

Chemistry, an ontology-free science?

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Abstract

It is often assumed that chemistry was a typical positivistic science as long as chemists used atomic and molecular models as mere fictions and denied any concern with their real existence. Even when they use notions such as molecular orbitals chemists do not reify them and often claim that they are mere models or instrumental artefacts.

However a glimpse on the history of chemistry in the *longue durée* suggests that such denials of the ontological status of chemical entities do not testify for any specific allegiance of chemists to positivism. Rather it suggests that the dilemma positivism vs realism is inappropriate for characterizing the ontology of chemistry. This alternative shaped at the turn of the twentieth century in the context of controversies about atomic physics does not take into account the major concern of chemists, i.e. making up things. Only by considering what matters for chemists, their matters of concern rather than their matter theories, can we expect to get an insight on their ontological assumptions. The argumentation based on historical data is twofold.

Generating new substances out of initial ingredients which is the *raison d'être* of chemistry raised a vexing puzzle which has been alternatively solved with the Aristotelian notion of mixt and the Lavoisieran notion of compound. I will argue that an essential tension remains intrinsic in chemistry between the two conceptual frameworks.

But how are we to make sense of the long tradition of ontological non-commitment in chemistry? I argue that what is usually considered as a denial of the existence of the basic units of matter is better characterized as a focus on more important actors on the chemical stage.

I Credo or denial?

Nineteenth century chemists were caught in a dilemma: they could not dispense with the notions of atoms and molecules but they did not want to assume the existence of atoms. They followed a general rule of non-commitment, an epistemic “vow of chastity”. This attitude often labeled as “positivist” has raised a lot of misunderstandings. From a present day perspective it is clear that the controversy between equivalentists and atomists was a controversy between conservative and progressive minds. The chemists who rejected atoms and molecules and instead used the equivalent weights of substances engaged in combinations of substitutions are described as positivists who wanted to deal exclusively

with observable entities and rejected metaphysical entities. By contrast, atomists are often described as people who assumed that the structural formulas and molecular models used for the synthesis of organic compounds in the second half of the nineteenth century represented the real architecture of matter. However a closer examination at the controversy as it developed in the late nineteenth century, suggests that the philosophical assumptions underlying the controversy are much more complex. I will confine this paper to the last stage of the controversy.

First remark : the first international conference of chemists was organized in 1860 precisely for deciding upon the issue of atoms and molecules. Charles A Wurtz and August von Kekulé wgo organized the meeting intended to put an end to “the deep differences on words and symbols that harm communication and discussion, which are essential springs of scientific progress”. The question of atoms was thus raised as a language issue (naming and writing the formulas of organic compounds) without any ontological claim. It was thus expected that the question of atoms and molecules could be decided by a convention, by a popular vote of the assembly of chemists.

Second remark: it is well-known that no consensus was reached although most chemists in Europe – Lothar Meyer and D. Mendeleev in particular - and the United States adopted the system of atomic weights based on Avogadro hypothesis and the distinction between atoms and molecules advocated by Stanislao Cannizzaro. However a number of leading chemists rejected the atomistic notation such as the Germans Jakob Volhard and Hermann Kolbe and the French Marcellin Berthelot. Many historians of chemistry argue that the French long-lasting resistance to atomism was due to the overarching influence of Auguste Comte’s positivism in France. I have deconstructed this wrong interpretation elsewhere. Now I just want to argue that the controversy did not run on ontological issues. The dividing line was not between people assuming the existence of atoms or molecules and people rejecting them as metaphysical entities.

To be sure the champions of equivalentism tried to use the argument of the unobservability of atoms and molecules. Henri Sainte-Claire Deville opened the debate at the French Académie des sciences by declaring that Avagadro’s law, was an unfounded hypothesis. And Berthelot ridiculed the atomist position by saying: ‘who has ever seen a gaseous molecule or an atom?’¹ However his attempt to impose such naive epistemological standards for scientific reality, was easily defeated by Wurtz who pointed out the hypocrisy in Berthelot’s position: ‘At its base, your notation in terms of equivalents covers the same idea of small particles, and you believe in them like we do [...] without repudiating hypotheses entirely as no science can do without them, no scientist can refrain from making them.’²

On the atomists’ side, some of the champions of Avogadro’s law and structural formulas held strictly positivist views. For instance Charles Gerhardt who promoted the notion of types of compounds conscientiously avoided any realist representation of the internal architecture of these compounds and

¹ Marcellin Berthelot (1877), *Comptes-rendus de l’Académie des sciences*, 84, p. 1194.

² Wurtz Charles Adolphe (1877) ‘Réponse à M. Berthelot sur l’atome’ *Comptes-rendus de l’Académie des sciences*, 84, N° 23, pp. 1264-68, on p. 1268.

refused to think of radicals as bodies that could be isolated in any permanent, stable form. For him, a radical was simply ‘the rule according to which certain elements or groups of elements are substituted for one another or are transported from one body to another in the event of a double decomposition’. Gerhardt was careful to point out that his radical had no material reality, and was just a taxonomic schema, suitable for revealing analogies and homologies between chemical compounds. To underline the fact that his formulae had no ontological import, he named them ‘rational formulae’ and even accepted that the same substance could have several different formulae.

August von Kekulé who conjectured the hexagonal structure of benzene and who realized that this structure allegedly visualized in a dream provided the basis for the synthesis of most artificial organic compounds manufactured by the end of the nineteenth century, should have been a staunch believer in the real existence of atoms and molecules. However, he rejected the ontological issue out of chemistry, as belonging to the realm of metaphysics. When he was prepared to enter onto this metaphysical terrain, however, Kekulé was inclined to believe that atoms did not exist.

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"The question whether atoms exist or not has little significance in a chemical point of view : its discussion belongs to metaphysics. In chemistry we have to decide whether the assumption of atoms is a hypothesis adapted to the explanation of chemical phenomena. More especially have we to consider the question whether a further development of the atomic hypothesis promises to advance our knowledge of the mechanism of chemical phenomena. I have no hesitation in saying that, from a philosophical point of view, I do not believe in the actual existence of atoms, taking the word in its literal signification of indivisible particles of matter. I rather expect that we shall some day find, for what we now call atoms, a mathematico-physical explanation, which will render an account of atomic weights, of atomicity, and of numerous properties of so-called atoms. As a chemist, however, I regard the assumption of atoms, not only advisable, but as absolutely necessary in chemistry."³

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Thus chemists made an extensive use of atoms and molecular models while denying their existence or claiming that atoms were fictions. Even in the twentieth-century some chemists who knew about the electronic structure of atoms and witnessed the radioactive decay of atoms continued to claim that atoms were fictions. For instance the French chemist Georges Urbain continued to treat the atom as a symbol, a simple representation, and rejected the ontological question of the real existence of atoms as beyond his competence as a chemist.

The current atomic theory, like all good physical theories, provides an economic way of thinking and relieves our memory. The theory is useful because these images provide a synthesis of a considerable number of relationships that exist between sensible qualities. It is useful because the language that evokes these images is clear and adapted to the facts with an adequate degree of precision. These images are like a form of writing composed of symbols that evokes the laws obeyed by the facts. Philosophers can discuss the question of whether atoms have a reality external to us. The study of objects in themselves is not part of science. Science only establishes the

³A. Kekulé, ‘On some points of chemical philosophy’, *The Laboratory*, I, July 27, 1867. Reprint in R. Anschütz, *August Kekulé*, Vol. 2, Berlin, 1929. See also Britta Görs (1999)

relationships that exist between the sensible properties of the delimited portions of space that we call bodies.⁴

Even in quantum chemistry, according to Ana Simoes, the ontological status of bonds and orbitals has been discussed among the founders. Some of them denied their physical reality in an effort to demarcate the chemical approach of concepts borrowed from physicists, such as resonance for instance.⁵ Chemistry thus appears as a science bound to ontological non-commitment by contrast with the attitude of modern physicists.

If we resist the temptation of identifying the philosophy of physics as the “right model” for all sciences, how are we to describe the strange attitude of unbeliever chemists?

For Meyerson, the chemists who denied the existence of atoms simply lacked authenticity.⁶ He claimed that all chemists professed a naive realism, a belief in the existence of things such as barium sulphide, for instance. Scientists are no different from common sense in their robust realism. Electrons and atoms are even more things than ordinary things because they are more persistent than the objects of our sense data. Postulating the reality of atoms and electrons is as necessary to chemists as breathing.⁷ Scientists cannot help ascribing experimental laws to nature itself, because there are no “rapports” without “supports”.⁸ Therefore, Meyerson could not take the chemists’ scepticism about atoms seriously. He simply distrust their positivist claims of ontological non-commitment.

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“He (Kekulé) sometimes expressed reserves but as one can feel it was just to pay lip service, as a formality. In his heart, he strongly believed in the existence of atoms, of their molecules and of their bonds, as he manipulated them rough and ready exactly as if they were objects of common sense.”⁹

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How are we to decide upon the two opposite interpretations? A sceptical credo on the side of chemists or an attitude of duplicity and denial of the evidence?

II Matters of concern

Meyerson is right: chemistry is certainly not ontology-free. However he misunderstood its ontology. The assumptions underlying chemical practices do not concern things such as barium sulphide. More precisely, 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 action.

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⁴ Georges Urbain *Les disciplines d'une science* (1921), p. 9.

⁵ Simoes, Gavrolu (2001)^o

⁶ E Meyerson, Conférence du 23 avril 1911 sur « Evolution de la pensée allemande dans le domaine de la philosophie des sciences » p. 22. (archives A 408/11)

⁷ Meyerson *De l'explication dans les sciences*, 1921, chapter 1.

⁸ Meyerson, *Le cheminement de la pensée*, Paris, Alcan 1931, p. 138

⁹ E Meyerson, Conférence du 23 avril 1911 sur « Evolution de la pensée allemande dans le domaine de la philosophie des sciences » p. 22. (archives A 408/11)

i) Relations

To be sure chemists deal with individual substances, and pay attention to their molecular structures. However these things are only of interest to them in so far as they enter in relations with other units. Nineteenth-century structural formulas were not meant as images of reality. They were not however pure conventions. Rather they displayed capacities of bonding, the so-called atomicity or valence. Even when Wilhelm August Hofmann introduced molecular models made of sticks and balls to visualize the spatial arrangement of carbon compounds, chemists used such models – both physical and pictorial – for didactic purposes with a tacit understanding that they were purely symbolic rather than being representative of any substantial reality. They were also treated as heuristic tools that could be manipulated, a way of reflecting on the relationship between the elements that composed a molecule. As the German philosopher Ernst Cassirer convincingly argued, it is only apparently that an atom is considered as the “absolute substrate” of properties in chemistry. In fact, the concept of atom is just a mediator for mapping out a network of interdependent relations between objects.¹⁰

Gaston Bachelard also emphasized that chemists were concerned with relations rather with their substrate. Since relations imply at least two terms, chemistry necessarily presupposes various kinds of beings. Plural and relational are the two features that Bachelard selected to define the rationalism of modern chemistry that he dubbed “non lavoisian”.

If atoms for chemists are above all units capable of being related to other units, their physical reality is not a matter of concern. Georges Urbain could still consider atoms as fictions in the 1920s, although he had supported atomism against equivalentists. The fictional status was his way of emphasizing the specificity of the discipline of chemistry. In his view, atomic theories were just like tools in the hands of craftsmen so that two rival theories – such as energetism and atomism - could work together.¹¹

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. For Pauling, both double bonds and resonance were man-made concepts. The theory of resonance involved “the same amounts of idealization and arbitrariness” as the valence-bond theory”. “The theory of resonance in chemistry is an essentially qualitative theory which, like the classical structure theory, depends for its successful application largely upon a chemical feeling that is developed through practice”.¹² Thus time and again chemists claim originality through their rejection of the physical meaning of the concepts they are using while they play with all sorts of interactions to make things.

¹⁰ Cassirer (1910) chapter “Conceptualization in natural science”

¹¹ Urbain (1921) p. 21-24 Later on in the 1930s, Urbain never adopted the electronic theories of chemical bond because he had forged an alternative theory of the chemical bond, based on Werner’s theory of complex that better suited his own practice of chemistry.

¹² Pauling, L. “The nature of the theory of resonance”, *Perspectives in Organic Chemistry*, 6-7, quoted in Simões, Gavrolu (2001) p. 66.

ii) Agencies

For chemists molecular structures are above all conditions of properties, which themselves are viewed as dispositions for desired or undesired performances. While chemists do not care for matter, they are looking for materials, i.e. substances useful for something. Remarkably eighteenth-century chemists used to present the four elements - fire, air, water and earth -, as natural instruments of the chemist's laboratory, along with artificial instruments - menstrues and vessels.. Later on, although the compositional paradigm prevailed after the reform of chemical language, and the structural paradigm with the emergence of organic chemistry, chemical names and formulas have been mainly used as "paper tools" for predicting operations and substitutions.¹³ They display the possible uses of the 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 experimenting.¹⁴ Therefore nineteenth-century chemists could deny any ontological commitment with atoms and molecules, while using them just as plumbers use screws, nails, and joints. They refused to bestow the atomic theory with the power for representing the world, as they were concerned with powers for intervening. Atoms and molecules are just potential actors in chemical drama.

Ian Hacking's comments on the way physicists use electrons typically suit the way chemists view the constituents of matter.¹⁵ Electrons are less explanatory notions, as they are instruments for acting or creating phenomena. Hacking's distinction between "realism about theories" and "realism about entities" could thus apply 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 agencies.

Chemical substances have to be clearly redefined by their intrinsic properties as well as by the dispositions they acquire in acquired in specific circumstances, or the affections they cause on human tissues or senses. This is important to understand the current debates raised by the implementation of a system of control of chemicals in the European Community (REACH). When it comes to current environmental and societal issues, definitions of chemical substances in terms of their molecular structure are not adequate. Rather it is what they do on human tissues or could do that is meaningful. For setting the standards of toxicity and correlative responsibility of industrial companies, distinctions between natural stable capacities, and dispositions really matter.

The chemists' art of synthesis takes advantage of the whole spectrum of qualities in order to put molecules at work, to make them do what humans cannot do with their fingers. In a 2003 conference, Susan Linquist, a biologist from MIT Whitehead Institute, said: "About 10,000 years ago, [humans]

¹³Klein ed, 2001.

¹⁴ Bachelard, 1940, p. 60

¹⁵ Hacking, 1983

began to domesticate plant and animals. Now it's time to domesticate molecules."¹⁶ But domesticating molecules is what chemists have been doing for centuries. At the cost of repeated experimental trials, they 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. However domesticated beings never work like man-made tools or machines. They operate according to their own nature, even when they are chemical "creatures". Through a number of more or less spectacular hazards and deplorable accidents, chemists have learned that they are still at the mercy of unexpected circumstances and that reagents do not always behave in a predictable way.

In addition, chemists usually work with huge populations of molecules in their flasks or vats. Unlike nanoscientists who are trying to domesticate isolated molecules, they have no control on individual molecules, although they may know a good deal about the species of molecules, especially when they are their own creations. In fact, the shift in length scale determines radically different relations 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 inspires nanotechnology. Individual molecules are supposed to be reliable entities, responding to precise signals. So deep is the contrast between this culture of precision and the more crude style of chemists, that to Eric K Drexler, the champion of nanotechnology, chemical synthesis is an improbable adventure, that he compares to putting together automotive parts in a large box, shaking it with the expectation of finding an assembled car when the shaking is finished.¹⁷ Such miraculous achievements are nevertheless daily practices in chemical factories. But the car they manufacture is a new whole thing, the parts of which are no longer visible or tangible. In their art of making molecules work for them, chemists are not like Plato's *demiurgos*, who builds up a world by imposing his own rules and rationality on a passive matter. Rather they are like the ship-pilot at sea, who conducts or guides forces and processes supplied by nature, thus revealing the powers inherent in it.

References

- Bachelard, Gaston (1940) *La philosophie du non*, Paris, Presses universitaires de France. transl. The Philosophy of No: A Philosophy of the Scientific Mind (1968) New York, Orion Press.
- Bachelard, Gaston (1952) *Le matérialisme rationnel*, Paris, Presses universitaires de France
- Baird, Davis, Scerri, Eric, McIntyre, Lee (eds) (2006), *Philosophy of Chemistry. Synthesis of a New Discipline*, Dordrecht, Springer.
- Bensaude-Vincent, Bernadette, Stengers, Isabelle *A History of Chemistry*, Cambridge, Harvard University Press, 1996.
- Bensaude-Vincent, Bernadette (1997), *Eloge du mixte. Matériaux nouveaux et philosophie ancienne*. Paris, Hachette Littératures.
- Bensaude-Vincent, Bernadette (1999), "Atomism and Positivism : A Legend about French Chemistry", *Annals of Science*, 56, p. 81-94.
- Bensaude-Vincent, Bernadette (2005), "Chemistry in the French tradition of philosophy of science: "Duhem, Meyerson, Metzger and Bachelard", *Studies in History and Philosophy of Science*, 36, p. 627-648.

¹⁶ Susan Linquist quoted by Zhang, S. (2003) p. 1177.

¹⁷ Drexler (1995) p. 2

Cassirer Ernst (1910) *Substanzbegriff und Funktionbegriff: untersuchungen über die Grundfragen der Erkenntniskritik*, Berlin, Engl tr., *Substance and Function and Einstein's Theory of Relativity*, New York, Dover, 1953.

Drexler, Eric (1995) "Introduction to nanotechnology" in Markus Krummenacker, James Lewis (eds) *Prospects in Nanotechnology. Proceedings of the 1st general conference on nanotechnology: developments, applications, and opportunities* nov 11-14, 1992, Palo-Alto, John Wiley & Sons 1995.

Duhem, P. (1902) *Le mixte et la combinaison chimique*, Paris, re-edition Paris, Fayard, 1985 ; Eng transl. By P. Needham, *Mixture and Chemical Combination and Related Essays*, Dordrecht, Kluwer academic, 2002.

Hacking Ian (1983) *Representing and Intervening*, Cambridge, Cambridge University Press.

Meyerson, E. (1921) *De l'explication dans les sciences*, Paris : Payot. 2 vols. *Explanation in the Sciences* transl. by Mary-Alice and A. Sipfle, Dordrecht: Kluwer, 1991.

Meyerson, E. (1931) *Du cheminement de la pensée*, Paris : Alcan, 3 vols

Meyerson, E. (1933) *Réel et déterminisme dans la physique quantique*. Paris : Hermann.

Simões, Ana, Gavrolu, Kostas (2001) "Issues in the History of theoretical and Quantum Chemistry (1927-1960)", in Carsten Reinhardt ed., *Chemical Sciences in the 20th century*, Weinheim, New York, Wiley-VCH, p.51-74.

Urbain, Georges (1921) *Les disciplines d'une science, la chimie*, Paris, Doin.

Zhang, Shuguang: 2003, 'Fabrication of Novel Biomaterials Through Molecular Self-assembly', *Nature Biotechnology*, 21, N°10, 1171-78.

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