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PHILOSOPHY OF CHEMISTRY

Bernadette Bensaude-Vincent

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The notion of “philosophy of chemistry” challenges the singular in the phrase “philosophy of science”, which is the standard term for the discipline in the English language. This linguistic peculiarity has undoubtedly favored the tacit equation science = physics that has characterized mainstream philosophy of science during the course of the twentieth-century. The hegemony of physics has had profound consequences that have subsequently become identifiable. One of them is the increasing gap between philosophical reflection and science in action. As Joachim Schummer has pointed out: “Had those philosophers without prejudice gone into the laboratories, then they would have stumbled on chemistry almost everywhere”¹. For there is a striking contrast between the philosophers’ neglect of chemistry and the quantitative data, which show that chemistry is by far the largest scientific discipline in terms of the number of publications indexed by the major journals of abstracts. Thus, philosophers have virtually ignored the major part of scientific activity choosing instead to focus on theoretical physics, which seemed more appropriate in light of the “linguistic turn”.

The situation is slightly different in the European tradition. The plural “*philosophie des sciences*” which has prevailed in the French language may be due to Auguste Comte’s longstanding influence, since he strongly advocated a regional epistemology. The result is that chemistry has not been totally neglected. As I have argued elsewhere, chemistry helped shape the French tradition, especially in what can be labeled its “historical turn” and its focus on theories of matter². Whether French philosophers interacted more with active scientists than their Anglo-Saxon counterparts

or shared the scientists' interests remains a matter of debate for historians of the philosophy of science.

After decades of neglect of chemistry in mainstream philosophy of science, however, the late twentieth century witnessed an impressive revival of philosophical interest in the discipline. Philosophy of chemistry has become a dynamic research field, establishing itself as a sub-discipline in the 1990s. An *International Society for the Philosophy of Chemistry*, founded in 1997, has organized an annual summer conference. Two journals have been launched, *Hyle* in 1995 and *Foundations of Chemistry* in 1999. Chemists and chemistry teachers have been the prime movers behind this renaissance of the philosophy of chemistry. For them, the hegemony of physics in the philosophy of science resonated with the reductionist ambitions of quantum physicists, who denied the very existence of any independent theoretical foundations of chemistry. For chemistry teachers, Paul Dirac's famous 1929 claim that "the underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known", had always been a trauma, as it meant that their discipline could be taught as a sort of applied physics³. Their concern with the philosophical implications of Dirac's statement was not shared by working chemists, who knew that the reductionist research agenda was impossible to achieve because the calculations would always be too complex. However, when digital computers allowed *ab initio* calculations, theoretical chemists started to worry once again about reductionism and became more interested in philosophy. Chemists felt the need to demonstrate that chemical concepts could not be deduced from quantum mechanical principles, giving rise to a flood of technical publications about reductionism in the 1980s.⁴ Chemists, advocates of the autonomy of their discipline, tend to use philosophy as a battlefield for their heroic struggle against the imperialism of quantum physics. As a consequence, reductionism and foundational issues have been the main concern over the last decade. Subtle conceptual distinctions became strategic to limit the dominion of quantum mechanics over chemistry: "quantitative reduction" does not mean "conceptual reduction", "ontological dependence" does not imply "epistemic dependence"⁵. The notion of supervenience referring to asymmetric dependence has been envisaged as a possible substitute for the notion of reduction⁶. In this perspective, only a few aspects of chemistry – such as the interpretation of the

periodic system – have drawn philosophical attention, while concepts and practices in daily use by laboratory chemists have been overlooked. Ironically the overwhelming concern with reductionism threatens to lead to a reduction of the emerging field of philosophy of chemistry to theoretical issues. If this trend continues, chemistry would paradoxically be bound in philosophical allegiance to physics, condemned to spend its existence ruminating over Dirac's arrogant claim.

It is time for philosophers to face up to what is the most evident feature of chemistry, that it is not only a natural science but also a cornucopia of material technologies. Explaining and modeling are just two of its many facets. Chemistry is also about making, testing, measuring, improving yields... The dual face of chemistry demands a specific philosophical approach. It is not enough to revisit philosophical notions that have been sanctified in the context of a tradition of philosophy of science that has modeled its categories around theoretical physics. Indeed, to try to accommodate these notions to chemistry understood in its entirety is a hopeless task.

Chemistry needs a philosophy of its own. A number of French philosophers – Pierre Duhem, Émile Meyerson, Hélène Metzger – have paved the way for such an approach. In particular, Gaston Bachelard has suggested an alternative philosophy that he termed “metachemistry”⁷. Bachelard's aim in *The Philosophy of No*, was to describe a new trend in science embracing non-Euclidian geometries, non-Aristotelian logics, non-Cartesian physics, non-Lavoisierian chemistry. The prefix “non” means i) that today's science is not the continuation of the past and rather questions and challenges established knowledge through a polemical process; ii) the non-sciences are not however negations of past theories and rather include them as particular cases in a dialectical process. Since Bachelard's aim was to promote a new updated “scientific spirit” rather than digging into the singularity of the philosophy of chemistry, here I will try to explore what Alfred Nordmann presented as “the promise of metachemistry”⁸. This aim cannot be achieved without a move away from the “linguistic turn” that has prevailed in the logical-positivist tradition, aligning instead with the “practical turn” that characterizes more recent philosophical trends.⁹ In this respect, I am merely following a path opened by Roald Hoffmann, Nobel laureate for chemistry in 1981, and adding a historical dimension to his philosophical essays¹⁰. I will first consider the impact of

laboratory practices on chemical explanations and theories, before turning my attention to the issue of the ontological burden of chemistry.

KNOWING THROUGH MAKING

Any philosophical examination of chemistry should take into account the fact that chemistry is and always has been a laboratory science. The word “laboratory” itself, originally referred to the place where chemists worked and only gradually spread to include the spaces used for other kinds of experimental practice. Frederic Larry Holmes, a leading historian of eighteenth-century chemistry, insisted on the importance of this physical setting:

The problems and objects of study of chemistry have been provided by and limited by the operations that could be performed on materials in a chemical laboratory [...]. As theoretical structures changed and new objectives supplemented or displaced older ones, the stable setting of the chemical laboratory both identified chemists and distinguished them from other natural philosophers who dealt with some of the same phenomena that concerned them¹¹.

This physical niche determines both the object of chemical investigation and a specific way of knowing that is the chemists'. As the etymology of the term reminds us, the laboratory is a place of labour, of manual work rather than of inductive or deductive reasoning. The practice of chemistry is as much a physical activity as a mental exercise. Joan Baptista Van Helmont used to say that “God sells the arts in return for sweat”, meaning that knowledge of nature was to be obtained only at the cost of painstaking experiments¹². Chemists attempt to know substances by transforming them by means of manipulations and physical operations. Whatever the importance of chemical theory, chemistry is first and foremost concerned with making. Historically it was an art and craft before it became an academic science.¹³ Nowadays, if we look at scientometric studies, we can see that making new molecules remains a major part of the work found in academic publications¹⁴.

Historically, chemistry provided the grounds for criticizing the *esprit de système*, embodied by scholars “speechifying” in their doctoral robes. As an illustration, we can cite Diderot’s blistering offensive launched against speculative and abstract knowledge in *De l’interprétation de la nature*, an attack echoed in Gabriel François Venel’s heroic

portrait of the chemist as an “artist”, in his article “*chymie*” in the *Encyclopédie*¹⁵. More recently, Roald Hoffmann has written:

The reliable knowledge gained of the molecular world came from the hot and cool work of our hands and mind combined. Sensory data, yes, but we did not wait for Scanning Tunnelling Microscopes to show us molecules; we gleaned their presence, their stoichiometry, the connectivity of the atoms in them and eventually their metrics, shapes and dynamics by indirect experiments¹⁶.

Indeed, “indirect” may be a key word for understanding the chemists’ way of knowing nature. They use the detour of the laboratory to access nature. This does not simply mean that they use the mediation of instruments to understand natural phenomena, like experimental physicists do. Rather, they take mediating practices much further by insisting that only man-made, artificial products provide information about natural substances. To know the nature and properties of substances, chemists proceed by analysis and synthesis. Since the Renaissance, decomposition or the resolution of bodies into their components, combined with recombination or the recombination of the purported components to give the original substance, has provided the key to understanding material substances¹⁷. Joan Baptista Vico’s famous statement *Verum et factum convertuntur*, established that we can get rational knowledge only about what we have done¹⁸. For chemists, we can know only what we have produced through technological processes. As Bachelard noted, even when they extract plants or minerals from nature, chemists first submit them to a number of purifying processes¹⁹. Thus, they rely on facticity to understand nature. This is how Bachelard interpreted Marcelin Berthelot’s famous statement: “Chemistry creates its object”²⁰. Making things and making them as pure as artefacts is the chemist’s approach to nature.

Bachelard also emphasized the asymmetry between analysis and synthesis. Indeed analysis can provide chemists with some *evidence* about the nature and proportion of the constituents of substances. However, it will never give them *confidence*, for there remains the suspicion that the results of analysis were produced by the analytical tools rather than being preexistent in the compound. Analysis lacks definitive demonstrative power. While it may serve the purposes of falsification, only synthesis has the power to confirm. There is no way to overcome objections apart from recomposing the original compound from its purported components. Synthesis thus stands as the realization of a conjecture about the composition or the structure of a

substance. Chemical proofs depend on the reciprocity of analysis and synthesis, which are both indissociably intellectual and experimental processes. Their reciprocity is at the root of Immanuel Kant's admiration for Georg Ernst Stahl, who "transformed metals into calx and calx into metals"²¹.

"MAKING UP STORIES WHILE MAKING MOLECULES"²²

Making is the chemists' major activity, and it is more than simply a material practice. It also characterizes an intellectual practice. As Hoffmann put it, they are "making up stories" about what they are doing with their hands and flasks. Chemical theories, unlike theories in physics, are not really aimed at explaining phenomena. Rather, they try to make sense of phenomenological data using stories about tiny invisible atoms or molecules. As early as the seventeenth century, Nicolas Lemery forged hooked and spiny atoms to account for the behaviour of acids and alkalis, while modern chemists use molecular models to predict new compounds. In so doing, they do not claim to provide a causal explanation, and their theory is closer to being a narrative. Just as early-modern hooked and spiny atoms were a "Cartesian novel", modern electronic orbitals could be regarded as a "quantum novel". Similarly, the structural formulas invented by nineteenth-century chemists were not meant as representations of the real world of atoms and molecules. Thus, Charles Gerhardt, who was a staunch advocate of atomic notation, drew the formulas of organic compounds according to three molecular "types". He used these types to interpret a great many reactions, and even predicted unknown compounds by substituting radicals for hydrogen in each of the types. But he never suggested that his formulas reflected the internal architecture of the compounds he was representing and refused to view the radicals as isolable and real bodies. They were useful and indispensable fictions.

Nevertheless, speaking of "fictions" does not necessarily mean that chemical theories have no truth-value at all or that they should be viewed as mere instruments for prediction and classification²³. Instead we need to redefine what counts as the truth-value of chemical statements. The dilemma of instrumentalism (or positivism) versus realism is a pitfall that chemists need strenuously to avoid. If by realism we mean the

representation of an external reality, it is just as inadequate a label as instrumentalism. Chemists make extensive use of visual images but these are not intended to refer to real individual molecules. Rather they are better thought of as icons representing relations between individual entities. Chemists seem to share the conviction that the bedrock of chemical properties does not lie at the ultimate level of matter. In other words, they do not strive to reach the roots, or to unveil the ultimate building blocks of matter. They make up plausible narratives to account for the properties observed in individual substances that they use, or to predict and make new substances with desired properties. In so doing, they are constantly shifting from the macro- to the micro-level²⁴. Thus, they never settle on a scale for their reflection, with the constant shifting between levels determining their characteristic expository style. Chemistry textbooks, whether from the seventeenth century or most recent ones, tend to juxtapose narratives of experiments performed at the macro-level with narratives about relationships between microscopic invisible entities. The two kinds of narrative run in parallel but neither alone accounts for the ultimate causation.

Rather than being ideal accurate representations of nature, these narratives display meanings, with atoms and molecules best described as actors in a story. Even when these invisible entities are visualized using imaging techniques, they do not mirror the ultimate reality underlying phenomenological appearances, although they do *mean* something for the chemists. In certain cases they may mean that there is a possibility of breaking a bond, or of substituting a functional group or of encapsulating certain atoms within a cage molecule, etc. In addition stories require a temporal structure: temporality plays a prominent role in chemical narratives as the kinetics determines whether the reaction will be a success story or not. Wilhelm Ostwald was, like Berthollet, concerned with incomplete reactions whose outcome depends on subtle equilibriums, and proposed new narratives of chemical experiments based on the frequency of collisions. Thus, for example, catalytic materials that prompt the advancement of a reaction in a specific direction play a similar role to that of the hero's companion in epic narratives.

REQUIREMENTS AND OBLIGATIONS

Hoffmann's metaphor of story telling suggests that chemical theories have very weak explanatory power. In fact, Hoffmann makes the case for the "power of poor theories" and insists that two alternative theories, belonging to different paradigms, are not necessarily incommensurable²⁵. A standard example is Linus Pauling's theory of the chemical bond, associating Lewis's notion of a shared electron pair with the quantum mechanical notion of a covalent wave function, which proved to be extremely useful in heuristic terms. Hoffman comments:

I think incommensurability is no problem whatsoever to chemists. Differences in language are there, the result of different paradigms, but more so of history, and of education. Yet people, eager to make things, with no handwringing on how problematic it all is, graft one way of understanding onto another.

Making up stories does not, however, mean that chemists rely on fanciful and arbitrary accounts. It just means that chemists do not claim to reach the roots, or the ultimate cause of phenomenological data. Chemistry, like other experimental sciences, is a normative activity. But if its ruling norm is not to provide *the* perfect representation of reality, we may nevertheless demand what kind of norms are in use in this science.

The distinction between requirements and obligations forged by Isabelle Stengers in her "ecological" approach to practices in science is particularly helpful for characterizing chemical practices²⁶. Experimental scientists like to see their activities as conforming to a number of criteria or standards, including logical rules, experimental controls, peer review, etc. Conforming to such general widely accepted rules allows them to draw a clear demarcation line between their practices and others that are generally considered to be non-scientific or at least less scientific. Fulfilling such criteria is thus indispensable for defining the identity of a scientific practice, and in this respect chemists are no exception. They comply with the canons of the so-called scientific method, which shows that they are full members of the scientific tribe. However, Stengers argues, experimental practices are also governed by a number of more elusive and tacit norms – dubbed "obligations" – instituted by active scientists in specific contexts. The chemists' obligations are the collective standards that they have adopted over the centuries in order to learn something about nature from their

experimental practices, while at the same time never forgetting about making, and producing new artefacts or drugs.

Galileo's major obligation – that only matters-of-fact can tell us about the truth – led him to question nature in a mathematical language in his experiments on falling bodies. By contrast, the chemists' major obligations seem to be caution and skepticism. Crystals, liquids or gases in flasks behave in unpredictable and sometimes positively dangerous ways. These behaviors are so puzzling that chemists had to forge an arsenal of obligations: purifying, synthesizing, submitting them to standard reactants to settle their identity and characterize their properties. For this purpose of identification they rely on a wide range of different tests. In medieval times, chemists tested everything with fire, but since then they have come to use all sorts of chemical reactants and physical techniques of measurement, ranging from traditional balances, hydrometers, gasometers, to modern spectrometers. They have to pay particular attention to the conditions of their experiments – in some cases even more than experimental physicists – as slight modifications in temperature, pressure, concentration etc., can alter the course of a reaction, thereby changing the composition of the product. Since Robert Boyle's famous publication, 'sceptical' has often been associated with the word 'chemist'. It does not mean that chemists are stubborn unbelievers. Rather it is because what they know about chemical substances and chemical reactions justify a cautious attitude concerning any conclusions they might be tempted to draw from their experiments.

Identifying, naming, and classifying are the chemists' principal responses to their major obligation. Due to their "creativity" – millions of new molecules are reported in the *Chemical Abstracts* each year – chemists are continuously under pressure, as they have to find a name and a place for all these newcomers in their databases. In 1787, when a group of French academicians designed a "method for naming", they assumed that by formulating the major requirements for a chemical nomenclature, they would provide subsequent generations with reliable guidelines for naming any newly discovered substances²⁷. They formulated general rules for coining systematic names based on composition, and banished names based on the substance's qualities, its uses, or the circumstances of its discovery. In doing so, they were acting as 'architects of matter', designing and planning future chemical edifices. The growing

number of organic compounds in the nineteenth century nevertheless generated a chaotic situation with dozens of different names for the same substance. Standardization and systematization were the two leading requirements reiterated at the end of the nineteenth century by the first International Conference on chemical nomenclature held in Geneva in 1892. The concerted response was to give each substance an official name, but most of them were never used by chemists in their daily chemical practices. Indeed, this ideal of standard and systematic names has been continuously challenged, and linguistic customs established within scientific journals tended to prevail, meaning that the standard names in common use no longer complied with the original ideal of a systematic nomenclature. Regular international meetings and a permanent commission on nomenclature at the International Union for Pure and Applied Chemistry continue periodically to revise the rules. Still, the current nomenclature is by no means as systematic as the 1787 reformers had envisioned. Trivial names – names that do not refer to the structure of the compound – coexist with the systematic names that conform to the rules. In fact, both in organic and inorganic chemistry, most names are semi-trivial, mixing informal parts with those constructed following the systematic rules. Thus, the difficulty of keeping up with systematic names for extremely complex compounds proved so difficult that chemists had to renounce their ambition of submitting the molecular world to their ideal of rational systematization. This obligation may be considered a fundamental weakness, a sign of the imperfection of the chemical sciences. But what Stengers means by “obligation” suggests a more charitable reading. This term suggests a kind of binding agreement between chemists and the object of their investigations. Chemists are “obliged”, in the dual sense of the word, bound by and indebted to the growing population of molecules they both create and investigate. They are less “architects of matter” than dusty laborers trying to discipline a jungle of diverse molecules.

The repeated attempts to classify chemical elements during the nineteenth century provide another illustration of the interplay between requirements and obligations. The official requirement was to group simple substances according to their common properties. Nevertheless, chemists soon realized that the ideal of a “natural classification” reflecting all the similarities between the elements would be impossible to achieve. They consequently adopted “artificial classifications”, based on one or two

properties arbitrarily selected among the wide variety of candidates. They even combined artificial classifications for metals with natural classifications for non-metals while admitting that the division between metals and non-metals was itself artificial. Such hybrid arrangements are far from the rational ideal and might therefore be considered a major defect. Chemists were, however, “obliged” to adopt and teach such imperfect solutions, as they were aware that their picture of the material world was inevitably biased, that between the exigencies of an operational system and an ideal one something had to give. Emile Meyerson, a chemist turned philosopher, argued that although the distinction between metals and non-metals was arbitrary, chemists used it because they had to draw strong distinctions, to artificially introduce rigid demarcations into the flux of complex inter-relations, in order to be able to refute conjectures. Rigidity and falsification add truth-value to the story invented by chemists. Meyerson used a suggestive metaphor, borrowed from Arthur Balfour, to characterize the chemist’s approach to nature: they are “drawing a fiber” out of the magma of reality. Chemical classifications seem to be based on the assumption that nature is composed of a “fibrous structure” in which they select a specific region in order to disentangle the local network of relations.²⁸ Focusing on a fiber, they start reasoning about its connections with the whole fabric, while all the time looking at the landscape created by the extraction of this one fiber. They never claim that this fiber is the root of the structure, or the unique entry into the puzzle. But drawing out a fiber is their obligation, which means, on the one hand, that they must not break it, and that they must use it as a robust guideline. On the other hand, they are not to treat the fiber as a completely secure element that would permit safe deductions. “If...then” is a forbidden leap in a jungle where unexpected surprises are strewn on every pathway. Thus, chemical classification remains an open field. More than a century after Mendeleev’s periodic system came to be considered “the chart of nature” a view subsequently justified by atomic physics, chemists are still unsure about the best way to represent the periodic function. There is no ideal chart. Each year, new systems are designed and new graphic representations are submitted for publication, some of them concocted by obscure chemical practitioners, suggesting that classifying elements remains a work in progress, a communal and endless task²⁹.

“NO NATURAL BODY CONSISTS OF MATTER *PER SE*”

An aura of materialism surrounds the image of chemistry, which derives as much from the chemist's concern with material things as from the abundance of material goods generated by the chemical industry.

Ironically, however, chemists do not care very much for matter. They have used the terms “substances” or “bodies” for centuries but, as Venel noted in Diderot's *Encyclopédie*, “no natural body consists of matter *per se*”.³⁰ Rather than being concerned with matter in general, chemists want to know why only one particular acid dissolves gold or why spirit of niter joined to salt of tartar produces true saltpeter. They pay attention to individual properties, with reference to a jungle of different materials and their potentialities.

Chemistry is concerned with the stuff things are made of, but we need to ask what concept of substance they use. In *The Philosophy of No*, Bachelard argued that the metaphysical notion of substance inherited from the Ancient Greek quest for permanence has been modeled on classical physics. Since Descartes, matter has been regarded as an essentially homogeneous substance defined in geometrical terms, with the diverse sensory properties that characterize the multiplicity of the phenomenal world being merely “secondary qualities” arising from the spatial arrangements and rearrangements of indistinguishable elements. This metaphysical notion of substance as a permanent and pervasive substrate underlying phenomenological change is, however, completely inappropriate for chemistry. What might a “metachemical” notion of substance look like? The stuff that chemists call ‘substances’ is always in the plural.³¹ For chemists, substances are concrete entities with individual properties. Explanations of chemical phenomena rely on a few immutable elements responsible for the individual properties of compounds. They may be irremediably invisible but they can be traced by means of the sensible effects that they cause at the phenomenological level, or by means of their circulation from one combination to another.

The dichotomy concerning this issue outlined above suggests that as far as the philosophy of matter is concerned, physics and chemistry are heirs to two different ancient traditions, with physics deriving from Democritus and Epicurus and chemistry

from Empedocles and Aristotle. In the former case, the endless variety of substances with their individual specific properties is referred to essentially similar atoms, only distinguishable with respect to their figures and movements, while in the latter case, the variety of individual properties is attributed to strongly individualized principles. In *Le Mixte et la combinaison chimique*, Pierre Duhem suggested a similar distinction between two “research schools”. The first was the “corpuscular school” – Cartesian and then Newtonian – which one could characterize by Boyle’s assumption of a “catholic matter”, and which would lead to the mechanistic models of the nineteenth century that Duhem rejected. The second was the “Aristotelian school”, taken to be characterized by its rejection of all “systems”, all *a priori* reasoning, as well as its firm attachment to irreducible qualities.³²

This dual genealogy is, however, superficial and in the end misleading. The so-called rival paradigms – the monist, atomistic, mechanistic philosophy versus the pluralist, qualitative doctrine of elementary principles – were not incommensurable. Most chemical theories managed to combine them in some fashion. As historians of early modern chemistry have shown, a corpuscular theory was embedded in the alchemical tradition, and was, in fact, crucial for justifying the possibility of transmutation.³³ It is now well established that Boyle’s corpuscular philosophy, for example, stemmed from this longstanding alchemical tradition transmitted via Daniel Sennert. Thus, Boyle’s corpuscular philosophy was not the grafting of a physical theory onto a previously incoherent body of alchemy or iatrochemistry³⁴. Later on, Georg-Ernst Stahl also assumed that material bodies were constituted by the *mixta*, *composita* and *supercomposita* of constituent particles. He assumed a corpuscular view of matter meshed with a view of individual principles acting as the vehicles of the properties. Such combinations suggest that atomist views and the principle theories were deployed for different purposes and did not address the same issues. Neither of them holds the secret of matter. For chemists, there is no privileged ultimate level of reality; instead they adopt what Bachelard termed a “laminated reality” since laboratory practice gives access to substances at multiple levels simultaneously³⁵.

Stahl used a clear-cut distinction to differentiate the territory of chemistry from that of physics. He acknowledged that mechanical physics could account for one species of material compounds, namely “aggregates”, whereas only chemistry could deal with “mixts”³⁶. Aggregation was a juxtaposition of units, and could be understood in mechanical terms such as mass and movement. Mixtion, however, was the union of principles involving individual affinities. The decomposition of an aggregate would not affect the properties of its components whereas the dissociation of a mixt entailed changing the properties of its elements.

This conceptual distinction echoed the issue raised by Aristotle in *De generatione and corruptione I* about the mode of presence of the constituents in a mixt. The problem emerged from a critical review of atomism. If atomist doctrines were right, then a mixt would be just a collection of atoms placed side by side, like grains of wheat and grains of barley. “To the eye of the Lynx nothing would be combined”³⁷; Constituents would be physically present in the compound although not visible at first glance. Thus, they can be recovered without changing the properties of the compound. Aristotle insisted that if the components are preserved unchanged then the mixt is only apparent. By contrast, a true process of mixture involves the interaction of qualitatively differentiated ingredients in such a manner that they do not persist unchanged in the resulting compound. A true mixt is not, therefore, composed of constituents sticking together. Something new is created, with properties not possessed by the original ingredients. The emergence of a new ‘stuff’ implies that the ingredients no longer coexist with the mixt. Consequently, a true mixt can be characterized by an *either...or* condition. Either you get a compound and you lose the properties of the initial ingredients, or you recover the original ingredients and you lose the properties of the mixt. By contrast, the atomic conception of chemical combination does not demand such a disjunction.

Paul Needham, who offered a detailed analysis of Aristotle’s conception of mixts, has convincingly argued that Aristotle raised the fundamental issue of chemistry, i.e. the generation of new substances out of initial ingredients³⁸. This clear recognition of the problem should not, however, be used to suggest that Aristotle conceived a

“theory of chemical reaction and chemical substances”, as Paul Neeham seems to argue, since chemistry did not exist as an identifiable branch of knowledge at this time.

Avoiding such anachronisms is important for grasping the concept that I have dubbed the chemists’ “essential tension”. By referring to the title of Thomas Kuhn’s famous book, I want to draw attention to the specificity of chemistry. Indeed the tension that Kuhn found implicit in scientific research between tradition and revolution, between conformism and iconoclasm is also at work in chemistry, although its identity has been shaped by a more specific tension between two competing views of chemical combination³⁹. At the turn of the eighteenth century, Stahl’s distinction between aggregates and mixts was aimed at circumscribing a territory for chemistry, centered on the notion of the mixt, in a defense against attempts at annexation by mechanism. So successful was this conceptual strategy, that Stahl was proclaimed the founder of chemistry throughout the eighteenth century. A century later, however, chemists no longer used the word mixt, as the notion of composition prevailed. In particular, Lavoisier’s famous definition of elements as undecomposable substances was an integral part of a reorganization of chemistry along the lines of another distinction, that between simple and compound. Lavoisier, who came to earn the title of the founder of “modern chemistry”, redefined it as the science that aimed at decomposing natural bodies and “examining separately the various substances entering into their combination”⁴⁰. To be sure the compositional perspective was nothing new, but with the reform of chemical language it became the dominant paradigm⁴¹. In the new language, names of compounds were coined by simple juxtaposition of the names of their components, and were considered as “mirror images” of the actual composition of the material bodies in question⁴². Lavoisier, who admired and extensively quoted Etienne Bonnot de Condillac’s *Logic*, adopted his views of languages as analytical methods as well as his notion of analysis as a two-way process, from simple to compound and from compound to simple. According to Condillac, analysis is a mental process involving the successive visualization of the individual elements of a picture presented simultaneously as a whole to the senses. Condillac used the metaphor of sight-seeing from the window of a castle. Immediately I see a landscape, then by analysis the mind will distinguish and name each element of the landscape pre-existing in the global view.⁴³ Condillac’s logic, inspired by algebra, in turn inspired Lavoisier’s use

of equations to describe chemical reactions. A compound is described as the addition of two constituent elements. It is entirely characterized by the nature and proportion of its constituents. The use of the sign “equals” in the equation clearly indicates that chemists are no longer thinking in terms of the either/or condition. The puzzling issue raised by Aristotle about the mode of the presence of ingredients in the compound has been laid aside, discarded rather than being solved.

Reinforced by John Dalton’s atomic hypothesis, the compositional paradigm has proved very successful. By the middle of the nineteenth century, the definition of a compound according to the nature and proportion of its constituents was being challenged by a structural paradigm that emphasized the importance of the arrangement of the atoms in molecules. Nevertheless, empirical and structural formulas both eliminate the either/or condition. The actual presence of the constituent elements suffices to account for the properties of the compound.

Pierre Duhem’s return to Aristotle’s notion in the title of *Le mixte et la combinaison chimique* (1902) was clearly intended to undermine the prevailing atomist interpretations. The familiar example of sugared water in his introductory chapter summarized Aristotle’s theory in a few words, and restored the legitimacy of the either/or condition:

What in general, then, is a mixt? Some bodies, the ones different from the others, are brought into contact. Gradually they disappear, they cease to exist, and in their place a new body is formed, distinguished by its properties from each of the elements that produced it by their disappearance. In this mixt, the elements no longer have any actual existence. They exist there only potentially, because upon destruction the mixt can regenerate them⁴⁴.

Duhem mainly reproached atomistic explanations for assuming that the properties of a compound could be deduced from those of its constituent elements or atoms. His criticism also encompassed Lavoisier’s compositional paradigm, since elements are not conserved as such in chemical reactions.

Emile Meyerson indirectly addressed the same issue although, unlike Duhem, he claimed that chemists could not do without atoms. He nevertheless pointed to the either/or issue involved in chemical equations, starting with the observation that when chemists write the equation $\text{Na} + \text{Cl} = \text{Na Cl}$, they obviously presuppose the conservation of matter⁴⁵. He observed that, interpreted literally, a chemical equation is a non-sense. In asserting that the addition of a soft metal like sodium to a greenish gas

like chlorine equates to a colorless salt, chemists seem to be oblivious of the very conditions of their laboratory practice. Although they continuously play on the potentialities of various individual substances and take advantage of their differences, they admit that the compound “equals” the sum of its initial ingredients.

Thus chemistry seems to be moved by two antagonist forces. On the one hand, chemists aim at reducing the qualitative diversity of substances to identity. They would like to deduce their empirical data from an ultimate hidden cause in order to “satisfy their rational tendency to identification”, to use Meyerson’s terminology. Chemical equations balancing the inputs and outputs of chemical reactions are the best expression of this effort aimed at identification. They presuppose subsistence throughout chemical change, or the conservation of elements in chemical reactions, even though the diversity of substances and their idiosyncratic behaviours constitute the very *raison d’être* of chemical practices. Without a diversity of substances with their own individual properties and without a diversity of processes of reaction, there would be no chemical reactions and so no chemistry. Thus, chemists have no choice but to face “irrationals” (again using Meyerson’s terminology). They sense that it is useless to try and reach the ultimate reality, and hopeless to try reducing everything to sameness⁴⁶.

The tension between the two conflicting views of chemical combinations is not necessarily to be understood as a fight between the rational and the irrational, or as a contrast between a rational tendency and a more pragmatic one. After all, atomic theories do not hold a monopoly over rationality⁴⁷. Moreover, atomic notions, and molecular models are man-made “artifacts”, tools forged for theoretical and practical purposes. Nevertheless, the tension is an essential one, as neither of the perspectives is sufficient to account for chemical combinations, while the two descriptions do not work harmoniously together. Chemical combinations thus offer a new case of complementarity in Niels Bohr’s sense; two necessary but nevertheless exclusive descriptions of a phenomenon⁴⁸.

Because chemists are not really concerned with understanding the fine structure of matter, they have regularly dismissed all hypotheses concerning the real existence of atoms. For instance, August von Kekulé, who conjectured the hexagonal structure of benzene that formed the basis of most artificial organic compounds manufactured in the second half of the nineteenth century, denied the existence of atoms. More precisely, he banished the ontological issue from chemistry, claiming that it belonged to metaphysics. Thus, chemists made extensive use of atoms and molecular models while denying their existence or claiming that they were simply fictions. This apparently inconsistent attitude survived (in France at least) long after the first demonstrations of molecular reality and the founding of atomic physics. For instance, the French chemist Georges Urbain wrote in 1921: “It is not absurd to suppose that the atomic model is identical with absolute reality. However, we know nothing positively about it. This model is a work of art”.⁴⁹ Such claims have sometimes been viewed as evidence for the theory that, under the pernicious influence of Auguste Comte, French chemists were sticking to strictly positivist positions, and consequently lagging behind modern chemistry.⁵⁰ This apparently inconsistent attitude was not, however, confined to the small circle of French chemists. The ontological status of bonds and orbitals was discussed at length by the founders of quantum chemistry, with some of them denying their physical reality in an effort to demarcate the chemical approach to concepts such as resonance borrowed from physicists.⁵¹ Chemistry thus appears as a science bound to ontological non-commitment, an attitude not shared by modern physicists.

If we resist the temptation of identifying the philosophy of physics as the “right model” for all of the sciences, how are we to understand the strange attitude of these non-committal chemists? For Meyerson, the chemists who denied the existence of atoms simply lacked authenticity⁵². He assumed that all chemists professed a naive realism, a belief in the existence of things such as barium sulphide, for instance. Meyerson is right: chemistry is certainly not ontology-free, although he misunderstood its ontology. The assumptions underlying chemical practices do not concern things such as barium sulphide, or rather, to be more precise, this sort of “thingism” (*chosisme*) is not typical of chemists. Two major matters of concern more adequately characterize their ontology: i) a concern for relations, and ii) a concern for agency.

i) Relations

There is no question that chemists deal with individual substances and pay attention to their molecular structures, but these things are of interest to them only in so far as they enter into relation with other units. Nineteenth-century structural formulas were not meant to be images of reality, and yet nor were they pure conventions. Rather they depicted capacities for bonding, the so-called atomicity or valence. Similarly, series of compounds were essentially viewed as potential combinations or syntheses. Ernst Cassirer has emphasized the functional determination of the concept of atoms in *Substance and Function* where he convincingly argued that the treatment of an atom as the “absolute substrate” of properties is only apparent. In fact, the concept of atom serves as a mediator for mapping out a network of interdependent relations between objects⁵³.

Bachelard also emphasized chemists’ concern with relations rather than with substrates. Since relations imply at least two terms, chemistry necessarily presupposes various kinds of beings. The two features that Bachelard selected to define the rationalism of modern chemistry, which he dubbed “non-lavoisieran”, were that it was plural and relational. For him, Mendeleev’s system epitomized the shift from realism to rationalism, because “law prevailed over matter of fact”⁵⁴.

The focus on relations allows chemists to choose the unit of matter that best suits their views. For instance, in Pauling’s valence bond theory, atoms are the combining units, and their interaction results in the formation of molecules. By contrast, in Mulliken’s molecular orbital approach, the atom is no longer the relevant concept for understanding chemical bonds. Molecules are taken as the basic building blocks, formed by feeding electrons into molecular orbitals⁵⁵.

After quantum chemistry had drawn physics and chemistry into cooperation, chemists continued to debate about the ontological status of relations themselves. In this context, we can cite the debate that took place between G. W. Wheland and Pauling about double bonds and resonance.⁵⁶ Thus, time and again, chemists set themselves apart by rejecting the physical meaning of the concepts they are using. They champion artificiality or “facticity” not only in their experimental practice but also in their intellectual practice. If today’s chemists are no longer noncommittal, it is mainly

because they assemble atoms and molecules like Lego blocks. They believe in orbitals as long as they can explain things with them and design reactions. According to Hoffmann “The reifying power of synthesis, when you do it with your hands, time and again, is incredibly strong”⁵⁷.

ii) *Agencies*

The chemists’ “things” are implicitly described in terms of structures, properties and functions. Molecular structures are above all conditions for the emergence of properties, which themselves are viewed as dispositions for desired performances. While chemists do not care for matter, they are by contrast always searching for materials, i.e. substances useful for something. Thus, in the eighteenth century, Hermann Boerhaave and Guillaume-François Rouelle redefined the four elements in terms of agents, conceiving them as both the constituent units of compounds, responsible for the conservation and transport of individual properties through chemical change, and instruments of chemical reactions. Rouelle introduced his four-element theory under the heading “Instruments” that included “natural instruments” - fire, air, water and earth -, and two artificial instruments - menstrua and vessels. The ancient radical distinction between nature and human artifacts was thereby being blurred in favor of an instrumental view of matter as an active operational process. Material principles were always at work, circulating from mixt to mixt, whether in laboratory vessels or in the depths of the earth or the heights of the heavens. Subsequently, following the rise of the compositional paradigm after the reform of chemical language, and later the structural paradigm linked with the emergence of organic chemistry, chemical names and formulas have been mainly used as “paper tools” for predicting operations and substitutions.⁵⁸ They display the possible uses of compounds through their structure. This action-oriented language inspired Bachelard’s description of structural formulas as “rational substitutes”, providing a clear account of the possibilities for experimentation⁵⁹. This is why nineteenth-century chemists could reject all ontological commitment concerning atoms and molecules, while using them like plumbers use pipes, valves, and joints. Even today chemists refuse to endow the atomic theory with the power of representing the world, as long as they are concerned with

powers for intervening in the world. Atoms and molecules are just potential actors in the drama of chemical transformation.

Ian Hacking's reflections on the way the physicists use electrons in electron microscopy is similar to the way chemists view the constituents of matter⁶⁰. Electrons are less explanatory notions than instruments for acting or creating phenomena. Hacking's distinction between "realism about theories" and "realism about entities" can thus be applied to chemistry. To be sure, chemists are realists; they believe in the reality of entities, which allow them to operate on the outside world or to be affected by it. "Operational realism" would thus be the right phrase to characterize the chemists' philosophy. The material world is a theater for operations; the entities underlying observable macroscopic phenomena are above all agents.

In this respect, the three categories of structures, properties, and functions are not the most appropriate for the philosophy of chemistry. Aristotle provides better resources by the addition of his notion of potential, which remains appropriate for characterizing the modality of constituent elements in combinations⁶¹; The dual nature of chemistry – science and technology – requires the whole panoply of subtler distinctions found in Aristotle's treatise on *Categories*, δ ⁶². Properties belong to the category of quality, but there are many varieties of qualities. States (for instance, hard or soft) differ from dispositions. The former are stable and durable "possessed" qualities, whereas the latter are ephemeral and easily altered. Both possessions and dispositions being acquired in specific circumstances differ from natural capacities embedded in the subject. They all differ from "affections" (bitterness, sweetness), which simply refer to sensory properties. The chemists' art of synthesis takes advantage of the whole spectrum of capacities in order to put molecules to work, to make the molecules do what chemists cannot do with their own hands.

In 2003, Susan Linquist, a biologist from MIT's Whitehead Institute, announced at a conference that: "about 10,000 years ago, [humans] began to domesticate plant and animals. Now it's time to domesticate molecules"⁶³. But domesticating molecules is what chemists have been doing for centuries. At the cost of repeated experimental trial and error, they have managed to tame an incredible number of molecules, to get sufficient control over their reactions to be able to use them as agents for performing specific tasks. Nevertheless, this domesticated stuff has never worked in the same way

as man-made tools or machines. Substances operate according to their own nature, even when they are chemical “creatures”. Through a number of more or less spectacular chance events and deplorable accidents, chemists have learned that they are still at the mercy of unexpected outcomes and that reactants do not always behave in a foreseeable way.

In addition, chemists usually work with huge populations of molecules in their vessels. Unlike nanoscientists, who are trying to domesticate molecules one at a time, chemists have no control over individual molecules, although they may know a good deal about the species of molecules in question, especially when they have created the substance themselves. Nevertheless, the shift in scale of the operations has radically changed the relationship between men and materials. The slogan of the nano-initiative, “shaping the world atom by atom” expresses the ideal of control and full command that lies behind nanotechnology. Individual molecules are supposed to be reliable entities, responding predictably to precise signals. So deep is the contrast between this culture of precision and the more crude tradition of chemists, that for Eric K Drexler, a champion of nanotechnology, chemical synthesis is an inexplicable enterprise, which he compares to trying to assemble a car by putting all the necessary parts in a large box and shaking them up together.⁶⁴ Nevertheless, such miraculous processes constitute the everyday functioning of the world’s chemical factories. The ‘cars’ that the chemists have managed to assemble by such ham-fisted methods are new things, with the constituent parts no longer accessible or even visible. When deploying their art, that of making molecules work for them, chemists are not like Plato’s demiurge, who builds up a world by imposing his own rules and rationality on passive matter. Rather, they are like a ship’s pilot at sea, who, constrained by the force of the ocean and atmosphere, is obliged to channel or guide the forces and processes given by nature, and ultimately exhibits the powers inherent in nature in the outcome.

In guise of a conclusion, I want to offer a few reflexive remarks on the functions of history in this philosophical essay on chemistry. In his paper on “The relations between the history and the philosophy of science”, Kuhn argued that bringing them together could be subversive, because philosophy and history were two distinct mental sets like the rabbit and duck in the famous Gestalt ‘duck-rabbit’ figure⁶⁵. Although this mutual exclusion seems quite alien to French scholars trained in a tradition that

promotes the conviction that: “there is no epistemology that is not historical”⁶⁶, the functions of history in this essay have to be clarified. History is not a source of examples that serve to illustrate and confirm philosophical claims about the “essence of chemistry”. There is no such thing as an immutable essence of chemistry that would fit this kind of strong philosophical program anyway. Instead, history is used here as a source of problems. The historical materials are not meant to allow us to reconstruct the past, rather they are an indispensable detour for grasping the problems at stake and the philosophical views shaped by chemists themselves in their investigative and productive practices.⁶⁷ For chemistry *is* a historical process. The journey into chemistry proposed in this essay should be thought of like a trip on a rocket ship that is continuously in motion, but changes direction in response to its environment and other circumstances, although overall retaining a more or less direct trajectory. The purpose was to identify the kind of problems and projects that have guided generations of chemists in defining this trajectory over time, thereby (unconsciously) reconfiguring the identity of their science.

Centuries of chemical practices oriented towards cognition and action have generated a set of specific obligations, which can be characterized as both epistemological and ethical rules. Caution, utility, and efficiency have been as highly valued as the quest for truth in the sense of *adaequatio rei et intellectus*. The chemical sciences are not aimed at unveiling the underlying reality beneath the surface. Instead, they deal with a jungle of molecules and strive to take advantage of their dispositions. Chemists are put under an obligation by these substances, by their structures, properties and capacities, meaning that respect, as much as responsibility, should be at the base of a chemist’s ethics.

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NOTES

¹ Schummer, 2006, p. 21.

² Bensaude-Vincent, 2005.

³ Simões, 2002.

⁴ See for instance Lévy, 1979, Primas, 1983, Liegener & Del Re, 1987, Scerri, 1991, 1994, 1997.

⁵ Primas, 1983, Scerri, 2000.

⁶ Scerri, 2000.

⁷ Bachelard, 1940.

⁸ Nordmann, 2006.

⁹ Schatzki et al., 2001.

¹⁰ Hoffmann, 1995, Grosholz, Hoffmann, 2000; see also Berson, 2003.

¹¹ Holmes, 1993, p. 478.

¹² Van Helmont, J.B. De febribus, Opuscula chap. 15, N°26, p. 58 quoted in Newman & Principe, 200, p. 180.

¹³ Bensaude and Stengers, 1993.

¹⁴ Joachim Schummer's survey of 300 papers on synthesis from 1980 to 1995 concluded that most of them were aimed more at syntheses rather than at classification or theoretical reflection (Schummer, 1997).

¹⁵ Diderot, *De l'interprétation de la nature*, 1753. Venel, Gabriel-François article "chymie", in Diderot, d'Alembert eds, *Encyclopédie ou Dictionnaire raisonné des sciences, des arts et des métiers*, vol. 3, 1753, p. 420b. Diderot, *De l'interprétation de la nature*, 1753.

¹⁶ Hoffmann, 2005.

¹⁷ In the Renaissance, chemistry was often referred to as *spagyria* or spagyric art, a term which, according to a dubious etymology spread in seventeenth-century chymical textbooks, derived from the Greek *span* (to pull apart) and *ageirein* (to put together), Newman and Principe, 2002, p. 90

¹⁸ Literally "The true and the made are interconvertible", Vico, J.B., 1725.

¹⁹ Bachelard, 1952, p. 22.

²⁰ Berthelot, Marcellin, 1867, p. 275.

²¹ Kant, *Critique de la raison pure*, Preface to the second edition, transl. Tremesaygues and Pacaud, PUF, 1968, p. 17

²² Hoffmann, 2005.

²³ Duhem, however, viewed chemical theory as a kind of natural classification.

²⁴ Grosholz and Hoffmann, 2000, analyzed this shift from macro and micro in terms of a motion between symbolic and iconic representations.

²⁵ Hoffmann, 2005.

²⁶ Stengers, 2006, p. 67-70. I am very indebted to Isabelle Stengers for this section.

²⁷ Crosland, 1962, Bensaude-Vincent, 2003.

²⁸ As Meyerson put it in a letter to André Lalande dated 1930: "Ce terme de *fibres* montre d'ailleurs clairement de quoi il s'agit en l'espèce; il faut déterminer, dans la masse confuse et troublante du réel, une région qu'il est possible d'en isoler suffisamment pour en déterminer le comportement". (Meyerson archives, A 408/60).

²⁹ Bensaude-Vincent, 2001.

³⁰ "Mais nul corps de la nature n'est de la matière proprement dite", Venel, article « principes », D'Alembert, Diderot, *Encyclopédie ou Dictionnaire raisonné des sciences, des arts et des métiers*, vol.3

³¹ Bachelard, 1940, Engl translation.

³² Duhem, 1902, chapter 1.

³³ As early as the end of the thirteenth century, the *Summa perfectionis*, falsely ascribed to Geber, developed corpuscular views intertwined with the doctrine of principles. The pseudo-Geber described the combination of *minima partes* or "small particles", which come together in a "strong composition" to form the two constituent principles of metals: sulphur and mercury. Newman William R., 1991.

³⁴ Clericuzio, 1990, Principe L., 1998.

³⁵ Bachelard, 1940, p. 46, 76. According to Bachelard, chemists work with three layers of reality: the "naïve" identification of particular substance; a "rationalized" and intellectual notion of substance; and the third layer of 'non-substantialism'. Nordman convincingly argues that Whitehead and Latour later developed similar notions. (Nordman, 2006)

³⁶ I use the ancient term "mixt" (derived from the Greek *mixis*, rather than the standard term "mixture" in order to avoid confusions with the modern notion of mixture, which is clearly distinguished from "combination".

³⁷ Aristotle, *De generatione et corruptione* I.10, 328^a13f.

³⁸ Needham 1996, 2006.

