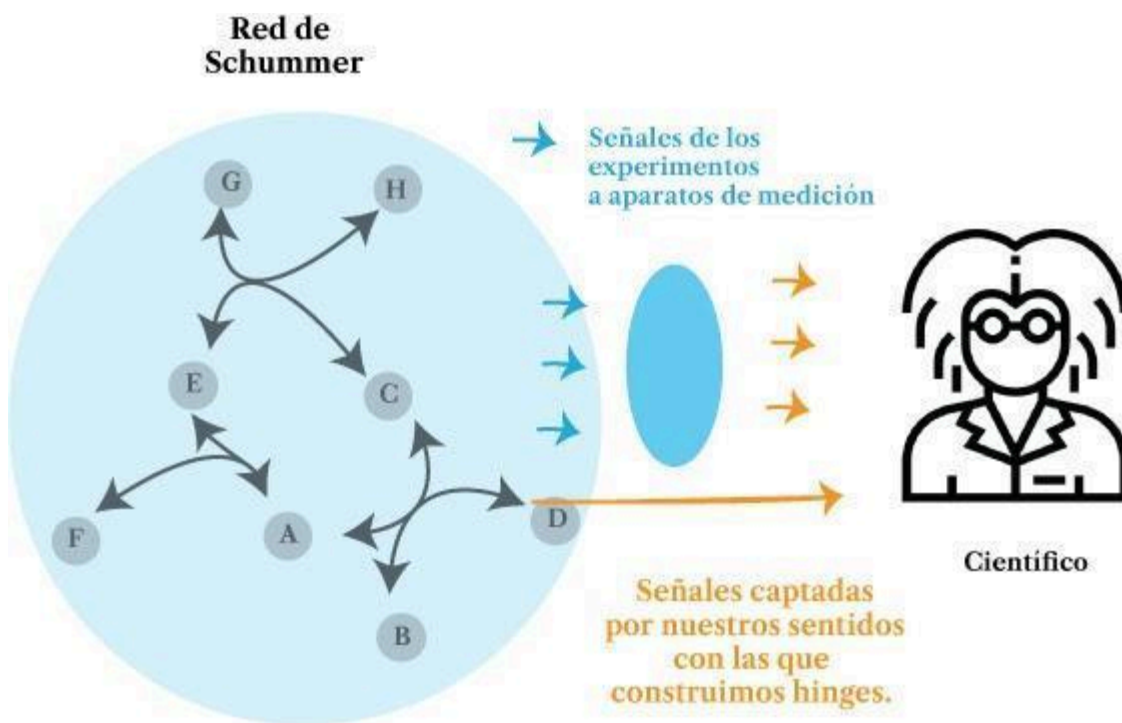


Figura 7 - Representación del conocimiento químico a partir de propiedades de bisagra

2.4.3 Mereological Fallacies

A specific type of mereological fallacy was introduced by M. R. Bennett and Peter Hacker (Bennett & Hacker, 2003, as cited in Harré, 2014, p. 80) in the context of evaluating neuroscience: they argued that it is a fallacy to attribute properties manifested by an entire animal to any one of its parts. For example, while it is valid to say that a person thinks, it is fallacious to assume that the brain alone thinks, or that its parts think on their own.

In chemistry, this kind of fallacious reasoning is often common in practice, as when we assume that an individual molecule or a small group of molecules will possess the same Gibson properties as the substance conceived as a conglomerate of molecules at the scale of several moles. At the same time, it is recognized that the properties of a molecule are not limited to the sum of the properties of the atoms that compose it.

The phenomenon known as *transduction* consists of making projections and drawing inferences about invisible, microscopic events based on observations at the macroscopic level. This phenomenon has



been common among chemists since the nineteenth century, with the rise of chemical atomism (Ochiai, 2013, p. 143).

Although models of chemical systems are often powerful, the ontology used to describe the phenomena within those models should not necessarily be taken as a realistic representation of reality (Schummer, 1998, p. 149). In presenting his network, Schummer takes a moment to clarify that he is not referring to the same thing when he thinks about the properties of a substance as a conglomerate (a node) and when he thinks about atomic or molecular entities as individuals. These concepts are often used interchangeably in chemical practice, overlooking or disregarding the fallacy being committed—sometimes for practical reasons.

In this segment of Schummer's network, it is shown that G and E have the Gibson property of producing H and C, or, in more familiar terms, that G and E react to produce H and C.

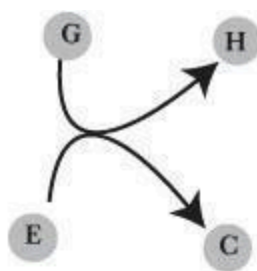


Figure 8

Substance **G**, as shown in the following illustration, may be composed of many individual molecules *g*, according to standard chemical models.

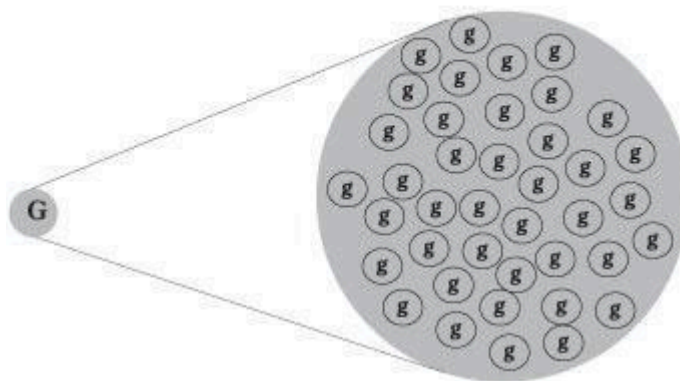


Figure 9



Schummer avoids the fallacy of proposing that individual entities possess the same Gibson properties as substances considered as conglomerates, a distinction he represents graphically in the following image.



Figure 10

G may exhibit emergent properties that arise from the interactions (represented by green arrows) among its component entities g , which would not display such properties individually. These properties, depending on the nature of the components and their interactions, may vary according to the number of entities that make up the conglomerate.

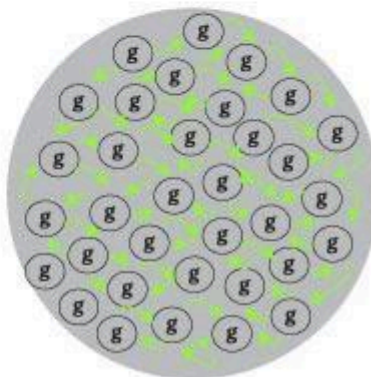


Figure 11

Having different quantities of the same substance G , represented as G_n and G_{n+m} :

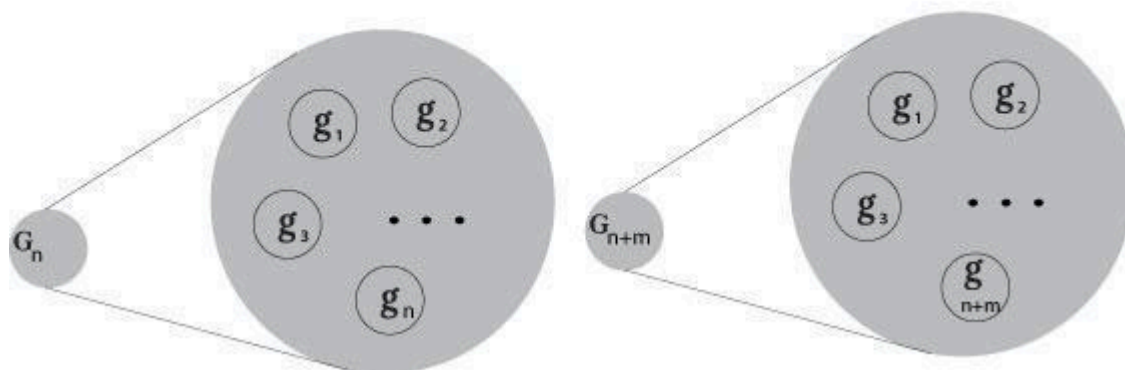


Figure 12

In chemical practice, it is assumed that the properties of G_n with respect to a particular observer—namely, the scientist—are approximately identical to those of G_{n+m} .

$$P(G_n) \approx P(G_{n+m})$$

Figure 13

Although G_n and G_{n+m} may differ in the number of constituent entities, if the observer cannot in fact distinguish their properties, then from a pragmatist perspective it is correct to say that they are equivalent within the observer's frame of reference.

$$P(G_n) = P(G_{n+m})$$

Figure 14

It is clear that the properties of a substance GG , considered as a conglomerate of n entities, are identical to the properties of the same substance composed of $n+m$ entities, for a wide range of values of m , as long as n corresponds to the quantity scales typically used in chemistry. Although chemical practice deals almost exclusively with substances at the level of conglomerates, Schummer remains aware of the risk of committing a mereological fallacy and avoids projecting the properties exhibited at this scale onto other scales, such as individual molecules or oligomolecular aggregates.

We close this chapter by concluding that these new tools for the philosophy of chemistry offer an opportunity to revolutionize how chemistry itself is conceived. The next chapter will address the concept of emergence, a notion deeply interconnected with mereological fallacies and one that



becomes a key component in laying the groundwork for this potential revolution in the philosophy of chemistry.

2.5 Emergence

The concept of emergence is actually one that chemists are familiar with from the earliest years of studying the discipline, even though it is not usually examined formally, nor is it common to refer to it explicitly by the name *emergence*. We know, for instance, that water is composed of molecules made up of hydrogen and oxygen, yet its properties differ significantly from the properties of hydrogen or oxygen in isolation. In molecules, *“the way electrons and nuclei join together matters, and the ‘connections’ (chemical bonds) determine the properties of the whole.”* (Del Re, 1998, p. 7)

An emergent behavior or property arises when a set of simple entities interact within an environment, giving rise to more complex behaviors as a collective. In other words, an emergent property of a system is a property that the system exhibits *as a whole* and that cannot be reduced to its components individually. It is important to emphasize that emergence is a concept used across many other areas of knowledge. Both philosophers and scientists employ the term *emergence* in relation to different levels of reality. (Manafu, 2015, p. 39)

“Emergence has commonly been described as representing the opposite tendency to reduction. To be an emergentist is to hold that certain phenomena, forms of organization, etc., emerge at certain levels, beyond what one would expect from the system’s constituents.” (Scerri, 2007, p. 77)

In the philosophy of chemistry, it is important to develop theories of emergence, as the concept is essential for defending the ontological autonomy of chemistry. The prevailing paradigm still maintains that chemistry is reducible to physics. Because chemistry is, in some ways, the science closest to physics, it is the first domain outside of physics where functional properties—as well as emergence and irreducibility, if they truly exist—are observed. (Manafu, 2015, pp. 46–47)

During the twentieth century, the success of quantum mechanics in accurately describing the behavior of simple molecules led to the widespread idea that chemistry was nothing more than applied physics (Dirac, 1929, p. 714). This success theoretically justifies the use of quantum mechanics to model chemical phenomena and predict reactivities. However, in contemporary chemical practice, many of the core concepts that emerged independently of quantum mechanics remain in active use. An example is the concept of the *orbital*, which has not been reducible to—or derivable directly from—quantum-mechanical calculations, yet possesses significant predictive value within chemical theory. In response to this tension, Manafu reflects:



“If the entities spoken about in chemistry are composed of nothing more than the entities spoken about in quantum mechanics, then why do we have chemistry and not merely applied quantum mechanics? (...) Does chemistry deal with genuine properties of the world, which inhabit a distinct ontological level? Or are chemical properties and laws merely useful instruments for prediction and explanation, but ultimately not fundamental truths about nature, which reside at the microphysical level? If chemistry is emergent, then these questions may find satisfactory answers. If one can show that there are, in fact, chemical entities, properties, laws, and explanations, then the ontological autonomy of chemistry is secured.” (Manafu, 2015, p. 47)

Among chemists, as previously noted, it is widely accepted that the properties of “free” atoms in an element are not the same as the properties of those atoms when they are part of a compound. As Del Re states: *“The structure of a molecule is distinct from the atoms that compose it, given that the physical and chemical properties of the molecule depend not only on the nature of these atoms but also on the way in which the atoms are connected.”* (Del Re, 1998, p. 95) Manafu further argues that what is emergent “are not the entities themselves, but properties, laws, and explanations.” (Manafu, 2015, pp. 53–54)

In chemistry, however, since the conceptual framework through which the identity of an object arises is preceded by the properties we perceive—properties that are themselves emergent—the identity we can distinguish and attribute from within our human perspective is also emergent. Emergence is consistent with an ontological view of chemistry in which objects are defined by their reactivity, achieved when those objects perform their efficient roles. It is important to emphasize that chemical knowledge originates at the moment the scientist is able to observe, and moreover, that the emergent properties resulting from the interactions between the scientist and the observational apparatus may be inseparable, irreducible, and not attributable to either part independently.

Regarding emergence, Manafu highlights the importance of focusing on a particular type: *functional emergence*. In his words (my translation): *“Functional emergence begins with the observation that many chemical properties are defined not in terms of their constitutive microphysical structures, but functionally, in terms of their efficient roles.”* (Manafu, 2015, p. 47)

Under this lens, chemistry could benefit from approaches that prioritize emergent properties rather than the “real” composition that supposedly generates the phenomena (i.e., the properties that grant identity). What allows us to construct the conceptual framework within which chemistry develops depends more on perceptible properties—including emergent ones—since the perception of these properties enables us to delimit and classify objects in order to assign them identities within that conceptual framework.



These notions can be represented in the following diagram. In order to develop knowledge about chemistry, the scientist has nothing but hinge properties; it is through these that they begin to develop concepts and divide reality into objects with relevant and useful properties (for example, distinguishing one substance from another). These hinge properties are functions of the properties exhibited by the portion of reality under study—properties that may themselves be emergent.

2.6 Time

2.6.1 Newtonian Time in Chemistry

As previously mentioned, chemistry has historically adopted the philosophy of physics under the assumption that chemistry is entirely reducible to physics. The concept of time in physics has evolved and been redefined multiple times (Maudlin, 2014, p. 21), whereas in chemistry, by contrast, developments related to time mostly concern chemical kinetics, which studies the temporal evolution of chemical reactions and the factors that influence that evolution. However, this does not entail any deeper exploration of time as a concept; it is simply adopted from physics.

In fact, the concept of time is generally not studied in depth in chemistry, at least at the undergraduate level. Instead, students are given introductory physics courses, and although it is not acknowledged explicitly, the conception of time used in chemical practice is the one developed by Newton, which emerged alongside the concept of space when Newton formulated the laws of motion.

For Newton, time—like space—was an invisible and constant structure within which physical phenomena occur:

“Newton believed in the existence of a spatial stage whose geometric structure was that of E^3 . He thought that this infinite three-dimensional space exists at every moment of time. And he also believed something much more subtle and controversial, namely that exactly the same points of space persist through time.” (Maudlin, 2014, p. 33)

Newton assumes that the existence of objects is separable from the temporal dimension and persists through time, with objects existing as such regardless of how long they endure. Newton also assumes that time can be divided into instants—intervals of time whose magnitude approaches zero—and even defines time itself in terms of these instants, as Tim Maudlin explains:



“Newtonian time is one-dimensional: a single sequence of instants that forms the totality of history. That set of instants possesses a topology determined by their order in time.” (Maudlin, 2014, p. 35)

Without making it explicit, Newton’s concept of time *requires* an observer, since it is also defined through comparisons of the magnitudes of intervals:

“Between any two instants, a certain amount of absolute time elapses, and this amount can be compared with any other in terms of its magnitude.

If a certain amount of time elapses between instant 1 and instant 2, and a certain amount of time elapses between instant 2 and instant 3, there is a fact of the matter about whether those intervals have the same magnitude or not, and a fact of the matter about the exact ratio between the intervals.”

(Maudlin, 2014, p. 35)

These are some of the assumptions embedded in Newton’s spatiotemporal conception. Time is conceived as a dimension in which phenomena occur, but one that is separable from the existence of objects. For Newton, time can be conceived in infinitely small or infinitely large intervals, because objects retain their identity as such over infinitely small and infinitely large durations. If reality does not depend on time, it follows that reality is both eternal and instantaneous.

This is a useful conception of reality—one that has resulted in remarkable progress in physics (and science more broadly), which in turn has enabled major technological advances. However, it is a *realist* conception of time, in which reality is singular. As mentioned in the first chapter, pragmatism rejects such conceptions because they require the “God’s-eye view,” or in other words, they are epistemologically inaccessible to any human. Pragmatism offers, as an alternative, the adoption of ontological pluralism.

2.6.2 Time as a Criterion of Existence in Chemical Identity: An Opportunity for Ontological Pluralism

The criterion of existence for chemical species, according to the literature, is that they persist long enough for there to be evidence of their existence; that is, that they interact with a measurement system (Earley, 1998, p. 107).

In chemistry, emergence seriously challenges the Newtonian conception of time by proposing that emergent properties—functions of interactions—precede the identity of matter and even any conception of matter, no matter how eternal or immutable it may seem in everyday experience. This implies that, within a pragmatist ontological framework, the processes that give rise to chemical identity cannot occur in an instant. In other words, the instant as a concept is an extrapolation in



which an observer could not experience any chemical phenomenon, since emergent properties dependent on interactions could not be exhibited. Chemical objects emerge or exist only in time intervals greater than zero.

2.6.3 For Reflection: Time in Contemporary Philosophy of Physics

Up to this point, we have contrasted our view with a reductionist view in physics. Although this contrast has been useful for the purposes of this work, it is important to recognize that contemporary philosophers of physics generally support a conception of time that is in harmony with the pluralist perspective that predominates here—and that, interestingly, is often contrasted with an atomistic and static view of matter.

Lee Smolin is a contemporary philosopher of physics who criticizes the scientific paradigm that seeks to eliminate time or consider it separable from the identity of the objects that make up reality, including atoms: *“This view diminishes time in many ways. There can be no surprises, no truly novel phenomena, since everything that happens is just a rearrangement of atoms. The properties of the atoms themselves are timeless, as are the laws that govern them; none of these change.”*(Smolin, 2013, p. 1)

Lee Smolin argues that time is an inseparable dimension of the world we conceive: what composes our world exists through time. Our experience unfolds in the temporal dimension: *“(...) neither individuals, systems, nor the universe as a whole can be conceived as things that simply exist. All of them are composed of processes that take place in time.”*(Smolin, 2013, p. 21)

Even time itself requires an interval—not an instant—of time in order to emerge as a concept: *“Time must be a consequence of change; without alterations in the world there can be no time.”* (Smolin, 2013, p. 20)



3. Discussion



3.1 The Identity of Chemical Substances as a Concept Defined by Their Affordances

Within the ontological frameworks with which we study chemistry, substances (S) emerge as portions of reality through a specific set of properties (P), by which we notice and differentiate them from one another. These properties are also affordances and are defined relative to an observer.

The set of properties that an observer (O) perceives and assigns to a given substance S can be represented as follows:

$$P_s^O$$

Figure 15

The set of properties P is composed of properties represented by the letter p.

$$P_s^O = \begin{pmatrix} p_1 & p_2 & p_3 \\ & \dots & \\ & & p_n \end{pmatrix}$$

Figure 16

Different substances may exhibit the same property p; however, the set P is unique for each substance and is, in fact, the criterion of identity by which substances are distinguished from one another.

$$P_g^O \neq P_c^O$$

Figure 17

Substances (S) are conceived as a collection of nn entities (ee), which can be atoms or molecules of the same type:

$$S_n^O = \begin{pmatrix} e_1 & e_2 & e_3 \\ & \dots & \\ & & e_n \end{pmatrix}$$

Figure 18

3.1.1 Possible Mereological Fallacies



Fallacies of Division and Composition

The fallacy of division is a logical error in which it is assumed that what is true for a whole must also be true for each of its parts, or in other words, that a property assigned to a whole is assigned to its parts on their own. This type of fallacy occurs when making statements such as: “Since water is transparent, the water molecules are transparent” or “Since water wets, a water molecule wets.” The inverse of the fallacy of division is known as the fallacy of composition.

In chemistry, it is assumed that a substance as a collection of $n+m$ entities behaves in the same way as the collection of n entities:

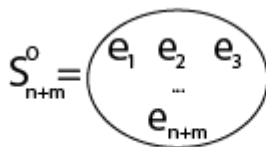


Figure 19

It could be said that the set of properties P of each of these systems is practically the same:

$$P_{S_n}^0 \approx P_{S_{n+m}}^0$$

Figure 20

In fact, for a sufficiently wide interval between n and $n+m$, the properties that an observer perceives may be exactly the same, which would imply:

$$P_{S_n}^0 = P_{S_{n+m}}^0$$

Figure 21

This is usually the case for practically any quantity of substance studied in chemical practice, and this is why mereological fallacies have only received attention in recent times in the philosophy of chemistry. Pushing this situation to the extreme, there could be a case in which the set of n entities exhibits different properties than the set of $n+m$ entities:

$$P_{S_n}^0 \neq P_{S_{n+m}}^0$$

Figure 22



This case is one of the possible novelties of interest for study, as it would represent a mereological fallacy that could potentially be observed and/or simulated given contemporary technological progress. Even Schummer warns the reader that the nodes of his network represent substances, not individual entities (molecular or atomic). In a substance G with entities g , this would mean that the set of properties of G would be different from the set of properties of g , a situation represented as follows:

$$P_G^o \neq P_g^o$$

Figure 23

This would be due to the emergent properties that G can exhibit, unlike g , because of the nature of the interactions among the g 's that make up G .



3.2 The Temporal Dimension of Emergent Properties

I ask this

<p>Niqitoa ni Nezahualcoyotl:</p> <p>¿Cuix oc nelli nemohua in tlalticpac?</p> <p>An nochipa tlalticpac: zan achica ya nican.</p> <p>Tel ca chalchihuitl no xamani, no teocuitlatl in tlapani, no quetzalli poztequi.</p> <p>An nochipa tlalticpac: zan achica ye nican.</p>	<p>I, Nezahualcoyotl, ask this:</p> <p>Do we truly live rooted in the earth? Not forever on the earth: only a little while here.</p> <p>Even if it is jade, it breaks, even if it is gold, it shatters, even if it is quetzal feathers, they tear.</p> <p>Not forever on the earth: only a little while here.</p>
---	--

- Nezahualcoyotl

Emergent properties arise from interactions, but these interactions also include interactions with the measuring device or instrument. Measurement is an affordance for this instrument, and since we consider them real properties of objects—given that their history depends on what happens with them—there are affordances that do not emerge until the moment they occur. In our language, this would translate to saying that it is only valid to attribute properties to objects at the moment they exhibit them, or only after they have done so. This type of interaction is far from trivial; in fact, it is the most important type of interaction, since it allows us, as scientists, to observe, conceptualize, and include objects within an ontological framework.

An axe, for example, is defined as an object that has the property of cutting. We can imagine a hypothetical axe whose blade is composed of a particular type of magnet that repels all objects it might cut; in that case, it would not be able to cut them, and we could not grant it the identity of an axe, since an axe must cut. This identity could not be granted, even if, given its shape (a material property at the level of color or material composition), we could imagine in our minds that it could cut objects.



For an observer to define the axe based on its functional properties, it must exhibit that affordance—the ability to cut—which defines, within a conceptual framework, what an axe is. Now, we can imagine that the material changes over time, going from repellent to non-repellent. If it remains non-repellent for a period long enough to allow the observer to perceive the affordance of cutting, then the functional property granting the identity of an axe is exhibited. If the time interval is too short relative to the act of cutting, the agent could not observe the functional property of cutting and would lack grounds to assign the object the identity of an axe, since identity is preceded by functional properties.

Now we can think of the example of the color wheel, which appears white when it is spun.



Figure 24 - Images taken from YouTube (Steve Spangler, Inc., 2021)

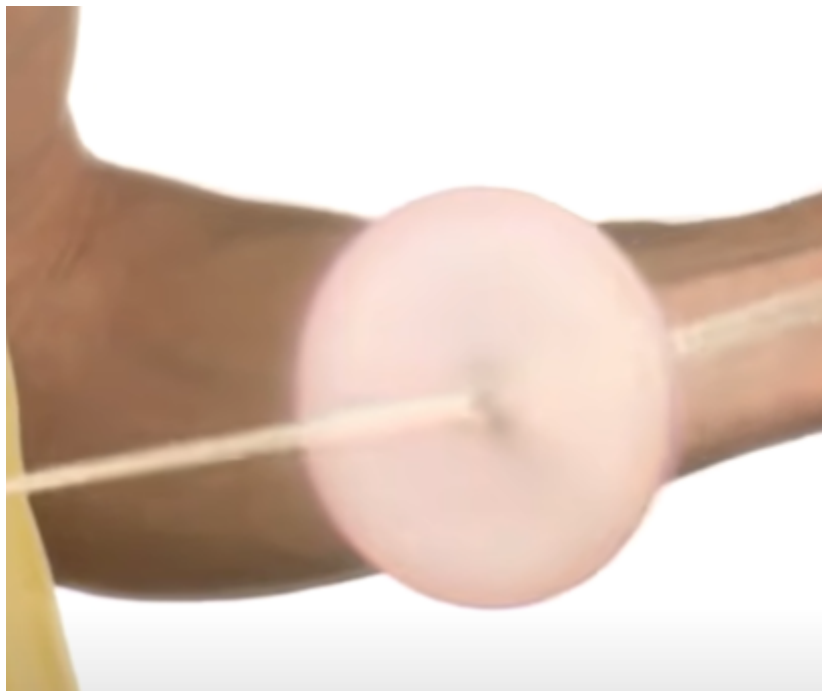


Figure 25 - Images taken from YouTube (Steve Spangler, Inc., 2021)

In this case, the color white can be considered a time-dependent emergent property. In the hypothetical scenario in which the wheel kept spinning forever and never stopped, would it be correct to say that it is white or that it is multicolored? Perhaps we could take a photo with enough resolution and capture the wheel with its colors separated, but if this possibility did not exist, we could say that the wheel's color is white with the same confidence with which we say that the sky is blue.

These kinds of examples are important for beginning to imagine how these questions apply in chemistry.

3.2.1 Mereological fallacies as a function of time

In addition to the mereological fallacies that arise from ignoring the difference between a conglomerate of chemical entities and the chemical entities considered separately, there are also time-dependent mereological fallacies.

Emergent properties are exhibited over a continuous span of time, since they depend on interactions, which imply changes, which in turn define the passage of time. Time here is defined in relation to the observer, who perceives the emergent properties with which they divide their reality into ontological objects, constructing conceptual frameworks.



In time intervals that are too short for the interactions through which properties emerge (emergent, by definition) and that define the identity of certain substances to occur, it is correct to assert that such substances do not exist within an appropriate ontological framework.

An illustrative example of the exhibition of time-dependent emergent properties is the previously mentioned color wheel that appears white when spun.

Analogously, over longer time spans, new properties emerge and additional criteria become available to define identities and/or differentiate them, if applicable. This implies that, across time intervals of sufficiently different magnitudes, the chemical network (and consequently the identities) may differ.

The fallacies of division and composition are errors in reasoning concerning assertions about the properties of a system based on the number of entities that compose it. Without forgetting that properties depend on an observer in order to emerge, one can similarly speak of mereological fallacies as a function of the magnitude of the time intervals in which the observer and the system interact. I will illustrate these possible mereological fallacies below.



Ambiente

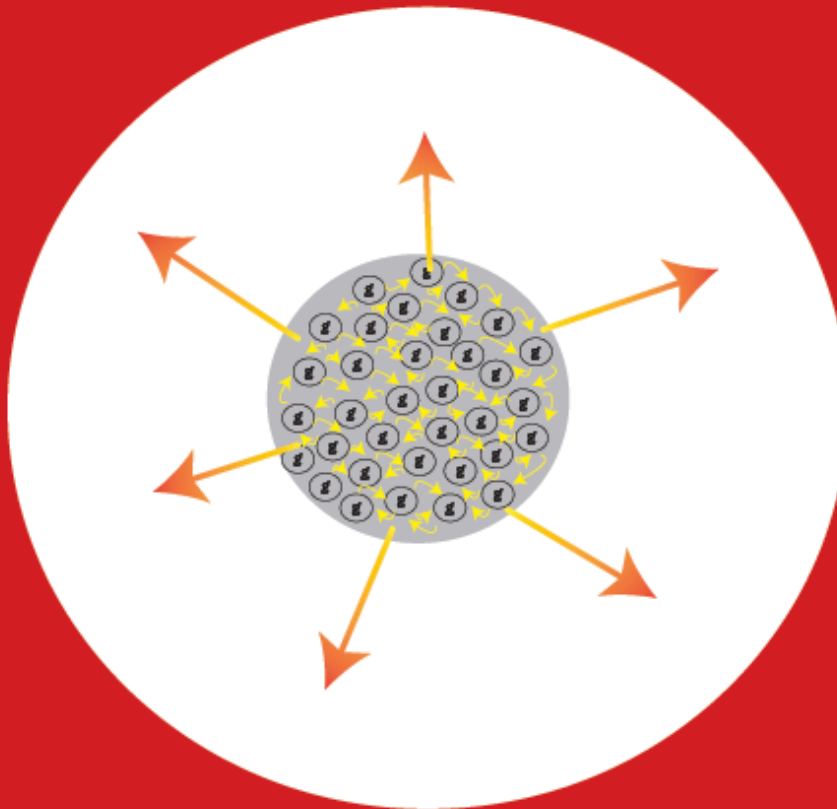


Figure 26

The properties that a substance (G), understood as a set of entities (g), exhibits to an observer can be emergent and depend on the interactions among its parts (g), as well as on the interactions between G and the environment. In Figure 6, the interactions among the parts of the substance (the “interior” of the substance) are represented with small yellow arrows; the emergent properties of the substance are represented with the red-tipped arrows pointing outward. Note that this latter type of arrow, by representing interactions with the environment (emergent properties exhibited to the environment), can also represent the interactions of the substance with the measuring apparatus.



Since interactions imply changes and occur in continuous spans of time, and emergent properties, in turn, imply multiple interactions, we can deduce that there may be time intervals so short that certain interactions cannot occur, as well as time intervals sufficiently long to give rise to the emergence of emergent properties.

The observational mechanism as a process allows the observer to perceive temporally local phenomena— that is, those phenomena whose temporality is such that an interaction can occur between the observational mechanism and the phenomenon to be observed. Earlier it was explained that the criterion for the existence of chemical substances is their persistence through time. Given that the criterion for the existence of chemical species is their ability to exhibit their properties, which are emergent, they must persist long enough for the interactions that give rise to those properties to occur.

Time gains meaning for an observer through the susceptibility to experience changes in what they are able to perceive. The color bars shown below represent time intervals of different magnitudes with respect to an observer.



Figure 27

The shortest time interval, the yellow one, could allow G to exhibit certain emergent properties derived from the interactions both among its components (the g's) and between G and the environment (double-headed arrows).

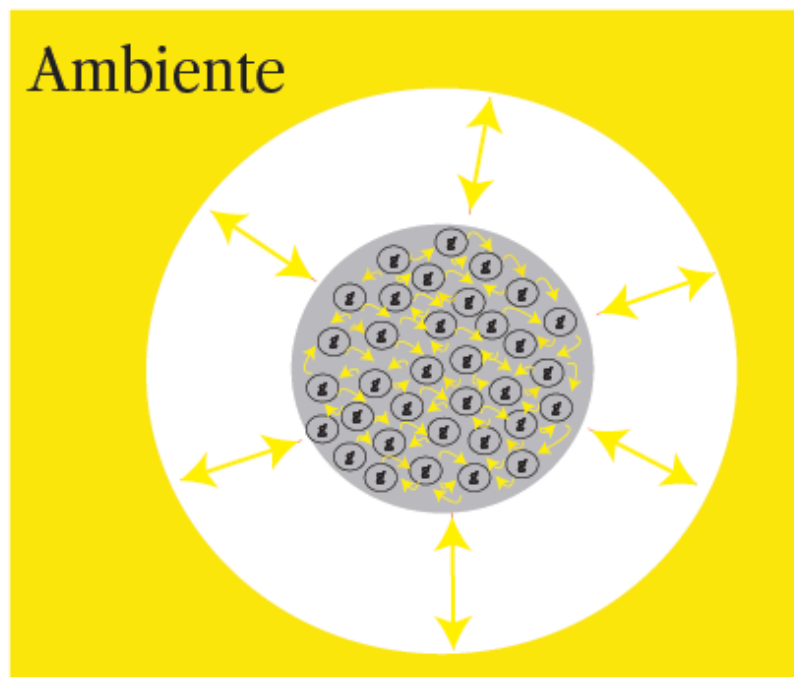


Figure 28

A longer interval, represented in green, would allow for more interactions and, consequently, for new emergent properties, represented with green arrows.

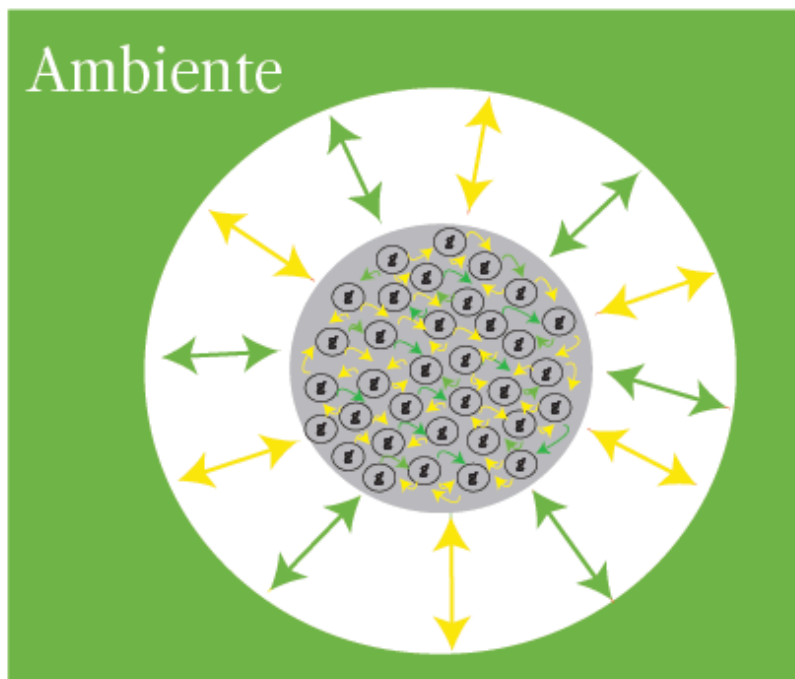


Figure 29

In the same way, more and more properties can be conceived the larger the time interval is, and the more opportunity there is for interactions that give rise to emergent properties. If the time span involved in the interaction process—given the nature of the observational mechanism—is shorter than the interval represented in blue, the blue emergent properties would not be perceptible to the observer and, as such, could not form part of an ontological framework that describes chemical reality, except in a purely hypothetical way.

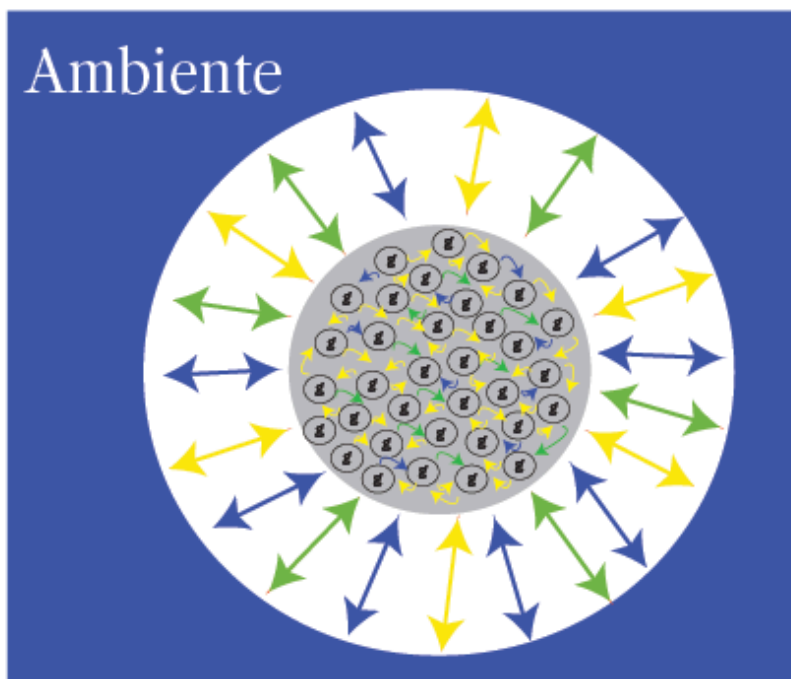


Figure 30

3.2.3 Implications of Temporal Mereological Fallacies in Chemistry

In Schummer's chemical network, substances are identified by their connections or relationships, which can also be interpreted through their temporal history. A substance is generated from other substances that existed before it, and it, in turn, later reacts and generates other substances, which also places them within the network. Chemical reactions occur over time intervals, so a representation of reactions can only take place over intervals of time, not at instants. In other words, chemistry unfolds in time.

Another interesting facet of chemical entities is that they not only acquire their identity over spans of time, but also *toward the future*, since identity is determined by the way a substance reacts.

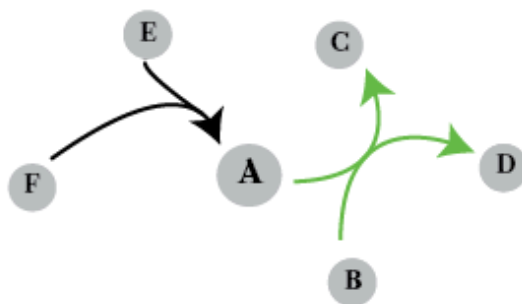


Figure 31

A can be obtained, for example, by reacting E and F; however, the identity of A is defined by its Gibson properties (green arrows), that is, its characteristic reactions. The identity of A—and of any chemical substance in general—is exhibited temporally in a forward direction.

Recalling that chemistry and its elements exist in reality within conceptual frameworks defined for an observer, and that the Gibson properties that define substances are exhibited within the temporal dimension, it follows that Schummer's chemical network is, in fact, temporally local, and that one can conceive distinct chemical ontologies—at least mentally—across time intervals whose magnitudes differ from the interval with which we conceive our chemistry. In other words, the chemical network is defined as a function of the magnitude of the time spans over which reactions are observed.

As illustrated in the diagram, the same underlying matter can give rise to different chemical networks (substances with different properties and identities) over time intervals that differ sufficiently, as represented here in blue and green.

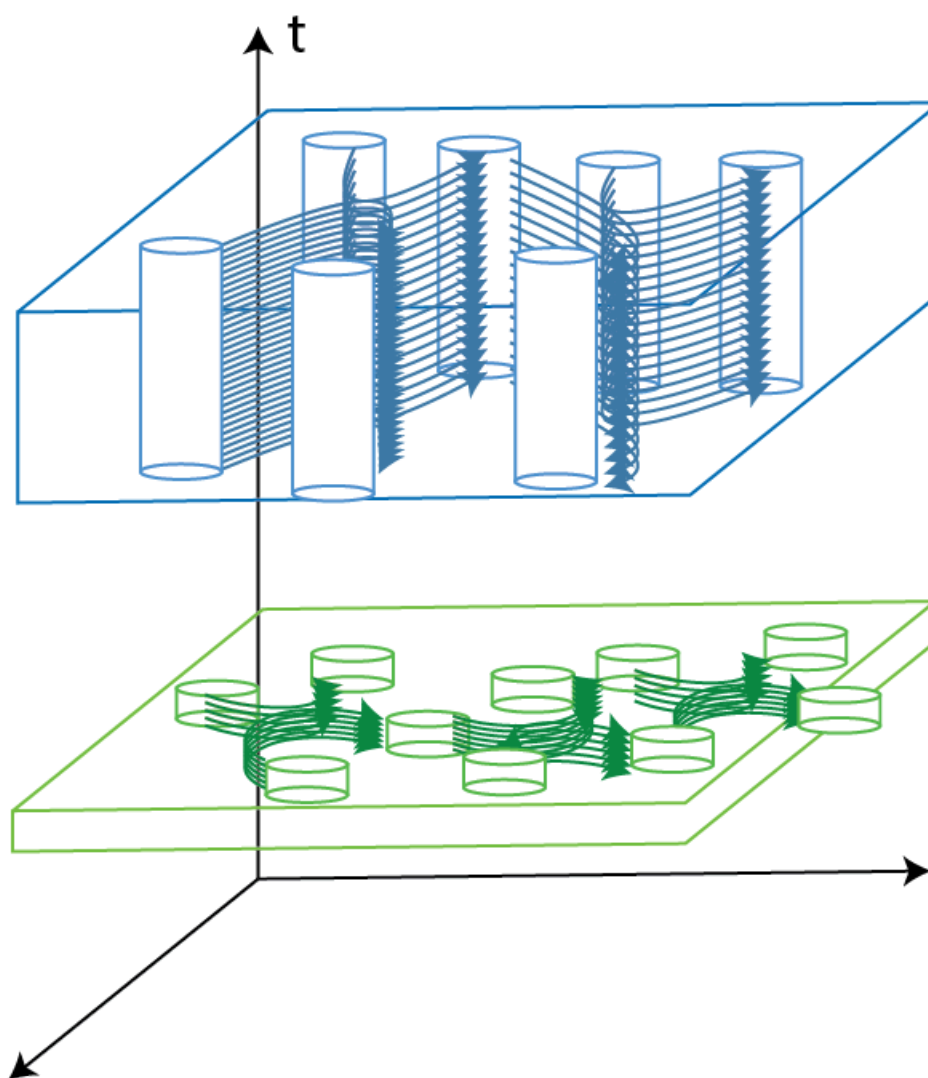


Figure 32

This locality is not only a function of time intervals, but also of the position or location on the timeline. That is, the emergent properties that define substances depend on events situated in the past, and it would not be correct to separate completely the identity or nature of substances from their history (or past), even though doing so is practical when modeling chemical phenomena and, furthermore, verifying it would be an unattainable task for *contemporary humanity*.

Graphically, this could be represented as follows:

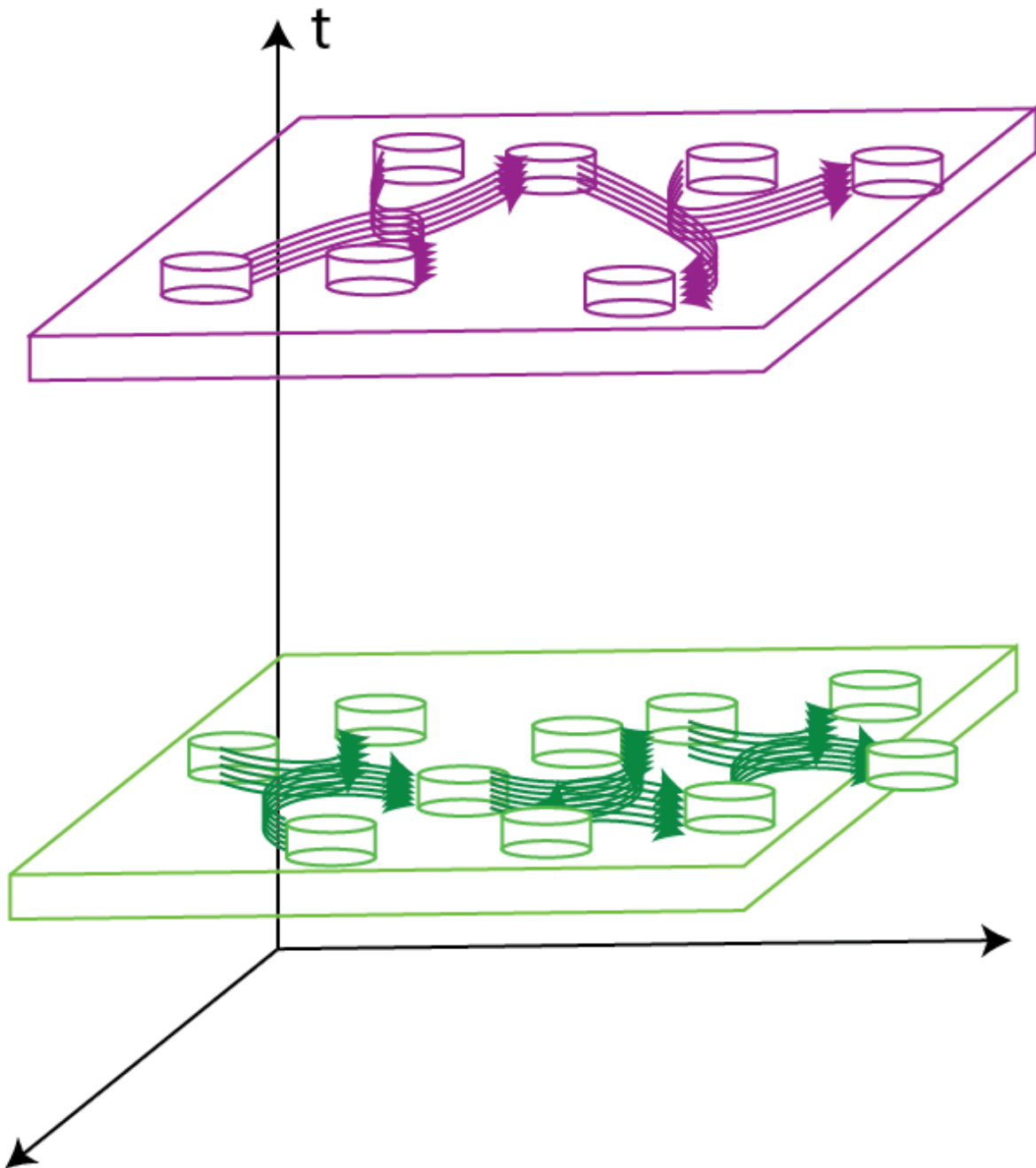


Figure 33





3.2.4 Allowing for Novelty in Chemistry: Corpuscularism vs. an Ontology of Internal Relations

Corpuscularism

Corpuscularism involves assuming that the properties substances exhibit are caused by their material and timeless composition. This conception becomes inconvenient when new properties are discovered and explained by making modifications to those structures—usually by adding more and more factors to consider—which ultimately violates Occam’s razor.

In the following diagram, we have a chemical reaction between substances C and H that results in the formation of G and E. The grid-like dots represent timeless and intrinsic characteristics used to explain the reactivity of each substance. If we assume that the structures of substances depend on internal factors, then their composition (structure) is such that it allows them to follow the appropriate process to form G and E, a process represented with colored arrows (green for C, blue for H). Continuing with the corpuscularist view, this structure must also cause the processes by which they react with any other substance (the other dots); in other words, the timeless structure (represented by dots) explains all of their behavior. As mentioned earlier, this results in the need to consider more and more variables as the number of reactions (or processes to explain) increases, resulting in a violation of Occam’s razor. Corpuscularism assigns more and more “dots” to the identity of entities as more behaviors are observed.

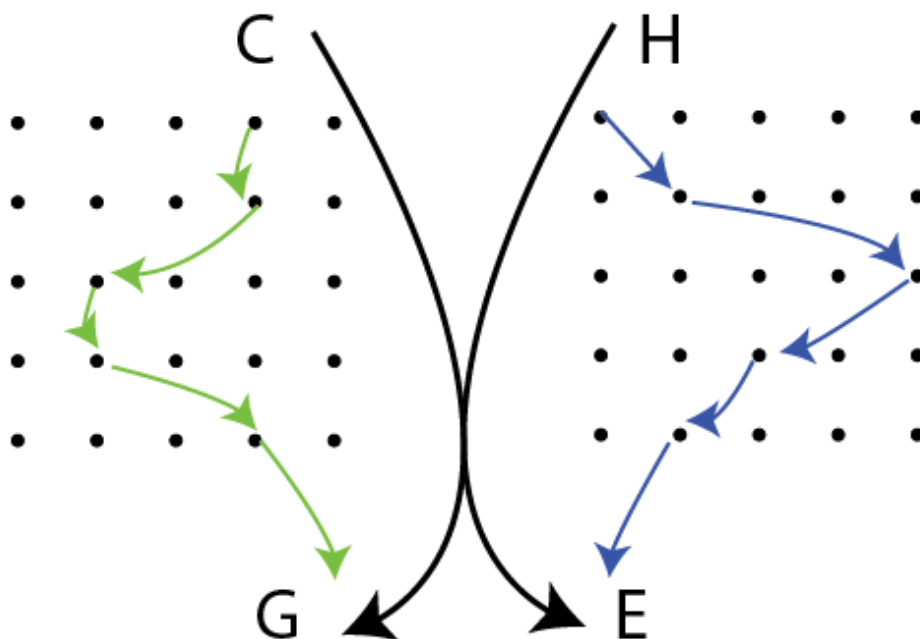


Figure 34

Ontology of Internal Relations

The ontology of internal relations recognizes that what causes the behavior of substances does not depend solely on their material composition, but is also affected by factors external to them, such as their relations with other substances. **It is important to contrast this with the corpuscularist conception, which implies eternal or timeless structures, whereas the ontology of internal relations—conceiving identity as a function of interactions or relations—must, consequently, consider time as a variable.**

This ontology allows us to recognize that the process by which C and H react to yield G and E originates from variables that may not influence the processes by which C and/or H react with other substances. Likewise, the causes of those other processes need not influence the process through which C and H form G and E. *This frees us from the obligation of considering those causes in this process, and, more generally, frees us from having to consider **all causes** (all the points representing structure) **at all times or in all processes.***

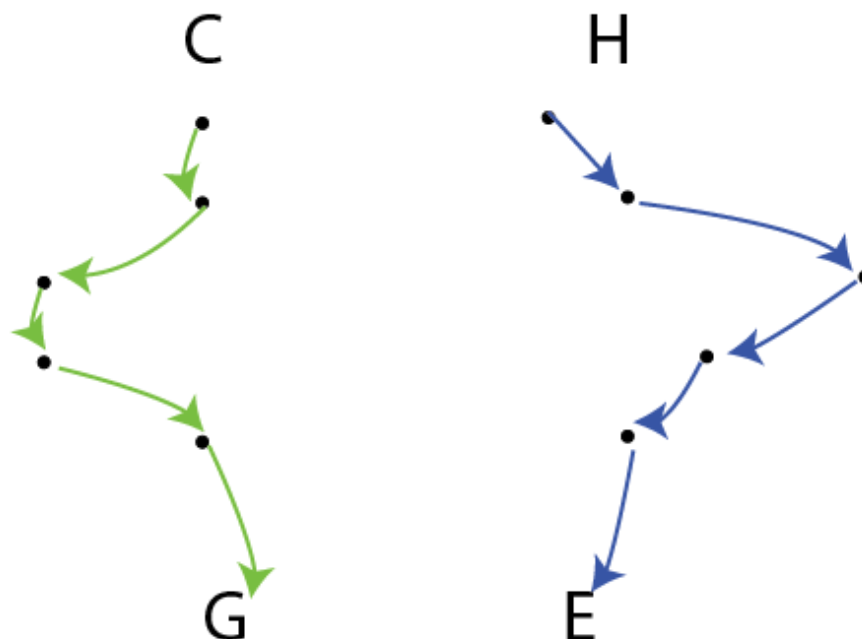


Figure 35

In conclusion, assuming that a substance “is the same” across a continuum of time, and that the cause of all its properties remains constant across that continuum, eventually leads us to violate Occam’s razor. Such an assumption ignores the fact that new or different contexts give rise to new or different Gibson properties, which in turn give rise to new or different emergent properties. In this case, the “points” that enable the property of going from C to G and from H to E arise as a function of the particular situations or the history (the “path” followed) of the entities, which allows the properties (and identity) of those entities to be conceived in terms of particular contexts and also in terms of time.



4. Conclusions



Regarding chemistry, particularly chemical identity, there are several conclusions I reach in this work:

- The emergent properties of substances as conglomerates also derive from interactions among their individual entities, meaning that the properties of those entities by themselves or in different environments may be different. Schummer is careful when structuring his network and avoids committing this fallacy by establishing the distinction between the properties of a molecule and those of the substance as a set of molecules.
- Chemical properties—and consequently, chemical identity—exist in a continuum of time. The underlying matter has historically been conceived as eternal and as preserving its identity both in instants and in infinitely large time intervals. This underlying matter may or may not exist, but chemical substances as such, with their distinctive properties, emerge in the sense that they can be distinguished and integrated into a conceptual framework that is constructed within temporal continuums.
- Because chemical identity is defined by the environment, it should not be conceived as something static or inherent, but can instead begin to be conceived as variable depending on the processes in which species participate. That is, the Gibson properties (affordances) that define chemical identity vary as a function of the interactions in which they are involved—which in other words means they vary depending on their environment and on the time at which they are exhibited.
- Chemical identity and properties are in fact exhibited locally in both temporal and spatial terms. At intervals far larger or smaller than those perceptible through human experience (extrapolating the concept), we must be prepared to observe unpredictable phenomena, including possible restructurings of the chemical network.
- The temporal locality in which chemistry emerges as epistemologically accessible to us is not only a function of the *extent* (the magnitude) of intervals, but also of position on the temporal line. Emergent properties are not only a function of what may occur during the interval in which substances exist as such, but also a function of the past of the underlying matter, depending on the interactions we have with it. If emergent properties are temporally preceded by certain interactions, then they depend on the past—and therefore, if the pasts of two systems are different, it is possible that their emergent properties will also be different.
- A pragmatist and dynamic ontological framework gives chemistry the advantage of approaching these novelties through ontological pluralism, no longer subordinated to the philosophy of physics.

Philosophical pragmatism applied to science is undoubtedly an opportunity that is only just beginning to be explored. Propositions such as those above reveal themselves after a bit of analysis, and it will be a matter of time before the scope of their practical applications in computational models can be determined.



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