On the Epistemological and Ontological Status of Chemical Relations

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Abstract: Following several authors, we point out the importance of relations in the conceptual frame of chemistry. We propose that an important characteristic of chemistry is given by the epistemological challenge associated with selectively related entities. We also suggest that internal relation ontologies have been seen by chemists as better suited for assessing this challenge, and that this ontological perspective has played an important role in shaping chemical concepts.

Keywords: *Chemical relations, external relations, internal relations, chemical atomism*.

1. Introduction

In the present, the relationship between chemistry and philosophy of chemistry often seems to be unilateral. Philosophers of chemistry look at the practice of chemistry to characterize its epistemological and ontological foundations, its logical structure, or its ethical implications. However the converse is seldom true: practitioners of chemistry are mostly uninterested in the philosophical dimension of their discipline. This seems to us like an impoverishing bias. The philosophy of chemistry can make important contributions to understanding the foundations of this science, and in that way offer guidelines for the development of chemical theory. In a period that emphasizes multidisciplinary approaches in scientific research, chemists would do well acknowledging the role that philosophical ideas can play in their research activities.

Some philosophers of chemistry advocate an autonomous approach, separating themselves from the physicalist tradition that dominated the philosophy of science during the twentieth century (see *e.g.* Schummer 2003, Baird et al. 2006, Bensaude-Vincent & Simon 2008). A recurrent element in many of these works is the acknowledgement of the central role that *relations* play

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in chemistry; the characterization of chemistry as “a science of peculiar relations” (Schummer 1997) that constructs its knowledge through or into a “network of relations” among substances regarded as “chemical actors”.[1]

However, Soukup’s assertion that “the relational character of chemical concepts is what distinguishes chemistry from physics as a discipline operating in a clearly different manner” (Soukup 2005, p. 804) might be too far-reaching. It sounds like a simplification of Turner’s definition of chemistry as “a science, the object of which is to examine the relations that affinity establishes between the bodies” (Turner 1840, quoted in Kim 1992, p. 85). That can offer a sharp characterization of the discipline only in as much as it is accompanied by a clear understanding of the particularities of ‘affinity’ relations. Therefore, we deem necessary to deepen the understanding of the ‘peculiar’ nature of the relations that chemistry deals with in order to characterize it as an autonomous discipline.

In this contribution we argue that chemistry is characterized by phenomena involving selective interaction and transformation among substances. The pursuit of knowledge of these selectively related entities favors an ontology of internal relations which permeates the language and classification schemes that are central to the chemical enterprise. Furthermore, we will argue that such an ontology directly opposes some atomistic ontologies, most notably corpuscularism but also those deriving from Newtonian mechanism, thus explaining the failure of known seventeenth and eighteenth-century atomistic systems of chemistry.

The first section introduces the main thesis of the paper, touching on the topic of the distinction between physicalist and chemical approaches to the study of materiality. First we introduce the problem of dealing with selective relations as a characteristic of the chemical approach. Second, we show how the corpuscularian perspective of members of the *Académie royale des sciences* in the seventeenth century was unable to deal with this problem, while Geoffroy’s affinity table achieved remarkable success. Then we identify corpuscularism as an ontology of external relations, and propose the incompatibility between the selectivity of relations and this ontological approach as an explanation for the failure of corpuscularian mechanism. The second section advances the characterization of chemistry as a science where the entities are internally related. To do so, we identify traces of this approach in chemical atomism, nomenclature, formulas, and classification schemes. Finally, we draw some conclusions on the consequences of these ideas for modern research in theoretical chemistry.

2. Selective relations in chemistry

Chemistry deals with relations established among substances as they undergo radical change (Schummer 1998). Thus, chemical properties are relational, they characterize the relations between substances and other substances they interact with and transform into (*ibid.*). This conceptualization of chemical properties appears as a core element quite early in the history of chemistry.[2] Though this focus on relational concepts has been seen by philosophers as a defining quality of chemistry (most explicitly in Soukup 2005), relations have arguably been also in the spotlight of many other scientific traditions. For instance, the law of gravitation in Newtonian mechanics characterizes the relation between bodies with masses, and the laws of electromagnetism describe the relations between charged bodies. Similarly, Boyle's clockwork universe is completely determined by relations among objects with figure, motion, and size. In order to clearly distinguish the chemical perspective, we have to look deeper into its peculiar relations.

One point that has been outlined before is the notorious complexity of chemical relations from a logical perspective: while physical laws, like those mentioned before, establish symmetric binary relations between atomic entities, chemical reactions establish "asymmetrical *dynamical relations* with two classes of *relata*: initial chemical substances before the change and different chemical substances afterwards" (Schummer 1998). Here we will not consider this logical aspect of chemical relations and discuss a different characteristic that, we believe, can help in accounting for the epistemological difference between chemical and physicalist approaches, explaining why some ontological perspectives that succeeded *e.g.* in mechanics mostly failed when imported to chemistry. That characteristic is the notorious *selectivity* of chemical relations.

Following Newton's and Coulomb's laws, any given mass interacts with any other mass, and any given charge interacts with any other charge. Both deal with *non-selective* interactions that exist between all bodies considered. Such is never the case in chemistry: even the most reactive substance is limited to interact, by means of chemical reactions, with a very restricted and characteristic set of substances. There is a vast complexity in the different ways compounds *select* their reaction partners and generate new products. This complexity sets a difference between chemistry and mechanics regarding the questions that need to be solved. As Kim asserted, "chemist needed to know *what* quantities of various substances should be mixed together to make successful products, *which* substances reacted together, and *which* did not" (Kim 2003, p. 5, our italics). These 'what' and 'which' questions make no sense in research fields characterized by non-selective interactions. If certain bodies are found to attract each other, and a domain of research is defined as that encompassing those bodies, it is pointless to ask *which* attract each other and which do not. Relation selectivity plays an important role in determining the knowledge that is to be gained; and, as we are about to argue, what knowledge is to be gained can prefigure the inadequacy of certain ontological perspectives.

2.1 The failure of corpuscularian ontologies

During the seventeenth century, chemistry came under the focus of natural philosophers "seeking to domesticate this rich empirical field in order to refurbish their systems of philosophical knowledge" (*ibid.,* p. 3). Central to this enterprise was the introduction of popular philosophical perspectives on matter into the discourse of chemistry, in order to transform this discourse "to conform to chemists' analytic practice", but also to give it a "level of respectability and legitimacy" (*ibid.,* p. 37). Boyle's corpuscularian program constitutes a notably explicit example of this phenomenon.

While corpuscularianism would achieve significant success regarding the second point, functioning as "the legitimating discourse of chemical practice in the emerging public sphere of the early Enlightenment" (*ibid.,* p. 47), it arguably failed regarding the first. The intrinsic selectivity of chemical phenomena was at the center of this failure, as revealed by modern studies in the history of seventeenth-century chemistry at the *Académie royale des sciences* (see Kim 2003, chap. 2-3; Bensaude-Vincent & Simon 2008, chap. 8). During this period, for instance, Kim (2003) identifies a shift from distillation to solution methods as the preferred analytical technique, which would result in a significant transformation in French chemistry. The new emphasis in solution methods took the problem of *selective* dissolution and *selective* displacement of metals to the front of chemical philosophy (*ibid.,* p. 112). In this way, in 1677 a prominent figure, Nicolas Lemery, identified metallic dissolutions and displacement as "one of the most difficult [questions] to resolve well, of any in Natural Philosophy" and attempted to give a corpuscularian answer (*ibid.,* p. 55). The corpuscularian language, however, was more impeding than helpful in constructing an explanation of these phenomena. Lemery's discourse was promptly saturated with a multitude of different shapes and sizes that he had to attribute to the corpuscles in order to encompass the complexity of selective dissolution. "This multitude of different corpuscles – smooth and round, jagged, or hooked – proposed by Lemery provoked the satirical scorn of a number of chemists" (Bensaude-Vincent & Simon 2008, p. 142).

The problem of selective dissolution and displacement remained open and would go on to become a prevalent challenge for corpuscularian accounts of chemical phenomena at the *académie*. After unsuccessfully trying to account for selectivity in acid-alkali reactions through a principalist approach, Wilhelm Homberg would resort to a "speculative corpuscular ontology" (Kim 2003, p. 78) with no better results than Lemery's (*ibid.*, pp. 75-79). In the early eighteenth century, Louis Lemery worked extensively on the matter that by the time had acquired a "theoretical urgency" (*ibid.*, p. 132). Arguably, his lengthy speculations on the corpuscular mechanism of metallic displacement did not help chemists predict the outcome of dissolution reactions anymore than those of Homberg or his father (see *ibid.*, pp. 121-123).

Etienne-Francois Geoffroy performed significantly better with a radically different approach (*ibid.*, pp. 132-146). He shared the concern over the theoretical foundations of solution chemistry, but he "did not care much for the corpuscular ontology his colleagues employed for the purpose" (*ibid.*, p. 134). He was more interested in the fact that chemical substances "offered *a certain preferences in reactions*" (*ibid.*, our italics). Abandoning all forms of corpuscular speculation, he instead devoted himself to the construction of a *Table des differents rapports observés entre different substances*. At first glance, this *affinity table* only summarized known reactions in solution chemistry, allowing easy access to a cumulus of data collected through years of chemical practice. But it did much more: it evidenced inconsistencies in current classifications of substances, allowing subtle differentiations that had not been possible before (see *e.g. ibid.*, p. 141), and even provided a solid ground for predicting other reactions (Kim 1992). It was, properly speaking, a powerful theory of solution chemistry, much more than the corposcularian model – unlike the later, the affinity table directly addressed Kim's *which* questions.

Geoffroy was able to assess the challenge of selective relations that so far had defeated corpuscularian ontologies. This was a key success in the development of chemistry. We uphold that the rejection of corpuscularism was fundamental in achieving this success, because the way it conceived relations turned selectivity into a growing and soon insurmountable problem. Geoffroy's interest in the substances' "preferences in reactions", on the contrary, led to an approach that tacitly conceived relations in a way that allowed selectivity to become the main source of its epistemic power.

2.2 Internal relation versus external relation ontologies

Corpuscularism belongs to a class of ontologies that conceive relations as being *external*, *i.e.* that the things related have a reality independent of their relations and are prior to being related (Ferrater-Mora 2004, pp. 3054-5). Thus, relations do not fundamentally affect the identity of the things related or to be related. This allows for the qualities of the things – *e.g.* shape and size – to determine their relations.

This ontological conception of relations can support powerful deductive theories when mostly non-selective relations are involved, because then one could take advantage of this homogeneity to derive a law that reduces the relations between objects to the fundamental qualities of the objects. This is what happens *e.g.* in the Coulombian approach to the study of electrostatic phenomena, where each object is identified with a property (here: charge) that can be conceived and thought of before it interacts with other objects, and that determines its behavior when interacting. This is also what Boyle attempted to achieve with his clockwork universe, where all phenomena are reduced to interactions between microscopic bodies, which in turn are determined by figure, size, and motion of the bodies.

However, such an approach is undermined by selective relations. When strong relation selectivity is involved, a complex variety of behaviors arises that can hardly be subsumed under a unique law that describes the system through a proper set of attributes of the individual objects. If attributes of the objects are supposed to account for their relations in a reasonably simple way, but the objects display complex, varied 'preferences' in what they relate with, external relation ontologies force the researcher to ascribe more and more attributes to the objects, in order to account for their different preferences. This is what happened to Nicolas Lemery when he attempted to account for selective dissolution from a corpuscularian ontology: common properties of the acids, *e.g.* their ability to dissolve metals, were explained by attributing the quality of being pointed to their particles. But then, to explain the preferences of some acid preparations for certain metals, additional attributes of the particles were required. Each new observation of selective interaction required an *ad hoc* mechanism and/or a new attribute of the bodies. That led to the proliferation of different corpuscles which gained him the scorn of his colleagues. Adopting a corpuscularian ontology for the study of chemical phenomena is problematic because the mixture of external relations and selective relations easily leads to a violation of Occam's razor principle.

External relation ontologies abstract the identity of an object from its relations. When relations are selective, this turns into a hard and unrewarding enterprise. In such a situation, by prioritizing epistemology we acknowledge that after all the purpose of the scientist is to characterize the object *in relation*, that the idea of an unrelated object is but a useful abstraction that now has ceased to be useful. An *ontology of internal relations* is then preferred, as it naturally uses relation selectivity as a mean to describe the entities being related.

When relations are conceived as internal relations, it is supposed that the things related are not independent of their relations. Thus, relations are 'internal' to the things themselves (*ibid*). In an ontology of internal relations there is no object previous to its relations, as they constitute the thing.

Qualities of the object cannot play any role in determining its relations, as the latter precede the former. Instead, relations of the object are used to construct its qualities. A theory about internal relations exploits complex relation patterns to construct rich characterizations of the entities. Thus, 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 but that all objects are alike; but when there is high selectivity, internal relations become a powerful source of knowledge regarding the entities. This is the root of Geoffroy's success: "Instead of musing upon the causes of selectivity, he represented the order of selectivity visually in his 1718 table des rapports." (Kim 2003, p. 113).

In Geoffroy's discourse, the smooth, round and small corpuscles of Lemery are replaced by simple letters designating each substance: "If among the substances [...] two were found united (A, B) and subsequently mixed with another (C), either the third substance (C) would join one of the substances (A) and shake the other (B) loose or it would not join either of the substances originally in combination (A or B). If C joined A, one could conclude with sufficient probability that C had 'more rapport of union or disposition to unite' with A than B did" (*ibid.*, p. 135). Like Lemery's corpuscles, substances here were regarded as fundamental units; unlike Lemery's corpuscles, they were primarily devoid of qualities, they existed only as anchor points for relations. In Geoffroy's approach, qualities of the substances (or of its ultimate corpuscular constituents) needed not and could not explain the selectivity of their relations: relation selectivity determined the identity and qualities of the substances. External and internal relations are at opposite extremes, from the ontological but also from the epistemological point of view. External relation ontologies are closer to the reductionist, deductive theories proper of the physicalist approach. They could not be further from the holistic, inductive approach adopted by Geoffroy in constructing his affinity table. In this sense, one can see why he had to reject corpuscularism to succeed where Homberg and the Lemeries had not.

The distance between physicalist ontologies and chemistry's has recently been developed in depth by Bensaude-Vincent & Simon (2008, pp. 132-151). The authors acknowledge the importance of epistemological concerns in the pursuit of a proper ontology by chemists.[3] They discard the idea that "the discontinuity [or] the homogeneity of matter implied by atomism provides sufficient grounds to distinguish a philosophical view characteristic of the physicist from that of a chemist" (*ibid.*, p. 133). Instead, they conclude that "the point of dissent is rather the reduction of qualities to other parameters considered fundamental, such as figure or shape or motion" (*ibid.*, p. 140), that chemists "object to the idea that one can reduce the diverse specific qualities of bodies to motion and form, or any such simple geometrical parameters" (*ibid.*, p. 144).

Chemical reactions "imply the transformation of the reactants, giving rise to qualitative change, and a fundamental shift in the identity of matter". In consequence, "no explanation in terms of the simple physical juxtaposition of particles can conceivably be adequate to the phenomena involved" (*ibid.,* p. 142). How could one explain phenomena that change the fundamental qualities of matter in terms of the qualities being transformed? How could those qualities define identity in the context of their change? The chemical approach thus diverges from the physicalist by adopting an "anti-essentialist" perspective, by disposing of the "mechanical puppet-master behind the scenes that explains the phenomenal world" and replacing it by "material agents that allow new properties to emerge through their different relationships with one another." (*ibid.*, p. 209) We propose two modifications on this thesis:

(1) The point of dissent may be seen not as much as regarding the reduction of sensorial qualities to other intangible, essential qualities, but as regarding the reduction of the complex network of relations among the substances to *any quality that ontologically precedes them*. For instance, the "metric approach" to chemistry with which Lavoisier attempted to reduce chemistry to the measurement of specific weights (Kim 2003, pp. 297-303) did not demand any "mechanical puppet-master". Yet this unsuccessful enterprise has been seen by historians as foreign to the chemical tradition, either the work of an amateur chemist or of someone insensitive to "the usual protocols of chemical practice" (*ibid.,* pp. 300-1 and references). This approach was alien to chemistry not because it reduced other qualities of matter to specific weight, but because it intended to detect substances in a solution through the metric measurement of a single quality, instead of doing it through "a web of chemical operations" (*ibid.,* p. 301). In the chemical approach, specific weight, or *any other quality of matter*, should come into being *after* the relations between substances.

(2) Relation selectivity is fundamental in understanding the rejection of this form of physical reductionism. Bensaude-Vincent and Simon build an interesting argument in terms of the problem of dealing with radical change, but we think that this problem is not enough to support the inadequacy of corpuscularian ontologies. We point to the fact that, if anything could transform into anything else, corpuscularian mechanism could easily deal with radical change: the transmutability of all substances into each other was one consequence of Boylean corpuscularianism, and no overly complicated elaborations on the different kinds of particles were necessary to support it (Kuhn 1952). On the other hand, as we said above, as soon as the selective character of chemical transformations is considered, the types and attributes of the

corpuscles are multiplied. Relation selectivity is useful to complete the argument because it is due to relation selectivity that corpuscularian mechanism in chemistry cannot succeed.

3. Chemistry as a science of internal relations

We have argued that corpuscularism conceives relations as external, explaining the relative theoretical sterility of this approach in seventeenth-century chemistry, despite the efforts of several members of the *académie*. A similar argument could enrich our understanding of the rejection of Boylean philosophy of matter, or of the assimilation of some elements of Newtonian philosophy in eighteenth-century chemistry.[4] For now we leave such analyses of the divergence between physicalism and the chemical perspective, and focus on the later. Thus, in what remains of this article, we intend to show how core chemical concepts, instruments, and methods carry some features proper of the internal conception of relations.

3.1 Chemical atomism

Though corpuscularian and Newtonian atomistic approaches were unsuccessful in chemistry, not all forms of atomism failed in the same extent. As Bensaude-Vincent and Simon remind, the discontinuity implied by atomism fits quite well with the phenomena of chemical combination (Bensaude-Vincent & Simon 2008, pp. 139-140). In this section, we claim that atomism can be introduced as an internal relation ontology that is more coherent and valuable to the chemical approach. Daltonian atomism offers an example that supports this claim.

On its most chemical vein, Daltonian atomism can be formulated as the assumption that "each chemical element has least parts that are all alike and which *combine* in simple and characteristic ways to form the least parts of compounds" (Chalmers 2008, p. 159, our italics). Those "least parts" are so in reference to experimental chemical methods, not to any underlying Newtonian reality. This formulation of atomism in nineteenth-century chemistry has been popularized by Alan Rocke under the name of "chemical atomism" (Rocke 1984).

Unlike the physical atoms, chemical atoms are fundamental units of *chemical combination*. Their atomic character is bounded not to their status as indivisible particles, but to their appearance as 'minimum factors' arising from the laws of proportions. Furthermore, they are devoid of intrinsic properties other than the potential to combine. Properties of the chemical atoms "are not specified in advance by embedding them in some physical theory but *are to be discerned as a result of chemical research*" (Chalmers 2008, p. 162, our italics). They arise as the substances are mixed and transformed, they come into being *after* they are put in relation with each other. This is true even for atomic weight. Notice that Dalton's proposal of atomic weight as the fundamental property of the elements did not mark the birth of a deductive theory of reactivity, but of the long experimental enterprise of discerning atomic weights "as a result of chemical research" and their implications on synthesis and analysis of chemical substances. Chemical atomism, then, can be seen as an ontology of internal relations, since its atomic entities are devoid of any property that precedes their relations.

Recently, Needham (2004) and Chalmers (2008) have posed strong doubts on the theoretical relevance of Daltonian atomism in the nineteenth century. Chalmers argues that it only explains the laws of proportions, and compares its status with that of aether in nineteenth century physics. Needham says it explains nothing new and argues that it is epistemically viable to interpret the laws of chemical combination without resource to Daltonian atomism. Our thesis regarding the epistemic value of Daltonian atomism as an internal relation ontology needs to address these criticisms.

It seems to us that the authors' demands for explanations are calling for a deductive theory that, as we have argued, is not natural to chemistry's conception of relations as internal.[5] The expectation of a cause-consequence relation between the atoms and chemical combination goes back to the physicalist face of Daltonian atomism. In chemical atomism, the relation between atomic weights and chemical combination is more sophisticated: atomic weights are inductively determined by chemical reactions, but at the same time the former modify the latter. Ever since Dalton the writing of chemical formulas has depended heavily on atomic weights, a matter that has severe theoretical implications.[6] The interdependence between the formulation of chemical relations and atomic weights is what gave them a central place in nineteenth-century chemistry. Rather than regarding Daltonian atomism as an explanatory tool, we think of it as a proper framework for speaking about chemical combination, a framework that other atomistic ontologies could not offer.[7]

3.2 Nomenclature

Nomenclature has been one of the nuclear elements of chemistry at least since the chemical revolution of the eighteenth-century. The central role of language is stated quite explicitly in the preliminary discourse of Lavoisier's *Traité eléméntaire de chimie* (Lavoisier 1864 [1789], pp. 1-2), which supposedly would have derived from an effort to reform chemical nomenclature.

Though insignificantly small when compared with modern IUPAC nomenclature, it is worth noting that most of this reformed nomenclature has subsisted until the present day (IUPAC 2010). We doubt that this persistence can be understood as the consequence of a force of habit. Such could be the case for some particular names, but by no means could we expect the same for the whole system. The nomenclature of the chemical revolution reveals fundamental aspects of the one we use today (Bensaude-Vincent & Simon 2008, pp. 204-5). In consequence, we briefly analyze the nomenclature of the group of the Arsenal to show how this chemical language evidences that the entities being named are internally related.

Let us consider, then, the case of *oxygène* (oxygen) and *azote*. Both names have Greek roots: 'oxygen' comes from the Greek words ξύς (sharp, for the taste of acids) and γένος (producer, begetter). Oxygen is then the generator of acids. '*Azote*', on the other hand, comes from the Greek word ζωή, meaning lifeless, as this gas cannot sustain the life of the animals that breathe it. Both names were proposed within the group of the Arsenal, but at least Lavoisier's attitude towards them was very different: while the first was a good name, a "name that comports a systematic idea", the second "presented something extraordinary" in that it did not actually fit the chemical system being built (Lavoisier 1864, p. 48).

'Generator of acids', for instance, summarizes the role of oxygen in chemical transformations: to combine with radicals to yield acid substances. It expresses what is fundamental of this substance to chemistry by relating it to the radicals it interacts with and to the acids it transforms into. 'Oxygen' is seen as a proper name because it defines the identity of the substance by its relations to other substances: oxygen is a material whose reactions yield materials of the acid type.

'*Azote*', on the other hand, does not express other facts than that an animal immersed in this gas will die after a short time. It says nothing about the way the substance relates to others substances. It does not express any fact of chemical relevance, as Lavoisier acknowledged:

> The chemical properties of the non-breathable part of air not being well-known yet, we have settled for deducing the name of its base from the property of this gas of depriving of life the animals that breathe it, and we have named it azote […] We have not hidden that this is a somewhat extraordinary name […] For a long time, in fact, we looked for a better name […] we were tempted to name it alkaligen gas, as it has been proven, by M. Berthollet's experiences, […] that this gas enters in the composition of the volatile alkali, or ammonia […] it is in fact proven that it enters equally in the combination of nitric acid; it would be equally proper then to name it nitrigen principle […] In the end, we have been forced to reject a name that comports a systematic idea, and we have not risked a mistake by adopting the name of azote and azo-

> tic gas, which expresses nothing but a fact, or better a property: that of depriving of life those animals that breathe this gas. [*Ibid.*, pp. 48-49].

The dissatisfaction in this paragraph is evident, and contrasts his defense of the also newly proposed name of ‘oxygen’: after criticizing common substance names (*ibid.*, pp. 8-12) and declaring that “we have not taken any difficulty to modify them in such a manner as to convey more determinate ideas” (*ibid.*, p. 47), he says regarding oxygen: “We have given the base of the breathable part of air the name of oxygen, [...] because in fact *one of the most general properties* of this base is that of forming acids *by combining with most substances*” (*ibid.*, p. 48 , our italics).

‘Oxygen’ is a meaningful name, a name that speaks of its chemical identity, and chemists would do well getting used to it. ‘*Azote*’ is a name taken out of caution, matching the stubborn empiricism of the French school. It is a temporary visitor in the chemical language, pending replacement as soon as enough facts have been collected to determine the chemical identity of the corresponding substance.[8] Lavoisier follows the ideas of his predecessors in the early eighteenth century (if not earlier) by regarding elements as “actors in chemical operations” that are “defined by how they act and react in a network of relations with other chemical actors” (Bensaude-Vincent & Simon 2008, p. 203). In consequence, simple substances were designated by names pointing to their potential to combine with substances of certain kinds to produce new compounds. Compound substances, as well, received compound names pointing to the interaction of two substances that combine to produce the one being named: acids and oxides are given names that invoke oxygen, a radical, and the oxygen-saturation level; and the names of salts recall the acid and oxide that produced it. The project of the new nomenclature configures a theory of internal relations, since it identifies each and every substance precisely by its relations with other substances and nothing more.

3.3 Formulas

Formulas are among the ‘trademarks’ of chemistry (Klein 2003, p. 2, in reference to a quote by Hoffmann and Laszlo). Though not the first to propose chemical formulas, the ones chemists use today are descendants of those introduced by Berzelius and copied, exploited and enriched by organic chemists in the nineteenth-century (Klein 2003). Klein has emphasized the power and complexity of chemical formulas by challenging the view that “Berzelian formulas were merely a shorthand for names” (*ibid.*, p. 11). This challenge presupposes the assumption that chemical names are nothing but simple conventions, which as we argued, is not exactly the case. Chemical formulas in organic chemistry inherit and extend the spirit of the nomenclature introduced in the eighteenth century, and a significant part of their power lies therein. The debate between Laurent and Berzelius regarding the phenomenon of organic substitutions serves as an example to illustrate this point.

Following Dumas discovery of the substitution of hydrogen by chlorine, Laurent proceeded to test and characterize this phenomenon in several compounds. While working with unsaturated hydrocarbons, he found two different kinds of chlorine substitution: one where equivalent quantities of hydrogen were substituted by chlorine, and a second where the amount of hydrogen displaced was not equivalent to the amount of chlorine absorbed. He called the compounds resulting from the latter hyper-chlorides, and those resulting from the former chlorides. Furthermore, when characterizing them, he found that

> 1. All the halides […] can be distilled without alteration. 2. All the hyper-halides […] are decomposed by distillation. 3. All the halides are undecomposable by potash. 4. All the hyper-halydes are decomposable by potash. [Laurent, 1963 (1855), p. 48]

It is this invariance which caught his attention:

> The first fact which struck me in these substitutions, was the stable condition of equilibrium of the halides […]. I perceived these groups, however great the quantity of chlorine they contained, resist, contrary to all previous experience, the action of alkalies. [*Ibid.*, p. 57]

Such behavior resembled that of the hydrocarbons themselves rather than that of previously known compounds of chlorine. Laurent furthered the experiments and found similar phenomena regarding the naphtalines and the carboxylic acids.

The root of the controversy lay precisely in Laurent's referring to chlorine compounds as if they were hydrogen compounds. In the early days of organic chemistry, Berzelius pleaded for initial analogy with the theory of inorganic chemistry as the optimal method for constructing a theory of organic chemistry. As a consequence, chemists should begin by assuming that the structure of organic compounds was consistent with the electrical dualism of inorganic chemistry (Hedley 1971, pp. 380-1), and reflect that dualism in their formulas. Now, since chlorine and hydrogen occupied distant positions in the electro-chemical series, their electrical polarities were expected to be highly different: chlorine was expected to be negative relative to carbon, while hydrogen was expected to be positive. In the dualist electrochemical theory, hydrogen and chlorine were to play opposite roles in carbon compounds, so that the formulas of the chlorides should significantly differ from those of the hydrocarbons. While Laurent's formulas for the halides closely resembled those of the corresponding hydrocarbons, Berzelius proposed formulas that radically diverged from them. Thus in order to preserve dualism, Berzelius identified chloride of benzoyle as a benzoic oxy-chloride

$(C^{14}H^{10}O^{3})+(C^{14}H^{10}Cl^{3})$ (Laurent 1963, p. 60), and tri-chloro acetic acid as $(C^{2}O^{3})+H^{2}O+C^{2}Cl^{6}$, "a combination of oxalic acid with an unknown oxalic chloride" (*ibid.,* p. 63).

Intending to present further evidence in favor of the phenomenon of chlorine substitution, Laurent produced chlorine-substituted derivatives of the recently discovered isatine whose behavior resembled that of isatine itself. Upon receiving Laurent's memory, Berzelius "endeavored to show that the chloro-derivatives of isatine, isathyde, &c, were, the one a sub-porrindinous sub-hypochlorite, the other a fluvidinous hypochlorite, and a third and acid of rubindene, &c." (*Ibid.*, p. 65) To which Laurent replied:

> A sub-hypochlorite volatile without decomposition! A sub-hypochlorite undecomposable by sulphuric acid! A sub-hypochlorite without action upon vegetable colouring matters! A sub-hypochlorite of an unknown oxide of an unknown porrindene! [...] It is almost incredible. [*Ibid*].

Just as we saw in the nomenclature introduced by the chemical revolution, Laurent's formulas insisted in respecting the status of chemical relations among the substances as determinants of their identity. He regarded this as a more fundamental principle than electrical dualism, not just in organic chemistry but in chemistry as a whole. Berzelius' dualistic formulas were meaningless because they no longer said anything about this chemical identity of substances. 'Sub-porrindinous' and 'sub-hypochlorite' became empty words, and the corresponding formulas became meaningless, the moment they stopped referring to a family of compounds that decomposed by the action of sulfuric acid or heat, that bleached vegetable colorants, that could be obtained from oxides of porrindene. He even declared quite explicitly his adherence to this principle, putting it above any atomistic concerns:

> In reply to the question, what is meant by the words: 'The chloro-ether continues an ether?' I might repeat, what I have just said, namely, that the arrangement of its atoms is the same as that of the normal ether. But I prefer to leave hypotheses aside, and say simply, that *an ether* [i.e. a modern ester] *is a body obtained by the reaction of an acid upon an alcohol, with an elimination of water, and that under certain circumstances that ether can be divided, either by regenerating the alcohol and acid which gave it birth, or by forming products which belong to the families of the alcohol and of the acid* [...] Whether or not the halides exist as such in the hyperhalides, aldehydes, and chloracids, is a matter of but little consequence. Whatever atomic arrangement we may please to imagine, we cannot destroy the fact, that certain substances may experience chlorine substitutions *without losing their fundamental properties*. [Laurent 1963, our italics].

The first part makes clear what the "fundamental properties" of chemical substances are, while the second formulates the phenomenon of substitution that guided his writing of formulas not in reference to an atomic reality, but to the preservation of those fundamental properties. Laurent conceived compounds not as “concatenations of elementary building blocks” but as “chemical agents” that participated in reactions (Bensaude-Vincent & Simon 2008, p. 204). These reactions thus characterized the chemical identity of a compound that was imprinted in its corresponding formula; if that identity was no longer consistent with the dualism of inorganic chemistry, then the analogy had to be dropped.[9]

It is true that many other developments took place between the work of Laurent and today’s formulas. We believe that the internal conception of relations reflected in chemical formulas can be traced through many of these developments, particularly through the invention of chemical graphs, which today constitute a valuable tool for chemists.[10] Even though we will not advance an analysis that supports this belief here, we hope that the short example we presented illustrates an attribute of chemical formulas that chemists can recognize in the tools of their trade.

3.4 Classification

Classification of substances is one of the principal goals and means of chemistry. Chemical formulas, in fact, are to a large extent lexical and visual representations of classificatory schemes that summarize our knowledge regarding reactivity.[11] This classificatory schemes are very peculiar in their recursiveness: just as substance identity is determined by its relations to other substances and not by its own qualities in isolation, when building chemical classifications the same approach leads to an entangled, recursive system, where no class can be defined in isolation. Such classificatory systems can be seen not only in the formulas of organic chemistry, but even in the nomenclature of the eighteenth-century French chemical revolution.

Since a material is named and characterized by its relations to substances of different kinds, such kinds need to be defined in the same terms in order to fully characterize the material. Consider, for instance, the concept of oxygen in the context of Lavoisier’s *Traité*. Previously we discussed how, by characterizing this substance as the generator of acids, it is being identified in the relations it establishes with two kinds of substances: radicals and acids. But then, one is forced to ask what an acid is, and to answer in the same terms of invoking the chemical relations of substances of that kind. Precisely, in the *Traité* the chapter on ‘The nomenclature of the different constituents of the air’, where oxygen is introduced, is promptly followed by a chapter ‘On the nomenclature of acids’, that deals with this issue by naming an acid as the concatenation of the names of the two substances that produced it (a radical and oxygen). In the following chapters, oxides and salts are once more defined by the act of giving them a name that references their precursors;

oxygen and a metal in the first case, an acid and an oxide in the second. In this way, the class of acids is defined by its relations to the class of radicals and to the unitary class of oxygen as precursors, to the class of oxides as reaction partners, and to the class of salts as derivatives. This comports a form of recursiveness, wherein no class can be defined prior to the others: only after the whole classification scheme is completed can we strictly say what an acid is.

Substance classes are thus constructed from the relational pattern of the network of substances.[12] In other words, they are characterized within the same internal relation ontology that characterizes the substances: they have no property that precedes that of being related with each other. In the end, a relational structure results that lets the chemist tell what kinds of substances combine to produce what kinds. In this way, the chemist constructs a reduced representation of the original network of substances that summarizes his current knowledge regarding their chemical behavior.

The same approach is kept in organic chemistry, though the amount and complexity of the phenomena accounted for increases. Recall Laurent's distinction between halides and hyper-halides (Laurent 1963, pp. 48-60). This classification of the products of halogen substitution of hydrocarbons obeys to the fact that products of the first class mimic the chemical behavior of the original hydrocarbon, while those of the second do not. This relation-driven classification was to be reflected in chemical formulas, as defenders of type theory as Laurent himself reiterated: chlorine in halides should occupy the same place of hydrogen in the formulas of the corresponding hydrocarbons, in order to express the fact that both substances where of the same *type*, that the way they reacted with other substances was equivalent (Bensaude-Vincent & Simon 2008, p. 204); but the same demand was not made for the hyper-halides, as they reacted in a very different manner. Even today, the basic classification of organic compounds according to their functional group goes in the same direction: we use lexical invariants in our formulas (-OH, -COOH, -CHO) to express the inclusion of the corresponding compounds in recursively defined classes: alcohols (a class of substances coded by the -OH motif) are defined as substances that react with carboxylic acids (-COOH, another class) to produce esters (-COO-, another class), etc; carboxylic acids in turn are substances that can react with certain halogenated compounds to produce acyl-halydes, and so on.

Beyond inorganic nomenclature and organic formulas, the most distinctive image of the success of chemical classification is probably Mendeleev's periodic table. The main information content of the periodic classification is arguably primarily relational: while physical constants that characterize the elements (*e.g.* boiling point, melting point, density) vary over a large range in any given group, each and every element of the group 1 interacts violently with any element of the group 17, yielding binary compounds of similar reactivity. The principle is the same as identified before: classes are defined by the ability of their members to react with members of a given class, producing members of another specific class.[13] Following the same vein of organic and inorganic classifications of compound substances, the periodic system of elements shows the prevalence of the internal conception of relations among the entities that we propose as a characteristic of the chemical approach. Modern studies on the periodic system support this assertion by showing the dominant character of descriptors of reaction selectivity in reconstructing and transcending the periodic table through the use of cluster analysis and topology (Restrepo et al. 2004, Leal & Restrepo 2009).[14]

This dominant character of the ontological conception of the elements as internally related in the periodic system can also be seen in community reactions to the first reports on the noble gases. Upon their discovery, the existence of these substances was regarded a threat to the periodic system (Bensaude-Vincent 1986). In fact, when Lord Rayleigh gave his 1895 lecture before the Royal Institution on the matter of the newly discovered argon (Rayleigh 1895), his tone was both confident regarding the novelty and elemental character of the substance that he and Ramsey had characterized, and apologetic regarding the disconcerting awkwardness of its properties. Rayleigh even declared that "the facts were too much for us; and all we can do now is to apologise for ourselves and for the gas" (*ibid*).

The properties of the gas were, indeed, surprising. For example, it had an exceptionally high ratio of specific heats, approaching the theoretical limit. This fact implied some extraordinary energetic properties. However surprising, it was not this property which met the skepticism of chemists, but the astonishing inability of the gas to react with any matter under any known conditions. Regarding this point Rayleigh did not content himself with an apology: he categorically denied that either he or Ramsay had ever thought the gas to be completely inert.[15]

The peculiar thermal properties of the gas were just that: peculiar. Its inactivity, on the other hand, was an oddity that had to be attributed to insufficient experiments. Rayleigh even went as far as quoting Berthelot as having announced a successful attempt to make argon react with benzene with the assistance of an electric discharge, though no reference was given (*ibid*). This suggests a powerful intention of settling the matter as soon as possible.

This resilience towards the existence of an inert matter can be explained in terms of the ideas we have introduced so far: if chemical substances are conceived as internally related, a substance incapable of interacting or transforming seems devoid of chemical identity. Being inert, the gas "*did not exhibit any chemical property*" (Bensaude-Vincent 1986, p. 16), which forced the use of physical properties for characterizing the substance within the periodic system, an enterprise that brought such difficulties that Mendeleev even denied its elemental character (*ibid.*). With this move, Mendeleev was trying to move the disconcerting argon away from the realm of the chemical elements, in an attempt to protect his oeuvre. The issue here, then, was not whether noble gases could exist in absolute terms, but if they existed within the scope of chemistry.

Of course, a closer look reveals that inert substances can have a proper and important place in chemical theory. In characterizing a chemical substance the occurrence of certain characteristic reactions is just as important as the absence of others (Schummer 1998). The inert character of the noble gases then can be thought of as a chemical property. The nature and raise of noble gases in chemistry can, in this sense, be understood as analogous to the number zero in mathematics: at first it is disconcerting, seemingly counter-natural and hard to grasp; but once one has, it promptly becomes a fundamental element in algebra. Noble gases were put at the end of Mendeleev's periodic system, and eventually came to be considered legitimate.

Now, following Bartlett's report of the synthesis of $Xe^+[PtF6]^-$ (Bartlett 1962), the first compound of a noble gas ever known, a frenzy possessed the chemical community, so large that within two years more than sixty papers relating to noble gas compounds were published (Gay 1977). In stark contrast with the situation sixty years earlier, the idea that the previously thought-to-be-inert gases could actually be active faced no resistance at all.

This fact might be presented as a success of the ideas introduced by Pauling and Coulson regarding the quantum-mechanical foundations of chemistry, which promptly offered an explanation to the newly found phenomenon. However, as Gay (1977) points out, the theoretical tools necessary for predicting the existence of noble gas compounds had been available for some years, and in fact, they had been used with that purpose. These predictions, however, were mostly overlooked: at the time, quantum chemistry was more of an explanation device than a predictive tool and could not be put to use before the facts had been accepted (*ibid.*, p. 63). Thus, we doubt that the enthusiasm following Bartlett's article could be attributed to the power of a new theory. Instead, we believe that after several generations conceiving their entities as internally related, his discovery found chemists readily prepared to accept it.

4. Conclusion

Nomenclature and formulas in chemistry speak of a peculiar classification scheme, one which is determined by chemical reactions. This shows the prevalence of relations between the substances over any quality that can be ascribed to them, a prevalence that distances chemistry from physicalist approaches. This ontological option needs not to be taken in response to a belief in an ultimate microscopic reality, but neither in opposition to it. Instead, it is advisable in order to address the epistemological challenge posed by the selectivity proper of the empirical phenomena that has drawn the attention of chemists. That challenge prefigures the initial inadequacy of several atomistic ontologies; not due to their being atomic, or even to their belief in an essential, imperceptible reality, but to their conception of relations as external: external relations promote a sub-optimal methodological approach to the project of achieving knowledge on selective relations. Chemical atomism, on the other hand, constructs all properties of its atoms through the reactivity of substances; its success in nineteenth-century chemistry can then be understood in terms of its status as an ontology of internal relations.

We believe that this analysis of the philosophical foundations of chemical relations is of relevance to chemistry as it is practiced today. Consider the QSAR paradigm that occupies a prevalent place in modern chemistry: chemical activity of materials is a function of their structure. Here 'structure' refers to the intimate constitution of matter and determines 'activity', which refers to the behavior of substances in chemical reactions. As overly-simplistic as this picture is, it stills serves to see how the paradigm mixes two opposing perspectives, and to raise a concern therein: the 'structure' part has engendered several approaches, including quantum-mechanical images (*e.g.* Carbó-Dorca et al. 2001), graph-theoretical representations of structural formulas,[16] matrix representations derived from spectroscopic data, and hybrids thereof (*e.g.* Marín et al. 2008). These models of significant ontological variety and complexity contrast with the overly simplified approach frequently used for the 'activity' part: properties as phase transition constants (Randic 1975) or a kinetic constant of a particular reaction of interest[17] are used as the unique representation of each substance in activity space. These simplistic pictures hardly say anything about the complex set of relations established by chemical reactions. A simple numeric index cannot pretend to talk about the selectivity of chemical relations that 'activity' references.

The recent raise of network analysis in chemistry opposes this take on the problem. Overlooking any concerns for the intimate structure of matter as it broadens the perspective to encompass a large universe of chemical reactions, this approach looks at substances as mere nodes interlinked in a network of chemical reactions. Qualities of the isolated entities are forgotten, emphasis is shifted back to their relations. Interestingly, many network models introduced in chemistry come from its biological frontier.[18] This reminds us of Bensaude-Vincent's recent assertion that "biology teaches chemists that success comes with improving the art of mixing heterogeneous components and working out elegant solutions to complex problems. Consequently, the focus is less on the ultimate components of matter, than on the relations between them." (Bensaude-Vincent, 2006, pp. 18-19) It is amazing that at the beginning of the twenty-first century biologists have to give chemists this reminder.

Notes

[1] Bensaude-Vincent & Simon 2008. Regarding the relational character of chemistry, see also Soukup 2005 and Cassirer 1923, pp. 203-219.

[2] "'Chemical property' [in eighteenth-century chemistry] referred to observable phenomena that were created when a substance was heated or mixed with a reagent" (Klein & Lefèvre 2007, p. 27); "elements [...] are defined by how they act and react in a network of relations with other chemical actors. This second sense of operational definition is more fundamental than the first, and was characteristic of chemistry even before Lavoisier introduced this explicitly pragmatic definition of the element." (Bensaude-Vincent & Simon 2008, p. 203).

[3] "Based on a positivist principle that science should limit itself to observable facts, these French anti-atomists condemned the approach because it went beyond experience. Although Duhem discussed this argument, it was not his principle criticism [...]. The problem that Duhem sees with atomism is, therefore, not so much its status as a metaphysical hypothesis, *but its weak explanatory power*" (*ibid.*, p. 127, our italics). "In his discussion of chemistry and physics, he [Béguin] argues on the basis of *an epistemological principle* that the specific properties of material bodies need to be reduced to the smallest possible number of discrete ontological principles" (*ibid.*, pp. 137-138, our italics).

[4] It has been suggested that Newtonianism approached atomism to the cause of chemistry when it was used to replace the hooked, pointed, rounded, etc. attributes of the corpuscles with the simple idea of an occult attraction, that approached the concept of affinity and stimulated the elemental perspective, but it moved away again when that attraction was reduced to attributes of the particles such as figure (see e.g. Kim 2003, pp. 246-252, regarding the case of Guyton's Newtonian model of chemical action, and Kuhn 1952, p. 35). On the first case, qualities of the entities are forgotten and emphasis is displaced to a relation that demands no explanation, thus moving us towards an ontology of internal relations; on the second, there is a throwback to the enterprise of explaining selective affinities in terms of essential qualities of the bodies, thus moving towards an ontology of external relations.

[5] This is clearer in Needham, whose main criticism concerns demands for Daltonian atomism to explain chemical affinity (Needham 2004, p. 1044). Chalmers is more measured, understanding 'explanation' in a way that accepts Daltonian atomism as an explanation of the laws of proportions. The root of our disagreement might be in Chalmers' demand that Daltonian atomism also explains physical properties of matter (Chalmers 2008, p. 160), or in his apparent belief that formulas before the revolution of organic chemistry have a lower epistemological status than after (*ibid.*, 160-1).

[6] Examples of this theoretical implications abound; Hedley (1971, p. 385) offers a sophisticated but illustrative one: powerful analogies between organic compounds and inorganic compounds that guided research in the challenging field of organic chemistry and that were central to the emergence of a unified discipline faded with each restatement of the proper empirical formulas for the compounds involved. For instance, the analogy between acetic acid ($C^4H^6O^3+H^2O$) and sulfuric acid (SO^3+H^2O) faded if Gerhardt's suggestion that $C^2H^4O^2$ is the correct empirical formula for acetic acid was accepted – such formula cannot be written in the RO^3+H^2O form.

[7] We have not questioned Chalmers' assertion that many nineteenth-century chemists did not commit to atomism at all, and that there was a rationale to that decision (*ibid.*, p. 162). We agree with this assertion as long as we attach it to a definition of atomism restricted enough to clearly identify those chemists' beliefs as non-atomistic. But we would rather not go deeper into this matter: regardless, we have shown how Daltonian atomism could provide an ontology consistent with the pursuit of chemical knowledge, and that is far more than what corpuscularian mechanism could achieve.

[8] The fact that it was ultimately named *nytrogen* further supports this view on the matter.

[9] It is very likely that Berzelius was not insensitive to this argument, as by 1843 the controversy had shifted from the rejection of the dualist analogy to Laurent's inversion of the direction of analogy between organic and inorganic chemistry (Hedley 1971, pp. 383-4).

[10] Chemical graph theory is a very active field of research. For a recent review see García 2008.

[11] Kim 1992, p. 69; also Chalmers 2008, p. 161. Regarding the interplay between chemical formulas and modern reaction classification methods see Chen 2003.

[12] At this point it is interesting to return for a moment to the comparison between physicalist and chemical approaches. At the beginning we pointed out that when relations are non-selective it does not make much sense to ask *which* objects are related. In this sense, relations do not establish a rich classification scheme among the entities. This remark gives a rationale for the contrast between the complexity and central role of classifications in chemistry, and the relative homogeneity of the particles in mechanism.

[13] Schummer 1998 has formulated this principle in terms of chemical similarity.

[14] In this discussion we have avoided reference to the fact that elements in Mendeleev's system are defined as *basic substances*, as opposed to elements regarded as *simple substances* (Paneth 2003 [1931]); an innovation that some authors have considered central and perhaps unavoidable when discussing the periodic system (*e.g.* Bensaude-Vincent 1986). In reply, we note that basic substances are unavoidably combined and completely devoid of any other quality. So a case can be made for basic substances being a perfect instance of internally related entities.

[15] "We never have asserted, and we do not now assert, that argon can under no circumstances be got to combine. That would, indeed, be a rash assertion for any one to venture upon." (*Ibid.*)

[16] Randic 1975 is one of the seminal works on this area.

[17] Cramer et al. 1988 sets one of the standards for validating QSAR models, which consist in evaluating the capability of the structural model to produce a predictor

that correlates with the kinetic constants of a single biochemical reaction on a set of 31 steroids.

[18] See e.g. Barabási & Oltvai 2004, Dittrich et al. 2001, 2007, Klamt & Gilles 2004. Benkö et al. 2003 integrates some elements from quantum mechanics and structural formulas. Daza & Bernal 2008 and Restrepo & Leal 2009 use similar models for approaching the old problem of substance classification.

References

Baird, D.; Scerri, E.; McIntyre, L. (eds.): 2006, *Philosophy of chemistry: Synthesis of a new discipline*, Dordrecht: Springer.

Barabási, A.; Oltvai, Z.: 2004, 'Network biology: understanding cell's functional organization', *Nature reviews: genetics*, **5**, 101-114.

Bartlett, N.: 1962, 'Xenon hexafluoroplatinate $Xe^{+}[PtF_{6}]^{-}$', *Proceedings of the chemical society of London*, **6**, 218.

Benkö, G.; Flamn, C.; Stadler, P.: 2003, 'A graph-based toy model of chemistry', *Journal of chemical information and computer science*, **43**, 1085-93.

Bensaude-Vincent, B.: 1986, 'Mendeleev's periodic system', *The British Journal for the History of Science*, **19**, 3-17.

Bensaude-Vincent, B.: 2006, 'Two cultures of nanotechnology?' in: J. Schummer and D. Baird (eds.), *Nanotechnology challenges: Implications for philosophy, ethics and society*, Singapore: World Scientific.

Bensaude-Vincent, B.; Simon, J.: 2008, *Chemistry: The impure science*, London: Imperial College Press.

Carbó-Dorca, R.; Amat, L.; Besalú, E.; Gironés, X.; Robert, D.: 2001, 'Quantum molecular similarity: theory and applications to the evaluation of molecular properties, biological activities and toxicity' in: R. Carbó-Dorca, X. Gironés and P. Mezy (eds.), *Fundamentals of molecuar similarity*, New York: Plenum.

Cassirer, E.: 1923, *Substance and function and Einstein's theory of relativity*, Chicago: Open Court.

Chalmers, A.: 2008, 'Atom and aether in nineteenth-century physical science', *Foundations of chemistry*, **10**, 157-166.

Chen, L.: 2003, 'Reaction classification and knowledge acquisition' in: J. Gasteiger (ed.), *Handbook of chemoinformatics*, Weinheim: Wiley-VCH.

Cramer, R.; Patterson, D.; Bunce, J.: 1988, 'Comparative Molecular Field Analysis (CoMFA) 1. Effect of shape on binding of steroids to carrier proteins, *Journal of the American Chemical Society*, **110**, 5959-67.

Daza, E.E.; Bernal, A.: 2008, 'A hyperdigraphic model of chemical activity: acid-basic behavior from a network model', presentation at the *23rd Math/Chem/Comp, 10-13 June 2008*, Verbania, Italy.

Dittrich, P.; Ziegler, J.; Banzhaf, W.: 2001, 'Artificial chemistries – a review', *Artificial Life*, **7**, 225-275.

Dittrich, P.; Speroni, P.: 2007, 'Chemical organization theory: towards a theory of constructive dynamical systems', *Bulletin of Mathematical Biology*, **69**, 1199-1231.

Ferrater-Mora, J.: 2004, *Diccionario de Filosofía*, Madrid: Ariel.

García, R.: 2008, 'Some new trends in chemical graph theory', *Chemical Review*, **108**, 1127-69.

Gay, H.: 1977, 'Noble gas compounds: A case study of scientific conservatism and opportunism', *Studies in History and Philosophy of Science Part A*, **8**, 61-70.

Hedley, J.H.: 1971, 'Organic synthesis and the unification of chemistry: a reappraisal', *The British Journal for the History of Science*, **5**, 363-392.

IUPAC: 2010, 'Nomenclature of Inorganic Chemistry' [http://old.iupac.org/reports/provisional/abstract04/connelly_310804.html], last visited, 25 May 2010.

Kim, Mi Gyung: 1992, 'The layers of chemical language I: Constitution of bodies v. structure of matter', *History of Science*, **30**, 69-96.

Kim, Mi Gyung: 2003, *Affinity, that elusive dream: A genealogy of the chemical revolution*, Cambridge, MA: MIT Press.

Klamt, S.; Gilles, E.: 2004, 'Minimal cut sets in biochemical reaction networks', *Bioinformatics*, **20**, 226-234.

Klein, U.: 2003, *Experiments, models, paper tools: Cultures of organic chemistry in the nineteenth century*, Stanford: Stanford University Press.

Klein, U. & W. Lefèvre: 2007, *Materials in eighteenth century science: A historical ontology*, Cambridge, MA: MIT Press.

Kuhn, T.S.:. 1952, 'Robert Boyle and structural chemistry in the seventeenth century', *Isis*, **43**, 12-37.

Laurent, A.: 1963 (1855), 'Translator's preface (by William Odling); Carbon, metallic and hydrogen, oxygen, and chlorine substitutions; theory of chlorine substitutions; nitrogen substitutions', in: T. Benfey (ed.), *Classics in the theory of chemical combination*, New York: Dover, pp. 40-68.

Lavoisier, A.: 1864 (1789), *Oeuvres de Lavoisier. Tome premier. Traité élémentaire de chimie,* Imprimerie impériale [available online at http://histsciences.univ-paris1.fr/i-corpus/lavoisier/book-detail.php?bookId=89] last visited 25 Sep. 2009.

Leal, W.; Restrepo, G.: 2009, 'Chemical elements, their sociology', *Journal of Scientific Education*, **10**, 126-7.

Marín, R.; Aguirre, N.; Daza, E.: 2008, 'Graph theoretical similarity approach to compare molecular electrostatic potentials', *Journal of Chemical Information and Modelling*, **48**, 109-118.

Needham, P.: 2004, 'Has daltonian atomism provided chemistry with any explanations?', *Philosophy of Science*, **71**, 1038-47.

Randic, M.: 1975, 'On characterization of molecular branching', *Journal of the American Chemical Society*, **97**, 6609-15.

Rayleigh: 1895, 'Argon', *Royal Institution Proceedings*, **14**, 524-537 [available online at http://web.lemoyne.edu/~giunta/Rayleigh.html] last visited 25 Oct 2009.

Restrepo, G.; Mesa, H.; Llanos, E.; Villaveces, J.: 2004, 'Topological study of the periodic system', *Journal of Chemical Information and Computer Science*, **44**, 68-75.

Rocke, A.: 1984, *Chemical atomism in the nineteenth century: from Dalton to Cannizzaro*, Columbus: Ohio State Univ. Press.

Schummer, J.: 1997, 'Towards a philosophy of chemistry', *Journal for General Philosophy of Science*, **28**, 307-336.

Schummer, J.: 1998, 'The chemical core of chemistry, I: A conceptual approach', *HYLE: International Journal for Philosophy of Chemistry*, **4**, 129-162.

Schummer, J.: 2003, 'The philosophy of chemistry', *Endeavour*, **27**, 37-41.

Soukup, R.W.: 2005, 'Historical aspects of the chemical bond: Chemical relationality versus physical objectivity', *Monatshefte für Chemie*, **136**, 803-813.

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